Chemical Information Review Document

for

Vinpocetine
[CAS No. 42971-09-5]

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Abstract

Vinpocetine is a semi-synthetic derivative of vincamine, an alkaloid derived from the *Vinca minor L.* plant, that has been used since the 1970s in Japan, Europe, Mexico, and Russia for the treatment of cerebrovascular and cognitive disorders. Vinpocetine can also be derived from tabersonine, the alkaloid extract of Voacanga seeds found mostly in West Africa. In the United States, it is commonly sold as a dietary supplement for the general population either alone or with other ingredients. Its numerous proposed uses include for improvement of brain function, rapid weight/fat loss, increases in energy, enhancement in focus and visual acuity, prevention of motion sickness, and treatment of menopausal symptoms, chronic fatigue syndrome, and hearing and eye disorders. According to the *Physicians' Desk Reference for Nutritional Supplements*, doses may range from 5-20 mg/day. Adverse reactions associated with its consumption include nausea, dizziness, dry mouth, transient hypo- and hyper-tension, headaches, heartburn, and changes in blood pressure and blood glucose levels. Pharmacokinetic absorption, distribution, metabolism, and excretion studies have been conducted in humans as well as rats via the oral, intravenous (i.v.), and/or intraperitoneal (i.p.) route. Vinpocetine and apovincaminic acid, the main metabolite, have been detected. Acute toxicity values (LD_{50}s) for vinpocetine were similar for mice and rats. Oral LD_{50}s were 534 and 503 mg/kg, respectively. For both species, values ranged from 43-59 mg/kg via the i.v. route and from 117-240 mg/kg via the i.p. route; lethal doses of vinpocetine produced ataxia and clonic convulsions. In short-term studies with rats, effects of oral administration of vinpocetine for up to five weeks included a decrease in bronchial blood flow and increases in salivation, urine volume, and liver and thyroid weights. When 25 mg/kg vinpocetine was given via i.v. injection for up to three months, 3/8 males and 2/8 females died; death was attributed to severe confluent fibroblastic peritonitis and ascites. However, doses of 25-100 mg/kg vinpocetine given via gastric intubation for up to six months did not result in mortality or adverse effects on a variety of endpoints. Vinpocetine inhibits cell proliferation in human breast cancer cell lines (i.e., MDA-MB-231, MDA-MB-468, MCF-7, and ZR-75-1). Additionally, it inhibited tumor growth in a xenograft model of breast cancer in nude mice. Vinpocetine did not affect male or female mating ability or fertility when orally administered for eight weeks prior to mating, but uterine bleeding was a common finding in studies with pregnant rats.

Executive Summary

Nontoxicological Data

Vinpocetine is a semi-synthetic derivative of vincamine, an alkaloid derived from the *Vinca minor L.* plant, that has been used since the 1970s in Japan, Europe, Mexico, and Russia for the treatment of cerebrovascular and cognitive disorders. An example of synthesis is transesterification of vincamine in ethanol using Lewis acids. It can also be derived from tabersonine, the alkaloid extract of Voacanga seeds found mostly in West Africa. In general, analysis of vinpocetine in matrices is via high-performance liquid chromatography. Vinpocetine is available from countries all around the world, from the United States to China to Italy to Korea. Although a pharmaceutical agent in Japan, Europe, and Mexico, it is commonly sold as a dietary supplement for the U.S. general population either alone or as one of several ingredients in dietary supplement products. Similar standards for identity and quality of vinpocetine products have been specified by the United States, British, and European Phamacopoeias. The marketed uses include improvement of brain function, rapid weight/fat loss, increases in energy, and enhancement in visual acuity, memory, and focus. These make vinpocetine a product for athletes too. Additional reported uses of vinpocetine are the prevention of motion sickness and the treatment of menopausal symptoms, chronic fatigue syndrome, seizure disorders, and hearing and eye disorders. Patents also claim additional applications of vinpocetine, such as its use in a topical application to increase female sexual response. Despite these uses, no regulatory body has approved vinpocetine for the treatment of cognitive impairment. In the United States, it is regulated under the Dietary Supplement Health and Education Act of 1994.

Human Data

Vinpocetine exposure typically occurs through oral consumption. According to the *Physicians' Desk Reference for Nutritional Supplements*, doses may range from 5-20 mg/day.

Adverse reactions associated with vinpocetine consumption include nausea, dizziness, dry mouth, transient hypo- and hyper-tension, headaches, and heartburn. Alterations in blood pressure and blood glucose levels were observed with prolonged use. Potential for development of tachycardia was also noted. In an elder Japanese man, vinpocetine was reported to produce agranulocytosis.

In absorption, distribution, metabolism, and excretion (ADME) studies, volunteers were orally exposed to radiolabeled vinpocetine. Radioactivity concentration decreased in the stomach and increased in the liver, blood, and kidneys. Unchanged vinpocetine levels in urine decreased to 4% after 60 minutes. Heterogenous brain distribution was noted; greatest uptake was observed in the thalamus, occipital cortex, basal ganglia, and some cortical structures. After intravenous (i.v.) administration of vinpocetine, vinpocetine and apovincaminic acid were detected in cerebrospinal fluid. In another i.v. study, total brain uptake of vinpocetine, peaked 2 minutes after administration and represented 3.71% of the total radioactivity administered. The greatest amount was present in the thalamus.

Pharmacokinetic studies on vinpocetine and apovincaminic acid, the main metabolite after vinpocetine consumption, have been conducted after oral consumption and i.v. administration of vinpocetine. The half-life of vinpocetine after oral administration ranged from 1.73 to 2.9 hours, while the half-life of apovincaminic acid after oral vinpocetine administration was calculated to be 1.25 hours. After intravenous vinpocetine administration, the half-lives of vinpocetine and apovincaminic acid were 2.1 to 17 hours and 2.8 hours, respectively.

Toxicological Data

Studies regarding carcinogenicity, initiation/promotion, genotoxicity, cogenotoxicity, cytotoxicity, and immunotoxicity were not located.

Chemical Disposition, Metabolism, and Toxicokinetics

In rats orally administered tritiated-vinpocetine, the majority of the urinary radioactivity was associated with apovincaminic acid. Unchanged vinpocetine was also identified in urine. In plasma, the majority of the radioactivity was excreted as either apovincaminic acid or vinpocetine. In a separate study in which male and female Wistar rats were orally administered tritiated-vinpocetine, maximal concentrations occurred approximately two hours after administration, with the greatest amounts in the liver and small intestine. By 48 hours after administration, vinpocetine levels were minimal in most organs except the liver and kidneys. Within 48 hours of administration 80% of the administered radioactivity was recovered in the feces and urine and <5% in the bile after nine hours. In blood, a majority of the vinpocetine was present in the plasma fraction bound to proteins. When Wistar rats were orally administered vinpocetine for five days and then tritiated-vinpocetine on day 5, ~75% of the administered radiolabel was excreted in the urine and feces within 48 hours. This was also seen following intraperitoneal (i.p.) injection of vinpocetine. Additionally, four metabolites were identified: ethyl vincaminate, 10-hydroxyvinpocetine, and a dihydroxylated, glycine-conjugate of apovincaminic acid; one could not be structurally identified.

Pharmacokinetic studies have been conducted after oral consumption and i.v. administration of vinpocetine. In rats, the half-life of vinpocetine after oral administration ranged from 1.73-2.9 hours. Comparatively, the half-life of vinpocetine after i.v. administration ranged from 15.2 minutes to 17 hours.

Acute Exposure

Acute toxicity values (LD_{50}s) for vinpocetine were similar for mice and rats. Oral LD_{50}s were 534 and 503 mg/kg, respectively. For both species, values ranged from 43-59 mg/kg via the i.v. route and from 117-240 mg/kg via the i.p. route; lethal doses of vinpocetine produced ataxia and clonic convulsions. At doses of 0.5-8 mg/kg, i.p. injection of vinpocetine resulted in increased sensitivity to environmental stimuli; at higher doses (16-64 mg/kg), clonic convulsions and decreases in spontaneous motility, orientation hypermotility, and locomotor activity were seen. When rats were orally administered 1-30 mg/kg vinpocetine, mean arterial pressure was increased at the highest dose, while cerebral blood flow was decreased at the lowest dose.

Short-Term and Subchronic Exposure

When male CD rats were orally administered 25 or 100 mg/kg vinpocetine over a four-week period, no deaths or changes in body weight gain were noted. At the higher dose, increases in salivation and liver and thyroid weights were observed. In Sprague-Dawley rats orally administered 3, 10, or 30 mg/kg vinpocetine for five days, mean arterial pressure was not altered, but cardiac output was increased at the high dose. Additionally, decreased bronchial blood flow and increased splanchnic blood flow were noted after administration of the low and high dose, respectively. In rats orally administered vinpocetine [dose n.p.] for five weeks, observed effects included fluid intake, increased urine volume, and weight loss or decreased weight gain.

Male and female Wistar rats were administered 5 or 25 mg/kg vinpocetine by i.p. injection five times per week for three months. At the high dose, three of eight males and two of eight females died; death was attributed to severe confluent fibroblastic peritonitis and ascites.

Chronic Exposure

Male and female CFY rats were administered 25, 50, or 100 mg/kg vinpocetine by gastric intubation five times per week for six months. No vinpocetine associated deaths, adverse effects, or changes in relative organ weights were observed. During treatment, animals were agitated. Mild tubular degeneration was observed in some mid-dose animals. In a separate study, rats were orally administered vinpocetine for 26 weeks. Observed effects included changes in liver and adrenal weight and increased urine volume.

Synergistic/Antagonistic Effects

Synergistic and antagonistic effects of vinpocetine have been described in a variety of systems. Vinpocetine was reported to antagonize liver injury induced by carbon tetrachloride in rats and the effects produced by postnatal alcohol exposure in mice and rats. Vinpocetine antagonized lead-induced hyperactivity in female mice pups, electroshock- and metrazol-induced convulsions in mice, and streptozotocin-induced effects on learning and memory in male rats.

Reproductive and Teratological Effects

Vinpocetine had no effects on male or female CFY rat fertility and mating ability after oral administration of 10 or 50 mg/kg vinpocetine for eight weeks prior to mating. However, high-dose males did have a decreased relative prostate weight. Although vinpocetine had no teratogenic effect in rats, uterine bleeding and death was observed in pregnant rats administered vinpocetine.

Other Data

Vinpocetine inhibited tumor necrosis factor (TNF)-α induced activation of nuclear factor-κB. In a xenograft model of breast cancer, i.p. administration inhibited tumor growth *in vivo*. *In vitro*, vinpocetine inhibited migration of MDA-MB-231 cells. Vinpocetine was active in 52 tests from 917 different bioassays indexed by PubChem. Protein targets included the KCNQ potassium channel family and euchromatic histone-lysine *N*-methyltransferase 2. Vinpocetine inhibited the cellular proliferation of four human breast cancer cell lines: MDA-MB-231, MDA-MB-468, MCF-7, and ZR-75-1. It also induced apoptosis in MDA-MB-231 and MCF-7 cells. Comparatively, it did not affect proliferation of murine thymus and spleen cells *in vitro*.

Structure Activity Relationships

Vincamine [CAS No. 1617-90-9]

Vincamine, an alkaloid derived from *Vinca minor* L., is used as a vasodilator but has been reported to cause cardiovascular effects such as hypotension and central nervous system effects such as sedation in patients. In mice, LD_{50} values were 48-75, 215, 1000, and >1000 mg/kg via the i.v., i.p., oral, and subcutaneous routes, respectively. In rats, an i.p. LD_{50} of 253 mg/kg was calculated. A single i.p. injection of vincamine produced disorganized and irregularly arranged tight junctions and irregularly shaped gap junctions in mouse liver. Rats administered 6.6-100 mg/kg vincamine daily for up to three months exhibited no adverse effects. In a reproductive study in mice, vincamine administered via stomach tube and daily from one week prior to mating until sacrifice or birth increased fetal resorptions. When a lower dose was administered from mating to the end of lactation, no adverse effects were noted. In rats, i.v. administration of 5 mg/kg daily from eight days prior to mating to two-thirds through gestation or end of gestation did not affect fertility and was not embryotoxic or teratogenic, but an oral administration of 2.25-37.5 mg/kg daily from gestation days 6-16 caused increased placental hemorrhages at 7.5 mg/kg; decreased body weight, reduced number of fetuses, smaller and lighter fetuses, and delayed ossification at 22.5 mg/kg; and fetotoxicity at 37.5 mg/kg. In male rats, 225 mg/kg vincamine (orally) had no effect on reproductive function. Vincamine was negative in several assays for genotoxicity.

GeneGo

Eight vinpocetine metabolites were predicted after first-pass metabolism. The metabolites could be classified as those produced after (a) aliphatic hydroxylation, (b) aromatic hydroxylation, and (d) *O*-dealkylation. Ten minor first-pass metabolites, 4 first-pass conjugated metabolites, 30 major second-pass metabolites, 8 minor second-pass metabolites, and 36 second-pass conjugated metabolites also were predicted. None of the predicted aliphatic hydroxylation metabolites were identified in human or rat urine. The main metabolite of vinpocetine in human and rodent studies is apovincaminic acid, which is identified as an *O*-dealkylation metabolite by GeneGo.

Inhibitory cytochrome P450 (CYP) models predicted that vinpocetine would have inhibitory activity against CYP2D6. It was also predicted to be a substrate for CYP2D6 and human P-glycoprotein transporters. Vinpocetine was predicted to have activity against heart failure, hypertension, osteoporosis, pain, and Parkinson's disease. Several of the proposed targets for vinpocetine were based on literature reports describing inhibitory effects on phosphoidesterase 1A, 1B, 1C, and E1, interaction with the peripheral benzodiazepine receptor, and inhibition of sodium channels.

Leadscope

Vinpocetine was classified as positive in two *in vivo* rat carcinogenicity models, three *in vitro* carcinogenicity models, two mutagenicity models, five developmental toxicity models, four cardiac models, and two urine models. Nitrogen- and oxygen-containing moieties were identified as playing a role in activity in many of the models.

Toxtree

A structural alert associated with micronucleus formation in rodents ("H-acceptor-path3-H-acceptor") was identified in vinpocetine. DNA and protein binding structural alerts were reported in the vinpocetine structure. Vinpocetine was classified as not corrosive to the skin or eye. However, the presence of a structural alert associated with skin sensitization (Michael acceptor) was reported. Vinpocetine was classified as belonging to Class III, "substances are those that permit no strong initial presumption of safety, or may even suggest significant toxicity or have reactive functional groups.", based on the presence of a heterocycle with complex substituents within vinpocetine. Vinpocetine was predicted to be reactive by Michael addition. .

Low specificity structural groups were an aldehyde or ketone, ether, carboxylic acid derivative, aromatic compound, and heterocyclic compound. The high specificity groups were a dialkylether, alkylarylether, tertiary aliphatic amine, carboxylic acid ester, and carbonic acid diester. Another functional group identified was enolether.

SMARTCyp

This program evaluates chemicals for sites that may be metabolized by CYP isoforms. The results are applicable to isoforms CYP1A2, CYP2A6, CYP2B6, CYP2C8, CYP2C19, CYP2E1, and CYP3A4. Additionally, two specific models for metabolism by CYP2C9 and CYP2D6 are provided. The initial model and the model for CYP2C9 both predicted atoms 6, 12, and 8 would be the primary, secondary, and tertiary sites for metabolism. While atoms 6 and 12 were predicted to be the primary and secondary metabolic sites for CYP2D6, the tertiary site was predicted to be atom 26.

Table of Contents

Chemical Information Review Document for Vinpocetine [CAS No. 42971-09-5]

Abstract i
Executive Summary ii
1.0 Introduction 1
1.1 Chemical Identification and Analysis 1
1.2 Physical-Chemical Properties 3
1.3 Commercial Availability 3
2.0 Production Processes 4
3.0 Production and Import Volumes 4
4.0 Uses 4
5.0 Environmental Occurrence and Persistence 6
6.0 Human Exposure 6
7.0 Regulatory Status 11
8.0 Toxicological Data 11
8.1 General Toxicology 11
8.1.1 Human Data 11
8.1.2 Chemical Disposition, Metabolism, and Toxicokinetics 18
8.1.3 Acute Exposure 21
8.1.4 Short-Term and Subchronic Exposure 22
8.1.5 Chronic Exposure 22
8.1.6 Synergistic/Antagonistic Effects 23
8.1.7 Cytotoxicity 24
8.2 Reproductive and Teratological Effects 24
8.3 Carcinogenicity 26
8.4 Initiation/Promotion Studies 26
8.5 Genotoxicity 26
8.6 Cogenotoxicity 26
8.7 Immunotoxicity 26
8.8 Other Data 26
9.0 Structure-Activity Relationships 29
9.1 Vincamine [CAS No. 1617-90-9; PubChem CID:15376] 29
9.2 GeneGo 30
9.3 Leadscope 31
9.4 Toxtree 32
9.5 SMARTCyp 33
10.0 Online Databases and Secondary References Searched 33
10.1 Online Databases 33
10.2 Secondary References 34
11.0 References 34
12.0 References Considered But Not Cited 43
Units and Abbreviations 44
Acknowledgements 46
Appendix A: Description of Search Strategy and Results 47
Appendix B: PubChem BioAssay Results 49

Appendix C: GeneGo Structure-Activity Relationship Analyses for Vinpocetine 207
Appendix D: Leadscope Structure-Activity Relationship Analyses for Vinpocetine 235
Appendix E: Toxtree Structure-Activity Relationship Analyses for Vinpocetine 248

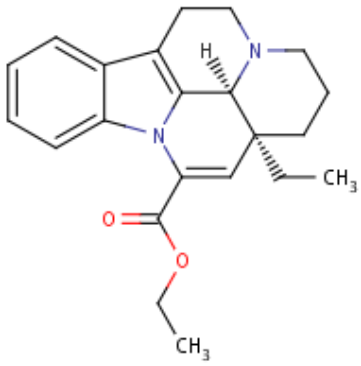
Tables:

Table 1. Pharmacopeian Standards for Vinpocetine 5
Table 2. Reported Side/Adverse Effects Associated with Vinpocetine Consumption 8
Table 3. Vinpocetine Pharmacokinetic Parameters after Oral Human Consumption of Vinpocetine 13
Table 4. Apovincaminic Acid Pharmacokinetic Parameters after Oral Human Consumption of Vinpocetine 15
Table 5. Vinpocetine Pharmacokinetic Parameters after Intravenous Human Exposure of Vinpocetine 16
Table 6. Apovincaminic Acid Pharmacokinetic Parameters after Intravenous Human Exposure of Vinpocetine 17
Table 7. Vinpocetine Pharmacokinetic Parameters after Oral Rodent Exposure of Vinpocetine 19
Table 8. Apovincaminic Acid Pharmacokinetic Parameters after Oral Rodent Exposure of Vinpocetine 19
Table 9. Vinpocetine and Apovincaminic Acid Pharmacokinetic Parameters after Intravenous Rodent Exposure of Vinpocetine 20
Table 10. Acute Toxicity Values for Vinpocetine 21
Table 11. Positive Results of Vinpocetine in PubChem BioAssays 28
Table 12. Leadscope Results 31

1.0 Introduction

Vinpocetine is a semi-synthetic derivative of vincamine, an alkaloid derived from the *Vinca minor L.* plant (Hendler and Rorvik, 2001). It has been used since the 1970s in Japan, Europe, Mexico, and Russia for the treatment of cerebrovascular and cognitive disorders (Hendler and Rorvik, 2001; Jha et al., 2012). Additional clinical indications and proposed mechanisms of action for vinpocetine are discussed in **Section 4.0**.

Vinpocetine
[42971-09-5]



1.1 Chemical Identification and Analysis

Vinpocetine ($C_{22}H_{26}N_2O_2$; mol. wt. = 350.46) is also called:

(+)-Apovincaminic acid ethyl ester
(+)-cis-Apovincaminic acid ethyl ester
(+)-Vinpocetine
1H-Indolo[3,2,1-de]pyrido[3,2,1-ij][1,5]naphthyridine, eburnamenine-14-carboxylic acid deriv.
3-α,16-α-Apovincaminic acid ethyl ester
Apovincaminic acid ethyl ester
Bravinton
Cavinton
Ceractin
cis-Apovincaminic acid ethyl ester
Eburnamenine-14-carboxylic acid, ethyl ester, (3.alpha.,16.alpha.)-
Ethyl (+)-apovincaminate
Ethyl (+)-cis-apovincaminate
Ethyl apovincamin-22-oate
Ethyl apovincaminate
RGH 4405
TCV-3B
Ultra-Vinca
Vinpocetinum
Vinporal

PubChem CID: 443955
InChI: 1S/C22H26N2O2/c1-3-22-11-7-12-23-13-10-16-15-8-5-6-9-17(15)24(19(16)20(22)23)18(14-22)21(25)26-4-2/h5-6,8-9,14,20H,3-4,7,10-13H2,1-2H3/t20-,22+/m1/s1
Canonical SMILES: CCC12CCCN3C1C4=C(CC3)C5=CC=CC=C5N4C(=C2)C(=O)OCC

Sources: ChemIDplus (undated); PubChem (undated); Registry (2012)

Several different methods have been developed to detect the presence of vinpocetine in a variety of matrices (e.g., plasma). These include high performance, thin layer, and gas chromatography (GC), and ^{1}H nuclear magnetic resonance (NMR). Select methods have been described below. Additional methods may be reviewed in articles discussing absorption, distribution, metabolism, and excretion (ADME) of vinpocetine by humans and rodents. [See **Sections 8.1.1** and **8.1.2**.] Furthermore, the *U.S. Pharmacopeia* describes a liquid chromatography method for analysis of formulations.

A majority of the detection methods described the use of high performance liquid chromatography (HPLC). For example, HPLC coupled to an ultraviolet (UV) detector was used by several groups for detection of vinpocetine in human plasma. HPLC was coupled to a UV detector with detection performed at 274 nm. Vinpocetine was extracted from plasma with acetonitrile. The method detection limit and lower limit of quantification (LOQ) were not provided, but 90% recovery was obtained from plasma samples spiked with 0.01 µg/mL (Elbary et al., 2002). An HPLC coupled to a UV detector (detection at 274 nm) was also used to identify vinpocetine in rat plasma. In the described protocol, vinpocetine was extracted with cyclohexane (Sozanski et al., 2011). An HPLC-UV method, with detection at 280 nm, was used for identification of vinpocetine in tablet preparations. The vinpocetine was extracted from the tables using acetonitrile. The LOQ and limit of detection (LOD) of the method were 0.2904 and 0.0968 µg/mL, respectively with linearity in response at concentrations ranging from 160 to 240 µg/mL (Bhadra et al., 2011).

HPLC-UV was used for separation of the enantiomers of the two diastereomers of vinpocetine. The column used was a Chiral-AGP column and detection was performed at 315 nm. The optimized mobile phase consisted of phosphate buffer (pH 7.73) and 2-propanol; ratios of the two constituents were varied over the course of the chromatographic run. Order of separation of the enantiomers was the following: *cis*-(+), *trans*-(-), *cis*-(-), and *trans*-(+) (Herenyi and Gorog, 1992).

An HPLC method described the identification of vinpocetine in plasma using a mass spectrometer (MS) for detection. The MS was operated in the positive ion detection mode and the turbo spray voltage was set to 5500 V. The multiple reaction monitoring mode was used for quantitation. Under optimized conditions, the LOD and LOQ were 0.25 and 0.5 ng/mL, respectively (Xia et al., 2010 [PMID:20561830]).

GC techniques have also been used for identification of vinpocetine. GC-MS was used to identify vinpocetine in human plasma. The plasma was initially extracted with *n*-hexane and evaporated. The residue was dissolved in 2-propanol. The LOD was 0.08 ng/mL plasma (Lohmann and Dingler, 1990). An earlier GC-MS method described the use of a quadrupole spectrometer operating in the selected ion monitoring mode with an electron ionization voltage

of 70 eV. Vinpocetine was extracted with *n*-hexane and the residue was dissolved in methanol. The LOD was 0.1 ng/mL (Hammes and Weyhenmeyer, 1987). [Note: A critique of the Lohmann and Dingler method was published by Hammes and Weyhenmeyer (1991).]

Two gas liquid chromatography methods were described for identification of vinpocetine in plasma and cerebrospinal fluid (Miskolczi et al., 1987 [PMID:3691609]; Polgar and Vereczkey, 1983; Polgar et al., 1985 [PMID:16867695]). A standardless NMR method was described for analytical identification of vinpocetine (Monakhova et al., 2012 [PMID:22550015]).

1.2 Physical-Chemical Properties

Property	Information	Reference(s)
Physical State	Crystals from benzene	Merck Index (2012)
Odor	Not located	
Boiling Point (°C)*	419.5 ± 45.0 @ 760 Torr	Registry (2012)
Melting Point (°C)	147-153 (decomposes), 148-151	Merck Index (2012); Registry (2012)
Flash Point (°C)*	207.5 ± 28.7	Registry (2012)
Vapor Pressure (mm Hg)*	3.02×10^{-7} @ 25 °C	Registry (2012)
Density (g/cm^3)*	1.28 ± 0.1 @ 20 °C and 760 Torr	Registry (2012)
Water Solubility	Not located	
Octanol-Water Partition Coefficient (Log K_{OW})	Not located	
Log P*	3.978 ± 0.577	Registry (2012)
Bioconcentration Factors (@ 25 °C)	1.0 @ pH 1-4, 1.33 @ pH 5, 8.75 @ pH 6, 74.19 @ pH 7, 356.80 @ pH 8, 578.40 @ pH 9, and 616.73 @ pH 10	Registry (2012)

*calculated properties using Advanced Chemistry Development (ACD/Labs) Software V11.02 (©1994-2012 ACD/Labs)

1.3 Commercial Availability

China is the major country when it comes to the number of companies producing and supplying vinpocetine. Producers include Beijing Ribio Biotech Co., Ltd., Chemieliva Pharmaceutical Co., Ltd., Hisunny Chemical Co., Ltd., and Simagchem Corporation, and examples of the numerous suppliers are AOKBIO Co., Ltd., Atomax Chemicals Co., Ltd., and Kinbester Co., Ltd. Other producers of vinpocetine are Santa Cruz Biotechnology, Inc. in the United States and Clearsynth Labs (P) Ltd. in India. Outside of China, suppliers are located in the United States (e.g., AIDP, Inc., AK Scientific, Inc., CellMark USA, LLC, Gallade Chemical, Inc., Kingston Chemistry, and Sigma-Aldrich Corporation), Canada (TLC PharmaChem, Inc.), Germany (e.g., Chemos GmbH and Chemical Point UG), India (Alchem International Ltd.), Korea (InterChem Engineering), the United Kingdom (e.g., Leancare Ltd. and Molekula Group), Switzerland (e.g., BIOTREND Chemicals AG), and Italy (Allorachem) (BuyersGuideChem, 2012; ChemBuyersGuide.com, undated; ChemExper, 2012).

Vinpocetine is available as a dietary supplement for the general population. The Dietary Supplements Labels Database lists 19 products currently on the market containing vinpocetine as an active ingredient. The amounts of vinpocetine range from 1 mg (two products: Irwin Naturals Ginkgo Smart Liquid Soft-Gels and Physician Formulas Mind Power Rx) to 15 mg (Life Enhancements CerebroPlex). Manufacturers of these products include Avesthagen, Inc., BioNatures, Gaia Herbs, Jarrow Formulas, and Xymogen (U.S. NLM, 2012). However, web searches (e.g., Google Products) for the chemical show that it is available as products (powder,

capsules, etc.) from other companies and in higher dose amounts via the Internet and health food and drug stores. For example, the product Triple-Strength Vinpocetine 30 mg can be purchased from Swanson Superior Herbs, while bulk powder, up to 1 kg, is available from Health Supplement Wholesalers (Amazon.com, Inc., 2012; Swanson Health Products, 2012). Additionally, vinpocetine is an ingredient in other dietary supplements. For instance, it is in trunature® Ginkgo Biloba with Vinpocetine [5 mg vinpocetine] (Costco, 2012). It is also available in the energy drink Redline Xtreme RTD and the fat burner Xyience Xelerate capsules (BodyBuilding.com, LLC, 2012). [See **Section 4.0**.] Covex, a Spanish company marketed as "the leader in the production of Vinca alkaloids," is currently expanding its activity towards the dietary supplements and energy drinks sector in the United States and other countries (Covex S.A., 2010).

The Pharmaceutical and Healthcare Online Databases provide a listing of 38 vinpocetine products. Among the manufacturers of the products are Covex, North Star, Gedeon Richter, Makiz-Pharma, Deko Company, and Biohimik (Catalog.md, 2012).

2.0 Production Processes

Vinpocetine is synthesized from vincamine, an alkaloid from the periwinkle plant (MSKCC, 2011). Several methods have been described for vinpocetine synthesis. One report described heating (+)-14-oxo-15-hydroxyimino-*E*-homo-eburnane with ethanol and sulfuric acid in a water bath for five hours. The reaction mixture was then poured into ice-water, and ammonium hydroxide was added until a pH of 9 was obtained. The reaction was extracted with methylene chloride and then the organic phase was dried, filtered, and evaporated. The residual oil was recrystallized in ethanol, yielding 67.6% vinpocetine (Szabo et al. 1983).

Using a "one-pot" synthesis, two pathways were described that led to vinpocetine formation from vincamine. Vinpocetine was synthesized via transesterification and/or dehydration of vincamine in ethanol using Lewis acids. Ferric chloride catalyzed both processes. At a temperature of 130 °C, an 80% product yield was reported (Kuge et al., 1994).

Patents have also proposed synthetic methods. For example, one claimed method described reaction of apovincaminic acid with ethanol in the presence of 2-fluoro-1,3,5-trinitrobenzene and 4-dimethylaminopyridine. The reaction was proposed to occur at room temperature for 3-5 hours. In a provided example, the reaction produced a yield of 92% (Mondelo, 1989 pat.).

Vinpocetine can also be derived from tabersonine, the alkaloid extract of Voacanga seeds found mostly in West Africa (Linnea Inc., undated).

3.0 Production and Import Volumes

No data were located.

4.0 Uses

Vinpocetine has therapeutic use as a vasodilator (Merck Index, 2012). Since the late 1970s, it has been used in Japan, Hungary, Germany, Poland, and Russia for the treatment of cerebrovascular-related diseases (Thorne Research, Inc., 2002). Currently, it is reportedly used in the "management of psychic and neurological symptoms (memory disorder, aphasia, apraxia,

motor disorders, dizziness and headache) and acute and chronic cerebral circulatory disorders of various origins (post-apoplectic, post-traumatic or sclerotic)" (Linnea SA, undated).

In the United States, vinpocetine is available as a dietary supplement to improve brain function (MSKCC, 2011). In addition to the general population, athletes use vinpocetine supplements and report significant enhancements in visual acuity, memory, and focus as well as rapid loss of body fat (South, 2001). Vinpocetine's use in the body building community is also evident with its own guide on the website BodyBuilding.com, providing a list of vinpocetine products. The products include fat burning capsules and energy enhancing products (e.g., energy drinks) (BodyBuilding.com, LLC, 2012). Additional reported uses of vinpocetine are prevention of motion sickness and treatment of menopausal symptoms, chronic fatigue syndrome, and seizure disorders. Vinpocetine has also been used to treat various forms of hearing disorders (e.g., tinnitus and Meniere's disease) as well as eye disorders (e.g., macular degeneration, glaucoma, and visual loss secondary to arteriosclerosis) (Linnea Inc., undated; Thorne Research, Inc., 2002; WebMD, 2012). Patents claim additional applications of vinpocetine, such as its use in a topical application to increase female sexual response and a primary ingredient in a nutritional supplement to improve "sleep and lucid dreaming" (Crosby and Bennett, 2004 pat., 2012 pat.; Luciano, 2012 pat.).

The biological effects of vinpocetine include relaxing smooth muscle, dilating blood vessels, inhibiting ion channels, improving blood flow, and protecting nerve cells deprived of oxygen and nutrients and from oxidative stress when restoring blood flow. Its use in patients with chronic cerebral vascular ischemia has been reported in various studies, while evidence for potential use in treating acute ischemic stroke, dementia, urinary incontinence, and Alzheimer's disease is increasing. [Note: One small study in Alzheimer's patients showed no improvements with vinpocetine supplementation] (Goepp, 2006; MSKCC, 2011).

Vinpocetine is a pharmaceutical agent in Europe, Japan, and Mexico used for the treatment of cerebrovascular and cognitive disorders (Anti-Aging-Meds.com, undated; Khulbe and Juyal, 2012). Furthermore, it is available as a prescription drug in Europe and Japan (Wong, 2007). Similar standards for identity and quality of vinpocetine products have been specified by the United States, British, and European Phamacopoeias (**Table 1**).

Table 1. Pharmacopeian Standards for Vinpocetine

	U.S. Pharmacopeia	British Pharmacopoeia	European Pharmacopoeia
Definition	≥98.5% and ≤101.5% vinpocetine, calculated on dried basis	≥98.5% and ≤101.5% vinpocetine, calculated based on dried substance	≥98.5% and ≤101.5% vinpocetine, calculated based on dried substance
Appearance		White or slightly yellow, crystalline powder	White or slightly yellow, crystalline powder
Organic Impurity	≤0.6% ethyl vincaminate ≤0.5% apovincamine ≤0.3% methoxyvinpocetine ≤0.5% dihydrovinpocetine ≤0.1% unspecified individual impurities ≤1.0% total impurities [as determined on liquid chromatograph]	≤0.6% ethyl vincaminate ≤0.5% apovincamine ≤0.3% methoxyvinpocetine ≤0.5% dihydrovinpocetine ≤0.1% unspecified individual impurities ≤1.0% total impurities [as determined on liquid chromatograph]	≤0.6% ethyl vincaminate ≤0.5% apovincamine ≤0.3% methoxyvinpocetine ≤0.5% dihydrovinpocetine ≤0.1% unspecified individual impurities ≤1.0% total impurities [as determined on liquid chromatograph]

	U.S. Pharmacopeia	British Pharmacopoeia	European Pharmacopoeia
Inorganic Impurity	Residue on ignition*: ≤0.1% Heavy metals: 10 ppm	Sulfated ash: ≤0.1% (determined on 1.0 g)	Sulfated ash: ≤0.1% (determined on 1.0 g)
Loss on Drying	≤0.5% (in vacuum at 100 °C for 3 hours)	≤0.5% (in vacuum at 100 °C for 3 hours)	≤0.5% (in vacuum at 100 °C for 3 hours)
Optical Rotation	+127.0° to +134.0° (10 mg/mL in dimethylformamide sample solution at 20°)	+127 to +134 (dried substance; "Dissolve 0.25 g in *dimethylformamide* R and dilute to 25.0 ml with the same solvent.")	+127 to +134 (dried substance; "Dissolve 0.25 g in *dimethylformamide* R and dilute to 25.0 ml with the same solvent.")
Reference Standards	Vinpocetine RS Vinpocetine Related Compound A RS Vinpocetine Related Compound B RS Vinpocetine Related Compound C RS Vinpocetine Related Compound D RS		Vinpocetine Vinpocetine impurity A – ethyl vincaminate Vinpocetine impurity B – apovincamine Vinpocetine impurity C – methoxyvinpocetine Vinpocetine impurity D – dihydrovinpocetine**

Sources: British Pharmacopoeia Commission (2009); European Pharmacopoeia Commission (2008); U.S. Pharmacopeial Convention (2012)
*Amount of residual substance not volatilized after ignition in the presence of sulfuric acid (U.S. Pharmacopeia, 2012)
**Council of Europe (2012)

Use Precautions

Reviews have indicated that vinpocetine may impact anticoagulant effects of some drugs (e.g., warfarin) (Hendler and Rorvik; Jha et al., 2012; MSKCC, 2011). Marginal changes in prothrombin time were observed after vinpocetine was added to a warfarin dosing regimen (Hitzenberger et al., 1990 [PMID:2272713]). Vinpocetine may also increase the hypotensive effects of antihypertensive agents (MSKCC, 2011).

5.0 Environmental Occurrence and Persistence

Vinpocetine is not a naturally occurring compound. No studies measuring vinpocetine in environmental media were located.

6.0 Human Exposure

Human exposure to vinpocetine typically occurs through oral consumption. Vinpocetine dosages in the United States range from 1-30 mg. [See **Section 1.3**.] One review reported that oral dosages may be 1-2 tablets (5 mg/tablet) three times per day with a maintenance dose of 3-5 mg tablets taken daily. Parenteral initial dose of 20 mg in a slow drip infusion could be used. This daily dose could then be increased up to 1 mg/kg (Anonymous, 1984). According to the *Physicians' Desk Reference (PDR) for Nutritional Supplements*, supplement doses may range from 5-20 mg/day. Higher doses were not advised (Hendler and Rorvik, 2001). A dose of 0.5 mg/kg/day is included in the U.S. Food and Drug Administration's Maximum Recommended Therapeutic Dose database (U.S. FDA, 2009).

In the *PDR for Nutritional Supplements*, adverse reactions associated with its consumption included nausea, dizziness, effects on wakefulness, dry mouth, transient hypo- and hypertension, headaches, and flushing. Alterations in blood pressure and blood glucose levels were noted with prolonged use (Hendler and Rorvik, 2001). Potential development of hypotension and tachycardia were reported in a separate review (Anonymous, 1984). A review of two articles to assess efficacy of vinpocetine in decreasing fatalities and dependency when

administered within two weeks of an ischemic stroke indicated that no adverse effects were reported (Bereczki and Fekete, 2008).

One case report described the development of agranulocytosis in a 73-year-old Japanese man. Fifty days after initiation of vinpocetine therapy (15 mg/day), he developed a high fever. Blood analysis indicated a white blood cell count of 600 mm^{-3} with no neutrophils. Vinpocetine treatment was discontinued and the patient was administered granulocyte colony-stimulating factor. White blood cell and neutrophil count remained in the normal range for the following two years, in the absence of vinpocetine (Shimizu et al., undated).

The data in **Table 2** summarize selected studies where the occurrence, or lack of occurrence, of side/adverse effects was reported. The studies include those that assessed the efficacy of vinpocetine treatment for a variety of disease states, efficacy in treatment of experimentally induced motion sickness, vasodilator effects in patients, and pharmacokinetic studies.

Table 2. Reported Side/Adverse Effects Associated with Vinpocetine Consumption

Patient Population	Dosing Regimen	Side/Adverse Effects Reported	Reference
20M and 64F with chronic cerebral dysfunction, 78.3 ± 9.8 years old; 42 received vinpocetine	Two 5 mg tablets three times per day for 30 days, then one 5 mg tablet three times per day for next 60 days	Difficulty swallowing or digesting, dry mouth, acidity, epigastric pain, vomiting, facial flushing, and palpitations [frequency not provided]; one patient developed multifocal extra systoles and another developed atrial fibrillation	Balestreri et al. (1987 [PMID:3553281])
30 healthy volunteers, 18-22 years old; vinpocetine effectiveness as an antimotion drug was assessed	10 mg three times per day for 7 days	Heartburn [article notes a "few cases" were reported]	Bodo et al. (1979; cited by Matsnev and Bodo, 1984 [PMID:6732678])
180M and 108F patients with cerebrovascular disorders, 37-85 years old	5 mg three times per day for <1 month to >6 months	Definitely treatment related: urticarial (whole body) [1 patient] Probably treatment related: eruption (stem) [1 patient] Possibly treatment related: diarrhea, dizziness, epileptiform convulsion, flushing, abnormal electrocardiography, increased glutamate pyruvate transaminase, increased γ-glutamate pyruvate transaminase, and stool occult blood [first four side effects occurred in 1 patient; 1 patient each for the remaining side effects] Unknown if treatment related: gastrointestinal symptoms; altered blood pressure, pulse, red and white blood cell count, hemoglobin, hematocrit, glutamate oxalacetate transaminase, glutamate pyruvate transaminase, increased γ-glutamate pyruvate transaminase, alkaline phosphatase, lactate dehydrogenase, total protein, blood urea nitrogen, creatinine, and urinary sugar [total of 17 patients reported at least one side effect]	Ebi (1985)
10M and 5F patients with acute ischemic stroke, 60.8 years old [mean]	10 mg once day i.v. for 5-7 days, then 10 mg three times per day for 30 days	Non-statistically significant increase in deaths noted	Feigin et al. (2001 [PMID:11509086])
26M and 18F neurosurgical cases, 44.3 years old [mean]	10 mg vinpocetine administered i.v. after electroencephalography; some patients were administered vinpocetine in three 5 mg doses for 1 to 2 months [Note: Presumed that the route of administration was oral for the longer term dosing.]	Allergic hypersensitivity was not noted after either dosing route. No adverse effects or effects on laboratory examinations were noted.	Fenyes et al. (1976 [PMID:1037223])
15M and 40F with mild cognitive impairment, 68.4 ± 1.1 years old	5 mg three times per day for 4 weeks; each course was repeated two times a year for three years	Acute respiratory disease [2], diarrhea [1], arthrosis of right hip joint [1], prostate tumor [1], breast tumor [1], angina [1]. [Note: The text suggests that the noted side effects were associated with treatment, but no further information is provided and the authors note that "Most side effects were mild or moderate. Serious side effects requiring hospitalization or termination of the study occurred in … two of group 2."	Gavrilova et al. (2011)
10M and 10F volunteers, 67.6 (M) and 70 (F) years old [means]	20 mg three times per day for 7 days, then 10 mg by i.v. infusion on day 8	No effect on heart rate or blood pressure; significant changes in some laboratory parameters (e.g., decreased hematocrit) were not "considered relevant with respect to clinical evaluation."	Grandt et al. (1989 [PMID:2624613])

Patient Population	Dosing Regimen	Side/Adverse Effects Reported	Reference
16M and 14F patients with cerebral infarction or cerebral ischemia, 30-80 years old	1 mg/mL vinpocetine by slow i.v. infusion (3-5 minutes)	Transient decrease in systolic and mean blood pressure values (6 and 5 mm Hg, respectively) 15 minutes after administration; "few patients" reported "warmth" during administration	Hadjiev and Yancheva (1976 [PMID:1037222])
6M and 14F with cerebrovascular insufficiencies	5 mg three times per day for 1 month	No effect on blood pressure, no side effects reported	Hadjiev and Yancheva (1976 [PMID:1037222])
18M and 12F stroke patients, 68 years old [mean]	10 mg three times per day for 3 months	No adverse effects reported. No consistent effect on blood pressure, pulse, or respiration.	Hayakawa (1992 [PMID:1642666])
21 patients with retinopathies	Six 5 mg tablets daily for 1 week, then three 5 mg tablets for three weeks	Significant decrease in baseline diastolic blood pressure [9/14]	Imre and Nemeth (1981)
6M volunteers, 25-47 years old	20 mg by i.v. infusion [Note: Crossover design used with vincamine and placebo administered during other weeks of study.]	Significant decrease in mean pulse rate. Adverse effects reported included dizziness and "faintness" on standing [1 volunteer] and mild facial flushing [1 volunteer].	Lim et al. (1980 lett.)
4M and 4F, 23-28 years old	10 mg once either before or after breakfast [Note: See **Section 8.1.1** for additional details on experiment.]	Treatment related effects were identified as headache and nausea; additional effects reported included diarrhea, stomachache, tiredness, dizziness, and cold hands/feet [1 volunteer each]	Lohmann et al. (1992 [PMID:1418055])
22 patients with neurological disorders	Two 10 mg tablets three times per day for 30 days, then one 5 mg tablet three times per day for next 60 days	Decreased baseline systolic and diastolic blood pressure on treatment days 60 and 90, decreased serum glucose in treatment group, one treated patient reported facial flushing	Manconi et al. (1986)
5 patients with parkinsonism (3), epilepsy (1), and familial myoclonus (1)	10 mg vinpocetine by i.v. administration with 5-, 10-, and 15-minute washout periods between treatments	No adverse effects noted, no decrease in blood pressure by >15 mm Hg, one patient reported "warmth" after administration	Orosz et al. (1976 [PMID:798588])
125M and 82F with cerebrovascular disorders, 34-86 years old	5 mg three times per day for 4 weeks	Anorexia [2 patients], urticaria and epigastric pain [1 patient], and hot flashes [1 patient]; no significant changes in blood pressure or pulse when compared to baseline; 3 patients with altered laboratory values	Otomo et al. (1985)
20 patients with cerebrovascular and/or central nervous system degenerative disorders	Two 5 mg tablets three times per day for 30 days, then one 5 mg tablet three times per day for next 60 days	Decreased systolic pressure vs. placebo group on treatment days 14 and 60, increased mean red blood cell count and aspartate transaminase levels vs. placebo, decreased baseline hemoglobin, red blood cell count, and serum glutamic pyruvic transaminase levels were not considered clinically significant, two patients also reported hyperirritability	Peruzza and DeJacobis (1986)

Patient Population	Dosing Regimen	Side/Adverse Effects Reported	Reference
Three groups evaluated: 1. 84 patients with cerebral circulatory disorders 2. 12 patients with lesions of the optic nerve 3. 4 additional patients (2 tabetic paralysis, 1 cerebral atrophy, 1 diabetic and ischemic polyneuropathy).	Dosing was either orally or orally and intramuscularly. For oral only administration: 15 mg on the first day then increased to 35-40 mg for 3-20 weeks. For oral and intramuscular administration: 10-20 mg/day by intramuscular injection with 15-30 mg orally each day	No effect on laboratory tests conducted (e.g., urinalysis, blood sugar, and liver function). Toxicoderma developed in one patient. A "collapse feeling" was reported by a hypertensive patient (accompanied by decreased blood pressure).	Szobor and Klein (1976 [PMID:1037230])
Patients with vertigo, 18-76 years old	15 mg/day for 4 weeks	Side effect noted in one patient, but not described	Taiji and Kanzaki (1986)
15 patients with Alzheimer's disease	10 mg three times per day for 8 weeks, then 15 mg three times per day for 8 weeks, then 20 mg three times per day for 24 weeks, then 10 mg three times per day for 12 weeks	No significant adverse effects reported	Thal et al. (1989 [PMID:2715559])
9M and 10F with urge incontinence and low compliance bladder, age n.p.	5 mg three times per day for 2 weeks	Lichen ruber planus [1 patient], dry mouth [1 patient], residual urine [2 patients]	Truss et al. (2000 [PMID:11204266])

Abbreviations: F = female(s); i.v. = intravenous(ly); M = male(s); n.p. = not provided

7.0 Regulatory Status

Vinpocetine is regulated under the Dietary Supplement Health and Education Act of 1994. This act identified a new dietary ingredient as one that was not marketed in the United States prior to October 15, 1994. The first notification regarding intent to market vinpocetine as a dietary supplement was filed in July 1997 by Amrion, Inc. (U.S. FDA, 1997). Since then, six other companies have filed: Leiner Health Products (October 1998 and March 1999), General Nutrition Corporation (April 1999), Pharmavite Corporation (May 1999), Genexis™ (May 2010), Nutraceutical Sciences Institute (November 2010), and Healthy Solutions LLC (June 2010) (Genexis, 2010; Healthy Solutions LLC, 2010; U.S. FDA, 2001; Vitacost.com, 2010). Additionally, The Amen Solution, ProCaps Laboratories, Cyanotech Corporation, and Jarrow Formulas, Inc. filed notifications in 2010 to market a dietary supplement product that contained vinpocetine (Cyanotech, 2010; Jarrow Formulas, Inc., 2010; ProCaps Laboratories, 2010; The Amen Solution, 2010).

A recent Cochrane review stated, "Although used in human treatment for over twenty years, it has not been approved by any regulatory body for the treatment of cognitive impairment" (Szatmari and Whitehouse, 2009).

8.0 Toxicological Data

8.1 General Toxicology

8.1.1 Human Data

ADME: Oral Administration

Six male volunteers were exposed to radiolabeled vinpocetine orally, and distribution was followed using positron emission tomography (PET). Radioactivity concentration decreased over a time period of 30 minutes from the stomach of two participants. Radioactivity was present in the liver within 15 minutes of exposure and increased during the evaluation, while levels in the blood increased steadily with time. Radioactivity was also detected in the kidneys of two volunteers. By the end of the evaluation (120 minutes after administration), 19.30% of total radioactivity was present in the blood and 17.25% in the plasma. Unchanged vinpocetine levels decreased in urine from 38% after 15 minutes to 4% after 60 minutes. Variable brain distribution was noted; greatest uptake was observed in the thalamus, occipital cortex, basal ganglia, and some cortical structures (Gulyas et al., 2002a [PMID:12173017]).

Additional oral consumption studies that evaluated the pharmacokinetics of vinpocetine and apovincaminic acid, the main vinpocetine metabolite, are summarized in **Tables 3** and **4**, respectively.

ADME: Intravenous Administration

Studies that evaluated the pharmacokinetics of vinpocetine and apovincaminic acid are summarized in **Tables 5** and **6**, respectively.

In the studies conducted by Polgar and colleagues (1985 [PMID:16867695]), vinpocetine and apovincaminic acid were both detected in cerebrospinal fluid. Peak vinpocetine concentrations were determined 30 to 45 minutes after start of administration. Cerebral blood flow measurements indicated a significant increase 32 minutes after start of the infusion.

PET studies were conducted in three male volunteers. Volunteers were administered [^{11}C]-vinpocetine in a single i.v. injection followed by saline. Total brain uptake of vinpocetine peaked 2 minutes after administration and represented 3.71% (mean) of the total radioactivity administered. Brain distribution indicated the greatest amount was present in the thalamus, followed by the putamen, occipital cortex, and other neocortical regions. The fraction of labeled vinpocetine decreased from 70-80% at 4 minutes to 25-30% at 50 minutes after administration (Gulyas et al., 2002b [PMID:12460136]).

Table 3. Vinpocetine Pharmacokinetic Parameters after Oral Human Consumption of Vinpocetine

	Elbary et al. (2002)[a]	Elbary et al. (2002)[a]	Grandt et al. (1989) [PMID:2624613]	Miskolczi et al. (1990)[a] [PMID:2384112]	Miskolczi et al. (1990)[a,b] [PMID:2384112]
Volunteer Characteristics (Sex, Number, and Age)	24M, 23.91 years old [mean]	24M, 23.91 years old [mean]	10M and 10F, 67.61 and 69.99 years old [means], respectively	5M, 20-21 years old	5M, 20-21 years old
Dose and Dosing Period	10 mg of Product A	10 mg of Product B	20 mg for 7 days	5 mg for 7 days	10 mg for 7 days
Dosing Regimen	1×	1×	8 am, 2 pm, and 8 pm after meals	8 h on 1st day, 8, 14, and 20 h on days 2-6, 8 h on 7th day	8 h on 1st day, 8, 14, and 20 h on days 2-6, 8 h on 7th day
Blood Sample Collection Times	0.25, 0.5, 1, 1.5, 2, 2.5, 3, 4, 6, 8, and 24 h after administration	0.25, 0.5, 1, 1.5, 2, 2.5, 3, 4, 6, 8, and 24 h after administration	0.25, 0.5, 0.75, 1, 1.5, 2, 4, 6, 6.25, 6.5, 6.75, 7, 7.5, 8, 10, and 12 h after 8 am dose	0, 0.25, 0.5, 0.75, 1, 1.5, 2, 3, 4, 6, 8, 10, 12, and 24 h after administration on 1st and 7th days, 1.33 and 2.16 h after first dosage on days 2-6	0, 0.25, 0.5, 0.75, 1, 1.5, 2, 3, 4, 6, 8, 10, 12, and 24 h after administration on 1st and 7th days, 1.33 and 2.16 h after first dosage on days 2-6
Pharmacokinetic Model				Non-compartmental	Non-compartmental
AUC	519.8 ± 8.2 ng × h/mL	514.6 ± 10.7 ng × h/mL	4.6×10^{-8} mol × h/L	5.4 ± 1.4 ng × h/mL (1st day) 5.8 ± 0.6 ng × h/mL (7th day)	10.7 ± 3.4 ng × h/mL (1st day) 10.2 ± 2.6 ng × h/mL (7th day)
MRT				1.93 ± 0.37 h (1st day) 2.48 ± 0.50 h (7th day)	2.62 ± 0.81 h (1st day) 2.11 ± 0.28 h (7th day)
$t_{1/2}$	2.09 ± 0.27 h	2.20 ± 0.35 h		1.22 ± 0.32 h (1st day) 1.71 ± 0.30 h (7th day)	1.69 ± 0.70 h (1st day) 1.30 ± 0.17 h (7th day)
MAT				0.81 ± 0.38 h (1st day) 1.36 ± 0.43 h (7th day)	1.45 ± 0.83 h (1st day) 0.94 ± 0.19 h (7th day)
C_{max}	64.3 ± 1.6 ng/mL	63.5 ± 1.3 ng/mL	1.71×10^{-8} mol/L		
t_{max}	1.50 ± 0.00 h	1.50 ± 0.00 h	2.33 h		
Bioavailability			6.7%		

Abbreviations: AUC = area under the curve; C_{max} = peak plasma concentration; F = female(s); h = hour(s); M = male(s); MAT = mean absorption time; MRT = mean residence time; n.p. = not provided; $t_{1/2}$ = elimination half-life; t_{max} = time to reach peak plasma concentration

[a]Crossover design used. A period of 1 (Elbary et al.) or 2 (Miskolczi et al.) weeks was allowed between different treatments.

[b]Data were also presented on i.v. administration of vinpocetine. However, limited information was provided on the dosing regimen used. Therefore, these data were not extracted.

Table 3. Vinpocetine Pharmacokinetic Parameters after Oral Human Consumption of Vinpocetine (Continued)

	Lohmann et al. (1992) [PMID:1418055])	Lohmann et al. (1992) [PMID:1418055])	Lohmann et al. (1992) [PMID:1418055])	Lohmann et al. (1992) [PMID:1418055])	Vereczkey et al. (1979a) [PMID:582791]
Volunteer Characteristics (Sex, Number, and Age)	4M and 4F, 23-28 years old	4M and 4F, 23-28 years old	4M and 4F, 23-28 years old	4M and 4F, 23-28 years old	2M and 1F, 28, 20, and 29 years old, respectively
Dose and Dosing Period	10 mg	10 mg	10 mg	10 mg	10 mg
Dosing Regimen	1× at 7:06 am, no breakfast consumed	1× at 7:06 am, breakfast consumed at 7:15 am	1× at 7:24 am, breakfast consumed at 7:15 am	1× at 7:57 am, breakfast consumed at 7:15 am	1×
Blood Sample Collection Times	Between 7 and 8 am	Between 7 and 8 am	Between 7 and 8 am	Between 7 and 8 am	0.083, 0.25, 0.5, 1, 2, 4, 6, and 8 h after administration
Pharmacokinetic Model					Two-compartment open system
AUC	27.26 ± 18.08 ng × h/mL	42.78 ± 27.04 ng × h/mL	46.48 ± 23.51 ng × h/mL	54.33 ± 38.42 ng × h/mL	
MRT	3.03 ± 1.20 h	2.65 ± 0.57 h	2.20 ± 0.36 h	2.68 ± 0.52 h	
$t_{1/2}$					
MAT					
C_{max}	15.23 ± 12.62 ng/mL	25.12 ± 19.24 ng/mL	34.90 ± 26.22 ng/mL	28.41 ± 28.19 ng/mL	20-63 ng/mL
t_{max}	0.91 ± 0.23 h	0.78 ± 0.21 h	0.72 ± 0.16 h	1.44 ± 0.46 h	1 - 1.5 h
Bioavailability					56.6 ± 8.9% (mean)

Abbreviations: AUC = area under the curve; C_{max} = peak plasma concentration; F = female(s); h = hour(s); M = male(s); MAT = mean absorption time; MRT = mean residence time; n.p. = not provided; $t_{1/2}$ = elimination half-life; t_{max} = time to reach peak plasma concentration

Table 4. Apovincaminic Acid Pharmacokinetic Parameters after Oral Human Consumption of Vinpocetine

	Chen et al. (2006) [PMID:16321580]	Grandt et al. (1989) [PMID:2624613]	Miskolczi et al. (1990)* [PMID:2384112]	Miskolczi et al. (1990)* [PMID:2384112]	Vlase et al. (2005)* [PMID:16366040]
Volunteer Characteristics (Sex, Number, and Age)	20M (Chinese), 18-24 years old	10M and 10F, 67.61 and 69.99 years old [means], respectively	5M, 20-21 years old	5M, 20-21 years old	24M (Caucasian), 22.5 ± 2.6 years old
Vinpocetine Dose and Dosing Period	10 mg once	20 mg for 7 days	5 mg for 7 days	10 mg for 7 days	10 mg (manufacturer: Vim Spectrum [test preparation]) 10 mg (local pharmacy [reference preparation])
Dosing Regimen	1x	8 am, 2 pm, and 8 pm after meals	8 h on 1st day, 8, 14, and 20 h on days 2-6, 8 h on 7th day	8 h on 1st day, 8, 14, and 20 h on days 2-6, 8 h on 7th day	1x
Blood Sample Collection Times	0, 0.25, 0.5, 0.75, 1, 1.5, 2, 2.5, 3, 4, 5, 6, 8 h after consumption	0.25, 0.5, 0.75, 1, 1.5, 2, 4, 6, 6.25, 6.5, 6.75, 7, 7.5, 8, 10, and 12 h after 8 am dose	0, 0.25, 0.5, 0.75, 1, 1.5, 2, 3, 4, 6, 8, 10, 12, and 24 h after administration on 1st and 7th days, 1.33 and 2.16 h after first dosage on days 2-6	0, 0.25, 0.5, 0.75, 1, 1.5, 2, 3, 4, 6, 8, 10, 12, and 24 h after administration on 1st and 7th days, 1.33 and 2.16 h after first dosage on days 2-6	0.5, 0.83, 1.16, 1.5, 2, 2.5, 3, 4, 6, 8, 10, and 12 h after consumption
Pharmacokinetic Model			Non-compartmental	Non-compartmental	Non-compartmental
AUC	238 ± 51 ng × h/mL	1.92×10^{-6} mol × h/L	240.7 ± 34.5 ng × h/mL (1st day) 214.0 ± 57.1 ng × h/mL (7th day)	383.3 ± 163.4 ng × h/mL (1st day) 232.5 ± 67.5 ng × h/mL (7th day)	95.1 ± 29.2 ng/mL × h [test] 96.9 ± 26.2 ng/mL × h [reference]
MRT			9.3 ± 2.0 h (1st day) 8.5 ± 3.5 h (7th day)	9.2 ± 1.5 h (1st day) 6.8 ± 2.3 h (7th day)	2.01 ± 0.36 h [test] 1.96 ± 0.36 h [reference]
$t_{1/2}$	1.8 ± 0.5 h (terminal elimination phase)		6.5 ± 1.3 h (1st day) 6.1 ± 2.7 h (7th day)	6.8 ± 0.7 h (1st day) 5.5 ± 1.9 h (7th day)	0.97 ± 0.27 h [test] 0.96 ± 0.28 h [reference]
C_{max}	99.9 ± 29.8 ng/mL	6.39×10^{-7} mol/L			49.5 ± 16.1 ng/mL [test] 51.4 ± 14.0 ng/mL [reference]
t_{max}	1.3 ± 0.5 h	2.41 h			1.11 ± 0.36 h [test] 1.02 ± 0.35 h [reference]
V_d/F					138 ± 74 L [test] 114.3 ± 47 L [reference]
t_{lag}					0.55 ± 0.22 h [test] 0.58 ± 0.2 [reference]

Abbreviations: AUC = area under the curve; C_{max} = peak plasma concentration; F = female(s); h = hour(s); M = male(s); MAT = mean absorption time; MRT = mean residence time; n.p. = not provided; $t_{1/2}$ = elimination half-life; t_{max} = time to reach peak plasma concentration; t_{lag} = lag time; V_d/F = apparent volume of distribution
*Crossover design used. A period of 2 weeks (Miskolczi et al.) or 1 week (Vlase et al.) was allowed between different dosages.

Table 5. Vinpocetine Pharmacokinetic Parameters after Intravenous Human Exposure of Vinpocetine

	Grandt et al. (1989) [PMID:2624613]	Miskolczi et al. (1987) [PMID:3691609]	Miskolczi et al. (1987) [PMID:3691609]	Polgar et al. (1985) [PMID:16867695]	Vereczkey et al. (1979a)* [PMID:582791]
Volunteer Characteristics (Sex, Number, and Age)	10M and 10F, 67.61 and 69.99 years old [means], respectively	7 subjects (sex n.p.), 63-79 years old	Number and sex of volunteers n.p., 21-26 years old	11M and 1F, 35-56 years old, either had stenosis or occlusion of internal carotid arteries	5M and 1F, 20-68 years old
Dose	10 mg	10 mg	10 mg	1 mg/kg	10 mg
Dosing Regimen	8 am and 2 pm	1×	1×	1× at 4 mL/min	1×
Blood Sample Collection Times	0.25, 0.5, 0.75, 1, 1.5, 2, 4, 6, 6.25, 6.5, 6.75, 7, 7.5, 8, 10, and 12 h after 8 am dose	0.08, 0.17, 0.2, 0.25, 0.33, 0.5, 0.67, 0.92, 1.17, 1.67, 2.17, 3.17, 4.17, 8.17, 8, 10, and 12 h after infusion [Note: Graphs suggest that time point is not 8.17, but 6.17 hours.]	0.08, 0.17, 0.2, 0.25, 0.33, 0.5, 0.67, 0.92, 1.17, 1.67, 2.17, 3.17, 4.17, 8.17, 8, 10, and 12 h after infusion [Note: Graphs suggest that time point is not 8.17, but 6.17 hours.]	0.08, 0.17, 0.33, 0.42, 0.5, 0.75, 1, 1.5, 2, 3, 4, 8, 10, 12, and 24 h after start of the infusion (from 6 patients)	0.083, 0.25, 0.5, 1, 2, 4, 6, and 8 h after administration
Pharmacokinetic Model				First-pass three compartment open model	Two-compartment open systems
AUC	3.42×10^{-7} mol × h/L	81.6 ± 32.1 ng × h/mL	157.8 ± 39.1 ng × h/mL	1269 ± 151 ng × h/mL	460.11 ± 188.22 ng × h/mL
$t_{1/2}$		2.12 ± 0.51 h	2.54 ± 0.48 h	0.044 ± 0.00 h 0.456 ± 0.08 h 4.71 ± 2.13 h	0.136 ± 0.02 h (distribution phase) 4.83 ± 1.29 h (elimination phase)
C_{max}	2.58×10^{-7} mol/L				
t_{max}	0.86 h				
V_d or V_d/F		6.7 ± 3.7 L/kg	3.2 ± 0.9 L/kg	407 ± 259 L	2.87 ± 2.74 L/kg
CL		2.20 ± 0.90 L/h/kg	0.88 ± 0.20 L/h/kg	0.79 ± 0.10 L/h/kg	0.366 ± 0.240 L/h/kg
Vd_{SS}					2.079 ± 2.39 L/kg

Abbreviations: AUC = area under the curve; C_{max} = peak plasma concentration; CL = clearance; F = female(s); h = hour(s); M = male(s); n.p. = not provided; $t_{1/2}$ = elimination half-life; t_{max} = time to reach peak plasma concentration; V_d = volume of distribution; V_d/F = apparent volume of distribution; Vd_{SS} = volume at steady state
*Data were also presented on multiple i.v. dosing of vinpocetine. However, limited information was provided on the dosing regimen used. Therefore, these data were not extracted.

Table 6. Apovincaminic Acid Pharmacokinetic Parameters after Intravenous Human Exposure of Vinpocetine

	Grandt et al. (1989) [PMID:2624613]	Miskolczi et al. (1987)* [PMID:3691609]	Miskolczi et al. (1987)* [PMID:3691609]	Polgar et al. (1985) [PMID:16867695]
Volunteer Characteristics (Sex, Number, and Age)	10M and 10F, 67.61 and 69.99 years old [means], respectively	7 subjects (sex n.p.), 63-79 years old	Number and sex of volunteers n.p., 21-26 years old	11M and 1F, 35-56 years old, either had stenosis or occlusion of internal carotid arteries
Dose	10 mg	10 mg	10 mg	1 mg/kg
Dosing Regimen	8 am and 2 pm	1×	1×	1× at 4 mL/min
Blood Sample Collection Times	0.25, 0.5, 0.75, 1, 1.5, 2, 4, 6, 6.25, 6.5, 6.75, 7, 7.5, 8, 10, and 12 h after 8 am dose	0.08, 0.17, 0.2, 0.25, 0.33, 0.5, 0.67, 0.92, 1.17, 1.67, 2.17, 3.17, 4.17, 8.17, 8, 10, and 12 h after infusion [Note: Graphs suggest that time point is not 8.17, but 6.17 hours]	0.08, 0.17, 0.2, 0.25, 0.33, 0.5, 0.67, 0.92, 1.17, 1.67, 2.17, 3.17, 4.17, 8.17, 8, 10, and 12 h after infusion [Note: Graphs suggest that time point is not 8.17, but 6.17 hours]	0.08, 0.17, 0.33, 0.42, 0.5, 0.75, 1, 1.5, 2, 3, 4, 8, 10, 12, and 24 h after start of the infusion (from 6 patients)
Pharmacokinetic Model				First-pass three compartment open model
AUC	1.69×10^{-6} mol × h/L	644.4 ± 152.7 ng × h/mL	431.0 ± 135.0 ng × h/mL	3386 ± 1143 ng × h/mL
$t_{1/2}$		5.83 ± 1.56 h	2.30 ± 1.20 h	3.9 ± 1.6 h
C_{max}	5.45×10^{-7} mol/L			
t_{max}	1.25 h			
V_d or V_d/F		0.53 ± 0.27 L/kg	0.26 ± 0.11 L/kg	
CL		0.07 ± 0.03 L/h/kg	0.11 ± 0.04 L/h/kg	

Abbreviations: AUC = area under the curve; C_{max} = peak plasma concentration; CL = clearance; F = female(s); h = hour(s); M = male(s); n.p. = not provided; $t_{1/2}$ = elimination half-life; t_{max} = time to reach peak plasma concentration; V_d = volume of distribution; V_d/F = apparent volume of distribution
*Dose used for calculation of pharmacokinetic parameters was taken as the amount measured in urine collected from 0-24 hours after vinpocetine exposure.

8.1.2 Chemical Disposition, Metabolism, and Toxicokinetics

Oral Administration

Rats [sex and strain not provided (n.p.)] were orally administered 10 mg/kg tritiated-vinpocetine. Plasma was collected two hours after administration. Urine was also collected for metabolite evaluation. Metabolite evaluation indicated the majority of the urinary radioactivity was associated with a single compound, which was identified as apovincaminic acid. Unchanged vinpocetine was also identified in the urine. Two additional metabolites were present in some urine samples, but they were not structurally identified. Analyses of the collected plasma indicated that the majority of the radioactivity was excreted as either apovincaminic acid or vinpocetine (Vereczkey and Szporny, 1976 [PMID:1037219]). [Note: Chromatograph of urine shown indicates data were obtained after oral administration. However, it is unclear whether similar metabolites were obtained using intraperitoneal (i.p.) injection (see below).]

Male and female Wistar rats were orally administered 10 mg/kg tritiated-vinpoctine. Rats were killed at selected time points and blood and organs were collected up to 48 hours after vinpocetine administration. Urine and feces were also collected for evaluation up to 48 hours after treatment. Evaluation of vinpocetine concentrations in collected organs indicated maximal concentrations occurred approximately two hours after administration. The organs with the greatest amounts were the liver and small intestine, followed by the lung, stomach, kidney, and adrenals. By 48 hours after administration, vinpocetine levels were minimal in most organs except the liver and kidneys. Within 48 hours of administration; 46.7% and 33.5% of the administered radioactivity were recovered from the urine and feces, respectively. Bile excretion studies indicated that <5% of administered vinpocetine was excreted in the bile after nine hours, while blood analyses indicated that a majority of the vinpocetine was present in the plasma fraction (86%) compared to the blood cell fraction (14%). Additionally, a majority of the vinpocetine present in the plasma fraction was bound to proteins (Vereczkey et al., 1976 [PMID:1037218]).

Wistar rats were orally administered 10 mg/kg vinpocetine for five days. On the last day, rats were also administered 10 mg/kg tritiated-vinpocetine. Excretion studies indicated that ~75% of the administered radiolabel was excreted within 48 hours; 46.9% and 28.3% were excreted in the urine and feces, respectively (Vereczkey et al., 1976 [PMID:1037218]).

Pharmacokinetic parameters calculated from rodent oral administration studies for vinpocetine and apovincaminic acid are provided in **Tables 7** and **8**, respectively.

Intravenous Administration

Pharmacokinetic parameters calculated from rodent i.v. administration studies for vinpocetine and apovincaminic acid are provided in **Table 9**.

Table 7. Vinpocetine Pharmacokinetic Parameters after Oral Rodent Exposure of Vinpocetine

	Sozanski et al. (2011)	Vereczkey et al. (1979b) [PMID:582790]	Xia et al. (2010) [PMID:20561830]
Species, Strain, Sex, Age, and Number	Rat, Wistar, M, age n.p., 12	Rat, Wistar, M&F, age and number n.p.	Rat, Sprague-Dawley, M&F, 14 weeks old, number, n.p.
Vinpocetine Dose	2 mg/kg	2.5 mg/kg tritiated vinpocetine	1 mg/kg
Blood Sample Collection Times	0.25, 0.5, 1, 1.5, 2, 3, 4, 5, 6, 8, 10, and 12 h after administration	Up to 10 hours after administration	0.083, 0.25, 0.5, 0.75, 1, 2, 3, 4, 8, and 12 h after administration
Pharmacokinetic Model	Non-compartmental	Two-compartment open system	
C_{max}	135.33 ± 11.71 ng/mL		23.8 ± 6.3 ng/mL
t_{max}	1.50 ± 0.0 h	1 h	0.75 ± 0.25 h
$t_{1/2}$	1.73 ± 0.5 h	141 min	2.9 ± 0.6 h
MRT	3.62 ± 0.21 h		
AUC_{0-t}	504.03 ± 57.28 ng × h/mL		57.4 ± 10.3 ng × h/mL
$AUC_{0-\infty}$	524.60 ± 56.67 ng × h/mL	39,250 ng/mL/min	
AUC_r	3.95 ± 2.45 % $AUC_{0-\infty}$		
CL	37.03 ± 4.73 mL/min; 80.43 ± 8.92 mL/min/kg		
V_d	5.60 ± 1.55 L; 12.25 ± 3.53 L/kg		
Bioavailability		52%	

Table 8. Apovincaminic Acid Pharmacokinetic Parameters after Oral Rodent Exposure of Vinpocetine

	Vereczkey et al. (1979b) [PMID:582790]	Xia et al. (2010) [PMID:20561830]
Species, Strain, Sex, Age, and Number	Rat, Wistar, M&F, age and number n.p.	Rat, Sprague-Dawley, M&F, 14 weeks old, number, n.p.
Vinpocetine Dose	2.5 mg/kg tritiated vinpocetine	1 mg/kg
Blood Sample Collection Times	Up to 24 hours after administration	0.083, 0.25, 0.5, 0.75, 1, 2, 3, 4, 8, and 12 h after administration
Pharmacokinetic Model	Two-compartment open system	
C_{max}		86.6 ± 22.6 ng/mL
t_{max}		1.25 ± 0.7 h
$t_{1/2}$	570 min	3.2 ± 0.6 h
AUC_{0-t}		471.6 ± 89.0 ng × h/mL
$AUC_{0-\infty}$	463,300 ng/mL/min	

Abbreviations: AUC = area under the curve (0-t: time 0 to last measureable time point, 0-∞: total, r: relative); C_{max} = peak plasma concentration; CL = clearance; F = female(s); h = hour(s); M = male(s); MRT = mean residence time; n.p. = not provided; $t_{1/2}$ = elimination half-life; t_{max} = time to reach peak plasma concentration; V_d = volume of distribution

Table 9. Vinpocetine and Apovincaminic Acid Pharmacokinetic Parameters after Intravenous Rodent Exposure of Vinpocetine

	Vereczkey et al. (1976) [PMID:1037218]	Vereczkey et al. (1979b) [PMID:582790]	Xia et al. (2010) [PMID:20561830]	Xia et al. (2010) [PMID:20561830]
Chemical	Vinpocetine	Vinpocetine	Vinpocetine	Apovincaminic Acid
Species, Strain, Sex, Age, and Number	Rat, Wistar, M&F, age and number n.p.	Rat, Wistar, M&F, age and number n.p.	Rat, Sprague-Dawley, M&F, 14 weeks old, number, n.p.	Rat, Sprague-Dawley, M&F, 14 weeks old, number, n.p.
Vinpocetine Dose	1 mg/kg tritiated vinpocetine	2.5 mg/kg tritiated vinpocetine	1 mg/kg	1 mg/kg
Blood Sample Collection Times	Up to 48 hours after administration	Up to 10 hours after administration	0.083, 0.25, 0.5, 0.75, 1, 2, 3, 4, 8, and 12 h after administration	0.083, 0.25, 0.5, 0.75, 1, 2, 3, 4, 8, and 12 h after administration
Pharmacokinetic Model		Two-compartment open system		
$t_{1/2}$	17 h	15.2 min ($T^{\alpha}_{1/2}$) 125 min ($T^{\beta}_{1/2}$)	3.0 ± 0.6 h	2.8 ± 0.6 h
AUC_{0-t}			315.4 ± 79.4 ng × h/mL	1253.6 ± 259.6 ng × h/mL
AUC		76,100 ng/mL/min		
Vd_{SS}		528 mL		
V_d		830 mL		
V_1		208 mL		
Notes	Blood concentrations decreased rapidly after administration followed by a slower elimination phase.	Regression curve analysis of the concentration-time curve indicated that the data fit best to a two-compartment model. Evaluation of vinpocetine levels indicated two phases: rapid distribution phase followed by a slower elimination phase. [Note: The $t_{1/2}$ for apovincaminic acid is 360 min, and the AUC is 241,500 ng/mL/min.]		

Abbreviations: AUC = area under the curve (0-t: time 0 to last measureable timepoint); F = female(s); h = hour(s); M = male(s); n.p. = not provided; $t_{1/2}$ = elimination half-life; V_1 = volume of central compartment; V_d = volume of distribution; Vd_{SS} = volume at steady state

Intraperitoneal Administration

Rats [sex and strain n.p.] were administered tritiated-vinpocetine [dose n.p.] by i.p. injection. Bile was collected for metabolite evaluation. Four metabolites were identified, none of which was apovincaminic acid. One of the metabolites could not be structurally identified. Two of the metabolites were identified as ethyl vincaminate and hydroxyvinpocetine, with the hydroxylation occurring on the A-ring. The remaining metabolite was identified as a dihydroxylated, glycine-conjugate of apovincaminic acid (Vereczkey and Szporny, 1976 [PMID:1037219]). A recent study identified the structure of the hydroxyvinpocetine as 10-hydroxyvinpocetine. An *N*-oxide derivative of vinpocetine was also identified as a novel minor metabolite (Nemes et al., 2008).

Male and female Wistar rats were administered 10 mg/kg tritiated-vinpocetine by i.p. injection. Feces and urine were collected up to 48 hours after administration. Results indicated that 76% of the administered radioactivity was excreted in the urine and feces within 48 hours (54.7% and 21.3%, respectively). Bile elimination studies showed that ~20% of the administered radioactivity was excreted in bile within nine hours (Vereczkey et al., 1976 [PMID:1037218]).

8.1.3 Acute Exposure

Acute toxicity values for vinpocetine are presented in **Table 10**.

Table 10. Acute Toxicity Values for Vinpocetine

Route	Species (Strain and Sex)	LD_{50} (mg/kg)	Reference(s)
p.o.	Mouse (CFLP, M&F)	534	Cholnoky and Dömök (1976 [PMID:1037220]); Palosi and Szporny (1976 [PMID:1037217])
p.o.	Rat (Wistar, M&F)	503.3	Cholnoky and Dömök (1976 [PMID:1037220]); Palosi and Szporny (1976 [PMID:1037217])
i.v.	Mouse (CFLP, M&F)	58.7	Cholnoky and Dömök (1976 [PMID:1037220]); Palosi and Szporny (1976 [PMID:1037217])
i.v.	Mouse (strain and sex n.p.)	45	RTECS (2012)
i.v.	Rat (Wistar, M&F)	42.6	Cholnoky and Dömök (1976 [PMID:1037220]); Palosi and Szporny (1976 [PMID:1037217])
i.v.	Rat (strain and sex n.p.)	32	RTECS (2012)
i.p.*	Mouse (CFLP, M&F)	161.2	Cholnoky and Dömök (1976 [PMID:1037220])
i.p.	Mouse (CFLP, M&F)	240	Palosi and Szporny (1976 [PMID:1037217])
i.p.	Mouse (strain and sex n.p.)	117	RTECS (2012)
i.p.*	Rat (Wistar, M&F)	133.8	Cholnoky and Dömök (1976 [PMID:1037220]); Palosi and Szporny (1976 [PMID:1037217])
i.p.	Rat (strain and sex n.p.)	119	RTECS (2012)

Abbreviations: F = female(s); i.p. = intraperitoneal; i.v. = intravenous; p.o. = *per os*; LD_{50} = lethal dose for 50% of test animals; M = male(s)

*Text indicates that an intramuscular injection was performed, while a summary table indicates that an i.p. injection was performed.

Ataxia and clonic convulsions were noted in mice and rats administered "lethal doses" of vinpocetine (Cholnoky and Dömök, 1976 [PMID:1037220]). [Note: No additional information was provided on the dose that produced the noted effects.]

Increased sensitivity to environmental stimuli was observed in mice and rats administered 0.5-8 mg/kg vinpocetine by i.p. injection. Spontaneous motility was decreased at higher doses (16-32 mg/kg). At 64 mg/kg, reduced spontaneous motility was followed by clonic convulsions. Reduced orientation hypermotility and locomotor activity were also associated with the highest dose (Palosi and Szporny, 1976 [PMID:1037217]).

Sprague-Dawley rats were orally administered 1, 10, or 30 mg/kg vinpocetine to assess hemodynamic effects. The high dose increased mean arterial pressure by 12 mm Hg. Comparatively, cerebral blood flow was decreased only at the low dose. Renal blood flow decreased after administration of the low and mid doses. No significant changes in cardiac output, total peripheral resistance, or heart rate were noted (Ferrone et al., 1986 abstr.).

8.1.4 Short-Term and Subchronic Exposure

Male CD rats were orally administered 25 or 100 mg/kg vinpocetine over a four-week period [dosing interval n.p.]. No deaths or changes in body weight gain were noted at either dose. Increased salivation was seen at the higher dose. Increases in liver and thyroid weights were also observed at the higher dose tested; however, there were no histopathological changes in these organs. No other effects (e.g., altered liver function, altered blood glucose levels, and altered serum chemistry) were observed (Cholnoky and Dömök, 1976 [PMID:1037220]).

Sprague-Dawley rats were orally administered 3, 10, or 30 mg/kg vinpocetine for five days to assess hemodynamic effects. Mean arterial pressure was not altered at any of the doses tested. Comparatively, cardiac output was increased in high-dose rats. Decreased bronchial blood flow was noted after administration of the low dose, and increased splanchnic blood flow was noted after administration of the high dose (Ferrone et al., 1986 abstr.).

A short-term rat toxicity study in a Japanese-language journal was indexed by RTECS (2012). According to the abstracted data, rats were orally administered vinpocetine for five weeks. Observed effects included fluid intake, increased urine volume, and weight loss or decreased weight gain. The lowest toxic dose (TD_{Lo}) was 4375 mg/kg.

Male and female Wistar rats were administered 5 or 25 mg/kg vinpocetine by i.p. injection for three months. Animals were dosed five times per week during the dosing period. At the higher dose, three of eight males and two of eight females died; death was attributed to severe confluent fibroblastic peritonitis and ascites. In remaining animals, no effect on erythropoiesis, leukopoiesis, or bromosulfalein excretion (as an indicator of liver function) was observed. Histopathological changes associated with exposure to vinpocetine were not noted (Cholnoky and Dömök, 1976 [PMID:1037220]).

8.1.5 Chronic Exposure

Male and female CFY rats were administered 25, 50, or 100 mg/kg vinpocetine by gastric intubation. Animals were administered vinpocetine five times per week for six months. No

deaths associated with vinpocetine exposure were observed. Animals were identified as agitated during treatment. Body weight gain changes were not related to the administered dose. No adverse effects were noted on a variety of endpoints evaluated (e.g., erythropoiesis, liver or kidney function, glucose metabolism, or thrombocytopoiesis). Relative organ weights were unaffected. Mild tubular degeneration was observed in some mid-dose animals. Minor nuclear swelling was also noted in the liver (Cholnoky and Dömök, 1976 [PMID:1037220]). [Note: It is unclear from the text if the swelling occurred only in the mid-dose animals.]

A long-term rat toxicity study in a Japanese-language journal was indexed by RTECS (2012). According to the abstracted data, rats were orally administered vinpocetine for 26 weeks. Observed effects included changes in liver and adrenal weight and increased urine volume. The TD_{Lo} was 14,560 mg/kg.

8.1.6 Synergistic/Antagonistic Effects

Reviews that discuss antagonistic and/or synergistic effects include articles by Thorne Research, Inc. (2002), Medina (2011), and Patyar and colleagues (2011). The following section summarizes selected findings from these reviews.

Postnatal exposure to vinpocetine antagonized lead-induced hyperactivity in female Swiss mice pups. Mice were exposed to lead acetate in water starting two months prior to mating until postnatal day (PND) 10. On PND 30, pups were administered 20 mg/kg vinpocetine by i.p. injection. The ambulatory activity of control female pups was 25.3% higher than those that received vinpocetine. There was no difference in the ambulatory activity between control groups and those that received lead and vinpocetine (Nunes et al., 2011 abstr.).

Vinpocetine antagonized convulsions induced by electroshock and metrazol in mice after i.p. administration; the median effective doses were 18.3 and 62.1 mg/kg, respectively. Vinpocetine antagonized hexobarbital-induced sleeping time at 16 and 32 mg/kg, but increased hexobarbital-induced sleeping time at 64 mg/kg in mice (Palosi and Szporny, 1976 [PMID:1037217]).

Vinpocetine antagonized liver injury induced by carbon tetrachloride (CCl_4) in male and female Sprague-Dawley rats. Rats were orally administered 2.1, 4.2, or 8.4 mg/kg vinpocetine together with CCl_4 for 15 days. Vinpocetine co-administration was associated with dose-dependent reduction of CCl_4-induced increases in alanine aminotransferase, aspartate aminotransferase, and alkaline phosphatase. In rats only treated with CCl_4, changes in hepatic architecture were noted (e.g., degeneration of hepatocytes). Co-administration of vinpocetine produced a protective effect on the liver. Dilation of blood vessels and proliferation and hypertrophy were noted in bile duct, but an improvement in hepatocyte structure was also seen. Quantitative analysis indicated >72% reduction in the area of damage when vinpocetine was administered compared to control animals (Salam et al., 2006, 2007).

The use of vinpocetine has been shown to antagonize the effects produced by postnatal alcohol exposure in rats. Long Evans rats were administered ethanol on alternate days from PND 4 to PND 10. Rats were then administered 20 mg/kg vinpocetine by i.p. injection on PND 25, 27, and 29, or PND 25 and 27 to assess effects on memory and learning as measured in the Morris water maze. Ethanol significantly increased the time needed by rats to locate a hidden-escape

platform when compared to control animals. Vinpocetine treatment significantly decreased the time rats needed to locate the platform, when compared to ethanol-treated rats. However, there was no difference between control and vinpocetine-treated rats in the time needed to locate the platform (Filguiras and Medina, 2013 abstr.; Filgueiras et al., 2009 abstr., 2010). Acute i.p. vinpocetine administration (20 mg) antagonized hyperactivity associated with alcohol exposure in mice (Nunes et al., 2011 [PMID:21689896]). A more recent study showed that vinpocetine administration antagonized ethanol effects on ocular dominance plasticity (Lantz et al., 2012).

Vinpocetine antagonized the effects produced by streptozotocin on learning and memory. Vinpocetine (5, 10, or 20 mg/kg) was administered by i.p. injection to male Wistar rats for 21 days after intracerebroventricular administration of streptozotocin. Similar to the results noted above, vinpocetine decreased the time needed for rats to locate a hidden platform in the Morris water maze when compared to rats that only received streptozotocin. Vinpocetine treatment was also associated with improved memory, as measured in a passive avoidance test. Vinpocetine treatment decreased streptozotocin-induced brain acetylcholinesterase activity and levels of lactate dehydrogenase, malondialdehyde, glutathione, and nitrate (Deshmukh et al., 2009 [PMID:19699735]).

In addition to learning and memory, a recent study showed that vinpocetine also antagonized the effects produced by rotenone on movement in rats. Vinpocetine treatment significantly reversed the rotenone-induced locomotor effects and increased dopamine levels in the striatum. Decreased levels of malondialdehyde and reduced glutathione were also observed (Zaitone et al., 2012).

In vitro studies using primary rat cerebrocortical cultures showed that vinpocetine blocked veratridine-induced cell death in a dose-dependent manner. The calculated IC_{50} for vinpocetine was 490 nM (Lakics et al., 1995 [PMID:7746503]).

8.1.7 Cytotoxicity

No data were located.

8.2 Reproductive and Teratological Effects

All of the following studies were obtained from a single source, Cholnoky and Dömök (1976). The source provided limited details on the experimental methods used for each of the studies described and provided limited information on the experimental results and findings.

Male CFY rats were orally administered 10 or 50 mg/kg vinpocetine for eight weeks prior to mating with untreated females. Mating ability and fertility were not affected by treatment. Relative prostate weight was decreased in the high-dose group (Cholnoky and Dömök, 1976 [PMID:1037220]).

Female CFY were orally administered 10 or 50 mg/kg vinpocetine for eight weeks prior to mating with untreated males. No effects on estrous cycle, mating ability, and fertility were observed (Cholnoky and Dömök, 1976 [PMID:1037220]).

Pregnant CD rats were orally administered 12.5, 25, or 50 mg/kg vinpocetine on gestation days (GD) 6-15. Animals were examined on GD 6, 8, 10, 12, 14, 15, and 21. All dams were euthanized on GD 21. Piloerection, impaired grooming, and a reduction in body weight gain were observed at the high dose. No adverse effects were noted in the low- or mid-dose groups. "In litters that survived to term, no adverse effects were observed on litter size or foetal weight that could be attributed to treatment" (Cholnoky and Dömök, 1976 [PMID:1037220]). [Note: It is unclear from the text how many litters may not have survived to term in each dose group.]

Pregnant rats were orally administered 15, 50, or 150 mg/kg vinpocetine on GD 7-15. [Note: Animals identified as "home colony."] Dams were euthanized on GD 20. Uterine bleeding was noted in animals administered 50 or 150 mg/kg vinpocetine; bleeding started on day 2-3 of treatment and lasted for 10 days. Fetal mortality was "particularly high" in animals administered 150 mg/kg vinpocetine. Significantly increased fetal retardation was also noted in the mid- and high-dose groups (Cholnoky and Dömök, 1976 [PMID:1037220]). [Note: It is unclear from the text how many litters may not have survived to term in each dose group.]

Pregnant CFY rats were orally administered 15, 45, or 135 mg/kg vinpocetine on GD 7-14. Animals were examined and weighed daily and euthanized on GD 21. Three of 18 dams died after administered 135 mg/kg vinpocetine. Body weight gain was decreased 40% when compared to control animals. Additionally, one dam had an abortion and ten had complete fetal loss. Increased fetal death was noted in the mid-dose animals but not in the low-dose animals. Retardation was noted in all dose groups, but no significant malformations were observed (Cholnoky and Dömök, 1976 [PMID:1037220]). [Note: No information is provided on what a "significant malformation" would encompass.]

Pregnant CFY rats were orally administered 15, 45, or 135 vinpocetine for eight days starting on GD 14. Dams were weighed daily during treatment. Offspring were examined daily and weighed weekly until 30 days old. Two of 18 high-dose animals died. [Note: Text states "… all fetuses were dead, uterine bleeding was observed." It is presumed that the statement refers to all surviving animals.] No adverse effects were noted in offspring up to day 30 (Cholnoky and Dömök, 1976 [PMID:1037220]).

Pregnant CFY rats were administered 3.13, 6.25, or 12.5 mg/kg vinpocetine by i.v. injection on GD 7-14. Animals were examined and weighed daily and euthanized on GD 21. Uterine bleeding occurred at all doses. One high-dose dam had an abortion. Fetal growth was decreased in all dose groups by 10%, when compared to controls. There was a dose-related decrease in fetal death but no significant malformations at any of the tested doses (Cholnoky and Dömök, 1976 [PMID:1037220]). [Note: No information is provided on what a "significant malformation" would encompass.]

Pregnant CFY rats were administered 3.15, 6.25, 12.5, or 25.0 mg/kg vinpocetine by i.v. injection for eight days starting on GD 14. All high-dose rats died within 30 minutes of treatment. Additionally, three of 20 dams administered 12.5 mg/kg vinpocetine died by treatment day 2 and two of 20 had abortions by treatment day 6. One of 18 females administered 3.15 mg/kg vinpocetine had no live offspring. [Note: Conflicting information on dose present in reference. One location states dose was 3.13 mg/kg, while the other states the dose was 3.15

mg/kg.] Offsprings of mid-dose females had significantly decreased body weights on day 30 (Cholnoky and Dömök, 1976 [PMID:1037220]).

A rat reproductive toxicity study in a Japanese-language journal was indexed by RTECS (2012). According to the abstracted data, pregnant rats were orally administered vinpocetine on GD 7-15. Observed fetal effects included altered litter size, fetal death, and fetotoxicity. Musculoskeletal system abnormalities, altered live birth index, and altered viability index were also reported. The TD_{Lo} was 1 g/kg.

8.3 Carcinogenicity
No data were located.

8.4 Initiation/Promotion Studies
No data were located.

8.5 Genotoxicity
No data were located.

8.6 Cogenotoxicity
No data were located.

8.7 Immunotoxicity
No data were located.

8.8 Other Data
Anti-Inflammatory Effects

Vinpocetine inhibited tumor necrosis factor (TNF)-α induced activation of nuclear factor-κB. The observed inhibition was through direct inhibition of IκB kinase and not through effects on phosphodiesterase activity or Ca^{+2} channels (Jeon et al., 2010). A single dose of vinpocetine also decreased interleukin-1β and TNF messenger ribonucleic acid expression in rat hippocampus (Gomez et al., 2013 abstr.).

Anticarcinogenicity

In a xenograft model of breast cancer in nude mice (using MDA-MB-231), i.p. administration of vinpocetine inhibited tumor growth (Huang et al., 2012 [PMID:22729609]).

Cell Proliferation

Vinpocetine inhibited the cellular proliferation of four human breast cancer cell lines: MDA-MB-231, MDA-MB-468, MCF-7, and ZR-75-1. IC_{50} values ranged from 23.5 to 32.2 µM. Vinpocetine induced apoptosis in MDA-MB-231 and MCF-7 cells (Huang et al., 2012 [PMID:22729609]). Comparatively, it did not affect proliferation of murine thymus and spleen cells *in vitro* (Banner et al., 1996 [PMID:8843508]).

Vinpocetine inhibited lipopolysaccharide-induced proliferation of mouse spleen cells. The calculated half maximal inhibitory concentration (IC_{50}) was 7.2 µM. Comparatively, vinpocetine had minimal inhibitory effect on phytohemagglutinin- and concanavalin A-induced proliferation

of mouse spleen cells (IC_{50} values >10 µM) (Banner et al., 1996 [PMID:8843508]).

Cell Migration

In vitro, vinpocetine inhibited migration of MDA-MB-231 cells at concentrations ≥15 µM (Huang et al., 2012 [PMID:22729609]).

PubChem BioAssay Results

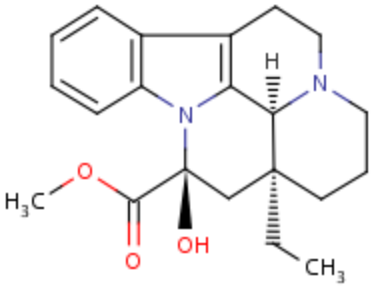
Vinpocetine has been evaluated in 1101 unique tests in 917 different bioassays. Of these tests, it was identified as active in 52 tests (PubChem BioAssay, undated). The tests where vinpocetine was classified as positive and the protein target, when specified, are provided in the table below. Protein targets for vinpocetine included the KCNQ potassium channel family, D_{1A} dopamine receptors, and euchromatic histone-lysine *N*-methyltransferase 2. Active results are summarized in **Table 11** and all results are provided in **Appendix B**.

Table 11. Positive Results of Vinpocetine in PubChem BioAssays

BioAssay	Protein Target
MDR-1	ABCB1 gene product [Homo sapiens][gi:42741659]
Measurement of GPCR-mediated thallium flux through GIRK channels: Primary Screen	
Discovery of Novel Allosteric Agonists of the M4 Muscarinic Receptor: Primary Screen	
Discovery of Novel Allosteric Agonists of the M4 Muscarinic Receptor: Confirmation Screen	cholinergic receptor, muscarinic 4 [Mus musculus][gi:6680940]
Measurement of GPCR-mediated thallium flux through GIRK channels: Confirmation Screen	
DSSTox (FDAMDD) FDA Maximum (Recommended) Daily Dose Database	
qHTS for differential inhibitors of proliferation of Plasmodium falciparum lines 7G8, GB4, W2, and HB3	
Aqueous Solubility from MLSMR Stock Solutions	
Primary cell-based high-throughput screening assay for identification of compounds that potentiate KCNQ2 potassium channels	Kcnq2 gene product [Rattus norvegicus][gi:18959272]
Specificity screen against KCNQ1 for compounds that potentiate KCNQ2 potassium channels	KCNQ1 gene product [Homo sapiens][gi:32479527]
Confirmatory screen for compounds that potentiate KCNQ2 potassium channels	Kcnq2 gene product [Rattus norvegicus][gi:18959272]
Fluorescence Polarization Cell-Free Homogeneous Primary HTS to Identify Inhibitors of the LANA Histone H2A/H2B Interaction	LANA [Human herpesvirus 8][gi:139472804]
Luminescence Microorganism Primary HTS to Identify Inhibitors of the SUMOylation Pathway Using a Temperature Sensitive Growth Reversal Mutant Mot1-301	
Evaluated for inhibitory activity against Phosphodiesterase 1 (PDE1) purified from bovine aorta	
Inhibition of human phosphodiesterase 1	Calcium/calmodulin-dependent 3',5'-cyclic nucleotide phosphodiesterase 1A [gi:1705942]
HTS Assay for Allosteric Agonists of the Human D1 Dopamine Receptor: Primary Screen for Potentiators	D(1A) dopamine receptor [Homo sapiens][gi:4503383]
qHTS Assay for Inhibitors of Histone Lysine Methyltransferase G9a	euchromatic histone-lysine N-methyltransferase 2 [Homo sapiens][gi:168985070]
qHTS profiling for inhibitors of Plasmodium falciparum proliferation [19 tests]	
qHTS for inhibitors of KCHN2 3.1: Mutant qHTS	potassium voltage-gated channel subfamily H member 2 isoform a [Homo sapiens][gi:342840031]
qHTS for inhibitors of KCHN2 3.1: Wildtype qHTS	Potassium voltage-gated channel subfamily H member 2 isoform a [Homo sapiens][gi:342840031]
Primary qHTS for delayed death inhibitors of the malarial parasite plastid, 48 hour [1 test] and 96 hour [2 tests] incubations	
HTS to Find Inhibitors of Pathogenic Pemphigus Antibodies	
qHTS Assay for Small Molecule Inhibitors of the Human hERG Channel Activity	KCNH2 gene product [Homo sapiens] [gi:325651834]
Antiplasmodial activity against Plasmodium falciparum GB4, 7G8, D10, 3D7, HB3, and W2 after 72 hrs by SYBR green assay	

9.0 Structure-Activity Relationships

9.1 Vincamine [CAS No. 1617-90-9; PubChem CID:15376]



Vincamine is an alkaloid derived from *Vinca minor* L. (Vas and Gulyas, 2005). It is used as a vasodilator but has been reported to cause cardiovascular effects such as hypotension and central nervous system effects such as sedation in patients. Other reported effects of vincamine include a hemodynamic effect in the ischemic regions of the brain in humans and increased paradoxical sleep in cats (HSDB, 2004; Vas and Gulyas, 2005).

In radiolabel studies, an oral dose of 10 mg/kg vincamine given to rats showed the compound to be almost completely metabolized with 6-7% of unchanged vincamine excreted in urine (HSDB, 2004; Vas and Gulyas, 2005). V incamine was either (1) hydrolyzed by plasma esterases to unstable vincaminic acid, which was then decarboxylized and oxidized to eburnamenine or (2) hydroxylated to 6α- and 6β-hydroxyvincamine (β being 40% of total urinary and biliary radioactivity) and their oxidized metabolite 6-keto-vincamine, which was eliminated by conjugation. These three latter metabolites were detected in man, rabbits, and dogs. vincamine generally follows a one-compartment kinetic model in humans and a two-compartment open model in rats (HSDB, 2004).

In mice, LD_{50} values were 48-75, 215, 1000, and >1000 mg/kg via the i.v., i.p., oral, and subcutaneous routes, respectively. In rats, an i.p. LD_{50} of 253 mg/kg was calculated. Vincamine effectively treats cyanide toxicity in mice. Rats administered 6.6-100 mg/kg vincamine daily for up to three months exhibited no adverse effects. [Note: Acute and subchronic exposure studies in dogs, cats, gerbils, and rabbits have also been conducted] (HSDB, 2004).

In a reproductive study in mice, 50 mg/kg vincamine administered via stomach tube and daily from one week prior to mating until sacrifice or birth resulted in increased fetal resorptions. When a lower dose (22.5 mg/kg) was administered from mating to the end of lactation, no adverse effects were noted. In rats, i.v. administration of 5 mg/kg daily from eight days prior to mating to two-thirds through gestation or end of gestation did not affect fertility and was not embryotoxic or teratogenic, but an oral administration of 2.25-37.5 mg/kg daily on GD days 6-16 caused increased placental hemorrhages at 7.5 mg/kg; decreased body weight, reduced number of fetuses, smaller and lighter fetuses, and delayed ossification at 22.5 mg/kg; and fetotoxicity (i.e., 1 fetus/6 gravid females) at 37.5 mg/kg. In male rats, 225 mg/kg vincamine (orally) had no effect on reproductive function. [Note: Studies in rabbits are also available] (HSDB, 2004).

Vincamine was negative in a *Salmonella typhimurium* assay in the presence and absence of metabolic activation (S9), the mouse lymphoma cell assay with and without S9, and the micronucleus test using male and female mice bone marrow (HSDB, 2004). Vincamine also possesses antimicrobial (antibacterial and antifungal) and antiviral activity; test species included the herpes simplex virus (type-1), *Escherichia coli*, *Bacillus subtilis*, *Acinetobacter baumannii*, and the fungi *Candida albicans* and *C. parapsilosis* (Özçelik et al., 2011 [PMID:21391841]).

9.2 GeneGo

For each GeneGo model, a quantitative structure-activity relationship (QSAR) value was calculated. Cutoffs for the definition of active molecules are model dependent. For many non-binary models, the calculated values ranged between two threshold values to be classified as active in the model. These threshold values corresponded to the negative logarithm of the activity for the most active compound in the training set and the negative logarithm of 50 µM (-1.7). For binary models (e.g., AMES mutagenicity binary model), the definition of an active chemical is model dependent, but was typically ≥0.5. In addition to a QSAR value, a Tanimoto similarity percentage (TP) was calculated for each model; TP indicates the percentage of similarity of vinpocetine to the most similar compound in the training set. Detailed results are provided in **Appendix C**.

ADME QSARs

Eight vinpocetine metabolites were predicted after first-pass metabolism. The metabolites could be classified as those produced after (a) aliphatic hydroxylation, (b) aromatic hydroxylation, and (d) *O*-dealkylation. In addition to these metabolites, 10 minor first-pass metabolites, 4 first-pass conjugated metabolites, 30 major second-pass metabolites, 8 minor second-pass metabolites, and 36 second-pass conjugated metabolites were predicted.

Inhibitory cytochrome P450 (CYP) models predicted that vinpocetine would have inhibitory activity against CYP2D6 (TP = 54.71). It was also predicted that vinpocetine would be a substrate for CYP2D6 (0.59, TP = 52.89). No data were located to support or contradict these predictions.

Protein Binding QSARs

Protein binding QSAR models predicted that vinpocetine could be a substrate for human P-glycoprotein transporters (0.68, TP = 52.89). No studies were located that support or contradict this prediction.

Therapeutic Activity QSARs

Five models predicted that vinpocetine would have therapeutic activity (>0.5). Vinpocetine was predicted to have activity against heart failure (0.68, TP = 99.10), hypertension (0.62, TP = 63.78), osteoporosis (0.52, TP = 55.39), pain (0.73, TP = 53.97), and Parkinson's disease (0.60, TP = 52.94).

Toxic Effects QSARs

Of the 22 models evaluated, four predicted that vinpocetine would produce a toxic effect. However, the TP value for each model was <50%. Vinpocetine was predicted to be negative in the AMES mutagenicity binary model (0.36 [0 defined as nonmutagenic], TP = 51.90) and

exhibit some toxicity towards MCF7 cells (4.92 [values <3 were less toxic and <6 were "preferable"], TP = 52.89). No studies were located that support or contradict these predictions.

Possible Targets

Along with vinpocetine, 15 a dditional compounds within the database were identified as structurally similar to vinpocetine. Proposed vinpocetine targets were based on studies reporting vinpocetine inhibition of phosphotidesterase 1A, 1B, 1C, and E1. Vinpocetine also interacted with the peripheral benzodiazepine receptor and inhibited sodium channels. Based on t he interactions of the structurally similar compound 1-ethyl-2,3,4,5,11a,11b-hexahydro-1H-3a,9b-diazabenzo[cd]fluoranthene-10-carboxylic acid ethyl ester, phosphodiesterase 3A and 3B were identified as possible targets for vinpocetine.

9.3 Leadscope

For each Leadscope model suite evaluated, a positive prediction probability (ranging from 0-1) was calculated. Values ≥0.5 were defined as positive. If the test compound was not at least 30% similar to one in the training set and at least one model feature was not present in the test compound, the chemical was defined as "not in the domain" and prediction probability was not determined. A summary of the models where positive prediction values were obtained or where the prediction is contradictory to literature is provided in **Table 12**. Additional details on the model features and chemicals identified as structurally similar for each of the models which were predicted to be positive may be reviewed in **Appendix D**.

Table 12. Leadscope Results

Model	Positive Probability Prediction Value[1]	Unique Model Features[2]	Training Set Chemicals with ≥30% Similarity	Literature Results
Carcinogenicity				
Carcinogenicity Rat	0.504	14	1	No data were located that support or contradict the prediction.
Carcinogenicity Rat Male	0.673	25	1	No data were located that support or contradict the prediction.
Cell transformation	0.887	12	1	No data were located that support or contradict the prediction.
SHE	0.861	8	1	No data were located that support or contradict the prediction.
BALB/c-3T3	0.742	10	1	No data were located that support or contradict the prediction.
Genotoxicity				
Chromosome aberrations *in vivo* rat	0.815	12	1	No data were located that support or contradict the prediction.
SCE *in vitro* CHO	0.681	14	1	No data were located that support or contradict the prediction.
Developmental Toxicity				
Structural dysmorphogenesis mouse	0.677	9	2	No data were located that support or contradict the prediction.
Fetal death rat	0.5185	10	7	No data were located that support or contradict the prediction.

Model	Positive Probability Prediction Value[1]	Unique Model Features[2]	Training Set Chemicals with ≥30% Similarity	Literature Results
Fetal death rabbit	0.8495	12	8	No data were located that support or contradict the prediction.
Post implantation loss rat	0.5115	9	8	No data were located that support or contradict the prediction.
Post implantation loss rabbit	0.8503	22	8	No data were located that support or contradict the prediction.
Human Cardiological Adverse Effects				
Coronary artery disorder	0.8173	14	6	No data were located that support or contradict the prediction.
Myocardial infarct disorder	0.749	18	6	No data were located that support or contradict the prediction.
Palpitations	0.534	16	6	No data were located that support or contradict the prediction.
Rate rhythm disorder	0.5577	11	6	No data were located that support or contradict the prediction.
Human Adverse Urinary Tract Effects				
Blood in urine disorders	0.7293	9	6	No data were located that support or contradict the prediction.

[1]Values ≥0.5 were defined as positive by the Leadscope analysis.
[2]Several models identified the same structural model feature multiple times as being associated with the predicted activity. The results presented above indicate the number of unique model features that were associated with the predicted activity. Details on the features that were identified more than one time are presented in **Appendix D**.
Abbreviations: CHL = Chinese hamster lung; CHO = Chinese hamster ovary; chrom. ab. = chromosomal aberration(s); dec = decreased; SCE = sister chromatid exchange; SHE = Syrian hamster embryo

9.4 Toxtree

Toxtree (V2.6.0) is an application provided by the European Union Joint Research Centre that places chemicals into categories and predicts toxicity for a variety of endpoints using a decision tree model. Toxicity endpoints evaluated included: eye and skin irritation/corrosion, skin sensitization, *in vivo* micronucleus formation, carcinogenicity, and mutagenicity. Additional models include toxicity mode of action, biodegradation, and CYP metabolism potential. Additional details on the model features and chemicals identified as structurally similar for each of the models which were predicted to be positive may be reviewed in **Appendix E**.

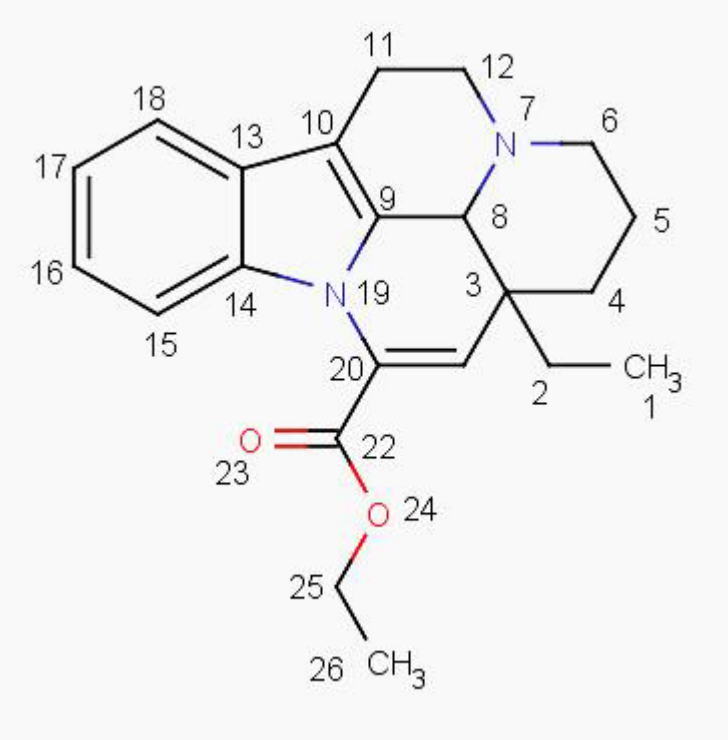
A structural alert associated with micronucleus formation in rodents ("H-acceptor-path3-H-acceptor") was identified in vinpocetine. DNA and protein binding structural alerts were reported in the vinpocetine structure. Vinpocetine was classified as not corrosive to the skin or eye. However, the presence of a structural alert associated with skin sensitization (Michael acceptor) was reported. Vinpocetine was classified as belonging to Class III, "substances are those that permit no strong initial presumption of safety, or may even suggest significant toxicity or have reactive functional groups." based on the presence of a heterocycle with complex substituents within vinpocetine. Vinpocetine was predicted to be reactive by Michael addition.

Low specificity structural groups were an aldehyde or ketone, ether, carboxylic acid derivative, aromatic compound, and heterocyclic compound. The high specificity groups were a dialkylether, alkylarylether, tertiary aliphatic amine, carboxylic acid ester, and carbonic acid diester. Another functional group identified was enolether.

9.5 SMARTCyp

This program (Version 2.4.2) evaluates chemicals for sites that may be metabolized by CYP isoforms. The results are applicable to isoforms CYP1A2, CYP2A6, CYP2B6, CYP2C8, CYP2C19, CYP2E1, and CYP3A4. Additionally, two specific models for metabolism by CYP2C9 and CYP2D6 are provided. The models use the two-dimensional structure of a compound to assess potential metabolism sites. The models calculate the energy needed to oxidize each atom and atom accessibility is assessed as the relative distance of the atom from the center of the molecule. The final score is based on these two values (SMARTCyp, undated).

Based on the numbering scheme in the chemical structure shown below, it was predicted that atoms 6, 12, and 8 would be the primary, secondary, and tertiary sites of metabolism in the model applicable to seven different CYP isoforms. For the CYP2C9 model, the predicted primary, secondary, and tertiary sites of metabolism were also atoms 6, 12, and 8, respectively. While atoms 6 and 12 were predicted to be the primary and secondary metabolic sites for CYP2D6, the tertiary site was predicted to be atom 26 (SMARTCyp, undated).



10.0 Online Databases and Secondary References Searched

10.1 Online Databases

National Library of Medicine Databases

PubMed

ChemIDplus – chemical information database that provides links to other databases such as CCRIS, DART, GENE-TOX, HSDB, IRIS, and TRI. A full list of databases and resources searched are available at http://www.nlm.nih.gov/databases/.

STN International Files

AGRICOLA	IPA	MEDLINE
BIOSIS	CABA	NAPRALERT
BIOTECHNO	EMBASE	TOXCENTER

Information on the content, sources, file data, and producer of each of the searched STN International Files is available at http://www.cas.org/support/stngen/dbss/index.html.

Government Printing Office
Code of Federal Regulations (CFR)

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Units and Abbreviations

ºC = degrees Celsius
µg/ mL = microgram(s) per milliliter
µM = micromolar
ADME = absorption, distribution, metabolism, and excretion
AUC = area under the curve
C_{max} = peak plasma concentration
CAS = Chemical Abstracts Service
CCl_4 = carbon tetrachloride
CHL = Chinese hamster lung
CHO = Chinese hamster ovary
chrom. ab. = chromosomal aberration(s)
CID = chemical identification
CL = clearance
CYP = cytochrome P450

dec = decreased
DNA = deoxyribonucleic acid
eV = electron volt(s)
F = female(s)
FDA = U.S. Food and Drug Administration
g = gram(s)
g/cm^3 = gram(s) per cubic centimeter
GC = gas chromatography
GD = gestation day(s)
h = hour(s)
HPLC = high performance liquid chromatography
IC_{50} = half maximal inhibitory concentration
i.p. = intraperitoneal(ly)
i.v. = intravenous(ly)
L/h/kg = liter(s) per hour per kilogram
L/kg = liter(s) per kilogram
LD_{50} = lethal dose for 50% of test animals
LOD = limit of detection
LOQ = limit of quantification
M = male(s)
MAT = mean absorption time
MRT = mean residence time
mg = milligram(s)
mg/kg = milligram(s) per kilogram
mg/mL = milligram(s) per milliliter
mm Hg = millimeter(s) of mercury
mm^{-3} = per cubic millimeter
mol×h/L = mole(s) per hour per liter
mol/L = mole(s) per liter
mol. wt. = molecular weight
MS = mass spectrometer
ng = nanogram(s)
ng×h/mL = nanogram(s) times hour per milliliter
ng/mL = nanogram(s) per milliliter
nM = nanomolar
NMR = nuclear magnetic resonance
n.p. = not provided
PDR = Physicians' Desk Reference
PET = positron emission tomography
PMID = PubMed identification
PND = postnatal day(s)
p.o. = *per os*
ppm = part(s) per million
QSAR = quantitative structure-activity relationship
S9 = metabolic activation
SCE = sister chromatid exchange

SHE = Syrian hamster embryo
$t_{1/2}$ = elimination half-life
t_{max} = time to reach peak plasma concentration
t_{lag} = lag time
TD_{Lo} = toxic dose low; lowest published toxic dose
TNF = tumor necrosis factor
TP = Tanimoto similarity percentage
UV = ultraviolet
V_1 = volume of central compartment
V_d = volume of distribution
V_d/F = apparent volume of distribution
Vd_{SS} = volume at steady state

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Appendix A: Description of Search Strategy and Results

STN International files MEDLINE, AGRICOLA, CABA, IPA, BIOSIS, TOXCENTER, EMBASE, BIOTECHNO, and NAPRALERT were searched simultaneously on June 14, 2012, for vinpocetine, and major and minor metabolites. RTECS and REGISTRY files were also searched for these compounds on the same day. To aid in subsequent selection for full record retrieval, PubMed was searched for reviews and other titles were scanned. The online history for the STN database search is shown below.

```
L1         3086 S VINPOCETINE OR ETHYL(3A)(APOVINCAMINATE OR APOVINCAMIN(W)22(W)OATE)
                  OR 42971-09-5
L2          772 S BRAVINTON OR CAVINTON OR CERACTIN OR RGH(W)4405 OR TCV(W)3B
L3            5 S ULTRA(W)VINCA OR VINPORAL OR AY(W)27255
L4          531 S 42971-12-0 OR ETHYL(W)EBURNAMENINE-14-CARBOXYLATE
L5         3150 S L1-L3
L6            1 S L4 NOT L5
L7         3151 S L1-L4
L8          267 S 27773-65-5 OR APOVINCAMINIC(W)ACID
L9           28 S 40163-56-2 OR ETHYL(3A)VINCAMINATE
L10         295 S L8 OR L9
L11          69 S L10 NOT L7
                SET DUPORDER FILE
L12          41 DUP REM L11 (28 DUPLICATES REMOVED)
              6 ANSWERS '1-6' FROM FILE MEDLINE
              1 ANSWER '7' FROM FILE IPA
             20 ANSWERS '8-27' FROM FILE BIOSIS
              3 ANSWERS '28-30' FROM FILE TOXCENTER
              7 ANSWERS '31-37' FROM FILE EMBASE
              4 ANSWERS '38-41' FROM FILE NAPRALERT
L13          41 SORT L12 1-41 TI
                SAVE L13 X902EXTRA/A
L14        2925 S L7 NOT L10
L15        1502 DUP REM L14 (1423 DUPLICATES REMOVED)
            570 ANSWERS '1-570' FROM FILE MEDLINE
              5 ANSWERS '571-575' FROM FILE CABA
             28 ANSWERS '576-603' FROM FILE IPA
            242 ANSWERS '604-845' FROM FILE BIOSIS
            229 ANSWERS '846-1074' FROM FILE TOXCENTER
            420 ANSWERS '1075-1494' FROM FILE EMBASE
              2 ANSWERS '1495-1496' FROM FILE BIOTECHNO
              6 ANSWERS '1497-1502' FROM FILE NAPRALERT
L16        1502 SORT L15 1-1502 TI
                SAVE L16 X902BIOMED/A
```

The principal investigator became aware of studies that did not appear in the STN International results while reading some original vinpocetine journal articles. However, they did appear in PubMed. (Differences in the coverage of MEDLINE versus PubMed may be found on this web page: http://www.nlm.nih.gov/pubs/factsheets/dif_med_pub.html.) On July 5, 2012, a PubMed search that included the following query: vinpocetine OR 42971-09-5 OR cavinton OR ("apovincaminic acid" AND "ethyl ester") OR "ethyl apovincaminate" retrieved 615 records, 177 of which EndNote did not recognize as duplicates based on the titles alone. Manual comparison of the 177 with the STN International titles led to identification of an additional 39 records; 27 were selected for downloading (human ADME or pharmacokinetics, 7; clinical trials, 1; other human, 3; whole rat or mouse studies, 6; analytical determination, 8; physical-chemical properties, 2). Google Scholar searches were conducted in June 2012 for "determination of vinpocetine" OR "vinpocetine determination," at least six more studies that were not in the STN or PubMed results were located.

2013 Update Search

STN International files MEDLINE, AGRICOLA, CABA, IPA, BIOSIS, TOXCENTER, EMBASE, BIOTECHNO, and NAPRALERT were searched simultaneously on August 8, 2013, with the following strategy:

```
=> ACTIVATE X902EXTRA/A
L1 (      3086)SEA VINPOCETINE OR ETHYL(3A)(APOVINCAMINATE OR APOVINCAMIN(W) 2
L2 (       772)SEA BRAVINTON OR CAVINTON OR CERACTIN OR RGH(W) 4405 OR TCV(W)
L3 (         5)SEA ULTRA(W) VINCA OR VINPORAL OR AY(W) 27255
L4 (       531)SEA 42971-12-0 OR ETHYL(W) EBURNAMENINE-14-CARBOXYLATE
L5 (      3151)SEA (L1 OR L2 OR L3 OR L4)
L6 (       267)SEA 27773-65-5 OR APOVINCAMINIC(W) ACID
L7 (        28)SEA 40163-56-2 OR ETHYL(3A) VINCAMINATE
L8 (       295)SEA L6 OR L7
L9 (        69)SEA L8 NOT L5
L10 (       41)DUP REM L9 (28 DUPLICATES REMOVED)
L11         41 SOR L10 1-41 TI

L12        212 S L5 AND (2012-2013)/PY
L13          2 S L9 AND (2012-2013)/PY
L14          2 S L13 NOT L12  [The two titles were duplicates.]
L15        214 L12 OR L13
L16        139 DUP REM L15 (75 DUPLICATES REMOVED)
               ANSWERS '1-30' FROM FILE MEDLINE
               ANSWERS '31-33' FROM FILE CABA
               ANSWER '34' FROM FILE IPA
               ANSWERS '35-44' FROM FILE BIOSIS
               ANSWERS '45-85' FROM FILE TOXCENTER
               ANSWERS '86-139' FROM FILE EMBASE
L17        139 SORT L16 1-139 TI
               L17 SAVED AS 'X902UPDATE/A
```

The 139 titles of answer set L17 were compared with the selected titles from the 2012 search results in the EndNote library and with the 19 new titles that resulted when PubMed was searched on August 8, 2013, with the same strategy used on July 5, 2012. Results were limited to database entries since July 6, 2012. One of the 19 PubMed results was not in the 2013 STN International results. Twenty-nine STN International records were selected for downloading. Their database distribution was MEDLINE, 18; TOXCENTER and EMBASE, each 4; and BIOSIS, 3.

Appendix B: PubChem BioAssay Results

AID	Outcome	Activity Concentration Name	Activity Concentration [uM]	BioAssay	Target	PMID
588834	Active	Potency	0.1413	qHTS Assay for Small Molecule Inhibitors of the Human hERG Channel Activity	KCNH2 gene product [Homo sapiens][gi:325651834]	19583963
588834	Active	Potency	0.1413	qHTS Assay for Small Molecule Inhibitors of the Human hERG Channel Activity	KCNH2 gene product [Homo sapiens][gi:325651834]	19583963
588834	Active	Potency	0.1413	qHTS Assay for Small Molecule Inhibitors of the Human hERG Channel Activity	KCNH2 gene product [Homo sapiens][gi:325651834]	19583963
588834	Active	Potency	0.1413	qHTS Assay for Small Molecule Inhibitors of the Human hERG Channel Activity	KCNH2 gene product [Homo sapiens][gi:325651834]	19583963
588834	Active	Potency	0.1413	qHTS Assay for Small Molecule Inhibitors of the Human hERG Channel Activity	KCNH2 gene product [Homo sapiens][gi:325651834]	19583963
488982	Active	Potency	3.2641	HTS Assay for Allosteric Agonists of the Human D1 Dopamine Receptor: Primary Screen for Potentiators	D(1A) dopamine receptor [Homo sapiens][gi:4503383]	
488982	Active	Potency	3.2641	HTS Assay for Allosteric Agonists of the Human D1 Dopamine Receptor: Primary Screen for Potentiators	D(1A) dopamine receptor [Homo sapiens][gi:4503383]	
488982	Active	Potency	3.2641	HTS Assay for Allosteric Agonists of the Human D1 Dopamine Receptor: Primary Screen for Potentiators	D(1A) dopamine receptor [Homo sapiens][gi:4503383]	
488982	Active	Potency	3.2641	HTS Assay for Allosteric Agonists of the Human D1 Dopamine Receptor: Primary Screen for Potentiators	D(1A) dopamine receptor [Homo sapiens][gi:4503383]	
504834	Active	Potency	3.6964	Primary qHTS for delayed death inhibitors of the malarial parasite plastid, 96 hour incubation		
504832	Active	Potency	5.2213	Primary qHTS for delayed death inhibitors of the malarial parasite plastid, 48 hour incubation		

AID	Outcome	Activity Concentration Name	Activity Concentration [uM]	BioAssay	Target	PMID
504834	Active	Potency	6.7456	Primary qHTS for delayed death inhibitors of the malarial parasite plastid, 96 hour incubation		
1815	Active	Potency	7.0795	qHTS for differential inhibitors of proliferation of Plasmodium falciparum line 7G8		
524794	Active	IC50	7.94328	Antiplasmodial activity against Plasmodium falciparum GB4 after 72 hrs by SYBR green assay		19734910
1816	Active	Potency	7.9433	qHTS for differential inhibitors of proliferation of Plasmodium falciparum line GB4		
524791	Active	IC50	10	Antiplasmodial activity against Plasmodium falciparum 7G8 after 72 hrs by SYBR green assay		19734910
524792	Active	IC50	12.5892	Antiplasmodial activity against Plasmodium falciparum D10 after 72 hrs by SYBR green assay		19734910
524795	Active	IC50	12.5892	Antiplasmodial activity against Plasmodium falciparum HB3 after 72 hrs by SYBR green assay		19734910
524796	Active	IC50	12.5892	Antiplasmodial activity against Plasmodium falciparum W2 after 72 hrs by SYBR green assay		19734910
524790	Active	IC50	12.5892	Antiplasmodial activity against Plasmodium falciparum 3D7 after 72 hrs by SYBR green assay		19734910
1886	Active	Potency	12.5893	qHTS for differential inhibitors of proliferation of Plasmodium falciparum line HB3		
238292	Active	Ki	14	Inhibition of human phosphodiesterase 1	Calcium/calmodulin-dependent 3',5'-cyclic nucleotide phosphodiesterase 1A[gi:1705942]	15887951

AID	Outcome	Activity Concentration Name	Activity Concentration [uM]	BioAssay	Target	PMID
1883	Active	Potency	14.1254	qHTS for differential inhibitors of proliferation of Plasmodium falciparum line W2		
158752	Active	IC50	19	Evaluated for inhibitory activity against Phosphodiesterase 1 (PDE1) purified from bovine aorta		9216839
504332	Active	Potency	22.3872	qHTS Assay for Inhibitors of Histone Lysine Methyltransferase G9a	euchromatic histone-lysine N-methyltransferase 2 [Homo sapiens][gi:168985070]	
2283	Active			Specificity screen against KCNQ1 for compounds that potentiate KCNQ2 potassium channels	KCNQ1 gene product [Homo sapiens][gi:32479527]	
377	Active			MDR-1	ABCB1 gene product [Homo sapiens][gi:42741659]	
377	Active			MDR-1	ABCB1 gene product [Homo sapiens][gi:42741659]	
377	Active			MDR-1	ABCB1 gene product [Homo sapiens][gi:42741659]	
643	Active			Discovery of Novel Allosteric Agonists of the M4 Muscarinic Receptor: Confirmation Screen	cholinergic receptor, muscarinic 4 [Mus musculus][gi:6680940]	
643	Active			Discovery of Novel Allosteric Agonists of the M4 Muscarinic Receptor: Confirmation Screen	cholinergic receptor, muscarinic 4 [Mus musculus][gi:6680940]	
504749_4	Active			qHTS profiling for inhibitors of Plasmodium falciparum proliferation		21817045
1996	Active			Aqueous Solubility from MLSMR Stock Solutions		
2716	Active			Luminescence Microorganism Primary HTS to Identify Inhibitors of the SUMOylation Pathway Using a Temperature Sensitive Growth Reversal Mutant Mot1-301		
1195	Active			DSSTox (FDAMDD) FDA Maximum (Recommended) Daily Dose Database		

AID	Outcome	Activity Concentration Name	Activity Concentration [uM]	BioAssay	Target	PMID
624	Active			Measurement of GPCR-mediated thallium flux through GIRK channels: Primary Screen		
625	Active			Discovery of Novel Allosteric Agonists of the M4 Muscarinic Receptor: Primary Screen		
780	Active			Measurement of GPCR-mediated thallium flux through GIRK channels: Confirmation Screen		
504749_48	Active			qHTS profiling for inhibitors of Plasmodium falciparum proliferation		21817045
588358	Active			HTS to Find Inhibitors of Pathogenic Pemphigus Antibodies		
504749_15	Active			qHTS profiling for inhibitors of Plasmodium falciparum proliferation		21817045
504749_19	Active			qHTS profiling for inhibitors of Plasmodium falciparum proliferation		21817045
504749_29	Active			qHTS profiling for inhibitors of Plasmodium falciparum proliferation		21817045
504749_34	Active			qHTS profiling for inhibitors of Plasmodium falciparum proliferation		21817045
504749_39	Active			qHTS profiling for inhibitors of Plasmodium falciparum proliferation		21817045
504749_42	Active			qHTS profiling for inhibitors of Plasmodium falciparum proliferation		21817045
504749_52	Active			qHTS profiling for inhibitors of Plasmodium falciparum proliferation		21817045
504749_54	Active			qHTS profiling for inhibitors of Plasmodium falciparum proliferation		21817045
504749_56	Active			qHTS profiling for inhibitors of Plasmodium falciparum proliferation		21817045
504749_57	Active			qHTS profiling for inhibitors of Plasmodium falciparum proliferation		21817045

AID	Outcome	Activity Concentration Name	Activity Concentration [uM]	BioAssay	Target	PMID
504749_53	Active			qHTS profiling for inhibitors of Plasmodium falciparum proliferation		21817045
504749_55	Active			qHTS profiling for inhibitors of Plasmodium falciparum proliferation		21817045
504749_2	Active			qHTS profiling for inhibitors of Plasmodium falciparum proliferation		21817045
504749_20	Active			qHTS profiling for inhibitors of Plasmodium falciparum proliferation		21817045
504749_60	Active			qHTS profiling for inhibitors of Plasmodium falciparum proliferation		21817045
504749_33	Active			qHTS profiling for inhibitors of Plasmodium falciparum proliferation		21817045
504749_36	Active			qHTS profiling for inhibitors of Plasmodium falciparum proliferation		21817045
720551	Active	Potency		qHTS for Inhibitors of KCHN2 3.1: Wildtype qHTS	potassium voltage-gated channel subfamily H member 2 isoform a [Homo sapiens][gi:342840031]	
720553	Active	Potency		qHTS for Inhibitors of KCHN2 3.1: Mutant qHTS	potassium voltage-gated channel subfamily H member 2 isoform a [Homo sapiens][gi:342840031]	
2629	Active			Fluorescence Polarization Cell-Free Homogeneous Primary HTS to Identify Inhibitors of the LANA Histone H2A/H2B Interaction	LANA [Human herpesvirus 8][gi:139472804]	
2287	Active			Confirmatory screen for compounds that potentiate KCNQ2 potassium channels	Kcnq2 gene product [Rattus norvegicus][gi:18959272]	
2287	Active			Confirmatory screen for compounds that potentiate KCNQ2 potassium channels	Kcnq2 gene product [Rattus norvegicus][gi:18959272]	
2239	Active			Primary cell-based high-throughput screening assay for identification of compounds that potentiate KCNQ2 potassium channels	Kcnq2 gene product [Rattus norvegicus][gi:18959272]	

AID	Outcome	Activity Concentration Name	Activity Concentration [uM]	BioAssay	Target	PMID
2239	Active			Primary cell-based high-throughput screening assay for identification of compounds that potentiate KCNQ2 potassium channels	Kcnq2 gene product [Rattus norvegicus][gi:18959272]	
540804	Unspecified	IC50	7.94328	GRAC: human PDE1A selective inhibitor	Calcium/calmodulin-dependent 3',5'-cyclic nucleotide phosphodiesterase 1A[gi:1705942]	
540723	Unspecified	IC50	50.1187	GRAC: human PDE1C selective inhibitor	Calcium/calmodulin-dependent 3',5'-cyclic nucleotide phosphodiesterase 1C[gi:2499445]	
312786	Unspecified	IC50	137	Inhibition of NADH-induced lipid peroxidation in rat brain microsome		18183943
312787	Unspecified	IC50	209	Inhibition of Fe2+-induced lipid peroxidation in rat brain homogenate		18183943
159196	Unspecified	IC50	300	Inhibitory activity against phosphodiesterase 3 (PDE3) purified from bovine heart		9216839
157927	Unspecified	IC50	300	Evaluated for inhibitory activity against Phosphodiesterase 5 (PDE5) purified from bovine lung		9216839
60591	Unspecified			Effect on femoral blood flow (FBF) was studied, after intraarterial administration in anesthetized dogs relative to vinpocetine		8464035
60592	Unspecified			Effect on vertebral blood flow (VBF) was studied, after intraarterial administration in anesthetized dogs relative to vinpocetine		8464035
312788	Unspecified			Inhibition of diazepam-induced amnesia in NMRI mouse at 0.1 mg/kg, po by one-trial passive avoidance test		18183943
312789	Unspecified			Inhibition of diazepam-induced amnesia in NMRI mouse at 10 mg/kg, po by one-trial passive avoidance test		18183943

AID	Outcome	Activity Concentration Name	Activity Concentration [uM]	BioAssay	Target	PMID
312791	Unspecified			Protective effect against diazepam-induced learning-deficit in Wistar rat at 5 mg/kg, po by water labyrinth test		18183943
697754	Unspecified			Octanol-water partition coefficient, log P of cationic form of compound at 0.15 M ionic strength by stir flask method		22793155
697757	Unspecified			Octanol-water partition coefficient, log P of noncharged form of compound at 0.15 M ionic strength by stir flask method		22793155
697758	Unspecified			Octanol-water distribution coefficient, log D of the compound at pH 0.82 by stir flask method		22793155
504749	Unspecified			qHTS profiling for inhibitors of Plasmodium falciparum proliferation		21817045
504749	Unspecified			qHTS profiling for inhibitors of Plasmodium falciparum proliferation		21817045
2675	Unspecified	Potency		qHTS Assay for Inhibitors of MBNL1-poly(CUG) RNA binding	muscleblind-like protein 1 isoform a [Homo sapiens][gi:41281591]	
624178	Unspecified	Potency		qHTS for Inhibitors of Human Acid Sphingomyelinase Assay: Native Substrate	acid sphingomyelinase [Homo sapiens][gi:179095]	
624178	Unspecified	Potency		qHTS for Inhibitors of Human Acid Sphingomyelinase Assay: Native Substrate	acid sphingomyelinase [Homo sapiens][gi:179095]	
311932	Unspecified			Inhibition of ASM in human H4 cells assessed as residual activity at 10 uM	Sphingomyelin phosphodiesterase[gi:224471897]	18027916
311932	Unspecified			Inhibition of ASM in human H4 cells assessed as residual activity at 10 uM	Sphingomyelin phosphodiesterase[gi:224471897]	18027916
697852	Unspecified			Inhibition of electric eel AChE at 2 mg/ml by Ellman's method	Acetylcholinesterase[gi:14916521]	23062825
697853	Unspecified			Inhibition of horse BChE at 2 mg/ml by Ellman's method	Cholinesterase[gi:21362409]	23062825

AID	Outcome	Activity Concentration Name	Activity Concentration [uM]	BioAssay	Target	PMID
504332	Inactive	Potency	0.0224	qHTS Assay for Inhibitors of Histone Lysine Methyltransferase G9a	euchromatic histone-lysine N-methyltransferase 2 [Homo sapiens][gi:168985070]	
651633	Inactive	Potency	0.1059	qHTS assay for small molecule agonists of the p53 signaling pathway - cell viability		
651633	Inactive	Potency	0.2113	qHTS assay for small molecule agonists of the p53 signaling pathway - cell viability		
624297	Inactive	Potency	0.2909	A quantitative high throughput screen for small molecules that induce DNA re-replication in SW480 colon adenocarcinoma cells.	GMNN gene product [Homo sapiens][gi:7705682]	
2288	Inactive	Potency	1.0399	qHTS Assay for Modulators of miRNAs and/orActivators of miR-21		
1458	Inactive	Potency	2.5119	qHTS Assay for Enhancers of SMN2 Splice Variant Expression	survival motor neuron protein isoform d [Homo sapiens][gi:10937869]	
1458	Inactive	Potency	2.5119	qHTS Assay for Enhancers of SMN2 Splice Variant Expression	survival motor neuron protein isoform d [Homo sapiens][gi:10937869]	
651634	Inactive	Potency	4.7308	qHTS assay for small molecules that induce genotoxicity in human embryonic kidney cells expressing luciferase-tagged ATAD5 - cell viability		
720538	Inactive	Potency	37.933	qHTS screen for enhancers of Arylsulfatase A (ASA1): LOPAC Validation Assay	arylsulfatase A [Homo sapiens][gi:220983390]	
2382	Inactive	EC50	195	Luminescence Cell-Based Dose Confimation HTS to Identify Inhibitors of Heat Shock Factor 1 (HSF1)	Hsf1 protein [Mus musculus][gi:62740231]	
2382	Inactive	EC50	195	Luminescence Cell-Based Dose Confimation HTS to Identify Inhibitors of Heat Shock Factor 1 (HSF1)	Hsf1 protein [Mus musculus][gi:62740231]	

AID	Outcome	Activity Concentration Name	Activity Concentration [uM]	BioAssay	Target	PMID
463199	Inactive	AC50	420	Luminescence Whole-Organism Secondary Assay to Identify Compounds Inducing Growth of Temperature Sensitive Mutant Burl-1		
463204	Inactive	AC50	420	Luminescence Whole-Organism Dose Retest to Confirm Inhibitors of the SUMOylation Pathway Using a Temperature Sensitive Growth Reversal Mutant Mot1-301		
463096	Inactive	Potency		Validation screen for inhibitors of Lassa infection		
540256	Inactive	Potency		qHTS for Inhibitors of binding or entry into cells for Lassa Virus		
488862	Inactive			Inhibitors of Prion Protein 5' UTR mRNA Measured in Cell-Based System Using Plate Reader - 2078-01_Inhibitor_SinglePoint_HTS_Activity		
488966	Inactive	IC50		Primary and Confirmatory Screening for Inhibitors of Bacterial Capsule Biogenesis		
493004	Inactive	AC50		SUMO pathway Measured in Whole Organism System Using Plate Reader - 2059-03_Inhibitor_Dose_CherryPick_Activity		
504648	Inactive	Potency		Nrf2 qHTS screen for inhibitors: counterscreen for cytotoxicity		
540267	Inactive			Small Molecules that selectively kill Giardia lamblia: qHTS		
540364	Inactive			Luminescence-based cell-based primary high throughput screening assay to identify activators of the GAA850 frataxin (FXN) promoter		
588334	Inactive			MITF Measured in Cell-Based System Using Plate Reader - 2084-01_Activator_SinglePoint_HTS_Activity		

AID	Outcome	Activity Concentration Name	Activity Concentration [uM]	BioAssay	Target	PMID
588335	Inactive			Counterscreen for inhibitors of the fructose-bisphosphate aldolase (FBA) of M. tuberculosis: Absorbance-based biochemical high throughput Glycerophosphate Dehydrogenase-Triosephosphate Isomerase (GDH-TPI) full deck assay to identify assay artifacts		
588436	Inactive			Cholera Quorum: HTS for inducers of light production in the absence ofautoinducers using BH1578 (luxS deficient, cqsA deficient) Measured in Microorganism System Using Plate Reader - 2132-01_Agonist_SinglePoint_HTS_Activity		
588466	Inactive			HTS to Find Inhibitors of Pathogenic Pemphigus Antibodies, using Cherry Pick 1 compounds		
588492	Inactive			uHTS identification of small molecule modulators of myocardial damage		
588674	Inactive			Schnurri-3 Inhibitors: specific inducers of adult bone formation Measured in Cell-Based System Using Plate Reader - 2134-01_Inhibitor_SinglePoint_HTS_Activity_Set2		
588727	Inactive	IC50		A Cell-Based Confirmatory Screen for Compounds that Inhibit VEEV, TC-83		
588692	Inactive			Luciferase Reporter Cell Based HTS to identify inhibitors of N-linked Glycosylation Measured in Cell-Based System Using Plate Reader - 2146-01_Inhibitor_SinglePoint_HTS_Activity_Set2		
602141	Inactive			uHTS determination of small molecule cytotoxicity in a fluorescence assay to identify cystic fibrosis induced NFkb Inhibitors		

AID	Outcome	Activity Concentration Name	Activity Concentration [uM]	BioAssay	Target	PMID
588856	Inactive	Potency		qHTS for Inhibitors of TGF-b: Cytotox Counterscreen		
602247	Inactive			Full deck counterscreen for positive allosteric modulators (PAMs) of the human M1 muscarinic receptor (CHRM1): Fluorescence-based cell-based high throughput screening assay to identify nonselective activators and assay artifacts using the parental CHOK1 cell line		
602248	Inactive			Full deck counterscreen for agonists of the human M1 muscarinic receptor (CHRM1): Fluorescence-based cell-based high throughput screening assay to identify nonselective activators and assay artifacts using the parental CHOK1 cell line		
602250	Inactive			Full deck counterscreen for antagonists of the human M1 muscarinic receptor (CHRM1): Fluorescence-based cell-based high throughput screening assay to identify nonselective inhibitors and assay artifacts using the parental CHOK1 cell line		
602274	Inactive			uHTS luminescent assay for identification of compounds that enhance the survival of human induced pluripotent stem cells when cultured as single cells		
602340	Inactive			HTS for suppressors of simvastatin-induced mytoxicity in differentiated C2C12 cells Measured in Cell-Based System Using Plate Reader - 2112-01_Suppressor_SinglePoint_HTS_Activity		
602342	Inactive			Small molecule inhibitors of miR122 Measured in Cell-Based System Using Plate Reader - 2144-01_Inhibitor_SinglePoint_HTS_Activity		

AID	Outcome	Activity Concentration Name	Activity Concentration [uM]	BioAssay	Target	PMID
602363	Inactive			Whole cell Yeast HTS to identify compounds modulating the fidelity of the start codon recognition in eukaryotes. Measured in Whole Organism System Using Plate Reader - 2155-01_Other_SinglePoint_HTS_Activity		
602449	Inactive			uHTS identification of small molecule inhibitors of the mitochondrial permeability transition pore via an absorbance assay		
623901	Inactive			Small molecule inhibitors of miR122 Measured in Cell-Based System Using Plate Reader - 2144-01_Activator_SinglePoint_HTS_Activity		
624256	Inactive			HTS to identify compounds that promote myeloid differentiation with MLPCN compound set		
624418	Inactive	Potency		qHTS of GLP-1 Receptor Inverse Agonists: Cytotox Screen		
624483	Inactive			Counterscreen of compound fluorescence effects on High-throughput multiplex microsphere screening for inhibitors of toxin protease		
463189	Inactive			96-well format Chlamydomonas reinhardtii Algae Gravitaxis Assay to measure the difference in the absorbance between the small compact plug of WT swimming algae versus the MUT algae lacking cilia.		
624151	Inactive			Luminescence Cell-Based Primary HTS to Identify Re-Activators of the P53 Mutant Pathway Measured in Cell-Based System Using Plate Reader - 2071-01_Activator_SinglePoint_HTS_Activity		

AID	Outcome	Activity Concentration Name	Activity Concentration [uM]	BioAssay	Target	PMID
624156	Inactive			Fluorescence Cell-Based Primary HTS to Identify Reactive Oxygen Species Inducers in Cancer Cells Measured in Cell-Based System Using Plate Reader and Imaging Combination - 2044-01_Activator_SinglePoint_HTS_Activity		
624349	Inactive			A screen for compounds that inhibit liver stage malaria		
493140	Inactive			Screening small molecules to find regulators of human embryonic stem cell survival.		
720533	Inactive	Potency		qHTS for Inhibitors of binding or entry into cells for Lassa Virus		
624349	Inactive			A screen for compounds that inhibit liver stage malaria		
651582	Inactive			uHTS identification of small molecule Triacylglycerol inhbitors in a fluoresence assay		
651640	Inactive			DENV2 CPE-Based HTS Measured in Cell-Based and Microorganism Combination System Using Plate Reader - 2149-01_Other_SinglePoint_HTS_Activity		
651654	Inactive			HTS for the detection of C. neoformans cell lysis via adenylate kinase (AK) release Measured in Microorganism System Using Plate Reader - 2162-01_Inhibitor_SinglePoint_HTS_Activity		
651661	Inactive			Luminescence Cell-Based Primary HTS to identify inhibitors of the oncoprotein EWS/Fli transcriptional activity Measured in Cell-Based System Using Plate Reader - 7014-01_Inhibitor_SinglePoint_HTS_Activity		

AID	Outcome	Activity Concentration Name	Activity Concentration [uM]	BioAssay	Target	PMID
651687	Inactive			MLPCN PGC1a Modulators Measured in Cell-Based System Using Plate Reader - 2139-01_Inhibitor_SinglePoint_HTS_Activity		
651702	Inactive			Flow Cytometric HTS Screening for Inhibitors of Lytic Granule Exocytosis with MLPCN Compound Library		
651820	Inactive	Potency		qHTS Assay for Inhibitors of Hepatitis C Virus (HCV)		
651820	Inactive	Potency		qHTS Assay for Inhibitors of Hepatitis C Virus (HCV)		
651821	Inactive			Fluorescence-based biochemical primary high throughput screening assay to identify molecules that bind r(CAG) RNA repeats		
651723	Inactive			MLPCN PGC1a Modulators Measured in Cell-Based System Using Plate Reader - 2139-01_Activator_SinglePoint_HTS_Activity		
686971	Inactive	Potency		qHTS for induction of synthetic lethality in tumor cells producing 2HG: qHTS for the HT-1080-IDH1KD cell line		
504749_31	Inactive			qHTS profiling for inhibitors of Plasmodium falciparum proliferation		21817045
588349	Inactive	Potency		qHTS for Inhibitors of ATXN expression: Validation of Cytotoxic Assay		
624349	Inactive			A screen for compounds that inhibit liver stage malaria		
624349	Inactive			A screen for compounds that inhibit liver stage malaria		
624349	Inactive			A screen for compounds that inhibit liver stage malaria		

AID	Outcome	Activity Concentration Name	Activity Concentration [uM]	BioAssay	Target	PMID
521220	Inactive			Inhibition of neurosphere proliferation of mouse neural precursor cells by MTT assay		17417631
651634	Inactive	Potency		qHTS assay for small molecules that induce genotoxicity in human embryonic kidney cells expressing luciferase-tagged ATAD5 - cell viability		
540276	Inactive	Potency		qHTS for inhibitors of binding or entry into cells for Marburg Virus	gene 4 small orf - Marburg virus[gi:420597]	
540276	Inactive	Potency		qHTS for inhibitors of binding or entry into cells for Marburg Virus	gene 4 small orf - Marburg virus[gi:420597]	
540276	Inactive	Potency		qHTS for inhibitors of binding or entry into cells for Marburg Virus	gene 4 small orf - Marburg virus[gi:420597]	
687037	Inactive			Fluorescence-based counterscreen assay of HCV NS3 helicase-DNA binding inhibitors in LOPAC1280: biochemical high-throughput screening assay to identify compounds that enhance or quench fluorescence of a Cy5-DNA-NS3h complex		22740655
651828	Inactive			A screen for compounds that inhibit nucleocapsid/RNA interactions in Rift Valley Fever Virus	Nucleoprotein[gi:127925]	
651828	Inactive			A screen for compounds that inhibit nucleocapsid/RNA interactions in Rift Valley Fever Virus	Nucleoprotein[gi:127925]	
559	Inactive			RNA polymerase	RNA polymerase beta subunit (EC 2.7.7.6)[gi:147728]	
1020	Inactive			Counter Screen for Glucose-6-Phosphate Dehydrogenase-based Primary Assay	glucose-6-phosphate dehydrogenase [Leuconostoc mesenteroides][gi:149631]	
411	Inactive	Potency		qHTS Assay for Inhibitors of Firefly Luciferase	Luciferase [Photinus pyralis][gi:160794]	

AID	Outcome	Activity Concentration Name	Activity Concentration [uM]	BioAssay	Target	PMID
624030	Inactive	Potency		Biochemical firefly luciferase enzyme assay for NPC	Luciferase [Photinus pyralis][gi:160794]	
588342	Inactive	Potency		qHTS profiling assay for firefly luciferase inhibitor/activator using purifed enzyme and Km concentrations of substrates (counterscreen for miR-21 project)	Luciferase [Photinus pyralis][gi:160794]	
1870	Inactive			Multiplex HTS Screen of TOR pathway GFP-fusion proteins in Saccharomyes cerevisiae_specifically_CIT2	citrate synthase 2 [Saccharomyces cerevisiae][gi:171229]	
2029	Inactive			Multiplex HTS Screen of TOR pathway GFP-fusion proteins in Saccharomyes cerevisiae_specifically_ CIT2_MLPCN.	citrate synthase 2 [Saccharomyces cerevisiae][gi:171229]	
1708	Inactive	Potency		Counterscreen for APE1 Inhibitors: qHTS Validation Assay for Inhibitors of Endonuclease IV	endonuclease IV [Escherichia coli][gi:405898]	
540276	Inactive	Potency		qHTS for inhibitors of binding or entry into cells for Marburg Virus	gene 4 small orf - Marburg virus[gi:420597]	
540276	Inactive	Potency		qHTS for inhibitors of binding or entry into cells for Marburg Virus	gene 4 small orf - Marburg virus[gi:420597]	
2023	Inactive			Multiplex HTS Screen of TOR pathway GFP-fusion proteins in Saccharomyes cerevisiae_specifically_ LAP4_MLPCN.	LAP4 [Saccharomyces cerevisiae][gi:486173]	
1873	Inactive			Multiplex HTS Screen of TOR pathway GFP-fusion proteins in Saccharomyes cerevisiae_specifically_LAP4	LAP4 [Saccharomyces cerevisiae][gi:486173]	
361	Inactive			Pyruvate Kinase	pyruvate kinase [Geobacillus stearothermophilus][gi:285623]	
1862	Inactive			Multiplex HTS Screen of TOR pathway GFP-fusion proteins in Saccharomyes cerevisiae_specifically_RPL19A	RPL19A [Saccharomyces cerevisiae][gi:536029]	

AID	Outcome	Activity Concentration Name	Activity Concentration [uM]	BioAssay	Target	PMID
2025	Inactive			Multiplex HTS Screen of TOR pathway GFP-fusion proteins in Saccharomyes cerevisiae_specifically_ RPL19A_MLPCN	RPL19A [Saccharomyces cerevisiae][gi:536029]	
504894	Inactive	Potency		Activators of T cell receptors: qHTS campaign	T cell receptor [Homo sapiens][gi:553160]	
2016	Inactive			Multiplex HTS Screen of TOR pathway GFP-fusion proteins in Saccharomyes cerevisiae_specifically_ MEP2_MLPCN.	MEP2 [Saccharomyces cerevisiae][gi:1302091]	
1867	Inactive			Multiplex HTS Screen of TOR pathway GFP-fusion proteins in Saccharomyes cerevisiae_specifically_MEP2	MEP2 [Saccharomyces cerevisiae][gi:1302091]	
817	Inactive			Identification and characterization of compounds for addressing human bone marrow failure	unnamed protein product [Saccharomyces cerevisiae][gi:1360328]	
565	Inactive			HIV-1 RT-RNase H MLSCN HTS MH077605	Chain A, Hiv-1 Reverse Transcriptase Mol_id: 1; Molecule: Hiv-1 Reverse Transcriptase; Chain: A, B; [gi:1431733]	
1379	Inactive	Potency		Counterscreen for Luciferase (Kinase-Glo TM) Inhibition	luciferase [Photuris pennsylvanica][gi:1669525]	
1379	Inactive	Potency		Counterscreen for Luciferase (Kinase-Glo TM) Inhibition	luciferase [Photuris pennsylvanica][gi:1669525]	
651965	Inactive	Potency		qHTS Assay for Activators of ClpP	ClpP [Bacillus subtilis][gi:2668494]	
429	Inactive			HTS for Tumor Hsp90 Inhibitors	90-kda heat shock protein beta HSP90 beta [Homo sapiens][gi:4261762]	
429	Inactive			HTS for Tumor Hsp90 Inhibitors	90-kda heat shock protein beta HSP90 beta [Homo sapiens][gi:4261762]	

AID	Outcome	Activity Concentration Name	Activity Concentration [uM]	BioAssay	Target	PMID
2177	Inactive			Counterscreen for PME1 inhibitors: fluorescence polarization-based primary biochemical high throughput screening assay to identify inhibitors of lysophospholipase 2 (LYPLA2)	lysophospholipase II [Homo sapiens][gi:4581413]	
2517	Inactive	Potency		qHTS Assay for Inhibitors of the Human Apurinic/apyrimidinic Endonuclease 1 (APE1)	Chain A, Human Ape1 Endonuclease With Bound Abasic Dna And Mn2+ Ion[gi:6980812]	
2517	Inactive	Potency		qHTS Assay for Inhibitors of the Human Apurinic/apyrimidinic Endonuclease 1 (APE1)	Chain A, Human Ape1 Endonuclease With Bound Abasic Dna And Mn2+ Ion[gi:6980812]	
1705	Inactive	Potency		qHTS Validation Assay for Inhibitors of the Human Apurinic/apyrimidinic Endonuclease 1 (APE1)	Chain A, Human Ape1 Endonuclease With Bound Abasic Dna And Mn2+ Ion[gi:6980812]	
624204	Inactive			uHTS identification of small molecule inhibitors of the catalytic domain of the SUMO protease, SENP1 in a FRET assay	SENP1 gene product [Homo sapiens][gi:7657550]	
1018	Inactive	IC50		Chemical Antagonists IAP-family anti-apoptotic proteins	X-linked inhibitor of apoptosis [Homo sapiens][gi:8744934]	
1066	Inactive			High Throughput Screen to Identify Compounds that Inhibit Class II HMG-CoA Reductases - Primary Screen	acetyl-CoA acetyltransferase/HMG-CoA reductase [Enterococcus faecalis][gi:9937384]	
1242	Inactive			C. albicans biofilm killing---Mixture HTS	glycosyl-phosphatidylinositol protein [Candida albicans][gi:11094021]	
1490	Inactive	Potency		qHTS Assay for Inhibitors of Bacillus subtilis Sfp phosphopantetheinyl transferase (PPTase)	phosphopantetheinyl transferase [Bacillus subtilis][gi:10954339]	
1490	Inactive	Potency		qHTS Assay for Inhibitors of Bacillus subtilis Sfp phosphopantetheinyl transferase (PPTase)	phosphopantetheinyl transferase [Bacillus subtilis][gi:10954339]	

AID	Outcome	Activity Concentration Name	Activity Concentration [uM]	BioAssay	Target	PMID
504690	Inactive			uHTS identification of small molecule inhibitors of Plasmodium falciparum Glucose-6-phosphate dehydrogenase via a fluorescence intensity assay	glucose-6-phosphate dehydrogenase-6-phosphogluconolactonase [Plasmodium berghei][gi:12381848]	
686996	Inactive			VEID(2) R110 Enzymatic Primary HTS to identify Inhibitors of Caspase 6 Measured in Biochemical System Using Plate Reader - 7052-01_Inhibitor_SinglePoint_HTS_Activity_Set2	Caspase 6, apoptosis-related cysteine peptidase [Homo sapiens][gi:13325293]	
591	Inactive			qHTS Assay for Spectroscopic Profiling in A488 Spectral Region		
592	Inactive			qHTS Assay for Spectroscopic Profiling in A647 Spectral Region		
1463	Inactive	Potency		Counterscreen qHTS for Inhibitors of Tau Fibril Formation, Fluorescence Polarization		
1477	Inactive	Potency		qHTS Assay for Compounds Blocking the Interaction Between CBF-beta and RUNX1 for the Treatment of Acute Myeloid Leukemia		
1519	Inactive	Potency		qHTS Assay for Lipid Storage Modulators		
1707	Inactive	Potency		Counterscreen for APE1 Inhibitors: Fluorescent Dye Displacement Validation Assay		
1865	Inactive	Potency		Quantitative High-Throughput Screen for Regulators of Epigenetic Control		
371	Inactive			Human A549 Lung Tumor Cell Growth Inhibition Assay		
430	Inactive	EC50		Fluorescent HTS Cytotoxicity/Cell viability assay (HPDE-C7 cells)		

AID	Outcome	Activity Concentration Name	Activity Concentration [uM]	BioAssay	Target	PMID
431	Inactive	EC50		Fluorescent HTS Cytotoxicity/Cell viability assay (HPDE-C7K cells)		
594	Inactive			qHTS Assay for Spectroscopic Profiling in Rhodamine Spectral Region		
597	Inactive			qHTS Assay for Epigenetic Modulators		
598	Inactive			Human H69AR Lung Tumor Cell Growth Inhibition Assay - 86K Screen		
601	Inactive			Identification of Molecular Probes that Reverse MRP-Mediated Drug Resistance Pilot Screen		
602	Inactive			Identification of Molecular Probes that Reverse MRP-Mediated Drug Resistance		
609	Inactive			Chemical Complementation Assay for MKP-3		
2391	Inactive	IC50		A Cell Based HTS Approach for the Discovery of New Inhibitors of Respiratory syncytial virus (RSV)		
2380	Inactive			uHTS identification of small molecules that induce b-cell replication in the MIN-6 cell line		
2685	Inactive	Potency		qHTS Assay for Lipid Storage Modulators in Drosophila S3 Cells		
2690	Inactive			A yeast HTS for caloric restriction mimetics that inhibit age-related superoxide		
2706	Inactive			A yeast HTS for caloric restriction mimetics that inhibit age-related superoxide for Validation Compound Set		
2716	Inactive			Luminescence Microorganism Primary HTS to Identify Inhibitors of the SUMOylation Pathway Using a Temperature Sensitive Growth Reversal Mutant Mot1-301		

AID	Outcome	Activity Concentration Name	Activity Concentration [uM]	BioAssay	Target	PMID
2717	Inactive			Luminescence Cell-Based Primary HTS to Identify Inhibitors of Cancer Stem Cells		
434955	Inactive	IC90		Screen to Identify Novel Compounds That Sensitize Mycobacterium Tuberculosis to Beta-lactam Antibiotics		
435003	Inactive			uHTS luminescence assay for the identification of chemical inhibitors of T-cell specific antigen receptor-induced NF-kB activation		
435005	Inactive			Luminescence Cell-Based Primary HTS to Identify Inhibitors of Beta Cell Apoptosis.		
435022	Inactive			uHTS luminescence assay for the identification of chemical inhibitors of B-cell specific antigen receptor-induced NF-kB activation		
449728	Inactive			Counterscreen for inhibitors of AddAB: absorbance-based bacterial cell-based high throughput screening assay to identify inhibitors of bacterial viability		
449762	Inactive	IC50		High Throughput Screening Assay used to Identify Novel Compounds that Inhibit Mycobacterium Tuberculosis in 7H9 Media		
449763	Inactive			uHTS identification of small molecule activators of the apoptotic arm of the Unfolded Protein response via a luminescent-based reporter assay		
732	Inactive			In Vivo Angiogenesis Assay for HTS		
463104	Inactive			uHTS identification of small molecule activators of the adaptive arm of the Unfolded Protein response via a luminescent-based reporter assay		
463187	Inactive			384-well Z-Lyte format Hck-Nef inhibitor HTS run at the PMLSC		

AID	Outcome	Activity Concentration Name	Activity Concentration [uM]	BioAssay	Target	PMID
463189	Inactive			96-well format Chlamydomonas reinhardtii Algae Gravitaxis Assay to measure the difference in the absorbance between the small compact plug of WT swimming algae versus the MUT algae lacking cilia		
485275	Inactive			Phenotypic HTS multiplex for antifungal efflux pump inhibitors		
485298	Inactive	Potency		qHTS Assay for Small Molecule Inhibitors of Mitochondrial Division or Activators of Mitochondrial Fusion		
463079	Inactive			Fluorescence-based counterscreen for orexin 1 receptor (OX1R) antagonists: cell-based assay to identify antagonists of the parental CHO cell line		
463075	Inactive			HTS to identify inhibitors of TNF-alpha Induced Cell Death in Jurkat FADD-/- Cells.		
488890	Inactive	IC50		Elucidation of physiology of non-replicating, drug-tolerant Mycobacterium tuberculosis		
2275	Inactive			Luminescence Cell-Based Primary HTS to Measure Viability of BJeLR cells		
1948	Inactive	Potency		qHTS Assay for Compounds that Induce Erasure of Genomic Imprints		
2322	Inactive			Luminescence Homogenous Primary HTS to Identify Inhibitors of STK33 Activity		
2774	Inactive			LOPAC Circadian Assay		
434959	Inactive			Fluorescence Cell-Based Primary HTS to Measure Inhibition of Y box Binding Protein 1 Expression		
504408	Inactive			Heat Shock Factor-1 (HSF-1) Measured in Cell-Based System Using Plate Reader - 2038-01_Activator_SinglePoint_HTS_Activity		

AID	Outcome	Activity Concentration Name	Activity Concentration [uM]	BioAssay	Target	PMID
588368	Inactive			HTS to Find Inhibitors of Pathogenic Pemphigus Antibodies from validation set		
588460	Inactive			High-throughput multiplex microsphere screening for inhibitors of toxin protease, specifically Botulinum neurotoxin light chain A protease, Validation Compound Set		16604538
588506	Inactive			Phenotypic HTS multiplex for antifungal efflux pump inhibitors with Validation compound Set		
588685	Inactive			HTS to identify compounds that promote myeloid differentiation with Validation compound set		
750	Inactive			Luminescent HTS for small molecule activators of MT1-MMP transcription		
751	Inactive			Disassembly of the 26S Proteasome (ATP Hydrolysis-dependent)		
795	Inactive			MLSCN Assay for Activators of Prostate Cell Differentiation		
804	Inactive			Screen for Chemicals that Shorten Yeast Lifespan		
834	Inactive			C. albicans biofilm killing		
841	Inactive			Non-Nucleoside Inhibitor of Measles Virus RNA-Dependent RNA Polymerase Complex Activity HTS Single Point (MLSMR Library)		
847	Inactive			Human SK-BR-3 Breast Tumor Cell Growth Inhibition In a 24- Hour Assay		
818	Inactive			High Throughput Screen to Identify Compounds that Suppress the Growth of Human Colon Tumor Cells Lacking Oncogenic Beta Catenin Expression		

AID	Outcome	Activity Concentration Name	Activity Concentration [uM]	BioAssay	Target	PMID
827	Inactive			High Throughput Screen to Identify Compounds that Suppress the Growth of Cells with a Deletion of the PTEN Tumor Suppressor		
868	Inactive			Screen for Chemicals that Inhibit the RAM Network		
878	Inactive			NIH Compound Library Profiling: Compound and DTT Dependent Redox Cycling H2O2 Generation		
1006	Inactive			Counter Screen for Luciferase-based Primary Inhibition Assays		
1027	Inactive			Counter Screen for Luciferase-based Primary Stimulation Assays		
1063	Inactive			Leishmania major promastigote HTS		
1222	Inactive	EC50		High Throughput Screen for Inhibitors of ER Stress-induced Cell Death in a 384 well format		
1235	Inactive			Alternative Pathway ELISA_orthogonal screening		
1251	Inactive			Anti-Viral Drugs Against Arbovirus Infections, a Primary Screen		
1362	Inactive			Chemical Genetic Screen to Identify Inhibitors of Mitochondrial Fusion - Primary Screen		
1377	Inactive			HTS to identify inhibitors of zVAD Induced Cell Death in L929 Cells		
1381	Inactive			HCS to Identify Inhibitors of Dynein Mediated Cargo Transport on Microtubules.		
1463	Inactive	Potency		Counterscreen qHTS for Inhibitors of Tau Fibril Formation, Fluorescence Polarization		
1465	Inactive	EC50		Screen for small molecule probes relevant to Friedreich's ataxia, Single Dose and Dose Response		

AID	Outcome	Activity Concentration Name	Activity Concentration [uM]	BioAssay	Target	PMID
1477	Inactive	Potency		qHTS Assay for Compounds Blocking the Interaction Between CBF-beta and RUNX1 for the Treatment of Acute Myeloid Leukemia		
1486	Inactive			Counterscreen for inhibitors of Janus kinase 2 mutant JAK2V617F: Cell-based high throughput assay to identify inhibitors of parental Ba/F3 cell viability		
1532	Inactive			Rml C and D inhibition 384-well mixture HTS		
1554	Inactive			MLPCN Ras selective lethality-BJeLR viability		
1621	Inactive	IC50		A Cell Based Assay for the Identification of Lead Compounds with Anti-Viral Activity Against West Nile Virus		
1626	Inactive	IC50		High Throughput Screen to Identify Inhibitors of Mycobacterium tuberculosis H37Rv		
1663	Inactive			MLPCN Platelet Activation -Dense Granule Release		
1656	Inactive			High Throughput Imaging Assay for Hepatic Lipid Droplet Formation		
1775	Inactive			Profiling compound fluorescence on Avidin Beads with 488 nm excitation and 530 nm emission		
1776	Inactive			Profiling compound fluorescence on GSH Beads with 488 nm excitation and 530 nm emission		
1813	Inactive			MLPCN Alpha-Synuclein 5'UTR - 5'-UTR binding - inhibitors		
1814	Inactive			MLPCN Alpha-Synuclein 5'UTR - 5'-UTR binding - activators		

AID	Outcome	Activity Concentration Name	Activity Concentration [uM]	BioAssay	Target	PMID
1825	Inactive			Luminescence-based counterscreen assay for KLF5 inhibitors: cell-based high throughput screening assay to identify cytotoxic compounds using the IEC-6 intestinal epithelial cell line		
1850	Inactive	IC50		A small molecule screen for inhibitors of the PhoP regulon in Salmonella typhi		
1863	Inactive	IC50		A small molecule screen for inhibitors of the PhoP regulon in Salmonella Typhimurium		
1865	Inactive	Potency		Quantitative High-Throughput Screen for Regulators of Epigenetic Control		
1875	Inactive			Luminescence Cell-Based Primary HTS to Identify Inhibitors of Polyadenylation		
1885	Inactive			Luminescence Cell-Based/Microorganism Primary HTS to Identify Inhibitors of T.Cruzi Replication		
1910	Inactive			Luminescence Cell-Based Primary HTS to Identify Transcriptional Activators of Hypoxia-Inducible Factor Pathway		
1956	Inactive	Conc @ Max Fold Increase		A high-throughput screen to identify small molecule compounds that augment HSV replication		
2099	Inactive			Fluorescence Biochemical Primary HTS to Identify Inhibitors of GASC-1 Activity		
2216	Inactive			Fluorescence Cell-Free Homogeneous Primary HTS to Identify Inhibitors of the RanGTP-Importin-beta complex		
626	Inactive			Discovery of Novel Allosteric Modulators of the M1 Muscarinic Receptor: Agonist Primary Screen		
620	Inactive	EC50		Fluorescent HTS Cytotoxicity/Cell viability assay (HT1080 cells)		

AID	Outcome	Activity Concentration Name	Activity Concentration [uM]	BioAssay	Target	PMID
636	Inactive			Modulators of Post-Golgi Transport - 384-well pilot screen		
637	Inactive			Modulators of Post-Golgi Transport - 1536-well pilot screen		
641	Inactive			Allosteric Modulators of D1 Receptors: Primary Screen		
645	Inactive			Isolation of Inhibitors of Her-Kinase Expression - 66K library screen		
648	Inactive			Human Endothelial Cell Proliferation Assay in 384-well format		
708	Inactive			Profiling the NIH Molecular Libraries Small Molecule Repository: Absorbance at 340 nm		
709	Inactive			Profiling the NIH Molecular Libraries Small Molecule Repository: Autofluorescence at 339/460 nm		
719	Inactive			Human Lung Fibroblast Proliferation Assay		
686	Inactive			Zebrafish Lipid Metabolism Assay---Primary Screen		
770	Inactive			Cell Growth High Content Screening Assay of Human HT29 Colon Tumor Cells (24 Hour Treatment Protocol)		
771	Inactive			Cell Growth High Content Screening Assay of Human HT29 Colon Tumor Cells (48 Hour Treatment Protocol)		
772	Inactive			Cell Growth High Content Screening Assay of Human HT29 Colon Tumor Cells (72 Hour Treatment Protocol)		
774	Inactive			Profiling the NIH Molecular Libraries Small Molecule Repository: Inhibition of Enzymes Frequently Used to reach a NAD/NADH Endpoint		

AID	Outcome	Activity Concentration Name	Activity Concentration [uM]	BioAssay	Target	PMID
775	Inactive			Screen for Chemicals that Extend Yeast Lifespan		
446	Inactive			Stat Signaling Pathway		
454	Inactive			VCAM-1 Plate Reader Assay in Pooled HUVECs: Inhibition of TNFa induced VCAM-1 cell surface expression		
455	Inactive			VCAM-1 Plate Reader Assay in Pooled HUVECs: Augmentation of TNFa induced VCAM-1 cell surface expression		
456	Inactive			VCAM-1 Imaging Assay in Pooled HUVECs: Inhibition of TNFa induced VCAM-1 cell surface expression		
457	Inactive			VCAM-1 Imaging Assay in Pooled HUVECs: Augmentation of TNFa induced VCAM-1 cell surface expression.		
487	Inactive			TNFalpha Induced E-Selectin Expression - Primary screen		
364	Inactive			Cell Proliferation & Viability (Cytotoxicity) Assay		
527	Inactive			Primary HTS Assay for Inhibitors of Bacterial Quorum Sensing		
552	Inactive			Antimicrobial HTS Assay for E. coli BW25113 (wild type)		
572	Inactive			Human SK-BR-3 Breast Tumor Cell Growth Inhibition In a 24- Hour Assay (Pilot Screen)		
573	Inactive			Primary Antimicrobial Assay for E. coli BW25113 ∆tolC::kan Protocol for 384-well HTS		
575	Inactive			Human Endothelial Cell Proliferation Assay		
580	Inactive			Human H69AR Lung Tumor Cell Growth Inhibition Assay		

AID	Outcome	Activity Concentration Name	Activity Concentration [uM]	BioAssay	Target	PMID
587	Inactive			qHTS Assay for Spectroscopic Profiling in Texas Red Spectral Region		
588	Inactive			qHTS Assay for Spectroscopic Profiling in Resorufin Spectral Region		
589	Inactive			qHTS Assay for Spectroscopic Profiling in 4-MU Spectral Region		
588664	Inactive			TRFRET-based biochemical primary high throughput screening assay to identify inhibitors of the interaction of the Ras and Rab interactor 1 protein (Rin1) and the c-abl oncogene 1, non-receptor tyrosine kinase (Abl)	ABL1 gene product [Homo sapiens][gi:62362414]	
588664	Inactive			TRFRET-based biochemical primary high throughput screening assay to identify inhibitors of the interaction of the Ras and Rab interactor 1 protein (Rin1) and the c-abl oncogene 1, non-receptor tyrosine kinase (Abl)	ABL1 gene product [Homo sapiens][gi:62362414]	
651560	Inactive			uHTS identification of small molecule inhibitors of Low Molecular Weight Protein Tyrosine Phosphatase, LMPTP, via a fluorescence intensity assay	Low molecular weight phosphotyrosine protein phosphatase[gi:1709543]	
651560	Inactive			uHTS identification of small molecule inhibitors of Low Molecular Weight Protein Tyrosine Phosphatase, LMPTP, via a fluorescence intensity assay	Low molecular weight phosphotyrosine protein phosphatase[gi:1709543]	
504459	Inactive			HTS for Beta-2AR agonists via FAP method from Validation Set	ADRB2 gene product [Homo sapiens][gi:4501969]	
504459	Inactive			HTS for Beta-2AR agonists via FAP method from Validation Set	ADRB2 gene product [Homo sapiens][gi:4501969]	
504459	Inactive			HTS for Beta-2AR agonists via FAP method from Validation Set	ADRB2 gene product [Homo sapiens][gi:4501969]	

AID	Outcome	Activity Concentration Name	Activity Concentration [uM]	BioAssay	Target	PMID
504459	Inactive			HTS for Beta-2AR agonists via FAP method from Validation Set	ADRB2 gene product [Homo sapiens][gi:4501969]	
492947	Inactive	Potency		qHTS assay of beta-arrestin-biased ligands of beta2-adrenergic receptor	ADRB2 gene product [Homo sapiens][gi:4501969]	
492947	Inactive	Potency		qHTS assay of beta-arrestin-biased ligands of beta2-adrenergic receptor	ADRB2 gene product [Homo sapiens][gi:4501969]	
492947	Inactive	Potency		qHTS assay of beta-arrestin-biased ligands of beta2-adrenergic receptor	ADRB2 gene product [Homo sapiens][gi:4501969]	
492947	Inactive	Potency		qHTS assay of beta-arrestin-biased ligands of beta2-adrenergic receptor	ADRB2 gene product [Homo sapiens][gi:4501969]	
504454	Inactive			HTS for Beta-2AR agonists via FAP method	ADRB2 gene product [Homo sapiens][gi:4501969]	
504454	Inactive			HTS for Beta-2AR agonists via FAP method	ADRB2 gene product [Homo sapiens][gi:4501969]	
504454	Inactive			HTS for Beta-2AR agonists via FAP method	ADRB2 gene product [Homo sapiens][gi:4501969]	
504454	Inactive			HTS for Beta-2AR agonists via FAP method	ADRB2 gene product [Homo sapiens][gi:4501969]	
485366	Inactive	Potency		qHTS validation assay of beta-arrestin-biased ligands of beta2-adrenergic receptor	ADRB2 gene product [Homo sapiens][gi:4501969]	
485366	Inactive	Potency		qHTS validation assay of beta-arrestin-biased ligands of beta2-adrenergic receptor	ADRB2 gene product [Homo sapiens][gi:4501969]	
485366	Inactive	Potency		qHTS validation assay of beta-arrestin-biased ligands of beta2-adrenergic receptor	ADRB2 gene product [Homo sapiens][gi:4501969]	
485366	Inactive	Potency		qHTS validation assay of beta-arrestin-biased ligands of beta2-adrenergic receptor	ADRB2 gene product [Homo sapiens][gi:4501969]	
488806	Inactive			RNA aptamer-based validation for inhibitors of GRK2	beta-adrenergic receptor kinase 1 [Homo sapiens][gi:148539876]	
488847	Inactive			RNA aptamer-based HTS for inhibitors of GRK2	beta-adrenergic receptor kinase 1 [Homo sapiens][gi:148539876]	

AID	Outcome	Activity Concentration Name	Activity Concentration [uM]	BioAssay	Target	PMID
2520	Inactive			uHTS identification of small molecule agonists of the APJ receptor via a luminescent beta-arrestin assay	APLNR gene product [Homo sapiens][gi:4885057]	
2520	Inactive			uHTS identification of small molecule agonists of the APJ receptor via a luminescent beta-arrestin assay	APLNR gene product [Homo sapiens][gi:4885057]	
2521	Inactive			uHTS identification of small molecule antagonists of the APJ receptor via a luminescent beta-arrestin assay	APLNR gene product [Homo sapiens][gi:4885057]	
2521	Inactive			uHTS identification of small molecule antagonists of the APJ receptor via a luminescent beta-arrestin assay	APLNR gene product [Homo sapiens][gi:4885057]	
652010	Inactive			Luminescence-based cell-based primary high throughput screening assay for inhibitors of the orphan nuclear receptor subfamily 0, group B, member 1 (DAX1; NR0B1): repression of SF-1 (NR5A1) activated StAR promoter by full-length DAX-1	NR0B1 gene product [Homo sapiens][gi:5016090]	
504766	Inactive			Luminescence-based primary cell-based high throughput screening assay to identify inhibitors of the orphan nuclear receptor subfamily 0, group B, member 1 (DAX1; NR0B1)	NR0B1 gene product [Homo sapiens][gi:5016090]	
2796	Inactive			Luminescence-based primary cell-based high throughput screening assay to identify activators of the Aryl Hydrocarbon Receptor (AHR)	AHR gene product [Homo sapiens][gi:4502003]	
2796	Inactive			Luminescence-based primary cell-based high throughput screening assay to identify activators of the Aryl Hydrocarbon Receptor (AHR)	AHR gene product [Homo sapiens][gi:4502003]	
2796	Inactive			Luminescence-based primary cell-based high throughput screening assay to identify activators of the Aryl Hydrocarbon Receptor (AHR)	AHR gene product [Homo sapiens][gi:4502003]	

AID	Outcome	Activity Concentration Name	Activity Concentration [uM]	BioAssay	Target	PMID
651550	Inactive			HTS Assay for Inhibitors of Akt Phophorylation: Primary Screen	RAC-alpha serine/threonine-protein kinase[gi:60391226]	
651550	Inactive			HTS Assay for Inhibitors of Akt Phophorylation: Primary Screen	RAC-alpha serine/threonine-protein kinase[gi:60391226]	
651550	Inactive			HTS Assay for Inhibitors of Akt Phophorylation: Primary Screen	RAC-alpha serine/threonine-protein kinase[gi:60391226]	
1030	Inactive	Potency		qHTS Assay for Inhibitors of Aldehyde Dehydrogenase 1 (ALDH1A1)	aldehyde dehydrogenase 1 family, member A1 [Homo sapiens][gi:30582681]	
1030	Inactive	Potency		qHTS Assay for Inhibitors of Aldehyde Dehydrogenase 1 (ALDH1A1)	aldehyde dehydrogenase 1 family, member A1 [Homo sapiens][gi:30582681]	
485290	Inactive	Potency		qHTS Assay for Inhibitors of Tyrosyl-DNA Phosphodiesterase (TDP1)	Chain A, Crystal Structure Of Human Tyrosyl-Dna Phosphodiesterase (Tdp1)[gi:20150581]	
485290	Inactive	Potency		qHTS Assay for Inhibitors of Tyrosyl-DNA Phosphodiesterase (TDP1)	Chain A, Crystal Structure Of Human Tyrosyl-Dna Phosphodiesterase (Tdp1)[gi:20150581]	
720542	Inactive	Potency		qHTS for Inhibitors of AMA1-RON; Towards Development of Antimalarial Drug Lead: Primary Screen	apical membrane antigen 1, AMA1 [Plasmodium falciparum 3D7][gi:23496270]	
1556	Inactive			Epi-absorbance primary biochemical high throughput screening assay to identify inhibitors of IMP-1 metallo-beta-lactamase	metallo-beta-lactamase IMP-1 [Pseudomonas aeruginosa][gi:27368096]	
720508	Inactive			Fluorescence polarization-based biochemical primary high throughput screening assay to identify inhibitors that disrupt the binding of a cyclic peptide (Tn7) to the fibrin proteolytic product D-Dimer and fragment E complex [DD(E)]	Chain E, Fragment Double-D From Human Fibrin[gi:28373962]	

AID	Outcome	Activity Concentration Name	Activity Concentration [uM]	BioAssay	Target	PMID
720509	Inactive			Fluorescence polarization-based biochemical primary high throughput screening assay to identify inhibitors that disrupt the binding of a cyclic peptide (Tn6) to the fibrin proteolytic product D-Dimer and fragment E complex [DD(E)]	Chain E, Fragment Double-D From Human Fibrin[gi:28373962]	
485295	Inactive	Potency		qHTS Validation Assay for the Inhibitors of DNA Replication in Gram-Positive Bacteria	DNA polymerase III [Bacillus subtilis][gi:30027657]	
2314	Inactive			Cycloheximide Counterscreen for Small Molecule Inhibitors of Shiga Toxin	shiga toxin 1 variant A subunit [Escherichia coli O157:H7][gi:32400299]	
2315	Inactive			A qHTS for Small Molecule Inhibitors of Shiga Toxin	shiga toxin 1 variant A subunit [Escherichia coli O157:H7][gi:32400299]	
2674	Inactive			HTS for Identification of VLA-4 Allosteric Modulators from Validation Compound Set.	Chain A, The Crystal Structure Of The I-Domain Of Human Integrin Alpha1beta1[gi:34810098]	
1986	Inactive	IC50		uHTS fluorescence assay for the identification of Human Immunodeficiency Virus Fusion Inhibitors.	envelope glycoprotein [Human immunodeficiency virus 1][gi:45357394]	
588519	Inactive			A screen for compounds that inhibit viral RNA polymerase binding and polymerization activities	Chain A, Poliovirus Polymerase With Gtp[gi:52695378]	21722674
588519	Inactive			A screen for compounds that inhibit viral RNA polymerase binding and polymerization activities	Chain A, Poliovirus Polymerase With Gtp[gi:52695378]	21722674
861	Inactive			Primary cell-based high-throughput screening assay for inhibitors of TLR4-MyD88 binding	toll-like receptor 4 [Homo sapiens][gi:55662034]	
1906	Inactive			QFRET-based counterscreen for PFM18AAP inhibitors: biochemical high throughput screening assay to identify inhibitors of the Cathepsin L proteinase (CTSL1)	cathepsin L1 [Homo sapiens][gi:55958172]	

AID	Outcome	Activity Concentration Name	Activity Concentration [uM]	BioAssay	Target	PMID
463210	Inactive			Counterscreen for procaspase-3 activators: absorbance-based primary biochemical high throughput screening assay to identify activators of procaspase-7	caspase 7, apoptosis-related cysteine peptidase [Homo sapiens][gi:55960760]	
761	Inactive			HTS to identify specific small molecule inhibitors of Ras and Ras-related GTPases specifically Cdc42 wildtype	cell division cycle 42 (GTP binding protein, 25kDa) [Homo sapiens][gi:56202836]	
624173	Inactive	Potency		qHTS of Trypanosoma Brucei Inhibitors	hypothetical protein, conserved [Trypanosoma brucei][gi:62359610]	
624173	Inactive	Potency		qHTS of Trypanosoma Brucei Inhibitors	hypothetical protein, conserved [Trypanosoma brucei][gi:62359610]	
624147	Inactive	Potency		qHTS of Trypanosoma Brucei Inhibitors: LOPAC Validation	hypothetical protein, conserved [Trypanosoma brucei][gi:62359610]	
2094	Inactive			Plate Read Microorganism-Based Primary HTS to Identify Modulators of the AI-2 Quorum Sensing System	Chain A, Crystal Structure Of The Apo Form Of Vibrio Harveyi Luxp Complexed With The Periplasmic Dom[gi:67463988]	
1706	Inactive			QFRET-based primary biochemical high throughput screening assay to identify inhibitors of the SARS coronavirus 3C-like Protease (3CLPro)	3C-like protease [Infectious bronchitis virus][gi:73745819]	
602405	Inactive			PgID: DNTB colorimetric HTS to detect inhibitor of PgID Measured in Biochemical System Using Plate Reader - 2164-01_Inhibitor_SinglePoint_HTS_Activity	WlaI protein (PglD)[gi:75495260]	
493033	Inactive			A screen for compounds that inhibit the bacterial siderophore biosynthetic enzyme MbtI	Isochorismate synthase/isochorismate-pyruvate lyase mbtI[gi:81706979]	
493033	Inactive			A screen for compounds that inhibit the bacterial siderophore biosynthetic enzyme MbtI	Isochorismate synthase/isochorismate-pyruvate lyase mbtI[gi:81706979]	

AID	Outcome	Activity Concentration Name	Activity Concentration [uM]	BioAssay	Target	PMID
1899	Inactive			TR-FRET-based primary biochemical high-throughput screening assay to identify inhibitors of Hepatitis C Virus (HCV) core protein dimerization	core protein [Hepatitis C virus][gi:83779224]	
720511	Inactive			Identification of Small Molecule Correctors of the Cystic Fibrosis Transmembrane Conductance Regulator (CFTR) Delta508 Mutation Function in Human Bronchial Epithelial Cells. Measured in Cell-Based System Using Plate Reader - 7017-01_Other_SinglePoint_HTS_Activity	cystic fibrosis transmembrane conductance regulator ATP-binding cassette sub-family C member 7 [Homo[gi:89348172]	
375	Inactive			Mycobacterium tuberculosis Pantothenate Synthetase Assay	Chain A, Crystal Structure Of A Pantothenate Synthetase, Apo Enzyme In C2 Space Group[gi:90108679]	
687016	Inactive			Counterscreen for inhibitors of 5-meCpG-binding domain protein 2 (MBD2): TRFRET-based biochemical primary high throughput screening assay to identify inhibitors of binding of ubiquitin-like with PHD and ring finger domains 1 (UHRF1) to methylated oligonucleotide	UHRF1 gene product [Homo sapiens][gi:115430235]	
485294	Inactive	Potency		qHTS Inhibitors of AmpC Beta-Lactamase (assay with detergent)	Chain A, Ampc Beta-Lactamase In Complex With 4-Methanesulfonylamino Benzoic Acid[gi:119389684]	
485341	Inactive	Potency		qHTS Inhibitors of AmpC Beta-Lactamase (assay without detergent)	Chain A, Ampc Beta-Lactamase In Complex With 4-Methanesulfonylamino Benzoic Acid[gi:119389684]	
504803	Inactive			Fluorescence polarization-based primary biochemical high throughput screening assay to identify inhibitors of the HTRA serine peptidase 1 (HTRA1)	HTRA1 protein[gi:121945198]	

AID	Outcome	Activity Concentration Name	Activity Concentration [uM]	BioAssay	Target	PMID
2451	Inactive	Potency		qHTS Assay for Inhibitors of Fructose-1,6-bisphosphate Aldolase from Giardia Lamblia	Chain A, Structure Of Giardia Fructose-1,6-Biphosphate Aldolase In Complex With Phosphoglycolohydrox[gi:122920737]	
2451	Inactive	Potency		qHTS Assay for Inhibitors of Fructose-1,6-bisphosphate Aldolase from Giardia Lamblia	Chain A, Structure Of Giardia Fructose-1,6-Biphosphate Aldolase In Complex With Phosphoglycolohydrox[gi:122920737]	
583	Inactive	IC50		High Throughput Screening Assay for Hsp70 Inhibitors	heat shock 70kDa protein 1A [Homo sapiens][gi:123271505]	
1845	Inactive			Fluorescence-based counterscreen assay for HCV NS3 helicase inhibitors: biochemical high-throughput screening assay to identify compounds that cause fluorescent intercalator displacement (FID)	NS3 [Hepatitis C virus][gi:125541954]	
1800	Inactive			Fluorescence-based primary biochemical high throughput screening assay to identify inhibitors of the Hepatitis C Virus non-structural protein 3 helicase (NS3)	NS3 [Hepatitis C virus][gi:125541954]	
687035	Inactive			Fluorescence polarization based primary biochemical high throughput screening assay of LOPAC1280 to identify inhibitors of hepatitis C non-structural protein 3 helicase	NS3 [Hepatitis C virus][gi:125541954]	22740655
602438	Inactive			uHTS identification of modulators of interaction between CendR and NRP-1 using Fluorescence Polarization assay	Chain A, Crystal Structure Of The B1b2 Domains From Human Neuropilin- 1[gi:160877737]	
504339	Inactive	Potency		qHTS Assay for Inhibitors of JMJD2A-Tudor Domain	Chain A, Jmjd2a Tandem Tudor Domains In Complex With A Trimethylated Histone H4-K20 Peptide[gi:162330054]	
2241	Inactive			Luminescence Cell-Based Primary HTS to Identify Inhibitors of A1	Chain A, Human Bcl2-A1 In Complex With Bim-Bh3 Peptide[gi:167013344]	

AID	Outcome	Activity Concentration Name	Activity Concentration [uM]	BioAssay	Target	PMID
588459	Inactive			High-throughput multiplex microsphere screening for inhibitors of toxin protease, specifically Botulinum neurotoxin light chain F protease, Validation compound set	botulinum neurotoxin type F, BoNT/F [Clostridium botulinum Bf][gi:168184763]	16604538
588497	Inactive			High-throughput multiplex microsphere screening for inhibitors of toxin protease, specifically Botulinum neurotoxin light chain F protease, MLPCN compound set	botulinum neurotoxin type F, BoNT/F [Clostridium botulinum Bf][gi:168184763]	16604538
602332	Inactive	Potency		qHTS for Inducers of the Endoplasmic Reticulum Stress Response (ERSR) in Human Glioma: qHTS	heat shock 70kDa protein 5 (glucose-regulated protein, 78kDa) [Homo sapiens][gi:168984549]	
504836	Inactive	Potency		Inducers of the Endoplasmic Reticulum Stress Response (ERSR) in human glioma: Validation	heat shock 70kDa protein 5 (glucose-regulated protein, 78kDa) [Homo sapiens][gi:168984549]	11836247
602332	Inactive	Potency		qHTS for Inducers of the Endoplasmic Reticulum Stress Response (ERSR) in Human Glioma: qHTS	heat shock 70kDa protein 5 (glucose-regulated protein, 78kDa) [Homo sapiens][gi:168984549]	
602332	Inactive	Potency		qHTS for Inducers of the Endoplasmic Reticulum Stress Response (ERSR) in Human Glioma: qHTS	heat shock 70kDa protein 5 (glucose-regulated protein, 78kDa) [Homo sapiens][gi:168984549]	
2528	Inactive	Potency		qHTS Assay for Inhibitors of Bloom's syndrome helicase (BLM)	BLM gene product [Homo sapiens][gi:4557365]	
2528	Inactive	Potency		qHTS Assay for Inhibitors of Bloom's syndrome helicase (BLM)	BLM gene product [Homo sapiens][gi:4557365]	
624202	Inactive	Potency		qHTS Assay to Identify Small Molecule Activators of BRCA1 Expression	BRCA1 [Homo sapiens][gi:1698399]	
624202	Inactive	Potency		qHTS Assay to Identify Small Molecule Activators of BRCA1 Expression	BRCA1 [Homo sapiens][gi:1698399]	
1700	Inactive			Primary cell-based high throughput screening assay to identify inhibitors of kruppel-like factor 5 (KLF5)	Kruppel-like factor 5 [Homo sapiens][gi:124263658]	

AID	Outcome	Activity Concentration Name	Activity Concentration [uM]	BioAssay	Target	PMID
538	Inactive			Complement factor C1s	complement component 1, s subcomponent [Homo sapiens][gi:4502495]	
538	Inactive			Complement factor C1s	complement component 1, s subcomponent [Homo sapiens][gi:4502495]	
463141	Inactive			Absorbance-based primary biochemical high throughput screening assay to identify activators of procaspase-3	CASP3 gene product [Homo sapiens][gi:14790119]	
463141	Inactive			Absorbance-based primary biochemical high throughput screening assay to identify activators of procaspase-3	CASP3 gene product [Homo sapiens][gi:14790119]	
463141	Inactive			Absorbance-based primary biochemical high throughput screening assay to identify activators of procaspase-3	CASP3 gene product [Homo sapiens][gi:14790119]	
463141	Inactive			Absorbance-based primary biochemical high throughput screening assay to identify activators of procaspase-3	CASP3 gene product [Homo sapiens][gi:14790119]	
1434	Inactive	IC50		uHTS identification of compounds inhibiting the binding between the RUNX1 Runt domain and CBFb-SMMHC via a fluorescence resonance energy transfer (FRET) assay	core-binding factor subunit beta isoform 1 [Homo sapiens][gi:13124881]	
1434	Inactive	IC50		uHTS identification of compounds inhibiting the binding between the RUNX1 Runt domain and CBFb-SMMHC via a fluorescence resonance energy transfer (FRET) assay	core-binding factor subunit beta isoform 1 [Homo sapiens][gi:13124881]	
1496	Inactive			uHTS identification of compounds inhibiting the binding between the RUNX1 Runt domain and CBFb via a fluorescence resonance energy transfer (FRET) assay	core-binding factor subunit beta isoform 1 [Homo sapiens][gi:13124881]	
1496	Inactive			uHTS identification of compounds inhibiting the binding between the RUNX1 Runt domain and CBFb via a fluorescence resonance energy transfer (FRET) assay	core-binding factor subunit beta isoform 1 [Homo sapiens][gi:13124881]	

AID	Outcome	Activity Concentration Name	Activity Concentration [uM]	BioAssay	Target	PMID
368	Inactive			Cdc25B Catalytic Domain protein tyrosine phosphatase HTS	cell division cycle 25B isoform 2 [Homo sapiens][gi:4757950]	
368	Inactive			Cdc25B Catalytic Domain protein tyrosine phosphatase HTS	cell division cycle 25B isoform 2 [Homo sapiens][gi:4757950]	
588850	Inactive			uHTS identification of cystic fibrosis induced NFkb Inhibitors in a fluoresence assay	CFTR gene product [Homo sapiens][gi:90421313]	
588850	Inactive			uHTS identification of cystic fibrosis induced NFkb Inhibitors in a fluoresence assay	CFTR gene product [Homo sapiens][gi:90421313]	
588852	Inactive			Fluorescence-based cell-based primary high throughput screening assay to identify antagonists of the human M1 muscarinic receptor (CHRM1)	CHRM1 gene product [Homo sapiens][gi:37622910]	
588852	Inactive			Fluorescence-based cell-based primary high throughput screening assay to identify antagonists of the human M1 muscarinic receptor (CHRM1)	CHRM1 gene product [Homo sapiens][gi:37622910]	
588814	Inactive			Fluorescence-based cell-based primary high throughput screening assay to identify agonists of the human cholinergic receptor, muscarinic 1 (CHRM1)	CHRM1 gene product [Homo sapiens][gi:37622910]	
588814	Inactive			Fluorescence-based cell-based primary high throughput screening assay to identify agonists of the human cholinergic receptor, muscarinic 1 (CHRM1)	CHRM1 gene product [Homo sapiens][gi:37622910]	
588819	Inactive			Fluorescence-based cell-based primary high throughput screening assay to identify positive allosteric modulators (PAMs) of the human M1 muscarinic receptor (CHRM1)	CHRM1 gene product [Homo sapiens][gi:37622910]	
588819	Inactive			Fluorescence-based cell-based primary high throughput screening assay to identify positive allosteric modulators (PAMs) of the human M1 muscarinic receptor (CHRM1)	CHRM1 gene product [Homo sapiens][gi:37622910]	

AID	Outcome	Activity Concentration Name	Activity Concentration [uM]	BioAssay	Target	PMID
624125	Inactive			Fluorescence-based cell-based primary high throughput screening assay to identify antagonists of the human cholinergic receptor, muscarinic 4 (CHRM4)	CHRM4 gene product [Homo sapiens][gi:52426748]	
624125	Inactive			Fluorescence-based cell-based primary high throughput screening assay to identify antagonists of the human cholinergic receptor, muscarinic 4 (CHRM4)	CHRM4 gene product [Homo sapiens][gi:52426748]	
624125	Inactive			Fluorescence-based cell-based primary high throughput screening assay to identify antagonists of the human cholinergic receptor, muscarinic 4 (CHRM4)	CHRM4 gene product [Homo sapiens][gi:52426748]	
624126	Inactive			Fluorescence-based cell-based primary high throughput screening assay to identify positive allosteric modulators (PAMs) of the human cholinergic receptor, muscarinic 4 (CHRM4)	CHRM4 gene product [Homo sapiens][gi:52426748]	
624126	Inactive			Fluorescence-based cell-based primary high throughput screening assay to identify positive allosteric modulators (PAMs) of the human cholinergic receptor, muscarinic 4 (CHRM4)	CHRM4 gene product [Homo sapiens][gi:52426748]	
624126	Inactive			Fluorescence-based cell-based primary high throughput screening assay to identify positive allosteric modulators (PAMs) of the human cholinergic receptor, muscarinic 4 (CHRM4)	CHRM4 gene product [Homo sapiens][gi:52426748]	
624127	Inactive			Fluorescence-based cell-based primary high throughput screening assay to identify agonists of the human cholinergic receptor, muscarinic 4 (CHRM4)	CHRM4 gene product [Homo sapiens][gi:52426748]	
624127	Inactive			Fluorescence-based cell-based primary high throughput screening assay to identify agonists of the human cholinergic receptor, muscarinic 4 (CHRM4)	CHRM4 gene product [Homo sapiens][gi:52426748]	
624127	Inactive			Fluorescence-based cell-based primary high throughput screening assay to identify agonists of the human cholinergic receptor, muscarinic 4 (CHRM4)	CHRM4 gene product [Homo sapiens][gi:52426748]	
624037	Inactive			Fluorescence-based cell-based primary high throughput screening assay to identify agonists of the human cholinergic receptor, muscarinic 5 (CHRM5)	CHRM5 gene product [Homo sapiens][gi:7108336]	

AID	Outcome	Activity Concentration Name	Activity Concentration [uM]	BioAssay	Target	PMID
624037	Inactive			Fluorescence-based cell-based primary high throughput screening assay to identify agonists of the human cholinergic receptor, muscarinic 5 (CHRM5)	CHRM5 gene product [Homo sapiens][gi:7108336]	
624037	Inactive			Fluorescence-based cell-based primary high throughput screening assay to identify agonists of the human cholinergic receptor, muscarinic 5 (CHRM5)	CHRM5 gene product [Homo sapiens][gi:7108336]	
624037	Inactive			Fluorescence-based cell-based primary high throughput screening assay to identify agonists of the human cholinergic receptor, muscarinic 5 (CHRM5)	CHRM5 gene product [Homo sapiens][gi:7108336]	
624038	Inactive			Fluorescence-based cell-based primary high throughput screening assay to identify positive allosteric modulators (PAMs) of the human cholinergic receptor, muscarinic 5 (CHRM5)	CHRM5 gene product [Homo sapiens][gi:7108336]	
624038	Inactive			Fluorescence-based cell-based primary high throughput screening assay to identify positive allosteric modulators (PAMs) of the human cholinergic receptor, muscarinic 5 (CHRM5)	CHRM5 gene product [Homo sapiens][gi:7108336]	
624038	Inactive			Fluorescence-based cell-based primary high throughput screening assay to identify positive allosteric modulators (PAMs) of the human cholinergic receptor, muscarinic 5 (CHRM5)	CHRM5 gene product [Homo sapiens][gi:7108336]	
624038	Inactive			Fluorescence-based cell-based primary high throughput screening assay to identify positive allosteric modulators (PAMs) of the human cholinergic receptor, muscarinic 5 (CHRM5)	CHRM5 gene product [Homo sapiens][gi:7108336]	
624040	Inactive			Fluorescence-based cell-based primary high throughput screening assay to identify antagonists of the human cholinergic receptor, muscarinic 5 (CHRM5)	CHRM5 gene product [Homo sapiens][gi:7108336]	
624040	Inactive			Fluorescence-based cell-based primary high throughput screening assay to identify antagonists of the human cholinergic receptor, muscarinic 5 (CHRM5)	CHRM5 gene product [Homo sapiens][gi:7108336]	
624040	Inactive			Fluorescence-based cell-based primary high throughput screening assay to identify antagonists of the human cholinergic receptor, muscarinic 5 (CHRM5)	CHRM5 gene product [Homo sapiens][gi:7108336]	

AID	Outcome	Activity Concentration Name	Activity Concentration [uM]	BioAssay	Target	PMID
624040	Inactive			Fluorescence-based cell-based primary high throughput screening assay to identify antagonists of the human cholinergic receptor, muscarinic 5 (CHRM5)	CHRM5 gene product [Homo sapiens][gi:7108336]	
493098	Inactive			uHTS identification of small molecule antagonists of the CCR6 receptor via a luminescent beta-arrestin assay	CCR6 gene product [Homo sapiens][gi:37187860]	
493098	Inactive			uHTS identification of small molecule antagonists of the CCR6 receptor via a luminescent beta-arrestin assay	CCR6 gene product [Homo sapiens][gi:37187860]	
588473	Inactive			uHTS identification of agonists of the CRF-binding protein and CRF-R2 receptor complex	corticotropin releasing factor-binding protein [Homo sapiens][gi:30219]	
588473	Inactive			uHTS identification of agonists of the CRF-binding protein and CRF-R2 receptor complex	corticotropin releasing factor-binding protein [Homo sapiens][gi:30219]	
588475	Inactive			uHTS identification of antagonists of the CRF-binding protein and CRF-R2 receptor complex	corticotropin releasing factor-binding protein [Homo sapiens][gi:30219]	
588475	Inactive			uHTS identification of antagonists of the CRF-binding protein and CRF-R2 receptor complex	corticotropin releasing factor-binding protein [Homo sapiens][gi:30219]	
1665	Inactive	IC50		High Throughput Imaging Assay for Beta-Catenin	catenin beta-1 [Homo sapiens][gi:4503131]	
1665	Inactive	IC50		High Throughput Imaging Assay for Beta-Catenin	catenin beta-1 [Homo sapiens][gi:4503131]	
453	Inactive			Cathepsin B	Cathepsin B [Homo sapiens][gi:63102437]	
453	Inactive			Cathepsin B	Cathepsin B [Homo sapiens][gi:63102437]	

AID	Outcome	Activity Concentration Name	Activity Concentration [uM]	BioAssay	Target	PMID
488	Inactive			Cathepsin B compound mixture screening	Cathepsin B [Homo sapiens][gi:63102437]	
488	Inactive			Cathepsin B compound mixture screening	Cathepsin B [Homo sapiens][gi:63102437]	
581	Inactive			Cathepsin G	Cathepsin G [Homo sapiens][gi:15680217]	
581	Inactive			Cathepsin G	Cathepsin G [Homo sapiens][gi:15680217]	
460	Inactive			Cathepsin L	cathepsin L1 preproprotein [Homo sapiens][gi:4503155]	
460	Inactive			Cathepsin L	cathepsin L1 preproprotein [Homo sapiens][gi:4503155]	
501	Inactive			Cathepsin S	cathepsin S preproprotein [Homo sapiens][gi:23110962]	
501	Inactive			Cathepsin S	cathepsin S preproprotein [Homo sapiens][gi:23110962]	
1217	Inactive			uHTS Identification of Diaphorase Inhibitors and Chemcical Oxidizers: Counter Screen for Diaphorase-based Primary Assays	Dihydrolipoamide dehydrogenase [Homo sapiens][gi:17391426]	
1229	Inactive			uHTS Identification of Diaphorase Activators and Chemical Reducers: Counter Screen for Diaphorase-based Primary Assays	Dihydrolipoamide dehydrogenase [Homo sapiens][gi:17391426]	
588458	Inactive			uHTS identification of DNMT1 inhibitors in a Fluorescent Molecular Beacon assay	DNA (cytosine-5)-methyltransferase 1 isoform b [Homo sapiens][gi:4503351]	
588458	Inactive			uHTS identification of DNMT1 inhibitors in a Fluorescent Molecular Beacon assay	DNA (cytosine-5)-methyltransferase 1 isoform b [Homo sapiens][gi:4503351]	
504651	Inactive			Potentiators of Human D1 Dopamine Receptor: qHTS	D(1A) dopamine receptor [Homo sapiens][gi:4503383]	

AID	Outcome	Activity Concentration Name	Activity Concentration [uM]	BioAssay	Target	PMID
504651	Inactive			Potentiators of Human D1 Dopamine Receptor: qHTS	D(1A) dopamine receptor [Homo sapiens][gi:4503383]	
504651	Inactive			Potentiators of Human D1 Dopamine Receptor: qHTS	D(1A) dopamine receptor [Homo sapiens][gi:4503383]	
504651	Inactive			Potentiators of Human D1 Dopamine Receptor: qHTS	D(1A) dopamine receptor [Homo sapiens][gi:4503383]	
504652	Inactive			Antagonist of Human D 1 Dopamine Receptor: qHTS	D(1A) dopamine receptor [Homo sapiens][gi:4503383]	
504652	Inactive			Antagonist of Human D 1 Dopamine Receptor: qHTS	D(1A) dopamine receptor [Homo sapiens][gi:4503383]	
504652	Inactive			Antagonist of Human D 1 Dopamine Receptor: qHTS	D(1A) dopamine receptor [Homo sapiens][gi:4503383]	
504652	Inactive			Antagonist of Human D 1 Dopamine Receptor: qHTS	D(1A) dopamine receptor [Homo sapiens][gi:4503383]	
504660	Inactive			Allosteric Agonists of the Human D1 Dopamine Receptor: qHTS	D(1A) dopamine receptor [Homo sapiens][gi:4503383]	
504660	Inactive			Allosteric Agonists of the Human D1 Dopamine Receptor: qHTS	D(1A) dopamine receptor [Homo sapiens][gi:4503383]	
504660	Inactive			Allosteric Agonists of the Human D1 Dopamine Receptor: qHTS	D(1A) dopamine receptor [Homo sapiens][gi:4503383]	
504660	Inactive			Allosteric Agonists of the Human D1 Dopamine Receptor: qHTS	D(1A) dopamine receptor [Homo sapiens][gi:4503383]	
488981	Inactive	Potency		HTS Assay for Allosteric Agonists of the Human D1 Dopamine Receptor: Primary Screen for Agonists	D(1A) dopamine receptor [Homo sapiens][gi:4503383]	
488981	Inactive	Potency		HTS Assay for Allosteric Agonists of the Human D1 Dopamine Receptor: Primary Screen for Agonists	D(1A) dopamine receptor [Homo sapiens][gi:4503383]	

AID	Outcome	Activity Concentration Name	Activity Concentration [uM]	BioAssay	Target	PMID
488981	Inactive	Potency		HTS Assay for Allosteric Agonists of the Human D1 Dopamine Receptor: Primary Screen for Agonists	D(1A) dopamine receptor [Homo sapiens][gi:4503383]	
488981	Inactive	Potency		HTS Assay for Allosteric Agonists of the Human D1 Dopamine Receptor: Primary Screen for Agonists	D(1A) dopamine receptor [Homo sapiens][gi:4503383]	
624455	Inactive	Potency		HTS Assay for Allosteric Antagonists of the Human D2 Dopamine Receptor: Hit Validation in HTRF	dopamine D1 receptor [Homo sapiens][gi:299681]	
624455	Inactive	Potency		HTS Assay for Allosteric Antagonists of the Human D2 Dopamine Receptor: Hit Validation in HTRF	dopamine D1 receptor [Homo sapiens][gi:299681]	
624455	Inactive	Potency		HTS Assay for Allosteric Antagonists of the Human D2 Dopamine Receptor: Hit Validation in HTRF	dopamine D1 receptor [Homo sapiens][gi:299681]	
624455	Inactive	Potency		HTS Assay for Allosteric Antagonists of the Human D2 Dopamine Receptor: Hit Validation in HTRF	dopamine D1 receptor [Homo sapiens][gi:299681]	
624463	Inactive			Beta-Arrestin HTS for Positive Allosteric Modulators of the Human D2 Dopamine Receptor: Antagonists	DRD2 gene product [Homo sapiens][gi:4503385]	
624463	Inactive			Beta-Arrestin HTS for Positive Allosteric Modulators of the Human D2 Dopamine Receptor: Antagonists	DRD2 gene product [Homo sapiens][gi:4503385]	
624463	Inactive			Beta-Arrestin HTS for Positive Allosteric Modulators of the Human D2 Dopamine Receptor: Antagonists	DRD2 gene product [Homo sapiens][gi:4503385]	
624463	Inactive			Beta-Arrestin HTS for Positive Allosteric Modulators of the Human D2 Dopamine Receptor: Antagonists	DRD2 gene product [Homo sapiens][gi:4503385]	
624463	Inactive			Beta-Arrestin HTS for Positive Allosteric Modulators of the Human D2 Dopamine Receptor: Antagonists	DRD2 gene product [Homo sapiens][gi:4503385]	

AID	Outcome	Activity Concentration Name	Activity Concentration [uM]	BioAssay	Target	PMID
624464	Inactive			Beta-Arrestin HTS for Positive Allosteric Modulators of the Human D2 Dopamine Receptor: Potentiators	DRD2 gene product [Homo sapiens][gi:4503385]	
624464	Inactive			Beta-Arrestin HTS for Positive Allosteric Modulators of the Human D2 Dopamine Receptor: Potentiators	DRD2 gene product [Homo sapiens][gi:4503385]	
624464	Inactive			Beta-Arrestin HTS for Positive Allosteric Modulators of the Human D2 Dopamine Receptor: Potentiators	DRD2 gene product [Homo sapiens][gi:4503385]	
624464	Inactive			Beta-Arrestin HTS for Positive Allosteric Modulators of the Human D2 Dopamine Receptor: Potentiators	DRD2 gene product [Homo sapiens][gi:4503385]	
624464	Inactive			Beta-Arrestin HTS for Positive Allosteric Modulators of the Human D2 Dopamine Receptor: Potentiators	DRD2 gene product [Homo sapiens][gi:4503385]	
624465	Inactive			Beta-Arrestin HTS for Positive Allosteric Modulators of the Human D2 Dopamine Receptor: Agonists	DRD2 gene product [Homo sapiens][gi:4503385]	
624465	Inactive			Beta-Arrestin HTS for Positive Allosteric Modulators of the Human D2 Dopamine Receptor: Agonists	DRD2 gene product [Homo sapiens][gi:4503385]	
624465	Inactive			Beta-Arrestin HTS for Positive Allosteric Modulators of the Human D2 Dopamine Receptor: Agonists	DRD2 gene product [Homo sapiens][gi:4503385]	
624465	Inactive			Beta-Arrestin HTS for Positive Allosteric Modulators of the Human D2 Dopamine Receptor: Agonists	DRD2 gene product [Homo sapiens][gi:4503385]	
624465	Inactive			Beta-Arrestin HTS for Positive Allosteric Modulators of the Human D2 Dopamine Receptor: Agonists	DRD2 gene product [Homo sapiens][gi:4503385]	
485344	Inactive			HTS Assay for Allosteric Antagonists of the Human D2 Dopamine Receptor: Primary Screen for Antagonists	DRD2 gene product [Homo sapiens][gi:4503385]	

AID	Outcome	Activity Concentration Name	Activity Concentration [uM]	BioAssay	Target	PMID
485344	Inactive			HTS Assay for Allosteric Antagonists of the Human D2 Dopamine Receptor: Primary Screen for Antagonists	DRD2 gene product [Homo sapiens][gi:4503385]	
485344	Inactive			HTS Assay for Allosteric Antagonists of the Human D2 Dopamine Receptor: Primary Screen for Antagonists	DRD2 gene product [Homo sapiens][gi:4503385]	
485344	Inactive			HTS Assay for Allosteric Antagonists of the Human D2 Dopamine Receptor: Primary Screen for Antagonists	DRD2 gene product [Homo sapiens][gi:4503385]	
485344	Inactive			HTS Assay for Allosteric Antagonists of the Human D2 Dopamine Receptor: Primary Screen for Antagonists	DRD2 gene product [Homo sapiens][gi:4503385]	
485347	Inactive			HTS Assay for Positive Allosteric Modulators of the Human D2 Dopamine Receptor: Primary Screen for Potentiators	DRD2 gene product [Homo sapiens][gi:4503385]	
485347	Inactive			HTS Assay for Positive Allosteric Modulators of the Human D2 Dopamine Receptor: Primary Screen for Potentiators	DRD2 gene product [Homo sapiens][gi:4503385]	
485347	Inactive			HTS Assay for Positive Allosteric Modulators of the Human D2 Dopamine Receptor: Primary Screen for Potentiators	DRD2 gene product [Homo sapiens][gi:4503385]	
485347	Inactive			HTS Assay for Positive Allosteric Modulators of the Human D2 Dopamine Receptor: Primary Screen for Potentiators	DRD2 gene product [Homo sapiens][gi:4503385]	
485347	Inactive			HTS Assay for Positive Allosteric Modulators of the Human D2 Dopamine Receptor: Primary Screen for Potentiators	DRD2 gene product [Homo sapiens][gi:4503385]	
485358	Inactive			HTS Assay for Allosteric Agonists of the Human D2 Dopamine Receptor: Primary Screen for Agonists	DRD2 gene product [Homo sapiens][gi:4503385]	
485358	Inactive			HTS Assay for Allosteric Agonists of the Human D2 Dopamine Receptor: Primary Screen for Agonists	DRD2 gene product [Homo sapiens][gi:4503385]	

AID	Outcome	Activity Concentration Name	Activity Concentration [uM]	BioAssay	Target	PMID
485358	Inactive			HTS Assay for Allosteric Agonists of the Human D2 Dopamine Receptor: Primary Screen for Agonists	DRD2 gene product [Homo sapiens][gi:4503385]	
485358	Inactive			HTS Assay for Allosteric Agonists of the Human D2 Dopamine Receptor: Primary Screen for Agonists	DRD2 gene product [Homo sapiens][gi:4503385]	
485358	Inactive			HTS Assay for Allosteric Agonists of the Human D2 Dopamine Receptor: Primary Screen for Agonists	DRD2 gene product [Homo sapiens][gi:4503385]	
652048	Inactive			qHTS of D3 Dopamine Receptor Agonist: qHTS	DRD3 gene product [Homo sapiens][gi:89191863]	
652048	Inactive			qHTS of D3 Dopamine Receptor Agonist: qHTS	DRD3 gene product [Homo sapiens][gi:89191863]	
652048	Inactive			qHTS of D3 Dopamine Receptor Agonist: qHTS	DRD3 gene product [Homo sapiens][gi:89191863]	
652048	Inactive			qHTS of D3 Dopamine Receptor Agonist: qHTS	DRD3 gene product [Homo sapiens][gi:89191863]	
652051	Inactive			qHTS of D3 Dopamine Receptor Potentiators: qHTS	DRD3 gene product [Homo sapiens][gi:89191863]	
652051	Inactive			qHTS of D3 Dopamine Receptor Potentiators: qHTS	DRD3 gene product [Homo sapiens][gi:89191863]	
652051	Inactive			qHTS of D3 Dopamine Receptor Potentiators: qHTS	DRD3 gene product [Homo sapiens][gi:89191863]	
652051	Inactive			qHTS of D3 Dopamine Receptor Potentiators: qHTS	DRD3 gene product [Homo sapiens][gi:89191863]	

AID	Outcome	Activity Concentration Name	Activity Concentration [uM]	BioAssay	Target	PMID
652054	Inactive			qHTS of D3 Dopamine Receptor Antagonist: qHTS	DRD3 gene product [Homo sapiens][gi:89191863]	
652054	Inactive			qHTS of D3 Dopamine Receptor Antagonist: qHTS	DRD3 gene product [Homo sapiens][gi:89191863]	
652054	Inactive			qHTS of D3 Dopamine Receptor Antagonist: qHTS	DRD3 gene product [Homo sapiens][gi:89191863]	
652054	Inactive			qHTS of D3 Dopamine Receptor Antagonist: qHTS	DRD3 gene product [Homo sapiens][gi:89191863]	
652048	Inactive			qHTS of D3 Dopamine Receptor Agonist: qHTS	DRD3 gene product [Homo sapiens][gi:89191863]	
652048	Inactive			qHTS of D3 Dopamine Receptor Agonist: qHTS	DRD3 gene product [Homo sapiens][gi:89191863]	
652048	Inactive			qHTS of D3 Dopamine Receptor Agonist: qHTS	DRD3 gene product [Homo sapiens][gi:89191863]	
652048	Inactive			qHTS of D3 Dopamine Receptor Agonist: qHTS	DRD3 gene product [Homo sapiens][gi:89191863]	
652051	Inactive			qHTS of D3 Dopamine Receptor Potentiators: qHTS	DRD3 gene product [Homo sapiens][gi:89191863]	
652051	Inactive			qHTS of D3 Dopamine Receptor Potentiators: qHTS	DRD3 gene product [Homo sapiens][gi:89191863]	
652051	Inactive			qHTS of D3 Dopamine Receptor Potentiators: qHTS	DRD3 gene product [Homo sapiens][gi:89191863]	
652051	Inactive			qHTS of D3 Dopamine Receptor Potentiators: qHTS	DRD3 gene product [Homo sapiens][gi:89191863]	
652048	Inactive			qHTS of D3 Dopamine Receptor Agonist: qHTS	DRD3 gene product [Homo sapiens][gi:89191863]	
652048	Inactive			qHTS of D3 Dopamine Receptor Agonist: qHTS	DRD3 gene product [Homo sapiens][gi:89191863]	
652048	Inactive			qHTS of D3 Dopamine Receptor Agonist: qHTS	DRD3 gene product [Homo sapiens][gi:89191863]	

AID	Outcome	Activity Concentration Name	Activity Concentration [uM]	BioAssay	Target	PMID
652048	Inactive			qHTS of D3 Dopamine Receptor Agonist: qHTS	DRD3 gene product [Homo sapiens][gi:89191863]	
652051	Inactive			qHTS of D3 Dopamine Receptor Potentiators: qHTS	DRD3 gene product [Homo sapiens][gi:89191863]	
652051	Inactive			qHTS of D3 Dopamine Receptor Potentiators: qHTS	DRD3 gene product [Homo sapiens][gi:89191863]	
652051	Inactive			qHTS of D3 Dopamine Receptor Potentiators: qHTS	DRD3 gene product [Homo sapiens][gi:89191863]	
652051	Inactive			qHTS of D3 Dopamine Receptor Potentiators: qHTS	DRD3 gene product [Homo sapiens][gi:89191863]	
374	Inactive			In vitro Primary HTS Assay for MKP-1	dual specificity phosphatase 1 [Homo sapiens][gi:4758204]	
374	Inactive			In vitro Primary HTS Assay for MKP-1	dual specificity phosphatase 1 [Homo sapiens][gi:4758204]	
1654	Inactive	IC50		uHTS absorbance assay for the identification of compounds that inhibit VHR1.	dual specificity protein phosphatase 3 [Homo sapiens][gi:4758208]	
1654	Inactive	IC50		uHTS absorbance assay for the identification of compounds that inhibit VHR1.	dual specificity protein phosphatase 3 [Homo sapiens][gi:4758208]	
651636	Inactive			uHTS identification of small molecule antagonists of the EBI2 receptor via a luminescent beta-arrestin assay	GPR183 gene product [Homo sapiens][gi:4826706]	
449	Inactive			Primary HTS and Confirmation Assays for S1P1 Agonists and Agonism Potentiators	S1PR1 gene product [Homo sapiens][gi:13027636]	
449	Inactive			Primary HTS and Confirmation Assays for S1P1 Agonists and Agonism Potentiators	S1PR1 gene product [Homo sapiens][gi:13027636]	
485	Inactive			Primary HTS Assay for S1P3 Antagonists	sphingosine 1-phosphate receptor 3 [Homo sapiens][gi:38788193]	
485	Inactive			Primary HTS Assay for S1P3 Antagonists	sphingosine 1-phosphate receptor 3 [Homo sapiens][gi:38788193]	

AID	Outcome	Activity Concentration Name	Activity Concentration [uM]	BioAssay	Target	PMID
485	Inactive			Primary HTS Assay for S1P3 Antagonists	sphingosine 1-phosphate receptor 3 [Homo sapiens][gi:38788193]	
373	Inactive			S1P3 Agonist Primary HTS and Confirmation Assays	sphingosine 1-phosphate receptor 3 [Homo sapiens][gi:38788193]	
373	Inactive			S1P3 Agonist Primary HTS and Confirmation Assays	sphingosine 1-phosphate receptor 3 [Homo sapiens][gi:38788193]	
373	Inactive			S1P3 Agonist Primary HTS and Confirmation Assays	sphingosine 1-phosphate receptor 3 [Homo sapiens][gi:38788193]	
624352	Inactive			uHTS identification of HIF-2a Inhibitors in a luminesence assay	EPAS1 gene product [Homo sapiens][gi:40254439]	
624352	Inactive			uHTS identification of HIF-2a Inhibitors in a luminesence assay	EPAS1 gene product [Homo sapiens][gi:40254439]	
624246	Inactive	Potency		qHTS for Small Molecule Inhibitors of the ERG Ets/DNA interaction	ERG gene product [Homo sapiens][gi:343478176]	
624246	Inactive	Potency		qHTS for Small Molecule Inhibitors of the ERG Ets/DNA interaction	ERG gene product [Homo sapiens][gi:343478176]	
694	Inactive			HTS of LOPAC library for Estrogen Receptor-alpha Coactivator Binding inhibitors	Estrogen receptor 1 [Homo sapiens][gi:118764400]	
694	Inactive			HTS of LOPAC library for Estrogen Receptor-alpha Coactivator Binding inhibitors	Estrogen receptor 1 [Homo sapiens][gi:118764400]	
694	Inactive			HTS of LOPAC library for Estrogen Receptor-alpha Coactivator Binding inhibitors	Estrogen receptor 1 [Homo sapiens][gi:118764400]	
694	Inactive			HTS of LOPAC library for Estrogen Receptor-alpha Coactivator Binding inhibitors	Estrogen receptor 1 [Homo sapiens][gi:118764400]	
629	Inactive			HTS of Estrogen Receptor- alpha Coactivator Binding inhibitors	Estrogen receptor 1 [Homo sapiens][gi:118764400]	
629	Inactive			HTS of Estrogen Receptor- alpha Coactivator Binding inhibitors	Estrogen receptor 1 [Homo sapiens][gi:118764400]	

AID	Outcome	Activity Concentration Name	Activity Concentration [uM]	BioAssay	Target	PMID
629	Inactive			HTS of Estrogen Receptor- alpha Coactivator Binding inhibitors	Estrogen receptor 1 [Homo sapiens][gi:118764400]	
629	Inactive			HTS of Estrogen Receptor- alpha Coactivator Binding inhibitors	Estrogen receptor 1 [Homo sapiens][gi:118764400]	
639	Inactive			HTS of Estrogen Receptor- alpha Coactivator Binding Potentiators	Estrogen receptor 1 [Homo sapiens][gi:118764400]	
639	Inactive			HTS of Estrogen Receptor- alpha Coactivator Binding Potentiators	Estrogen receptor 1 [Homo sapiens][gi:118764400]	
639	Inactive			HTS of Estrogen Receptor- alpha Coactivator Binding Potentiators	Estrogen receptor 1 [Homo sapiens][gi:118764400]	
639	Inactive			HTS of Estrogen Receptor- alpha Coactivator Binding Potentiators	Estrogen receptor 1 [Homo sapiens][gi:118764400]	
633	Inactive			HTS for Estrogen Receptor-beta Coactivator Binding inhibitors	estrogen receptor beta isoform 1 [Homo sapiens][gi:10835013]	
633	Inactive			HTS for Estrogen Receptor-beta Coactivator Binding inhibitors	estrogen receptor beta isoform 1 [Homo sapiens][gi:10835013]	
633	Inactive			HTS for Estrogen Receptor-beta Coactivator Binding inhibitors	estrogen receptor beta isoform 1 [Homo sapiens][gi:10835013]	
488837	Inactive	Potency		qHTS Assay for Inhibitors of the Phosphatase Activity of Eya2	EYA2 gene product [Homo sapiens][gi:26667227]	
488837	Inactive	Potency		qHTS Assay for Inhibitors of the Phosphatase Activity of Eya2	EYA2 gene product [Homo sapiens][gi:26667227]	
1046	Inactive			Thrombin 1536 HTS	prothrombin [Homo sapiens][gi:339641]	
1046	Inactive			Thrombin 1536 HTS	prothrombin [Homo sapiens][gi:339641]	
687	Inactive			Factor XIa Single Well HTS	coagulation factor XI[gi:180352]	
687	Inactive			Factor XIa Single Well HTS	coagulation factor XI[gi:180352]	
680	Inactive			Factor XIa Mixture HTS	coagulation factor XI[gi:180352]	

AID	Outcome	Activity Concentration Name	Activity Concentration [uM]	BioAssay	Target	PMID
680	Inactive			Factor XIa Mixture HTS	coagulation factor XI[gi:180352]	
798	Inactive			Factor XIa 1536 HTS	coagulation factor XI[gi:180352]	
798	Inactive			Factor XIa 1536 HTS	coagulation factor XI[gi:180352]	
800	Inactive			Factor XIIa 1536 HTS	Coagulation factor XII[gi:317373446]	
701	Inactive			Factor XIIa Single Well HTS	Coagulation factor XII[gi:317373446]	
684	Inactive			Factor XIIa Mixture HTS	Coagulation factor XII[gi:317373446]	
602261	Inactive			uHTS identification of small molecule inhibitors of the thioesterase domain of fatty acid synthase via a fluorescence intensity assay	FASN gene product [Homo sapiens][gi:41872631]	
602261	Inactive			uHTS identification of small molecule inhibitors of the thioesterase domain of fatty acid synthase via a fluorescence intensity assay	FASN gene product [Homo sapiens][gi:41872631]	
602261	Inactive			uHTS identification of small molecule inhibitors of the thioesterase domain of fatty acid synthase via a fluorescence intensity assay	FASN gene product [Homo sapiens][gi:41872631]	
488816	Inactive	Potency		qHTS Validation Assay for the Inhibitors of Human Flap endonuclease 1 (FEN1)	FEN1 gene product [Homo sapiens][gi:4758356]	
588795	Inactive	Potency		qHTS Assay for the Inhibitors of Human Flap endonuclease 1 (FEN1)	FEN1 gene product [Homo sapiens][gi:4758356]	
588795	Inactive	Potency		qHTS Assay for the Inhibitors of Human Flap endonuclease 1 (FEN1)	FEN1 gene product [Homo sapiens][gi:4758356]	
440	Inactive			Primary HTS Assay for Formylpeptide Receptor (FPR) Ligands and Primary HTS Counter-Screen Assay for Formylpeptide-Like-1 (FPRL1) Ligands	formyl peptide receptor 1 [Homo sapiens][gi:4503779]	

AID	Outcome	Activity Concentration Name	Activity Concentration [uM]	BioAssay	Target	PMID
440	Inactive			Primary HTS Assay for Formylpeptide Receptor (FPR) Ligands and Primary HTS Counter-Screen Assay for Formylpeptide-Like-1 (FPRL1) Ligands	formyl peptide receptor 1 [Homo sapiens][gi:4503779]	
441	Inactive			Primary HTS Assay for Formylpeptide Receptor-Like-1 (FPRL1) Ligands and Primary HTS Counter-Screen Assay for Formylpeptide Receptor (FPR) Ligands	FPR2 gene product [Homo sapiens][gi:54112388]	
441	Inactive			Primary HTS Assay for Formylpeptide Receptor-Like-1 (FPRL1) Ligands and Primary HTS Counter-Screen Assay for Formylpeptide Receptor (FPR) Ligands	FPR2 gene product [Homo sapiens][gi:54112388]	
2660	Inactive	Potency		Cytometric Cell-Based qHTS for Inhibitors of the mTORC1 Signaling Pathway in MEF (Tsc2-/-, p53-/-) Cells	MTOR gene product [Homo sapiens][gi:4826730]	
2660	Inactive	Potency		Cytometric Cell-Based qHTS for Inhibitors of the mTORC1 Signaling Pathway in MEF (Tsc2-/-, p53-/-) Cells	MTOR gene product [Homo sapiens][gi:4826730]	
2666	Inactive	Potency		High Content Imaging Cell-Based qHTS for Inhibitors of the mTORC1 Signaling Pathway in MEF (Tsc2-/-, p53-/-) Cells	MTOR gene product [Homo sapiens][gi:4826730]	
2666	Inactive	Potency		High Content Imaging Cell-Based qHTS for Inhibitors of the mTORC1 Signaling Pathway in MEF (Tsc2-/-, p53-/-) Cells	MTOR gene product [Homo sapiens][gi:4826730]	
2667	Inactive	Potency		High Content Imaging Cell-Based qHTS for Inhibitors of the mTORC1 Signaling Pathway in MEF Cells	MTOR gene product [Homo sapiens][gi:4826730]	
2667	Inactive	Potency		High Content Imaging Cell-Based qHTS for Inhibitors of the mTORC1 Signaling Pathway in MEF Cells	MTOR gene product [Homo sapiens][gi:4826730]	
2668	Inactive	Potency		Cytometry Cell-Based qHTS for Inhibitors of the mTORC1 Signaling Pathway in MEF cells	MTOR gene product [Homo sapiens][gi:4826730]	
2668	Inactive	Potency		Cytometry Cell-Based qHTS for Inhibitors of the mTORC1 Signaling Pathway in MEF cells	MTOR gene product [Homo sapiens][gi:4826730]	

AID	Outcome	Activity Concentration Name	Activity Concentration [uM]	BioAssay	Target	PMID
602396	Inactive			Luminescence-based cell-based primary high throughput screening assay to identify inverse agonists of the liver receptor homolog-1 (LRH-1; NR5A2)	NR5A2 gene product [Homo sapiens][gi:4504343]	
602396	Inactive			Luminescence-based cell-based primary high throughput screening assay to identify inverse agonists of the liver receptor homolog-1 (LRH-1; NR5A2)	NR5A2 gene product [Homo sapiens][gi:4504343]	
525	Inactive			Primary Cell-based High Throughput Screening assay for inhibitors of the nuclear receptor Steroidogenic Factor 1 (SF-1)	NR5A1 gene product [Homo sapiens][gi:20070193]	
525	Inactive			Primary Cell-based High Throughput Screening assay for inhibitors of the nuclear receptor Steroidogenic Factor 1 (SF-1)	NR5A1 gene product [Homo sapiens][gi:20070193]	
525	Inactive			Primary Cell-based High Throughput Screening assay for inhibitors of the nuclear receptor Steroidogenic Factor 1 (SF-1)	NR5A1 gene product [Homo sapiens][gi:20070193]	
522	Inactive			Primary Cell-based High Throughput Screening assay for activators of the nuclear receptor Steroidogenic Factor 1 (SF-1)	NR5A1 gene product [Homo sapiens][gi:20070193]	
522	Inactive			Primary Cell-based High Throughput Screening assay for activators of the nuclear receptor Steroidogenic Factor 1 (SF-1)	NR5A1 gene product [Homo sapiens][gi:20070193]	
522	Inactive			Primary Cell-based High Throughput Screening assay for activators of the nuclear receptor Steroidogenic Factor 1 (SF-1)	NR5A1 gene product [Homo sapiens][gi:20070193]	
2112	Inactive	Potency		qHTS Assay for Inhibitors and Activators of Human alpha-Glucosidase From Spleen Homogenate	lysosomal alpha-glucosidase preproprotein [Homo sapiens][gi:119393891]	
2112	Inactive	Potency		qHTS Assay for Inhibitors and Activators of Human alpha-Glucosidase From Spleen Homogenate	lysosomal alpha-glucosidase preproprotein [Homo sapiens][gi:119393891]	
2112	Inactive	Potency		qHTS Assay for Inhibitors and Activators of Human alpha-Glucosidase From Spleen Homogenate	lysosomal alpha-glucosidase preproprotein [Homo sapiens][gi:119393891]	

AID	Outcome	Activity Concentration Name	Activity Concentration [uM]	BioAssay	Target	PMID
2242	Inactive	Potency		qHTS Assay for Activators of Human alpha-Glucosidase as a Potential Chaperone Treatment of Pompe Disease	lysosomal alpha-glucosidase preproprotein [Homo sapiens][gi:119393891]	
2242	Inactive	Potency		qHTS Assay for Activators of Human alpha-Glucosidase as a Potential Chaperone Treatment of Pompe Disease	lysosomal alpha-glucosidase preproprotein [Homo sapiens][gi:119393891]	
2242	Inactive	Potency		qHTS Assay for Activators of Human alpha-Glucosidase as a Potential Chaperone Treatment of Pompe Disease	lysosomal alpha-glucosidase preproprotein [Homo sapiens][gi:119393891]	
2112	Inactive	Potency		qHTS Assay for Inhibitors and Activators of Human alpha-Glucosidase From Spleen Homogenate	lysosomal alpha-glucosidase preproprotein [Homo sapiens][gi:119393891]	
2112	Inactive	Potency		qHTS Assay for Inhibitors and Activators of Human alpha-Glucosidase From Spleen Homogenate	lysosomal alpha-glucosidase preproprotein [Homo sapiens][gi:119393891]	
2112	Inactive	Potency		qHTS Assay for Inhibitors and Activators of Human alpha-Glucosidase From Spleen Homogenate	lysosomal alpha-glucosidase preproprotein [Homo sapiens][gi:119393891]	
2100	Inactive	Potency		qHTS Assay for Inhibitors and Activators of Human alpha-Glucosidase Cleavage of Glycogen	lysosomal alpha-glucosidase preproprotein [Homo sapiens][gi:119393891]	
2100	Inactive	Potency		qHTS Assay for Inhibitors and Activators of Human alpha-Glucosidase Cleavage of Glycogen	lysosomal alpha-glucosidase preproprotein [Homo sapiens][gi:119393891]	
2100	Inactive	Potency		qHTS Assay for Inhibitors and Activators of Human alpha-Glucosidase Cleavage of Glycogen	lysosomal alpha-glucosidase preproprotein [Homo sapiens][gi:119393891]	
1466	Inactive	Potency		qHTS Assay for Inhibitors of Human alpha-Glucosidase as a Potential Chaperone Treatment of Pompe Disease	lysosomal alpha-glucosidase preproprotein [Homo sapiens][gi:119393891]	
1466	Inactive	Potency		qHTS Assay for Inhibitors of Human alpha-Glucosidase as a Potential Chaperone Treatment of Pompe Disease	lysosomal alpha-glucosidase preproprotein [Homo sapiens][gi:119393891]	

AID	Outcome	Activity Concentration Name	Activity Concentration [uM]	BioAssay	Target	PMID
1466	Inactive	Potency		qHTS Assay for Inhibitors of Human alpha-Glucosidase as a Potential Chaperone Treatment of Pompe Disease	lysosomal alpha-glucosidase preproprotein [Homo sapiens][gi:119393891]	
1868	Inactive	Potency		qHTS Assay for Inhibitors of Human Galactokinase (GALK)	galactokinase [Homo sapiens][gi:4503895]	
1868	Inactive	Potency		qHTS Assay for Inhibitors of Human Galactokinase (GALK)	galactokinase [Homo sapiens][gi:4503895]	
493189	Inactive	Potency		qHTS Validation Assay for Inhibitors of Human Galactokinase (GALK)	galactokinase [Homo sapiens][gi:4503895]	
493189	Inactive	Potency		qHTS Validation Assay for Inhibitors of Human Galactokinase (GALK)	galactokinase [Homo sapiens][gi:4503895]	
2472	Inactive			qHTS Assay for Inhibitors of Fructose-1,6-bisphosphate Aldolase from Giardia Lamblia: Coupling assay counterscreen	glyceraldehyde-3-phosphate dehydrogenase [Homo sapiens][gi:7669492]	
2472	Inactive			qHTS Assay for Inhibitors of Fructose-1,6-bisphosphate Aldolase from Giardia Lamblia: Coupling assay counterscreen	glyceraldehyde-3-phosphate dehydrogenase [Homo sapiens][gi:7669492]	
2101	Inactive	Potency		qHTS Assay for Inhibitors and Activators of N370S glucocerebrosidase as a Potential Chaperone Treatment of Gaucher Disease	glucocerebrosidase [Homo sapiens][gi:496369]	
2101	Inactive	Potency		qHTS Assay for Inhibitors and Activators of N370S glucocerebrosidase as a Potential Chaperone Treatment of Gaucher Disease	glucocerebrosidase [Homo sapiens][gi:496369]	
2101	Inactive	Potency		qHTS Assay for Inhibitors and Activators of N370S glucocerebrosidase as a Potential Chaperone Treatment of Gaucher Disease	glucocerebrosidase [Homo sapiens][gi:496369]	
2101	Inactive	Potency		qHTS Assay for Inhibitors and Activators of N370S glucocerebrosidase as a Potential Chaperone Treatment of Gaucher Disease	glucocerebrosidase [Homo sapiens][gi:496369]	
784	Inactive			Primary Cell Based High Throughput Screening Assay for Enhancers of Beta-Glucosidase Activity	Glucosylceramidase[gi:55584151]	

AID	Outcome	Activity Concentration Name	Activity Concentration [uM]	BioAssay	Target	PMID
784	Inactive			Primary Cell Based High Throughput Screening Assay for Enhancers of Beta-Glucosidase Activity	Glucosylceramidase[gi:55584151]	
504327	Inactive	Potency		qHTS Assay for Inhibitors of GCN5L2	histone acetyltransferase KAT2A [Homo sapiens][gi:153791535]	
504327	Inactive	Potency		qHTS Assay for Inhibitors of GCN5L2	histone acetyltransferase KAT2A [Homo sapiens][gi:153791535]	
504327	Inactive	Potency		qHTS Assay for Inhibitors of GCN5L2	histone acetyltransferase KAT2A [Homo sapiens][gi:153791535]	
504327	Inactive	Potency		qHTS Assay for Inhibitors of GCN5L2	histone acetyltransferase KAT2A [Homo sapiens][gi:153791535]	
2107	Inactive	Potency		qHTS Assay for Inhibitors and Activators of Human alpha-Galactosidase From Spleen Homogenate	alpha-galactosidase [Homo sapiens][gi:757912]	
2107	Inactive	Potency		qHTS Assay for Inhibitors and Activators of Human alpha-Galactosidase From Spleen Homogenate	alpha-galactosidase [Homo sapiens][gi:757912]	
2107	Inactive	Potency		qHTS Assay for Inhibitors and Activators of Human alpha-Galactosidase From Spleen Homogenate	alpha-galactosidase [Homo sapiens][gi:757912]	
2107	Inactive	Potency		qHTS Assay for Inhibitors and Activators of Human alpha-Galactosidase From Spleen Homogenate	alpha-galactosidase [Homo sapiens][gi:757912]	
1467	Inactive	Potency		qHTS Assay for Inhibitors of Human alpha-Galactosidase at pH 4.5	alpha-galactosidase [Homo sapiens][gi:757912]	
1467	Inactive	Potency		qHTS Assay for Inhibitors of Human alpha-Galactosidase at pH 4.5	alpha-galactosidase [Homo sapiens][gi:757912]	
624172	Inactive	Potency		qHTS of GLP-1 Receptor Agonists	glp-1 receptor [Homo sapiens][gi:1724069]	
624172	Inactive	Potency		qHTS of GLP-1 Receptor Agonists	glp-1 receptor [Homo sapiens][gi:1724069]	

AID	Outcome	Activity Concentration Name	Activity Concentration [uM]	BioAssay	Target	PMID
624148	Inactive	Potency		qHTS of GLP-1 Receptor Agonists: LOPAC Validation	glp-1 receptor [Homo sapiens][gi:1724069]	
624148	Inactive	Potency		qHTS of GLP-1 Receptor Agonists: LOPAC Validation	glp-1 receptor [Homo sapiens][gi:1724069]	
624172	Inactive	Potency		qHTS of GLP-1 Receptor Agonists	glp-1 receptor [Homo sapiens][gi:1724069]	
624172	Inactive	Potency		qHTS of GLP-1 Receptor Agonists	glp-1 receptor [Homo sapiens][gi:1724069]	
624417	Inactive	Potency		qHTS of GLP-1 Receptor Inverse Agonists (Inhibition Mode)	glp-1 receptor [Homo sapiens][gi:1724069]	
624417	Inactive	Potency		qHTS of GLP-1 Receptor Inverse Agonists (Inhibition Mode)	glp-1 receptor [Homo sapiens][gi:1724069]	
624170	Inactive	Potency		qHTS for Inhibitors of Glutaminase (GLS)	GLS protein [Homo sapiens][gi:71051501]	
624146	Inactive	Potency		qHTS for Inhibitors of Glutaminase (GLS): LOPAC Validation	GLS protein [Homo sapiens][gi:71051501]	
624170	Inactive	Potency		qHTS for Inhibitors of Glutaminase (GLS)	GLS protein [Homo sapiens][gi:71051501]	
493083	Inactive	AC50		HSF-1 induced GFP reporter and Doxycycline induced RFP reporter Measured in Cell-Based System Using Plate Reader - 2038-03_Inhibitor_DoseNoFile_CherryPick_Activity_Set3	Hsf1 protein [Mus musculus][gi:62740231]	
493083	Inactive	AC50		HSF-1 induced GFP reporter and Doxycycline induced RFP reporter Measured in Cell-Based System Using Plate Reader - 2038-03_Inhibitor_DoseNoFile_CherryPick_Activity_Set3	Hsf1 protein [Mus musculus][gi:62740231]	

AID	Outcome	Activity Concentration Name	Activity Concentration [uM]	BioAssay	Target	PMID
493085	Inactive	AC50		HSF-1 induced GFP reporter and Doxycycline induced RFP reporter Measured in Cell-Based System Using Plate Reader - 2038-03_Inhibitor_DoseNoFile_CherryPick_Internal-Standard_Set3	Hsf1 protein [Mus musculus][gi:62740231]	
493085	Inactive	AC50		HSF-1 induced GFP reporter and Doxycycline induced RFP reporter Measured in Cell-Based System Using Plate Reader - 2038-03_Inhibitor_DoseNoFile_CherryPick_Internal-Standard_Set3	Hsf1 protein [Mus musculus][gi:62740231]	
588827	Inactive	AC50		HSF-1 induced GFP reporter and Doxycycline induced RFP reporter Measured in Cell-Based System Using Plate Reader - 2038-03_Inhibitor_Dose_CherryPick_Activity_Set4	Hsf1 protein [Mus musculus][gi:62740231]	
588827	Inactive	AC50		HSF-1 induced GFP reporter and Doxycycline induced RFP reporter Measured in Cell-Based System Using Plate Reader - 2038-03_Inhibitor_Dose_CherryPick_Activity_Set4	Hsf1 protein [Mus musculus][gi:62740231]	
624169	Inactive			Luminescence-based cell-based primary high throughput screening assay to identify agonists of the mouse 5-hydroxytryptamine (serotonin) receptor 2A (HTR2A)	Htr2a gene product [Mus musculus][gi:27753985]	
624169	Inactive			Luminescence-based cell-based primary high throughput screening assay to identify agonists of the mouse 5-hydroxytryptamine (serotonin) receptor 2A (HTR2A)	Htr2a gene product [Mus musculus][gi:27753985]	
652025	Inactive	Potency		qHTS of IL-2 Activators	Il2 gene product [Mus musculus][gi:7110653]	
2523	Inactive			HTS of MLPCN Validation Compound Set for developing T Cell Immune Modulators	integrin alpha-L [Mus musculus][gi:124486680]	
2523	Inactive			HTS of MLPCN Validation Compound Set for developing T Cell Immune Modulators	integrin alpha-L [Mus musculus][gi:124486680]	
2523	Inactive			HTS of MLPCN Validation Compound Set for developing T Cell Immune Modulators	integrin alpha-L [Mus musculus][gi:124486680]	
2052	Inactive			HTS for developing T Cell Immune Modulators	integrin alpha-L [Mus musculus][gi:124486680]	

AID	Outcome	Activity Concentration Name	Activity Concentration [uM]	BioAssay	Target	PMID
2052	Inactive			HTS for developing T Cell Immune Modulators	integrin alpha-L [Mus musculus][gi:124486680]	
2052	Inactive			HTS for developing T Cell Immune Modulators	integrin alpha-L [Mus musculus][gi:124486680]	
2345	Inactive			Specificity screen against Kir2.1 for compounds that potentiate KCNQ2	inward rectifier potassium channel 2 [Mus musculus][gi:6680530]	
1672	Inactive			Primary cell-based high-throughput screening assay for identification of compounds that inhibit/block inward-rectifying potassium ion channel Kir2.1	inward rectifier potassium channel 2 [Mus musculus][gi:6680530]	
1984	Inactive	IC50		Fluorescence for the identification of compounds that decrease p/CIP protein stability	nuclear receptor coactivator 3 [Mus musculus][gi:118026946]	
504707	Inactive			Fluorescence polarization-based biochemical primary high throughput screening assay to identify activators of the Protein Kinase A-R1A (PKA-R1A) complex	cAMP-dependent protein kinase catalytic subunit beta isoform 1 [Mus musculus][gi:6755076]	
540303	Inactive	Potency		qHTS for Inhibitors of Cell Surface uPA Generation	urokinase-type plasminogen activator [Mus musculus][gi:6679377]	
540303	Inactive	Potency		qHTS for Inhibitors of Cell Surface uPA Generation	urokinase-type plasminogen activator [Mus musculus][gi:6679377]	
493164	Inactive	Potency		qHTS for Inhibitors of Cell Surface uPA Generation: Validation Assay	urokinase-type plasminogen activator [Mus musculus][gi:6679377]	
493164	Inactive	Potency		qHTS for Inhibitors of Cell Surface uPA Generation: Validation Assay	urokinase-type plasminogen activator [Mus musculus][gi:6679377]	
2546	Inactive	Potency		VP16 counterscreen qHTS for inhibitors of ROR gamma transcriptional activity	nuclear receptor ROR-gamma [Mus musculus][gi:188536040]	
2551	Inactive	Potency		qHTS for inhibitors of ROR gamma transcriptional activity	nuclear receptor ROR-gamma [Mus musculus][gi:188536040]	

AID	Outcome	Activity Concentration Name	Activity Concentration [uM]	BioAssay	Target	PMID
2732	Inactive			HTS for small molecule inhibitors of CHOP to regulate the unfolded protein response to ER stress	Ddit3 gene product [Mus musculus][gi:160707929]	
2732	Inactive			HTS for small molecule inhibitors of CHOP to regulate the unfolded protein response to ER stress	Ddit3 gene product [Mus musculus][gi:160707929]	
782	Inactive			uHTS for Small Molecule Inhibitors of Eukaryotic Translation Initiation	eukaryotic translation initiation factor 4E [Mus musculus][gi:83627717]	
782	Inactive			uHTS for Small Molecule Inhibitors of Eukaryotic Translation Initiation	eukaryotic translation initiation factor 4E [Mus musculus][gi:83627717]	
493131	Inactive			Activator for delta FosB/delta FosB homodimer Measured in Biochemical System Using Plate Reader - 2072-01_Activator_SinglePoint_HTS_Activity	protein fosB [Mus musculus][gi:6679827]	
588413	Inactive			uHTS identification of Gli-Sufu Antagonists in a luminescence reporter assay	Gli1 [Mus musculus][gi:6009644]	
588413	Inactive			uHTS identification of Gli-Sufu Antagonists in a luminescence reporter assay	Gli1 [Mus musculus][gi:6009644]	
2098	Inactive			Luminescence Cell-Based Primary HTS to Identify Inhibitors of Heat Shock Factor 1 (HSF1)	Hsf1 protein [Mus musculus][gi:62740231]	
2098	Inactive			Luminescence Cell-Based Primary HTS to Identify Inhibitors of Heat Shock Factor 1 (HSF1)	Hsf1 protein [Mus musculus][gi:62740231]	
720552	Inactive	Potency		qHTS assay for small molecule agonists of the p53 signaling pathway: Summary	Cellular tumor antigen p53[gi:269849759]	
720552	Inactive	Potency		qHTS assay for small molecule agonists of the p53 signaling pathway: Summary	Cellular tumor antigen p53[gi:269849759]	
720552	Inactive	Potency		qHTS assay for small molecule agonists of the p53 signaling pathway: Summary	Cellular tumor antigen p53[gi:269849759]	

AID	Outcome	Activity Concentration Name	Activity Concentration [uM]	BioAssay	Target	PMID
720552	Inactive	Potency		qHTS assay for small molecule agonists of the p53 signaling pathway: Summary	Cellular tumor antigen p53[gi:269849759]	
2546	Inactive	Potency		VP16 counterscreen qHTS for inhibitors of ROR gamma transcriptional activity	nuclear receptor ROR-gamma [Mus musculus][gi:188536040]	
602393	Inactive			Screen for inhibitors of the SWI/SNF chromatin remodeling complex (esBAF) in mouse embryonic stem cells with Luciferase reporter assay Measured in Cell-Based System Using Plate Reader - 2141-01_Inhibitor_SinglePoint_HTS_Activity	transcription activator BRG1 isoform 1 [Mus musculus][gi:291463269]	
504775	Inactive			HTS using DiI-HDL to assay lipid transfer in ldlA[SR-BI] cells Measured in Cell-Based System Using Plate Reader - 2085-01_Activator_SinglePoint_HTS_Activity	Scarb1 gene product [Mus musculus][gi:14389423]	
488896	Inactive			HTS using DiI-HDL to assay lipid transfer in ldlA[SR-BI] cells Measured in Cell-Based System Using Plate Reader - 2085-01_Inhibitor_SinglePoint_HTS_Activity	Scarb1 gene product [Mus musculus][gi:14389423]	
2237	Inactive			Primary cell-based screen for identification of compounds that activate transient receptor potential cation channel C4 (TRPC4)	alternatively spliced Trp4 [Mus musculus][gi:2935630]	
2227	Inactive			Primary cell-based high-throughput screening assay for identification of compounds that allosterically potentiate transient receptor potential cation channel C4 (TRPC4)	alternatively spliced Trp4 [Mus musculus][gi:2935630]	
2247	Inactive			Primary cell-based screen for identification of compounds that inhibit transient receptor potential cation channel C4 (TRPC4).	alternatively spliced Trp4 [Mus musculus][gi:2935630]	
2553	Inactive			High throughput screening of inhibitors of transient receptor potential cation channel C6 (TRPC6)	short transient receptor potential channel 6 [Mus musculus][gi:160333370]	
2550	Inactive			High throughput screening of activators of transient receptor potential cation channel C6 (TRPC6)	short transient receptor potential channel 6 [Mus musculus][gi:160333370]	

AID	Outcome	Activity Concentration Name	Activity Concentration [uM]	BioAssay	Target	PMID
2071	Inactive			Colorimetric Assay for Inhibitors for NALP1	NACHT, LRR and PYD domains-containing protein 1 isoform 1 [Homo sapiens][gi:14719829]	
504462	Inactive			uHTS fluorescent assay for identification of inhibitors of ATG4B	cysteine protease ATG4B isoform a [Homo sapiens][gi:47132611]	
652115	Inactive			MLPCN SirT-5 Measured in Biochemical System Using Imaging - 7044-01_Inhibitor_SinglePoint_HTS_Activity_Set5	NAD-dependent protein deacylase sirtuin-5, mitochondrial[gi:38258652]	
652115	Inactive			MLPCN SirT-5 Measured in Biochemical System Using Imaging - 7044-01_Inhibitor_SinglePoint_HTS_Activity_Set5	NAD-dependent protein deacylase sirtuin-5, mitochondrial[gi:38258652]	
652104	Inactive	Potency		qHTS of TDP-43 Inhibitors	TAR DNA-binding protein 43[gi:20140568]	
485272	Inactive			Fluorescence polarization-based primary biochemical high throughput screening assay to identify inhibitors of Protein Arginine Deiminase 4 (PAD4) (1536 HTS)	PADI4 gene product [Homo sapiens][gi:216548487]	
485272	Inactive			Fluorescence polarization-based primary biochemical high throughput screening assay to identify inhibitors of Protein Arginine Deiminase 4 (PAD4) (1536 HTS)	PADI4 gene product [Homo sapiens][gi:216548487]	
463073	Inactive			Fluorescence polarization-based primary biochemical high throughput screening assay to identify inhibitors of Protein Arginine Deiminase 4 (PAD4)	PADI4 gene product [Homo sapiens][gi:216548487]	
463073	Inactive			Fluorescence polarization-based primary biochemical high throughput screening assay to identify inhibitors of Protein Arginine Deiminase 4 (PAD4)	PADI4 gene product [Homo sapiens][gi:216548487]	
624032	Inactive	Potency		S16 Schwann cell PMP22 intronic element firefly luciferase assay	Pmp22 gene product [Rattus norvegicus][gi:8393992]	
624044	Inactive	Potency		S16 Schwann cell PMP22 intronic element beta-lactamase assay	Pmp22 gene product [Rattus norvegicus][gi:8393992]	
628	Inactive			Discovery of novel allosteric modulators of the M1 muscarinic receptor: Antagonist Primary Screen	Muscarinic acetylcholine receptor M[gi:113121]	

AID	Outcome	Activity Concentration Name	Activity Concentration [uM]	BioAssay	Target	PMID
628	Inactive			Discovery of novel allosteric modulators of the M1 muscarinic receptor: Antagonist Primary Screen	Muscarinic acetylcholine receptor M[gi:113121]	
628	Inactive			Discovery of novel allosteric modulators of the M1 muscarinic receptor: Antagonist Primary Screen	Muscarinic acetylcholine receptor M[gi:113121]	
504441	Inactive			Dyrk1 A HTS Measured in Biochemical System Using Plate Reader - 2124-01_Inhibitor_SinglePoint_HTS_Activity	dual specificity tyrosine-phosphorylation-regulated kinase 1A [Rattus norvegicus][gi:6978787]	
504441	Inactive			Dyrk1 A HTS Measured in Biochemical System Using Plate Reader - 2124-01_Inhibitor_SinglePoint_HTS_Activity	dual specificity tyrosine-phosphorylation-regulated kinase 1A [Rattus norvegicus][gi:6978787]	
873	Inactive			Kallikrein 5 1536 HTS	kallikrein-related peptidase 5 preproprotein [Homo sapiens][gi:6912644]	
873	Inactive			Kallikrein 5 1536 HTS	kallikrein-related peptidase 5 preproprotein [Homo sapiens][gi:6912644]	
485360	Inactive	Potency		qHTS Assay for the Inhibitors of L3MBTL1	lethal(3)malignant brain tumor-like protein 1 isoform I [Homo sapiens][gi:117938328]	
485360	Inactive	Potency		qHTS Assay for the Inhibitors of L3MBTL1	lethal(3)malignant brain tumor-like protein 1 isoform I [Homo sapiens][gi:117938328]	
2599	Inactive			uHTS Luminescent assay for identification of inhibitors of Sentrin-specific protease 6 (SENP6)	SUMO-1-specific protease [Homo sapiens][gi:6166485]	
606	Inactive			HTS for LYP Inhibitors-an Autoimmunity Target - Primary screen	PTPN22 gene product [Homo sapiens][gi:224586929]	
606	Inactive			HTS for LYP Inhibitors-an Autoimmunity Target - Primary screen	PTPN22 gene product [Homo sapiens][gi:224586929]	

AID	Outcome	Activity Concentration Name	Activity Concentration [uM]	BioAssay	Target	PMID
606	Inactive			HTS for LYP Inhibitors-an Autoimmunity Target - Primary screen	PTPN22 gene product [Homo sapiens][gi:224586929]	
1779	Inactive	IC50		uHTS identification of small molecule inhibitors of LYP via a fluorescence intensity assay	PTPN22 gene product [Homo sapiens][gi:224586929]	
1779	Inactive	IC50		uHTS identification of small molecule inhibitors of LYP via a fluorescence intensity assay	PTPN22 gene product [Homo sapiens][gi:224586929]	
1779	Inactive	IC50		uHTS identification of small molecule inhibitors of LYP via a fluorescence intensity assay	PTPN22 gene product [Homo sapiens][gi:224586929]	
588489	Inactive			uHTS identification of microRNA-mediated mRNA deadenylation inhibitors by fluoresence polarization assay	polyadenylate-binding protein 1 [Homo sapiens][gi:46367787]	
2014	Inactive	IC50		uHTS fluorescence polarization assay for the identification of translation initiation inhibitors (PABP)	polyadenylate-binding protein 1 [Homo sapiens][gi:46367787]	
651658	Inactive			Small Molecule Inhibitors of FGF22-Mediated Excitatory Synaptogenesis & Epilepsy Measured in Biochemical System Using RT-PCR - 7012-01_Inhibitor_SinglePoint_HTS_Activity	FGF22 gene product [Homo sapiens][gi:10190672]	
624330	Inactive	IC50		Discovery of small molecule inhibitors of the oncogenic and cytokinetic protein MgcRacGAP - Primary and Confirmatory Screens	RACGAP1 gene product [Homo sapiens][gi:21361397]	
622	Inactive			Voltage-Dependent Potassium Channel Beta Subunit (KvBeta) Negative Modulator Primary Screen	RCKbeta2 [Rattus norvegicus][gi:499328]	
623	Inactive			Voltage-Dependent Potassium Channel Beta Subunit (KvBeta) Positive Modulator: Primary Screen	RCKbeta2 [Rattus norvegicus][gi:499328]	
1481	Inactive			Primary biochemical high-throughput screening assay to measure P97 ATPase inhibition	Valosin-containing protein [Homo sapiens][gi:111305821]	

AID	Outcome	Activity Concentration Name	Activity Concentration [uM]	BioAssay	Target	PMID
1481	Inactive			Primary biochemical high-throughput screening assay to measure P97 ATPase inhibition	Valosin-containing protein [Homo sapiens][gi:111305821]	
504847	Inactive	Potency		Inhibitors of the vitamin D receptor (VDR): qHTS	vitamin D3 receptor isoform VDRA [Homo sapiens][gi:63054845]	
504847	Inactive	Potency		Inhibitors of the vitamin D receptor (VDR): qHTS	vitamin D3 receptor isoform VDRA [Homo sapiens][gi:63054845]	
504847	Inactive	Potency		Inhibitors of the vitamin D receptor (VDR): qHTS	vitamin D3 receptor isoform VDRA [Homo sapiens][gi:63054845]	
504847	Inactive	Potency		Inhibitors of the vitamin D receptor (VDR): qHTS	vitamin D3 receptor isoform VDRA [Homo sapiens][gi:63054845]	
504847	Inactive	Potency		Inhibitors of the vitamin D receptor (VDR): qHTS	vitamin D3 receptor isoform VDRA [Homo sapiens][gi:63054845]	
504847	Inactive	Potency		Inhibitors of the vitamin D receptor (VDR): qHTS	vitamin D3 receptor isoform VDRA [Homo sapiens][gi:63054845]	
504847	Inactive	Potency		Inhibitors of the vitamin D receptor (VDR): qHTS	vitamin D3 receptor isoform VDRA [Homo sapiens][gi:63054845]	
504847	Inactive	Potency		Inhibitors of the vitamin D receptor (VDR): qHTS	vitamin D3 receptor isoform VDRA [Homo sapiens][gi:63054845]	
504847	Inactive	Potency		Inhibitors of the vitamin D receptor (VDR): qHTS	vitamin D3 receptor isoform VDRA [Homo sapiens][gi:63054845]	
504847	Inactive	Potency		Inhibitors of the vitamin D receptor (VDR): qHTS	vitamin D3 receptor isoform VDRA [Homo sapiens][gi:63054845]	

AID	Outcome	Activity Concentration Name	Activity Concentration [uM]	BioAssay	Target	PMID
504847	Inactive	Potency		Inhibitors of the vitamin D receptor (VDR): qHTS	vitamin D3 receptor isoform VDRA [Homo sapiens][gi:63054845]	
504847	Inactive	Potency		Inhibitors of the vitamin D receptor (VDR): qHTS	vitamin D3 receptor isoform VDRA [Homo sapiens][gi:63054845]	
488979	Inactive	Potency		HTS Assay for Compounds that Act as Enhancers of the Vanilloid Receptor 1	TRPV1 gene product [Homo sapiens][gi:74315350]	
488979	Inactive	Potency		HTS Assay for Compounds that Act as Enhancers of the Vanilloid Receptor 1	TRPV1 gene product [Homo sapiens][gi:74315350]	
540277	Inactive			HTS Assay for Compounds that Act as Potentiators of the Vanilloid Receptor 1	TRPV1 gene product [Homo sapiens][gi:74315350]	
540277	Inactive			HTS Assay for Compounds that Act as Potentiators of the Vanilloid Receptor 1	TRPV1 gene product [Homo sapiens][gi:74315350]	
540275	Inactive			HTS Assay for Compounds that Act as Agonists of the Vanilloid Receptor 1	TRPV1 gene product [Homo sapiens][gi:74315350]	
540275	Inactive			HTS Assay for Compounds that Act as Agonists of the Vanilloid Receptor 1	TRPV1 gene product [Homo sapiens][gi:74315350]	
2012	Inactive	IC50		uHTS fluorescence polarization assay for the identification of translation initiation inhibitors (eIF4H)	Eukaryotic translation initiation factor 4H [Homo sapiens][gi:45219878]	
1321	Inactive			Primary Cell-based High Throughput Screening Assay for Inhibitors of Wee1 Degradation	WEE1 homolog (S. pombe) [Homo sapiens][gi:47123300]	
1321	Inactive			Primary Cell-based High Throughput Screening Assay for Inhibitors of Wee1 Degradation	WEE1 homolog (S. pombe) [Homo sapiens][gi:47123300]	

AID	Outcome	Activity Concentration Name	Activity Concentration [uM]	BioAssay	Target	PMID
1321	Inactive			Primary Cell-based High Throughput Screening Assay for Inhibitors of Wee1 Degradation	WEE1 homolog (S. pombe) [Homo sapiens][gi:47123300]	
651768	Inactive	Potency		qHTS for Inhibitors of WRN Helicase	WRN [Homo sapiens][gi:3719421]	
422	Inactive			HTS for 14-3-3 protein interaction modulators	tyrosine 3-monooxygenase/tryptophan 5-monooxygenase activation protein, gamma polypeptide [Homo sapi[gi:21464101]	
422	Inactive			HTS for 14-3-3 protein interaction modulators	tyrosine 3-monooxygenase/tryptophan 5-monooxygenase activation protein, gamma polypeptide [Homo sapi[gi:21464101]	
652154	Inactive			HTS for PAX8 inhibitors using PAX8 luciferase reporter gene assay in RMG-I cells Measured in Cell-Based System Using Plate Reader - 7054-01_Inhibitor_SinglePoint_HTS_Activity	PAX8 [Homo sapiens][gi:998701]	
463082	Inactive			Fluorescence polarization-based primary biochemical high throughput screening assay to identify inhibitors of the plasma platelet activating factor acetylhydrolase (pPAFAH)	PLA2G7 gene product [Homo sapiens][gi:270133071]	
463082	Inactive			Fluorescence polarization-based primary biochemical high throughput screening assay to identify inhibitors of the plasma platelet activating factor acetylhydrolase (pPAFAH)	PLA2G7 gene product [Homo sapiens][gi:270133071]	
588352	Inactive			Luminescence-based cell-based primary high throughput screening assay to identify inhibitors of the Steroid Receptor Coactivator 3 (SRC3; NCOA3)	nuclear receptor coactivator 3 isoform a [Homo sapiens][gi:32307126]	
436	Inactive			HTS for BAP1 Enzyme inhibitors	Ubiquitin carboxyl-terminal hydrolase BAP1 (BRCA1-associated protein 1) (Cerebral protein 6)[gi:68565074]	

AID	Outcome	Activity Concentration Name	Activity Concentration [uM]	BioAssay	Target	PMID
436	Inactive			HTS for BAP1 Enzyme inhibitors	Ubiquitin carboxyl-terminal hydrolase BAP1 (BRCA1-associated protein 1) (Cerebral protein 6)[gi:68565074]	
602329	Inactive			Identification of inhibitors of RAD54 Measured in Biochemical System Using Plate Reader - 2159-01_Inhibitor_SinglePoint_HTS_Activity	RAD54L gene product [Homo sapiens][gi:216548193]	
588354	Inactive			Luminescence-based cell-based primary high throughput screening assay to identify inhibitors of the Steroid Receptor Coactivator 1 (SRC1; NCOA1)	nuclear receptor coactivator 1 isoform 1 [Homo sapiens][gi:22538455]	
588354	Inactive			Luminescence-based cell-based primary high throughput screening assay to identify inhibitors of the Steroid Receptor Coactivator 1 (SRC1; NCOA1)	nuclear receptor coactivator 1 isoform 1 [Homo sapiens][gi:22538455]	
1509	Inactive			Primary Cell-Based Assay to Identify Agonists of the Sphingosine 1-Phosphate Receptor 4 (S1P4)	Sphingosine-1-phosphate receptor 4 [Homo sapiens][gi:15929025]	
1509	Inactive			Primary Cell-Based Assay to Identify Agonists of the Sphingosine 1-Phosphate Receptor 4 (S1P4)	Sphingosine-1-phosphate receptor 4 [Homo sapiens][gi:15929025]	
1510	Inactive			Primary Cell-Based Assay to Identify Antagonists of the Sphingosine 1-Phosphate Receptor 4 (S1P4)	Sphingosine-1-phosphate receptor 4 [Homo sapiens][gi:15929025]	
1510	Inactive			Primary Cell-Based Assay to Identify Antagonists of the Sphingosine 1-Phosphate Receptor 4 (S1P4)	Sphingosine-1-phosphate receptor 4 [Homo sapiens][gi:15929025]	
1443	Inactive			uHTS for the identification of compounds that potentiate TRAIL-induced apoptosis of cancer cells	tumor necrosis factor ligand superfamily member 10 isoform 1 [Homo sapiens][gi:4507593]	
624267	Inactive			Fluorescence-based cell-based primary high throughput screening assay to identify inhibitors of the interaction of nucleotide-binding oligomerization domain containing 2 (NOD2) and the receptor-interacting serine-threonine kinase 2 (RIPK2)	RIPK2 gene product [Homo sapiens][gi:4506537]	

AID	Outcome	Activity Concentration Name	Activity Concentration [uM]	BioAssay	Target	PMID
624267	Inactive			Fluorescence-based cell-based primary high throughput screening assay to identify inhibitors of the interaction of nucleotide-binding oligomerization domain containing 2 (NOD2) and the receptor-interacting serine-threonine kinase 2 (RIPK2)	RIPK2 gene product [Homo sapiens][gi:4506537]	
624354	Inactive			uHTS identification of Caspase-8 TRAIL sensitizers in a luminesence assay	TNFRSF10B gene product [Homo sapiens][gi:224494019]	
624354	Inactive			uHTS identification of Caspase-8 TRAIL sensitizers in a luminesence assay	TNFRSF10B gene product [Homo sapiens][gi:224494019]	
803	Inactive			Primary cell-based high-throughput screening assay to identify agonists of Galanin Receptor 2 (GALR2)	Galanin receptor type 2[gi:6016094]	
828	Inactive			Primary cell-based high-throughput screening assay to identify antagonists of Galanin Receptor 2 (GALR2)	Galanin receptor type 2[gi:6016094]	
2718	Inactive			Fluorescence Cell-Free Homogeneous Primary HTS to Identify Inhibitors of Histone Deacetylase 3	histone deacetylase 3 [Homo sapiens][gi:13128862]	
2718	Inactive			Fluorescence Cell-Free Homogeneous Primary HTS to Identify Inhibitors of Histone Deacetylase 3	histone deacetylase 3 [Homo sapiens][gi:13128862]	
488839	Inactive			Development of CDK5 inhibitors Measured in Biochemical System Using Plate Reader - 2083-01_Inhibitor_SinglePoint_HTS_Activity	Cyclin-dependent kinase 5, regulatory subunit 1 (p35) [Homo sapiens][gi:20072248]	
488839	Inactive			Development of CDK5 inhibitors Measured in Biochemical System Using Plate Reader - 2083-01_Inhibitor_SinglePoint_HTS_Activity	Cyclin-dependent kinase 5, regulatory subunit 1 (p35) [Homo sapiens][gi:20072248]	
488839	Inactive			Development of CDK5 inhibitors Measured in Biochemical System Using Plate Reader - 2083-01_Inhibitor_SinglePoint_HTS_Activity	Cyclin-dependent kinase 5, regulatory subunit 1 (p35) [Homo sapiens][gi:20072248]	

AID	Outcome	Activity Concentration Name	Activity Concentration [uM]	BioAssay	Target	PMID
651699	Inactive			uHTS identification of inhibitors of cullin neddylation in a TR-FRET assay	NAE1 gene product [Homo sapiens][gi:4502169]	
449739	Inactive			Inhibitors of Cav3 T-type Calcium Channels: Primary Screen	voltage-dependent T-type calcium channel subunit alpha-1H isoform a [Homo sapiens][gi:53832009]	
449739	Inactive			Inhibitors of Cav3 T-type Calcium Channels: Primary Screen	voltage-dependent T-type calcium channel subunit alpha-1H isoform a [Homo sapiens][gi:53832009]	
449739	Inactive			Inhibitors of Cav3 T-type Calcium Channels: Primary Screen	voltage-dependent T-type calcium channel subunit alpha-1H isoform a [Homo sapiens][gi:53832009]	
686964	Inactive			TRFRET-based biochemical primary high throughput screening assay to identify inhibitors of 5-meCpG-binding domain protein 2 (MBD2)-DBD binding to methylated oligonucleotide	Methyl-CpG binding domain protein 2 [Homo sapiens][gi:21595776]	
463106	Inactive	Potency		qHTS Validation Assay for Inhibitors of Ubiquitin-specific Protease USP2a Using CHOP2 as the Reporter	ubiquitin carboxyl-terminal hydrolase 2 isoform a [Homo sapiens][gi:188528692]	
463106	Inactive	Potency		qHTS Validation Assay for Inhibitors of Ubiquitin-specific Protease USP2a Using CHOP2 as the Reporter	ubiquitin carboxyl-terminal hydrolase 2 isoform a [Homo sapiens][gi:188528692]	
463254	Inactive	Potency		qHTS Assay for Inhibitors of Ubiquitin-specific Protease USP2a Using CHOP2 as the Reporter	ubiquitin carboxyl-terminal hydrolase 2 isoform a [Homo sapiens][gi:188528692]	
463254	Inactive	Potency		qHTS Assay for Inhibitors of Ubiquitin-specific Protease USP2a Using CHOP2 as the Reporter	ubiquitin carboxyl-terminal hydrolase 2 isoform a [Homo sapiens][gi:188528692]	
624168	Inactive			uHTS identification of small molecule activators of alpha dystroglycan glycosylation	LARGE [Homo sapiens][gi:47678551]	
2013	Inactive	IC50		Image-Based HTS for Selective Antagonists for GPR55	G-protein coupled receptor 55 [Homo sapiens][gi:33695107]	

AID	Outcome	Activity Concentration Name	Activity Concentration [uM]	BioAssay	Target	PMID
1961	Inactive	EC50		Image-based HTS for Selective Agonists of GPR55	G-protein coupled receptor 55 [Homo sapiens][gi:33695107]	
485297	Inactive	Potency		qHTS Assay for Rab9 Promoter Activators	RAB9A gene product [Homo sapiens][gi:4759012]	
485297	Inactive	Potency		qHTS Assay for Rab9 Promoter Activators	RAB9A gene product [Homo sapiens][gi:4759012]	
1325	Inactive			High-throughput multiplex screening for ABC transporter inhibitors: specifically ABCG2 screen, ABCB1 counter-screen	ATP-binding cassette sub-family G member 2 [Homo sapiens][gi:62526033]	
1325	Inactive			High-throughput multiplex screening for ABC transporter inhibitors: specifically ABCG2 screen, ABCB1 counter-screen	ATP-binding cassette sub-family G member 2 [Homo sapiens][gi:62526033]	
1974	Inactive			Fluorescence polarization-based counterscreen for RBBP9 inhibitors: primary biochemical high throughput screening assay to identify inhibitors of the oxidoreductase glutathione S-transferase omega 1(GSTO1).	glutathione S-transferase omega-1 isoform 1 [Homo sapiens][gi:4758484]	
1974	Inactive			Fluorescence polarization-based counterscreen for RBBP9 inhibitors: primary biochemical high throughput screening assay to identify inhibitors of the oxidoreductase glutathione S-transferase omega 1(GSTO1).	glutathione S-transferase omega-1 isoform 1 [Homo sapiens][gi:4758484]	
1416	Inactive			Primary cell-based high-throughput screening assay to measure PERK inhibition	eukaryotic translation initiation factor 2-alpha kinase 3 [Homo sapiens][gi:134304838]	
1416	Inactive			Primary cell-based high-throughput screening assay to measure PERK inhibition	eukaryotic translation initiation factor 2-alpha kinase 3 [Homo sapiens][gi:134304838]	
604	Inactive			Primary biochemical high-throughput screening assay for inhibitors of Rho kinase 2 (Rhok2)	rho-associated protein kinase 2 [Homo sapiens][gi:41872583]	

AID	Outcome	Activity Concentration Name	Activity Concentration [uM]	BioAssay	Target	PMID
604	Inactive			Primary biochemical high-throughput screening assay for inhibitors of Rho kinase 2 (Rhok2)	rho-associated protein kinase 2 [Homo sapiens][gi:41872583]	
2751	Inactive			Fluorescence polarization-based primary biochemical high throughput screening assay to identify inhibitors of the prolyl oligopeptidase-like enzyme (PREPL)	Prolyl endopeptidase-like [Homo sapiens][gi:153217451]	
504523	Inactive			Fluorescence polarization to screen for inhibitors that disrupt the protein-protein interaction between Keap1 and Nrf2 Measured in Biochemical System Using Plate Reader - 2119-01_Inhibitor_SinglePoint_HTS_Activity	KEAP1 gene product [Homo sapiens][gi:45269145]	
504523	Inactive			Fluorescence polarization to screen for inhibitors that disrupt the protein-protein interaction between Keap1 and Nrf2 Measured in Biochemical System Using Plate Reader - 2119-01_Inhibitor_SinglePoint_HTS_Activity	KEAP1 gene product [Homo sapiens][gi:45269145]	
602229	Inactive			Luminescence-based cell-based high throughput primary screening assay to identify agonists of nuclear receptor subfamily 2, group E, member 3 (NR2E3)	photoreceptor-specific nuclear receptor [Homo sapiens][gi:216409728]	
602229	Inactive			Luminescence-based cell-based high throughput primary screening assay to identify agonists of nuclear receptor subfamily 2, group E, member 3 (NR2E3)	photoreceptor-specific nuclear receptor [Homo sapiens][gi:216409728]	
602229	Inactive			Luminescence-based cell-based high throughput primary screening assay to identify agonists of nuclear receptor subfamily 2, group E, member 3 (NR2E3)	photoreceptor-specific nuclear receptor [Homo sapiens][gi:216409728]	
2300	Inactive			TR-FRET-based primary biochemical high throughput screening assay to identify agonists of nuclear receptor subfamily 2, group E, member 3 (NR2E3).	photoreceptor-specific nuclear receptor [Homo sapiens][gi:216409728]	
2300	Inactive			TR-FRET-based primary biochemical high throughput screening assay to identify agonists of nuclear receptor subfamily 2, group E, member 3 (NR2E3).	photoreceptor-specific nuclear receptor [Homo sapiens][gi:216409728]	

AID	Outcome	Activity Concentration Name	Activity Concentration [uM]	BioAssay	Target	PMID
2300	Inactive			TR-FRET-based primary biochemical high throughput screening assay to identify agonists of nuclear receptor subfamily 2, group E, member 3 (NR2E3).	photoreceptor-specific nuclear receptor [Homo sapiens][gi:216409728]	
951	Inactive			Multiplexed high-throughput screen for small molecule regulators of Bcl-2 family protein interactions, specifically Bim-Bcl-B.	Bcl-2-like protein 10[gi:23396469]	
951	Inactive			Multiplexed high-throughput screen for small molecule regulators of Bcl-2 family protein interactions, specifically Bim-Bcl-B.	Bcl-2-like protein 10[gi:23396469]	
951	Inactive			Multiplexed high-throughput screen for small molecule regulators of Bcl-2 family protein interactions, specifically Bim-Bcl-B.	Bcl-2-like protein 10[gi:23396469]	
2462	Inactive			Luminescence Cell-Based Primary HTS to Identify Inhibitors of A1 Apoptosis.	bcl-2-like protein 11 isoform 1 [Homo sapiens][gi:20336315]	
2462	Inactive			Luminescence Cell-Based Primary HTS to Identify Inhibitors of A1 Apoptosis.	bcl-2-like protein 11 isoform 1 [Homo sapiens][gi:20336315]	
2462	Inactive			Luminescence Cell-Based Primary HTS to Identify Inhibitors of A1 Apoptosis.	bcl-2-like protein 11 isoform 1 [Homo sapiens][gi:20336315]	
2462	Inactive			Luminescence Cell-Based Primary HTS to Identify Inhibitors of A1 Apoptosis.	bcl-2-like protein 11 isoform 1 [Homo sapiens][gi:20336315]	
602162	Inactive			Flow Cytometric HTS Screen for inhibitors of the ABC transporter ABCB6 for MLPCN Compound Set	ABCB6 gene product [Homo sapiens][gi:9955963]	
588550	Inactive			Flow Cytometric HTS Screen for inhibitors of the ABC transporter ABCB6 for Validation Compound Set	ABCB6 gene product [Homo sapiens][gi:9955963]	
540253	Inactive	Potency		qHTS Assay for Inhibitors of RanGTP induced Rango (Ran-regulated importin-beta cargo) - Importin beta complex dissociation	snurportin-1 [Homo sapiens][gi:5031833]	

AID	Outcome	Activity Concentration Name	Activity Concentration [uM]	BioAssay	Target	PMID
540263	Inactive	Potency		qHTS Assay for Inhibitors of Rango (Ran-regulated importin-beta cargo) - Importin beta complex formation	snurportin-1 [Homo sapiens][gi:5031833]	
651711	Inactive			Turbidometric Biochemical Primary HTS to identify inhibitors of ERp5 Measured in Biochemical System Using Plate Reader - 7002-01_Inhibitor_SinglePoint_HTS_Activity	Protein disulfide-isomerase A6[gi:2501205]	
588493	Inactive			uHTS identification of inhibitors of Rpn11 in a Fluorescent Polarization assay	PSMD14 protein [Homo sapiens][gi:16306916]	
1578	Inactive	EC50		uHTS luminescence assay for the identification of compounds that inhibit NOD1	nucleotide-binding oligomerization domain-containing protein 1 [Homo sapiens][gi:5174617]	
1578	Inactive	EC50		uHTS luminescence assay for the identification of compounds that inhibit NOD1	nucleotide-binding oligomerization domain-containing protein 1 [Homo sapiens][gi:5174617]	
2174	Inactive			Counterscreen for PME1 inhibitors: fluorescence polarization-based primary biochemical high throughput screening assay to identify inhibitors of lysophospholipase 1 (LYPLA1).	acyl-protein thioesterase 1 [Homo sapiens][gi:5453722]	
2174	Inactive			Counterscreen for PME1 inhibitors: fluorescence polarization-based primary biochemical high throughput screening assay to identify inhibitors of lysophospholipase 1 (LYPLA1).	acyl-protein thioesterase 1 [Homo sapiens][gi:5453722]	
651957	Inactive			Luminescence-based cell-based primary high throughput screening assay to identify inhibitors of the Steroid Receptor Coactivator 2 (SRC2; NCOA2)	NCOA2 gene product [Homo sapiens][gi:5729858]	
651957	Inactive			Luminescence-based cell-based primary high throughput screening assay to identify inhibitors of the Steroid Receptor Coactivator 2 (SRC2; NCOA2)	NCOA2 gene product [Homo sapiens][gi:5729858]	
504842	Inactive	Potency		Inhibitors of TCP-1 ring complex (TRiC) of Methanococcus maripaludis (MmCpn): qHTS	chaperonin-containing TCP-1 beta subunit homolog [Homo sapiens][gi:4090929]	

AID	Outcome	Activity Concentration Name	Activity Concentration [uM]	BioAssay	Target	PMID
602244	Inactive			uHTS identification of CXCR6 Inhibitors in a B-arrestin luminescence assay	CXCR6 gene product [Homo sapiens][gi:5730106]	
602244	Inactive			uHTS identification of CXCR6 Inhibitors in a B-arrestin luminescence assay	CXCR6 gene product [Homo sapiens][gi:5730106]	
1515	Inactive			Primary biochemical high throughput screening assay to identify inhibitors of Retinoblastoma binding protein 9 (RBBP9)	putative hydrolase RBBP9 [Homo sapiens][gi:24119166]	
540317	Inactive	Potency		HTS for Inhibitors of HP1-beta Chromodomain Interactions with Methylated Histone Tails	chromobox protein homolog 1 [Homo sapiens][gi:187960037]	
1468	Inactive	Potency		qHTS for Inhibitors of Tau Fibril Formation, Fluorescence Polarization	Microtubule-associated protein tau [Homo sapiens][gi:92096784]	
1468	Inactive	Potency		qHTS for Inhibitors of Tau Fibril Formation, Fluorescence Polarization	Microtubule-associated protein tau [Homo sapiens][gi:92096784]	
2642	Inactive			Primary cell-based high-throughput screening assay for identification of compounds that inhibit KCNQ1 potassium channels	KCNQ1 gene product [Homo sapiens][gi:32479527]	
2648	Inactive			Primary cell-based high-throughput screening assay for identification of compounds that potentiate/activate KCNQ1 potassium channels	KCNQ1 gene product [Homo sapiens][gi:32479527]	
1458	Inactive	Potency		qHTS Assay for Enhancers of SMN2 Splice Variant Expression	survival motor neuron protein isoform d [Homo sapiens][gi:10937869]	
1458	Inactive	Potency		qHTS Assay for Enhancers of SMN2 Splice Variant Expression	survival motor neuron protein isoform d [Homo sapiens][gi:10937869]	
504937	Inactive	Potency		Inhibitors of Secretory Acid Sphingomyelinase (S-ASM): qHTS	acid sphingomyelinase [Homo sapiens][gi:179095]	

AID	Outcome	Activity Concentration Name	Activity Concentration [uM]	BioAssay	Target	PMID
504937	Inactive	Potency		Inhibitors of Secretory Acid Sphingomyelinase (S-ASM): qHTS	acid sphingomyelinase [Homo sapiens][gi:179095]	
1326	Inactive			High-throughput multiplex screening for ABC transporter inhibitors: specifically ABCB1 screen, ABCG2 counter-screen	ABCB1 gene product [Homo sapiens][gi:42741659]	
1326	Inactive			High-throughput multiplex screening for ABC transporter inhibitors: specifically ABCB1 screen, ABCG2 counter-screen	ABCB1 gene product [Homo sapiens][gi:42741659]	
1326	Inactive			High-throughput multiplex screening for ABC transporter inhibitors: specifically ABCB1 screen, ABCG2 counter-screen	ABCB1 gene product [Homo sapiens][gi:42741659]	
504891	Inactive	Potency		qHTS Assay to Find Inhibitors of Pin1	PIN1 gene product [Homo sapiens][gi:5453898]	
504891	Inactive	Potency		qHTS Assay to Find Inhibitors of Pin1	PIN1 gene product [Homo sapiens][gi:5453898]	
504536	Inactive	Potency		qHTS Validation Assay to Find Inhibitors of Pin1	PIN1 gene product [Homo sapiens][gi:5453898]	
504536	Inactive	Potency		qHTS Validation Assay to Find Inhibitors of Pin1	PIN1 gene product [Homo sapiens][gi:5453898]	
652105	Inactive	Potency		qHTS for Inhibitors of phosphatidylinositol 5-phosphate 4-kinase (PI5P4K)	Phosphatidylinositol 5-phosphate 4-kinase type-2 alpha[gi:18266879]	
1631	Inactive	Potency		qHTS Assay for Activators of Human Muscle isoform 2 Pyruvate Kinase	PKM gene product [Homo sapiens][gi:33286418]	
1631	Inactive	Potency		qHTS Assay for Activators of Human Muscle isoform 2 Pyruvate Kinase	PKM gene product [Homo sapiens][gi:33286418]	
1631	Inactive	Potency		qHTS Assay for Activators of Human Muscle isoform 2 Pyruvate Kinase	PKM gene product [Homo sapiens][gi:33286418]	
1634	Inactive	Potency		qHTS Assay for Inhibitors of Human Muscle isoform 2 Pyruvate Kinase	PKM gene product [Homo sapiens][gi:33286418]	

AID	Outcome	Activity Concentration Name	Activity Concentration [uM]	BioAssay	Target	PMID
1634	Inactive	Potency		qHTS Assay for Inhibitors of Human Muscle isoform 2 Pyruvate Kinase	PKM gene product [Homo sapiens][gi:33286418]	
1634	Inactive	Potency		qHTS Assay for Inhibitors of Human Muscle isoform 2 Pyruvate Kinase	PKM gene product [Homo sapiens][gi:33286418]	
1817	Inactive	IC50		uHTS identification of small molecule antagonists of the binding of Siah-1 and a peptide ligand via a fluorescence polarization assay	plectin 1 [Homo sapiens][gi:40849930]	
720504	Inactive	Potency		qHTS for Inhibitors of PLK1-PDB (polo-like kinase 1 - polo-box domain): Primary Screen	PLK1 gene product [Homo sapiens][gi:21359873]	
720504	Inactive	Potency		qHTS for Inhibitors of PLK1-PDB (polo-like kinase 1 - polo-box domain): Primary Screen	PLK1 gene product [Homo sapiens][gi:21359873]	
2675	Inactive	Potency		qHTS Assay for Inhibitors of MBNL1-poly(CUG) RNA binding	muscleblind-like protein 1 isoform a [Homo sapiens][gi:41281591]	
540308	Inactive			Luminescence-based cell-based primary high throughput screening assay to identify biased ligands of the melanocortin 4 receptor (MC4R): agonists of MC4R	melanocortin receptor 4 [Homo sapiens][gi:119508433]	
540308	Inactive			Luminescence-based cell-based primary high throughput screening assay to identify biased ligands of the melanocortin 4 receptor (MC4R): agonists of MC4R	melanocortin receptor 4 [Homo sapiens][gi:119508433]	
540295	Inactive			TRFRET-based cell-based primary high throughput screening assay to identify biased ligands of the melanocortin 4 receptor (MC4R): antagonists of MC4R	melanocortin receptor 4 [Homo sapiens][gi:119508433]	
540295	Inactive			TRFRET-based cell-based primary high throughput screening assay to identify biased ligands of the melanocortin 4 receptor (MC4R): antagonists of MC4R	melanocortin receptor 4 [Homo sapiens][gi:119508433]	

AID	Outcome	Activity Concentration Name	Activity Concentration [uM]	BioAssay	Target	PMID
2057	Inactive			Fluorescence polarization-based primary biochemical high throughput screening assay to identify inhibitors of myeloid cell leukemia sequence 1 (MCL1) interactions with BIM-BH3 peptide.	Myeloid cell leukemia sequence 1 (BCL2-related) [Homo sapiens][gi:78070770]	
2057	Inactive			Fluorescence polarization-based primary biochemical high throughput screening assay to identify inhibitors of myeloid cell leukemia sequence 1 (MCL1) interactions with BIM-BH3 peptide.	Myeloid cell leukemia sequence 1 (BCL2-related) [Homo sapiens][gi:78070770]	
2057	Inactive			Fluorescence polarization-based primary biochemical high throughput screening assay to identify inhibitors of myeloid cell leukemia sequence 1 (MCL1) interactions with BIM-BH3 peptide.	Myeloid cell leukemia sequence 1 (BCL2-related) [Homo sapiens][gi:78070770]	
1009	Inactive			Multiplexed high-throughput screen for small molecule regulators of Bcl-2 family protein interactions, specifically Bim-Mcl-1	Mcl-1 [Homo sapiens][gi:7582271]	
1009	Inactive			Multiplexed high-throughput screen for small molecule regulators of Bcl-2 family protein interactions, specifically Bim-Mcl-1	Mcl-1 [Homo sapiens][gi:7582271]	
1009	Inactive			Multiplexed high-throughput screen for small molecule regulators of Bcl-2 family protein interactions, specifically Bim-Mcl-1	Mcl-1 [Homo sapiens][gi:7582271]	
1021	Inactive			uHTS of Mcl-1/Bid interaction inhibitors	Mcl-1 [Homo sapiens][gi:7582271]	
1021	Inactive			uHTS of Mcl-1/Bid interaction inhibitors	Mcl-1 [Homo sapiens][gi:7582271]	
1021	Inactive			uHTS of Mcl-1/Bid interaction inhibitors	Mcl-1 [Homo sapiens][gi:7582271]	
1022	Inactive			uHTS of Mcl-1/Noxa interaction inhibitors	Mcl-1 [Homo sapiens][gi:7582271]	
1022	Inactive			uHTS of Mcl-1/Noxa interaction inhibitors	Mcl-1 [Homo sapiens][gi:7582271]	
1022	Inactive			uHTS of Mcl-1/Noxa interaction inhibitors	Mcl-1 [Homo sapiens][gi:7582271]	

AID	Outcome	Activity Concentration Name	Activity Concentration [uM]	BioAssay	Target	PMID
485346	Inactive			uHTS for identification of Inhibitors of Mdm2/MdmX interaction in luminescent format.	protein Mdm4 isoform 1 [Homo sapiens][gi:88702791]	
485346	Inactive			uHTS for identification of Inhibitors of Mdm2/MdmX interaction in luminescent format.	protein Mdm4 isoform 1 [Homo sapiens][gi:88702791]	
1529	Inactive			Multiplex HTS Assay for Inhibitors of MEK Kinase PB1 Domains, specifically MEK5 MEK Kinase3 Wildtype	mitogen-activated protein kinase kinase kinase 3 isoform 1 [Homo sapiens][gi:42794767]	
1529	Inactive			Multiplex HTS Assay for Inhibitors of MEK Kinase PB1 Domains, specifically MEK5 MEK Kinase3 Wildtype	mitogen-activated protein kinase kinase kinase 3 isoform 1 [Homo sapiens][gi:42794767]	
1529	Inactive			Multiplex HTS Assay for Inhibitors of MEK Kinase PB1 Domains, specifically MEK5 MEK Kinase3 Wildtype	mitogen-activated protein kinase kinase kinase 3 isoform 1 [Homo sapiens][gi:42794767]	
1766	Inactive	Potency		qHTS Assay for Inhibitors Targeting the Menin-MLL Interaction in MLL Related Leukemias: Competition With Fluorescein Labeled MLL-derived Peptide	MEN1 gene product [Homo sapiens][gi:18860839]	
1768	Inactive	Potency		qHTS Assay for Inhibitors Targeting the Menin-MLL Interaction in MLL Related Leukemias: Competition With Texas Red Labeled MLL-derived Mutant Peptide	MEN1 gene product [Homo sapiens][gi:18860839]	
1766	Inactive	Potency		qHTS Assay for Inhibitors Targeting the Menin-MLL Interaction in MLL Related Leukemias: Competition With Fluorescein Labeled MLL-derived Peptide	MEN1 gene product [Homo sapiens][gi:18860839]	
1768	Inactive	Potency		qHTS Assay for Inhibitors Targeting the Menin-MLL Interaction in MLL Related Leukemias: Competition With Texas Red Labeled MLL-derived Mutant Peptide	MEN1 gene product [Homo sapiens][gi:18860839]	
1766	Inactive	Potency		qHTS Assay for Inhibitors Targeting the Menin-MLL Interaction in MLL Related Leukemias: Competition With Fluorescein Labeled MLL-derived Peptide	MEN1 gene product [Homo sapiens][gi:18860839]	

AID	Outcome	Activity Concentration Name	Activity Concentration [uM]	BioAssay	Target	PMID
1511	Inactive			Primary cell-based high-throughput screening assay for identification of compounds that protect hERG from block by proarrhythmic agents	putative potassium channel subunit [Homo sapiens][gi:487738]	
1511	Inactive			Primary cell-based high-throughput screening assay for identification of compounds that protect hERG from block by proarrhythmic agents	putative potassium channel subunit [Homo sapiens][gi:487738]	
1511	Inactive			Primary cell-based high-throughput screening assay for identification of compounds that protect hERG from block by proarrhythmic agents	putative potassium channel subunit [Homo sapiens][gi:487738]	
1511	Inactive			Primary cell-based high-throughput screening assay for identification of compounds that protect hERG from block by proarrhythmic agents	putative potassium channel subunit [Homo sapiens][gi:487738]	
1511	Inactive			Primary cell-based high-throughput screening assay for identification of compounds that protect hERG from block by proarrhythmic agents	putative potassium channel subunit [Homo sapiens][gi:487738]	
602410	Inactive			Primary cell-based screen for identification of compounds that inhibit the two-pore domain potassium channel KCNK3	Kcnk3 channel [Homo sapiens][gi:11093520]	
1459	Inactive	Potency		Validation of Assay for Modulators of Lamin A Splicing	prelamin-A/C isoform 3 [Homo sapiens][gi:27436948]	
1487	Inactive	Potency		qHTS Assay for Modulators of Lamin A Splicing	prelamin-A/C isoform 3 [Homo sapiens][gi:27436948]	
588855	Inactive	Potency		qHTS for Inhibitors of TGF-b	Smad3 [Homo sapiens][gi:18418623]	
588855	Inactive	Potency		qHTS for Inhibitors of TGF-b	Smad3 [Homo sapiens][gi:18418623]	

AID	Outcome	Activity Concentration Name	Activity Concentration [uM]	BioAssay	Target	PMID
630	Inactive			HTS of Smad transcription factor inhibitors	mothers against decapentaplegic homolog 3 [Homo sapiens][gi:5174513]	
630	Inactive			HTS of Smad transcription factor inhibitors	mothers against decapentaplegic homolog 3 [Homo sapiens][gi:5174513]	
1460	Inactive	Potency		qHTS for Inhibitors of Tau Fibril Formation, Thioflavin T Binding	Microtubule-associated protein tau [Homo sapiens][gi:92096784]	
1460	Inactive	Potency		qHTS for Inhibitors of Tau Fibril Formation, Thioflavin T Binding	Microtubule-associated protein tau [Homo sapiens][gi:92096784]	
652106	Inactive	Potency		qHTS of alpha-syn Inhibitors	Alpha-synuclein[gi:586067]	
652106	Inactive	Potency		qHTS of alpha-syn Inhibitors	Alpha-synuclein[gi:586067]	
652106	Inactive	Potency		qHTS of alpha-syn Inhibitors	Alpha-synuclein[gi:586067]	
652106	Inactive	Potency		qHTS of alpha-syn Inhibitors	Alpha-synuclein[gi:586067]	
920	Inactive			Primary cell-based high throughput screening assay to measure STAT1 inhibition	signal transducer and activator of transcription 1-alpha/beta isoform alpha [Homo sapiens][gi:6274552]	
920	Inactive			Primary cell-based high throughput screening assay to measure STAT1 inhibition	signal transducer and activator of transcription 1-alpha/beta isoform alpha [Homo sapiens][gi:6274552]	
932	Inactive			Primary cell-based high throughput screening assay to measure STAT1 activation	signal transducer and activator of transcription 1-alpha/beta isoform alpha [Homo sapiens][gi:6274552]	
932	Inactive			Primary cell-based high throughput screening assay to measure STAT1 activation	signal transducer and activator of transcription 1-alpha/beta isoform alpha [Homo sapiens][gi:6274552]	
862	Inactive			Primary cell-based high throughput screening assay to measure STAT3 inhibition	STAT3 [Homo sapiens][gi:13272532]	

AID	Outcome	Activity Concentration Name	Activity Concentration [uM]	BioAssay	Target	PMID
862	Inactive			Primary cell-based high throughput screening assay to measure STAT3 inhibition	STAT3 [Homo sapiens][gi:13272532]	
862	Inactive			Primary cell-based high throughput screening assay to measure STAT3 inhibition	STAT3 [Homo sapiens][gi:13272532]	
871	Inactive			Primary cell-based high throughput screening assay to measure STAT3 activation	STAT3 [Homo sapiens][gi:13272532]	
871	Inactive			Primary cell-based high throughput screening assay to measure STAT3 activation	STAT3 [Homo sapiens][gi:13272532]	
871	Inactive			Primary cell-based high throughput screening assay to measure STAT3 activation	STAT3 [Homo sapiens][gi:13272532]	
651800	Inactive			Fluorescence-based biochemical primary high throughput assay to identify inhibitors of T-cell receptor (TCR)-CD3 interaction using a TAMRA-labeled TCR probe	TCRAV4S1 [Homo sapiens][gi:2358024]	
686940	Inactive			Luminescence-based cell-based primary high throughput screening assay to identify inhibitors of COUP-TFII (NR2F2)	NR2F2 gene product [Homo sapiens][gi:14149746]	
686940	Inactive			Luminescence-based cell-based primary high throughput screening assay to identify inhibitors of COUP-TFII (NR2F2)	NR2F2 gene product [Homo sapiens][gi:14149746]	
1479	Inactive	Potency		Total Fluorescence Counterscreen for Inhibitors of the Interaction of Thyroid Hormone Receptor and Steroid Receptor Coregulator 2	thyroid hormone receptor beta [Homo sapiens][gi:189491771]	
1479	Inactive	Potency		Total Fluorescence Counterscreen for Inhibitors of the Interaction of Thyroid Hormone Receptor and Steroid Receptor Coregulator 2	thyroid hormone receptor beta [Homo sapiens][gi:189491771]	
1479	Inactive	Potency		Total Fluorescence Counterscreen for Inhibitors of the Interaction of Thyroid Hormone Receptor and Steroid Receptor Coregulator 2	thyroid hormone receptor beta [Homo sapiens][gi:189491771]	
1469	Inactive	Potency		qHTS for Inhibitors of the Interaction of Thyroid Hormone Receptor and Steroid Receptor Coregulator 2	thyroid hormone receptor beta [Homo sapiens][gi:189491771]	

AID	Outcome	Activity Concentration Name	Activity Concentration [uM]	BioAssay	Target	PMID
1469	Inactive	Potency		qHTS for Inhibitors of the Interaction of Thyroid Hormone Receptor and Steroid Receptor Coregulator 2	thyroid hormone receptor beta [Homo sapiens][gi:189491771]	
1469	Inactive	Potency		qHTS for Inhibitors of the Interaction of Thyroid Hormone Receptor and Steroid Receptor Coregulator 2	thyroid hormone receptor beta [Homo sapiens][gi:189491771]	
1469	Inactive	Potency		qHTS for Inhibitors of the Interaction of Thyroid Hormone Receptor and Steroid Receptor Coregulator 2	thyroid hormone receptor beta [Homo sapiens][gi:189491771]	
1469	Inactive	Potency		qHTS for Inhibitors of the Interaction of Thyroid Hormone Receptor and Steroid Receptor Coregulator 2	thyroid hormone receptor beta [Homo sapiens][gi:189491771]	
1469	Inactive	Potency		qHTS for Inhibitors of the Interaction of Thyroid Hormone Receptor and Steroid Receptor Coregulator 2	thyroid hormone receptor beta [Homo sapiens][gi:189491771]	
1479	Inactive	Potency		Total Fluorescence Counterscreen for Inhibitors of the Interaction of Thyroid Hormone Receptor and Steroid Receptor Coregulator 2	thyroid hormone receptor beta [Homo sapiens][gi:189491771]	
1479	Inactive	Potency		Total Fluorescence Counterscreen for Inhibitors of the Interaction of Thyroid Hormone Receptor and Steroid Receptor Coregulator 2	thyroid hormone receptor beta [Homo sapiens][gi:189491771]	
1479	Inactive	Potency		Total Fluorescence Counterscreen for Inhibitors of the Interaction of Thyroid Hormone Receptor and Steroid Receptor Coregulator 2	thyroid hormone receptor beta [Homo sapiens][gi:189491771]	
602276	Inactive			Novel Modifiers of Toll-like and RIG-like Receptor Signaling-SeV Stimulus	Toll-like receptor 3[gi:20140422]	
602277	Inactive			Novel Modifiers of Toll-like and RIG-like Receptor Signaling-Poly IC Stimulus	Toll-like receptor 3[gi:20140422]	
504706	Inactive	Potency		qHTS assay for re-activators of p53 using a Luc reporter	P53 [Homo sapiens][gi:23491729]	

AID	Outcome	Activity Concentration Name	Activity Concentration [uM]	BioAssay	Target	PMID
504706	Inactive	Potency		qHTS assay for re-activators of p53 using a Luc reporter	P53 [Homo sapiens][gi:23491729]	
504706	Inactive	Potency		qHTS assay for re-activators of p53 using a Luc reporter	P53 [Homo sapiens][gi:23491729]	
504706	Inactive	Potency		qHTS assay for re-activators of p53 using a Luc reporter	P53 [Homo sapiens][gi:23491729]	
720552	Inactive	Potency		qHTS assay for small molecule agonists of the p53 signaling pathway: Summary	Cellular tumor antigen p53[gi:269849759]	
720552	Inactive	Potency		qHTS assay for small molecule agonists of the p53 signaling pathway: Summary	Cellular tumor antigen p53[gi:269849759]	
720552	Inactive	Potency		qHTS assay for small molecule agonists of the p53 signaling pathway: Summary	Cellular tumor antigen p53[gi:269849759]	
720552	Inactive	Potency		qHTS assay for small molecule agonists of the p53 signaling pathway: Summary	Cellular tumor antigen p53[gi:269849759]	
493056	Inactive			qHTS for Small Molecule Agonists and Allosteric Enhancers of Human TRH Receptor: Primary Screen for Enhancers	thyrotropin-releasing hormone receptor [Homo sapiens][gi:4507681]	
493084	Inactive			qHTS for Small Molecule Agonists and Allosteric Enhancers of Human TRH Receptor: Primary Screen for Agonists.	thyrotropin-releasing hormone receptor [Homo sapiens][gi:4507681]	
493127	Inactive			qHTS for Small Molecule Agonists and Allosteric Enhancers of Human TRH Receptor: Validation Screen for Agonists	thyrotropin-releasing hormone receptor [Homo sapiens][gi:4507681]	
493005	Inactive	Potency		qHTS Assay for Iinhibitors of HIV-1 Budding by Blocking the Interaction of PTAP/TSG101	TSG101 gene product [Homo sapiens][gi:5454140]	
493005	Inactive	Potency		qHTS Assay for Iinhibitors of HIV-1 Budding by Blocking the Interaction of PTAP/TSG101	TSG101 gene product [Homo sapiens][gi:5454140]	
485342	Inactive	Potency		qHTS Validation Assay for Iinhibitors of HIV-1 Budding by Blocking the Interaction of PTAP/TSG101	TSG101 gene product [Homo sapiens][gi:5454140]	

AID	Outcome	Activity Concentration Name	Activity Concentration [uM]	BioAssay	Target	PMID
485342	Inactive	Potency		qHTS Validation Assay for Iinhibitors of HIV-1 Budding by Blocking the Interaction of PTAP/TSG101	TSG101 gene product [Homo sapiens][gi:5454140]	
488980	Inactive	Potency		qHTS Assay for Antagonists of the Thyroid Stimulating Hormone Receptor	thyroid stimulating hormone receptor [Homo sapiens][gi:38016895]	
488980	Inactive	Potency		qHTS Assay for Antagonists of the Thyroid Stimulating Hormone Receptor	thyroid stimulating hormone receptor [Homo sapiens][gi:38016895]	
488980	Inactive	Potency		qHTS Assay for Antagonists of the Thyroid Stimulating Hormone Receptor	thyroid stimulating hormone receptor [Homo sapiens][gi:38016895]	
504821	Inactive	Potency		Antagonists of the Thyroid Stimulating Hormone Receptor: Validation	thyroid stimulating hormone receptor [Homo sapiens][gi:38016895]	
504821	Inactive	Potency		Antagonists of the Thyroid Stimulating Hormone Receptor: Validation	thyroid stimulating hormone receptor [Homo sapiens][gi:38016895]	
504821	Inactive	Potency		Antagonists of the Thyroid Stimulating Hormone Receptor: Validation	thyroid stimulating hormone receptor [Homo sapiens][gi:38016895]	
504810	Inactive			Antagonists of the Thyroid Stimulating Hormone Receptor: HTS campaign	TSHR protein [Homo sapiens][gi:118341367]	20427476
504810	Inactive			Antagonists of the Thyroid Stimulating Hormone Receptor: HTS campaign	TSHR protein [Homo sapiens][gi:118341367]	20427476
504810	Inactive			Antagonists of the Thyroid Stimulating Hormone Receptor: HTS campaign	TSHR protein [Homo sapiens][gi:118341367]	20427476
504812	Inactive			Inverse Agonists of the Thyroid Stimulating Hormone Receptor: HTS campaign	TSHR protein [Homo sapiens][gi:118341367]	20427476

AID	Outcome	Activity Concentration Name	Activity Concentration [uM]	BioAssay	Target	PMID
504812	Inactive			Inverse Agonists of the Thyroid Stimulating Hormone Receptor: HTS campaign	TSHR protein [Homo sapiens][gi:118341367]	20427476
504812	Inactive			Inverse Agonists of the Thyroid Stimulating Hormone Receptor: HTS campaign	TSHR protein [Homo sapiens][gi:118341367]	20427476
504810	Inactive			Antagonists of the Thyroid Stimulating Hormone Receptor: HTS campaign	TSHR protein [Homo sapiens][gi:118341367]	20427476
504810	Inactive			Antagonists of the Thyroid Stimulating Hormone Receptor: HTS campaign	TSHR protein [Homo sapiens][gi:118341367]	20427476
504810	Inactive			Antagonists of the Thyroid Stimulating Hormone Receptor: HTS campaign	TSHR protein [Homo sapiens][gi:118341367]	20427476
504812	Inactive			Inverse Agonists of the Thyroid Stimulating Hormone Receptor: HTS campaign	TSHR protein [Homo sapiens][gi:118341367]	20427476
504812	Inactive			Inverse Agonists of the Thyroid Stimulating Hormone Receptor: HTS campaign	TSHR protein [Homo sapiens][gi:118341367]	20427476
504812	Inactive			Inverse Agonists of the Thyroid Stimulating Hormone Receptor: HTS campaign	TSHR protein [Homo sapiens][gi:118341367]	20427476
2006	Inactive	IC50		uHTS HTRF assay for identification of inhibitors of SUMOylation	SUMO-conjugating enzyme UBC9 [Homo sapiens][gi:4507785]	
485273	Inactive			uHTS identification of UBC13 Polyubiquitin Inhibitors via a TR-FRET Assay	UBE2N gene product [Homo sapiens][gi:4507793]	
485273	Inactive			uHTS identification of UBC13 Polyubiquitin Inhibitors via a TR-FRET Assay	UBE2N gene product [Homo sapiens][gi:4507793]	
602429	Inactive			uHTS identification of SUMO1-mediated protein-protein interactions	SUMO-1 [Homo sapiens][gi:1762973]	
686992	Inactive			Identification of agents that induce E-selectin on human endothelial cells Measured in Cell-Based System Using Imaging - 2152-01_Activator_SinglePoint_HTS_Activity	SELE gene product [Homo sapiens][gi:187960042]	

AID	Outcome	Activity Concentration Name	Activity Concentration [uM]	BioAssay	Target	PMID
2326	Inactive	Potency		qHTS Assay for Inhibitors of Influenza NS1 Protein Function	nonstructural protein 1 [Influenza A virus (A/WSN/1933(H1N1))][gi:194352380]	
2326	Inactive	Potency		qHTS Assay for Inhibitors of Influenza NS1 Protein Function	nonstructural protein 1 [Influenza A virus (A/WSN/1933(H1N1))][gi:194352380]	
588689	Inactive	IC50		Primary and Confirmatory Screening for Flavivirus Genomic Capping Enzyme Inhibition	Chain A, Crystal Structure Of Dengue-2 Virus Methyltransferase Complexed With S-Adenosyl-L-Homocyste[gi:219689243]	
2147	Inactive	Potency		qHTS Assay for Inhibitors of Human Jumonji Domain Containing 2E (JMJD2E)	Chain A, Crystal Structure Of The Human 2-Oxoglutarate Oxygenase Loc390245[gi:221046486]	
504329	Inactive	IC50		Discovery of Small Molecule Probes for H1N1 Influenza NS1A	nonstructural protein 1 [Influenza A virus (A/California/07/2009(H1N1))][gi:227977143]	
2323	Inactive	Potency		qHTS Validation Assay for Identification of Novel General Anesthetics	Chain A, Horse Spleen Apoferritin[gi:254220970]	
485281	Inactive	Potency		qHTS Assay for Identification of Novel General Anesthetics	Chain A, Horse Spleen Apoferritin[gi:254220970]	
1476	Inactive	Potency		qHTS Assay for Promiscuous and Specific Inhibitors of Cruzain (without detergent)	Chain A, Crystal Structure Of Cruzain Covalently Bound To A Purine Nitrile[gi:281307097]	
1478	Inactive	Potency		qHTS Assay for Promiscuous and Specific Inhibitors of Cruzain (with detergent)	Chain A, Crystal Structure Of Cruzain Covalently Bound To A Purine Nitrile[gi:281307097]	
1478	Inactive	Potency		qHTS Assay for Promiscuous and Specific Inhibitors of Cruzain (with detergent)	Chain A, Crystal Structure Of Cruzain Covalently Bound To A Purine Nitrile[gi:281307097]	
1476	Inactive	Potency		qHTS Assay for Promiscuous and Specific Inhibitors of Cruzain (without detergent)	Chain A, Crystal Structure Of Cruzain Covalently Bound To A Purine Nitrile[gi:281307097]	

AID	Outcome	Activity Concentration Name	Activity Concentration [uM]	BioAssay	Target	PMID
2353	Inactive	Potency		qHTS Validation Assay for Inhibitors of RecQ-Like Dna Helicase 1 (RECQ1)	Chain A, Structure Of Human Recq-Like Helicase In Complex With A Dna Substrate[gi:282403581]	
2549	Inactive	Potency		qHTS Assay for Inhibitors of RecQ-Like Dna Helicase 1 (RECQ1)	Chain A, Structure Of Human Recq-Like Helicase In Complex With A Dna Substrate[gi:282403581]	
2549	Inactive	Potency		qHTS Assay for Inhibitors of RecQ-Like Dna Helicase 1 (RECQ1)	Chain A, Structure Of Human Recq-Like Helicase In Complex With A Dna Substrate[gi:282403581]	
1721	Inactive	Potency		qHTS Assay for Inhibitors of Leishmania Mexicana Pyruvate Kinase (LmPK)	pyruvate kinase [Leishmania mexicana mexicana][gi:290753097]	
1722	Inactive	Potency		qHTS Assay for Activators of Leishmania Mexicana Pyruvate Kinase (LmPK)	pyruvate kinase [Leishmania mexicana mexicana][gi:290753097]	
720516	Inactive	Potency		qHTS assay for small molecules that induce genotoxicity in human embryonic kidney cells expressing luciferase-tagged ATAD5: Summary	ATPase family AAA domain-containing protein 5[gi:296439460]	
651632	Inactive	Potency		qHTS assay for small molecules that induce genotoxicity in human embryonic kidney cells expressing luciferase-tagged ATAD5	ATPase family AAA domain-containing protein 5[gi:296439460]	
651632	Inactive	Potency		qHTS assay for small molecules that induce genotoxicity in human embryonic kidney cells expressing luciferase-tagged ATAD5	ATPase family AAA domain-containing protein 5[gi:296439460]	
720516	Inactive	Potency		qHTS assay for small molecules that induce genotoxicity in human embryonic kidney cells expressing luciferase-tagged ATAD5: Summary	ATPase family AAA domain-containing protein 5[gi:296439460]	
504423	Inactive			C-LANA FP assay Measured in Biochemical System Using Plate Reader - 2117-01_Inhibitor_SinglePoint_HTS_Activity	LANA [Human herpesvirus 8][gi:312275222]	

AID	Outcome	Activity Concentration Name	Activity Concentration [uM]	BioAssay	Target	PMID
1452	Inactive	Potency		qHTS Assay for Inhibitors of 12-hLO (12-human lipoxygenase)	arachidonate 12-lipoxygenase, 12S-type [Homo sapiens][gi:154426292]	
1452	Inactive	Potency		qHTS Assay for Inhibitors of 12-hLO (12-human lipoxygenase)	arachidonate 12-lipoxygenase, 12S-type [Homo sapiens][gi:154426292]	
2524	Inactive			uHTS Luminescent assay for identification of activators of human intestinal alkaline phosphatase	Alkaline phosphatase, intestinal [Homo sapiens][gi:124376142]	
2524	Inactive			uHTS Luminescent assay for identification of activators of human intestinal alkaline phosphatase	Alkaline phosphatase, intestinal [Homo sapiens][gi:124376142]	
2544	Inactive			uHTS Luminescent assay for identification of inhibitors of human intestinal alkaline phosphatase	Alkaline phosphatase, intestinal [Homo sapiens][gi:124376142]	
2544	Inactive			uHTS Luminescent assay for identification of inhibitors of human intestinal alkaline phosphatase	Alkaline phosphatase, intestinal [Homo sapiens][gi:124376142]	
518	Inactive	IC50		TNAP luminescent HTS assay	alkaline phosphatase, tissue-nonspecific isozyme isoform 1 precursor [Homo sapiens][gi:116734717]	
518	Inactive	IC50		TNAP luminescent HTS assay	alkaline phosphatase, tissue-nonspecific isozyme isoform 1 precursor [Homo sapiens][gi:116734717]	
813	Inactive			HTS identification of compounds activating TNAP at intermediate concentration of phosphate acceptor detected in luminescent assay	alkaline phosphatase, tissue-nonspecific isozyme isoform 1 precursor [Homo sapiens][gi:116734717]	
813	Inactive			HTS identification of compounds activating TNAP at intermediate concentration of phosphate acceptor detected in luminescent assay	alkaline phosphatase, tissue-nonspecific isozyme isoform 1 precursor [Homo sapiens][gi:116734717]	

AID	Outcome	Activity Concentration Name	Activity Concentration [uM]	BioAssay	Target	PMID
614	Inactive			HTS colorimetric detection of phosphate released in TNAP reaction	alkaline phosphatase, tissue-nonspecific isozyme isoform 1 precursor [Homo sapiens][gi:116734717]	
614	Inactive			HTS colorimetric detection of phosphate released in TNAP reaction	alkaline phosphatase, tissue-nonspecific isozyme isoform 1 precursor [Homo sapiens][gi:116734717]	
615	Inactive			HTS colorimetric detection of p-nitrophenol released in TNAP reaction	alkaline phosphatase, tissue-nonspecific isozyme isoform 1 precursor [Homo sapiens][gi:116734717]	
615	Inactive			HTS colorimetric detection of p-nitrophenol released in TNAP reaction	alkaline phosphatase, tissue-nonspecific isozyme isoform 1 precursor [Homo sapiens][gi:116734717]	
1135	Inactive			uHTS identification of compounds inhibiting TNAP at a high concentration of phosphate acceptor detected in a luminescent assay	alkaline phosphatase, tissue-nonspecific isozyme isoform 1 precursor [Homo sapiens][gi:116734717]	
1135	Inactive			uHTS identification of compounds inhibiting TNAP at a high concentration of phosphate acceptor detected in a luminescent assay	alkaline phosphatase, tissue-nonspecific isozyme isoform 1 precursor [Homo sapiens][gi:116734717]	
1136	Inactive			uHTS identification of compounds activating TNAP at a high concentration of phosphate acceptor detected in a luminescent assay	alkaline phosphatase, tissue-nonspecific isozyme isoform 1 precursor [Homo sapiens][gi:116734717]	
1136	Inactive			uHTS identification of compounds activating TNAP at a high concentration of phosphate acceptor detected in a luminescent assay	alkaline phosphatase, tissue-nonspecific isozyme isoform 1 precursor [Homo sapiens][gi:116734717]	
1012	Inactive			uHTS identification of TNAP inhibitors in the absence of phosphate acceptor performed in luminescent assay	alkaline phosphatase, tissue-nonspecific isozyme isoform 1 precursor [Homo sapiens][gi:116734717]	
1012	Inactive			uHTS identification of TNAP inhibitors in the absence of phosphate acceptor performed in luminescent assay	alkaline phosphatase, tissue-nonspecific isozyme isoform 1 precursor [Homo sapiens][gi:116734717]	

AID	Outcome	Activity Concentration Name	Activity Concentration [uM]	BioAssay	Target	PMID
1001	Inactive	EC50		uHTS identification of compounds activating TNAP in the absence of phosphate acceptor performed in luminescent assay	alkaline phosphatase, tissue-nonspecific isozyme isoform 1 precursor [Homo sapiens][gi:116734717]	
1001	Inactive	EC50		uHTS identification of compounds activating TNAP in the absence of phosphate acceptor performed in luminescent assay	alkaline phosphatase, tissue-nonspecific isozyme isoform 1 precursor [Homo sapiens][gi:116734717]	
489030	Inactive			uHTS Fluorescent assay for identification of inhibitors of Apaf-1	Apoptotic peptidase activating factor 1 [Homo sapiens][gi:187952397]	
489031	Inactive			uHTS Fluorescent assay for identification of activators of Apaf-1	Apoptotic peptidase activating factor 1 [Homo sapiens][gi:187952397]	
720559	Inactive	Potency		qHTS for compounds that reverse cellular toxicity of Amyloid beta (A-beta) peptide in yeast: LOPAC Validation Assay	Amyloid beta A4 protein[gi:112927]	
720559	Inactive	Potency		qHTS for compounds that reverse cellular toxicity of Amyloid beta (A-beta) peptide in yeast: LOPAC Validation Assay	Amyloid beta A4 protein[gi:112927]	
720559	Inactive	Potency		qHTS for compounds that reverse cellular toxicity of Amyloid beta (A-beta) peptide in yeast: LOPAC Validation Assay	Amyloid beta A4 protein[gi:112927]	
1276	Inactive			Primary screen for compounds that activate Alzheimer's amyloid precursor	amyloid precursor protein; APP [Homo sapiens][gi:257380]	
1276	Inactive			Primary screen for compounds that activate Alzheimer's amyloid precursor	amyloid precursor protein; APP [Homo sapiens][gi:257380]	
1276	Inactive			Primary screen for compounds that activate Alzheimer's amyloid precursor	amyloid precursor protein; APP [Homo sapiens][gi:257380]	
1285	Inactive			Primary screen for compounds that inhibit Alzheimer's amyloid precursor protein (APP) translation	amyloid precursor protein; APP [Homo sapiens][gi:257380]	

AID	Outcome	Activity Concentration Name	Activity Concentration [uM]	BioAssay	Target	PMID
1285	Inactive			Primary screen for compounds that inhibit Alzheimer's amyloid precursor protein (APP) translation	amyloid precursor protein; APP [Homo sapiens][gi:257380]	
1285	Inactive			Primary screen for compounds that inhibit Alzheimer's amyloid precursor protein (APP) translation	amyloid precursor protein; APP [Homo sapiens][gi:257380]	
623870	Inactive			ARNT-TAC3: AlphaScreen HTS to detect disruption of ARNT/TAC3 interactions Measured in Biochemical System Using Plate Reader - 2158-01_Inhibitor_SinglePoint_HTS_Activity	aryl hydrocarbon receptor nuclear translocator [Homo sapiens][gi:2702319]	
623870	Inactive			ARNT-TAC3: AlphaScreen HTS to detect disruption of ARNT/TAC3 interactions Measured in Biochemical System Using Plate Reader - 2158-01_Inhibitor_SinglePoint_HTS_Activity	aryl hydrocarbon receptor nuclear translocator [Homo sapiens][gi:2702319]	
504490	Inactive			Assay for Inhibitors of the beta-Arrestin-Adaptor Protein 2 Interaction That Mediate GPCR Degradation and Recycling	Arrestin, beta 1 [Homo sapiens][gi:13177715]	
504541	Inactive			Assay for Inhibitors of the beta-Arrestin-Adaptor Protein 2 Interaction for Validation Set	Arrestin, beta 1 [Homo sapiens][gi:13177715]	
485349	Inactive	Potency		qHTS Assay for Identifying a Potential Treatment of Ataxia-Telangiectasia	serine-protein kinase ATM [Homo sapiens][gi:71902540]	
485349	Inactive	Potency		qHTS Assay for Identifying a Potential Treatment of Ataxia-Telangiectasia	serine-protein kinase ATM [Homo sapiens][gi:71902540]	
2797	Inactive			Counterscreen for Oxytocin Receptor (OXTR) agonists: Fluorescence-based primary cell-based high throughput assay to identify agonists of the vasopressin 1 receptor (V1R)	vasopressin V1a receptor [Homo sapiens][gi:4502331]	
2797	Inactive			Counterscreen for Oxytocin Receptor (OXTR) agonists: Fluorescence-based primary cell-based high throughput assay to identify agonists of the vasopressin 1 receptor (V1R)	vasopressin V1a receptor [Homo sapiens][gi:4502331]	

AID	Outcome	Activity Concentration Name	Activity Concentration [uM]	BioAssay	Target	PMID
2797	Inactive			Counterscreen for Oxytocin Receptor (OXTR) agonists: Fluorescence-based primary cell-based high throughput assay to identify agonists of the vasopressin 1 receptor (V1R)	vasopressin V1a receptor [Homo sapiens][gi:4502331]	
950	Inactive			Multiplexed high-throughput screen for small molecule regulators of Bcl-2 family protein interactions, specifically Bim-Bcl-2.	Apoptosis regulator Bcl- [gi:231632]	
950	Inactive			Multiplexed high-throughput screen for small molecule regulators of Bcl-2 family protein interactions, specifically Bim-Bcl-2.	Apoptosis regulator Bcl- [gi:231632]	
1008	Inactive			Multiplexed high-throughput screen for small molecule regulators of Bcl-2 family protein interactions, specifically Bim-Bfl-1	bcl-2-related protein A1 isoform 1 [Homo sapiens][gi:4757840]	
1008	Inactive			Multiplexed high-throughput screen for small molecule regulators of Bcl-2 family protein interactions, specifically Bim-Bfl-1	bcl-2-related protein A1 isoform 1 [Homo sapiens][gi:4757840]	
1007	Inactive			Multiplexed high-throughput screen for small molecule regulators of Bcl-2 family protein interactions, specifically Bim-Bcl-XL.	bcl-xL [Homo sapiens][gi:510901]	
1007	Inactive			Multiplexed high-throughput screen for small molecule regulators of Bcl-2 family protein interactions, specifically Bim-Bcl-XL.	bcl-xL [Homo sapiens][gi:510901]	
1007	Inactive			Multiplexed high-throughput screen for small molecule regulators of Bcl-2 family protein interactions, specifically Bim-Bcl-XL.	bcl-xL [Homo sapiens][gi:510901]	
2129	Inactive			Primary biochemical high throughput screening assay to identify inhibitors of BCL2-related protein, long isoform (BCLXL).	bcl-xL [Homo sapiens][gi:510901]	
2129	Inactive			Primary biochemical high throughput screening assay to identify inhibitors of BCL2-related protein, long isoform (BCLXL).	bcl-xL [Homo sapiens][gi:510901]	
2129	Inactive			Primary biochemical high throughput screening assay to identify inhibitors of BCL2-related protein, long isoform (BCLXL).	bcl-xL [Homo sapiens][gi:510901]	

AID	Outcome	Activity Concentration Name	Activity Concentration [uM]	BioAssay	Target	PMID
952	Inactive			Multiplexed high-throughput screen for small molecule regulators of Bcl-2 family protein interactions, specifically Bim-Bcl-W.	Bcl-w [Homo sapiens][gi:1572493]	
952	Inactive			Multiplexed high-throughput screen for small molecule regulators of Bcl-2 family protein interactions, specifically Bim-Bcl-W.	Bcl-w [Homo sapiens][gi:1572493]	
1441	Inactive			Multiplexed high-throughput screen for small molecule regulators of RGS family protein interactions, specifically RGS16-Galphao.	guanine nucleotide-binding protein G(o) subunit alpha isoform a [Homo sapiens][gi:10567816]	
1441	Inactive			Multiplexed high-throughput screen for small molecule regulators of RGS family protein interactions, specifically RGS16-Galphao.	guanine nucleotide-binding protein G(o) subunit alpha isoform a [Homo sapiens][gi:10567816]	
1441	Inactive			Multiplexed high-throughput screen for small molecule regulators of RGS family protein interactions, specifically RGS16-Galphao.	guanine nucleotide-binding protein G(o) subunit alpha isoform a [Homo sapiens][gi:10567816]	
1423	Inactive			Multiplexed high-throughput screen for small molecule regulators of RGS family protein interactions, specifically RGS8-Galphao.	guanine nucleotide-binding protein G(o) subunit alpha isoform a [Homo sapiens][gi:10567816]	
1423	Inactive			Multiplexed high-throughput screen for small molecule regulators of RGS family protein interactions, specifically RGS8-Galphao.	guanine nucleotide-binding protein G(o) subunit alpha isoform a [Homo sapiens][gi:10567816]	
1423	Inactive			Multiplexed high-throughput screen for small molecule regulators of RGS family protein interactions, specifically RGS8-Galphao.	guanine nucleotide-binding protein G(o) subunit alpha isoform a [Homo sapiens][gi:10567816]	
1415	Inactive			Multiplexed high-throughput screen for small molecule regulators of RGS family protein interactions, specifically RGS4-Galphao.	guanine nucleotide-binding protein G(o) subunit alpha isoform a [Homo sapiens][gi:10567816]	
1415	Inactive			Multiplexed high-throughput screen for small molecule regulators of RGS family protein interactions, specifically RGS4-Galphao.	guanine nucleotide-binding protein G(o) subunit alpha isoform a [Homo sapiens][gi:10567816]	
1415	Inactive			Multiplexed high-throughput screen for small molecule regulators of RGS family protein interactions, specifically RGS4-Galphao.	guanine nucleotide-binding protein G(o) subunit alpha isoform a [Homo sapiens][gi:10567816]	

AID	Outcome	Activity Concentration Name	Activity Concentration [uM]	BioAssay	Target	PMID
624288	Inactive	Potency		qHTS for Antagonists of gsp, the Etiologic Mutation Responsible for Fibrous Dysplasia/McCune-Albright Syndrome: qHTS	Guanine nucleotide-binding protein G(s) subunit alpha isoforms short[gi:52000961]	
1861	Inactive			Fluorescence-based primary cell-based high throughput screening assay to identify antagonists of the G-protein coupled receptor 7 (GPR7).	neuropeptides B/W receptor 1 [Homo sapiens][gi:119607128]	
1861	Inactive			Fluorescence-based primary cell-based high throughput screening assay to identify antagonists of the G-protein coupled receptor 7 (GPR7).	neuropeptides B/W receptor 1 [Homo sapiens][gi:119607128]	
2058	Inactive	IC50		Image-Based HTS for Selective Antagonists of GPR35	G-protein coupled receptor 35 isoform a [Homo sapiens][gi:33695097]	
2058	Inactive	IC50		Image-Based HTS for Selective Antagonists of GPR35	G-protein coupled receptor 35 isoform a [Homo sapiens][gi:33695097]	
2058	Inactive	IC50		Image-Based HTS for Selective Antagonists of GPR35	G-protein coupled receptor 35 isoform a [Homo sapiens][gi:33695097]	
450	Inactive			GR-GFP Redistribution	glucocorticoid receptor isoform gamma [Homo sapiens][gi:66528677]	
450	Inactive			GR-GFP Redistribution	glucocorticoid receptor isoform gamma [Homo sapiens][gi:66528677]	
450	Inactive			GR-GFP Redistribution	glucocorticoid receptor isoform gamma [Homo sapiens][gi:66528677]	
450	Inactive			GR-GFP Redistribution	glucocorticoid receptor isoform gamma [Homo sapiens][gi:66528677]	
2650	Inactive			Luminescence Cell-Free Homogenous Primary HTS to Identify Inhibitors of GSK-3 alpha	GSK3A gene product [Homo sapiens][gi:49574532]	

AID	Outcome	Activity Concentration Name	Activity Concentration [uM]	BioAssay	Target	PMID
2650	Inactive			Luminescence Cell-Free Homogenous Primary HTS to Identify Inhibitors of GSK-3 alpha	GSK3A gene product [Homo sapiens][gi:49574532]	
2097	Inactive			Cell-Free Homogeneous Primary HTS to Identify Inhibitors of GSK3beta Activity	GSK3B gene product [Homo sapiens][gi:21361340]	
2097	Inactive			Cell-Free Homogeneous Primary HTS to Identify Inhibitors of GSK3beta Activity	GSK3B gene product [Homo sapiens][gi:21361340]	
2097	Inactive			Cell-Free Homogeneous Primary HTS to Identify Inhibitors of GSK3beta Activity	GSK3B gene product [Homo sapiens][gi:21361340]	
485270	Inactive			FRET-based cell-based primary high throughput screening assay to identify antagonists of the orexin 1 receptor (OX1R; HCRTR1)	HCRTR1 gene product [Homo sapiens][gi:222080095]	
485270	Inactive			FRET-based cell-based primary high throughput screening assay to identify antagonists of the orexin 1 receptor (OX1R; HCRTR1)	HCRTR1 gene product [Homo sapiens][gi:222080095]	
434989	Inactive			Fluorescence-based cell-based primary high throughput screening assay to identify antagonists of the orexin 1 receptor (OX1R; HCRTR1)	HCRTR1 gene product [Homo sapiens][gi:222080095]	
434989	Inactive			Fluorescence-based cell-based primary high throughput screening assay to identify antagonists of the orexin 1 receptor (OX1R; HCRTR1)	HCRTR1 gene product [Homo sapiens][gi:222080095]	
483	Inactive			Aggregation and Clearance of Mutant Huntingtin Protein	Huntingtin[gi:296434520]	
483	Inactive			Aggregation and Clearance of Mutant Huntingtin Protein	Huntingtin[gi:296434520]	
1688	Inactive	Potency		qHTS Multiplex Assay to Identify Dual Action Probes in a Cell Model of Huntington: Aggregate Formation (GFP)	huntingtin [Homo sapiens][gi:90903231]	

AID	Outcome	Activity Concentration Name	Activity Concentration [uM]	BioAssay	Target	PMID
1688	Inactive	Potency		qHTS Multiplex Assay to Identify Dual Action Probes in a Cell Model of Huntington: Aggregate Formation (GFP)	huntingtin [Homo sapiens][gi:90903231]	
1471	Inactive			qHTS Multiplex Assay to Identify Dual Action Probes in a Cell Model of Huntington: Cytoprotection (ATP)	huntingtin [Homo sapiens][gi:90903231]	
1471	Inactive			qHTS Multiplex Assay to Identify Dual Action Probes in a Cell Model of Huntington: Cytoprotection (ATP)	huntingtin [Homo sapiens][gi:90903231]	
1688	Inactive	Potency		qHTS Multiplex Assay to Identify Dual Action Probes in a Cell Model of Huntington: Aggregate Formation (GFP)	huntingtin [Homo sapiens][gi:90903231]	
1688	Inactive	Potency		qHTS Multiplex Assay to Identify Dual Action Probes in a Cell Model of Huntington: Aggregate Formation (GFP)	huntingtin [Homo sapiens][gi:90903231]	
894	Inactive	Potency		qHTS Assay for Inhibitors of HPGD (15-Hydroxyprostaglandin Dehydrogenase)	15-hydroxyprostaglandin dehydrogenase [NAD+] isoform 1 [Homo sapiens][gi:31542939]	
894	Inactive	Potency		qHTS Assay for Inhibitors of HPGD (15-Hydroxyprostaglandin Dehydrogenase)	15-hydroxyprostaglandin dehydrogenase [NAD+] isoform 1 [Homo sapiens][gi:31542939]	
894	Inactive	Potency		qHTS Assay for Inhibitors of HPGD (15-Hydroxyprostaglandin Dehydrogenase)	15-hydroxyprostaglandin dehydrogenase [NAD+] isoform 1 [Homo sapiens][gi:31542939]	
894	Inactive	Potency		qHTS Assay for Inhibitors of HPGD (15-Hydroxyprostaglandin Dehydrogenase)	15-hydroxyprostaglandin dehydrogenase [NAD+] isoform 1 [Homo sapiens][gi:31542939]	
894	Inactive	Potency		qHTS Assay for Inhibitors of HPGD (15-Hydroxyprostaglandin Dehydrogenase)	15-hydroxyprostaglandin dehydrogenase [NAD+] isoform 1 [Homo sapiens][gi:31542939]	
894	Inactive	Potency		qHTS Assay for Inhibitors of HPGD (15-Hydroxyprostaglandin Dehydrogenase)	15-hydroxyprostaglandin dehydrogenase [NAD+] isoform 1 [Homo sapiens][gi:31542939]	

AID	Outcome	Activity Concentration Name	Activity Concentration [uM]	BioAssay	Target	PMID
759	Inactive			HTS to identify specific small molecule inhibitors of Ras and Ras-related GTPases specifically Ras wildtype	ras protein [Homo sapiens][gi:190938]	
759	Inactive			HTS to identify specific small molecule inhibitors of Ras and Ras-related GTPases specifically Ras wildtype	ras protein [Homo sapiens][gi:190938]	
759	Inactive			HTS to identify specific small molecule inhibitors of Ras and Ras-related GTPases specifically Ras wildtype	ras protein [Homo sapiens][gi:190938]	
652257	Inactive			Primary biochemical fluorescence polarization-based high throughput screening assay to identify inhibitors of protein arginine methyltransferase 1 (PRMT1)	PRMT1 protein [Homo sapiens][gi:32425330]	
652257	Inactive			Primary biochemical fluorescence polarization-based high throughput screening assay to identify inhibitors of protein arginine methyltransferase 1 (PRMT1)	PRMT1 protein [Homo sapiens][gi:32425330]	
1203	Inactive			Primary cell-based high-throughput screening assay to identify transcriptional activators of heat shock protein 70 (Hsp70)	Heat shock 70kDa protein 1A [Homo sapiens][gi:12803275]	
1203	Inactive			Primary cell-based high-throughput screening assay to identify transcriptional activators of heat shock protein 70 (Hsp70)	Heat shock 70kDa protein 1A [Homo sapiens][gi:12803275]	
568	Inactive	IC50		High Throughput Screening Assay for Hsc70 Inhibitors	heat shock cognate 71 kDa protein isoform 1 [Homo sapiens][gi:5729877]	
568	Inactive	IC50		High Throughput Screening Assay for Hsc70 Inhibitors	heat shock cognate 71 kDa protein isoform 1 [Homo sapiens][gi:5729877]	
568	Inactive	IC50		High Throughput Screening Assay for Hsc70 Inhibitors	heat shock cognate 71 kDa protein isoform 1 [Homo sapiens][gi:5729877]	
1789	Inactive			Luminescence-based primary biochemical high throughput screening assay to identify inhibitors of the Heat Shock Protein 90 (HSP90)	HSP90AA1 protein [Homo sapiens][gi:83318444]	

AID	Outcome	Activity Concentration Name	Activity Concentration [uM]	BioAssay	Target	PMID
1789	Inactive			Luminescence-based primary biochemical high throughput screening assay to identify inhibitors of the Heat Shock Protein 90 (HSP90)	HSP90AA1 protein [Homo sapiens][gi:83318444]	
1789	Inactive			Luminescence-based primary biochemical high throughput screening assay to identify inhibitors of the Heat Shock Protein 90 (HSP90)	HSP90AA1 protein [Homo sapiens][gi:83318444]	
567	Inactive			Primary HTS assay for 5-Hydroxytryptamine (Serotonin) Receptor Subtype 1a (5HT1a) agonists	HTR1A gene product [Homo sapiens][gi:55956923]	
567	Inactive			Primary HTS assay for 5-Hydroxytryptamine (Serotonin) Receptor Subtype 1a (5HT1a) agonists	HTR1A gene product [Homo sapiens][gi:55956923]	
567	Inactive			Primary HTS assay for 5-Hydroxytryptamine (Serotonin) Receptor Subtype 1a (5HT1a) agonists	HTR1A gene product [Homo sapiens][gi:55956923]	
574	Inactive			Primary Cell Based High Throughput Screening Assay for Agonists of the 5-Hydroxytryptamine Receptor Subtype 1E (5HT1E)	5-hydroxytryptamine receptor 1E[gi:112822]	
574	Inactive			Primary Cell Based High Throughput Screening Assay for Agonists of the 5-Hydroxytryptamine Receptor Subtype 1E (5HT1E)	5-hydroxytryptamine receptor 1E[gi:112822]	
571	Inactive			Primary Cell Based High Throughput Screening Assay for Antagonists of the 5-Hydroxytryptamine Receptor Subtype 1E (5HT1E)	5-hydroxytryptamine receptor 1E[gi:112822]	
571	Inactive			Primary Cell Based High Throughput Screening Assay for Antagonists of the 5-Hydroxytryptamine Receptor Subtype 1E (5HT1E)	5-hydroxytryptamine receptor 1E[gi:112822]	
504692	Inactive			Counterscreen for agonists of OPRM1-OPRD1 heterodimerization: luminescence-based cell-based full-deck high throughput screening assay to identify agonists of 5-hydroxytryptamine (serotonin) 5A receptor (HTR5A)	HTR5A gene product [Homo sapiens][gi:13236497]	

AID	Outcome	Activity Concentration Name	Activity Concentration [uM]	BioAssay	Target	PMID
504692	Inactive			Counterscreen for agonists of OPRM1-OPRD1 heterodimerization: luminescence-based cell-based full-deck high throughput screening assay to identify agonists of 5-hydroxytryptamine (serotonin) 5A receptor (HTR5A)	HTR5A gene product [Homo sapiens][gi:13236497]	
504692	Inactive			Counterscreen for agonists of OPRM1-OPRD1 heterodimerization: luminescence-based cell-based full-deck high throughput screening assay to identify agonists of 5-hydroxytryptamine (serotonin) 5A receptor (HTR5A)	HTR5A gene product [Homo sapiens][gi:13236497]	
504634	Inactive			Counterscreen for inverse agonists of OPRM1-OPRD1 heterodimerization: luminescence-based cell-based full-deck high throughput screening assay to identify inverse agonists of 5-hydroxytryptamine (serotonin) 5A receptor (HTR5A)	HTR5A gene product [Homo sapiens][gi:13236497]	
504634	Inactive			Counterscreen for inverse agonists of OPRM1-OPRD1 heterodimerization: luminescence-based cell-based full-deck high throughput screening assay to identify inverse agonists of 5-hydroxytryptamine (serotonin) 5A receptor (HTR5A)	HTR5A gene product [Homo sapiens][gi:13236497]	
504634	Inactive			Counterscreen for inverse agonists of OPRM1-OPRD1 heterodimerization: luminescence-based cell-based full-deck high throughput screening assay to identify inverse agonists of 5-hydroxytryptamine (serotonin) 5A receptor (HTR5A)	HTR5A gene product [Homo sapiens][gi:13236497]	
434962	Inactive			Fluorescence polarization-based cell-based primary high throughput screening assay to identify inhibitors of insulin-degrading enzyme (IDE)	IDE gene product [Homo sapiens][gi:155969707]	
493087	Inactive			Fluorescence polarization-based cell-based primary high throughput screening assay to identify activators of insulin-degrading enzyme (IDE)	IDE gene product [Homo sapiens][gi:155969707]	

AID	Outcome	Activity Concentration Name	Activity Concentration [uM]	BioAssay	Target	PMID
686970	Inactive	Potency		qHTS for induction of synthetic lethality in tumor cells producing 2HG: qHTS for the HT-1080-NT fibrosarcoma cell line	IDH1 [Homo sapiens][gi:49168486]	
686970	Inactive	Potency		qHTS for induction of synthetic lethality in tumor cells producing 2HG: qHTS for the HT-1080-NT fibrosarcoma cell line	IDH1 [Homo sapiens][gi:49168486]	
686970	Inactive	Potency		qHTS for induction of synthetic lethality in tumor cells producing 2HG: qHTS for the HT-1080-NT fibrosarcoma cell line	IDH1 [Homo sapiens][gi:49168486]	
624101	Inactive			Development of IDH1/2 inhibitors (CTD2project) Measured in Biochemical System Using Plate Reader - 2107-01_Inhibitor_SinglePoint_HTS_Activity	Isocitrate dehydrogenase 1 (NADP+), soluble [Homo sapiens][gi:62203298]	
624101	Inactive			Development of IDH1/2 inhibitors (CTD2project) Measured in Biochemical System Using Plate Reader - 2107-01_Inhibitor_SinglePoint_HTS_Activity	Isocitrate dehydrogenase 1 (NADP+), soluble [Homo sapiens][gi:62203298]	
624101	Inactive			Development of IDH1/2 inhibitors (CTD2project) Measured in Biochemical System Using Plate Reader - 2107-01_Inhibitor_SinglePoint_HTS_Activity	Isocitrate dehydrogenase 1 (NADP+), soluble [Homo sapiens][gi:62203298]	
602179	Inactive	Potency		qHTS for Inhibitors of mutant isocitrate dehydrogenase 1 (IDH1): qHTS	isocitrate dehydrogenase 1 [Homo sapiens][gi:89573979]	
602179	Inactive	Potency		qHTS for Inhibitors of mutant isocitrate dehydrogenase 1 (IDH1): qHTS	isocitrate dehydrogenase 1 [Homo sapiens][gi:89573979]	
602179	Inactive	Potency		qHTS for Inhibitors of mutant isocitrate dehydrogenase 1 (IDH1): qHTS	isocitrate dehydrogenase 1 [Homo sapiens][gi:89573979]	
1296	Inactive			Primary screen for compounds that activate Insulin promoter activity in TRM-6 cells	proinsulin [Homo sapiens][gi:59036749]	
1296	Inactive			Primary screen for compounds that activate Insulin promoter activity in TRM-6 cells	proinsulin [Homo sapiens][gi:59036749]	

AID	Outcome	Activity Concentration Name	Activity Concentration [uM]	BioAssay	Target	PMID
1273	Inactive			Primary screen for compounds that inhibit Insulin promoter activity in TRM-6 cells	proinsulin [Homo sapiens][gi:59036749]	
1273	Inactive			Primary screen for compounds that inhibit Insulin promoter activity in TRM-6 cells	proinsulin [Homo sapiens][gi:59036749]	
2557	Inactive			HTS for Identification of VLA-4 Allosteric Modulators from MLPCN library	integrin alpha-4 precursor [Homo sapiens][gi:67191027]	
2557	Inactive			HTS for Identification of VLA-4 Allosteric Modulators from MLPCN library	integrin alpha-4 precursor [Homo sapiens][gi:67191027]	
528	Inactive			Allosteric Agonists for the VLA-4 Integrin	integrin alpha-4 precursor [Homo sapiens][gi:67191027]	
528	Inactive			Allosteric Agonists for the VLA-4 Integrin	integrin alpha-4 precursor [Homo sapiens][gi:67191027]	
529	Inactive			Allosteric Antagonists for the VLA-4 Integrin	integrin alpha-4 precursor [Homo sapiens][gi:67191027]	
529	Inactive			Allosteric Antagonists for the VLA-4 Integrin	integrin alpha-4 precursor [Homo sapiens][gi:67191027]	
576	Inactive			Auto-fluorescence of compounds effecting screening of VLA-4 Integrin	integrin alpha-4 precursor [Homo sapiens][gi:67191027]	
576	Inactive			Auto-fluorescence of compounds effecting screening of VLA-4 Integrin	integrin alpha-4 precursor [Homo sapiens][gi:67191027]	
1446	Inactive			Primary cell-based high throughput assay for inhibitors of the Janus kinase 2 mutant JAK2V617F	Janus kinase 2 (a protein tyrosine kinase) [Homo sapiens][gi:119579178]	

AID	Outcome	Activity Concentration Name	Activity Concentration [uM]	BioAssay	Target	PMID
1446	Inactive			Primary cell-based high throughput assay for inhibitors of the Janus kinase 2 mutant JAK2V617F	Janus kinase 2 (a protein tyrosine kinase) [Homo sapiens][gi:119579178]	
1446	Inactive			Primary cell-based high throughput assay for inhibitors of the Janus kinase 2 mutant JAK2V617F	Janus kinase 2 (a protein tyrosine kinase) [Homo sapiens][gi:119579178]	
488899	Inactive			MITF Measured in Cell-Based System Using Plate Reader - 2084-01_Inhibitor_SinglePoint_HTS_Activity	Microphthalmia-associated transcription factor [Homo sapiens][gi:40807040]	
488899	Inactive			MITF Measured in Cell-Based System Using Plate Reader - 2084-01_Inhibitor_SinglePoint_HTS_Activity	Microphthalmia-associated transcription factor [Homo sapiens][gi:40807040]	
2240	Inactive			Luminescence Cell-Based Primary HTS to Identify Inhibitors of MITF	microphthalmia-associated transcription factor isoform 1 [Homo sapiens][gi:38156699]	
2240	Inactive			Luminescence Cell-Based Primary HTS to Identify Inhibitors of MITF	microphthalmia-associated transcription factor isoform 1 [Homo sapiens][gi:38156699]	
2662	Inactive	Potency		qHTS Fluorescence Polarization Assay for Inhibitors of MLL CXXC domain - DNA interaction	MLL gene product [Homo sapiens][gi:56550039]	
2662	Inactive	Potency		qHTS Fluorescence Polarization Assay for Inhibitors of MLL CXXC domain - DNA interaction	MLL gene product [Homo sapiens][gi:56550039]	
651704	Inactive			Inhibition of the MLL-AF4-AF9 Interaction in Pediatric Leukemia Measured in Biochemical System Using Plate Reader - 2160-01_Inhibitor_SinglePoint_HTS_Activity	MLLT3 gene product [Homo sapiens][gi:156104889]	
570	Inactive			Primary biochemical high-throughput screening assay for inhibitors of Matrix Metalloproteinase 13 (MMP13) activity	matrix metalloproteinase 13 preproprotein [Homo sapiens][gi:4505209]	
570	Inactive			Primary biochemical high-throughput screening assay for inhibitors of Matrix Metalloproteinase 13 (MMP13) activity	matrix metalloproteinase 13 preproprotein [Homo sapiens][gi:4505209]	

AID	Outcome	Activity Concentration Name	Activity Concentration [uM]	BioAssay	Target	PMID
618	Inactive	EC50		Luminescent HTS for small molecule inhibitors of MT1-MMP transcription	matrix metalloproteinase 1 [Homo sapiens][gi:6690534]	
618	Inactive	EC50		Luminescent HTS for small molecule inhibitors of MT1-MMP transcription	matrix metalloproteinase 1 [Homo sapiens][gi:6690534]	
618	Inactive	EC50		Luminescent HTS for small molecule inhibitors of MT1-MMP transcription	matrix metalloproteinase 1 [Homo sapiens][gi:6690534]	
651647	Inactive			uHTS identification of inhibitors of MT1-MMP activation in a fluoresence assay	MMP14 gene product [Homo sapiens][gi:4826834]	
651647	Inactive			uHTS identification of inhibitors of MT1-MMP activation in a fluoresence assay	MMP14 gene product [Homo sapiens][gi:4826834]	
651647	Inactive			uHTS identification of inhibitors of MT1-MMP activation in a fluoresence assay	MMP14 gene product [Homo sapiens][gi:4826834]	
1220	Inactive	IC50		HTS identification of compounds inhibiting phosphomannose isomerase (PMI) via a fluorescence intensity assay using a high concentration of mannose 6-phosphate	MPI protein [Homo sapiens][gi:16878311]	
1220	Inactive	IC50		HTS identification of compounds inhibiting phosphomannose isomerase (PMI) via a fluorescence intensity assay using a high concentration of mannose 6-phosphate	MPI protein [Homo sapiens][gi:16878311]	
1209	Inactive	IC50		HTS identification of compounds inhibiting phosphomannose isomerase (PMI) via a fluorescence intensity assay.	MPI protein [Homo sapiens][gi:16878311]	
1209	Inactive	IC50		HTS identification of compounds inhibiting phosphomannose isomerase (PMI) via a fluorescence intensity assay.	MPI protein [Homo sapiens][gi:16878311]	
1214	Inactive			HTS identification of compounds activating phosphomannose isomerase (PMI) via a fluorescence intensity assay.	MPI protein [Homo sapiens][gi:16878311]	

AID	Outcome	Activity Concentration Name	Activity Concentration [uM]	BioAssay	Target	PMID
1214	Inactive			HTS identification of compounds activating phosphomannose isomerase (PMI) via a fluorescence intensity assay.	MPI protein [Homo sapiens][gi:16878311]	
1216	Inactive			HTS identification of compounds activating phosphomannose isomerase (PMI) via a fluorescence intensity assay using a near-saturating concentration of mannose 6-phosphat	MPI protein [Homo sapiens][gi:16878311]	
1216	Inactive			HTS identification of compounds activating phosphomannose isomerase (PMI) via a fluorescence intensity assay using a near-saturating concentration of mannose 6-phosphat	MPI protein [Homo sapiens][gi:16878311]	
799	Inactive			Identification of Molecular Probes that Activate MRP-1	ATP-binding cassette, sub-family C, member 1 isoform 1 [Homo sapiens][gi:134142337]	
799	Inactive			Identification of Molecular Probes that Activate MRP-1	ATP-binding cassette, sub-family C, member 1 isoform 1 [Homo sapiens][gi:134142337]	
493153	Inactive	Potency		Nrf2 qHTS screen for inhibitors: Validation	NFE2L2 gene product [Homo sapiens][gi:224028257]	
493153	Inactive	Potency		Nrf2 qHTS screen for inhibitors: Validation	NFE2L2 gene product [Homo sapiens][gi:224028257]	
493153	Inactive	Potency		Nrf2 qHTS screen for inhibitors: Validation	NFE2L2 gene product [Homo sapiens][gi:224028257]	
493153	Inactive	Potency		Nrf2 qHTS screen for inhibitors: Validation	NFE2L2 gene product [Homo sapiens][gi:224028257]	
504444	Inactive	Potency		Nrf2 qHTS screen for inhibitors	NFE2L2 gene product [Homo sapiens][gi:224028257]	

AID	Outcome	Activity Concentration Name	Activity Concentration [uM]	BioAssay	Target	PMID
504444	Inactive	Potency		Nrf2 qHTS screen for inhibitors	NFE2L2 gene product [Homo sapiens][gi:224028257]	
504444	Inactive	Potency		Nrf2 qHTS screen for inhibitors	NFE2L2 gene product [Homo sapiens][gi:224028257]	
504444	Inactive	Potency		Nrf2 qHTS screen for inhibitors	NFE2L2 gene product [Homo sapiens][gi:224028257]	
624149	Inactive	Potency		qHTS of Nrf2 Activators: LOPAC Validation	Nrf2 [Homo sapiens][gi:693842]	
624149	Inactive	Potency		qHTS of Nrf2 Activators: LOPAC Validation	Nrf2 [Homo sapiens][gi:693842]	
624149	Inactive	Potency		qHTS of Nrf2 Activators: LOPAC Validation	Nrf2 [Homo sapiens][gi:693842]	
624149	Inactive	Potency		qHTS of Nrf2 Activators: LOPAC Validation	Nrf2 [Homo sapiens][gi:693842]	
624171	Inactive	Potency		qHTS of Nrf2 Activators	Nrf2 [Homo sapiens][gi:693842]	
624171	Inactive	Potency		qHTS of Nrf2 Activators	Nrf2 [Homo sapiens][gi:693842]	
624171	Inactive	Potency		qHTS of Nrf2 Activators	Nrf2 [Homo sapiens][gi:693842]	
624171	Inactive	Potency		qHTS of Nrf2 Activators	Nrf2 [Homo sapiens][gi:693842]	

AID	Outcome	Activity Concentration Name	Activity Concentration [uM]	BioAssay	Target	PMID
1239	Inactive			High Throughput Screen to Identify Compounds that increase expression of NF-kB in Human Neuronal Cells - Primary Screen	NFKB1 gene product [Homo sapiens][gi:34577122]	
1239	Inactive			High Throughput Screen to Identify Compounds that increase expression of NF-kB in Human Neuronal Cells - Primary Screen	NFKB1 gene product [Homo sapiens][gi:34577122]	
1239	Inactive			High Throughput Screen to Identify Compounds that increase expression of NF-kB in Human Neuronal Cells - Primary Screen	NFKB1 gene product [Homo sapiens][gi:34577122]	
1239	Inactive			High Throughput Screen to Identify Compounds that increase expression of NF-kB in Human Neuronal Cells - Primary Screen	NFKB1 gene product [Homo sapiens][gi:34577122]	
485313	Inactive	Potency		qHTS Assay for NPC1 Promoter Activators	NPC1 gene product [Homo sapiens][gi:255652944]	
485313	Inactive	Potency		qHTS Assay for NPC1 Promoter Activators	NPC1 gene product [Homo sapiens][gi:255652944]	
1304	Inactive			Primary cell-based high-throughput screening assay for potentiators or agonists of NPY-Y1	NPY1R gene product [Homo sapiens][gi:4505445]	
1304	Inactive			Primary cell-based high-throughput screening assay for potentiators or agonists of NPY-Y1	NPY1R gene product [Homo sapiens][gi:4505445]	
1040	Inactive			Primary cell-based high-throughput screening assay for antagonists of NPY-Y1	NPY1R gene product [Homo sapiens][gi:4505445]	
1040	Inactive			Primary cell-based high-throughput screening assay for antagonists of NPY-Y1	NPY1R gene product [Homo sapiens][gi:4505445]	
1359	Inactive			Primary cell-based high-throughput screening assay for potentiators or agonists of NPY-Y2	NPY2R gene product [Homo sapiens][gi:4505447]	

AID	Outcome	Activity Concentration Name	Activity Concentration [uM]	BioAssay	Target	PMID
1359	Inactive			Primary cell-based high-throughput screening assay for potentiators or agonists of NPY-Y2	NPY2R gene product [Homo sapiens][gi:4505447]	
793	Inactive			Primary cell based high-throughput screening assay for antagonists of neuropeptide Y receptor Y2 (NPY-Y2)	NPY2R gene product [Homo sapiens][gi:4505447]	
793	Inactive			Primary cell based high-throughput screening assay for antagonists of neuropeptide Y receptor Y2 (NPY-Y2)	NPY2R gene product [Homo sapiens][gi:4505447]	
493036	Inactive			Image-Based HTS for Selective Agonists for NTR1	NTSR1 gene product [Homo sapiens][gi:110611243]	
493036	Inactive			Image-Based HTS for Selective Agonists for NTR1	NTSR1 gene product [Homo sapiens][gi:110611243]	
504357	Inactive			Luminescence-based cell-based primary high throughput screening assay to identify inverse agonists of heterodimerization of the mu 1 (OPRM1) and delta 1 (OPRD1) opioid receptors	OPRD1 gene product [Homo sapiens][gi:63477962]	
504357	Inactive			Luminescence-based cell-based primary high throughput screening assay to identify inverse agonists of heterodimerization of the mu 1 (OPRM1) and delta 1 (OPRD1) opioid receptors	OPRD1 gene product [Homo sapiens][gi:63477962]	
504326	Inactive			Luminescence-based cell-based primary high throughput screening assay to identify agonists of heterodimerization of the mu 1 (OPRM1) and delta 1 (OPRD1) opioid receptors	OPRD1 gene product [Homo sapiens][gi:63477962]	
504326	Inactive			Luminescence-based cell-based primary high throughput screening assay to identify agonists of heterodimerization of the mu 1 (OPRM1) and delta 1 (OPRD1) opioid receptors	OPRD1 gene product [Homo sapiens][gi:63477962]	

AID	Outcome	Activity Concentration Name	Activity Concentration [uM]	BioAssay	Target	PMID
1777	Inactive	EC50		uHTS identification of small molecule agonists of the kappa opioid receptor via a luminescent beta-arrestin assay	OPRK1 gene product [Homo sapiens][gi:39725940]	
1777	Inactive	EC50		uHTS identification of small molecule agonists of the kappa opioid receptor via a luminescent beta-arrestin assay	OPRK1 gene product [Homo sapiens][gi:39725940]	
1777	Inactive	EC50		uHTS identification of small molecule agonists of the kappa opioid receptor via a luminescent beta-arrestin assay	OPRK1 gene product [Homo sapiens][gi:39725940]	
1777	Inactive	EC50		uHTS identification of small molecule agonists of the kappa opioid receptor via a luminescent beta-arrestin assay	OPRK1 gene product [Homo sapiens][gi:39725940]	
1778	Inactive	IC50		uHTS identification of small molecule antagonists of the kappa opioid receptor via a luminescent beta-arrestin assay	OPRK1 gene product [Homo sapiens][gi:39725940]	
1778	Inactive	IC50		uHTS identification of small molecule antagonists of the kappa opioid receptor via a luminescent beta-arrestin assay	OPRK1 gene product [Homo sapiens][gi:39725940]	
1778	Inactive	IC50		uHTS identification of small molecule antagonists of the kappa opioid receptor via a luminescent beta-arrestin assay	OPRK1 gene product [Homo sapiens][gi:39725940]	
1778	Inactive	IC50		uHTS identification of small molecule antagonists of the kappa opioid receptor via a luminescent beta-arrestin assay	OPRK1 gene product [Homo sapiens][gi:39725940]	
2435	Inactive			Fluorescence-based primary cell-based high throughput screening assay to identify agonists of the Oxytocin Receptor (OXTR).	oxytocin receptor [Homo sapiens][gi:32307152]	
2435	Inactive			Fluorescence-based primary cell-based high throughput screening assay to identify agonists of the Oxytocin Receptor (OXTR).	oxytocin receptor [Homo sapiens][gi:32307152]	
2435	Inactive			Fluorescence-based primary cell-based high throughput screening assay to identify agonists of the Oxytocin Receptor (OXTR).	oxytocin receptor [Homo sapiens][gi:32307152]	

AID	Outcome	Activity Concentration Name	Activity Concentration [uM]	BioAssay	Target	PMID
2445	Inactive			Fluorescence-based primary cell-based high throughput screening assay to identify potentiators of Oxytocin Receptor (OXTR)	oxytocin receptor [Homo sapiens][gi:32307152]	
2445	Inactive			Fluorescence-based primary cell-based high throughput screening assay to identify potentiators of Oxytocin Receptor (OXTR)	oxytocin receptor [Homo sapiens][gi:32307152]	
2445	Inactive			Fluorescence-based primary cell-based high throughput screening assay to identify potentiators of Oxytocin Receptor (OXTR)	oxytocin receptor [Homo sapiens][gi:32307152]	
588391	Inactive			Turbidometric Biochemical Primary HTS to identify inhibitors of Protein Disulfide Isomerase Measured in Biochemical System Using Plate Reader - 2137-01_Inhibitor_SinglePoint_HTS_Activity	Prolyl 4-hydroxylase, beta polypeptide [Homo sapiens][gi:14790033]	
588391	Inactive			Turbidometric Biochemical Primary HTS to identify inhibitors of Protein Disulfide Isomerase Measured in Biochemical System Using Plate Reader - 2137-01_Inhibitor_SinglePoint_HTS_Activity	Prolyl 4-hydroxylase, beta polypeptide [Homo sapiens][gi:14790033]	
463115	Inactive			High throughput fluorescence intensity-based biochemical assay to screen for small molecule inhibitors of Furin conducted by the Pittsburgh Molecular Library Screening Center.	furin (paired basic amino acid cleaving enzyme), isoform CRA_a [Homo sapiens][gi:119622516]	
463115	Inactive			High throughput fluorescence intensity-based biochemical assay to screen for small molecule inhibitors of Furin conducted by the Pittsburgh Molecular Library Screening Center.	furin (paired basic amino acid cleaving enzyme), isoform CRA_a [Homo sapiens][gi:119622516]	
492953	Inactive			Fluorescence polarization-based primary biochemical high throughput screening assay to identify inhibitors of human platelet-activating factor acetylhydrolase 1b, catalytic subunit 2 (PAFAH1B2)	platelet-activating factor acetylhydrolase IB subunit beta isoform b [Homo sapiens][gi:296080766]	
492972	Inactive			Fluorescence polarization-based primary biochemical high throughput screening assay to identify inhibitors of human platelet-activating factor acetylhydrolase 1B, catalytic subunit 3 (PAFAH1B3)	platelet-activating factor acetylhydrolase IB subunit gamma [Homo sapiens][gi:225543099]	

AID	Outcome	Activity Concentration Name	Activity Concentration [uM]	BioAssay	Target	PMID
492956	Inactive			Fluorescence polarization-based primary biochemical high throughput screening assay to identify inhibitors of human platelet activating factor acetylhydrolase 2 (PAFAH2)	platelet-activating factor acetylhydrolase 2, cytoplasmic [Homo sapiens][gi:4758878]	
492956	Inactive			Fluorescence polarization-based primary biochemical high throughput screening assay to identify inhibitors of human platelet activating factor acetylhydrolase 2 (PAFAH2)	platelet-activating factor acetylhydrolase 2, cytoplasmic [Homo sapiens][gi:4758878]	
624263	Inactive	Potency		A Quantitative High throughput Screen to Identify Chemical Modulators of PINK1 Expression	Parkin [Homo sapiens][gi:3063388]	
485314	Inactive	Potency		qHTS Assay for Inhibitors of DNA Polymerase Beta	DNA polymerase beta [Homo sapiens][gi:4505931]	
485314	Inactive	Potency		qHTS Assay for Inhibitors of DNA Polymerase Beta	DNA polymerase beta [Homo sapiens][gi:4505931]	
485314	Inactive	Potency		qHTS Assay for Inhibitors of DNA Polymerase Beta	DNA polymerase beta [Homo sapiens][gi:4505931]	
485314	Inactive	Potency		qHTS Assay for Inhibitors of DNA Polymerase Beta	DNA polymerase beta [Homo sapiens][gi:4505931]	
588591	Inactive	Potency		qHTS for Inhibitors of Polymerase Eta	POLH gene product [Homo sapiens][gi:5729982]	
588591	Inactive	Potency		qHTS for Inhibitors of Polymerase Eta	POLH gene product [Homo sapiens][gi:5729982]	
588591	Inactive	Potency		qHTS for Inhibitors of Polymerase Eta	POLH gene product [Homo sapiens][gi:5729982]	
588591	Inactive	Potency		qHTS for Inhibitors of Polymerase Eta	POLH gene product [Homo sapiens][gi:5729982]	

AID	Outcome	Activity Concentration Name	Activity Concentration [uM]	BioAssay	Target	PMID
631	Inactive			Primary biochemical High Throughput Screening assay for agonists of the steroid receptor coactivator 1 (SRC-1) recruitment by the peroxisome proliferator-activated receptor gamma (PPARgamma)	peroxisome proliferator-activated receptor gamma isoform 2 [Homo sapiens][gi:20336229]	
631	Inactive			Primary biochemical High Throughput Screening assay for agonists of the steroid receptor coactivator 1 (SRC-1) recruitment by the peroxisome proliferator-activated receptor gamma (PPARgamma)	peroxisome proliferator-activated receptor gamma isoform 2 [Homo sapiens][gi:20336229]	
631	Inactive			Primary biochemical High Throughput Screening assay for agonists of the steroid receptor coactivator 1 (SRC-1) recruitment by the peroxisome proliferator-activated receptor gamma (PPARgamma)	peroxisome proliferator-activated receptor gamma isoform 2 [Homo sapiens][gi:20336229]	
631	Inactive			Primary biochemical High Throughput Screening assay for agonists of the steroid receptor coactivator 1 (SRC-1) recruitment by the peroxisome proliferator-activated receptor gamma (PPARgamma)	peroxisome proliferator-activated receptor gamma isoform 2 [Homo sapiens][gi:20336229]	
731	Inactive			Primary biochemical High Throughput Screening assay for agonists of the steroid receptor coactivator 3 (SRC-3) recruitment by the peroxisome proliferator-activated receptor gamma (PPARgamma)	peroxisome proliferator-activated receptor gamma isoform 2 [Homo sapiens][gi:20336229]	
731	Inactive			Primary biochemical High Throughput Screening assay for agonists of the steroid receptor coactivator 3 (SRC-3) recruitment by the peroxisome proliferator-activated receptor gamma (PPARgamma)	peroxisome proliferator-activated receptor gamma isoform 2 [Homo sapiens][gi:20336229]	
731	Inactive			Primary biochemical High Throughput Screening assay for agonists of the steroid receptor coactivator 3 (SRC-3) recruitment by the peroxisome proliferator-activated receptor gamma (PPARgamma)	peroxisome proliferator-activated receptor gamma isoform 2 [Homo sapiens][gi:20336229]	
731	Inactive			Primary biochemical High Throughput Screening assay for agonists of the steroid receptor coactivator 3 (SRC-3) recruitment by the peroxisome proliferator-activated receptor gamma (PPARgamma)	peroxisome proliferator-activated receptor gamma isoform 2 [Homo sapiens][gi:20336229]	

AID	Outcome	Activity Concentration Name	Activity Concentration [uM]	BioAssay	Target	PMID
1032	Inactive			Primary biochemical High Throughput Screening assay for agonists of the steroid receptor coactivator 2 (SRC-2) recruitment by the peroxisome proliferator-activated receptor gamma (PPARgamma)	peroxisome proliferator-activated receptor gamma isoform 2 [Homo sapiens][gi:20336229]	
1032	Inactive			Primary biochemical High Throughput Screening assay for agonists of the steroid receptor coactivator 2 (SRC-2) recruitment by the peroxisome proliferator-activated receptor gamma (PPARgamma)	peroxisome proliferator-activated receptor gamma isoform 2 [Homo sapiens][gi:20336229]	
1032	Inactive			Primary biochemical High Throughput Screening assay for agonists of the steroid receptor coactivator 2 (SRC-2) recruitment by the peroxisome proliferator-activated receptor gamma (PPARgamma)	peroxisome proliferator-activated receptor gamma isoform 2 [Homo sapiens][gi:20336229]	
1032	Inactive			Primary biochemical High Throughput Screening assay for agonists of the steroid receptor coactivator 2 (SRC-2) recruitment by the peroxisome proliferator-activated receptor gamma (PPARgamma)	peroxisome proliferator-activated receptor gamma isoform 2 [Homo sapiens][gi:20336229]	
1048	Inactive			Measurement of TR-FRET detection format artefact in the screen for agonists of steroid receptor coactivator 3 (SRC-3) recruitment by the peroxisome proliferator-activated receptor gamma (PPARgamma)	peroxisome proliferator-activated receptor gamma isoform 2 [Homo sapiens][gi:20336229]	
1048	Inactive			Measurement of TR-FRET detection format artefact in the screen for agonists of steroid receptor coactivator 3 (SRC-3) recruitment by the peroxisome proliferator-activated receptor gamma (PPARgamma)	peroxisome proliferator-activated receptor gamma isoform 2 [Homo sapiens][gi:20336229]	
1048	Inactive			Measurement of TR-FRET detection format artefact in the screen for agonists of steroid receptor coactivator 3 (SRC-3) recruitment by the peroxisome proliferator-activated receptor gamma (PPARgamma)	peroxisome proliferator-activated receptor gamma isoform 2 [Homo sapiens][gi:20336229]	
1048	Inactive			Measurement of TR-FRET detection format artefact in the screen for agonists of steroid receptor coactivator 3 (SRC-3) recruitment by the peroxisome proliferator-activated receptor gamma (PPARgamma)	peroxisome proliferator-activated receptor gamma isoform 2 [Homo sapiens][gi:20336229]	

AID	Outcome	Activity Concentration Name	Activity Concentration [uM]	BioAssay	Target	PMID
1049	Inactive			Measurement of TR-FRET detection format artefact in the screen for agonists of steroid receptor coactivator 2 (SRC-2) recruitment by the peroxisome proliferator-activated receptor gamma (PPARgamma)	peroxisome proliferator-activated receptor gamma isoform 2 [Homo sapiens][gi:20336229]	
1049	Inactive			Measurement of TR-FRET detection format artefact in the screen for agonists of steroid receptor coactivator 2 (SRC-2) recruitment by the peroxisome proliferator-activated receptor gamma (PPARgamma)	peroxisome proliferator-activated receptor gamma isoform 2 [Homo sapiens][gi:20336229]	
1049	Inactive			Measurement of TR-FRET detection format artefact in the screen for agonists of steroid receptor coactivator 2 (SRC-2) recruitment by the peroxisome proliferator-activated receptor gamma (PPARgamma)	peroxisome proliferator-activated receptor gamma isoform 2 [Homo sapiens][gi:20336229]	
1049	Inactive			Measurement of TR-FRET detection format artefact in the screen for agonists of steroid receptor coactivator 2 (SRC-2) recruitment by the peroxisome proliferator-activated receptor gamma (PPARgamma)	peroxisome proliferator-activated receptor gamma isoform 2 [Homo sapiens][gi:20336229]	
1051	Inactive			Measurement of TR-FRET detection format artefact in the screen for agonists of steroid receptor coactivator 1 (SRC-1) recruitment by the peroxisome proliferator-activated receptor gamma (PPARgamma)	peroxisome proliferator-activated receptor gamma isoform 2 [Homo sapiens][gi:20336229]	
1051	Inactive			Measurement of TR-FRET detection format artefact in the screen for agonists of steroid receptor coactivator 1 (SRC-1) recruitment by the peroxisome proliferator-activated receptor gamma (PPARgamma)	peroxisome proliferator-activated receptor gamma isoform 2 [Homo sapiens][gi:20336229]	
1051	Inactive			Measurement of TR-FRET detection format artefact in the screen for agonists of steroid receptor coactivator 1 (SRC-1) recruitment by the peroxisome proliferator-activated receptor gamma (PPARgamma)	peroxisome proliferator-activated receptor gamma isoform 2 [Homo sapiens][gi:20336229]	
1051	Inactive			Measurement of TR-FRET detection format artefact in the screen for agonists of steroid receptor coactivator 1 (SRC-1) recruitment by the peroxisome proliferator-activated receptor gamma (PPARgamma)	peroxisome proliferator-activated receptor gamma isoform 2 [Homo sapiens][gi:20336229]	

AID	Outcome	Activity Concentration Name	Activity Concentration [uM]	BioAssay	Target	PMID
2235	Inactive			Counterscreen for inhibitors of PP5: fluorescence-based biochemical high throughput primary assay to identify inhibitors of Protein Phosphatase 1 (PP1).	PPP1CA gene product [Homo sapiens][gi:56790945]	
1987	Inactive			Fluorescence-based primary biochemical high throughput screening assay to identify inhibitors of Protein Phosphatase 5 (PP5).	PPP5C protein [Homo sapiens][gi:37589898]	
1987	Inactive			Fluorescence-based primary biochemical high throughput screening assay to identify inhibitors of Protein Phosphatase 5 (PP5).	PPP5C protein [Homo sapiens][gi:37589898]	
524	Inactive			Primary biochemical high-throughput screening assay for inhibitors of protein kinase A (PKA) activity	cAMP-dependent protein kinase catalytic subunit alpha isoform 1 [Homo sapiens][gi:4506055]	
524	Inactive			Primary biochemical high-throughput screening assay for inhibitors of protein kinase A (PKA) activity	cAMP-dependent protein kinase catalytic subunit alpha isoform 1 [Homo sapiens][gi:4506055]	
504700	Inactive			Fluorescence polarization-based biochemical primary high throughput screening assay to identify activators of the Protein Kinase A-R2B (PKA-R2B) complex	cAMP-dependent protein kinase catalytic subunit beta isoform 3 [Homo sapiens][gi:46909587]	
504700	Inactive			Fluorescence polarization-based biochemical primary high throughput screening assay to identify activators of the Protein Kinase A-R2B (PKA-R2B) complex	cAMP-dependent protein kinase catalytic subunit beta isoform 3 [Homo sapiens][gi:46909587]	
504700	Inactive			Fluorescence polarization-based biochemical primary high throughput screening assay to identify activators of the Protein Kinase A-R2B (PKA-R2B) complex	cAMP-dependent protein kinase catalytic subunit beta isoform 3 [Homo sapiens][gi:46909587]	
797	Inactive			Fluorescence polarization assay for PKD inhibitors	serine/threonine-protein kinase D1 [Homo sapiens][gi:115529463]	
797	Inactive			Fluorescence polarization assay for PKD inhibitors	serine/threonine-protein kinase D1 [Homo sapiens][gi:115529463]	
1454	Inactive	Potency		qHTS Assay for Inhibitors of the ERK Signaling Pathway using a Homogeneous Screening Assay; Stimulation with EGF	mitogen-activated protein kinase 1 [Homo sapiens][gi:66932916]	

AID	Outcome	Activity Concentration Name	Activity Concentration [uM]	BioAssay	Target	PMID
1454	Inactive	Potency		qHTS Assay for Inhibitors of the ERK Signaling Pathway using a Homogeneous Screening Assay; Stimulation with EGF	mitogen-activated protein kinase 1 [Homo sapiens][gi:66932916]	
1454	Inactive	Potency		qHTS Assay for Inhibitors of the ERK Signaling Pathway using a Homogeneous Screening Assay; Stimulation with EGF	mitogen-activated protein kinase 1 [Homo sapiens][gi:66932916]	
1454	Inactive	Potency		qHTS Assay for Inhibitors of the ERK Signaling Pathway using a Homogeneous Screening Assay; Stimulation with EGF	mitogen-activated protein kinase 1 [Homo sapiens][gi:66932916]	
1454	Inactive	Potency		qHTS Assay for Inhibitors of the ERK Signaling Pathway using a Homogeneous Screening Assay; Stimulation with EGF	mitogen-activated protein kinase 1 [Homo sapiens][gi:66932916]	
1454	Inactive	Potency		qHTS Assay for Inhibitors of the ERK Signaling Pathway using a Homogeneous Screening Assay; Stimulation with EGF	mitogen-activated protein kinase 1 [Homo sapiens][gi:66932916]	
746	Inactive			Primary biochemical high-throughput screening assay for inhibitors of the c-Jun N-Terminal Kinase 3 (JNK3)	Mitogen-activated protein kinase 10[gi:2507196]	
746	Inactive			Primary biochemical high-throughput screening assay for inhibitors of the c-Jun N-Terminal Kinase 3 (JNK3)	Mitogen-activated protein kinase 10[gi:2507196]	
652039	Inactive			Fluorescence Intensity-based biochemical primary high throughput screening assay to identify activators of kallikrein-7 (K7) zymogen	KLK7 gene product [Homo sapiens][gi:21327705]	
652039	Inactive			Fluorescence Intensity-based biochemical primary high throughput screening assay to identify activators of kallikrein-7 (K7) zymogen	KLK7 gene product [Homo sapiens][gi:21327705]	
2417	Inactive			High Content Assay for Compounds that inhibit the Assembly of the Perinucleolar Compartment	polypyrimidine tract-binding protein 1 isoform a [Homo sapiens][gi:4506243]	
940	Inactive			Modulators of the EP2 prostaglandin E2 receptor - Primary Screening	prostaglandin E receptor 2 (subtype EP2), 53kDa [Homo sapiens][gi:31881630]	

AID	Outcome	Activity Concentration Name	Activity Concentration [uM]	BioAssay	Target	PMID
940	Inactive			Modulators of the EP2 prostaglandin E2 receptor - Primary Screening	prostaglandin E receptor 2 (subtype EP2), 53kDa [Homo sapiens][gi:31881630]	
1422	Inactive			Inhibitors of the EP2 Prostaglandin E2 Receptor - Primary Screen	prostaglandin E receptor 2 (subtype EP2), 53kDa [Homo sapiens][gi:31881630]	
1422	Inactive			Inhibitors of the EP2 Prostaglandin E2 Receptor - Primary Screen	prostaglandin E receptor 2 (subtype EP2), 53kDa [Homo sapiens][gi:31881630]	
940	Inactive			Modulators of the EP2 prostaglandin E2 receptor - Primary Screening	prostaglandin E receptor 2 (subtype EP2), 53kDa [Homo sapiens][gi:31881630]	
940	Inactive			Modulators of the EP2 prostaglandin E2 receptor - Primary Screening	prostaglandin E receptor 2 (subtype EP2), 53kDa [Homo sapiens][gi:31881630]	
1422	Inactive			Inhibitors of the EP2 Prostaglandin E2 Receptor - Primary Screen	prostaglandin E receptor 2 (subtype EP2), 53kDa [Homo sapiens][gi:31881630]	
1422	Inactive			Inhibitors of the EP2 Prostaglandin E2 Receptor - Primary Screen	prostaglandin E receptor 2 (subtype EP2), 53kDa [Homo sapiens][gi:31881630]	
940	Inactive			Modulators of the EP2 prostaglandin E2 receptor - Primary Screening	prostaglandin E receptor 2 (subtype EP2), 53kDa [Homo sapiens][gi:31881630]	
940	Inactive			Modulators of the EP2 prostaglandin E2 receptor - Primary Screening	prostaglandin E receptor 2 (subtype EP2), 53kDa [Homo sapiens][gi:31881630]	
1422	Inactive			Inhibitors of the EP2 Prostaglandin E2 Receptor - Primary Screen	prostaglandin E receptor 2 (subtype EP2), 53kDa [Homo sapiens][gi:31881630]	
1422	Inactive			Inhibitors of the EP2 Prostaglandin E2 Receptor - Primary Screen	prostaglandin E receptor 2 (subtype EP2), 53kDa [Homo sapiens][gi:31881630]	

AID	Outcome	Activity Concentration Name	Activity Concentration [uM]	BioAssay	Target	PMID
521	Inactive	IC50		HTS Discovery of Chemical Inhibitors of HePTP, a Leukemia Target	tyrosine-protein phosphatase non-receptor type 7 isoform 2 [Homo sapiens][gi:18375660]	
521	Inactive	IC50		HTS Discovery of Chemical Inhibitors of HePTP, a Leukemia Target	tyrosine-protein phosphatase non-receptor type 7 isoform 2 [Homo sapiens][gi:18375660]	
521	Inactive	IC50		HTS Discovery of Chemical Inhibitors of HePTP, a Leukemia Target	tyrosine-protein phosphatase non-receptor type 7 isoform 2 [Homo sapiens][gi:18375660]	
1530	Inactive			Multiplex HTS Assay for Inhibitors of MEK Kinase PB1 Domains, specifically MEK5 MEK Kinase 2 mutant	mitogen-activated protein kinase kinase kinase kinase 2 [Homo sapiens][gi:22035600]	
1530	Inactive			Multiplex HTS Assay for Inhibitors of MEK Kinase PB1 Domains, specifically MEK5 MEK Kinase 2 mutant	mitogen-activated protein kinase kinase kinase kinase 2 [Homo sapiens][gi:22035600]	
1531	Inactive			Multiplex HTS Assay for Inhibitors of MEK Kinase PB1 Domains, specifically MEK5 binding to MEK Kinase 2 Wildtype	mitogen-activated protein kinase kinase kinase kinase 2 [Homo sapiens][gi:22035600]	
1531	Inactive			Multiplex HTS Assay for Inhibitors of MEK Kinase PB1 Domains, specifically MEK5 binding to MEK Kinase 2 Wildtype	mitogen-activated protein kinase kinase kinase kinase 2 [Homo sapiens][gi:22035600]	
757	Inactive			HTS to identify specific small molecule inhibitors of Ras and Ras-related GTPases specifically Rac wildtype	Rac1 protein [Homo sapiens][gi:8574038]	
757	Inactive			HTS to identify specific small molecule inhibitors of Ras and Ras-related GTPases specifically Rac wildtype	Rac1 protein [Homo sapiens][gi:8574038]	
764	Inactive			HTS to identify specific small molecule inhibitors of Ras and Ras-related GTPases specifically Rac activated mutant	Rac1 protein [Homo sapiens][gi:8574038]	
764	Inactive			HTS to identify specific small molecule inhibitors of Ras and Ras-related GTPases specifically Rac activated mutant	Rac1 protein [Homo sapiens][gi:8574038]	

AID	Outcome	Activity Concentration Name	Activity Concentration [uM]	BioAssay	Target	PMID
1385	Inactive			Homologous recombination - Rad 51	RAD51 [Homo sapiens][gi:49168602]	
1385	Inactive			Homologous recombination - Rad 51	RAD51 [Homo sapiens][gi:49168602]	
651710	Inactive			FRET-based HTS for detection of RAD52 Inhibitors Measured in Biochemical System Using Plate Reader - 7018-01_Inhibitor_SinglePoint_HTS_Activity_Set2	RAD52 gene product [Homo sapiens][gi:109637798]	
651660	Inactive			FRET-based HTS for detection of RAD52 Inhibitors Measured in Biochemical System Using Plate Reader - 7018-01_Inhibitor_SinglePoint_HTS_Activity	RAD52 gene product [Homo sapiens][gi:109637798]	
651724	Inactive			qHTS Assay for Inhibitors of the CtBP/E1A Interaction	CtBP interacting protein CtIP [Homo sapiens][gi:1730321]	
438	Inactive			Cellular assay for TNF alpha induced NFkappaB translocation	v-rel reticuloendotheliosis viral oncogene homolog A isoform 1 [Homo sapiens][gi:223468676]	
438	Inactive			Cellular assay for TNF alpha induced NFkappaB translocation	v-rel reticuloendotheliosis viral oncogene homolog A isoform 1 [Homo sapiens][gi:223468676]	
504845	Inactive	Potency		Inhibitors of Regulator of G Protein Signaling (RGS) 4: qHTS	regulator of G-protein signaling 4 [Homo sapiens][gi:86301163]	
504845	Inactive	Potency		Inhibitors of Regulator of G Protein Signaling (RGS) 4: qHTS	regulator of G-protein signaling 4 [Homo sapiens][gi:86301163]	
504845	Inactive	Potency		Inhibitors of Regulator of G Protein Signaling (RGS) 4: qHTS	regulator of G-protein signaling 4 [Homo sapiens][gi:86301163]	
504845	Inactive	Potency		Inhibitors of Regulator of G Protein Signaling (RGS) 4: qHTS	regulator of G-protein signaling 4 [Homo sapiens][gi:86301163]	

AID	Outcome	Activity Concentration Name	Activity Concentration [uM]	BioAssay	Target	PMID
504845	Inactive	Potency		Inhibitors of Regulator of G Protein Signaling (RGS) 4: qHTS	regulator of G-protein signaling 4 [Homo sapiens][gi:86301163]	
504845	Inactive	Potency		Inhibitors of Regulator of G Protein Signaling (RGS) 4: qHTS	regulator of G-protein signaling 4 [Homo sapiens][gi:86301163]	
463165	Inactive			Primary cell-based high-throughput screening assay for identification of compounds that inhibit regulator of G-protein signaling 4 (RGS4)	RGS4 gene product [Homo sapiens][gi:5032039]	
463165	Inactive			Primary cell-based high-throughput screening assay for identification of compounds that inhibit regulator of G-protein signaling 4 (RGS4)	RGS4 gene product [Homo sapiens][gi:5032039]	
463165	Inactive			Primary cell-based high-throughput screening assay for identification of compounds that inhibit regulator of G-protein signaling 4 (RGS4)	RGS4 gene product [Homo sapiens][gi:5032039]	
463111	Inactive			Primary cell-based high-throughput screening assay for identification of compounds that potentiate/activate regulator of G-protein signaling 4 (RGS4)	RGS4 gene product [Homo sapiens][gi:5032039]	
463111	Inactive			Primary cell-based high-throughput screening assay for identification of compounds that potentiate/activate regulator of G-protein signaling 4 (RGS4)	RGS4 gene product [Homo sapiens][gi:5032039]	
463111	Inactive			Primary cell-based high-throughput screening assay for identification of compounds that potentiate/activate regulator of G-protein signaling 4 (RGS4)	RGS4 gene product [Homo sapiens][gi:5032039]	
1439	Inactive			Multiplexed high-throughput screen for small molecule regulators of RGS family protein interactions, specifically RGS7-Galphao.	RGS7 [Homo sapiens][gi:1166512]	
880	Inactive			qHTS Assay for Inhibitors of RGS12 GoLoco Motif Activity (Red Fluorophore)	RGS12 [Homo sapiens][gi:3290016]	

AID	Outcome	Activity Concentration Name	Activity Concentration [uM]	BioAssay	Target	PMID
880	Inactive			qHTS Assay for Inhibitors of RGS12 GoLoco Motif Activity (Red Fluorophore)	RGS12 [Homo sapiens][gi:3290016]	
560	Inactive			Primary Cell-based High Throughput Screening assay for activators of the Retinoic Acid Receptor-related orphan receptor A (RORA)	Nuclear receptor ROR-alpha[gi:548814]	
560	Inactive			Primary Cell-based High Throughput Screening assay for activators of the Retinoic Acid Receptor-related orphan receptor A (RORA)	Nuclear receptor ROR-alpha[gi:548814]	
560	Inactive			Primary Cell-based High Throughput Screening assay for activators of the Retinoic Acid Receptor-related orphan receptor A (RORA)	Nuclear receptor ROR-alpha[gi:548814]	
560	Inactive			Primary Cell-based High Throughput Screening assay for activators of the Retinoic Acid Receptor-related orphan receptor A (RORA)	Nuclear receptor ROR-alpha[gi:548814]	
561	Inactive			Primary Cell-based High Throughput Screening assay for inhibitors of the Retinoic Acid Receptor-related orphan receptor A (RORA)	Nuclear receptor ROR-alpha[gi:548814]	
561	Inactive			Primary Cell-based High Throughput Screening assay for inhibitors of the Retinoic Acid Receptor-related orphan receptor A (RORA)	Nuclear receptor ROR-alpha[gi:548814]	
561	Inactive			Primary Cell-based High Throughput Screening assay for inhibitors of the Retinoic Acid Receptor-related orphan receptor A (RORA)	Nuclear receptor ROR-alpha[gi:548814]	
561	Inactive			Primary Cell-based High Throughput Screening assay for inhibitors of the Retinoic Acid Receptor-related orphan receptor A (RORA)	Nuclear receptor ROR-alpha[gi:548814]	
652163	Inactive			S100A4: HTS Measured in Biochemical System Using Plate Reader - 7045-01_Inhibitor_SinglePoint_HTS_Activity	S100A4 [Homo sapiens][gi:47496637]	

AID	Outcome	Activity Concentration Name	Activity Concentration [uM]	BioAssay	Target	PMID
588378	Inactive	Potency		qHTS for Inhibitors of ATXN expression: Validation	ATXN2 gene product [Homo sapiens][gi:171543895]	
651635	Inactive	Potency		qHTS for Inhibitors of ATXN expression	ATXN2 gene product [Homo sapiens][gi:171543895]	
651635	Inactive	Potency		qHTS for Inhibitors of ATXN expression	ATXN2 gene product [Homo sapiens][gi:171543895]	
651725	Inactive			qHTS Assay for Inhibitors of the Six1/Eya2 Interaction	six1 [Homo sapiens][gi:1246761]	
449768	Inactive			High Throughput Screening for Cocaine Antagonists: Primary Screen	dopamine transporter [Homo sapiens][gi:7108463]	
449768	Inactive			High Throughput Screening for Cocaine Antagonists: Primary Screen	dopamine transporter [Homo sapiens][gi:7108463]	
449768	Inactive			High Throughput Screening for Cocaine Antagonists: Primary Screen	dopamine transporter [Homo sapiens][gi:7108463]	
449768	Inactive			High Throughput Screening for Cocaine Antagonists: Primary Screen	dopamine transporter [Homo sapiens][gi:7108463]	
652017	Inactive			Luminescence-based cell-based primary high throughput screening assay to identify activators of the function of SWI/SNF related, matrix associated, actin dependent regulator of chromatin, subfamily a, member 2 (SMARCA2, BRM)	SWI/SNF related, matrix associated, actin dependent regulator of chromatin, subfamily a, member 2, i[gi:119579215]	
504364	Inactive	Potency		Validation screen for small molecules that induce DNA re-replication in SW480 colon adenocarcinoma cells	GMNN gene product [Homo sapiens][gi:7705682]	

AID	Outcome	Activity Concentration Name	Activity Concentration [uM]	BioAssay	Target	PMID
463097	Inactive	Potency		Validation screen for small molecules that induce DNA re-replication in MCF 10A normal breast cells	GMNN gene product [Homo sapiens][gi:7705682]	
624296	Inactive	Potency		A quantitative high throughput screen for small molecules that induce DNA re-replication in MCF 10a normal breast cells.	GMNN gene product [Homo sapiens][gi:7705682]	
624297	Inactive	Potency		A quantitative high throughput screen for small molecules that induce DNA re-replication in SW480 colon adenocarcinoma cells.	GMNN gene product [Homo sapiens][gi:7705682]	
602281	Inactive			Luminescence-based biochemical primary high throughput screening assay to identify inhibitors of the interaction of the lipase co-activator protein, abhydrolase domain containing 5 (ABHD5) with perilipin-5 (MLDP; PLIN5)	ABHD5 gene product [Homo sapiens][gi:31542303]	
493027	Inactive			Luminescence-based biochemical high throughput validation assay to identify inhibitors of the interaction of the lipase co-activator protein, abhydrolase domain containing 5 (ABHD5) with perilipin-1 (PLIN1)	ABHD5 gene product [Homo sapiens][gi:31542303]	
493035	Inactive			Luminescence-based biochemical high throughput validation assay to identify inhibitors of the interaction of the lipase co-activator protein, abhydrolase domain containing 5 (ABHD5) with perilipin-5 (MLDP; PLIN5)	ABHD5 gene product [Homo sapiens][gi:31542303]	
488922	Inactive			Primary cell-based screen for identification of compounds that inhibit the two-pore domain potassium channel KCNK9	KCNK9 gene product [Homo sapiens][gi:7706135]	
2130	Inactive			Fluorescence polarization-based primary biochemical high throughput screening assay to identify inhibitors of Protein Phosphatase Methylesterase 1 (PME-1).	protein phosphatase methylesterase 1 [Homo sapiens][gi:7706645]	
588579	Inactive	Potency		qHTS for Inhibitors of Polymerase Kappa	POLK gene product [Homo sapiens][gi:7705344]	

AID	Outcome	Activity Concentration Name	Activity Concentration [uM]	BioAssay	Target	PMID
588579	Inactive	Potency		qHTS for Inhibitors of Polymerase Kappa	POLK gene product [Homo sapiens][gi:7705344]	
588579	Inactive	Potency		qHTS for Inhibitors of Polymerase Kappa	POLK gene product [Homo sapiens][gi:7705344]	
588579	Inactive	Potency		qHTS for Inhibitors of Polymerase Kappa	POLK gene product [Homo sapiens][gi:7705344]	
588579	Inactive	Potency		qHTS for Inhibitors of Polymerase Kappa	POLK gene product [Homo sapiens][gi:7705344]	
588579	Inactive	Potency		qHTS for Inhibitors of Polymerase Kappa	POLK gene product [Homo sapiens][gi:7705344]	
652197	Inactive			MLPCN ERAP1 Measured in Biochemical System Using Plate Reader - 7016-01_Inhibitor_SinglePoint_HTS_Activity	ERAP1 protein [Homo sapiens][gi:21315078]	
652197	Inactive			MLPCN ERAP1 Measured in Biochemical System Using Plate Reader - 7016-01_Inhibitor_SinglePoint_HTS_Activity	ERAP1 protein [Homo sapiens][gi:21315078]	
504734	Inactive			Fluorescence-based cell-based primary high throughput screening assay to identify inhibitors of TLR9-MyD88 binding.	toll-like receptor 9 [Homo sapiens][gi:194068499]	
504734	Inactive			Fluorescence-based cell-based primary high throughput screening assay to identify inhibitors of TLR9-MyD88 binding.	toll-like receptor 9 [Homo sapiens][gi:194068499]	
651999	Inactive			uHTS identification of small molecule inhibitors of Csn-mediated Deneddylation of Cullin-Ring Ligases, vis a fluorescence polarization assay	COPS5 gene product [Homo sapiens][gi:38027923]	
588590	Inactive	Potency		qHTS for Inhibitors of Polymerase Iota	POLI gene product [Homo sapiens][gi:154350220]	

AID	Outcome	Activity Concentration Name	Activity Concentration [uM]	BioAssay	Target	PMID
588590	Inactive	Potency		qHTS for Inhibitors of Polymerase Iota	POLI gene product [Homo sapiens][gi:154350220]	
588590	Inactive	Potency		qHTS for Inhibitors of Polymerase Iota	POLI gene product [Homo sapiens][gi:154350220]	
588590	Inactive	Potency		qHTS for Inhibitors of Polymerase Iota	POLI gene product [Homo sapiens][gi:154350220]	
432	Inactive	IC50		HTS discovery of chemical inhibitors of anti-apoptotic protein Bfl-1	Bcl2a1a gene product [Mus musculus][gi:11024684]	
624377	Inactive			Fluorescence polarization-based biochemical primary high throughput screening assay to identify inhibitors of ArfGAP with SH3 domain, ankyrin repeat and PH domain 1 (ASAP1)	ASAP1 gene product [Homo sapiens][gi:351542238]	
624296	Inactive	Potency		A quantitative high throughput screen for small molecules that induce DNA re-replication in MCF 10a normal breast cells.	GMNN gene product [Homo sapiens][gi:7705682]	
624297	Inactive	Potency		A quantitative high throughput screen for small molecules that induce DNA re-replication in SW480 colon adenocarcinoma cells.	GMNN gene product [Homo sapiens][gi:7705682]	
624296	Inactive	Potency		A quantitative high throughput screen for small molecules that induce DNA re-replication in MCF 10a normal breast cells.	GMNN gene product [Homo sapiens][gi:7705682]	
488949	Inactive	Potency		qHTS Validation Assay for Inhibitors for MPP8 Chromodomain Interactions with Methylated Histone Tails	MPHOSPH8 gene product [Homo sapiens][gi:41055989]	
1448	Inactive			Primary cell-based high-throughput screening assay to identify agonists of the transient receptor potential channel ML3 (TRPML3)	MCOLN3 protein [Homo sapiens][gi:38174238]	

AID	Outcome	Activity Concentration Name	Activity Concentration [uM]	BioAssay	Target	PMID
602252	Inactive			Fluorescence Polarization with CAL-PDZ Measured in Biochemical System Using Plate Reader - 2109-02_Inhibitor_SinglePoint_HTS_Activity	Golgi-associated PDZ and coiled-coil motif-containing protein isoform b [Homo sapiens][gi:62868213]	
602252	Inactive			Fluorescence Polarization with CAL-PDZ Measured in Biochemical System Using Plate Reader - 2109-02_Inhibitor_SinglePoint_HTS_Activity	Golgi-associated PDZ and coiled-coil motif-containing protein isoform b [Homo sapiens][gi:62868213]	
504414	Inactive			Fluorescence Polarization with Cer CAL-PDZ Measured in Biochemical System Using Plate Reader - 2109-01_Inhibitor_SinglePoint_HTS_Activity	Golgi-associated PDZ and coiled-coil motif-containing protein isoform a [Homo sapiens][gi:9966877]	
504414	Inactive			Fluorescence Polarization with Cer CAL-PDZ Measured in Biochemical System Using Plate Reader - 2109-01_Inhibitor_SinglePoint_HTS_Activity	Golgi-associated PDZ and coiled-coil motif-containing protein isoform a [Homo sapiens][gi:9966877]	
624414	Inactive			qHTS for Agonists of the Human Mucolipin Transient Receptor Potential 1 (TRPML1)	MCOLN1 gene product [Homo sapiens][gi:10092597]	
624415	Inactive			qHTS for Inhibitors of the Human Mucolipin Transient Receptor Potential 1 (TRPML1)	MCOLN1 gene product [Homo sapiens][gi:10092597]	
434973	Inactive			uHTS Luminescent assay for identification of inhibitors of Sentrin-specific protease 7 (SENP7)	SUMO1/sentrin specific peptidase 7 [Homo sapiens][gi:120538355]	
1456	Inactive			Identification of Novel Modulators of Cl-dependent Transport Process via HTS: Primary Screen	electroneutral potassium-chloride cotransporter KCC2 [Homo sapiens][gi:12003227]	
493091	Inactive			uHTS Colorimetric assay for identification of inhibitors of Scp-1	carboxy-terminal domain RNA polymerase II polypeptide A small phosphatase 1 isoform 1 [Homo sapiens][gi:10864009]	
588453	Inactive	Potency		qHTS Assay for Inhibitors of Mammalian Selenoprotein Thioredoxin Reductase 1 (TrxR1): qHTS	thioredoxin reductase [Rattus norvegicus][gi:8659577]	

AID	Outcome	Activity Concentration Name	Activity Concentration [uM]	BioAssay	Target	PMID
588453	Inactive	Potency		qHTS Assay for Inhibitors of Mammalian Selenoprotein Thioredoxin Reductase 1 (TrxR1): qHTS	thioredoxin reductase [Rattus norvegicus][gi:8659577]	
588456	Inactive	Potency		qHTS Assay for Substrates of Mammalian Selenoprotein Thioredoxin Reductase 1 (TrxR1): qHTS	thioredoxin reductase [Rattus norvegicus][gi:8659577]	
588456	Inactive	Potency		qHTS Assay for Substrates of Mammalian Selenoprotein Thioredoxin Reductase 1 (TrxR1): qHTS	thioredoxin reductase [Rattus norvegicus][gi:8659577]	
488772	Inactive	Potency		qHTS Assay for Substrates of Mammalian Selenoprotein Thioredoxin Reductase 1 (TrxR1)	thioredoxin reductase [Rattus norvegicus][gi:8659577]	
488772	Inactive	Potency		qHTS Assay for Substrates of Mammalian Selenoprotein Thioredoxin Reductase 1 (TrxR1)	thioredoxin reductase [Rattus norvegicus][gi:8659577]	
488773	Inactive	Potency		qHTS Assay for Inhibitors of Mammalian Selenoprotein Thioredoxin Reductase 1 (TrxR1)	thioredoxin reductase [Rattus norvegicus][gi:8659577]	
488773	Inactive	Potency		qHTS Assay for Inhibitors of Mammalian Selenoprotein Thioredoxin Reductase 1 (TrxR1)	thioredoxin reductase [Rattus norvegicus][gi:8659577]	
588453	Inactive	Potency		qHTS Assay for Inhibitors of Mammalian Selenoprotein Thioredoxin Reductase 1 (TrxR1): qHTS	thioredoxin reductase [Rattus norvegicus][gi:8659577]	
588453	Inactive	Potency		qHTS Assay for Inhibitors of Mammalian Selenoprotein Thioredoxin Reductase 1 (TrxR1): qHTS	thioredoxin reductase [Rattus norvegicus][gi:8659577]	
588456	Inactive	Potency		qHTS Assay for Substrates of Mammalian Selenoprotein Thioredoxin Reductase 1 (TrxR1): qHTS	thioredoxin reductase [Rattus norvegicus][gi:8659577]	
588456	Inactive	Potency		qHTS Assay for Substrates of Mammalian Selenoprotein Thioredoxin Reductase 1 (TrxR1): qHTS	thioredoxin reductase [Rattus norvegicus][gi:8659577]	

AID	Outcome	Activity Concentration Name	Activity Concentration [uM]	BioAssay	Target	PMID
2676	Inactive	Potency		qHTS Assay for Agonists of the Relaxin Receptor RXFP1	relaxin receptor 1 isoform 1 [Homo sapiens][gi:85986601]	
2676	Inactive	Potency		qHTS Assay for Agonists of the Relaxin Receptor RXFP1	relaxin receptor 1 isoform 1 [Homo sapiens][gi:85986601]	
488975	Inactive			Primary cell-based screen for identification of compounds that inhibit the Choline Transporter (CHT)	SLC5A7 gene product [Homo sapiens][gi:11141885]	
488975	Inactive			Primary cell-based screen for identification of compounds that inhibit the Choline Transporter (CHT)	SLC5A7 gene product [Homo sapiens][gi:11141885]	
488977	Inactive			Primary cell-based screen for identification of compounds that allosterically activate the Choline Transporter (CHT)	SLC5A7 gene product [Homo sapiens][gi:11141885]	
488977	Inactive			Primary cell-based screen for identification of compounds that allosterically activate the Choline Transporter (CHT)	SLC5A7 gene product [Homo sapiens][gi:11141885]	
493012	Inactive			uHTS identification of APOBEC3G DNA Deaminase Inhibitors via a fluorescence-based single-stranded DNA deaminase assay	APOBEC3G gene product [Homo sapiens][gi:13399304]	
602310	Inactive	Potency		qHTS for Inhibitors of Vif-A3G Interactions: qHTS	APOBEC3G gene product [Homo sapiens][gi:13399304]	
1566	Inactive	EC50		uHTS luminescence assay for the identification of compounds that inhibit NOD2	nucleotide-binding oligomerization domain-containing protein 2 [Homo sapiens][gi:11545912]	
1566	Inactive	EC50		uHTS luminescence assay for the identification of compounds that inhibit NOD2	nucleotide-binding oligomerization domain-containing protein 2 [Homo sapiens][gi:11545912]	
1566	Inactive	EC50		uHTS luminescence assay for the identification of compounds that inhibit NOD2	nucleotide-binding oligomerization domain-containing protein 2 [Homo sapiens][gi:11545912]	

AID	Outcome	Activity Concentration Name	Activity Concentration [uM]	BioAssay	Target	PMID
2330	Inactive			Luminescence Cell-Based Primary HTS to Identify Inhibitors of STK33	serine/threonine kinase 33 [Homo sapiens][gi:12830367]	
2330	Inactive			Luminescence Cell-Based Primary HTS to Identify Inhibitors of STK33	serine/threonine kinase 33 [Homo sapiens][gi:12830367]	
2330	Inactive			Luminescence Cell-Based Primary HTS to Identify Inhibitors of STK33	serine/threonine kinase 33 [Homo sapiens][gi:12830367]	
2661	Inactive			Luminescence Cell-Free Homogenous Primary HTS to Identify Inhibitors of Serine/Threonine Kinase 33 Activity	serine/threonine-protein kinase 33 [Homo sapiens][gi:23943882]	
2661	Inactive			Luminescence Cell-Free Homogenous Primary HTS to Identify Inhibitors of Serine/Threonine Kinase 33 Activity	serine/threonine-protein kinase 33 [Homo sapiens][gi:23943882]	
2661	Inactive			Luminescence Cell-Free Homogenous Primary HTS to Identify Inhibitors of Serine/Threonine Kinase 33 Activity	serine/threonine-protein kinase 33 [Homo sapiens][gi:23943882]	
2805	Inactive			uHTS Luminescent assay for identification of activators of mouse intestinal alkaline phosphatase	intestinal alkaline phosphatase precursor [Mus musculus][gi:124487323]	
2806	Inactive			uHTS Luminescent assay for identification of inhibitors of mouse intestinal alkaline phosphatase	intestinal alkaline phosphatase precursor [Mus musculus][gi:124487323]	
504466	Inactive	Potency		qHTS screen for small molecules that induce genotoxicity in human embryonic kidney (HEK293T) cells expressing luciferase-tagged ELG1	ATAD5 protein [Homo sapiens][gi:116283940]	
2156	Inactive			Primary cell-based high-throughput screening assay for identification of compounds that inhibit KCNQ2 potassium channels	Kcnq2 gene product [Rattus norvegicus][gi:18959272]	
2156	Inactive			Primary cell-based high-throughput screening assay for identification of compounds that inhibit KCNQ2 potassium channels	Kcnq2 gene product [Rattus norvegicus][gi:18959272]	

AID	Outcome	Activity Concentration Name	Activity Concentration [uM]	BioAssay	Target	PMID
2558	Inactive			Mode of action - Automated patch clamp assay for KCNQ2 potentiators on Retigabine insensitive KCNQ2 Mutant W236L cell line	Kcnq2 gene product [Rattus norvegicus][gi:18959272]	
2558	Inactive			Mode of action - Automated patch clamp assay for KCNQ2 potentiators on Retigabine insensitive KCNQ2 Mutant W236L cell line	Kcnq2 gene product [Rattus norvegicus][gi:18959272]	
588405	Inactive			HTS Assay for Peg3 Promoter Inhibitors	Ppp1r15a gene product [Rattus norvegicus][gi:78486550]	
2280	Inactive			Fluorescence polarization-based primary biochemical high throughput screening assay to identify inhibitors of GLD-1 protein - TGE RNA interaction.	defective in Germ Line Development family member (gld-1) [Caenorhabditis elegans][gi:17507875]	
624304	Inactive			uHTS identification of SKN-1 Inhibitors in a fluoresence assay	Protein SKN-1, isoform b [Caenorhabditis elegans][gi:25148072]	
1832	Inactive			MLPCN maternal gene expression-MEX-5 TCR-2 binding assay-Primary Screen	Zinc finger protein mex- [gi:55976631]	
1832	Inactive			MLPCN maternal gene expression-MEX-5 TCR-2 binding assay-Primary Screen	Zinc finger protein mex- [gi:55976631]	
652126	Inactive			Luminescence-based cell-based primary high throughput screening assay to identify activators of the DAF-12 from the parasite S. stercoralis (ssDAF-12)	Protein DAF-12, isoform a [Caenorhabditis elegans][gi:71987181]	
652067	Inactive			Luminescence-based cell-based primary high throughput screening assay to identify activators of the DAF-12 from the parasite H. contortus (hcDAF-12)	Protein DAF-12, isoform a [Caenorhabditis elegans][gi:71987181]	
687014	Inactive			Luminescence-based cell-based primary high throughput screening assay to identify agonists of the DAF-12 from the parasite H. glycines (hgDAF-12).	Protein DAF-12, isoform a [Caenorhabditis elegans][gi:71987181]	
493011	Inactive			uHTS identification of APOBEC3A DNA Deaminase Inhibitors via a fluorescence-based single-stranded DNA deaminase assay	APOBEC3A gene product [Homo sapiens][gi:21955158]	

AID	Outcome	Activity Concentration Name	Activity Concentration [uM]	BioAssay	Target	PMID
602313	Inactive	Potency		qHTS for Inhibitors of Vif-A3F Interactions: qHTS	APOBEC3F gene product [Homo sapiens][gi:22907044]	
2205	Inactive			HCS assay for microtubule stabilizers	tubulin, beta [Homo sapiens][gi:29788785]	
2205	Inactive			HCS assay for microtubule stabilizers	tubulin, beta [Homo sapiens][gi:29788785]	
504411	Inactive			Fluorescence-based primary biochemical high throughput screening assay to identify inhibitors of human diacylglycerol lipase, beta (DAGLB)	sn1-specific diacylglycerol lipase beta isoform 1 [Homo sapiens][gi:218931251]	
504411	Inactive			Fluorescence-based primary biochemical high throughput screening assay to identify inhibitors of human diacylglycerol lipase, beta (DAGLB)	sn1-specific diacylglycerol lipase beta isoform 1 [Homo sapiens][gi:218931251]	
1947	Inactive			Fluorescence polarization-based counterscreen for RBBP9 inhibitors: primary biochemical high throughput screening assay to identify inhibitors of the serine hydrolase family member Fam108B.	Fam108b protein [Mus musculus][gi:21595511]	
1947	Inactive			Fluorescence polarization-based counterscreen for RBBP9 inhibitors: primary biochemical high throughput screening assay to identify inhibitors of the serine hydrolase family member Fam108B.	Fam108b protein [Mus musculus][gi:21595511]	
1947	Inactive			Fluorescence polarization-based counterscreen for RBBP9 inhibitors: primary biochemical high throughput screening assay to identify inhibitors of the serine hydrolase family member Fam108B.	Fam108b protein [Mus musculus][gi:21595511]	
651572	Inactive			Fluorescence polarization-based biochemical primary high throughput screening assay to identify inhibitors of ADP-ribosylation factor GTPase activating protein 1 (ARFGAP1)	Arfgap1 gene product [Rattus norvegicus][gi:21489979]	

AID	Outcome	Activity Concentration Name	Activity Concentration [uM]	BioAssay	Target	PMID
588627	Inactive			Primary cell-based high-throughput screening for identification of compounds that activate MrgX1 receptor signaling	MAS-related GPR member X1 [Homo sapiens][gi:195969650]	
588627	Inactive			Primary cell-based high-throughput screening for identification of compounds that activate MrgX1 receptor signaling	MAS-related GPR member X1 [Homo sapiens][gi:195969650]	
588675	Inactive			Primary cell-based high-throughput screening for identification of compounds that allosterically activate MrgX1 receptor signaling	MAS-related GPR member X1 [Homo sapiens][gi:195969650]	
588675	Inactive			Primary cell-based high-throughput screening for identification of compounds that allosterically activate MrgX1 receptor signaling	MAS-related GPR member X1 [Homo sapiens][gi:195969650]	
588676	Inactive			Primary cell-based high-throughput screening for identification of compounds that antagonize MrgX1 receptor signaling	MAS-related GPR member X1 [Homo sapiens][gi:195969650]	
588676	Inactive			Primary cell-based high-throughput screening for identification of compounds that antagonize MrgX1 receptor signaling	MAS-related GPR member X1 [Homo sapiens][gi:195969650]	
1019	Inactive			Luminescent assay for identification of inhibitors of bovine intestinal alkaline phosphatase	intestinal-type alkaline phosphatase [Bos taurus][gi:68299797]	
1019	Inactive			Luminescent assay for identification of inhibitors of bovine intestinal alkaline phosphatase	intestinal-type alkaline phosphatase [Bos taurus][gi:68299797]	
1016	Inactive			Luminescent assay for identification of activators of bovine intestinal alkaline phosphatase	intestinal-type alkaline phosphatase [Bos taurus][gi:68299797]	
1016	Inactive			Luminescent assay for identification of activators of bovine intestinal alkaline phosphatase	intestinal-type alkaline phosphatase [Bos taurus][gi:68299797]	
602163	Inactive			Absorbance-based biochemical primary high throughput screening assay to identify activators of Methionine sulfoxide reductase A (MsrA)	MSRA protein [Bos taurus][gi:73586699]	

AID	Outcome	Activity Concentration Name	Activity Concentration [uM]	BioAssay	Target	PMID
651718	Inactive			Absorbance-based biochemical primary high throughput screening assay to identify inhibitors of Methionine sulfoxide reductase A (MsrA)	MSRA protein [Bos taurus][gi:73586699]	
781	Inactive			uHTS for 14-3-3/Bad interaction inhibitors	tyrosine 3-monooxygenase/tryptophan 5-monooxygenase activation protein, zeta polypeptide [Bos taurus[gi:27807367]	
1424	Inactive			Primary cell-based high-throughput screening assay to identify agonists of the transient receptor potential channel N1 (TRPN1)	transient receptor potential cation channel, subfamily N, member 1 [Danio rerio][gi:34330186]	
1461	Inactive	Potency		qHTS Assay for Antagonists of the Neuropeptide S Receptor: cAMP Signal Transduction	NPSR1 gene product [Homo sapiens][gi:46395496]	
1461	Inactive	Potency		qHTS Assay for Antagonists of the Neuropeptide S Receptor: cAMP Signal Transduction	NPSR1 gene product [Homo sapiens][gi:46395496]	
1461	Inactive	Potency		qHTS Assay for Antagonists of the Neuropeptide S Receptor: cAMP Signal Transduction	NPSR1 gene product [Homo sapiens][gi:46395496]	
1461	Inactive	Potency		qHTS Assay for Antagonists of the Neuropeptide S Receptor: cAMP Signal Transduction	NPSR1 gene product [Homo sapiens][gi:46395496]	
1236	Inactive			uHTS for Calpain Inhibitors	calpain II [Sus scrofa][gi:1628587]	
1236	Inactive			uHTS for Calpain Inhibitors	calpain II [Sus scrofa][gi:1628587]	
758	Inactive			HTS to identify specific small molecule inhibitors of Ras and Ras-related GTPases specifically Rab7 wildtype	GTP-binding protein (rab7) [Canis lupus familiaris][gi:164058]	
760	Inactive			HTS to identify specific small molecule inhibitors of Ras and Ras-related GTPases specifically Rab2 wildtype	Ras-related protein Rab-2[gi:46577642]	

AID	Outcome	Activity Concentration Name	Activity Concentration [uM]	BioAssay	Target	PMID
1274	Inactive			uHTS of small molecular inhibitors for p47phox, a regulatory protein of NADPH oxidases (Noxs)	neutrophil cytosolic factor 1 [Homo sapiens][gi:115298672]	
504582	Inactive			In vivo-based yeast HTS to detect compounds rescuing yeast growth/survival of Plasmodium Falciparum HSP40-mediated toxicity Measured in Whole Organism System Using Plate Reader - 2120-01_Inhibitor_SinglePoint_HTS_Activity	HSP40, subfamily A, putative [Plasmodium falciparum 3D7][gi:124809271]	
504594	Inactive			Anti-Malarial Hsp90 Inhibitors Measured in Microorganism System Using Plate Reader - 2121-01_Inhibitor_SinglePoint_HTS_Activity	HSP90 [Plasmodium falciparum 3D7][gi:124809506]	
504621	Inactive			Anti-Malarial Hsp90 Inhibitors Measured in Microorganism System Using Plate Reader - 2121-01_Inhibitor_SinglePoint_HTS_Activity_Set2	HSP90 [Plasmodium falciparum 3D7][gi:124809506]	
1619	Inactive	IC50		Inhibitors of Plasmodium falciparum M17-Family Leucine Aminopeptidase (M17LAP)	M17 leucyl aminopeptidase [Plasmodium falciparum 3D7][gi:124809582]	
1619	Inactive	IC50		Inhibitors of Plasmodium falciparum M17-Family Leucine Aminopeptidase (M17LAP)	M17 leucyl aminopeptidase [Plasmodium falciparum 3D7][gi:124809582]	
1619	Inactive	IC50		Inhibitors of Plasmodium falciparum M17-Family Leucine Aminopeptidase (M17LAP)	M17 leucyl aminopeptidase [Plasmodium falciparum 3D7][gi:124809582]	
1822	Inactive			QFRET-based primary biochemical high throughput screening assay to identify inhibitors of the Plasmodium falciparum M18 Aspartyl Aminopeptidase (PFM18AAP).	M18 aspartyl aminopeptidase [Plasmodium falciparum 3D7][gi:23505220]	
1822	Inactive			QFRET-based primary biochemical high throughput screening assay to identify inhibitors of the Plasmodium falciparum M18 Aspartyl Aminopeptidase (PFM18AAP).	M18 aspartyl aminopeptidase [Plasmodium falciparum 3D7][gi:23505220]	
1445	Inactive	IC50		Inhibitors of Plasmodium falciparum M1-Family Alanyl Aminopeptidase (M1AAP)	m1-family aminopeptidase [Plasmodium falciparum 3D7][gi:124512980]	

AID	Outcome	Activity Concentration Name	Activity Concentration [uM]	BioAssay	Target	PMID
1445	Inactive	IC50		Inhibitors of Plasmodium falciparum M1-Family Alanyl Aminopeptidase (M1AAP)	m1-family aminopeptidase [Plasmodium falciparum 3D7][gi:124512980]	
1887	Inactive			Multiplex HTS Screen of TOR pathway GFP-fusion proteins in Saccharomyes cerevisiae_specifically_AGP1	Agp1p [Saccharomyces cerevisiae S288c][gi:85666113]	
2066	Inactive			Multiplex HTS Screen of TOR pathway GFP-fusion proteins in Saccharomyes cerevisiae_specifically_ AGP1_MLPCN.	Agp1p [Saccharomyces cerevisiae S288c][gi:85666113]	
2563	Inactive			Fluorescence Cell-Free Homogenous Primary HTS to Identify Inhibitors of the Ras-converting Enzyme	Rce1p [Saccharomyces cerevisiae S288c][gi:6323930]	
2563	Inactive			Fluorescence Cell-Free Homogenous Primary HTS to Identify Inhibitors of the Ras-converting Enzyme	Rce1p [Saccharomyces cerevisiae S288c][gi:6323930]	
463212	Inactive			uHTS identification of small molecule inhibitors of tim23-1 yeast via a luminescent assay	TPA: Tim23p [Saccharomyces cerevisiae S288c][gi:285814664]	
504577	Inactive			HTS of Small Molecules that Regulate V-ATPase Proton Transport in Yeast using pHLuorin	Vma11p [Saccharomyces cerevisiae S288c][gi:6325022]	
504600	Inactive			Validation of HTS of Small Molecules that Regulate V-ATPase Proton Transport in Yeast using pHLuorin	Vma11p [Saccharomyces cerevisiae S288c][gi:6325022]	
463190	Inactive			uHTS identification of small molecule inhibitors of tim10-1 yeast via a luminescent assay	TPA: Tim10p [Saccharomyces cerevisiae S288c][gi:285809906]	
463195	Inactive			uHTS identification of small molecule inhibitors of tim10 yeast via a luminescent assay	TPA: Tim10p [Saccharomyces cerevisiae S288c][gi:285809906]	
2606	Inactive			Fluorescence polarization-based primary biochemical high throughput screening assay to identify inhibitors of the membrane-associated serine protease Rv3671c in M.tuberculosis	membrane-associated serine protease [Mycobacterium tuberculosis H37Rv][gi:15610807]	

AID	Outcome	Activity Concentration Name	Activity Concentration [uM]	BioAssay	Target	PMID
1376	Inactive	IC50		Inhibitors of Mycobacterial Glucosamine-1-phosphate acetyl transferase (GlmU)	UDP-N-acetylglucosamine pyrophosphorylase glmU [Mycobacterium tuberculosis H37Rv][gi:15608158]	
504406	Inactive			Inhibitors of Mycobacterium tuberculosis UDP-galactopyranose mutase (UGM) enzyme - High throughput screening using Fluorescent polarization assay Measured in Biochemical System Using Plate Reader - 2105-01_Inhibitor_SinglePoint_HTS_Activity_Set6	glf gene product [Mycobacterium tuberculosis H37Rv][gi:15610945]	
588726	Inactive			Fluorescence-based biochemical primary high throughput screening assay to identify inhibitors of the fructose-bisphosphate aldolase (FBA) of M. tuberculosis	Probable fructose-bisphosphate aldolase Fba [Mycobacterium tuberculosis H37Rv][gi:15607504]	
540299	Inactive			A screen for compounds that inhibit the MenB enzyme of Mycobacterium tuberculosis	naphthoate synthase [Mycobacterium tuberculosis H37Rv][gi:15607688]	20850304
540299	Inactive			A screen for compounds that inhibit the MenB enzyme of Mycobacterium tuberculosis	naphthoate synthase [Mycobacterium tuberculosis H37Rv][gi:15607688]	20850304
2221	Inactive			Fluorescence Cell-Free Homogenous Primary HTS to Identify Inhibitors of RecA Intein Splicing Activity	DNA recombination protein RecA [Mycobacterium tuberculosis H37Rv][gi:15609874]	
435030	Inactive			Absorbance-based primary bacterial cell-based high throughput screening assay to identify inhibitors of AddAB recombination protein complex	hypothetical protein HP1089 [Helicobacter pylori 26695][gi:15645703]	
1662	Inactive			MLPCN Streptokinase Expression Inhibition	streptokinase A precursor [Streptococcus pyogenes M1 GAS][gi:15675770]	
653	Inactive			West Nile Virus NS2bNS3 Proteinase Inhibitor Dose Response Confirmation.	polyprotein precursor [West Nile virus][gi:11528014]	
577	Inactive			HTS to identify Inhibitors of West Nile Virus NS2bNS3 Proteinase	polyprotein precursor [West Nile virus][gi:11528014]	

AID	Outcome	Activity Concentration Name	Activity Concentration [uM]	BioAssay	Target	PMID
602123	Inactive			Fluorescence polarization-based primary biochemical high throughput screening assay to identify inhibitors of Escherichia coli DNA-binding ATP-dependent protease La (eLon)	DNA-binding ATP-dependent protease La [Escherichia coli str. K-12 substr. MG1655][gi:16128424]	
547	Inactive			HTS for inhibitors of bacterial DnaK	heat shock protein [Escherichia coli str. K-12 substr. MG1655][gi:16130533]	
504720	Inactive			uHTS identification of MazEF TA System activators via a fluorescence-based single-stranded RNase assay	mRNA interferase toxin, antitoxin is MazE [Escherichia coli str. K-12 substr. MG1655][gi:16130689]	
651602	Inactive			Absorbance-based primary bacterial cell-based high throughput screening assay to identify inhibitors of RecBCD (with phage)	exonuclease V (RecBCD complex), alpha chain [Escherichia coli str. K-12 substr. MG1655][gi:16130723]	
488895	Inactive			High Throughput Screen for Tat Transport Inhibitors Measured in Microorganism System Using Plate Reader - 2093-01_Inhibitor_SinglePoint_HTS_Activity	TatABCE protein translocation system subunit [Escherichia coli str. K-12 substr. MG1655][gi:90111653]	
602399	Inactive			uHTS identification of inhibitors of NadD in a Colorimetric assay	hypothetical protein SA1422 [Staphylococcus aureus subsp. aureus N315][gi:15927174]	
588501	Inactive			High-throughput multiplex microsphere screening for inhibitors of toxin protease, specifically Lethal Factor Protease, MLPCN compound set	lethal factor [Bacillus anthracis str. A2012][gi:21392848]	16604538
588461	Inactive			High-throughput multiplex microsphere screening for inhibitors of toxin protease, specifically Lethal Factor Protease, Validation compound set	lethal factor [Bacillus anthracis str. A2012][gi:21392848]	16604538
504884	Inactive			Inhibitors of Y. pestis Topo-I using cleavage product accumulation Measured in Biochemical System Using Plate Reader - 2123-01_Inhibitor_SinglePoint_HTS_Activity	DNA topoisomerase I [Yersinia pestis CO92][gi:115347926]	
898	Inactive			YopH HTS	YopH [Yersinia enterocolitica][gi:28373018]	

AID	Outcome	Activity Concentration Name	Activity Concentration [uM]	BioAssay	Target	PMID
1903	Inactive	IC50		Identification of SV40 T antigen inhibitors: A route to novel anti-viral reagents	large T antigen [Simian virus 40][gi:297591903]	
485353	Inactive			qHTS of Yeast-based Assay for SARS-CoV PLP	orf1ab polyprotein (pp1ab) [SARS coronavirus][gi:30124074]	
485353	Inactive			qHTS of Yeast-based Assay for SARS-CoV PLP	orf1ab polyprotein (pp1ab) [SARS coronavirus][gi:30124074]	
485353	Inactive			qHTS of Yeast-based Assay for SARS-CoV PLP	orf1ab polyprotein (pp1ab) [SARS coronavirus][gi:30124074]	
504770	Inactive			A screen for compounds that inhibit replication of Vibrio cholerae chromosome II	hypothetical protein VC_A0002 [Vibrio cholerae O1 biovar El Tor str. N16961][gi:9657380]	
686977	Inactive	IC50		Vibrio cholerae assay for pro-quorum sensing small molecules	cyclic AMP receptor protein [Vibrio cholerae O1 biovar El Tor str. N16961][gi:9657203]	
488978	Inactive	Potency		High-Throughput Screening for Modulators of Cytosolic Chaperonin Activity: MmCpn Primary Screen	chaperonin GroEL [Methanococcus maripaludis S2][gi:45359078]	
492967	Inactive			A screen for compounds that inhibit the CapD enzyme of Bacillus anthracis	gamma-glutamyltranspeptidase [Bacillus anthracis str. 'Ames Ancestor'][gi:47566732]	
651958	Inactive			Fluorescence-based biochemical high throughput screening primary assay to identify inhibitors of Crimean-Congo Hemorrhagic Fever (CCHF) viral ovarian tumor domain protease (vOTU): Pep-AMC substrate	putative polyprotein [Crimean-Congo hemorrhagic fever virus][gi:76364066]	
540336	Inactive			Rtt109/Vps75 Measured in Biochemical System Using Plate Reader - 2106-01_Inhibitor_SinglePoint_HTS_Activity	hypothetical protein CaO19.7491 [Candida albicans SC5314][gi:68474550]	
1962	Inactive			Fluorescence polarization-based primary biochemical high throughput screening assay to identify inhibitors of tRNA 2'-phosphotransferase (TPT1).	likely tRNA 2'-phosphotransferase [Candida albicans SC5314][gi:68476498]	

AID	Outcome	Activity Concentration Name	Activity Concentration [uM]	BioAssay	Target	PMID
485368	Inactive	Potency		qHTS Validation Assay to Find Inhibitors of T. brucei phosphofructokinase	ATP-dependent phosphofructokinase [Trypanosoma brucei][gi:72386991]	
485367	Inactive	Potency		qHTS Assay to Find Inhibitors of T. brucei phosphofructokinase	ATP-dependent phosphofructokinase [Trypanosoma brucei][gi:72386991]	
624268	Inactive			Luminescence-based biochemical primary high throughput screening assay to identify inhibitors of Trypanosoma brucei methionyl tRNA synthetase (MetRS)	methionyl-tRNA synthetase [Trypanosoma brucei brucei strain 927/4 GUTat10.1][gi:71746704]	
1430	Inactive			HTS assay for inhibitors of Trypanosoma brucei hexokinase 1	hexokinase [Trypanosoma brucei][gi:70832125]	
1950	Inactive			Fluorescence polarization-based primary biochemical high throughput screening assay to identify inhibitors of the Epstein-Barr virus nuclear antigen 1 (EBNA-1).	EBNA-1 protein [Human herpesvirus 4][gi:23893623]	
2234	Inactive			Counterscreen for inhibitors of EBNA-1: fluorescence polarization-based biochemical high throughput primary assay to identify inhibitors of the Epstein-Barr virus-encoded protein, ZTA.	BZLF1 [Human herpesvirus 4][gi:82503229]	
504558	Inactive			Inhibitors of Epstein-Barr LMP1 inducible NF-kappaB luciferase reporter Measured in Cell-Based System Using Plate Reader - 2122-01_Inhibitor_SinglePoint_HTS_Activity	LMP1 [Human herpesvirus 4][gi:23893668]	
504547	Inactive	Potency		qHTS Validation Assay to Find Inhibitors of Phosphoglycerate Kinase	phosphoglycerate kinase [Trypanosoma brucei][gi:115503961]	
602233	Inactive	Potency		qHTS Assay to Find Inhibitors of Phosphoglycerate Kinase	phosphoglycerate kinase [Trypanosoma brucei][gi:115503961]	
556	Inactive			Screening for Inhibitors of the Mevalonate Pathway in Streptococcus Pneumoniae - DPM-DC	diphosphomevalonate decarboxylase [Streptococcus pneumoniae D39][gi:116076351]	

AID	Outcome	Activity Concentration Name	Activity Concentration [uM]	BioAssay	Target	PMID
556	Inactive			Screening for Inhibitors of the Mevalonate Pathway in Streptococcus Pneumoniae - DPM-DC	diphosphomevalonate decarboxylase [Streptococcus pneumoniae D39][gi:116076351]	
539	Inactive			Screening for Inhibitors of the Mevalonate Pathway in Streptococcus Pneumoniae - PMK	phosphomevalonate kinase [Streptococcus pneumoniae D39][gi:116077694]	
555	Inactive			Screening for Inhibitors of the Mevalonate Pathway in Streptococcus Pneumoniae - MK	mevalonate kinase [Streptococcus pneumoniae D39][gi:116516899]	
652162	Inactive			C. difficile toxins: HTS for inhibitors of TcdB glycohydrolase activity Measured in Biochemical System Using Plate Reader - 7074-01_Inhibitor_SinglePoint_HTS_Activity	Toxin B [Clostridium difficile 630][gi:126698238]	
485350	Inactive			A screen for compounds that inhibit the bacterial siderophore biosynthetic enzyme BasE	enterobactin synthase subunit E [Acinetobacter baumannii ATCC 17978][gi:126642418]	
485350	Inactive			A screen for compounds that inhibit the bacterial siderophore biosynthetic enzyme BasE	enterobactin synthase subunit E [Acinetobacter baumannii ATCC 17978][gi:126642418]	
2629	Inactive			Fluorescence Polarization Cell-Free Homogeneous Primary HTS to Identify Inhibitors of the LANA Histone H2A/H2B Interaction	LANA [Human herpesvirus 8][gi:139472804]	
493244	Inactive			Fluorescence-based biochemical primary high throughput screening assay to identify inhibitors of the calcium sensitivity of cardiac Regulated Thin Filaments (RTF)	cardiac alpha tropomyosin [Sus scrofa][gi:1927]	
493008	Inactive			Fluorescence-based biochemical primary high throughput screening assay to identify activators of the calcium sensitivity of cardiac Regulated Thin Filaments (RTF)	cardiac alpha tropomyosin [Sus scrofa][gi:1927]	
493106	Inactive	Potency		Validation screen for small molecules that induce genotoxicity in human embryonic kidney (HEK293T) cells expressing luciferase-tagged ELG1	ATAD5 protein [Homo sapiens][gi:116283940]	

AID	Outcome	Activity Concentration Name	Activity Concentration [uM]	BioAssay	Target	PMID
1085	Inactive			uHTS for Small Molecule Inhibitiors of Epstein-Barr Virus Inhibitors	BZLF2 [Human herpesvirus 4 type 2][gi:139424501]	
588499	Inactive			High-throughput multiplex microsphere screening for inhibitors of toxin protease, specifically Botulinum neurotoxin light chain A protease, MLPCN compound set	botulinum neurotoxin type A [Clostridium botulinum A str. ATCC 3502][gi:148378801]	16604538
602314	Inactive			A screen for compounds that modulate the activity of the Staphylococcus aureus MgrA protein	MarR family regulatory protein [Staphylococcus aureus subsp. aureus str. Newman][gi:151220867]	
602314	Inactive			A screen for compounds that modulate the activity of the Staphylococcus aureus MgrA protein	MarR family regulatory protein [Staphylococcus aureus subsp. aureus str. Newman][gi:151220867]	
504548	Inactive	Potency		qHTS Validation Assay to Find Inhibitors of Phosphoglycerate Mutase	2,3-bisphosphoglycerate-independent phosphoglycerate mutase; 2,3-bisphosphoglycerate-independentphos[gi:157877932]	
488965	Inactive			Fluorescent Biochemical Primary HTS to Identify Inhibitors of P. aeruginosa PvdQ acylase Measured in Biochemical System Using Plate Reader and Imaging Combination - 2091-01_Inhibitor_SinglePoint_HTS_Activity	pvdQ gene product [Pseudomonas aeruginosa LESB58][gi:218891639]	
602481	Inactive			Mycobacterium tuberculosis BioA enzyme inhibitor Measured in Biochemical System Using Plate Reader - 2163-01_Inhibitor_SinglePoint_HTS_Activity	bioA [Mycobacterium tuberculosis UT205][gi:378544807]	
588549	Inactive			Fluorescence polarization to screen for inhibitor that competite the binding of FadD28 to bisubstrate Measured in Biochemical System Using Plate Reader - 2147-01_Inhibitor_SinglePoint_HTS_Activity	FATTY-ACID-CoA LIGASE FADD28 (FATTY-ACID-CoA SYNTHETASE) (FATTY-ACID-CoA SYNTHASE) [Mycobacterium tu[gi:1781172]	
1527	Inactive			Primary biochemical high throughput screening assay to identify inhibitors of VIM-2 metallo-beta-lactamase	metallo beta-lactamase [Pseudomonas aeruginosa][gi:7381449]	

AID	Outcome	Activity Concentration Name	Activity Concentration [uM]	BioAssay	Target	PMID
1527	Inactive			Primary biochemical high throughput screening assay to identify inhibitors of VIM-2 metallo-beta-lactamase	metallo beta-lactamase [Pseudomonas aeruginosa][gi:7381449]	
493160	Inactive			uHTS Fluorescent assay for identification of inhibitors of hexokinase domain containing I (HKDC1)	putative hexokinase HKDC1 [Homo sapiens][gi:156151420]	
493187	Inactive			uHTS Fluorescent assay for identification of activators of hexokinase domain containing I (HKDC1)	putative hexokinase HKDC1 [Homo sapiens][gi:156151420]	
1457	Inactive	Potency		qHTS Assay for Identifying the Cell-Membrane Permeable IMPase Inhibitors: Potentiation with Lithium	Inositol monophosphatase[gi:44888968]	
1457	Inactive	Potency		qHTS Assay for Identifying the Cell-Membrane Permeable IMPase Inhibitors: Potentiation with Lithium	Inositol monophosphatase[gi:44888968]	
1457	Inactive	Potency		qHTS Assay for Identifying the Cell-Membrane Permeable IMPase Inhibitors: Potentiation with Lithium	Inositol monophosphatase[gi:44888968]	
1457	Inactive	Potency		qHTS Assay for Identifying the Cell-Membrane Permeable IMPase Inhibitors: Potentiation with Lithium	Inositol monophosphatase[gi:44888968]	
2073	Inactive	IC50		Homogeneous Time-Resolved Fluorescence Resonance Energy Transfer (HTRF) Assay	Mint1 [Rattus norvegicus][gi:2625023]	
463193	Inactive			High-content cell-based screening for modulators of autophagy	microtubule-associated proteins 1A/1B light chain 3A isoform b [Homo sapiens][gi:31563518]	
588621	Inactive			uHTS identification of small molecule inhibitors of Striatal-Enriched Phosphatase via a fluorescence intensity assay	PTPN5 gene product [Homo sapiens][gi:90652859]	
588621	Inactive			uHTS identification of small molecule inhibitors of Striatal-Enriched Phosphatase via a fluorescence intensity assay	PTPN5 gene product [Homo sapiens][gi:90652859]	

AID	Outcome	Activity Concentration Name	Activity Concentration [uM]	BioAssay	Target	PMID
588511	Inactive			Primary cell-based high-throughput screening for identification of compounds that inhibit/block calcium-activated chloride channels (TMEM16A)	Ano1 gene product [Mus musculus][gi:334278898]	
623877	Inactive			Primary cell-based high-throughput screening for identification of compounds that activate/potentiate calcium-activated chloride channels (TMEM16A)	Ano1 gene product [Mus musculus][gi:334278898]	
720543	Inactive			Fluorescence polarization-based biochemical high throughput primary assay to identify inhibitors of alpha/beta hydrolase domain containing 4 (ABHD4).	Abhd4 gene product [Mus musculus][gi:326937491]	
720543	Inactive			Fluorescence polarization-based biochemical high throughput primary assay to identify inhibitors of alpha/beta hydrolase domain containing 4 (ABHD4).	Abhd4 gene product [Mus musculus][gi:326937491]	
2825	Inactive			uHTS Luminescent assay for identification of inhibitors of NALP3 in yeast	NLRP3 protein [Homo sapiens][gi:219518789]	
425	Inactive	IC50		MKP-3 in vitro HTS assay	dual specificity protein phosphatase 6 [Rattus norvegicus][gi:16758752]	
425	Inactive	IC50		MKP-3 in vitro HTS assay	dual specificity protein phosphatase 6 [Rattus norvegicus][gi:16758752]	
602440	Inactive			uHTS Fluorescent Assay Using Nedd8 Protein Substrate for Identification of Inhibitors of Sentrin-Specific Protease 8 (SENP8)	SENP8 gene product [Homo sapiens][gi:262118306]	
2540	Inactive			HTS Luminescent assay for identification of inhibitors of Sentrin-specific protease 8 (SENP8)	SENP8 gene product [Homo sapiens][gi:262118306]	
624466	Inactive			Fluorescence-based cell-based primary high throughput screening assay to identify antagonists of the human trace amine associated receptor 1 (TAAR1)	TAAR1 gene product [Homo sapiens][gi:21264324]	

AID	Outcome	Activity Concentration Name	Activity Concentration [uM]	BioAssay	Target	PMID
624466	Inactive			Fluorescence-based cell-based primary high throughput screening assay to identify antagonists of the human trace amine associated receptor 1 (TAAR1)	TAAR1 gene product [Homo sapiens][gi:21264324]	
624467	Inactive			Fluorescence-based cell-based primary high throughput screening assay to identify agonists of the human trace amine associated receptor 1 (TAAR1)	TAAR1 gene product [Homo sapiens][gi:21264324]	
624467	Inactive			Fluorescence-based cell-based primary high throughput screening assay to identify agonists of the human trace amine associated receptor 1 (TAAR1)	TAAR1 gene product [Homo sapiens][gi:21264324]	
651819	Inactive			High-Throughput Screening for Modulators of Cytosolic Chaperonin Activity	TRIC [Homo sapiens][gi:83758679]	
602346	Inactive			Identification of VIF Inhibitors Measured in Cell-Based System Using Imaging - 2108-01_Inhibitor_SinglePoint_HTS_Activity	Vif [Human immunodeficiency virus 1][gi:9629361]	
651644	Inactive	Potency		qHTS Assay for Inhibitors of the HIV-1 protein Vpr	Vpr [Human immunodeficiency virus 1][gi:28872817]	
624416	Inactive			TRFRET-based biochemical primary high throughput screening assay to identify small molecules that bind to the HIV-1-gp120 binding antibody, PG9	Envelope surface glycoprotein gp160, precursor [Human immunodeficiency virus 1][gi:9629363]	
1565	Inactive	IC50		uHTS absorbance assay for the identification of compounds that inhibit PHOSPHO1	phosphoethanolamine/phosphocholine phosphatase isoform 1 [Homo sapiens][gi:219689097]	
2282	Inactive			Counter screen for compounds that potentiate KCNQ2 potassium channels	Kcnq2 gene product [Rattus norvegicus][gi:18959272]	
2282	Inactive			Counter screen for compounds that potentiate KCNQ2 potassium channels	Kcnq2 gene product [Rattus norvegicus][gi:18959272]	
651631	Inconclusive	Potency	0.3758	qHTS assay for small molecule agonists of the p53 signaling pathway	Cellular tumor antigen p53[gi:269849759]	

AID	Outcome	Activity Concentration Name	Activity Concentration [uM]	BioAssay	Target	PMID
651631	Inconclusive	Potency	0.3758	qHTS assay for small molecule agonists of the p53 signaling pathway	Cellular tumor antigen p53[gi:269849759]	
651631	Inconclusive	Potency	0.3758	qHTS assay for small molecule agonists of the p53 signaling pathway	Cellular tumor antigen p53[gi:269849759]	
651631	Inconclusive	Potency	0.3758	qHTS assay for small molecule agonists of the p53 signaling pathway	Cellular tumor antigen p53[gi:269849759]	
2364	Inconclusive	Potency	0.7943	qHTS Validation Assay for Inhibitors of Bloom's syndrome helicase (BLM)	BLM gene product [Homo sapiens][gi:4557365]	
2528	Inconclusive	Potency	0.7943	qHTS Assay for Inhibitors of Bloom's syndrome helicase (BLM)	BLM gene product [Homo sapiens][gi:4557365]	
2289	Inconclusive	Potency	1.0399	qHTS Assay for Modulators of miRNAs and/or Inhibitors of miR-21		
540276	Inconclusive	Potency	1.2589	qHTS for inhibitors of binding or entry into cells for Marburg Virus	gene 4 small orf - Marburg virus[gi:420597]	
493014	Inconclusive	Potency	1.2995	qHTS Assay to Find Inhibitors of Chronic Active B-Cell Receptor Signaling		
504467	Inconclusive	Potency	1.4581	qHTS screen for small molecules that inhibit ELG1-dependent DNA repair in human embryonic kidney (HEK293T) cells expressing luciferase-tagged ELG1	ATAD5 protein [Homo sapiens][gi:116283940]	
686978	Inconclusive	Potency	2.9855	qHTS for Inhibitors of human tyrosyl-DNA phosphodiesterase 1 (TDP1): qHTS in cells in absence of CPT	TDP1 protein [Homo sapiens][gi:79154014]	
686978	Inconclusive	Potency	2.9855	qHTS for Inhibitors of human tyrosyl-DNA phosphodiesterase 1 (TDP1): qHTS in cells in absence of CPT	TDP1 protein [Homo sapiens][gi:79154014]	

AID	Outcome	Activity Concentration Name	Activity Concentration [uM]	BioAssay	Target	PMID
686978	Inconclusive	Potency	2.9855	qHTS for Inhibitors of human tyrosyl-DNA phosphodiesterase 1 (TDP1): qHTS in cells in absence of CPT	TDP1 protein [Homo sapiens][gi:79154014]	
651631	Inconclusive	Potency	3.3491	qHTS assay for small molecule agonists of the p53 signaling pathway	Cellular tumor antigen p53[gi:269849759]	
651631	Inconclusive	Potency	3.3491	qHTS assay for small molecule agonists of the p53 signaling pathway	Cellular tumor antigen p53[gi:269849759]	
651631	Inconclusive	Potency	3.3491	qHTS assay for small molecule agonists of the p53 signaling pathway	Cellular tumor antigen p53[gi:269849759]	
651631	Inconclusive	Potency	3.3491	qHTS assay for small molecule agonists of the p53 signaling pathway	Cellular tumor antigen p53[gi:269849759]	
540256	Inconclusive	Potency	3.6611	qHTS for Inhibitors of binding or entry into cells for Lassa Virus		
686979	Inconclusive	Potency	4.7318	qHTS for Inhibitors of human tyrosyl-DNA phosphodiesterase 1 (TDP1): qHTS in cells in presence of CPT	TDP1 protein [Homo sapiens][gi:79154014]	
686979	Inconclusive	Potency	4.7318	qHTS for Inhibitors of human tyrosyl-DNA phosphodiesterase 1 (TDP1): qHTS in cells in presence of CPT	TDP1 protein [Homo sapiens][gi:79154014]	
686979	Inconclusive	Potency	4.7318	qHTS for Inhibitors of human tyrosyl-DNA phosphodiesterase 1 (TDP1): qHTS in cells in presence of CPT	TDP1 protein [Homo sapiens][gi:79154014]	
588453	Inconclusive	Potency	6.3096	qHTS Assay for Inhibitors of Mammalian Selenoprotein Thioredoxin Reductase 1 (TrxR1): qHTS	thioredoxin reductase [Rattus norvegicus][gi:8659577]	
588453	Inconclusive	Potency	6.3096	qHTS Assay for Inhibitors of Mammalian Selenoprotein Thioredoxin Reductase 1 (TrxR1): qHTS	thioredoxin reductase [Rattus norvegicus][gi:8659577]	

AID	Outcome	Activity Concentration Name	Activity Concentration [uM]	BioAssay	Target	PMID
914	Inconclusive	Potency	6.3096	qHTS Assay for Identification of Small Molecule Agonists for Hypoxia Response Element Signaling Pathway	hypoxia-inducible factor 1, alpha subunit (basic helix-loop-helix transcription factor) [Homo sapien[gi:32879895]	
914	Inconclusive	Potency	6.3096	qHTS Assay for Identification of Small Molecule Agonists for Hypoxia Response Element Signaling Pathway	hypoxia-inducible factor 1, alpha subunit (basic helix-loop-helix transcription factor) [Homo sapien[gi:32879895]	
914	Inconclusive	Potency	6.3096	qHTS Assay for Identification of Small Molecule Agonists for Hypoxia Response Element Signaling Pathway	hypoxia-inducible factor 1, alpha subunit (basic helix-loop-helix transcription factor) [Homo sapien[gi:32879895]	
915	Inconclusive	Potency	6.3096	qHTS Assay for Identification of Small Molecule Antagonists for Hypoxia Response Element Signaling Pathway	hypoxia-inducible factor 1, alpha subunit (basic helix-loop-helix transcription factor) [Homo sapien[gi:32879895]	
915	Inconclusive	Potency	6.3096	qHTS Assay for Identification of Small Molecule Antagonists for Hypoxia Response Element Signaling Pathway	hypoxia-inducible factor 1, alpha subunit (basic helix-loop-helix transcription factor) [Homo sapien[gi:32879895]	
915	Inconclusive	Potency	6.3096	qHTS Assay for Identification of Small Molecule Antagonists for Hypoxia Response Element Signaling Pathway	hypoxia-inducible factor 1, alpha subunit (basic helix-loop-helix transcription factor) [Homo sapien[gi:32879895]	
504832	Inconclusive	Potency	8.4921	Primary qHTS for delayed death inhibitors of the malarial parasite plastid, 48 hour incubation		
488983	Inconclusive	Potency	8.9125	HTS Assay for Allosteric Agonists of the Human D1 Dopamine Receptor: Primary Screen for Antagonists	D(1A) dopamine receptor [Homo sapiens][gi:4503383]	
488983	Inconclusive	Potency	8.9125	HTS Assay for Allosteric Agonists of the Human D1 Dopamine Receptor: Primary Screen for Antagonists	D(1A) dopamine receptor [Homo sapiens][gi:4503383]	
488983	Inconclusive	Potency	8.9125	HTS Assay for Allosteric Agonists of the Human D1 Dopamine Receptor: Primary Screen for Antagonists	D(1A) dopamine receptor [Homo sapiens][gi:4503383]	

AID	Outcome	Activity Concentration Name	Activity Concentration [uM]	BioAssay	Target	PMID
488983	Inconclusive	Potency	8.9125	HTS Assay for Allosteric Agonists of the Human D1 Dopamine Receptor: Primary Screen for Antagonists	D(1A) dopamine receptor [Homo sapiens][gi:4503383]	
1468	Inconclusive	Potency	8.9125	qHTS for Inhibitors of Tau Fibril Formation, Fluorescence Polarization	Microtubule-associated protein tau [Homo sapiens][gi:92096784]	
1468	Inconclusive	Potency	8.9125	qHTS for Inhibitors of Tau Fibril Formation, Fluorescence Polarization	Microtubule-associated protein tau [Homo sapiens][gi:92096784]	
488745	Inconclusive	Potency	10.4179	Quantitative high throughput screen for delayed death inhibitors of the malarial parasite plastid, 96 hour incubation		
488752	Inconclusive	Potency	10.4179	Quantitative high throughput screen for delayed death inhibitors of the malarial parasite plastid, 48 hour incubation		
720532	Inconclusive	Potency	11.2202	qHTS for Inhibitors of binding or entry into cells for Marburg Virus	gene 4 small orf - Marburg virus[gi:420597]	
1487	Inconclusive	Potency	11.2202	qHTS Assay for Modulators of Lamin A Splicing	prelamin-A/C isoform 3 [Homo sapiens][gi:27436948]	
1882	Inconclusive	Potency	12.5893	qHTS for differential inhibitors of proliferation of Plasmodium falciparum line Dd2		
1876	Inconclusive	Potency	14.1254	qHTS for differential inhibitors of proliferation of Plasmodium falciparum line 3D7		
540276	Inconclusive	Potency	14.581	qHTS for inhibitors of binding or entry into cells for Marburg Virus	gene 4 small orf - Marburg virus[gi:420597]	
540276	Inconclusive	Potency	14.581	qHTS for inhibitors of binding or entry into cells for Marburg Virus	gene 4 small orf - Marburg virus[gi:420597]	

AID	Outcome	Activity Concentration Name	Activity Concentration [uM]	BioAssay	Target	PMID
720532	Inconclusive	Potency	15.8489	qHTS for Inhibitors of binding or entry into cells for Marburg Virus	gene 4 small orf - Marburg virus[gi:420597]	
1877	Inconclusive	Potency	15.8489	qHTS for differential inhibitors of proliferation of Plasmodium falciparum line D10		
485345	Inconclusive	Potency	18.3564	qHTS Validation Assay to Find Inhibitors of Chronic Active B-Cell Receptor Signaling		
1768	Inconclusive	Potency	19.9526	qHTS Assay for Inhibitors Targeting the Menin-MLL Interaction in MLL Related Leukemias: Competition With Texas Red Labeled MLL-derived Mutant Peptide	MEN1 gene product [Homo sapiens][gi:18860839]	
2551	Inconclusive	Potency	19.9526	qHTS for inhibitors of ROR gamma transcriptional activity	nuclear receptor ROR-gamma [Mus musculus][gi:188536040]	
485298	Inconclusive	Potency	23.1093	qHTS Assay for Small Molecule Inhibitors of Mitochondrial Division or Activators of Mitochondrial Fusion		
686978	Inconclusive	Potency	23.1093	qHTS for Inhibitors of human tyrosyl-DNA phosphodiesterase 1 (TDP1): qHTS in cells in absence of CPT	TDP1 protein [Homo sapiens][gi:79154014]	
686978	Inconclusive	Potency	23.1093	qHTS for Inhibitors of human tyrosyl-DNA phosphodiesterase 1 (TDP1): qHTS in cells in absence of CPT	TDP1 protein [Homo sapiens][gi:79154014]	
686978	Inconclusive	Potency	23.1093	qHTS for Inhibitors of human tyrosyl-DNA phosphodiesterase 1 (TDP1): qHTS in cells in absence of CPT	TDP1 protein [Homo sapiens][gi:79154014]	
686978	Inconclusive	Potency	23.715	qHTS for Inhibitors of human tyrosyl-DNA phosphodiesterase 1 (TDP1): qHTS in cells in absence of CPT	TDP1 protein [Homo sapiens][gi:79154014]	
686978	Inconclusive	Potency	23.715	qHTS for Inhibitors of human tyrosyl-DNA phosphodiesterase 1 (TDP1): qHTS in cells in absence of CPT	TDP1 protein [Homo sapiens][gi:79154014]	

AID	Outcome	Activity Concentration Name	Activity Concentration [uM]	BioAssay	Target	PMID
686978	Inconclusive	Potency	23.715	qHTS for Inhibitors of human tyrosyl-DNA phosphodiesterase 1 (TDP1): qHTS in cells in absence of CPT	TDP1 protein [Homo sapiens][gi:79154014]	
720533	Inconclusive	Potency	28.1838	qHTS for Inhibitors of binding or entry into cells for Lassa Virus		
493107	Inconclusive	Potency	29.081	Validation screen for small molecules that inhibit ELG1-dependent DNA repair in human embryonic kidney (HEK293T) cells expressing luciferase-tagged ELG1	ATAD5 protein [Homo sapiens][gi:116283940]	
686979	Inconclusive	Potency	29.0929	qHTS for Inhibitors of human tyrosyl-DNA phosphodiesterase 1 (TDP1): qHTS in cells in presence of CPT	TDP1 protein [Homo sapiens][gi:79154014]	
686979	Inconclusive	Potency	29.0929	qHTS for Inhibitors of human tyrosyl-DNA phosphodiesterase 1 (TDP1): qHTS in cells in presence of CPT	TDP1 protein [Homo sapiens][gi:79154014]	
686979	Inconclusive	Potency	29.0929	qHTS for Inhibitors of human tyrosyl-DNA phosphodiesterase 1 (TDP1): qHTS in cells in presence of CPT	TDP1 protein [Homo sapiens][gi:79154014]	
540256	Inconclusive	Potency	29.0929	qHTS for Inhibitors of binding or entry into cells for Lassa Virus		
624031	Inconclusive	Potency	32.1968	S16 Schwann cell viability assay (CellTiter-Glo assay)		
686979	Inconclusive	Potency	33.4983	qHTS for Inhibitors of human tyrosyl-DNA phosphodiesterase 1 (TDP1): qHTS in cells in presence of CPT	TDP1 protein [Homo sapiens][gi:79154014]	
686979	Inconclusive	Potency	33.4983	qHTS for Inhibitors of human tyrosyl-DNA phosphodiesterase 1 (TDP1): qHTS in cells in presence of CPT	TDP1 protein [Homo sapiens][gi:79154014]	
686979	Inconclusive	Potency	33.4983	qHTS for Inhibitors of human tyrosyl-DNA phosphodiesterase 1 (TDP1): qHTS in cells in presence of CPT	TDP1 protein [Homo sapiens][gi:79154014]	

AID	Outcome	Activity Concentration Name	Activity Concentration [uM]	BioAssay	Target	PMID
485364	Inconclusive	Potency	35.4813	qHTS Assay for the Inhibitors of Schistosoma Mansoni Peroxiredoxins	thioredoxin glutathione reductase [Schistosoma mansoni][gi:15149312]	
504332	Inconclusive	Potency	39.8107	qHTS Assay for Inhibitors of Histone Lysine Methyltransferase G9a	euchromatic histone-lysine N-methyltransferase 2 [Homo sapiens][gi:168985070]	
2147	Inconclusive	Potency	39.8107	qHTS Assay for Inhibitors of Human Jumonji Domain Containing 2E (JMJD2E)	Chain A, Crystal Structure Of The Human 2-Oxoglutarate Oxygenase Loc390245[gi:221046486]	
1030	Inconclusive	Potency	39.8107	qHTS Assay for Inhibitors of Aldehyde Dehydrogenase 1 (ALDH1A1)	aldehyde dehydrogenase 1 family, member A1 [Homo sapiens][gi:30582681]	
1030	Inconclusive	Potency	39.8107	qHTS Assay for Inhibitors of Aldehyde Dehydrogenase 1 (ALDH1A1)	aldehyde dehydrogenase 1 family, member A1 [Homo sapiens][gi:30582681]	
1460	Inconclusive	Potency	44.6684	qHTS for Inhibitors of Tau Fibril Formation, Thioflavin T Binding	Microtubule-associated protein tau [Homo sapiens][gi:92096784]	
1460	Inconclusive	Potency	44.6684	qHTS for Inhibitors of Tau Fibril Formation, Thioflavin T Binding	Microtubule-associated protein tau [Homo sapiens][gi:92096784]	
488949	Inconclusive	Potency	44.6684	qHTS Validation Assay for Inhibitors for MPP8 Chromodomain Interactions with Methylated Histone Tails	MPHOSPH8 gene product [Homo sapiens][gi:41055989]	
504865	Inconclusive	Potency	56.2341	Inhibitors of USP1/UAF1: Pilot qHTS	USP1 protein [Homo sapiens][gi:118600387]	
504333	Inconclusive	Potency	56.2341	qHTS Assay for Inhibitors of BAZ2B	bromodomain adjacent to zinc finger domain 2B [Homo sapiens][gi:6683500]	
488953	Inconclusive	Potency	63.0957	qHTS Validation Assay for Inhibitors of HP1-beta Chromodomain Interactions with Methylated Histone Tails	chromobox protein homolog 1 [Homo sapiens][gi:187960037]	

AID	Outcome	Activity Concentration Name	Activity Concentration [uM]	BioAssay	Target	PMID
1967	Inconclusive	Potency	75.6863	qHTS Assay for Modulators of Human Peripheral Myelin Protein 22 (PMP22) Expression/Activity	peripheral myelin protein 22 [Homo sapiens][gi:4505907]	
504865	Inconclusive	Potency	79.4328	Inhibitors of USP1/UAF1: Pilot qHTS	USP1 protein [Homo sapiens][gi:118600387]	
1440	Inconclusive			Multiplexed high-throughput screen for small molecule regulators of RGS family protein interactions, specifically RGS19-Galphao.	guanine nucleotide-binding protein G(o) subunit alpha isoform a [Homo sapiens][gi:10567816]	
1440	Inconclusive			Multiplexed high-throughput screen for small molecule regulators of RGS family protein interactions, specifically RGS19-Galphao.	guanine nucleotide-binding protein G(o) subunit alpha isoform a [Homo sapiens][gi:10567816]	
1440	Inconclusive			Multiplexed high-throughput screen for small molecule regulators of RGS family protein interactions, specifically RGS19-Galphao.	guanine nucleotide-binding protein G(o) subunit alpha isoform a [Homo sapiens][gi:10567816]	
504749_22	Inconclusive			qHTS profiling for inhibitors of Plasmodium falciparum proliferation		21817045
504749_23	Inconclusive			qHTS profiling for inhibitors of Plasmodium falciparum proliferation		21817045
504749_27	Inconclusive			qHTS profiling for inhibitors of Plasmodium falciparum proliferation		21817045
504749_28	Inconclusive			qHTS profiling for inhibitors of Plasmodium falciparum proliferation		21817045
504749_30	Inconclusive			qHTS profiling for inhibitors of Plasmodium falciparum proliferation		21817045
504749_3	Inconclusive			qHTS profiling for inhibitors of Plasmodium falciparum proliferation		21817045

AID	Outcome	Activity Concentration Name	Activity Concentration [uM]	BioAssay	Target	PMID
504749_41	Inconclusive			qHTS profiling for inhibitors of Plasmodium falciparum proliferation		21817045
504749_45	Inconclusive			qHTS profiling for inhibitors of Plasmodium falciparum proliferation		21817045
504749_50	Inconclusive			qHTS profiling for inhibitors of Plasmodium falciparum proliferation		21817045
504749_59	Inconclusive			qHTS profiling for inhibitors of Plasmodium falciparum proliferation		21817045
504749_38	Inconclusive			qHTS profiling for inhibitors of Plasmodium falciparum proliferation		21817045
504749_49	Inconclusive			qHTS profiling for inhibitors of Plasmodium falciparum proliferation		21817045
504749_51	Inconclusive			qHTS profiling for inhibitors of Plasmodium falciparum proliferation		21817045
504749_5	Inconclusive			qHTS profiling for inhibitors of Plasmodium falciparum proliferation		21817045
504749_9	Inconclusive			qHTS profiling for inhibitors of Plasmodium falciparum proliferation		21817045
504749_12	Inconclusive			qHTS profiling for inhibitors of Plasmodium falciparum proliferation		21817045
504749_14	Inconclusive			qHTS profiling for inhibitors of Plasmodium falciparum proliferation		21817045

AID	Outcome	Activity Concentration Name	Activity Concentration [uM]	BioAssay	Target	PMID
504749_58	Inconclusive			qHTS profiling for inhibitors of Plasmodium falciparum proliferation		21817045
504749_61	Inconclusive			qHTS profiling for inhibitors of Plasmodium falciparum proliferation		21817045
504749_43	Inconclusive			qHTS profiling for inhibitors of Plasmodium falciparum proliferation		21817045
504749_44	Inconclusive			qHTS profiling for inhibitors of Plasmodium falciparum proliferation		21817045
504749_46	Inconclusive			qHTS profiling for inhibitors of Plasmodium falciparum proliferation		21817045
504749_47	Inconclusive			qHTS profiling for inhibitors of Plasmodium falciparum proliferation		21817045
504749_1	Inconclusive			qHTS profiling for inhibitors of Plasmodium falciparum proliferation		21817045
504749_32	Inconclusive			qHTS profiling for inhibitors of Plasmodium falciparum proliferation		21817045
504749_40	Inconclusive			qHTS profiling for inhibitors of Plasmodium falciparum proliferation		21817045
504749_35	Inconclusive			qHTS profiling for inhibitors of Plasmodium falciparum proliferation		21817045
504749_37	Inconclusive			qHTS profiling for inhibitors of Plasmodium falciparum proliferation		21817045

AID	Outcome	Activity Concentration Name	Activity Concentration [uM]	BioAssay	Target	PMID
504749_21	Inconclusive			qHTS profiling for inhibitors of Plasmodium falciparum proliferation		21817045
504749_24	Inconclusive			qHTS profiling for inhibitors of Plasmodium falciparum proliferation		21817045
504749_25	Inconclusive			qHTS profiling for inhibitors of Plasmodium falciparum proliferation		21817045
504749_26	Inconclusive			qHTS profiling for inhibitors of Plasmodium falciparum proliferation		21817045
504749_16	Inconclusive			qHTS profiling for inhibitors of Plasmodium falciparum proliferation		21817045
504749_17	Inconclusive			qHTS profiling for inhibitors of Plasmodium falciparum proliferation		21817045
504749_18	Inconclusive			qHTS profiling for inhibitors of Plasmodium falciparum proliferation		21817045
504749_6	Inconclusive			qHTS profiling for inhibitors of Plasmodium falciparum proliferation		21817045
504749_7	Inconclusive			qHTS profiling for inhibitors of Plasmodium falciparum proliferation		21817045
504749_8	Inconclusive			qHTS profiling for inhibitors of Plasmodium falciparum proliferation		21817045
504749_10	Inconclusive			qHTS profiling for inhibitors of Plasmodium falciparum proliferation		21817045

AID	Outcome	Activity Concentration Name	Activity Concentration [uM]	BioAssay	Target	PMID
504749_11	Inconclusive			qHTS profiling for inhibitors of Plasmodium falciparum proliferation		21817045
504749_13	Inconclusive			qHTS profiling for inhibitors of Plasmodium falciparum proliferation		21817045
2313	Inconclusive			Luminescence Cell-Based Primary HTS to Identify Inhibitors of the Sonic Hedgehog Signaling Pathway		
1332	Inconclusive			High Throughput Screen to Identify Inhibitors of Mycobacterium tuberculosis H37Rv		
1828	Inconclusive			qHTS for Inhibitors of Plasmodium falciparum proliferation: Summary		
593	Inconclusive			qHTS Assay for Spectroscopic Profiling in Fluorescein Spectral Region		
444	Inconclusive			NFAT Signaling Pathway		
590	Inconclusive			qHTS Assay for Spectroscopic Profiling in A350 Spectral Region		
357	Inconclusive			AP1 Signaling Pathway		

Appendix C: GeneGo Structure-Activity Relationship Analyses for Vinpocetine

The GeneGo summary provides an overview of the MetaDrug™ analysis method (version 6.15 build 62452) and the results of the quantitative structure-activity relationship (QSAR) analysis conducted on vinpocetine on August 12, 2013. The background information provided in the GeneGo summary was obtained from the GeneGo Online Help Section (GeneGo, 2013a), unless otherwise noted.

1.1 Background and Overview of MetaDrug Analysis Methodology

MetaDrug, from GeneGo, Inc., combines chemical structural analysis tools (metabolite prediction, QSAR, structural similarity searching), a structure-activity database, and a systems biology database of molecular interactions (protein-protein, compound-protein, protein-enzymatic reaction, compound-enzymatic reaction), canonical signaling and metabolic pathways, and gene-biological property associations.

The MetaDrug analysis starts with uploading a chemical structure. Potential metabolites for the query compound are predicted and separated into major and minor phase 1 and phase 2 metabolites. A suite of pre-defined QSAR models is used to predict chemical and biological properties of the molecule (and, optionally, its metabolites). These include models for substrate affinity, inhibition of metabolic enzymes and transporters, water solubility, blood-brain barrier penetration, and plasma protein binding.

MetaDrug uses three methods with which to associate compounds to protein targets, which are subsequently subjected to functional analysis. The first method uses the MetaBase database, which contains compound-protein interactions. This database directly allows compounds with known biological activities to be incorporated into networks and their pharmacological properties further investigated. The second method uses QSAR predictions of protein target affinity from the included models that define a limited number of potential targets for novel molecules and/or their metabolites submitted for analysis. The third method performs a similarity search for the structure and its major metabolites against the database of existing structures and their targets. Potential targets for novel molecules are inferred through structurally similar compounds in the database (GeneGo, personal communication).

Having defined a list of known and predicted targets using the above approach, MetaDrug uses enrichment analysis (hypergeometric distribution) of the list across nine pre-defined biological ontologies to identify biological pathways, biological, metabolic, or toxicological processes, or diseases that may be affected by interaction of the query compound and its metabolites with biological systems. These are reported as enrichment scores (-log of the hypergeometric p-value) for the top 11 enriched categories in each ontology and, for canonical pathway maps, images of the top three enriched pathway maps with predicted targets of the query compound flagged (GeneGo, personal communication).

1.2 Metabolites

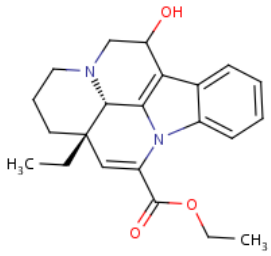
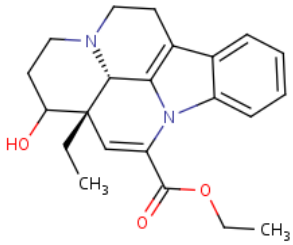
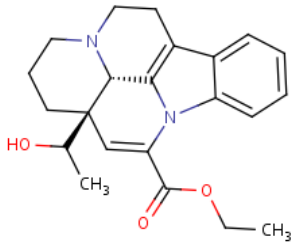
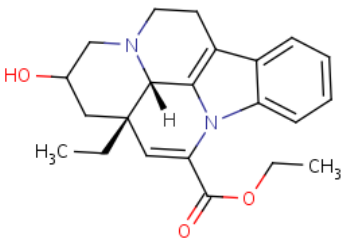
MetaDrug predicts first-pass and second-pass metabolites. Reactions are classified as Phase 1 and Phase 2, respectively. Phase 1 metabolic reactions typically include non-synthetic reactions (e.g., oxidation, reduction, and hydrolysis). These reactions are typically catalyzed by cytochrome P450 (CYP450) enzymes to increase chemical solubility. Phase 2 reactions include

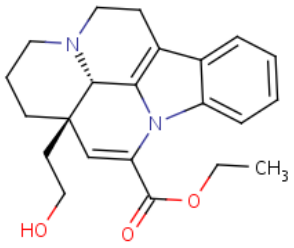
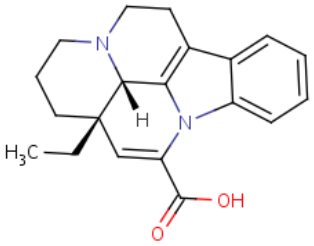
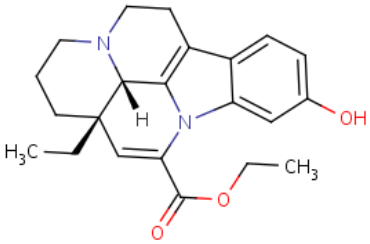
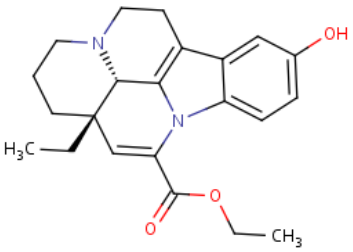
conjugation reactions with glucuronic acid, sulfate, glutathione, and amino acids. These reactions are proposed to target the chemical for excretion. The metabolic pathways describe "most likely metabolic reactions categorized according to the particular type of chemical transformation (e.g., aromatic hydroxylation or ester hydrolysis)." Phase 1 pathways include: C-oxidation, quinone formation, N-oxidation, S-oxidation, P-oxidation, spontaneous (e.g., ketone tautomerization, vicdiol to aldehyde), reduction, and hydrolysis. Phase 2 pathways include: glucuronide transfer, sulfate transfer, glutathione transfer, methyl transfer, cysteine transfer, other conjugation reactions (e.g., O-phosphate transfer), conjugation of amino acids, and N-acetyl transfer.

The metabolic pathways were derived from the analysis of a manually annotated human drug metabolism database that includes xenobiotic reactions, enzyme substrates, and enzyme inhibitors with kinetic data. MetaDrug also includes rules to predict and identify likely reactive metabolites (e.g., quinines and phenols).

In addition to classification as first-pass or second-pass metabolites, metabolites are further classified as predicted major or minor metabolites. The classification of major and minor metabolites is based on a score identified as the occurrence rate (OC). The OC is the "ratio of the occurrence of a particular metabolic reaction to the total number of metabolic reactions in the MetaCore™/MetaDrug™ database." The occurrence frequency is assigned to a metabolite as the negative log value. The greater the score, the higher the frequency the predicted metabolic reaction is present in the database. Major predicted metabolites have the highest OC values. Predicted metabolites are also identified as major metabolites "if they are produced by specific metabolic reactions, or when unique or highly reactive substructures undergo a transformation."

Eight first-pass major metabolites were predicted to occur with vinpocetine. In addition to these metabolites, 10 minor first-pass metabolites, 4 first-pass conjugated metabolites, 30 major second-pass metabolites, 8 minor second-pass metabolites, and 36 second-pass conjugated metabolites were predicted. The structures of the predicted first-pass major metabolites are provided below.

Metabolites					
Pass	**Name**	**Structure**	**SMILES**	**Formula**	**MW**
First pass Major metabolites	2_Aliphatic_hydroxylation1		[H][C@]12N3CCC[C@@]1(CC)C=C(N1C4=C(C=CC=C4)C(C(O)C3)=C21)C(=O)OCC	C22H26N2O3	366.4534
First pass Major metabolites	2_Aliphatic_hydroxylation2		[H][C@]12N3CCC(O)[C@@]1(CC)C=C(N1C4=C(C=CC=C4)C(CC3)=C21)C(=O)OCC	C22H26N2O3	366.4534
First pass Major metabolites	2_Aliphatic_hydroxylation3		[H][C@]12N3CCC[C@]1(C=C(N1C4=C(C=CC=C4)C(CC3)=C21)C(=O)OCC)C(C)O	C22H26N2O3	366.4534
First pass Major metabolites	2_Aliphatic_hydroxylation4		[H][C@@]12N3CCC4=C1N(C1=C4C=CC=C1)C(=C[C@]2(CC)CC(O)C3)C(=O)OCC	C22H26N2O3	366.4534

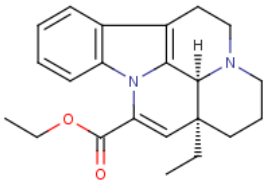
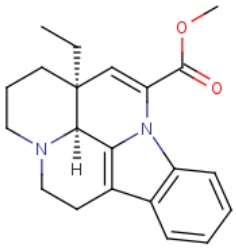
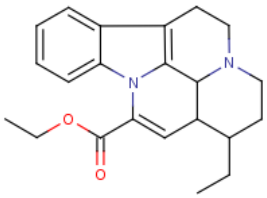
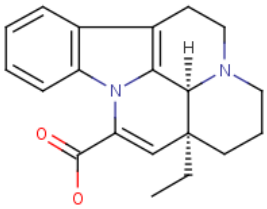
Metabolites					
Pass	**Name**	**Structure**	**SMILES**	**Formula**	**MW**
First pass Major metabolites	2_Aliphatic_hydroxylation5		[H][C@]12N3CCC[C@@]1(CCO)C=C(N1C4=C(C=CC=C4)C(CC3)=C21)C(=O)OCC	C22H26N2O3	366.4534
First pass Major metabolites	2_Aliphatic_hydroxylation6_O-dealkylation1A		[H][C@]12N3CCC[C@@]1(CC)C=C(N1C4=C(C=CC=C4)C(CC3)=C21)C(O)=O	C20H22N2O2	322.4009
First pass Major metabolites	2_Aromatic_hydroxylation1		[H][C@]12N3CCC[C@@]1(CC)C=C(N1C4=C(C=CC(O)=C4)C(CC3)=C21)C(=O)OCC	C22H26N2O3	366.4534
First pass Major metabolites	2_Aromatic_hydroxylation2		[H][C@]12N3CCC[C@@]1(CC)C=C(N1C4=C(C=C(O)C=C4)C(CC3)=C21)C(=O)OCC	C22H26N2O3	366.4534

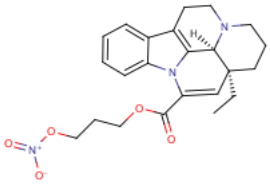
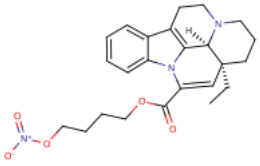
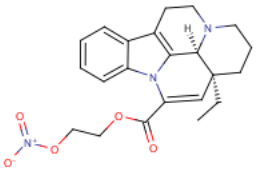
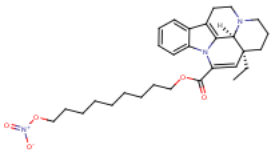
Compared to the predicted aliphatic hydroxylation metabolites, none were identified in human or rat urine. Human and rodent studies indicated that the main metabolite of vinpocetine is apovincaminic acid, which is identified as an *O*-dealkylation metabolite by GeneGo. Veresczkey and Szporny (1976 [PMID:1037219]) also suggested that an aromatic hydroxylated metabolite may be formed in rats; the position of the hydroxyl moiety was not known. Therefore, either or both of the compounds included under the Aromatic Hydroxylation classification by GeneGo could be present in rat urine.

1.3 Structurally Similar Chemicals in Database

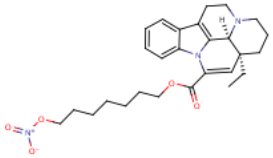
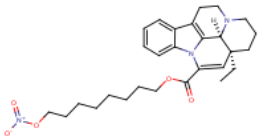
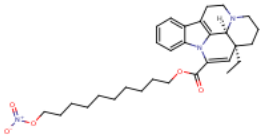
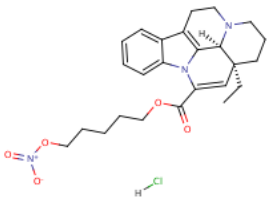
Based on the hypothesis that structurally similar compounds produce similar biological effects, similarity searches are conducted by searching the MetaCore™/MetaDrug™ database and results are ranked based on similarity (%). Two-dimensional fingerprints are developed for each chemical using the Accelrys Accord Cartridge. "Fingerprints are arrays generated for each molecule and containing as its elements binary hashes representing particular substructures (patterns) within that molecule." Similarity is quantified with the Tanimoto coefficient. The Tanimoto coefficient ranges from 0 to 1 and represents the ratio of the number of common fragments to the total number of fragments for two molecules. The greater the value, the greater degree of similarity noted. Seventeen chemicals, including vinpocetine itself, in the GeneGo database were identified as structurally similar to vinpocetine. Only two of the chemicals identified had known targets. Their names, structures, and degree of similarity to vinpocetine are provided below.

Similar compounds for input molecule

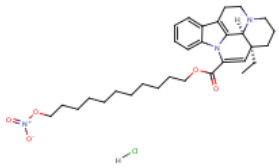
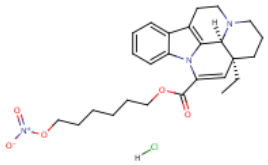
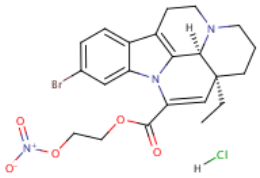
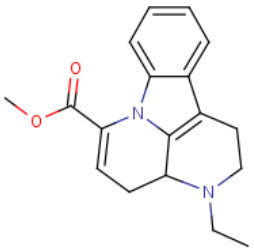
#	Compound in database	Structure	Drug	Input molecule	Similarity, %	Network
1	Vinpocetine		drug	Vinpocetine	100	Yes
2	Apovincamine		drug	Vinpocetine	99.1	
3	1-Ethyl-2,3,4,5,11a,11b-hexahydro-1H-3a,9b-diaza-benzo[cd]fluoranthene-10-carboxylic acid ethyl ester			Vinpocetine	98.81	Yes
4	3a-Ethyl-1,2,3,3a,10,11b-hexahydro-11H-5a,11a-diaza-benzo[cd]fluoranthene-5-carboxylic acid			Vinpocetine	95.48	

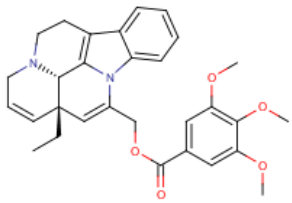
Similar compounds for input molecule						
#	Compound in database	Structure	Drug	Input molecule	Similarity, %	Network
5	(11aS,11bS)-11a-Ethyl-2,3,4,5,11a,11b-hexahydro-1H-3a,9b-diaza-benzo[cd]fluoranthene-10-carboxylic acid 3-nitrooxy-propyl ester			Vinpocetine	95.4	
6	(11aS,11bS)-11a-Ethyl-2,3,4,5,11a,11b-hexahydro-1H-3a,9b-diaza-benzo[cd]fluoranthene-10-carboxylic acid 4-nitrooxy-butyl ester			Vinpocetine	95.13	
7	(11aS,11bS)-11a-Ethyl-2,3,4,5,11a,11b-hexahydro-1H-3a,9b-diaza-benzo[cd]fluoranthene-10-carboxylic acid 2-nitrooxy-ethyl ester			Vinpocetine	95.13	
8	(11aS,11bS)-11a-Ethyl-2,3,4,5,11a,11b-hexahydro-1H-3a,9b-diaza-benzo[cd]fluoranthene-10-carboxylic acid 9-nitrooxy-nonyl ester			Vinpocetine	94.86	

Similar compounds for input molecule

#	Compound in database	Structure	Drug	Input molecule	Similarity, %	Network
9	(11aS,11bS)-11a-Ethyl-2,3,4,5,11a,11b-hexahydro-1H-3a,9b-diaza-benzo[cd]fluoranthene-10-carboxylic acid 7-nitrooxy-heptyl ester			Vinpocetine	94.86	
10	(11aS,11bS)-11a-Ethyl-2,3,4,5,11a,11b-hexahydro-1H-3a,9b-diaza-benzo[cd]fluoranthene-10-carboxylic acid 8-nitrooxy-octyl ester			Vinpocetine	94.86	
11	(11aS,11bS)-11a-Ethyl-2,3,4,5,11a,11b-hexahydro-1H-3a,9b-diaza-benzo[cd]fluoranthene-10-carboxylic acid 10-nitrooxy-decyl ester			Vinpocetine	94.86	
12	(11aS,11bS)-11a-Ethyl-2,3,4,5,11a,11b-hexahydro-1H-3a,9b-diaza-benzo[cd]fluoranthene-10-carboxylic acid 5-nitrooxy-pentyl ester			Vinpocetine	94.86	

Similar compounds for input molecule

#	Compound in database	Structure	Drug	Input molecule	Similarity, %	Network
13	(11aS,11bS)-11a-Ethyl-2,3,4,5,11a,11b-hexahydro-1H-3a,9b-diaza-benzo[cd]fluoranthene-10-carboxylic acid 11-nitrooxy-undecyl ester			Vinpocetine	94.59	
14	(11aS,11bS)-11a-Ethyl-2,3,4,5,11a,11b-hexahydro-1H-3a,9b-diaza-benzo[cd]fluoranthene-10-carboxylic acid 6-nitrooxy-hexyl ester			Vinpocetine	94.59	
15	(11aS,11bS)-8-Bromo-11a-ethyl-2,3,4,5,11a,11b-hexahydro-1H-3a,9b-diaza-benzo[cd]fluoranthene-10-carboxylic acid 2-nitrooxy-ethyl ester			Vinpocetine	90.96	
16	Vinconate		drug	Vinpocetine	89.76	

Similar compounds for input molecule						
#	Compound in database	Structure	Drug	Input molecule	Similarity, %	Network
17	Vinmegallate		drug	Vinpocetine	78.73	

1.4 Possible Targets for Vinpocetine

Compound-target associations are based on the premise that structurally similar compounds have similar biological function. Reported are the predicted target, the input compound (MD object), Tanimoto similarity score (%), MetaDrug database compound to which the input compound is similar, effect of MetaDrug database compound on the target, and references to the literature used to make the compound-target associations.

Several of the predicted targets were based on literature reports describing the noted effects of vinpocetine. Literature reports indicated that vinpocetine inhibited phosphotidesterase 1A, 1B, 1C, and E1. Literature studies also indicated that vinpocetine interacted with the peripheral benzodiazepine receptor and inhibited sodium channels. [Note: Results identify one of the targets as NaV1.6, while the cited reference refers to the sodium channel as $Na_V1.8$ (Zhou et al., 2003).] Based on the interactions of the identified structurally similar compound, phosphodiesterase 3A and 3B were identified as possible targets for vinpocetine.

Possible targets for input molecule						
#	Target	Type	MD object	Similarity, %	Metadrug compound	Effect
1	PDE1		Vinpocetine	100	Vinpocetine	Inhibition
2	Nav1.6		Vinpocetine	100	Vinpocetine	Inhibition
3	PDE1A		Vinpocetine	100	Vinpocetine	Inhibition
4	PDE1A		1-Ethyl-2,3,4,5,11a,11b-hexahydro-1H-3a,9b-diaza-benzo[cd]fluoranthene-10-carboxylic acid ethyl ester	98.81	Vinpocetine	Inhibition
5	PDE1C		Vinpocetine	100	Vinpocetine	Inhibition
6	PDE1C		1-Ethyl-2,3,4,5,11a,11b-hexahydro-1H-3a,9b-diaza-benzo[cd]fluoranthene-10-carboxylic acid ethyl ester	98.81	Vinpocetine	Inhibition
7	PBR		Vinpocetine	100	Vinpocetine	Unspecified
8	Tetrodotoxin-resistant Na(I) channel		Vinpocetine	100	Vinpocetine	Inhibition
9	PDE1B		Vinpocetine	100	Vinpocetine	Inhibition
10	PDE1B		1-Ethyl-2,3,4,5,11a,11b-hexahydro-1H-3a,9b-diaza-benzo[cd]fluoranthene-10-carboxylic acid ethyl ester	98.81	Vinpocetine	Inhibition
11	PDE3A		1-Ethyl-2,3,4,5,11a,11b-hexahydro-1H-3a,9b-diaza-benzo[cd]fluoranthene-10-carboxylic acid ethyl ester	98.81	Vinpocetine	Inhibition
12	PDE3B		1-Ethyl-2,3,4,5,11a,11b-hexahydro-1H-3a,9b-diaza-benzo[cd]fluoranthene-10-carboxylic acid ethyl ester	98.81	Vinpocetine	Inhibition
13	CYP2D6		CYP3A4-sub, prob	0	Vinpocetine	metabolized b
14	CYP1A2		CYP1A2-inh, prob	0	Vinpocetine	Inhibition
15	CYP2C19		CYP2C19-inh, prob	0	Vinpocetine	Inhibition
16	CYP2C9		CYP2C9-inh, prob	0	Vinpocetine	Inhibition
17	MDR1		Pgp-sub, prob	0	Vinpocetine	Inhibition
18	CYP3A4		CYP2D6-sub, prob	0	Vinpocetine	metabolized by

1.5 QSAR

MetaDrug uses the ChemTree™ (Golden Helix) software with recursive partitioning algorithm to calculate QSAR models. A suite of pre-defined QSAR models is used to predict chemical and biological properties of the molecule (and, optionally, its metabolites) such as absorption, metabolism, distribution, excretion, and toxicology. Each model is developed based on literature and/or manually annotated training sets from MetaCore™/MetaDrug™ database.

The recursive partitioning method used in the ChemTree software separates data based on relationships between independent (e.g., atom connectivity) and dependent (e.g., activity) variables. Data separation continues (into nodes) until no further partitions can be made based on pre-defined stopping rules. Parameters that may be adjusted include path length (minimum number of compounds that must be present for a descriptor to be included), maximum segments (maximum number of nodes for any data separation), p-value threshold (disallows any split where the p-value is greater than the threshold), and number of random trees (maximum number of trees that can be generated).

Predicted activity is classified as active or non-active based on calculated values. For non-binary QSAR algorithms, values must comply with two QSAR thresholds to be classified as active. One threshold corresponds to the negative logarithm of activity value of the most active compound of the training set, which defines the predictability limit of the model. The second threshold is the negative logarithm of 50 μM (-1.7), which is considered the lower limit for active chemicals. If the QSAR value falls within these two thresholds, the compound is considered active. For binary QSAR models, values range from 0 to 1.

For non-binary QSAR models, the ideal training set would contain data as similar as possible (e.g., from the same origin, cell line, and experiment type). For the best results in developing binary QSAR models, the training sets used contained approximately equal numbers of positives and negatives. Examples of positives for therapeutic effects included marketed drugs, drug candidates in clinical trials, and preclinical compounds with *in vivo* activity. Chemicals that produce specific adverse effects were defined as producing toxic effects. Chemicals present in the database that produced a particular effect were assigned an arbitrary value of 1, while those that did not produce those effects were assigned a value of 0.

The following tables summarize the results from the GeneGo analyses. The models evaluated included: effects on CYPP450s; protein binding potential; absorption, distribution, metabolism, and excretion; and predicted therapeutic and toxic activities.

CYP450 QSAR Models

Property	Model Description	Value	TP
CYP1A2-inh, prob	Potential to inhibit CYP1A2 at ≤10 μM, range from 0 to 1. Cutoff is 0.5. Values ≥0.5 indicate potential inhibitors.	0.19	54.71
CYP1A2-sub, prob	Potential to be metabolized by CYP1A2, range from 0 to 1. Cutoff is 0.5. Values ≥0.5 indicate that the compound is a substrate for CYP1A2.	0.60	45.38
CYP2B6-sub, prob	Potential to be metabolized by CYP2B6, range from 0 to 1. Cutoff is 0.5. Values ≥0.5 indicate that the compound is a substrate for CYP2B6.	0.34	45.38
CYP2C19-inh, prob	Potential to inhibit CYP2C19 at ≤10 μM, range from 0 to 1. Cutoff is 0.5. Values ≥0.5 indicate potential inhibitors.	0.34	54.71
CYP2C9-inh, prob	Potential to inhibit CYP2C19 at ≤10 μM, range from 0 to 1. Cutoff is 0.5. Values ≥0.5 indicate potential inhibitors.	0.25	54.71
CYP2D6-inh, prob	Potential to inhibit CYP2D6 at ≤10 μM, range from 0 to 1. Cutoff is 0.5. Values ≥0.5 indicate potential inhibitors.	0.62	54.71
CYP2D6-sub, prob	Potential to be metabolized by CYP2D6, range from 0 to 1. Cutoff is 0.5. Values ≥0.5 indicate that the compound is a substrate for CYP2D6.	0.59	52.89
CYP3A4-inh, prob	Potential to inhibit CYP3A4 at ≤10 μM, range from 0 to 1. Cutoff is 0.5. Values ≥0.5 indicate potential inhibitors.	0.38	54.71
CYP3A4-sub, prob	Potential to be metabolized by CYP3A4, range from 0 to 1. Cutoff is 0.5. Values ≥0.5 indicate that the compound is a substrate for CYP3A4.	0.32	52.89
sEH-inh, pIC50	Human soluble epoxide hydrolase inhibition, pIC50 (μM). Cutoff is -1.7. The higher the value, the higher the inhibition activity.	-2.08	33.42

Abbreviation: TP = Tanimoto similarity percentage
Sources: GeneGo (2013a,b)

QSAR modeling results indicate the following predicted properties of vinpocetine (Tanimoto Percentage [TP] values ≥50%):

- An inhibitor of CYP2D6 (0.62, TP = 54.71)
- Not an inhibitor of CYP1A2 (0.19, TP = 54.71), CYP2C19 (0.34, TP = 54.71), CYP2C9 (0.25, TP = 54.71), or CYP3A4 (0.38, TP = 54.71)
- A substrate of CYP2D6 (0.59, TP = 54.89)
- Not a substrate of CYP3A4 (0.32, TP = 52.89)

No data were located to support or contradict these predictions.

Protein Binding QSAR Models

Property	Model Description	Value	TP
5HT2B-act, prob	Potential to activate serotonin receptor 2B at ≤1 µM, range from 0 to 1. Cutoff is 0.5. Values ≥0.5 indicate active compounds.	0.65	49.62
ADR-lig, prob	Potential to bind to androgen receptor, range from 0 to 1. Cutoff is 0.5. Values ≥0.5 indicate potential ligands.	0.02	39.65
ESR-lig, prob	Potential to bind to estrogen receptor at ≤100 µM, range from 0 to 1. Cutoff is 0.5. Values ≥0.5 indicate potential ligands.	0.17	31.60
PXR-act, prob	Pregnane X receptor activation binary model, range from 0 to 1. Values ≥0.5 indicate potential PXR activators.	0.84	33.52
Pgp-inh, pIC50	Human P-glycoprotein transporter inhibition, pIC50 (µM). Cutoff is -1.7. The higher the value, the higher the inhibition activity.	-0.62	45.31
Pgp-sub, prob	Potential to be a substrate for the human P-glycoprotein transporter, range from 0 to 1. Cutoff is 0.5. Values closer to 1 indicate potential ligands.	0.68	52.89
SERT-inh, pKi	Human serotonin transporter inhibition, pKi (µM). Cutoff is -1.7. The higher the value, the higher the inhibition activity of the metabolite.	-0.57	32.45
hERG-inh, pKi	Human ether a-go-go-related gene channel inhibition, pKi (µM). Cutoff is -1.7. The higher the value, the higher the inhibition activity.	-0.49	45.38

Abbreviation: TP = Tanimoto similarity percentage
Sources: GeneGo (2013a,b)

QSAR modeling results indicate that vinpocetine (TP value ≥50%) could be a substrate for human P-glycoprotein transporters (0.68, TP = 52.89). No data were located to support or contradict these predictions.

ADME QSAR Models

Property	Model Description	Value	TP
BBB, log ratio	Blood brain barrier penetration model. The data are expressed as log values of the ratio of the metabolite concentrations in brain and plasma. Cutoff is -0.3. Larger values indicate that the metabolite is more likely to enter the brain.	0.28	44.56
G-logP	Lipophilicity, log of compound octanol-water distribution. Cutoffs are -0.4 to 5.6. Values >5.6 correspond to overly hydrophobic compounds.	3.69	NC
Prot-bind, %	Human serum protein binding, %. Cutoff is 50%. A value of >95% is highly bound and <50% is a low binding metabolite.	70.03	44.56
Prot-bind, log t	Affinity to human serum albumin, log value of the retention time. Cutoff is 0. Positive values correspond to higher protein binding.	-0.06	44.56
WSol, log mg/L	Water solubility at 25 °C, log mg/L. Cutoffs are from 2 to 4.	2.25	NC

Abbreviations: NC = not calculated; TP = Tanimoto similarity percentage
Sources: GeneGo (2013a,b)

The TP values for the ADME prediction models were 44.56, which is slightly below the 50% cutoff used by the system. The models predicted that vinpocetine has some probability of penetrating the blood-brain barrier (0.28), binding to human serum protein (70.03), and binding to human serum albumin (-0.06). [Note: The model description for the blood brain barrier model states "The data is [*sic*] expressed as log values of the ratio of the metabolite concentrations in brain and plasma. … Larger values indicate that the metabolite is more likely to enter the brain."]

PET studies support the prediction that that vinpocetine may penetrate the blood-brain barrier to enter the brain (Gulyas et al., 2002a [PMID:12173017], 2002b [PMID:12460136]). While human studies did not evaluate the binding of vinpocetine to serum proteins or albumin, rat

studies indicated that the majority of plasma vinpocetine after oral administration was protein bound (Vereczkey et al., 1976 [PMID:1037218]).

Prediction of Therapeutic Activity

Property	Model Description	Value	TP
Allergy	Potential antiallergenic activity. Cutoff is 0.5. Values ≥0.5 indicate potentially active compounds.	0.38	47.13
Alzheimer	Potential activity against Alzheimer's disease. Cutoff is 0.5. Values ≥0.5 indicate potentially active compounds.	0.24	44.14
Angina	Potential antianginal activity. Cutoff is 0.5. Values ≥0.5 indicate potentially active compounds.	0.20	44.83
Arthritis	Potential activity against arthritis. Cutoff is 0.5. Values ≥0.5 indicate potentially active compounds.	0.52	37.22
Asthma	Potential activity against asthma. Cutoff is 0.5. Values ≥0.5 indicate potentially active compounds.	0.32	44.14
Bacterial	Potential antibacterial activity. Cutoff is 0.5. Values ≥0.5 indicate potentially active compounds.	0.18	99.10
Cancer	Potential activity against cancer. Cutoff is 0.5. Values ≥0.5 indicate potentially active compounds.	0.36	63.78
Depression	Potential activity against depression. Cutoff is 0.5. Values ≥0.5 indicate potentially active compounds.	0.49	53.74
Diabetes	Potential antidiabetic activity. Cutoff is 0.5. Values ≥0.5 indicate potentially active compounds.	0.11	59.89
HIV	Potential activity against HIV. Cutoff is 0.5. Values ≥0.5 indicate potentially active compounds.	0.21	44.14
Heart failure	Potential activity against heart failure. Cutoff is 0.5. Values ≥0.5 indicate potentially active compounds.	0.68	99.10
Hyperlipidemia	Potential antihyperlipidemic activity. Cutoff is 0.5. Values ≥0.5 indicate potentially active compounds.	0.21	45.19
Hypertension	Potential antihypertensive activity. Cutoff is 0.5. Values ≥0.5 indicate potentially active compounds.	0.62	63.78
Inflammation	Potential anti-inflammatory activity. Cutoff is 0.5. Values ≥0.5 indicate potentially active compounds.	0.21	52.94
Migraine	Potential activity against migraine. Cutoff is 0.5. Values ≥0.5 indicate potentially active compounds.	0.29	44.14
Mycosis	Potential antifungal activity. Cutoff is 0.5. Values ≥0.5 indicate potentially active compounds.	0.29	51.90
Obesity	Potential activity against obesity. Cutoff is 0.5. Values ≥0.5 indicate potentially active compounds.	0.70	41.60
Osteoporosis	Potential anti-osteoporosis activity. Cutoff is 0.5. Values ≥0.5 indicate potentially active compounds.	0.51	55.39
Pain	Potential analgesic activity. Cutoff is 0.5. Values ≥0.5 indicate potentially active compounds.	0.73	53.97
Parkinson	Potential activity against Parkinson's disease. Cutoff is 0.5. Values ≥0.5 indicate potentially active compounds.	0.60	52.94
Psoriasis	Potential activity against psoriasis. Cutoff is 0.5. Values ≥0.5 indicate potentially active compounds.	0.40	38.03
Schizophrenia	Potential activity against schizophrenia. Cutoff is 0.5. Values ≥0.5 indicate potentially active compounds.	0.13	52.89
Skin diseases	Potential activity against skin diseases. Cutoff is 0.5. Values ≥0.5 indicate potentially active compounds.	0.33	53.39
Thrombosis	Potential antithrombotic activity. Cutoff is 0.5. Values ≥0.5 indicate potentially active compounds.	0.25	52.89
Viral	Potential antiviral activity. Cutoff is 0.5. Values ≥0.5 indicate potentially active compounds.	0.39	34.00

Abbreviation: TP = Tanimoto similarity percentage
Sources: GeneGo (2013a,b)

QSAR modeling results indicate the following predicted properties of vinpocetine (TP values ≥50%):

- Potential to treat heart failure (0.68, TP = 99.10)
- Potential to treat hypertension (0.62, TP = 63.78)
- Potential to treat osteoporosis (0.52, TP = 55.39)
- Potential analgesic activity (0.73, TP = 53.97)
- Potential activity against Parkinson's Disease (0.60, TP = 52.94)

No human studies have been identified which indicate that vinpocetine has been used for treatment of any of the endpoints noted above (e.g., hypertension, heart failure, or osteoporosis). Studies have shown that vinpocetine acts as a vasodilator and has been used in the treatment of cerebrovascular-related diseases (Merck Index, 2012; Thorne Research, Inc., 2002). While human studies have indicated that vinpocetine may produce transient hypotensive effects, no studies have been identified where it was evaluated for treatment of heart failure or hypertension. [See **Section 6.0**.] While the anti-inflammatory properties of vinpocetine have been proposed for potential use in the treatment of Parkinson's disease, no human studies assessing this potential have been identified (Medina, 2010). Similarly, while rat studies indicate that vinpocetine may have antinociceptive properties, no human studies have been identified (Salam, 2006). Additionally, no studies assessing the therapeutic potential for treatment of osteoporosis have been noted.

Prediction of Toxic Activity

Property	Model Description	Value	TP
AMES	Potential to be mutagenic (AMES positive), range from 0 to 1. Cutoff is 0.5. A value of 1 is positive (mutagenic).	0.36	51.90
Anemia	Potential for causing anemia. Cutoff is 0.5. Values ≥0.5 indicate potentially toxic compounds. Model organism: human.	0.22	37.22
Carcinogenicity	Potential for inducing cancer in rats and mice. Cutoff is 0.5. Values ≥0.5 indicate potentially toxic compounds.	0.06	99.10
Carcinogenicity Mouse Female	Potential for inducing cancer in female mice. Cutoff is 0.5. Values ≥0.5 indicate potentially toxic compounds.	0.07	48.11
Carcinogenicity Mouse Male	Potential for inducing cancer in male mice. Cutoff is 0.5. Values ≥0.5 indicate potentially toxic compounds.	0.10	59.89
Carcinogenicity Rat Female	Potential for inducing cancer in female rats. Cutoff is 0.5. Values ≥0.5 indicate potentially toxic compounds.	0.15	59.89
Carcinogenicity Rat Male	Potential for inducing cancer in male rats. Cutoff is 0.5. Values ≥0.5 indicate potentially toxic compounds.	0.11	59.89
Cardiotoxicity	Potential for inducing cardiotoxicity. Cutoff is 0.5. Values ≥0.5 indicate potentially toxic compounds. Model organisms: human, rat, mouse.	0.75	34.16
Cytotoxicity, -log GI50 (M)	Growth inhibition of MCF7 cells, pGI50. Cutoff is 6. Values from 6-8 indicate a toxic metabolite. Values below 6 are preferable.	4.92	52.89
Epididymis toxicity	Potential for inducing epididymis toxicity. Cutoff is 0.5. Values ≥0.5 indicate potentially toxic compounds. Model organisms: human, rat, mouse.	0.02	46.72
Genotoxicity	Potential for inducing gentoxicity. Cutoff is 0.5. Values ≥0.5 indicate potentially toxic compounds. Model organisms: rat, mouse.	0.41	48.11
Heptatotoxicity	Potential for inducing hepatoxicity. Cutoff is 0.5. Values ≥0.5 indicate potentially toxic compounds. Model organisms: human, rat, mouse.	0.25	52.89
Kidney necrosis	Potential for inducing kidney necrosis. Cutoff is 0.5. Values ≥0.5 indicate potentially toxic compounds. Model organisms: human, rat, mouse.	0.12	37.22
Kidney weight gain	Potential for inducing kidney weight gain. Cutoff is 0.5. Values ≥0.5 indicate potentially toxic compounds. Model organisms: rat, mouse.	0.06	46.12
Liver cholestasis	Potential for inducing liver cholestasis. Cutoff is 0.5. Values ≥0.5 indicate potentially toxic compounds. Model organisms: human, rat, mouse.	0.63	47.80

Property	Model Description	Value	TP
Liver lipid accumulation	Potential for inducing liver lipid accumulation. Cutoff is 0.5. Values ≥0.5 indicate potentially toxic compounds. Model organisms: human, rat, mouse.	0.15	52.89
Liver necrosis	Potential for inducing liver necrosis. Cutoff is 0.5. Values ≥0.5 indicate potentially toxic compounds. Model organisms: human, rat, mouse.	0.67	39.56
Liver weight gain	Potential for inducing liver weight gain. Cutoff is 0.5. Values ≥0.5 indicate potentially toxic compounds. Model organisms: rat, mouse.	0.54	47.80
MRTD	Maximum Recommended Therapeutic Dose, log mg/kg-bm/day, range from -5 to 3. Cutoff is 0.5. Chemicals with high log MRTDs can be classified as mildly toxic compounds, chemicals with low log MRTDs as highly toxic.	0.00	48.11
Nasal pathology	Potential for causing nasal pathology. Cutoff is 0.5. Values ≥0.5 indicate potentially toxic compounds. Model organisms: human, rat, mouse.	0.04	45.31
Nephron injury	Potential for inducing nephron injury. Cutoff is 0.5. Values ≥0.5 indicate potentially toxic compounds. Model organisms: human, rat, mouse.	0.19	45.78
Nephrotoxicity	Potential for inducing nephrotoxicity. Cutoff is 0.5. Values ≥0.5 indicate potentially toxic compounds. Model organisms: human, rat, mouse.	0.09	45.78
Neurotoxicity	Potential for inducing neurotoxicity. Cutoff is 0.5. Values ≥0.5 indicate potentially toxic compounds. Model organisms: human, rat, mouse.	0.45	46.72
Pulmonary toxicity	Potential for inducing pulmonary toxicity. Cutoff is 0.5. Values ≥0.5 indicate potentially toxic compounds. Model organisms: human, rat, mouse.	0.35	99.10
SkinSens, EC3	Skin sensitization potential expressed as effective concentration 3 (EC3 %). Values >10 indicate weak and moderate sensitizers.	43.05	29.08
Testicular toxicity	Potential for inducing testicular toxicity. Cutoff is 0.5. Values ≥0.5 indicate potentially toxic compounds. Model organisms: human, rat, mouse.	0.08	46.72

Abbreviation: TP = Tanimoto similarity percentage
Sources: GeneGo (2013a,b)

QSAR modeling results indicate the following predicted properties of vinpocetine (TP values ≥50%):

- Negative in the AMES assay (0.36 [0 defined as nonmutagenic], TP = 51.90)
- Exhibit some toxicity towards MCF7 cells (4.92 [values 6-8 were identified as toxic metabolites and values <6 were "preferable"], TP = 52.89).

Of the 22 models evaluated, four predicted that vinpocetine would produce a toxic effect. However, the TP value for each model was <50%.

1.6 GeneGo Functional Ontologies

Enrichment analysis of the identified target list is shown across seven functional biology ontologies; two ontologies (process networks and disease biomarker networks) were not provided since there were no targets provided. The enrichment calculation uses the Fisher's exact test or hypergeometric distribution to calculate the probability that the degree of overlap between the list of possible protein targets generated from the query compound analysis and the proteins represented in the functional ontology category can happen by chance given an identical number of proteins selected at random from the universe of proteins annotated within the ontology. The p-value generated is used to rank order the categories within each ontology by their significance to the list of targets, thereby identifying maps or biological processes likely to be affected by compound exposure (GeneGo, personal communication). Those entries with a p-value ≤0.01000 are highlighted in yellow.

Pathway Maps		
Name	**Map**	**pValue**
Vinpocetine	GTP metabolism	1.419e-07
Vinpocetine	Neurophysiological process_Delta-type opioid receptor in the nervous system	6.681e-06
Vinpocetine	G-protein signaling_Regulation of cAMP levels by ACM	9.571e-06
Vinpocetine	ATP metabolism	1.262e-04
Vinpocetine	Acetaminophen metabolism	3.550e-04
Vinpocetine	Estradiol metabolism	5.186e-04
Vinpocetine	Estradiol metabolism / Human version	5.488e-04
Vinpocetine	Estradiol metabolism / Rodent version	5.799e-04
Vinpocetine	PXR-mediated direct regulation of xenobiotic metabolizing enzymes / Rodent version	6.445e-04
Vinpocetine	CAR-mediated direct regulation of xenobiotic metabolizing enzymes / Rodent version	7.125e-04
Vinpocetine	CAR-mediated direct regulation of xenobiotic metabolizing enzymes / Human version	7.125e-04
Vinpocetine	PXR-mediated direct regulation of xenobiotic metabolizing enzymes / Human version	7.477e-04
Vinpocetine	Signal transduction_PKA signaling	1.102e-03
Vinpocetine	Retinol metabolism / Rodent version	1.952e-03
Vinpocetine	Retinol metabolism	2.185e-03
Vinpocetine	Transcription_Assembly of RNA Polymerase II preinitiation complex on TATA-less promoters	1.784e-02
Vinpocetine	SREBP1 cross-talk with PXR, CAR and LXR	2.568e-02
Vinpocetine	CAR signaling via cross-talk / Human Version	2.568e-02
Vinpocetine	CAR signaling via cross-talk / Rodent version	2.665e-02
Vinpocetine	SREBP1 cross-talk with PXR, CAR and LXR/ Rodent version	3.055e-02
Vinpocetine	Cortisol biosynthesis from Cholesterol	3.055e-02
Vinpocetine	Cholesterol and Sphingolipids transport / Distribution to the intracellular membrane compartments (normal and CF)	3.055e-02
Vinpocetine	Regulation of lipid metabolism_FXR-dependent negative-feedback regulation of bile acids concentration	3.055e-02
Vinpocetine	Estrone metabolism	3.443e-02
Vinpocetine	Estrone metabolism / Human version	3.540e-02
Vinpocetine	Vitamin D2 (ergocalciferol) metabolism	3.733e-02
Vinpocetine	Transport_FXR-regulated cholesterol and bile acids cellular transport	4.119e-02
Vinpocetine	Benzo[a]pyrene metabolism	4.119e-02
Vinpocetine	Niacin-HDL metabolism	4.215e-02
Vinpocetine	Estrogen biosynthesis	4.215e-02
Vinpocetine	Trichloroethylene metabolism/Rodent version	4.407e-02
Vinpocetine	Development_Leptin signaling via PI3K-dependent pathway	4.599e-02
Vinpocetine	Renal secretion of drugs / Rodent version	4.599e-02
Vinpocetine	Regulation of lipid metabolism_Insulin signaling:generic cascades	4.599e-02
Vinpocetine	Serotonin - melatonin biosynthesis and metabolism	4.982e-02
Vinpocetine	Development_Beta-adrenergic receptors signaling via cAMP	5.077e-02
Vinpocetine	Androstenedione and testosterone biosynthesis and metabolism p.1	5.172e-02
Vinpocetine	Regulation of lipid metabolism_Insulin regulation of glycogen metabolism	5.458e-02
Vinpocetine	Muscle contraction_Regulation of eNOS activity in cardiomyocytes	5.458e-02
Vinpocetine	Androstenedione and testosterone biosynthesis and metabolism p.1/ Rodent version	5.553e-02
Vinpocetine	Naphthalene metabolism	5.932e-02
Vinpocetine	Transcription_Role of VDR in regulation of genes involved in osteoporosis	5.932e-02
Vinpocetine	2-Naphthylamine and 2-Nitronaphtalene metabolism	5.932e-02
Vinpocetine	Renin-Angiotensin-Aldosterone System	6.027e-02
Vinpocetine	Transport_Macropinocytosis regulation by growth factors	6.121e-02
Vinpocetine	Catecholamine metabolism	6.968e-02
Vinpocetine	Catecholamine metabolism / Human version	7.062e-02
Vinpocetine	Regulation of lipid metabolism_Insulin regulation of fatty acid methabolism	8.549e-02
Vinpocetine	Transport_Intracellular cholesterol transport in norm	8.641e-02
Vinpocetine	NAD metabolism	1.137e-01

Process Networks		
Name	**Network**	**pValue**
Vinpocetine	Reproduction_Progesterone signaling	1.226e-02
Vinpocetine	Development_Blood vessel morphogenesis	1.397e-02
Vinpocetine	Transport_Sodium transport	1.409e-02
Vinpocetine	Transport_Bile acids transport and its regulation	5.659e-02
Vinpocetine	Regulation of metabolism_Bile acid regulation of lipid metabolism and neg	5.819e-02
Vinpocetine	Cytoskeleton_Macropinocytosis and its regulation	6.932e-02
Vinpocetine	Signal transduction_Leptin signaling	8.582e-02
Vinpocetine	Muscle contraction_Nitric oxide signaling in the cardiovascular system	1.005e-01
Vinpocetine	Development_Skeletal muscle development	1.150e-01
Vinpocetine	Muscle contraction	1.368e-01
Vinpocetine	Signal transduction_Insulin signaling	1.391e-01
Vinpocetine	Development_Neurogenesis_Synaptogenesis	1.420e-01

Disease Biomarker Networks		
Name	**Network**	**pValue**
Vinpocetine	Cystic Fibrosis (core network)	8.603e-02
Vinpocetine	Schizophrenia	9.177e-02
Vinpocetine	Crohn Disease (core network)	1.084e-01
Vinpocetine	Breast neoplasm_Calcium signaling	1.157e-01
Vinpocetine	Breast neoplasm_Gene transcription	1.279e-01
Vinpocetine	Breast neoplasm_PPAR regulation by TGF-beta	1.375e-01
Vinpocetine	Parkinson Disease (core network)	1.842e-01
Vinpocetine	Alzheimer disease (core network)	2.693e-01
Vinpocetine	Hepatitis (core network)	3.582e-01
Vinpocetine	Diabetes Mellitus, Type 2 (core network)	3.803e-01

Drug Target Networks

Name	Network	pValue
Vinpocetine	Metabolism_Cyclic phosphodiesterases_Nucleotide metabolism	2.161e-09
Vinpocetine	Transport_Sodium transport	8.021e-03
Vinpocetine	Metabolism_Steroid hormone metabolism (fragment)	1.642e-01
Vinpocetine	Cell adhesion_Collagen Prolyl 4-Hydroxylase activity	1.775e-01
Vinpocetine	Signal transduction_IGF-1, CREB1 signaling	1.948e-01
Vinpocetine	Signal transduction_TGF-beta signaling	2.034e-01
Vinpocetine	Signal transduction_GPCR, p53 signaling	2.245e-01
Vinpocetine	Signal transduction_CREBP1, p53, C_EBPbeta signaling	2.327e-01
Vinpocetine	Signal transduction_CCR1-SP1 signaling	2.450e-01
Vinpocetine	Transmission of nerve impulse_Voltage channels	2.651e-01

Toxicity Networks

Name	Network	pValue
Vinpocetine	Signal transduction_AMPK	3.104e-02
Vinpocetine	Transport_Monovalent cation transport	4.692e-02
Vinpocetine	Metabolism_Biogenic amine metabolism	6.000e-02
Vinpocetine	Metabolism_CYP's and Fanconi anemia group proteins	6.519e-02
Vinpocetine	Metabolism_Protein biosynthesis	6.907e-02
Vinpocetine	Metabolism_Lipid metabolism_Leptin regulation	6.907e-02
Vinpocetine	Metabolism_Xenobiotic metabolism	7.164e-02
Vinpocetine	Signal transduction_Carnitine palmitoyltransferase 1B (muscle)	8.318e-02

Metabolic Networks		
Name	**Network**	**pValue**
Vinpocetine	CYP3A4-9-IL1-CAR	6.514e-04
Vinpocetine	CYP3A4-6-WNT-HNF3	6.655e-04
Vinpocetine	Steroid metabolism_Estrone and Estradiol metabolism	6.798e-04
Vinpocetine	CYP3A4-5-WNT-HNF3	7.087e-04
Vinpocetine	CYP3A4-5-Insulin-C/EBP-IRS2	7.532e-04
Vinpocetine	CYP3A4-5-Insulin-C/EBP-IRS1	8.304e-04
Vinpocetine	CYP3A4-5-Leptin-C/EBP-IRS2	8.304e-04
Vinpocetine	CYP3A4-6-Leptin-C/EBP-IRS1	8.784e-04
Vinpocetine	Steroid metabolism_Pregnenolone and progesterone metabolism	8.948e-04
Vinpocetine	Steroid metabolism_Cortisol, cortisone and corticosterone metabolism	9.786e-04
Vinpocetine	1-alkyl-2-lyso-glycerophosphocholine pathway	2.382e-02
Vinpocetine	CYP3A4-5-Glucagon-HNF4	3.793e-02
Vinpocetine	(L)-carnitine pathway	3.887e-02
Vinpocetine	CYP3A4-2-Glucagon-HNF4	3.981e-02
Vinpocetine	CYP3A4-11-IL1-CAR	4.074e-02
Vinpocetine	CYP2D6-6-Glucagon-HNF4	4.074e-02
Vinpocetine	CYP3A4-5-Leptin-C/EBP-IRS1	4.121e-02
Vinpocetine	CYP2D6-5-Glucagon-HNF4	4.121e-02
Vinpocetine	CYP3A4-3-Glucagon-HNF4	4.121e-02
Vinpocetine	CYP3A4-1-IL1-CAR	4.214e-02
Vinpocetine	CYP2D6-3-Glucagon-HNF4	4.214e-02
Vinpocetine	CYP3A4-1-WNT-HNF3	4.214e-02
Vinpocetine	CYP3A4-1-LPS-CAR	4.261e-02
Vinpocetine	CYP3A4-9-Glucagon-HNF4	4.307e-02
Vinpocetine	CYP3A4-9-Leptin-C/EBP-IRS1	4.307e-02
Vinpocetine	CYP3A4-11-Glucagon-HNF4	4.307e-02
Vinpocetine	CYP3A4-9-Insulin-C/EBP-IRS1	4.307e-02
Vinpocetine	CYP3A4-9-Insulin-C/EBP-IRS2	4.354e-02
Vinpocetine	CYP3A4-12-IL1-CAR	4.354e-02
Vinpocetine	CYP3A4-12-Glucagon-HNF4	4.354e-02
Vinpocetine	CYP3A4-5-IL1-CAR	4.401e-02
Vinpocetine	CYP3A4-2-WNT-HNF3	4.401e-02
Vinpocetine	CYP3A4-1-Leptin-C/EBP-IRS2	4.401e-02
Vinpocetine	CYP3A4-11-WNT-HNF3	4.494e-02
Vinpocetine	CYP3A4-4-IL1-CAR	4.540e-02
Vinpocetine	CYP3A4-1-Insulin-C/EBP-IRS1	4.540e-02
Vinpocetine	CYP3A4-7-Glucagon-HNF4	4.540e-02
Vinpocetine	CYP3A4-2-IL1-CAR	4.540e-02
Vinpocetine	CYP3A4-2-LPS-CAR	4.540e-02
Vinpocetine	CYP3A4-2-Insulin-C/EBP-IRS2	4.540e-02
Vinpocetine	CYP3A4-1-Leptin-C/EBP-IRS1	4.540e-02
Vinpocetine	CYP3A4-8-WNT-HNF3	4.587e-02
Vinpocetine	CYP3A4-12-Leptin-C/EBP-IRS2	4.587e-02
Vinpocetine	CYP3A4-11-LPS-CAR	4.587e-02
Vinpocetine	CYP3A4-8-Leptin-C/EBP-IRS1	4.634e-02
Vinpocetine	CYP3A4-4-WNT-HNF3	4.634e-02
Vinpocetine	CYP3A4-3-Leptin-C/EBP-IRS1	4.634e-02
Vinpocetine	CYP3A4-9-WNT-HNF3	4.634e-02
Vinpocetine	CYP3A4-12-Insulin-C/EBP-IRS1	4.680e-02
Vinpocetine	CYP3A4-2-Leptin-C/EBP-IRS2	4.680e-02

GO Processes		
Name	**Process**	**pValue**
Vinpocetine	cAMP catabolic process	4.012e-16
Vinpocetine	cGMP catabolic process	9.334e-12
Vinpocetine	activation of phospholipase C activity	1.088e-07
Vinpocetine	negative regulation of insulin secretion	2.991e-06
Vinpocetine	fibroblast growth factor receptor signaling pathway	4.245e-06
Vinpocetine	cellular response to granulocyte macrophage colony-stimulating factor stimulus	4.941e-06
Vinpocetine	epidermal growth factor receptor signaling pathway	8.111e-06
Vinpocetine	alkaloid catabolic process	9.217e-06
Vinpocetine	cellular response to macrophage colony-stimulating factor stimulus	9.217e-06
Vinpocetine	regulation of smooth muscle cell apoptotic process	9.217e-06
Vinpocetine	blood coagulation	2.087e-05
Vinpocetine	regulation of smooth muscle cell proliferation	2.170e-05
Vinpocetine	drug catabolic process	2.170e-05
Vinpocetine	heterocycle metabolic process	2.170e-05
Vinpocetine	monoterpenoid metabolic process	2.170e-05
Vinpocetine	serotonin metabolic process	2.563e-05
Vinpocetine	regulation of dopamine metabolic process	3.448e-05
Vinpocetine	neurotrophin TRK receptor signaling pathway	3.901e-05
Vinpocetine	diterpenoid metabolic process	3.940e-05
Vinpocetine	regulation of neurotransmitter levels	3.940e-05
Vinpocetine	metabolic process	4.008e-05
Vinpocetine	locomotory behavior	4.127e-05
Vinpocetine	oxidative demethylation	4.464e-05
Vinpocetine	steroid metabolic process	1.276e-04
Vinpocetine	monocyte differentiation	1.831e-04
Vinpocetine	response to amphetamine	3.364e-04
Vinpocetine	drug metabolic process	3.664e-04
Vinpocetine	visual learning	5.919e-04
Vinpocetine	sodium ion transmembrane transport	8.010e-04
Vinpocetine	innate immune response	8.133e-04
Vinpocetine	negative regulation of cellular organofluorine metabolic process	1.199e-03
Vinpocetine	membrane depolarization involved in regulation of action potential	1.199e-03
Vinpocetine	response to vitamin B1	1.199e-03
Vinpocetine	response to calcium ion	1.740e-03
Vinpocetine	alkaloid metabolic process	1.799e-03
Vinpocetine	contact inhibition	1.799e-03
Vinpocetine	SA node cell to atrial cardiac muscle cell communication	1.799e-03
Vinpocetine	positive regulation of oocyte development	2.397e-03
Vinpocetine	isoquinoline alkaloid metabolic process	2.397e-03
Vinpocetine	cardiac ventricle development	2.397e-03
Vinpocetine	signal transduction	2.991e-03
Vinpocetine	cellular response to cGMP	2.996e-03
Vinpocetine	membrane depolarization involved in regulation of SA node cell action potential	2.996e-03
Vinpocetine	negative regulation of binding	2.996e-03
Vinpocetine	cellular hypotonic response	2.996e-03
Vinpocetine	regulation of atrial cardiac muscle cell membrane repolarization	2.996e-03
Vinpocetine	AV node cell to bundle of His cell communication	2.996e-03
Vinpocetine	sodium ion transport	3.152e-03
Vinpocetine	positive regulation of mitochondrial depolarization	3.594e-03
Vinpocetine	positive regulation of necrotic cell death	3.594e-03

GO Molecular Functions		
Name	**Function**	**pValue**
Vinpocetine	3',5'-cyclic-AMP phosphodiesterase activity	2.015e-14
Vinpocetine	3',5'-cyclic-nucleotide phosphodiesterase activity	1.347e-12
Vinpocetine	phosphoric diester hydrolase activity	6.540e-11
Vinpocetine	calmodulin-dependent cyclic-nucleotide phosphodiesterase activity	1.560e-10
Vinpocetine	calcium- and calmodulin-regulated 3',5'-cyclic-GMP phosphodiesterase ac	1.560e-10
Vinpocetine	cAMP binding	1.768e-07
Vinpocetine	cGMP-inhibited cyclic-nucleotide phosphodiesterase activity	3.209e-07
Vinpocetine	calmodulin binding	2.950e-06
Vinpocetine	cyclic-nucleotide phosphodiesterase activity	8.967e-06
Vinpocetine	catalytic activity	3.777e-05
Vinpocetine	voltage-gated sodium channel activity	3.833e-05
Vinpocetine	hydrolase activity	1.274e-04
Vinpocetine	sodium channel activity	1.677e-04
Vinpocetine	quinine 3-monooxygenase activity	5.941e-04
Vinpocetine	taurochenodeoxycholate 6alpha-hydroxylase activity	5.941e-04
Vinpocetine	albendazole monooxygenase activity	5.941e-04
Vinpocetine	voltage-gated sodium channel activity involved in regulation of SA node ce	5.941e-04
Vinpocetine	steroid 21-monooxygenase activity	1.781e-03
Vinpocetine	drug binding	1.925e-03
Vinpocetine	monooxygenase activity	2.315e-03
Vinpocetine	vitamin D 24-hydroxylase activity	2.374e-03
Vinpocetine	androgen binding	2.967e-03
Vinpocetine	vitamin D3 25-hydroxylase activity	2.967e-03
Vinpocetine	voltage-gated sodium channel activity involved in regulation of cardiac mus	2.967e-03
Vinpocetine	testosterone 6-beta-hydroxylase activity	2.967e-03
Vinpocetine	voltage-gated ion channel activity	3.507e-03
Vinpocetine	xenobiotic-transporting ATPase activity	3.560e-03
Vinpocetine	arachidonic acid monooxygenase activity	3.560e-03
Vinpocetine	benzodiazepine receptor activity	4.152e-03
Vinpocetine	caffeine oxidase activity	4.744e-03
Vinpocetine	heme binding	4.879e-03
Vinpocetine	iron ion binding	5.201e-03
Vinpocetine	protein kinase B binding	5.335e-03
Vinpocetine	sodium ion binding	5.926e-03
Vinpocetine	metal ion binding	6.215e-03
Vinpocetine	electron carrier activity	6.643e-03
Vinpocetine	ATPase activity, coupled	7.108e-03
Vinpocetine	cGMP binding	8.878e-03
Vinpocetine	steroid hydroxylase activity	1.182e-02
Vinpocetine	ankyrin binding	1.241e-02
Vinpocetine	enzyme binding	1.241e-02
Vinpocetine	fibroblast growth factor binding	1.476e-02
Vinpocetine	ion channel activity	1.530e-02
Vinpocetine	scaffold protein binding	1.768e-02
Vinpocetine	ATPase activity, coupled to transmembrane movement of substances	2.060e-02
Vinpocetine	cholesterol binding	2.177e-02
Vinpocetine	oxidoreductase activity, acting on paired donors, with incorporation or red	2.235e-02
Vinpocetine	oxygen binding	2.410e-02
Vinpocetine	phosphoprotein binding	2.526e-02
Vinpocetine	steroid binding	2.874e-02

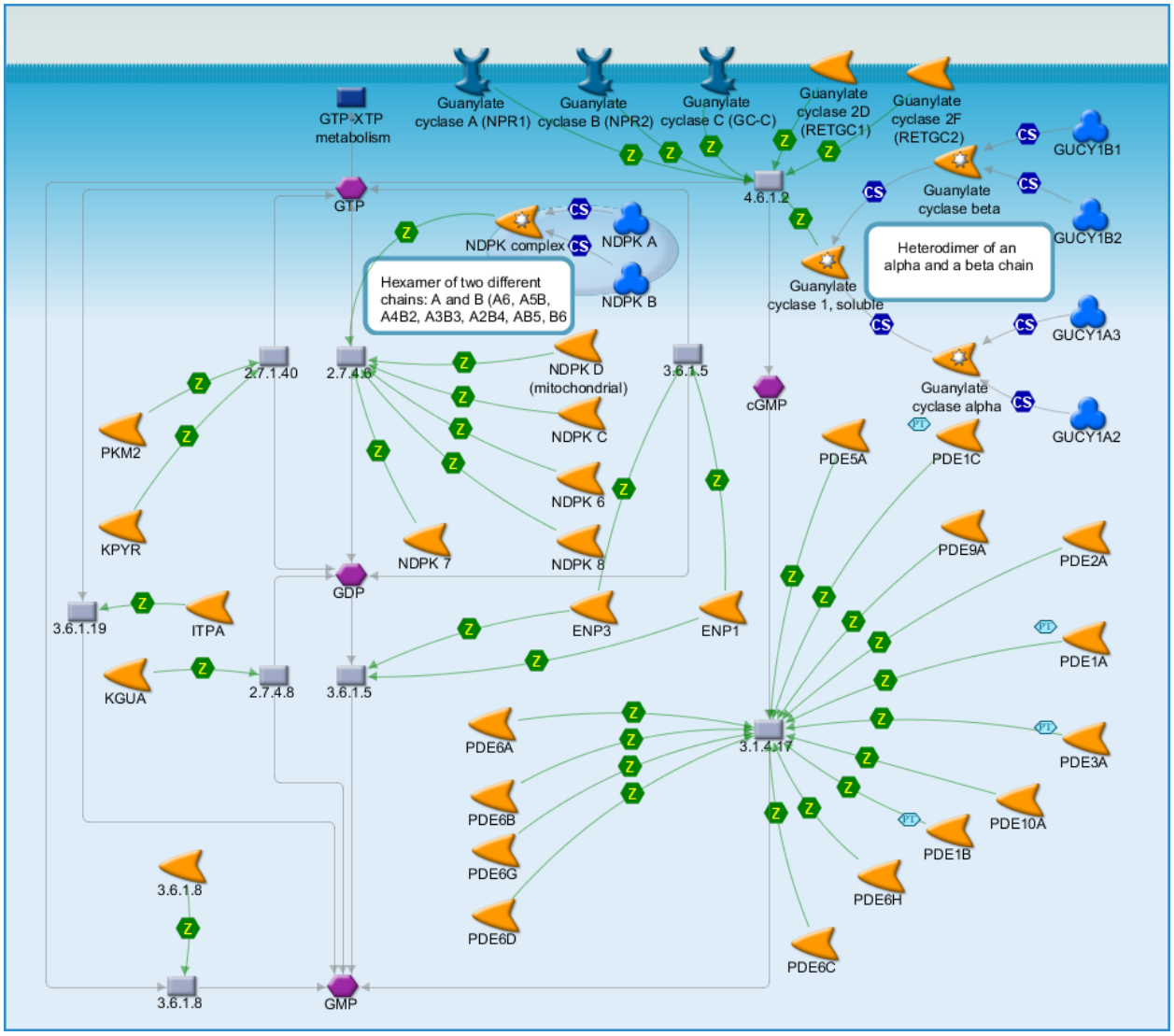
GO Localizations

Name	Localization	pValue
Vinpocetine	sodium channel complex	5.874e-06
Vinpocetine	voltage-gated sodium channel complex	2.540e-05
Vinpocetine	neuronal cell body	4.714e-05
Vinpocetine	organelle membrane	1.454e-03
Vinpocetine	cell surface	1.748e-03
Vinpocetine	guanyl-nucleotide exchange factor complex	3.313e-03
Vinpocetine	intercellular canaliculus	5.515e-03
Vinpocetine	axon initial segment	6.615e-03
Vinpocetine	node of Ranvier	7.714e-03
Vinpocetine	cytosol	1.069e-02
Vinpocetine	intercalated disc	2.027e-02
Vinpocetine	T-tubule	2.460e-02
Vinpocetine	endoplasmic reticulum	2.513e-02
Vinpocetine	integral to membrane	2.556e-02
Vinpocetine	caveola	3.909e-02
Vinpocetine	intracellular membrane-bounded organelle	4.434e-02
Vinpocetine	sarcolemma	5.444e-02
Vinpocetine	Z disc	5.811e-02
Vinpocetine	endoplasmic reticulum membrane	6.584e-02
Vinpocetine	mitochondrial outer membrane	7.421e-02
Vinpocetine	cytoplasmic membrane-bounded vesicle	7.575e-02
Vinpocetine	cilium	1.081e-01
Vinpocetine	membrane	1.309e-01
Vinpocetine	apical plasma membrane	1.457e-01
Vinpocetine	dendrite	1.656e-01
Vinpocetine	mitochondrion	2.466e-01
Vinpocetine	Golgi membrane	2.508e-01
Vinpocetine	cytoplasm	4.358e-01
Vinpocetine	Golgi apparatus	4.708e-01
Vinpocetine	plasma membrane	4.756e-01
Vinpocetine	nucleolus	6.179e-01
Vinpocetine	nucleus	9.193e-01

1.7 Top GeneGo Pathway Maps

GeneGo pathway maps comprise pictorial representations of human and rodent signaling and metabolic pathways. The three most significant maps are shown below. Compounds are represented by purple hexagons, proteins by colored shapes representing different classes of compound, and enzymatic reactions by gray rectangles. Protein-protein, compound-protein, and compound-reaction interactions are shown as unidirectional arrows, and a mechanism of interaction is represented by letters in hexagonal boxes over the arrows.

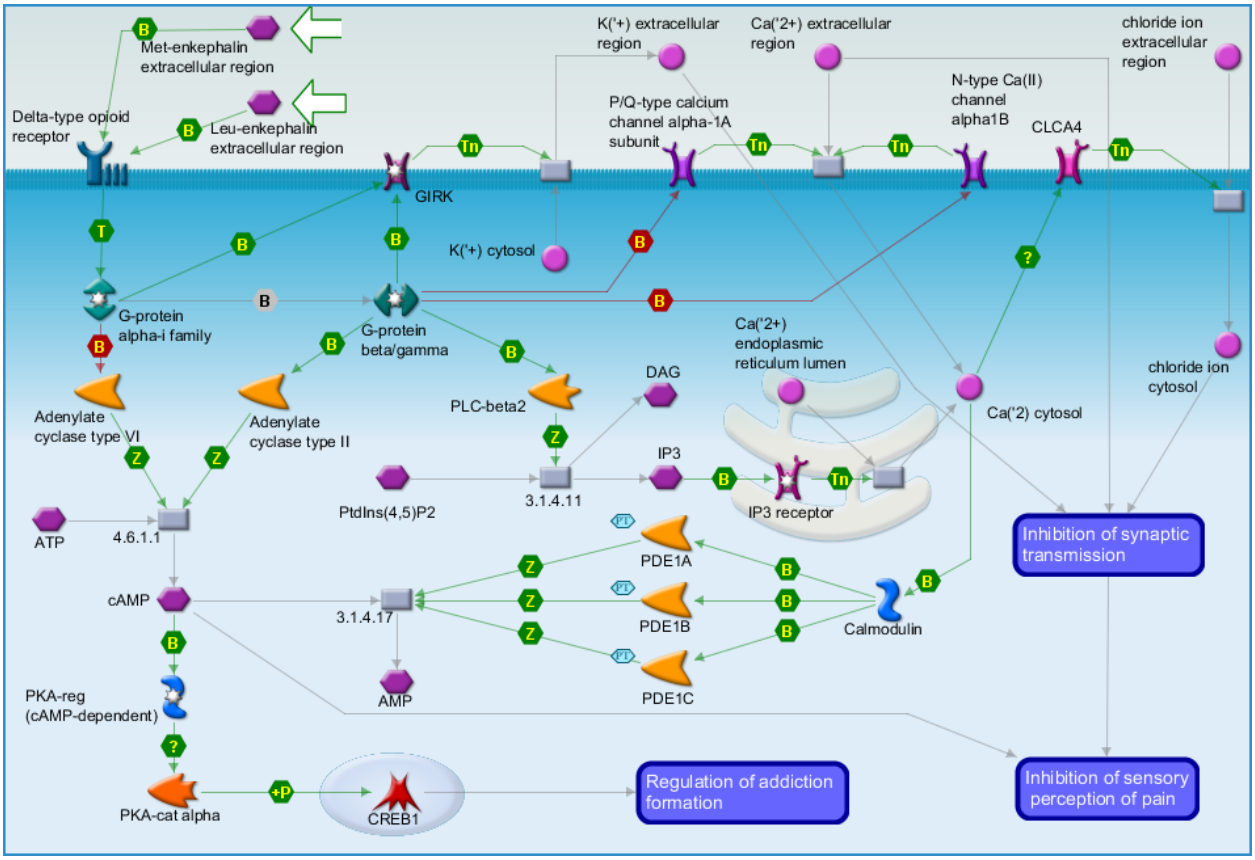
1.7.1 GTP Metabolism



Guanine triphosphate (GTP) may be metabolized through a variety of mechanisms. Activation of atrial natriuretic peptide receptor 1 or 2 or heat stable enterotoxin receptor, which has guanylyl cyclase activity, leads to formation of cyclic guanosine monophosphase (cGMP). Activation of various guanylate cyclase enzymes also lead to formation of cGMP. cGMP may then be further metabolized to gunosine monophosphate through actions of phophodiesterase enzymes. GTP

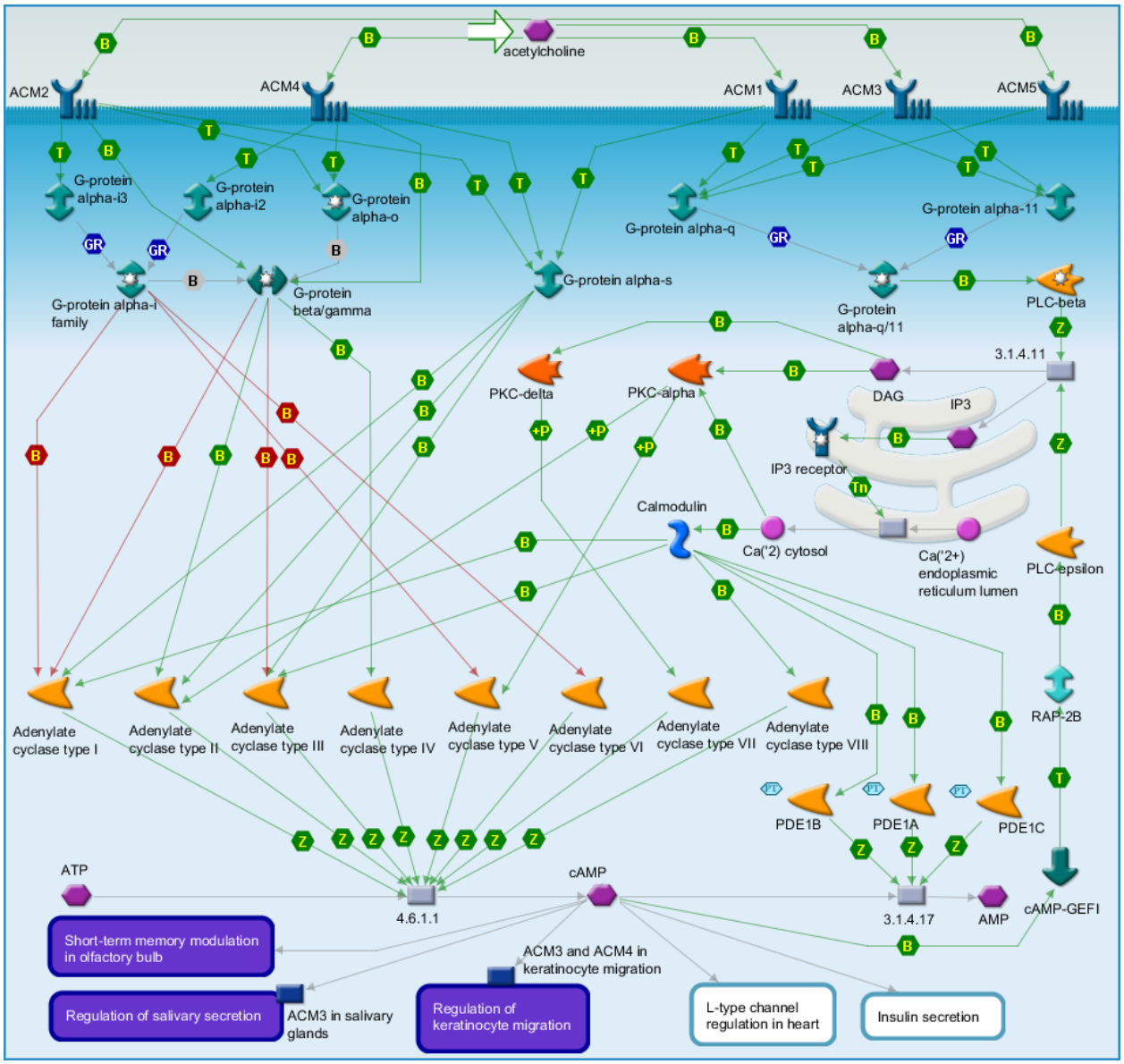
also may be metabolized by the action of ectonucleoside triphosphate diphosphohydrolase 1 or 3 or inosine triphosphate pyrophosphatase (GeneGo, 2012).

1.7.2 Neurophysiological Process_Delta-Type Opioid Receptor in the Nervous System



Delta-opioid receptors are encompassed within the class of guanine nucleotide binding protein (G-protein) coupled receptors (GPCRs). Endogenous ligands for the receptor are Met-enkephalin and Leu-enkephalin. Activation of the δ-opioid receptor is associated with inhibition of synaptic transmission which leads to inhibition of pain perception. Receptor activation leads to dissociation of the G-protein α subunit and β/γ subunits from the trimeric protein which then may activate the G-protein inwardly rectifying channel. The β/γ subunits also modulate cell surface calcium channels and activate phospholipase C β2, which leads to reduction of cell excitability and inhibition of synaptic transmission. The α subunit, as well as the β/γ subunits, modulate adenylate cyclase activity which leads to formation of cyclic adenosine monophosphate (cAMP), which leads to inhibition of pain perception. c AMP formation also leads to phosphorylation and activation of cAMP responsive element binding protein 1 (CREB1). CREB1 plays a role in addiction formation. cAMP may be metabolized by phosphodiesterase 1A, 1B, and/or 1C to form adenosine monophosphate. P hospodiesterase activity is regulated by intracellular calcium levels effects on calmodulin (GeneGo, 2013c).

1.7.3 G-protein Signaling_Regulation of cAMP levels by ACM



Muscarinic cholinergic receptors produce numerous effects through modulation of cAMP and internal calcium levels. cA MP levels are regulated through receptor-mediated modulate of adenylate cyclase isoforms. T he different muscarinic receptors modulate various adenylate cylcase isoforms differently (e.g., M2 inhibits adenylate cyclase type 5 while M1 activates adenylate cylcase type 1). Calcium levels are modulated through regulation of phopolipase C β activity, which leads to release of calcium from internal stores. C alcium levels modulate calmodulin activity which regulates adenylate cyclase and phosphodiesterase activity. cAMP is shown to play a role in regulation of salivary secretion, regulation of keratinocyte migration, and insulin secretion. cAMP may be metabolized by phosphodiesterase 1A, 1B, and/or 1C to form adenosine monophosphate (GeneGo, 2013d).

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Units and Abbreviations

μM = micromolar
cAMP = cyclic adenosime monophosphate
cGMP = cyclic guanosine monophosphase
CREB1 = cAMP responsive element binding protein 1
CYP450 = cytochrome P450
FDA = U.S. Food and Drug Administration
G-protein = guanine nucleotide binding protein
GPCRs = G-protein coupled receptors
GTP = guanine triphosphate
NC = not calculated
OC = occurrence rate
QSAR = quantitative structure-activity relationship
TP = Tanimoto (similarity) percentage

Appendix D: Leadscope Structure-Activity Relationship Analyses for Vinpocetine

This summary provides an overview of the Leadscope method and the results of the quantitative structure-activity relationship (QSAR) analysis conducted on vinpocetine on August 12, 2013. The background information provided in this summary was obtained from the *Leadscope Model Applier Documentation* (Leadscope Inc., 2009), unless otherwise noted.

1.1 Background and Overview of Leadscope Analysis Methodology

The QSAR model suites are divided into (1) human clinical endpoints and (2) non-human toxicity endpoints. The human clinical endpoint suites model potential adverse cardiac effects, adverse hepatobiliary effects, and adverse urinary tract effects. The non-human toxicity endpoints are comprised of rodent carcinogenicity, genetic toxicity, reproductive toxicity, developmental toxicity, and neurotoxicity.

Most of the QSAR models used in this analysis were based on public information, which included structures of the chemicals present in the training set and the biological/toxicological result for the particular endpoint being modeled. The exceptions are the rodent, rat, and mouse carcinogenicity models, which were developed using confidential data. The QSAR models were constructed by the Informatics and Computational Safety Analysis Staff at the U.S. Food and Drug Administration (FDA) within the Leadscope Prediction Data Miner software. In designing the models, all default settings were used.

The modeling strategy was described in six steps by Yang and colleagues (2004):

(1) diagnose the data set – data set is analyzed for structural diversity, similarity, and distribution
(2) assembly of macrostructures - macrostructures associated with activity are identified
(3) preselection of features – selection of a subset of features based on statistical analyses
(4) develop model – model is developed based on selected model building algorithms
(5) evaluate the model with chemical inference – evaluate results of known chemicals and evaluate why model worked or failed for particular chemicals
(6) refine model – based on evaluation, refine model with new features

Structural features and calculated properties are used to develop the models. "The structural features include Leadscope® default hierarchy features plus the predictive scaffolds generated with default settings." In addition to the structural features, calculated properties are used. These are: parent molecular weight, LogP, polar surface area, hydrogen bond acceptors, hydrogen bond donors, number of rotational bonds, and Lipinski score (rule violation). [Note: The *Leadscope Model Applier Documentation* notes that there were eight calculated properties used, but seven are listed. In reviewing an article discussing the prediction modeling methodology used, it was noted that in addition to the seven calculated properties that the calculated property of parent atom count was also noted (Yang et al., 2004).]

Predictive performance of a model is dependent on the ratio of active to inactive compounds present in the training set. Sub-models were developed for some of the models to improve predictive performance. The active/inactive compound ratios were between 0.30 and 0.35 for these sub-models. Overall prediction results were based on averaging the probabilities for the sub-models.

Output from the models includes a prediction status and a prediction probability. The prediction status of a test compound was defined as "positive," "negative," or "not-in-domain." Test compounds are defined as "not-in-domain" when they are not within the parameters of the specified model. "The model domain is defined within the Leadscope application for two factors: 1) containing structural model features in addition to property descriptors; 2) being within a similar structure group with at least 30 % similarity." The prediction probability is given as a value between 0 and 1. The greater the number, the greater the likelihood that the test compound is toxic for the evaluated model. Within the FDA, a probability ≥0.5 is defined as active.

In addition to the prediction status and prediction probability, the structural features and calculated properties associated with the predicted activity are provided for review. For the models that were developed using confidential data, the Leadscope default hierarchy is provided, but the scaffold structures are not revealed. Additionally, the structures of the compounds in the training data set for models developed using confidential data are encrypted and randomly generated numbers are presented as the compound names. [Note: All names for structurally similar chemicals identified in the Leadscope summary were based on chemical names identified based on structure drawn using ChemIDplus Advanced and then searched for in ChemSpider, PubChem, and/or ChemIDplus. Lack of chemical names for some of the structurally similar chemicals was due to the lack of clarity on the structure of these compounds.]

1.2 Suite Results

1.2.1 Rodent Carcinogenicity

This suite is composed of a total of 11 models, seven *in vivo* and four *in vitro*. The *in vivo* models are based on results from the two-year rodent bioassay; training sets were based on confidential data. The *in vitro* models are based on cell transformation studies. The table below (**Table 1**) provides the results for vinpocetine including the prediction call and prediction probability. The number of training compounds used to develop the models and the sensitivity and specificity of each model are also provided.

Table 1. Summary of Predicted Results for Carcinogenicity Models

Endpoint	Prediction Call[#]	Prediction Probability[#]	Number of Training Compounds*	Sensitivity*	Specificity*
Carcinogenicity Mouse	Negative	0.338	1132-1260	37.7-40.8	91.6-92.9
Carcinogenicity Male Mouse	Negative	0.1385	1106-1235	37.1-38.1	90.2-91.7
Carcinogenicity Female Mouse	Negative	0.2675	1110-1246	35.7-38.9	90.3-92.0
Carcinogenicity Rat	Positive	0.504	1206-1415	33.7-40.5	93.8-95.1
Carcinogenicity Male Rat	Positive	0.673	1155-1361	35.4-39.7	93.0-94.2
Carcinogenicity Female Rat	Negative	0.3045	1164-1356	37.9-40.1	93.2-94.1
Carcinogenicity Rodent	Negative	0.417	1153-1569	32.5-37.9	91.6-94.2
In Vitro Cell Transformation	Positive	0.887	640	87.8	50.8
SHE	Positive	0.861	425	88.8	55.8
BALB/c-3T3	Positive	0.742	316	87.8	54.7
C3H10T1/2	Not in domain		138	93.9	22.5

[#]For models where sub-models were included, the prediction calls and prediction probabilities are for the overall results.
*Ranges are provided for those models where sub-models were developed.

Vinpocetine was classified as positive in five models: carcinogenicity rat, carcinogenicity male rat, *in vitro* cell transformation, SHE, and BALB/c-3T3. All eight previously described property features (e.g., hydrogen bond donors) were identified as contributing to predicted chemical activity. The number of unique structural features identified as contributing to the predicted activity ranged from 8 to 25 (see **Table 2**), while a single chemical was identified as at least 30% structurally similar to vinpocetine for each of the models (see **Table 3**).

Table 2. Structural Features Identified as Associated with Predicted Carcinogenicity Activity†

Feature	Carcinogenicity Rat	Carcinogenicity Rat Male	Cell Transformation	SHE	BALB/c-3T3
1-Methoxy-2-butene				X	
2-Methylpentane					X
Amine, alkenyl-	X				
Amine, alkenyl, cyc-	X				X
Benzene					X
Butylethylamine			X		
Butylmethylamine			X	X	
Carboxylate				X	
Carboxylate, alkenyl					X*
Diethylmethylamine			X		
Ethyl acetate					X
Hexane			X	X	X
Hexene					X
N,2-Dimethyl-1-propanamine			X		
N,3-Dimethyl-1-propanamine			X		
N,N-Dimethyl-1-butanamine			X		
N,N-Dimethyl-1-propanamine			X	X	
N-Ethyl-2-propanamine				X	
N-Methylpentylamine			X		
Oxycarbonyl, O-(alkyl, acyc)-		X			
Oxycarbonyl, O-ethyl		X			
Pentylamine			X		
Piperidine, 2-aryl	X	X			
Propane	X	X	X	X	X
Propylethylamine			X	X	
Pyridine(H)	X	X			
Pyridine(H), 1-(alkyl, cyc)-	X				
Pyridine(H), 2-(alkyl, cyc)-		X			
Scaffold 216		X			
Scaffold 238		X			
Scaffold 313		X			
Scaffold 371		X			
Scaffold 392		X			
Scaffold 443		X			
Scaffold 457		X			
Scaffold 463		X			
Scaffold 475		X			
Scaffold 493	X				
Scaffold 498		X			
Scaffold 500		X			
Scaffold 521	X				
Scaffold 528		X			
Scaffold 529		X			
Scaffold 543		X			
Scaffold 551		X			
Scaffold 554		X			

Feature	Carcinogenicity Rat	Carcinogenicity Rat Male	Cell Transformation	SHE	BALB/c-3T3
Scaffold 556	X				
Scaffold 557	X				
Scaffold 571	X				
Scaffold 596	X				
Scaffold 601	X				
Scaffold 61	X				
Scaffold 650		X			
Scaffold 677		X			
Scaffold 98		X			
Tert-amine					X
Tert-amine, alkyl					X

†For models where sub-models were developed, the structural features identified are for the overall results.
*Identified twice as contributing to predicted activity

Since the rat carcinogenicity and rat male carcinogenicity models were developed using confidential data, most of the structural features are not revealed. Of those features that were identified, nitrogen- and oxygen-containing substructures were noted. For all of the positive *in vitro* models, the predicted activity was more highly associated with structural features of the molecule. For all three models, the propane and hexane moieties were negatively associated with the predicted activity. Overall, mono- and di-substituted amines were more positively associated with the predicted activity. Trisubstituted amines generally were either less positively associated or negatively associated with activity. In the SHE and BALB/c-3T3 predictions, oxygen-containing moieties were also positively associated with the predicted activity.

Table 3. Chemicals Identified as at Least 30% Structurally Similar to Vinpocetine for Each Positive Carcinogenicity Model

Structurally Similar Chemicals	Carcinogenicity Rat	Carcinogenicity Rat Male	Cell Transformation	SHE	BALB/c-3T3
LS-200748*			X	X	X
1286820055946#		X			
1286820264351#	X				

*Lack of chemical names for the structurally similar chemicals due to the lack of clarity on the structure of these compounds.
#Structure not provided since models were developed using confidential data

Additionally, the structures of the compounds in the *in vivo* training data set were encrypted and randomly generated numbers are presented as the compound names. A single chemical in the *in vitro* carcinogenicity model database was identified as at least 30% structurally similar to vinpocetine. The chemical contained several rings with at least two containing a nitrogen within the ring. Several methoxy substituents were also noted in the structure.

1.2.2 Genetic Toxicity

This suite is composed of 29 models. There are 12 *in vitro* mammalian and microbial mutagenicity models evaluated. Additionally, there is a mouse lymphoma mutagenicity model. Three *in vitro* unscheduled DNA synthesis models are used to assess DNA damage. Clastogenicity models are based on *in vivo* micronucleus and chromosomal aberration studies. Finally, three sister chromatid exchange models and five chromosomal aberration models are described using results from a variety of cell types. The table below (**Table 4**) provides the results for vinpocetine including the prediction call and prediction probability. The number of

training compounds used to develop the models and the sensitivity and specificity of each model are also provided.

Table 4. Summary of Predicted Results for Genotoxicity Models

Endpoint	Prediction Call[#]	Prediction Probability[#]	Number of Training Compounds*	Sensitivity*	Specificity*
Mutagenicity models					
In vitro microbial	Negative	0.198	3683	64.3	87.5
In vitro Salmonella	Negative	0.332	3575	62.0	89.5
In vitro E. coli	Not in domain		524	76.3	76.7
E. coli w strains	Not in domain		277	62.6	90.1
In vitro yeast	Not in domain		435-603	59.5-63.5	89.6-91.1
In vitro S. cerevisiae	Not in domain		356-473	65.5-66.5	89.6-90.8
In vivo Drosophila	Negative	0.471	595	73.0	81.9
In vivo Drosophila sex linked recessive lethal	Negative	0.297	588	71.6	82.8
In vivo Drosophila heritable translocations	Not in domain		118	77.4	84.6
In vivo mammalian	Not in domain		213	62.7	88.5
In vivo mammalian dominant lethal	Not in domain		182	61.5	90.6
In vitro CHO V79 hgprt	Not in domain		472-643	42.1-46.5	91.4-92.7
Mouse lymphoma mutagenicity model					
Mouse lymphoma 5178Y-tk	Not in domain		565-809	48.8-68.0	72.6-87.2
DNA damage models					
UDS *in vitro*	Negative	0.0497	374	61.5	90.0
UDS *in vitro* rat hepatocytes	Negative	0	143	63.6	90.9
UDS *in vitro* human lymphocytes	Not in domain		194	66.7	89.4
Clastogenicity models					
Micronucleus *in vivo*	Negative	0.106	824	41.3	95.4
Micronucleus *in vivo* mouse	Negative	0.404	624	45.7	90.7
Chromosome aberrations *in vivo*	Negative	0.00364	285	48.0	91.4
Chromosome aberrations *in vivo* rat	Positive	0.815	110	6.67	96.8
Chromosome aberrations *in vivo* other rodent	Negative	0.0689	153	48.1	86.9
Chromosomal aberrations models					
In vitro chrom. ab.	Negative	0.295	1182-1596	43.5-44.1	89.2-90.6
In vitro chrom. ab. CHO	Not in domain	0.251	591-688	42.8-46.9	91.0-91.5
In vitro chrom. ab. CHL	Negative	0.447	535-734	44.8-52.4	91.9-94.8
In vitro chrom. ab. HL	Not in domain		186	75.3	81.9
In vitro chrom. ab. Other cells	Not in domain		281	54.9	81.9
Sister chromatid exchange models					
SCE *in vitro*	Negative	0.1169	410-758	70.1-72.7	66.5-74.0
SCE *in vitro* CHO	Positive	0.681	624	87.7	42.4
SCE *in vitro* other cells	Not in domain		204	96.0	38.7

[#]For models where sub-models were included, the prediction calls and prediction probabilities are for the overall results.
*Ranges are provided for those models where sub-models were developed.

Vinpocetine was classified as positive in two models, chromosome aberrations *in vivo* rat and SCE *in vitro* CHO. The number of unique structural features identified as contributing to the predicted activity was 12 and 14, respectively (see **Table 5**). A single chemical (LS-200748) was identified as at least 30% structurally similar to vinpocetine for both models. The chemical contained several rings with at least two containing a nitrogen within the ring. Several methoxy substituents were also noted in the structure.

Table 5. Structural Features Identified as Associated with Predicted Genotoxicity Activity†

Feature	Chrom. ab. rat	SCE in vitro CHO
2-Methylpentane		X
3-Methylhexane		X
Amine, alkenyl	X	
Amine, alkenyl, cyc-	X	
Benzene		X
Butylmethylamine		X
Carbonyl, alkenyl, cyc-	X	
Carboxylate, alkenyl		X*
Hexane		X
Indole	X*	
N,1-Dimethyl-1-butanamine		X
N,1-Dimethyl-1-propanamine		X
N,N-Dimethyl-1-propanamine		X
N-Methyl-N-propyl-1-propanamine		X
Oxycarbonyl, O-(alkyl, acyc)-	X	
Oxycarbonyl, O-ethyl-	X	
Piperidine		X
Piperidine, 1-(alkyl, cyc)-	X	
Propane	X	X
Pyridine(H)		X
Pyridine(H), 3-(alkyl, acyc)-	X	
Pyridine(H), 4-(alkyl, cyc)-	X	
Pyrrole	X	
Quinolizine	X	
Tert-amine, alkyl-		X

†For models where sub-models were developed, the structural features identified are for the overall results.
*Identified twice as contributing to predicted activity

Comparison of the structural features identified as relevant to the predicted activity for these two models indicated very different features as being positively associated with the predicted activity. For the *in vivo* model, nitrogen-containing ring structures (e.g., indole and piperidine) were identified as having the greatest positive contribution to the predicted activity. Comparatively, a carboxylate substructure was most highly associated with *in vitro* activity. Amines were also identified as positively associated with *in vitro* activity. Of all the positively associated features for the SCE model, a piperidine moiety was the only nitrogen-containing ring tructure that was identified.

1.2.3 Reproductive Toxicity

A total of nine models are used to predict reproductive toxicity; six male and three female. The table below (**Table 6**) provides the results for vinpocetine including the prediction call and prediction probability. The number of training compounds used to develop the models and the sensitivity and specificity of each model are also provided.

Table 6. Summary of Predicted Results for Reproductive Toxicity Models

Endpoint	Prediction Call[#]	Prediction Probability[#]	Number of Training Compounds*	Sensitivity*	Specificity*
Repro Rodent Male	Negative	0.142	786	36.3	93.8
Repro Rat Male	Negative	0.0753	717	41.7	92.0
Repro Mouse Male	Negative	0.0666	146	63.8	83.9
Repro Rodent Female	Negative	0.4375	476-965	46.1-53.3	91.4-92.9
Repro Rat Female	Negative	0.1978	435-900	35.4-50.4	90.6-96.5
Repro Mouse Female	Negative	0.0187	150	62.5	90.2
Sperm Rodent	Negative	0.1315	684-910	44.0-50.4	88.1-89.8
Sperm Rat	Negative	0.4975	542-726	52.3-57.5	89.7-90.2
Sperm Mouse	Negative	0.0141	260	50.0	87.1

[#]For models where sub-models were included, the prediction calls and prediction probabilities are for the overall results.
*Ranges are provided for those models where sub-models have been developed.

Vinpocetine was classified as negative for all the models evaluated.

1.2.4 Developmental Toxicity

A total of 27 developmental toxicity models are included in this suite. The models can be classified as structural dysmorphogenesis (four models), visceral dysmorphogenesis (three models), fetal survival (12 models), and fetal growth (eight models). The table below (**Table 7**) provides the results for vinpocetine including the prediction call and prediction probability. The number of training compounds used to develop the models and the sensitivity and specificity of each model are also provided.

Table 7. Summary of Predicted Results for Developmental Toxicity Models[†]

Endpoint	Prediction Call[#]	Prediction Probability[#]	Number of Training Compounds*	Sensitivity*	Specificity*
Structural dysmorphogenesis					
Structural dysmorphogenesis rodent	Negative	0.144	2019	28.6	94.4
Structural dysmorphogenesis rat	Negative	0.442	1330-1759	40.7-43.4	88.7-89.8
Structural dysmorphogenesis mouse	Positive	0.677	979	34.6	90.5
Structural dysmorphogenesis rabbit	Negative	0.1917	432-1014	50.4-55.3	87.3-90.0
Visceral dysmorphogenesis					
Visceral dysmorphogenesis rodent	Negative	0.3372	1004-2019	35.6-38.0	89.4-92.3
Visceral dysmorphogenesis rat	Negative	0.45	743-1654	42.3-42.7	88.9-92.9
Visceral dysmorphogenesis mouse	Negative	0.07702	321-978	30.8-51.9	85.7-93.2
Fetal growth					
Fetal growth retardation rodent	Negative	0.277	2019	22.1	92.6
Fetal growth retardation rat	Negative	0.4775	1317-1759	33.3-34.9	89.4-89.8
Fetal growth retardation mouse	Negative	0.04235	727-978	39.1-40.4	89.8-90.3
Fetal growth retardation rabbit	Negative	0.4278	269-1013	29.4-52.9	87.2-89.7
Fetal weight decrease rodent	Negative	0.117	2019	30.8	91.8
Fetal weight decrease rat	Negative	0.3865	1325-1759	35.4-36.7	89.0-89.9
Fetal weight decrease mouse	Negative	0.053	732-978	39.3-43.9	89.8-91.4
Fetal weight decrease rabbit	Negative	0.1082	420-1013	26.6-48.4	87.2-95.3
Fetal survival					
Fetal death rodent	Negative	0.2905	1538-2019	27.7-29.8	89.8-92.1
Fetal death rat	Positive	0.5185	1519-1759	27.9-28.9	91.1-91.8
Fetal death mouse	Negative	0.1551	842-978	34.4-36.9	90.4-90.9
Fetal death rabbit	Positive	0.8495	760-1013	40.9-42.9	89.5-89.9
Post implantation loss rodent	Negative	0.309	2019	30.9	92.5

Endpoint	Prediction Call[#]	Prediction Probability[#]	Number of Training Compounds*	Sensitivity*	Specificity*
Post implantation loss rat	Positive	0.5115	1321-1759	30.0-32.3	89.5-91.3
Post implantation loss mouse	Negative	0.148	978	28.3	92.6
Post implantation loss rabbit	Positive	0.8503	432-1013	43.4-49.0	84.4-89.0
Pre implantation loss rodent	Negative	0.3415	1516-2019	31.3-32.3	90.2-90.6
Pre implantation loss rat	Negative	0.461	1059-1759	35.4-38.7	89.0-89.1
Pre implantation loss mouse	Negative	0.04219	589-978	43.3-51.2	89.7-90.2
Pre implantation loss rabbit	Negative	0.1611	323-1013	38.3-57.4	87.0-90.0

[#]For models where sub-models were included, the prediction calls and prediction probabilities are for the overall results.
*Ranges are provided for those models where sub-models have been developed.

Vinpocetine was positive in five models. All eight previously described property features (e.g., hydrogen bond donor s) were identified as contributing to predicted chemical activity. The structural features that were identified as playing a role in the predicted activity and chemicals identified as at least 30% structurally similar to vinpocetine are provided in **Tables 8** and **9**, respectively.

Table 8. Structural Features Identified as Contributing to Predicted Developmental Toxicity Activity[†]

Feature	Structural dysmorphogenesis mouse	Fetal death rat	Fetal death rabbit	Post implantation loss rat	Post implantation loss rabbit
1,5-Napthapyridine(H)			X		
Carbonyl, alkenyl		X	X		X
Ethyl acrylate					X
Amine, alkenyl		X			
Amine, alkenyl, cyc-		X			X
Benzene	X		X		X
Carbonyl, alkenyl, cyc-	X		X		X
Carboxylate					X
Carboxylate, alkenyl					X
Carboxylate, alkenyl, cyc-					X
Ethanolamine	X				
Indole	X			X	
Indole, 2-(alkyl, cyc)-				X	X
Indole, 2-aminomethyl			X		X
Indole, 3-(2-aminomethyl)-	X			X	
Indole, 3-(alkyl, cyc)-	X	X		X	X
Octahydroindolizine#		X		X	
Oxycarbonyl, O-(alkyl, acyc)-					X
Oxycarbonyl, O-alkyl					X
Piperidine			X		X
Piperidine, 1-(alkyl, cyc)-		X		X	X
Piperidine, 2-aryl-					X
Piperidine, 3-(alkyl, acyc)-		X			
Propane			X	X	
Pyridine(H)/Scaffold 5356	X	X*	X		X
Pyridine(H), 1-(alkyl, cyc)-		X			
Pyridine(H), 2-(alkyl, cyc)-					X
Pyridine(H), 2-aryl-				X	
Pyridine(H), 2-carbonyl		X		X	
Pyridine(H), 3-(alkyl, acyc)-					X
Pyridine(H), 3-alkylamino			X		

Feature	Structural dysmorphogenesis mouse	Fetal death rat	Fetal death rabbit	Post implantation loss rat	Post implantation loss rabbit
Pyridine(H), 3-amino-			X		X
Pyridine(H), 4-(alkyl, cyc)-	X				
Pyrrole	X				
Pyrrolo[2,3-c]pyridine(H)			X		
Quinolizine			X		X
Tert-amine, alkyl					X

†For models where sub-models were developed, the structural features identified are for the overall results.
*Substructure identified twice as contributing to predicted activity; percentage contributions were different for each entry.
#Identified as Pyrrolo[1,2-a]pyridine in Leadscope report. Name listed obtained from structure search in ChemIDplus.

For all of the evaluated models, the presence of an unsubstituted and/or substituted nitrogen-containing ring was positively associated with the predicted activity. The presence of an amino substructure was also positively associated with activities predicted in the fetal death rat and structural dysmorphogenesis mouse models.

Table 9. Chemicals Identified as at Least 30% Structurally Similar to Vinpocetine for Each Positive Developmental Toxicity Model

Structurally Similar Chemical	Structural dysmorphogenesis mouse	Fetal death rat	Fetal death rabbit	Post implantation loss rat	Post implantation loss rabbit
Ethyl eburnamenine-14-carboxylate		X	X	X	X
Methyl 11-bromo-14-hydroxy-14,15-dihydroeburnamenine-14-carboxylate		X	X	X	X
(-)-(12R*,13aR*,13bS*)-2,3,5,6,12,13,13a,13b-Octahydro-1H-indolo(3,2,1-de)pyrido(3,2,1-ij)(1,5)naphthyridin-12-ol			X	X	X
Methyl 17-hydroxyyohimban-16-carboxylate			X		
LS-200898		X	X	X	X
LS-200783		X	X	X	X
LS-200748	X	X	X	X	X
8-[(Methylsulfanyl)methyl]-6-propylergoline	X		X		X
Methyl 17-hydroxyyohimban-16-carboxylate		X		X	X
LS-194748		X		X	

*Lack of chemical names for the structurally similar chemicals due to the lack of clarity on the structure of these compounds.

All the positive models identified the same chemicals as being at least 30% structurally similar to vinpocetine. All the chemicals contained multiple rings with at least one heterocycle present. Several methoxy substituents were also noted in the structure.

1.2.5 Neurotoxicity

Neurotoxicity models were developed based on alterations in newborn rodent, rat, and mouse. The table below (**Table 10**) provides the results for vinpocetine including the prediction call and prediction probability. The number of training compounds used to develop the models and the sensitivity and specificity of each model are also provided.

Table 10. Summary of Predicted Results for Neurotoxicity Models

Endpoint	Prediction Call[#]	Prediction Probability[#]	Number of Training Compounds*	Sensitivity*	Specificity*
Behavioral toxicity newborn rodent	Negative	0.0761	502-671	55.8-60.7	86.4-89.7
Behavioral toxicity newborn rat	Negative	0.2367	466-628	52.5-58.2	90.2-91.4
Behavioral toxicity newborn mouse	Negative	0.00364	127-172	43.2-78.4	86.7-90.0

[#]For models where sub-models were included, the prediction calls and prediction probabilities are for the overall results.
*Ranges are provided for those models where sub-models have been developed.

Vinpocetine was classified as negative in all the evaluated models.

1.2.6 Human Adverse Cardiological Effects

A total of 13 models are used to assess potential human adverse cardiac effects of tested chemicals. The table below (**Table 11**) provides the results for vinpocetine including the prediction call and prediction probability. The number of training compounds used to develop the models and the sensitivity and specificity of each model are also provided.

Table 11. Summary of Predicted Results for Human Adverse Cardiological Effects Models

Endpoint	Prediction Call[#]	Prediction Probability[#]	Number of Training Compounds*	Sensitivity*	Specificity*
Conduction disorders	Negative	0.2185	370-1628	54.2-64.2	88.4-93.6
Coronary artery disorders	Positive	0.8173	700-1628	50.0-52.9	88.3-89.5
Electrocardiogram disorders	Negative	0.2993	535-1628	47.7-52.3	87.1-88.2
Heart failure disorders	Negative	0.148	679-1628	41.0-48.8	90.7-91.6
Arrhythmia disorders	Negative	0.4367	682-1509	43.8-54.3*	91.1-92.0
Bradycardia disorders	Negative	0.1842	324-1628	47.2-65.7	86.2-90.4
QT prolongation	Negative	0.1334	444-1628	52.0-61.3	88.5-88.9
Tachycardia disorders	Negative	0.3652	554-1628	48.7-60.3	86.4-89.1
Torsades	Negative	0.212	374-1628	53.6-61.0	86.9-88.8
Myocardial infarct disorders	Positive	0.749	366-1628	53.0-64.3	87.6-90.5
Myocardial disorders	Negative	0.3072	314-1629	38.1-57.7	85.8-93.2
Palpitations	Positive	0.534	548-1628	54.0-58.2	86.4-88.6
Rate rhythm disorders	Positive	0.5577	813-1628	32.1-40.2	87.7-90.8

[#]For models where sub-models were included, the prediction calls and prediction probabilities are for the overall results.
*Ranges are provided for those models where sub-models have been developed.

Vinpocetine was positive in four models. All eight previously described property features (e.g., hydrogen bond donors) were identified as contributing to predicted chemical activity. The structural features that were identified as playing a role in the predicted activity and chemicals identified as at least 30% structurally similar to vinpocetine provided in **Tables 12** and **13**, respectively.

Table 12. Structural Features Identified As Contributing To Predicted Human Adverse Cardiological Effects Activity†

Feature	Coronary artery disorder	Myocardial infarction disorders	Palpitations	Rate rhythm disorders
Amine, alkenyl-			X	
Amine, alkenyl, cyc-			X	
Carbonyl, alkenyl, cyc-		X		
Carboxylate		X		
Carboxylate, alkenyl-	X	X	X	
Carboxylate, alkenyl, cyc-	X	X	X	
Diethyl ether		X		
Ethyl acetate		X		
Glycine			X	X
Indole	X	X	X	X
Indole, 3-(2-aminoethyl)-	X	X	X	
Indole, 3-(alkyl, cyc)-	X	X	X	
Oxycarbonyl, O-ethyl-	X	X		X
Piperidine			X	X
Piperidine, 1-(alkyl, cyc)-			X	
Piperidine, 2-aryl-		X		
Propane	X	X	X	X
Pyridine(H)	X	X	X	X
Pyridine(H), 1-(alkyl, cyc)-			X	
Pyridine(H), 2-(alkyl, cyc)-	X	X		X
Pyridine(H), 2-carbonyl-	X			
Pyridine(H), 3-(alkyl, acyc)-	X			X
Pyridine(H), 4-(alkyl, acyc)-				X
Pyridine(H), 4-(alkyl, cyc)-		X		
Pyrrole	X	X	X	X
Pyrrole, 2-(alkyl, cyc)-	X			
Quinolizine		X		
Tert-amine			X	
Tert-amine, alkyl	X	X	X	X

†For models where sub-models were developed, the structural features identified are for the overall results.

For all of the evaluated models, the presence of an unsubstituted and/or substituted indole substructure was positively associated with the predicted activity. Additional nitrogen-containing substructures (e.g., pyrrole, piperidine, and quinolizine) were also positively associated with the activity predicted by the models. F urthermore, an ester moiety was associated with positive activity.

Table 13. Chemicals Identified As At Least 30% Structurally Similar To Vinpocetine for Each Positive Genotoxicty Model

Structurally Similar Chemical	Coronary artery disorder	Myocardial infarction disorders	Palpitations	Rate rhythm disorders
Methyl (16α,17α)-17-hydroxy-2,7-dihydroyohimban-16-carboxylate	X	X	X	X
LS-194748-copy-1*	X	X	X	X
LS-200747-copy-1*	X	X	X	X
LS-200783-copy-1*	X	X	X	X
LS-200748	X	X	X	X
8-[(Methylsulfanyl)methyl]-6-propylergoline	X	X	X	X

*Lack of chemical names for the structurally similar chemicals due to the lack of clarity on the structure of these compounds.

All the positive models identified the same chemicals as being at least 30% structurally similar to vinpocetine. All the chemicals contained multiple rings with at least one heterocycle present. Several methoxy substituents were also noted in the structure.

1.2.7 Human Adverse Hepatobiliary Effects

Five models are used to assess the potential for adverse human hepatobiliary effects produced by test compounds. The table below (**Table 14**) provides the results for vinpocetine including the prediction call and prediction probability. The number of training compounds used to develop the models and the sensitivity and specificity of each model are also provided.

Table 14. Summary of Predicted Results for Human Adverse Hepatobiliary Effects Models

Endpoint	Prediction Call[#]	Prediction Probability[#]	Number of Training Compounds*	Sensitivity*	Specificity*
Bile duct disorders	Negative	0.1278	567-1043	23.9-27.2	97.9
Gall bladder disorders	Negative	0.0881	607-1055	41.3-42.5	92.9-93.7
Liver jaundice disorders	Negative	0.1424	692-1604	49.6-51.7	91.4-92.7
Liver acute damage disorders	Negative	0.0482	646-1603	47.3-51.5	92.7-93.5
Liver enzyme release disorders	Negative	0.02223	624-1602	40.4-48.5	94.3-95.7

[#]For models where sub-models were included, the prediction calls and prediction probabilities are for the overall results.
*Ranges are provided for those models where sub-models have been developed.

Vinpocetine was classified as negative for all the models evaluated.

1.2.8 Human Adverse Urinary Tract Effects

Six models are used to assess the potential for adverse urinary tract effects produced by test compounds. The table below (**Table 15**) provides the results for vinpocetine including the prediction call and prediction probability. The number of training compounds used to develop the models and the sensitivity and specificity of each model are also provided.

Table 15. Summary of Predicted Results for Human Adverse Urinary Tract Effects Models

Endpoint	Prediction Call[#]	Prediction Probability[#]	Number of Training Compounds*	Sensitivity*	Specificity*
Bladder disorders	Negative	0.2603	689-1591	43.9-51.5	89.2-90.2
Blood in urine disorders	Positive	0.7293	638-1591	43.6-53.3	93.7-95.2
Kidney disorders	Negative	0.0951	625-1590	35.4-38.9	94.8-96.1
Kidney function tests	Negative	0.1152	687-1589	45.6-50.6	89.8-90.0
Nephropathy disorders	Negative	0.3711	667-1590	44.2-55.8	90.2-91.6
Urolithiasis disorders	Negative	0.05323	626-1591	34.5-48.3	94.2-95.5

[#]For models where sub-models were included, the prediction calls and prediction probabilities are for the overall results.
*Ranges are provided for those models where sub-models have been developed.

Vinpocetine was classified as positive in the blood in urine disorders model. Nine unique structural features were identified as being associated with the predicted activity: 1,2-dimethyl-1H-pyrrole; 1-ethyl-1H-pyrrole; 1-ethyl-2,3-dimethyl-1H-pyrrole; amine, alkenyl, cyc-; amine, alkenyl; carbonyl, alkenyl, cyc-; tert-amine, alkyl, hexane, and oxycarbonyl, O-alkyl. Six chemicals were identified as being at least 30% structurally similar to vinpocetine.

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Units and Abbreviations

CHL = Chinese hamster lung
CHO = Chinese hamster ovary
chrom. ab. = chromosomal aberration
DNA = deoxyribonucleic acid
FDA = U.S. Food and Drug Administration
QSAR = quantitative structure-activity relationship
SCE = sister chromatid exchange
SHE = Syrian hamster embryo
UDS = unscheduled DNA synthesis

Appendix E: Toxtree Structure-Activity Relationship Analyses for Vinpocetine

Toxtree (V2.6.0) is an application provided by the European Union Joint Research Centre that places chemicals into categories and predicts toxicity for a variety of endpoints using a decision tree model. Toxicity endpoints evaluated included: eye and skin irritation/corrosion, skin sensitization, *in vivo* micronucleus formation, carcinogenicity, and mutagenicity. Additional models include toxicity mode of action, biodegradation, and cytochrome P450 (CYP) metabolism potential.

1.2 Benigni/Bossa Rules for Carcinogenicity and Mutagenicity

Chemicals are evaluated for the presence of structural alerts associated with carcinogenic and/or mutagenic activity. Structural alerts for nongenotoxic and genotoxic compounds are evaluated. Structural alerts that are evaluated include acyl halides, hydrazine, nitro aromatics, thiocarbonyls, and halogenated benzene (Benigni et al., 2008). There were no structural alerts identified in vinpocetine for genotoxic or non-genotoxic carcinogenic activity.

[Note: Three quantitative structure-activity relationship (QSAR) models were included in the rules for this evaluation. The models focused on evaluating (1) mutagenic activity of aromatic amines in *Salmonella typhimurium* strain TA100, (2) mutagenic activity of α,β-unsaturated aldehydes in *S. typhimurium* strain TA100, and (3) carcinogenic activity of the aromatic amines in rodents. The applicability domains of the three QSAR models were (1) compounds containing (a) homocyclic amines (excluding aromatic amines containing aromatic nitro groups) and (b) diazo, isocyanate, and imine groups, (2) linear aldehydes, and (3) compounds containing (a) homocyclic amines (including aromatic amines containing aromatic nitro groups) and (b) diazo, isocyanate, and imine groups, respectively.]

1.3 Structural Alerts for the *In Vivo* Micronucleus Assay in Rodents

Chemicals are evaluated for the presence of structural alerts associated with micronucleus formation in rodents. Structural alerts that are evaluated include acyl halides, hydrazine, quinones, isocyanate and isothiocyanate groups, and nitro aromatic groups (Benigni et al., 2009). A review of the structure indicates the presence of a single structural alert which may predict *in vivo* micronucleus formation (H-acceptor-path3-H-acceptor). [Note: Much of the data used in the Toxtree analysis were obtained from the "FDA SAR Genetox Database" developed by Leadscope.]

1.4 *In Vitro* Mutagenicity (Ames Test)

Chemicals are evaluated for the presence of structural alerts associated with activity in the Ames assay. Structural alerts that are evaluated include quinones, hydrazine, isocyanate, and aliphatic N-nitro (Benigni and Bossa, 2011; Benigni et al., 2013 [PMID:23132285]). There were no structural alerts identified in vinpocetine for *S. typhimurium* mutagenicity.

1.5 DNA Binding Alerts

Chemicals are evaluated for the presence of structural alerts associated with covalent DNA binding. Structural alerts that are evaluated include imides, thiazoles, furans, aliphatic aldehydes, and imides (Enoch and Cronin, 2010 [PMID:20722585]). There were structural alerts for an SN1 reaction mechanism and Michael acceptor identified in vinpocetine.

1.6 Protein Binding Alerts

Chemicals are evaluated for the presence of structural alerts associated with covalent protein binding. Structural alerts that are evaluated include lactones, alkyl halides, piperizines, and pyranones (Enoch et al., 2011 [PMID:21809939]). There were structural alerts for an SN2 reaction and Michael acceptor identified in vinpocetine.

1.7 Structural Alerts for Eye Irritation and/or Corrosion

Based on general chemical class, chemicals are evaluated for physicochemical properties and the presence of structural alerts associated with eye irritation and/or corrosion. For the current evaluation, physicochemical properties were not included in the evaluation and vinpocetine was only evaluated for the presence of structural alerts. [Note: The user manual notes that exclusion of physicochemical properties may lead to a low quality prediction (Ideaconsult Ltd., 2011). Physicochemical properties were not included because data for all the necessary properties were not available (e.g., lipid solubility and water solubility).] Structural alerts that were evaluated included presence of aliphatic monoalcohol, pyrrolidine, and aliphatic carboxylic acid (Ideaconsult Ltd., 2011). Based on the calculated molecular weight of the chemical (>290.0), vinpocetine was classified as not corrosive to the skin. However, no further structural analysis was conducted to assess eye irritation or corrosion potential. [Note: A review of the original paper indicates that there are no structural features that would be predictive of eye irritation or corrosive potential (Gerner et al., 2005 [PMID:16180977]).]

1.8 Structural Alerts for Skin Irritation and/or Corrosion

This model estimates skin irritation and/or corrosion potential based on physicochemical properties and the presence of structural alerts. For the current evaluation, physicochemical properties were not included in the evaluation and vinpocetine was only evaluated for the presence of structural alerts. [Note: The user manual notes that exclusion of physicochemical properties may lead to a low quality prediction (Ideaconsult Ltd., 2011). Physicochemical properties were not included because data for all the necessary properties were not available (e.g., lipid solubility and water solubility).] Based on the calculated molecular weight of the chemical (>290.0), vinpocetine was classified as not corrosive to the skin.

1.9 Skin Sensitization

This model evaluates chemicals for the presence of structural alerts associated with skin sensitization. The model identified one alert (presence of a Michael acceptor) for skin sensitization in vinpocetine.

1.10 Cramer Classification Scheme and Kroes Threshold of Toxicological Concern Decision Tree

The Cramer Classification Scheme uses chemical structures and estimated total human intake to estimate the threshold of toxicological concern (TTC). The scheme also uses metabolic pathways, toxicity data, and the presence of the substance in foods or as an endogenous metabolite in developing a TTC. The chemical is then classified into one of three classes:

Class I contains substances of simple chemical structure with known metabolic pathways and innocuous end products which suggest a low order of oral toxicity.

Class II contains substances that are intermediate. They possess structures that are less innocuous than those in Class 1, but they do not contain structural features that are suggestive of toxicity like those in Class 3.

Class III contains substances with chemical structures that permit no strong initial impression of safety and may even suggest a significant toxicity (JRC, 2011).

The Kroes TTC Decision Tree incorporates daily intake rules with Cramer and Benigni/Bossa rules to determine whether chemicals may be assessed by TTC.

Based on the Cramer model, vinpocetine was classified as belonging to Class III, "substances are those that permit no strong initial presumption of safety, or may even suggest significant toxicity or have reactive functional groups" (Curios-IT, 2009). This classification was based on the presence of a heterocycle with complex substituents within vinpocetine. Since vinpocetine does not contain a "sodium, potassium, or calcium sulphonate or sulphamate for every 20 or fewer carbon atoms without any free primary amines except those adjacent to the sulphonate or suphamate," the chemical was classified as belonging to Group III (Cramer et al., 1978).

1.11 START Biodegradation and Persistence

Chemicals are evaluated for the presence of structural alerts associated with biodegradation and/or environmental persistence. Chemicals are then classified into one of three categories: Class 1 (easily biodegradable), Class 2 (persistent chemical), or Class 3 (unknown biodegradability) (Molecular Networks, 2008). Structural alerts that are evaluated include epoxides, two or more rings, and a tertiary amine. Vinpocetine was classified as a Class 2 chemical based on the presence of at least two rings in the structure.

1.12 Michael Acceptor

This model evaluates whether the chemical may be a Michael acceptor based on the presence of structural alerts. The model indicated that vinpocetine is reactive by Michael addition based on the presence of "vinyl or vinylene with a carbonyl" and an "α-carbon atom substituted with a second carbonyl" moieties within the structure.

1.13 Structural Alerts for Functional Groups

The model evaluates chemicals for the presence of classical organic functional groups (e.g., carbonyl). The functional groups can be subdivided into those with high specificity and those with low specificity. This low specificity group identifies structural features that could include a wide range of compounds (e.g., sulfonic acid derivatives). These groups are then divided into high specificity features (e.g., sulfonic acid, sulfonic acid ester, and sulfonamide). This classification allows for grouping a variety of chemicals by functional groups and allows for the potential of "read-across" analyses (Benigni et al., 2011). The low specificity structural features identified in vinpocetine were an aldehyde or ketone, ether, carboxylic acid derivative, aromatic compound, and heterocyclic compound. The high specificity structural groups identified in vinpocetine were a dialkylether, alkylarylether, tertiary aliphatic amine, carboxylic acid ester, and carbonic acid diester. Another functional group identified was enolether. [Note: Although tertiary aliphatic amine and carbonic acid diester were identified as high specificity functional groups present in vinpocetine, the respective low specific functional groups (amine and carbonic acid derivative, respectively) were not identified.]

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