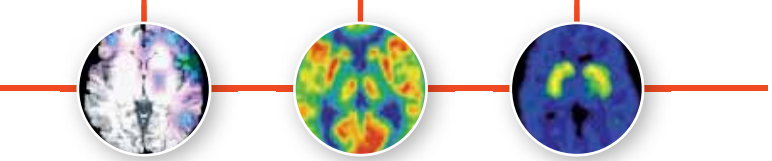
NIMH Chemical Synthesis and Drug Supply Program

Compound Catalog

October 2010

NIMH
National Institute of Mental Health



Purpose

The mission of the Molecular, Cellular, and Genomic Neuroscience Research Branch (MCGNRB) of the National Institute of Mental Health (NIMH) is to support fundamental research on the mechanisms underlying and influencing brain development, neuronal signaling, synaptic plasticity, signal transduction pathways, and the biochemical and behavioral actions of therapeutic agents in animals and humans. The goals of the MCGNRB include the identification of novel targets (genes or molecules) for therapeutic intervention; characterization of the behavioral effects of psychoactive agents; and design and development of novel ligands for functional brain imaging in humans, psychoactive agents for basic and clinical research, and potential therapeutic agents for the treatment of mental disorders.

Since 1959, the NIMH Chemical Synthesis and Drug Supply Program (CSDSP) has synthesized and distributed novel research chemicals, psychoactive drugs, and compounds that are unavailable from commercial sources to the scientific community working on research relevant to mental health. The purpose of the present NIMH CSDSP is to synthesize, purify, and distribute otherwise unavailable essential compounds to stimulate basic and clinical research in psychopharmacology relevant to mental health in areas such as the molecular pharmacology and signaling of central nervous system (CNS) receptors; longitudinal studies to evaluate the molecular, biochemical, and behavioral actions of psychoactive compounds; and functional brain imaging in both primates and humans. NIMH has contracted with RTI International to operate the NIMH CSDSP.

What Is Available?

- Ligands for CNS receptors, radiolabeled compounds for autoradiography and neuroimaging, biochemical markers, drug analogs and metabolites, and reference standards
- Synthesis (including GMP) of promising compounds for mental health research, including preclinical toxicology and safety studies, especially compounds for PET neuroimaging
- A listing of currently available NIMH CSDSP compounds is available online at www.nimh-repository.rti.org. RTI International scientists can provide investigators with technical assistance and additional information about the compounds on request. Data sheets containing purity, storage, and handling information are supplied with all NIMH CSDSP compounds.

Who Is Eligible?

Investigators involved in basic or clinical research relevant to mental health are eligible to submit requests. To learn more about current NIMH research areas, please visit the NIMH website at www.nimh.nih.gov. NIMH CSDSP compounds are free to qualified academic investigators, but payment may be required from nonacademic requestors.

How to Submit Requests

Requests for NIMH CSDSP compounds and for the synthesis of new compounds, together with supporting information, should be submitted on the order form available at the NIMH CSDSP website at www.nimh-repository.rti.org. Alternatively, requests may be emailed to Jamie Driscoll (NIMH) or Ken Rehder (RTI International) (see *Contact Information*).

Investigators who are interested in obtaining radiolabeled compounds but are uncertain about what type of label or specific activity would work best may obtain help by contacting Jamie Driscoll (NIMH) or Anita Lewin (RTI International) (see *Contact Information*).

Requests Should Include

- A brief summary of the significance of the compound to the investigator's research and an indication of the importance of the research to neuroscience
- A description of the protocols to be employed with the compounds, and the amounts required
- For synthesis requests, please include information on prior sources of the compound or related compounds, if available. Literature citations relevant to the synthesis of the target compound or related compounds are essential to the evaluation of the request. Requests for GMP synthesis will require additional information and review; contact Jamie Driscoll (NIMH) for more information
- Primary source of financial support for the proposed research
- For radiolabeled compounds, a copy of the institution's current Nuclear Regulatory Commission (NRC) license showing the authorized amount of the specific isotope and the license's expiration date will be required before shipment
- Current IACUC or institutional review board assurances, if appropriate.

CATALOG FIELD DEFINITIONS

HBA - Number of hydrogen-bond acceptor groups

HBD - Number of hydrogen-bond donor groups

RotB - Number of freely rotatable bonds

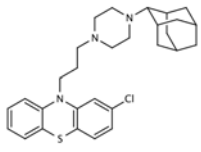
AlogP - Ghose-Crippen octanol-water partition coefficient
(Viswanadhan, V.N., Ghose, A.K., Revankar, G.R. & Robins, R.K. *J. Chem. Inf. Comput. Sci.*, **1989**, *29*, 163-172.)

TPSA - Topological Polar Surface Area
(Ertl, P.; Rohde, B.; Selzer, P., *J. Med. Chem.*, **2000**, *43*, 3714-3717.)

Structures -
The desalted or free base form of each compound is illustrated, unless the exact salt form is important in distinguishing related catalog items.

Catalog number : A-502A

Drug name : Adapiprazine dihydrochloride



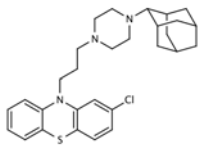
Mol. Formula : $C_{29}H_{38}Cl_3N_3S$ **FW :** 567.07 **HBA:** 5 **HBD:** 0 **RotB:** 5

PubChem ID : 62872 **CASRN :** 57942-72-0 **AlogP:** 6.40 **TPSA:** 35.0

Activity: Dopamine antagonist; antiemetic; antipsychotic agent

Catalog number : A-502B

Drug name : Adapiprazine



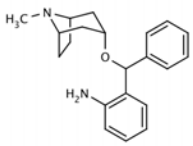
Mol. Formula : $C_{29}H_{36}ClN_3S$ **FW :** 494.13 **HBA:** 5 **HBD:** 0 **RotB:** 5

PubChem ID : 62872 **CASRN :** 57942-72-0 **AlogP:** 6.40 **TPSA:** 35.0

Activity: Dopamine antagonist; antiemetic; antipsychotic agent

Catalog number : A-503

Drug name : Aminobenztropine



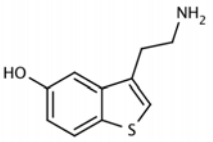
Mol. Formula : $C_{21}H_{26}N_2O$ **FW :** 322.45 **HBA:** 3 **HBD:** 1 **RotB:** 4

PubChem ID : 2143 **CASRN :** 88097-86-3 **AlogP:** 3.30 **TPSA:** 38.5

Activity: Muscarinic m_1 ligand

Catalog number : A-504

Drug name : 3-(β-Aminoethyl)-5-hydroxybenzo[b]thiophene



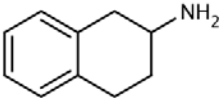
Mol. Formula : $C_{10}H_{11}NOS$ **FW :** 193.27 **HBA:** 3 **HBD:** 2 **RotB:** 2

PubChem ID : 25600 **CASRN :** 13012-93-6 **AlogP:** 1.14 **TPSA:** 74.5

Activity: Serotonin 5-HT_{1E} ligand

Catalog number : A-505

Drug name : 2-Aminotetralin hydrochloride



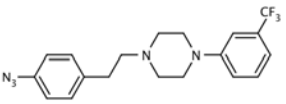
Mol. Formula : $C_{10}H_{14}ClN$ **FW :** 183.68 **HBA:** 1 **HBD:** 1 **RotB:** 0

PubChem ID : 34677 **CASRN :** 2954-50-9 **AlogP:** 1.86 **TPSA:** 26.0

Activity: Serotonin 5-HT_1 ligand

Catalog number : A-506

Drug name : p-Azido-PE-TFMPP hydrochloride



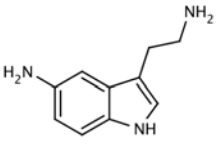
Mol. Formula : $C_{19}H_{21}ClF_3N_5$ **FW :** 411.86 **HBA:** 7 **HBD:** 0 **RotB:** 6

PubChem ID : 128737 **CASRN :** 105025-90-9 **AlogP:** 0.91 **TPSA:** 35.9

Activity: Serotonin 5-HT_{1A} receptor photoaffinity labeling probe

Catalog number : A-507

Drug name : 5-Aminotryptamine dipicrate



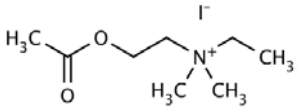
Mol. Formula : $C_{22}H_{19}N_9O_{14}$ **FW :** 633.44 **HBA:** 2 **HBD:** 3 **RotB:** 2

PubChem ID : 3083677 **CASRN :** 1078-00-8 **AlogP:** 0.73 **TPSA:** 67.8

Activity: Serotonin 5-HT agonist

Catalog number : A-508

Drug name : Acetoxyethyldimethylethylammonium iodide

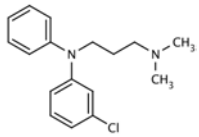


Mol. Formula : $C_8H_{18}INO_2$ **FW :** 287.14 **HBA:** 1 **HBD:** 0 **RotB:** 5

PubChem ID : **CASRN :** **AlogP:** -4.39 **TPSA:** 26.3

Catalog number : A-509

Drug name : *N*-(3-Chlorophenyl)-*N*-(γ-*N',N'*-dimethylaminopropyl)aniline hydrochloride

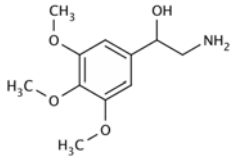


Mol. Formula : $C_{17}H_{22}Cl_2N_2$ **FW :** 325.28 **HBA:** 3 **HBD:** 0 **RotB:** 6

PubChem ID : **CASRN :** 82735-00-0 **AlogP:** 4.09 **TPSA:** 6.5

Catalog number : A-510

Drug name : 2-Amino-1-(3,4,5-trimethoxyphenyl)ethanol

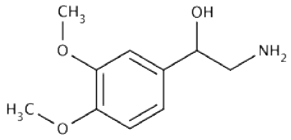


Mol. Formula : $C_{11}H_{17}NO_4$ **FW :** 227.26 **HBA:** 5 **HBD:** 2 **RotB:** 5

PubChem ID : 28894 **CASRN :** 18111-13-2 **AlogP:** -0.27 **TPSA:** 73.9

Catalog number : A-511

Drug name : 2-Amino-1-(3,4-dimethoxyphenyl)ethanol hydrochloride

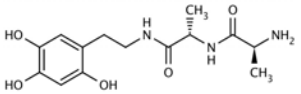


Mol. Formula : $C_{10}H_{16}ClNO_3$ **FW :** 233.70 **HBA:** 4 **HBD:** 2 **RotB:** 4

PubChem ID : 3863978 **CASRN :** **AlogP:** -0.01 **TPSA:** 64.7

Catalog number : A-512

Drug name : Alanylalanyl-6-hydroxydopamine hydrochloride

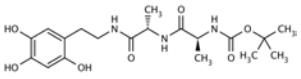


Mol. Formula : $C_{14}H_{22}ClN_3O_6$ **FW :** 347.80 **HBA:** 6 **HBD:** 6 **RotB:** 6

PubChem ID : **CASRN :** **AlogP:** -0.86 **TPSA:** 144.9

Catalog number : A-513

Drug name : *N*-(*t*-Butoxycarbonyl)-L-alanyl-*N*-[2-(2,4,5-trihydroxyphenyl)ethyl]-L-alaninamide

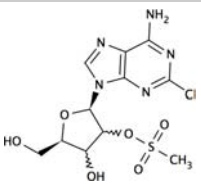


Mol. Formula : $C_{19}H_{29}N_3O_7$ **FW :** 411.46 **HBA:** 7 **HBD:** 6 **RotB:** 9

PubChem ID : **CASRN :** **AlogP:** 0.77 **TPSA:** 157.2

Catalog number : A-514

Drug name : 6-Amino-2-chloro-9-(2'-*O*-methylsulfonyl-β-D-xylofuranosyl)-9*H*-purine

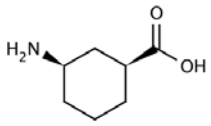


Mol. Formula : $C_{11}H_{14}ClN_5O_6S$ **FW :** 379.78 **HBA:** 10 **HBD:** 3 **RotB:** 4

PubChem ID : 254973 **CASRN :** **AlogP:** -1.36 **TPSA:** 171.1

Catalog number : A-701

Drug name : *cis*-3-Aminocyclohexanecarboxylic acid



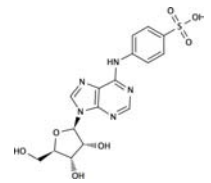
Mol. Formula : $C_7H_{13}NO_2$ **FW :** 143.19 **HBA:** 3 **HBD:** 2 **RotB:** 1

PubChem ID : 544887 **CASRN :** 38541-66-1 **AlogP:** -2.09 **TPSA:** 63.3

Activity: Neuronal GABA uptake inhibitor

Catalog number : A-702

Drug name : N_6-*p*-Sulfophenyladenosine triethylamine salt



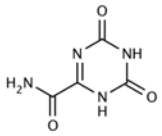
Mol. Formula : $C_{22}H_{32}N_6O_7S$ **FW :** 524.60 **HBA:** 11 **HBD:** 5 **RotB:** 5

PubChem ID : 9866960 **CASRN :** **AlogP:** -4.39 **TPSA:** 188.3

Activity: Adenosine A_1 water-soluble receptor agonist

Catalog number : A-703

Drug name : Allantoxanamide



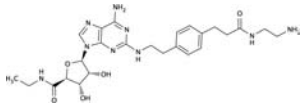
Mol. Formula : $C_4H_4N_4O_3$ **FW :** 156.10 **HBA:** 4 **HBD:** 3 **RotB:** 1

PubChem ID : 188244 **CASRN :** 69391-08-8 **AlogP:** -1.51 **TPSA:** 113.7

Activity: Uricase inhibitor

Catalog number : A-704

Drug name : APEC trifluoroacetate



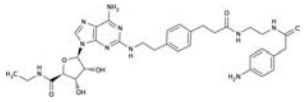
Mol. Formula : $C_{29}H_{37}F_6N_9O_9$ **FW :** 769.66 **HBA:** 11 **HBD:** 7 **RotB:** 12

PubChem ID : 3081741 **CASRN :** 126828-50-0 **AlogP:** -1.28 **TPSA:** 215.6

Activity: Adenosine A_2 receptor ligand

Catalog number : A-705

Drug name : p-Aminophenylacetyl-APEC



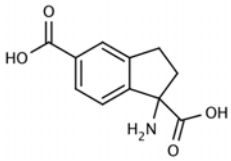
Mol. Formula : $C_{33}H_{42}N_{10}O_6$ **FW :** 674.76 **HBA:** 12 **HBD:** 8 **RotB:** 15

PubChem ID : 3081715 **CASRN :** 124190-27-8 **AlogP:** -0.39 **TPSA:** 244.7

Activity: Adenosine A_2 functionalized receptor ligand

Catalog number : A-801

Drug name : (±)-1-Aminoindan-1,5-dicarboxylic acid



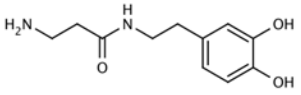
Mol. Formula : $C_{11}H_{11}NO_4$ **FW :** 221.21 **HBA:** 5 **HBD:** 3 **RotB:** 2

PubChem ID : 2071 **CASRN :** 168560-79-0 **AlogP:** -1.71 **TPSA:** 100.6

Activity: mGluR1 antagonist

Catalog number : A-802

Drug name : N-(β-Alanyl)dopamine formate



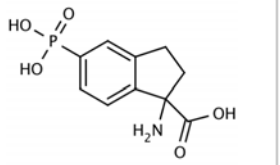
Mol. Formula : $C_{12}H_{18}N_2O_5$ **FW :** 270.29 **HBA:** 4 **HBD:** 4 **RotB:** 5

PubChem ID : 162755 **CASRN :** 54653-62-2 **AlogP:** -0.60 **TPSA:** 95.6

Activity: Sclerotin precursor

Catalog number : A-803

Drug name : (±)-1-Amino-5-phosphonoindan-1-carboxylic acid



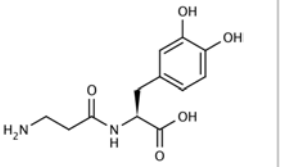
Mol. Formula : $C_{10}H_{12}NO_5P$ **FW :** 257.18 **HBA:** 6 **HBD:** 4 **RotB:** 2

PubChem ID : 4694355 **CASRN :** **AlogP:** -2.48 **TPSA:** 130.7

Activity: mGluR2 receptor ligand

Catalog number : A-804

Drug name : N-(β-Alanyl)-L-DOPA trifluoroacetate

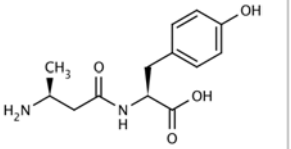


Mol. Formula : $C_{14}H_{17}F_3N_2O_7$ **FW :** 382.29 **HBA:** 6 **HBD:** 5 **RotB:** 6

PubChem ID : **CASRN :** **AlogP:** -3.24 **TPSA:** 132.9

Catalog number : A-805

Drug name : Sarcophagine trifluoroacetate; Alanyltyrosine trifluoroacetate

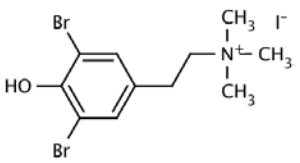


Mol. Formula : $C_{14}H_{17}F_3N_2O_6$ **FW :** 366.29 **HBA:** 5 **HBD:** 4 **RotB:** 6

PubChem ID : 92946 **CASRN :** 3061-88-9 **AlogP:** -2.54 **TPSA:** 112.7

Catalog number : A-806

Drug name : Autonomium iodide

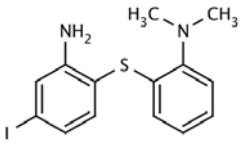


Mol. Formula : $C_{11}H_{16}Br_2INO$ **FW :** 464.97 **HBA:** 1 **HBD:** 1 **RotB:** 3

PubChem ID : **CASRN :** **AlogP:** -1.09 **TPSA:** 20.2

Catalog number : A-807

Drug name : ADAM



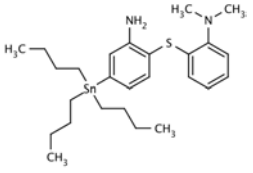
Mol. Formula : $C_{15}H_{17}IN_2S$ **FW :** 384.28 **HBA:** 3 **HBD:** 1 **RotB:** 3

PubChem ID : **CASRN :** **AlogP:** 5.03 **TPSA:** 54.6

Activity: Serotonin 5-HT transporter ligand

Catalog number : A-808

Drug name : Tributylstannyl-ADAM



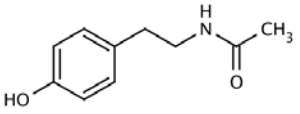
Mol. Formula : $C_{27}H_{44}N_2SSn$ **FW :** 547.42 **HBA:** 3 **HBD:** 1 **RotB:** 13

PubChem ID : **CASRN :** **AlogP:** 7.12 **TPSA:** 54.6

Activity: Radioiodinated ADAM precusor

Catalog number : A-901

Drug name : N-Acetyltyramine

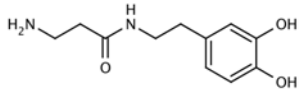


Mol. Formula : $C_{10}H_{13}NO_2$ **FW :** 179.22 **HBA:** 2 **HBD:** 2 **RotB:** 3

PubChem ID : 121051 **CASRN :** 1202-66-0 **AlogP:** 0.96 **TPSA:** 49.3

Catalog number : A-902

Drug name : N-(β-Alanyl)dopamine hydrochloride



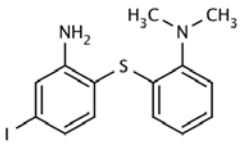
Mol. Formula : $C_{11}H_{17}ClN_2O_3$ **FW :** 260.72 **HBA:** 4 **HBD:** 4 **RotB:** 5

PubChem ID : 162755 **CASRN :** 54653-62-2 **AlogP:** -0.60 **TPSA:** 95.6

Activity: Sclerotin precursor

Catalog number : A-903

Drug name : ADAM dihydrochloride



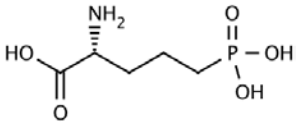
Mol. Formula : $C_{15}H_{19}Cl_2IN_2S$ **FW :** 457.20 **HBA:** 3 **HBD:** 1 **RotB:** 3

PubChem ID : **CASRN :** **AlogP:** 5.03 **TPSA:** 54.6

Activity: Serotonin 5-HT transporter ligand

Catalog number : A-904

Drug name : (*R*)-2-Amino-5-phosphonopentanoic acid



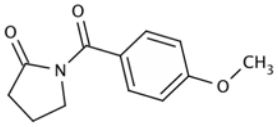
Mol. Formula : $C_5H_{12}NO_5P$ **FW :** 197.13 **HBA:** 6 **HBD:** 4 **RotB:** 5

PubChem ID : 135342 **CASRN :** 79088-68-8 **AlogP:** -3.54 **TPSA:** 130.7

Activity: NMDA receptor antagonist

Catalog number : A-905

Drug name : Aniracetam



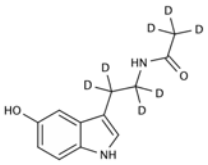
Mol. Formula : $C_{12}H_{13}NO_3$ **FW :** 219.24 **HBA:** 3 **HBD:** 0 **RotB:** 2

PubChem ID : 2196 **CASRN :** 72432-10-1 **AlogP:** 0.83 **TPSA:** 46.6

Activity: Antidepressive agent; nootropic Agent

Catalog number : A-906

Drug name : d_7-*N*-Acetylserotonin



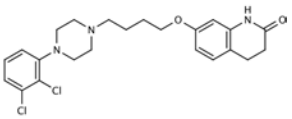
Mol. Formula : $C_{12}H_7D_7N_2O_2$. **FW :** 225.29 **HBA:** 2 **HBD:** 3 **RotB:** 3

PubChem ID : 903 **CASRN :** 1210-83-9 **AlogP:** 1.06 **TPSA:** 65.1

Activity: Stable isotope labeled melatonin receptor antagonist

Catalog number : A-907

Drug name : Aripiprazole



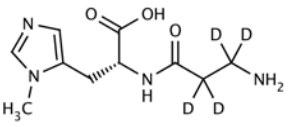
Mol. Formula : $C_{23}H_{27}Cl_2N_3O_2$ **FW :** 448.39 **HBA:** 6 **HBD:** 1 **RotB:** 7

PubChem ID : 60795 **CASRN :** 129722-12-9 **AlogP:** 4.79 **TPSA:** 44.8

Activity: Antipsychotic

Catalog number : A-908

Drug name : Anserine-d_4



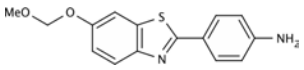
Mol. Formula : $C_{10}H_{12}D_4N_4O_3$ **FW :** 244.28 **HBA:** 5 **HBD:** 3 **RotB:** 6

PubChem ID : 11444 **CASRN :** 584-85-0 **AlogP:** -5.15 **TPSA:** 110.2

Activity: Stable isotope labeled Anserine LC/MS internal standard

Catalog number : A-909

Drug name : 6-MOMO-BTA-0



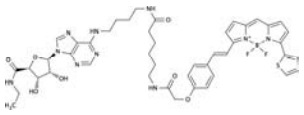
Mol. Formula : $C_{15}H_{14}N_2O_2S$ **FW :** 286.35 **HBA:** 5 **HBD:** 1 **RotB:** 4

PubChem ID : 11778756 **CASRN :** **AlogP:** 3.13 **TPSA:** 85.6

Activity: Aggregated amyloid protein ligand; Thioflavin-T analog

Catalog number : A-910

Drug name : ABEA-X-BY630



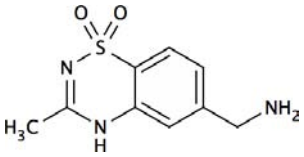
Mol. Formula : $C_{45}H_{51}BF_2N_{10}O_7S$ **FW :** 924.82 **HBA:** 14 **HBD:** 6 **RotB:** 21

PubChem ID : 16109359 **CASRN :** **AlogP:** -2.13 **TPSA:** 238.0

Activity: Fluorescent adenosine A_3 receptor agonist

Catalog number : A-911

Drug name : 6-Aminomethyl-3-methyl-4H-1,2,4-benzothiadazine-1,1-dioxide hydrochloride



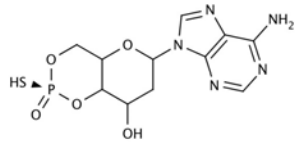
Mol. Formula : $C_9H_{12}ClN_3O_2S$ **FW :** 261.73 **HBA:** 5 **HBD:** 2 **RotB:** 1

PubChem ID : 121929 **CASRN :** 79987-38-5 **AlogP:** -0.48 **TPSA:** 92.9

Activity: Taurine antagonist

Catalog number : A-912 new

Drug name : (*Sp*)-cAMPS triethylammonium salt



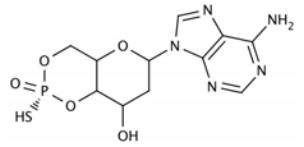
Mol. Formula : $C_{16}H_{27}N_6O_5PS$ **FW :** 446.46 **HBA:** 11 **HBD:** 3 **RotB:** 5

PubChem ID : 6858240 **CASRN :** 93602-66-5 **AlogP:** **TPSA:** 186.5

Activity: Protein kinase A agonist.

Catalog number : A-913 new

Drug name : (*Rp*)-cAMPS triethylammonium salt



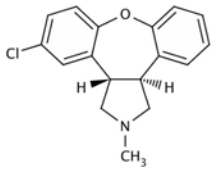
Mol. Formula : $C_{16}H_{27}N_6O_5PS$ **FW :** 446.46 **HBA:** 11 **HBD:** 3 **RotB:** 5

PubChem ID : 6858240 **CASRN :** **AlogP:** **TPSA:** 186.5

Activity: Protein kinase A inhibitor.

Catalog number : A-914 new

Drug name : Asenapine maleate



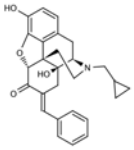
Mol. Formula : $C_{21}H_{20}ClNO_5$ **FW :** 401.84 **HBA:** 2 **HBD:** 0 **RotB:** 0

PubChem ID : 11954293 **CASRN :** 65576-45-6 **AlogP:** 4.31 **TPSA:** 12.5

Activity: Antipsychotic.

Catalog number : B-139

Drug name : (*E*)-7-Benzylidene-7-dehydronaltrexone hydrochloride



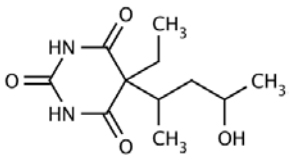
Mol. Formula : $C_{27}H_{28}ClNO_4$ **FW :** 465.97 **HBA:** 5 **HBD:** 2 **RotB:** 3

PubChem ID : 5310988 **CASRN :** 129468-28-6 **AlogP:** 3.49 **TPSA:** 70.0

Activity: Delta opioid δ_1 receptor antagonist

Catalog number : B-501

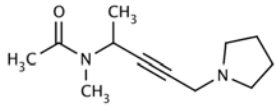
Drug name : 5-Ethyl-5-(3'-hydroxy-1'-methylbutyl)barbituric acid



Mol. Formula :	$C_{11}H_{18}N_2O_4$	**FW :** 242.28	**HBA:** 4	**HBD:** 3	**RotB:** 4
PubChem ID :	94288	**CASRN :** 4241-40-1		**AlogP:** 0.43	**TPSA:** 95.5
Activity:	Pentobarbitol metabolite				

Catalog number : B-504

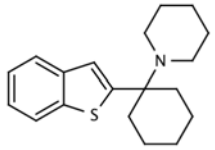
Drug name : *N*-Methyl-*N*-(1-methyl-4-pyrrolidino-2-butynyl)acetamide oxalate



Mol. Formula :	$C_{14}H_{22}N_2O_5$	**FW :** 298.33	**HBA:** 2	**HBD:** 0	**RotB:** 4
PubChem ID :	55005	**CASRN :** 83481-69-0		**AlogP:** 0.48	**TPSA:** 23.6
Activity:	Muscarinic partial agonist (oxotremorine analog)				

Catalog number : B-701

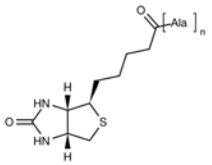
Drug name : N-[1-(2-Benzo[b]thiophenyl)cyclohexyl]piperidine hydrochloride



Mol. Formula :	$C_{19}H_{26}ClNS$	**FW :** 335.94	**HBA:** 2	**HBD:** 0	**RotB:** 2
PubChem ID :	123692	**CASRN :** 112726-66-6		**AlogP:** 4.88	**TPSA:** 31.5
Activity:	Dopamine uptake inhibitor with little affinity for PCP sites				

Catalog number : B-702

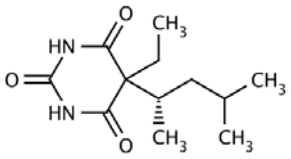
Drug name : Biotin-poly-DL-alanine



Mol. Formula :		**FW :**	**HBA:**	**HBD:**	**RotB:**
PubChem ID :		**CASRN :**		**AlogP:**	**TPSA:**

Catalog number : B-704

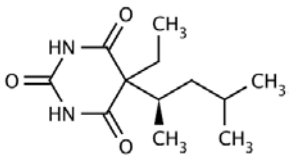
Drug name : (*S*)-(–)-5-(1,3-Dimethylbutyl)-5-ethylbarbituric acid; Diberal



Mol. Formula :	$C_{12}H_{20}N_2O_3$	**FW :** 240.30	**HBA:** 3	**HBD:** 2	**RotB:** 4
PubChem ID :	18079	**CASRN :** 2964-06-9		**AlogP:** 2.19	**TPSA:** 75.3
Activity:	Sedative, hypnotic				

Catalog number : B-705

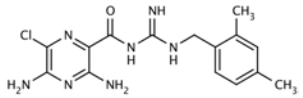
Drug name : (*R*)-(+)-5-(1,3-Dimethylbutyl)-5-ethylbarbituric acid; Diberal



Mol. Formula :	$C_{12}H_{20}N_2O_3$	**FW :** 240.30	**HBA:** 3	**HBD:** 2	**RotB:** 4
PubChem ID :	18079	**CASRN :** 2964-06-9		**AlogP:** 2.19	**TPSA:** 75.3
Activity:	Convulsant				

Catalog number : B-709

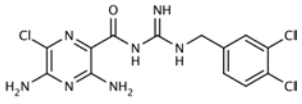
Drug name : 2',4'-Dimethylbenzamil hydrochloride



Mol. Formula :	$C_{15}H_{19}Cl_2N_7O$	**FW :** 384.27	**HBA:** 8	**HBD:** 5	**RotB:** 3
PubChem ID :	10247117	**CASRN :**		**AlogP:** 3.03	**TPSA:** 142.8
Activity:	Sodium/calcium exchanger inhibiter				

Catalog number : B-710

Drug name : 3',4'-Dichlorobenzamil hydrochloride



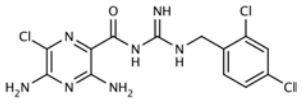
Mol. Formula : $C_{13}H_{13}Cl_4N_7O$ **FW :** 425.11 **HBA:** 10 **HBD:** 5 **RotB:** 3

PubChem ID : 114771 **CASRN :** 1166-01-4 **AlogP:** 3.13 **TPSA:** 142.8

Activity: Sodium/calcium exchanger inhibitor

Catalog number : B-711

Drug name : 2',4'-Dichlorobenzamil hydrochloride



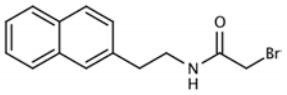
Mol. Formula : $C_{13}H_{13}Cl_4N_7O$ **FW :** 425.11 **HBA:** 10 **HBD:** 5 **RotB:** 3

PubChem ID : 6610300 **CASRN :** **AlogP:** 3.13 **TPSA:** 142.8

Activity: Sodium/calcium exchanger inhibitor

Catalog number : B-801

Drug name : N-Bromoacetylnapthalene-2-ethylamine

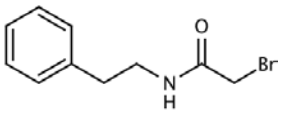


Mol. Formula : $C_{14}H_{14}BrNO$ **FW :** 292.17 **HBA:** 1 **HBD:** 1 **RotB:** 4

PubChem ID : 23626931 **CASRN :** **AlogP:** 2.90 **TPSA:** 29.1

Catalog number : B-802

Drug name : N-Bromoacetyl-β-phenethylamine

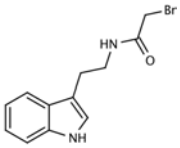


Mol. Formula : $C_{10}H_{12}BrNO$ **FW :** 242.12 **HBA:** 1 **HBD:** 1 **RotB:** 4

PubChem ID : 9881279 **CASRN :** **AlogP:** 1.90 **TPSA:** 29.1

Catalog number : B-803

Drug name : N-Bromoacetyltryptamine



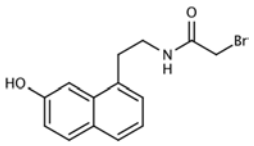
Mol. Formula : $C_{12}H_{13}BrN_2O$ **FW :** 281.16 **HBA:** 1 **HBD:** 2 **RotB:** 4

PubChem ID : 399698 **CASRN :** **AlogP:** 2.00 **TPSA:** 44.9

Activity: Reversible inhibitor of melatonin secretion in the pineal gland

Catalog number : B-804

Drug name : N-[2-(7-Hydroxy-1-napthyl)ethyl]-2-bromoacetamide

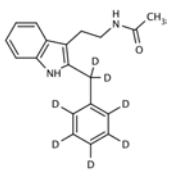


Mol. Formula : $C_{14}H_{14}BrNO_2$ **FW :** 308.18 **HBA:** 2 **HBD:** 2 **RotB:** 4

PubChem ID : **CASRN :** **AlogP:** 2.61 **TPSA:** 49.3

Catalog number : B-805

Drug name : (Benzyl-[$^2H_7$])-2-Benzyl-*N*-acetyltryptamine; Deuterated luzindole



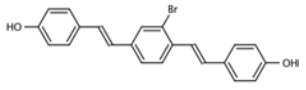
Mol. Formula : $C_{19}H_{13}D_7N_2O$ **FW :** 299.42 **HBA:** 1 **HBD:** 2 **RotB:** 5

PubChem ID : **CASRN :** **AlogP:** 3.04 **TPSA:** 44.9

Activity: Stable isotope labeled melatonin receptor antagonist luzindole

Catalog number : B-806

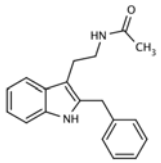
Drug name : 1-Bromo-2,5-bis(4-hydroxystyryl)benzene



Mol. Formula :	$C_{22}H_{17}BrO_2$	**FW :**	393.28	**HBA:**	2	**HBD:**	2	**RotB:**	4
PubChem ID :		**CASRN :**				**AlogP:**	7.70	**TPSA:**	40.5

Catalog number : B-807

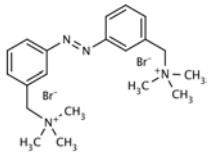
Drug name : Luzindole



Mol. Formula :	$C_{19}H_{20}N_2O$	**FW :**	292.38	**HBA:**	1	**HBD:**	2	**RotB:**	5
PubChem ID :	122162	**CASRN :**	117946-91-5			**AlogP:**	3.04	**TPSA:**	44.9
Activity:	Melatonin receptor antagonist								

Catalog number : B-901

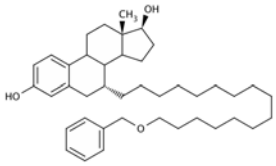
Drug name : *trans*-Bis-Q



Mol. Formula :	$C_{20}H_{30}Br_2N_4$	**FW :**	486.29	**HBA:**	2	**HBD:**	0	**RotB:**	6
PubChem ID :	133795	**CASRN :**	81931-05-7			**AlogP:**	-5.03	**TPSA:**	24.7
Activity:	Photochromic acetylcholine receptor activator								

Catalog number : B-902

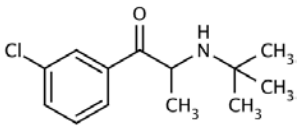
Drug name : 7α-(16-Benzyloxyhexadecyl)estra-1,3,5-trien-3,17β-diol



Mol. Formula :	$C_{41}H_{62}O_3$	**FW :**	602.94	**HBA:**	3	**HBD:**	2	**RotB:**	21
PubChem ID :		**CASRN :**				**AlogP:**	11.68	**TPSA:**	49.7

Catalog number : B-903

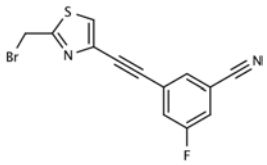
Drug name : Bupropion hydrochloride



Mol. Formula :	$C_{13}H_{19}Cl_2NO$	**FW :**	276.21	**HBA:**	3	**HBD:**	1	**RotB:**	4
PubChem ID :	62884	**CASRN :**	34841-36-6			**AlogP:**	2.75	**TPSA:**	29.1
Activity:	Dopamine uptake inhibitor								

Catalog number : B-904

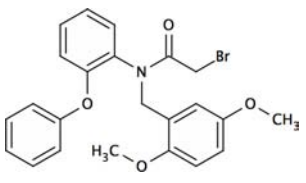
Drug name : 3-{2-[2-(Bromomethyl)thiazol-4-yl]ethynyl}-5-fluorobenzonitrile



Mol. Formula :	$C_{13}H_6BrFN_2S$	**FW :**	321.17	**HBA:**	4	**HBD:**	0	**RotB:**	4
PubChem ID :		**CASRN :**				**AlogP:**	3.67	**TPSA:**	64.9
Activity:	mGluR5 PET imaging ligand precursor								

Catalog number : B-905

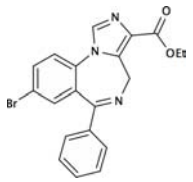
Drug name : 2-Bromo-*N*-[(2,5-dimethoxyphenyl)methyl]-*N*-(2-phenoxyphenyl)acetamide



Mol. Formula :	$C_{23}H_{22}BrNO_4$	**FW :**	456.34	**HBA:**	4	**HBD:**	0	**RotB:**	8
PubChem ID :		**CASRN :**				**AlogP:**	3.49	**TPSA:**	60.9
Activity:	Brain peripheral benzodiazepine receptor (TSPO) ligand								

Catalog number : B-906

Drug name : 8-Bromo-6-phenyl-4H-benzo[f]imidazo[1,5-a][1,4]diazepine-3-carboxylic acid ethyl ester



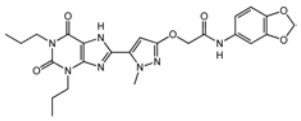
Mol. Formula : $C_{20}H_{16}BrN_3O_2$ **FW :** 410.26 **HBA:** 3 **HBD:** 0 **RotB:** 4

PubChem ID : 21930956 **CASRN :** **AlogP:** 3.28 **TPSA:** 56.5

Activity: Anxiolytic

Catalog number : B-907 new

Drug name : MRE 2029-F20

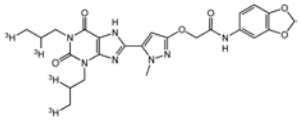


Mol. Formula : $C_{24}H_{27}N_7O_6$ **FW :** 509.52 **HBA:** **HBD:** **RotB:**

PubChem ID : **CASRN :** **AlogP:** **TPSA:**

Catalog number : B-908 new

Drug name : [^{3}H]MRE 2029-F20

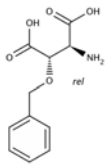


Mol. Formula : $C_{24}H_{27}N_7O_6$ **FW :** 509.51 **HBA:** **HBD:** **RotB:**

PubChem ID : **CASRN :** **AlogP:** **TPSA:**

Catalog number : B-909 new

Drug name : DL-TBOA



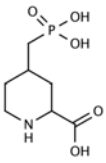
Mol. Formula : $C_{11}H_{13}NO_5$ **FW :** 239.23 **HBA:** 6 **HBD:** 4 **RotB:** 7

PubChem ID : 5311218 **CASRN :** **AlogP:** 2.49 **TPSA:** 65.1

Activity: Glutamate uptake inhibitor.

Catalog number : C-105

Drug name : CGS 19755; Selfotel



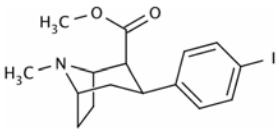
Mol. Formula : $C_7H_{14}NO_5P$ **FW :** 223.17 **HBA:** 6 **HBD:** 4 **RotB:** 3

PubChem ID : 68736 **CASRN :** 110347-85-8 **AlogP:** -3.56 **TPSA:** 116.7

Activity: Competitive NMDA receptor antagonist

Catalog number : C-148

Drug name : RTI-55



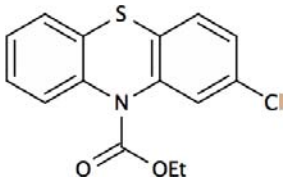
Mol. Formula : $C_{20}H_{26}INO_8$ **FW :** 535.32 **HBA:** 2 **HBD:** 0 **RotB:** 3

PubChem ID : 108220 **CASRN :** 133647-95-7 **AlogP:** 3.39 **TPSA:** 29.5

Activity: Dopamine transporter ligand

Catalog number : C-501

Drug name : 10-Carboethoxy-2-chlorophenothiazine

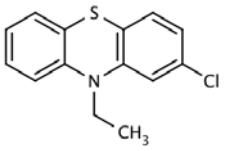


Mol. Formula : $C_{15}H_{12}ClNO_2S$ **FW :** 305.79 **HBA:** 5 **HBD:** 0 **RotB:** 2

PubChem ID : **CASRN :** **AlogP:** 4.77 **TPSA:** 54.8

Catalog number : C-502

Drug name : N-Ethyl-2-chlorophenothiazine

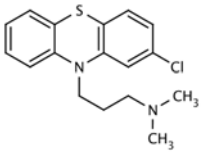


Mol. Formula : $C_{14}H_{12}ClNS$ **FW :** 261.78 **HBA:** 3 **HBD:** 0 **RotB:** 1

PubChem ID : **CASRN :** 56301-63-4 **AlogP:** 4.87 **TPSA:** 28.5

Catalog number : C-503

Drug name : Chlorpromazine hydrochloride



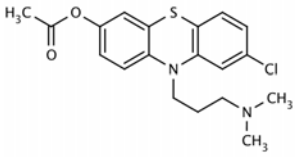
Mol. Formula : $C_{17}H_{20}Cl_2N_2S$ **FW :** 355.33 **HBA:** 4 **HBD:** 0 **RotB:** 4

PubChem ID : 2726 **CASRN :** 69-09-0 **AlogP:** 4.56 **TPSA:** 31.8

Activity: Dopamine receptor antagonist; serotonin receptor antagonist; histamine

Catalog number : C-504

Drug name : 7-Acetoxychlorpromazine hydrogen maleate

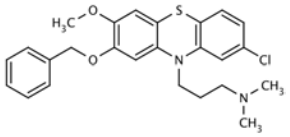


Mol. Formula : $C_{23}H_{25}ClN_2O_6S$ **FW :** 429.98 **HBA:** 5 **HBD:** 0 **RotB:** 6

PubChem ID : 547310 **CASRN :** **AlogP:** 4.05 **TPSA:** 58.1

Catalog number : C-505

Drug name : 8-Benzyloxy-7-methoxychlorpromazine

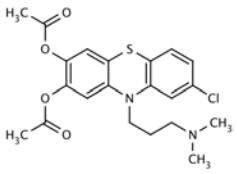


Mol. Formula : $C_{25}H_{27}ClN_2O_2S$ **FW :** 455.02 **HBA:** 6 **HBD:** 1 **RotB:** 7

PubChem ID : **CASRN :** **AlogP:** 5.61 **TPSA:** 61.2

Catalog number : C-506

Drug name : 7,8-Diacetoxychlorpromazine hydrogen maleate

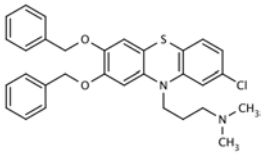


Mol. Formula : $C_{25}H_{27}ClN_2O_8S$ **FW :** 551.02 **HBA:** 6 **HBD:** 0 **RotB:** 8

PubChem ID : **CASRN :** **AlogP:** 3.55 **TPSA:** 84.4

Catalog number : C-508

Drug name : 7,8-Dibenzyloxychlorpromazine

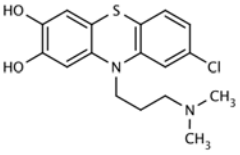


Mol. Formula : $C_{31}H_{31}ClN_2O_2S$ **FW :** 531.12 **HBA:** 6 **HBD:** 0 **RotB:** 10

PubChem ID : **CASRN :** **AlogP:** 7.60 **TPSA:** 50.2

Catalog number : C-511

Drug name : 7,8-Dihydroxychlorpromazine hydrochloride



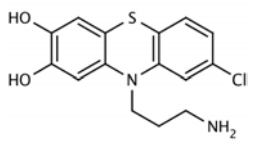
Mol. Formula : $C_{17}H_{20}Cl_2N_2O_2S$ **FW :** 387.33 **HBA:** 6 **HBD:** 2 **RotB:** 4

PubChem ID : 159916 **CASRN :** 21598-02-7 **AlogP:** 3.43 **TPSA:** 72.2

Activity: Chlorpromazine metabolite

Catalog number : C-512

Drug name : 7,8-Dihydroxy-N,N-didesmethylchlorpromazine hydrochloride



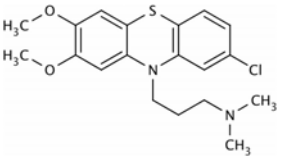
Mol. Formula : $C_{15}H_{16}C_2N_2O_2S$ **FW :** 359.29 **HBA:** 6 **HBD:** 3 **RotB:** 3

PubChem ID : 125358 **CASRN :** 95574-30-4 **AlogP:** 2.38 **TPSA:** 95.0

Activity: Chlorpromazine metabolite

Catalog number : C-513

Drug name : 7,8-Dimethoxychlorpromazine hydrochloride



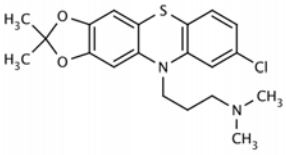
Mol. Formula : $C_{19}H_{24}Cl_2N_2O_2S$ **FW :** 415.39 **HBA:** 6 **HBD:** 0 **RotB:** 6

PubChem ID : 87327 **CASRN :** 17831-98-0 **AlogP:** 4.05 **TPSA:** 50.2

Activity: Chlorpromazine metabolite

Catalog number : C-514

Drug name : 7,8-(Dimethylmethylenedioxy)chlorpromazine



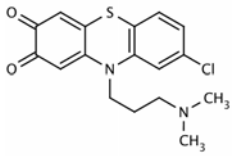
Mol. Formula : $C_{20}H_{23}ClN_2O_2S$ **FW :** 390.93 **HBA:** 6 **HBD:** 0 **RotB:** 4

PubChem ID : 114324 **CASRN :** 63834-02-6 **AlogP:** 4.87 **TPSA:** 50.2

Activity: Chlorpromazine metabolite

Catalog number : C-515

Drug name : 7,8-Dioxochlorpromazine hydrochloride



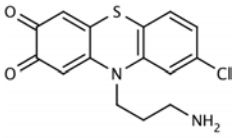
Mol. Formula : $C_{17}H_{18}Cl_2N_2O_2S$ **FW :** 385.31 **HBA:** 6 **HBD:** 0 **RotB:** 4

PubChem ID : 122845 **CASRN :** 52172-18-6 **AlogP:** 2.54 **TPSA:** 65.9

Activity: Chlorpromazine metabolite

Catalog number : C-516

Drug name : 7,8-Dioxo-N,N-didesmethylchlorpromazine hydrochloride

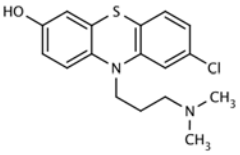


Mol. Formula : $C_{15}H_{14}Cl_2N_2O_2S$ **FW :** 357.26 **HBA:** 6 **HBD:** 1 **RotB:** 3

PubChem ID : 125595 **CASRN :** 95574-31-5 **AlogP:** 1.77 **TPSA:** 88.7

Catalog number : C-518

Drug name : 7-Hydroxychlorpromazine hydrochloride



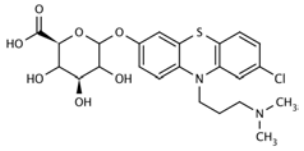
Mol. Formula : $C_{17}H_{20}Cl_2N_2OS$ **FW :** 371.33 **HBA:** 5 **HBD:** 1 **RotB:** 4

PubChem ID : 16414 **CASRN :** 2095-62-7 **AlogP:** 3.96 **TPSA:** 52.0

Activity: Dopamine antagonist

Catalog number : C-519

Drug name : 7-Hydroxychlorpromazine-*O*-β-D-glucuronide trifluoroacetate



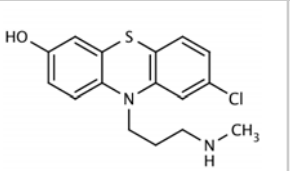
Mol. Formula : $C_{25}H_{28}ClF_3N_2O_9S$ **FW :** 625.02 **HBA:** 11 **HBD:** 4 **RotB:** 7

PubChem ID : **CASRN :** **AlogP:** -4.20 **TPSA:** 148.2

Activity: 7-Hydroxychlorpromazine metabolite

Catalog number : C-520

Drug name : 7-Hydroxy-*N*-desmethylchlorpromazine hydrochloride



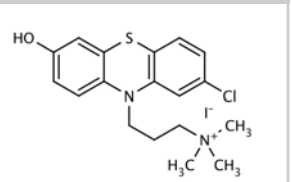
Mol. Formula : $C_{16}H_{18}Cl_2N_2OS$ **FW :** 357.31 **HBA:** 5 **HBD:** 2 **RotB:** 4

PubChem ID : 107410 **CASRN :** 3546-08-5 **AlogP:** 3.35 **TPSA:** 60.8

Activity: Chlorpromazine metabolite

Catalog number : C-521

Drug name : 7-Hydroxychlorpromazine methiodide



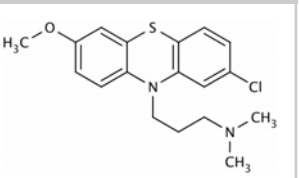
Mol. Formula : $C_{18}H_{22}ClIN_2OS$ **FW :** 476.81 **HBA:** 4 **HBD:** 1 **RotB:** 4

PubChem ID : **CASRN :** **AlogP:** -0.30 **TPSA:** 48.8

Activity: Dopamine antagonist

Catalog number : C-523

Drug name : 7-Methoxychlorpromazine hydrochloride



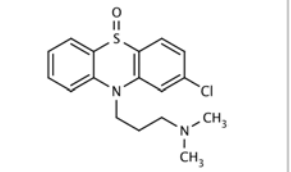
Mol. Formula : $C_{18}H_{22}Cl_2N_2OS$ **FW :** 385.36 **HBA:** 5 **HBD:** 0 **RotB:** 5

PubChem ID : 21115409 **CASRN :** 2752-11-6 **AlogP:** 4.30 **TPSA:** 41.0

Activity: Chlorpromazine metabolite

Catalog number : C-524

Drug name : Chlorpromazine sulfoxide hydrochloride



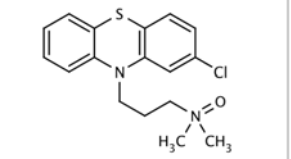
Mol. Formula : $C_{17}H_{20}Cl_2N_2OS$ **FW :** 371.33 **HBA:** 4 **HBD:** 0 **RotB:** 4

PubChem ID : 70413 **CASRN :** 969-99-30 **AlogP:** 2.58 **TPSA:** 42.8

Activity: Dopamine antagonist

Catalog number : C-525

Drug name : Chlorpromazine-*N*-oxide



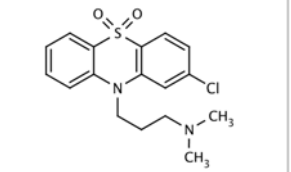
Mol. Formula : $C_{17}H_{19}ClN_2OS$ **FW :** 334.87 **HBA:** 0 **HBD:** 0 **RotB:** 4

PubChem ID : 443037 **CASRN :** 1672-76-0 **AlogP:** **TPSA:** 48.8

Activity: Dopamine antagonist

Catalog number : C-526

Drug name : Chlorpromazine sulfone hydrochloride

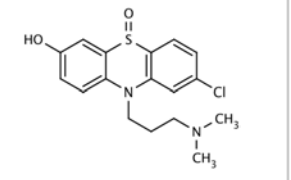


Mol. Formula : $C_{17}H_{20}Cl_2N_2O_2S$ **FW :** 387.33 **HBA:** 5 **HBD:** 0 **RotB:** 4

PubChem ID : 165214 **CASRN :** **AlogP:** 2.87 **TPSA:** 49.0

Catalog number : C-528

Drug name : 7-Hydroxychlorpromazine sulfoxide

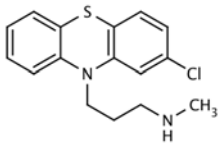


Mol. Formula : $C_{17}H_{19}ClN_2O_2S$ **FW :** 350.87 **HBA:** 5 **HBD:** 1 **RotB:** 4

PubChem ID : 21857538 **CASRN :** **AlogP:** 2.04 **TPSA:** 63.0

Catalog number : C-529

Drug name : *nor*-1-Chlorpromazine hydrochloride



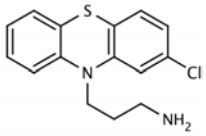
Mol. Formula : $C_{16}H_{18}Cl_2N_2S$ **FW :** 341.30 **HBA:** 4 **HBD:** 1 **RotB:** 4

PubChem ID : 520950 **CASRN :** 1225-64-5 **AlogP:** 4.19 **TPSA:** 40.6

Activity: Chlorpromazine metabolite

Catalog number : C-530

Drug name : *nor*-2-Chlorpromazine hydrochloride



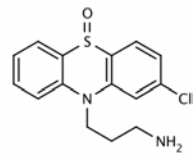
Mol. Formula : $C_{15}H_{16}Cl_2N_2S$ **FW :** 327.27 **HBA:** 4 **HBD:** 1 **RotB:** 3

PubChem ID : 197797 **CASRN :** 3763-80-2 **AlogP:** 3.79 **TPSA:** 54.6

Activity: Active metabolite of chlorpromazine.

Catalog number : C-531

Drug name : *nor*-2-Chlorpromazine sulfoxide hydrochloride



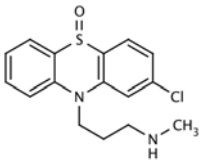
Mol. Formula : $C_{15}H_{16}Cl_2N_2OS$ **FW :** 343.27 **HBA:** 4 **HBD:** 1 **RotB:** 3

PubChem ID : 75220 **CASRN :** 2232-49-7 **AlogP:** 1.81 **TPSA:** 65.5

Activity: Chlorpromazine metabolite

Catalog number : C-532

Drug name : *nor*-1-Chlorpromazine sulfoxide hydrochloride

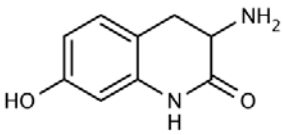


Mol. Formula : $C_{16}H_{18}Cl_2N_2OS$ **FW :** 357.30 **HBA:** 4 **HBD:** 1 **RotB:** 4

PubChem ID : 11723560 **CASRN :** **AlogP:** 2.22 **TPSA:** 51.6

Catalog number : C-535

Drug name : 3-Amino-3,4-dihydro-7-hydroxycarbostyril

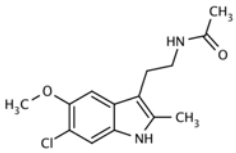


Mol. Formula : $C_9H_{10}N_2O_2$ **FW :** 178.19 **HBA:** 3 **HBD:** 3 **RotB:** 0

PubChem ID : **CASRN :** **AlogP:** 0.11 **TPSA:** 75.4

Catalog number : C-536

Drug name : 6-Chloro-2-methylmelatonin

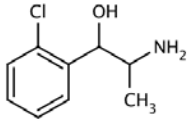


Mol. Formula : $C_{14}H_{17}ClN_2O_2$ **FW :** 280.76 **HBA:** 3 **HBD:** 2 **RotB:** 4

PubChem ID : **CASRN :** **AlogP:** 1.62 **TPSA:** 54.1

Catalog number : C-537

Drug name : 2-Chloropropadrine hydrochloride

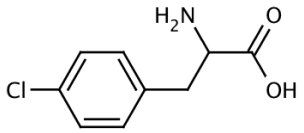


Mol. Formula : $C_9H_{13}Cl_2NO$ **FW :** 222.12 **HBA:** 3 **HBD:** 2 **RotB:** 2

PubChem ID : **CASRN :** **AlogP:** 1.42 **TPSA:** 46.3

Catalog number : C-538

Drug name : (±)-p-Chlorophenylalanine; Fenclonine



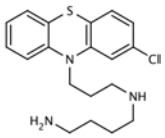
Mol. Formula : $C_9H_{10}ClNO_2$ **FW :** 199.64 **HBA:** 4 **HBD:** 2 **RotB:** 3

PubChem ID : 4652 **CASRN :** 7424-00-2 **AlogP:** -0.63 **TPSA:** 63.3

Activity: Serotonin 5-HT antagonist

Catalog number : C-701

Drug name : Chlorpromazine-10-spermidine dihydrochloride



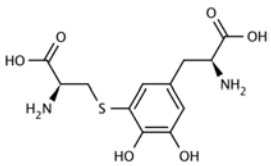
Mol. Formula : $C_{19}H_{26}Cl_3N_3S$ **FW :** 434.85 **HBA:** 5 **HBD:** 2 **RotB:** 8

PubChem ID : **CASRN :** **AlogP:** 3.91 **TPSA:** 66.6

Activity: Potential prodrug for polyamines

Catalog number : C-702

Drug name : 5-(*S*)-Cysteinyl-L-DOPA



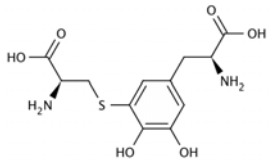
Mol. Formula : $C_{12}H_{16}N_2O_6S$ **FW :** 316.33 **HBA:** 9 **HBD:** 6 **RotB:** 7

PubChem ID : **CASRN :** **AlogP:** -4.66 **TPSA:** 192.4

Activity: Melanoma biomarker

Catalog number : C-702A

Drug name : 5-(*S*)-Cysteinyl-L-DOPA dihydrochloride



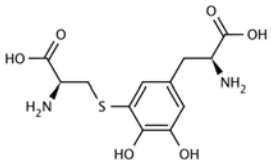
Mol. Formula : $C_{12}H_{18}Cl_2N_2O_6S$ **FW :** 389.25 **HBA:** 9 **HBD:** 6 **RotB:** 7

PubChem ID : **CASRN :** **AlogP:** -4.66 **TPSA:** 192.4

Activity: Melanoma biomarker

Catalog number : C-702B

Drug name : 5-(*S*)-Cysteinyl-L-DOPA trifluoroacetate



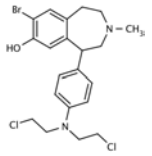
Mol. Formula : $C_{16}H_{18}F_6N_2O_{10}S$ **FW :** 544.38 **HBA:** 9 **HBD:** 6 **RotB:** 7

PubChem ID : **CASRN :** **AlogP:** -4.66 **TPSA:** 192.4

Activity: Melanoma biomarker

Catalog number : C-705

Drug name : (±)-*bis*-(2-Chloroethyl)amino-SKF-83566 hydrochloride



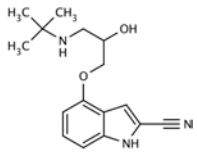
Mol. Formula : $C_{21}H_{26}BrCl_3N_2O$ **FW :** 508.72 **HBA:** 5 **HBD:** 1 **RotB:** 6

PubChem ID : **CASRN :** **AlogP:** 5.30 **TPSA:** 26.7

Activity: Dopamine D_1 receptor alkylating ligand

Catalog number : C-706

Drug name : Cyanopindolol fumarate



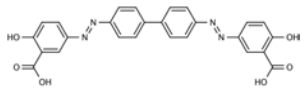
Mol. Formula : $C_{36}H_{46}N_6O_8$ **FW :** 690.80 **HBA:** 4 **HBD:** 3 **RotB:** 7

PubChem ID : 155346 **CASRN :** 69906-85-0 **AlogP:** 0.63 **TPSA:** 81.1

Activity: Adrenergic β-antagonist; serotonin 5-HTantagonist

Catalog number : C-707

Drug name : Chrysamine G



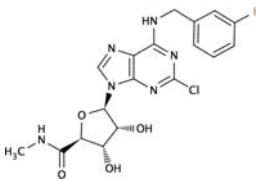
Mol. Formula : $C_{26}H_{18}N_4O_6$ **FW :** 482.46 **HBA:** 10 **HBD:** 4 **RotB:** 7

PubChem ID : 6506185 **CASRN :** 6472-91-9 **AlogP:** 8.10 **TPSA:** 164.5

Activity: Beta-amyloid ligand

Catalog number : C-708

Drug name : Chloro-IB-MECA



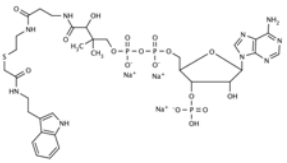
Mol. Formula : $C_{18}H_{18}ClIN_6O_4$ **FW :** 544.74 **HBA:** 9 **HBD:** 4 **RotB:** 5

PubChem ID : 393593 **CASRN :** 163042-96-4 **AlogP:** 1.47 **TPSA:** 134.4

Activity: Adenosine A_3 receptor ligand

Catalog number : C-711A

Drug name : Coenzyme A-*S*-acetyltryptamine

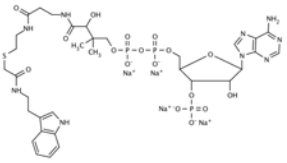


Mol. Formula : $C_{33}H_{45}N_9Na_3O_{17}P_3S$ **FW :** 1033.73 **HBA:** 18 **HBD:** 8 **RotB:** 24

PubChem ID : 2822 **CASRN :** **AlogP:** -5.83 **TPSA:** 454.7

Catalog number : C-711B

Drug name : Coenzyme A-*S*-acetyltryptamine

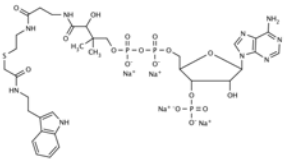


Mol. Formula : $C_{33}H_{44}N_9Na_4O_{17}P_3S$ **FW :** 1055.71 **HBA:** 18 **HBD:** 7 **RotB:** 24

PubChem ID : 2822 **CASRN :** **AlogP:** -5.83 **TPSA:** 457.5

Catalog number : C-711C

Drug name : Coenzyme A-*S*-acetyltryptamine

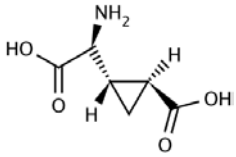


Mol. Formula : $C_{33}H_{44}N_9Na_4O_{17}P_3S$ **FW :** 1055.70 **HBA:** 18 **HBD:** 7 **RotB:** 24

PubChem ID : 2822 **CASRN :** **AlogP:** -5.83 **TPSA:** 457.5

Catalog number : C-801

Drug name : (2*S*,1'*S*,2'*S*)-2-(Carboxycyclopropyl)glycine



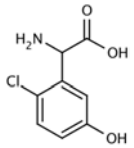
Mol. Formula : $C_6H_9NO_4$ **FW :** 159.14 **HBA:** 5 **HBD:** 3 **RotB:** 3

PubChem ID : 5310956 **CASRN :** 22255-17-0 **AlogP:** -3.19 **TPSA:** 100.6

Activity: mGluR2 agonist

Catalog number : C-802

Drug name : (*RS*)-2-Chloro-5-hydroxyphenylglycine



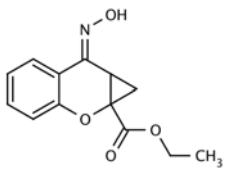
Mol. Formula : $C_8H_8ClNO_3$ **FW :** 201.61 **HBA:** 5 **HBD:** 3 **RotB:** 2

PubChem ID : 3645780 **CASRN :** **AlogP:** -1.16 **TPSA:** 83.6

Activity: mGlu5 agonist

Catalog number : C-803

Drug name : 7-(Hydroxyimino)cyclopropa[*b*]chromen-1a-carboxylate ethyl ester



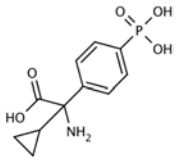
Mol. Formula : $C_{13}H_{13}NO_4$ **FW :** 247.25 **HBA:** 4 **HBD:** 1 **RotB:** 3

PubChem ID : 6278000 **CASRN :** 179067-99-3 **AlogP:** 1.00 **TPSA:** 68.1

Activity: mGluR1 antagonist

Catalog number : C-804

Drug name : (*RS*)-α-Cyclopropyl-4-phosphonophenylglycine



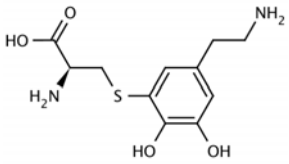
Mol. Formula : $C_{11}H_{14}NO_5P$ **FW :** 268.19 **HBA:** 6 **HBD:** 4 **RotB:** 4

PubChem ID : 2878 **CASRN :** **AlogP:** -2.11 **TPSA:** 130.7

Activity: mGlu3 antagonist

Catalog number : C-805A

Drug name : 5-(*S*)-Cysteinyldopamine trifluoroacetate



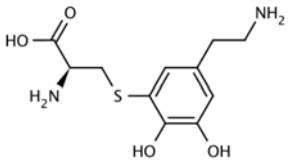
Mol. Formula : $C_{15}H_{18}F_6N_2O_8S$ **FW :** 500.36 **HBA:** 7 **HBD:** 5 **RotB:** 6

PubChem ID : 122084 **CASRN :** 99558-89-1 **AlogP:** -3.40 **TPSA:** 155.1

Activity: Antioxidant

Catalog number : C-805B

Drug name : 5-(*S*)-Cysteinyldopamine dihydrochloride



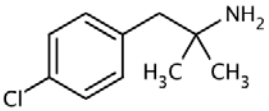
Mol. Formula : $C_{11}H_{18}Cl_2N_2O_4S$ **FW :** 345.24 **HBA:** 7 **HBD:** 5 **RotB:** 6

PubChem ID : 122084 **CASRN :** 99558-89-1 **AlogP:** -3.40 **TPSA:** 155.1

Activity: Anti-oxidant

Catalog number : C-806

Drug name : Chlorophentermine hydrochloride



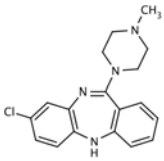
Mol. Formula : $C_{10}H_{15}Cl_2N$ **FW :** 220.14 **HBA:** 2 **HBD:** 1 **RotB:** 2

PubChem ID : 10007 **CASRN :** 151-06-4 **AlogP:** 2.42 **TPSA:** 26.0

Activity: Sympathomimetic

Catalog number : C-807

Drug name : Clozapine



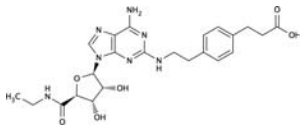
Mol. Formula : $C_{18}H_{19}ClN_4$ **FW :** 326.83 **HBA:** 5 **HBD:** 1 **RotB:** 0

PubChem ID : SID: 24277892 **CASRN :** 5786-21-0 **AlogP:** 3.39 **TPSA:** 30.9

Activity: Dopamine D_4 receptor antagonist

Catalog number : C-901

Drug name : CGS 21680 hydrochloride



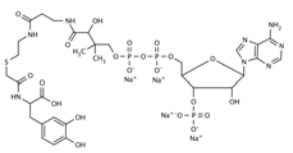
Mol. Formula : $C_{23}H_{30}ClN_7O_6$ **FW :** 535.99 **HBA:** 11 **HBD:** 6 **RotB:** 10

PubChem ID : 10256643 **CASRN :** 124182-57-6 **AlogP:** -1.28 **TPSA:** 197.7

Activity: Adenosine A_2 receptor agonist

Catalog number : C-902

Drug name : Coenzyme A-*S*-acetyl-L-DOPA

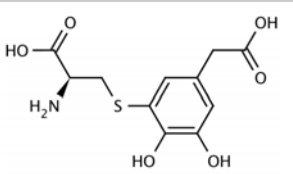


Mol. Formula : $C_{32}H_{43}N_8Na_4O_{21}P_3S$ **FW :** 1092.68 **HBA:** 22 **HBD:** 9 **RotB:** 25

PubChem ID : **CASRN :** **AlogP:** -6.63 **TPSA:** 519.5

Catalog number : C-903

Drug name : 5-(*S*)-Cysteinyl-DOPAC hydrochloride

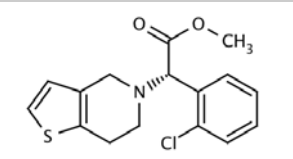


Mol. Formula : $C_{11}H_{14}ClNO_6S$ **FW :** 323.75 **HBA:** 8 **HBD:** 5 **RotB:** 6

PubChem ID : 128185 **CASRN :** 102986-13-0 **AlogP:** -1.93 **TPSA:** 166.4

Catalog number : C-904

Drug name : Clopidogrel hydrogen sulfate



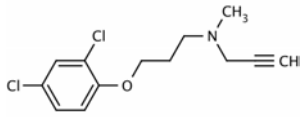
Mol. Formula : $C_{16}H_{18}ClNO_6S_2$ **FW :** 419.90 **HBA:** 4 **HBD:** 0 **RotB:** 4

PubChem ID : 115366 **CASRN :** 135046-48-9 **AlogP:** 3.80 **TPSA:** 57.8

Activity: Platelet aggregation inhibitor

Catalog number : C-905

Drug name : Clorgyline hydrochloride



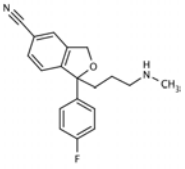
Mol. Formula : $C_{13}H_{16}Cl_3NO$ **FW :** 308.64 **HBA:** 4 **HBD:** 0 **RotB:** 7

PubChem ID : 28767 **CASRN :** 17780-75-5 **AlogP:** 3.13 **TPSA:** 12.5

Activity: Monoamine oxidase inhibitor

Catalog number : C-906

Drug name : N-Norcitalopram oxalate



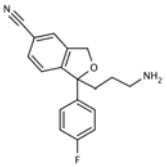
Mol. Formula : $C_{21}H_{21}FN_2O_5$ **FW :** 400.41 **HBA:** 4 **HBD:** 1 **RotB:** 6

PubChem ID : 162180 **CASRN :** 62498-67-3 **AlogP:** 3.20 **TPSA:** 45.1

Activity: Citalopram metabolite

Catalog number : C-907

Drug name : N,N-Dinorcitalopram oxalate



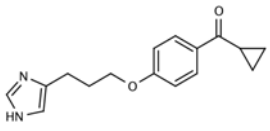
Mol. Formula : $C_{20}H_{19}FN_2O_5$ **FW :** 386.38 **HBA:** 4 **HBD:** 1 **RotB:** 5

PubChem ID : 162976 **CASRN :** 62498-69-5 **AlogP:** 2.79 **TPSA:** 59.0

Activity: Citalopram metabolite

Catalog number : C-908

Drug name : Ciproxifan



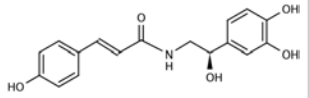
Mol. Formula : $C_{20}H_{22}N_2O_6$ **FW :** 386.40 **HBA:** 3 **HBD:** 1 **RotB:** 7

PubChem ID : 6422124 **CASRN :** 184025-19-2 **AlogP:** 1.85 **TPSA:** 55.0

Activity: Histamine H_3 receptor antagonist

Catalog number : C-909

Drug name : (*R*)-(+)-*N*-*trans*-*p*-Coumaroylnoradrenaline



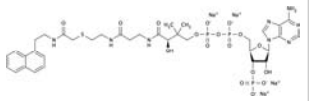
Mol. Formula : $C_{17}H_{17}NO_5$ **FW :** 315.32 **HBA:** 5 **HBD:** 5 **RotB:** 5

PubChem ID : **CASRN :** **AlogP:** 2.03 **TPSA:** 110.0

Activity: Plant metabolite implicated in tomato defense against pathogens

Catalog number : C-910

Drug name : Coenzyme A-*S*-acetyl-2-naphthylen-1-ylethylamine



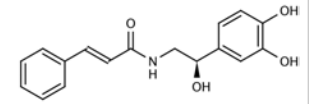
Mol. Formula : $C_{35}H_{45}N_8Na_4O_{17}P_3S$ **FW :** 1066.72 **HBA:** 18 **HBD:** 6 **RotB:** 24

PubChem ID : **CASRN :** **AlogP:** -4.93 **TPSA:** 441.7

Activity: Melatonin arylalkylamine-N-acetyltransferase rhythm enzyme ligand

Catalog number : C-911

Drug name : *N*-Cinnamoylnorepinephrine

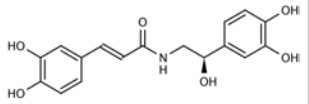


Mol. Formula : $C_{17}H_{17}NO_4$ **FW :** 299.32 **HBA:** 4 **HBD:** 4 **RotB:** 5

PubChem ID : **CASRN :** **AlogP:** 2.32 **TPSA:** 89.8

Catalog number : C-912

Drug name : *N*-Caffeoylnorepinephrine

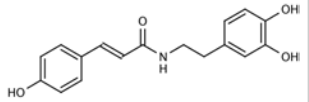


Mol. Formula : $C_{17}H_{17}NO_6$ **FW :** 331.32 **HBA:** 6 **HBD:** 6 **RotB:** 5

PubChem ID : **CASRN :** **AlogP:** 1.75 **TPSA:** 130.3

Catalog number : C-913

Drug name : *N*-Coumaroyldopamine

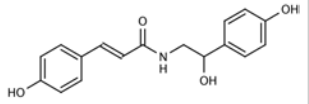


Mol. Formula : $C_{17}H_{17}NO_4$ **FW :** 299.32 **HBA:** 4 **HBD:** 4 **RotB:** 5

PubChem ID : 11630793 **CASRN :** **AlogP:** 2.96 **TPSA:** 89.8

Catalog number : C-914

Drug name : *N*-Coumaroyloctopamine

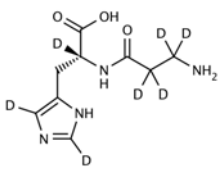


Mol. Formula : $C_{17}H_{17}NO_4$ **FW :** 299.32 **HBA:** 4 **HBD:** 4 **RotB:** 5

PubChem ID : 23874492 **CASRN :** **AlogP:** 2.32 **TPSA:** 89.8

Catalog number : C-915

Drug name : Carnosine-d7



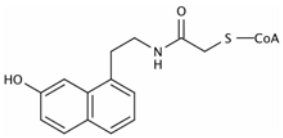
Mol. Formula : $C_9H_{14}N_4O_3$ **FW :** 226.23 **HBA:** 5 **HBD:** 4 **RotB:** 6

PubChem ID : 9369 **CASRN :** **AlogP:** -5.39 **TPSA:** 121.1

Activity: Stable isotope labeled Carnosine LC/MS internal standard

Catalog number : C-916

Drug name : Coenzyme A-*S*-acetyl-7-hydroxynaphthylethylamine



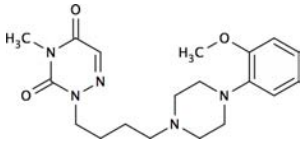
Mol. Formula : $C_{37}H_{49}N_8O_{17}P_3S_2$ **FW :** 1034.88 **HBA:** 19 **HBD:** 6 **RotB:** 25

PubChem ID : **CASRN :** **AlogP:** -3.41 **TPSA:** 467.0

Activity: Melatonin arylalkylamine-N-acetyltransferase rhythm enzyme ligand

Catalog number : C-917

Drug name : CUMI-101



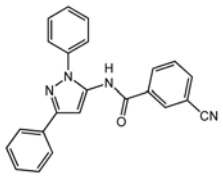
Mol. Formula : $C_{19}H_{27}N_5O_3$ **FW :** 373.45 **HBA:** 6 **HBD:** 0 **RotB:** 7

PubChem ID : 21830793 **CASRN :** **AlogP:** 1.79 **TPSA:** 68.7

Activity: Serotonin 5-HT_{1A} receptor ligand

Catalog number : C-918 new

Drug name : CDPPB



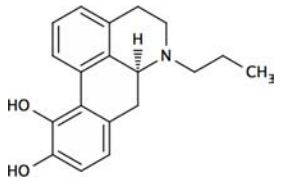
Mol. Formula : $C_{23}H_{16}N_4O$ **FW :** 364.41 **HBA:** 5 **HBD:** 1 **RotB:** 4

PubChem ID : 11245456 **CASRN :** 781652-57-1 **AlogP:** 2.72 **TPSA:** 70.7

Activity: Positive allosteric modulator of the mGlu5 receptor.

Catalog number : D-041

Drug name : (*S*)-(+)-*N*-Propylnorapomorphine hydrochloride



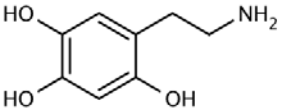
Mol. Formula : $C_{19}H_{22}ClNO_2$ **FW :** 331.84 **HBA:** 3 **HBD:** 2 **RotB:** 2

PubChem ID : 13533173 **CASRN :** 79703-31-4 **AlogP:** 3.62 **TPSA:** 43.7

Activity: Limbic-selective dopamine antagonist

Catalog number : D-501

Drug name : 6-Hydroxydopamine hydrobromide; Oxidopamine



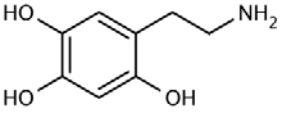
Mol. Formula : $C_8H_{12}BrNO_3$ **FW :** 250.09 **HBA:** 4 **HBD:** 4 **RotB:** 2

PubChem ID : 176170 **CASRN :** 636-00-0 **AlogP:** -0.18 **TPSA:** 86.7

Activity: Neurotoxin at catecholaminergic terminals

Catalog number : D-502

Drug name : 6-Hydroxydopamine hydrochloride; Oxidopamine



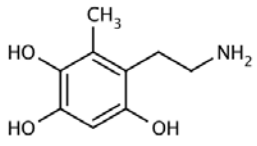
Mol. Formula : $C_8H_{12}ClNO_3$ **FW :** 205.64 **HBA:** 4 **HBD:** 4 **RotB:** 2

PubChem ID : 160157 **CASRN :** 28094-15-7 **AlogP:** -0.18 **TPSA:** 86.7

Activity: Neurotoxin at catecholaminergic terminals

Catalog number : D-503

Drug name : 2-Methyl-6-hydroxydopamine hydrobromide

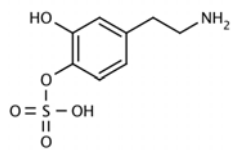


Mol. Formula : $C_9H_{14}BrNO_3$ **FW :** 264.12 **HBA:** 4 **HBD:** 4 **RotB:** 2

PubChem ID : **CASRN :** **AlogP:** 0.33 **TPSA:** 86.7

Catalog number : D-504

Drug name : Dopamine-4-O-sulfate

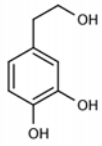


Mol. Formula :	$C_8H_{11}NO_5S$	**FW :**	233.24	**HBA:**	5	**HBD:**	3	**RotB:**	4
PubChem ID :	123932	**CASRN :**	38339-02-5			**AlogP:**	-1.75	**TPSA:**	118.2

Activity: Possible norepinephrine precursor

Catalog number : D-505

Drug name : Hydroxytyrosol

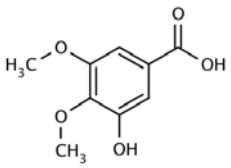


Mol. Formula :	$C_{14}H_{22}N_2O_3$	**FW :**	266.34	**HBA:**	3	**HBD:**	3	**RotB:**	2
PubChem ID :	82755	**CASRN :**	10597-60-1			**AlogP:**	0.89	**TPSA:**	60.7

Activity: Antioxidant; platelet aggregation inhibitor

Catalog number : D-506

Drug name : 3,4-Dimethoxy-5-hydroxybenzoic acid

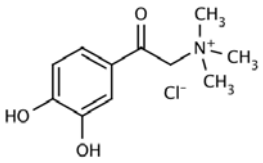


Mol. Formula :	$C_9H_{10}O_5$	**FW :**	198.18	**HBA:**	5	**HBD:**	2	**RotB:**	3
PubChem ID :	74709	**CASRN :**	1916-08-1			**AlogP:**	0.77	**TPSA:**	76.0

Activity: Thiopurine methyltransferase inhibitor

Catalog number : D-507

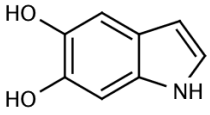
Drug name : α-Dimethylamino-3,4-dihydroxyacetophenone methachloride



Mol. Formula :	$C_{11}H_{16}ClNO_3$	**FW :**	245.71	**HBA:**	3	**HBD:**	2	**RotB:**	3
PubChem ID :	412800	**CASRN :**				**AlogP:**	-3.92	**TPSA:**	57.5

Catalog number : D-509

Drug name : 5,6-Dihydroxyindole

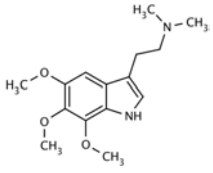


Mol. Formula :	$C_8H_7NO_2$	**FW :**	149.15	**HBA:**	2	**HBD:**	3	**RotB:**	0
PubChem ID :	114683	**CASRN :**	3131-52-0			**AlogP:**	1.58	**TPSA:**	56.3

Activity: Catechol O-methyltransferase (COMT) inhibitor

Catalog number : D-510

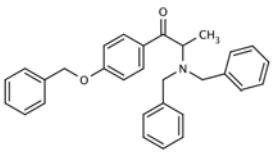
Drug name : 5,6,7-Trimethoxy-N,N-dimethyltryptamine



Mol. Formula :	$C_{15}H_{22}N_2O_3$	**FW :**	278.35	**HBA:**	4	**HBD:**	1	**RotB:**	6
PubChem ID :		**CASRN :**				**AlogP:**	1.53	**TPSA:**	46.7

Catalog number : D-511

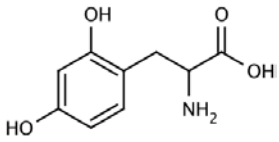
Drug name : 4'-Benzyloxy-2-dibenzylaminopropiophenone



Mol. Formula :	$C_{30}H_{29}NO_2$	**FW :**	435.59	**HBA:**	3	**HBD:**	0	**RotB:**	10
PubChem ID :		**CASRN :**				**AlogP:**	6.84	**TPSA:**	29.5

Catalog number : D-512

Drug name : (±)-2,4-Dihydroxyphenylalanine

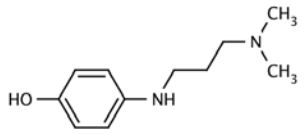


Mol. Formula : $C_9H_{11}NO_4$ **FW :** 197.19 **HBA:** 5 **HBD:** 4 **RotB:** 3

PubChem ID : 251462 **CASRN :** 582-34-3 **AlogP:** -1.71 **TPSA:** 103.8

Catalog number : D-513

Drug name : 4-(γ-N,N-Dimethylaminopropylamino)phenol dimaleate

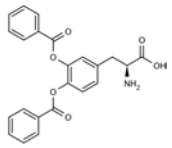


Mol. Formula : $C_{19}H_{26}N_2O_9$ **FW :** 426.43 **HBA:** 3 **HBD:** 2 **RotB:** 5

PubChem ID : **CASRN :** **AlogP:** 1.11 **TPSA:** 35.5

Catalog number : D-514

Drug name : L-3,4-Dibenzoyloxyphenylalanine



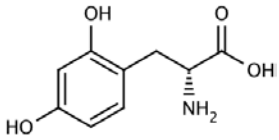
Mol. Formula : $C_{23}H_{19}NO_6$ **FW :** 405.41 **HBA:** 5 **HBD:** 2 **RotB:** 9

PubChem ID : 149369 **CASRN :** 120382-00-5 **AlogP:** 2.51 **TPSA:** 115.9

Activity: Na-K-ATPase inhibitor

Catalog number : D-515

Drug name : (+)-2,4-Dihydroxyphenylalanine

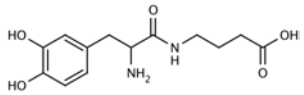


Mol. Formula : $C_9H_{11}NO_4$ **FW :** 197.19 **HBA:** 5 **HBD:** 4 **RotB:** 3

PubChem ID : 152670 **CASRN :** 24146-06-3 **AlogP:** -1.71 **TPSA:** 103.8

Catalog number : D-516

Drug name : (±)-3,4-Dihydroxyphenylalanyl-GABA

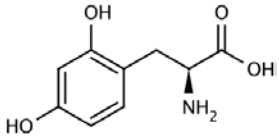


Mol. Formula : $C_{13}H_{18}N_2O_5$ **FW :** 282.30 **HBA:** 6 **HBD:** 5 **RotB:** 7

PubChem ID : **CASRN :** **AlogP:** -3.34 **TPSA:** 132.9

Catalog number : D-517

Drug name : (–)-2,4-Dihydroxyphenylalanine

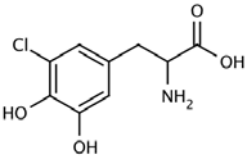


Mol. Formula : $C_9H_{11}NO_4$ **FW :** 197.19 **HBA:** 5 **HBD:** 4 **RotB:** 3

PubChem ID : 152670 **CASRN :** 24146-06-3 **AlogP:** -1.71 **TPSA:** 103.8

Catalog number : D-518

Drug name : (±)-3-Chloro-4,5-dihydroxyphenylalanine hydrobromide

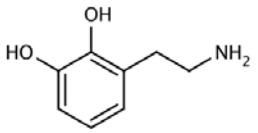


Mol. Formula : $C_9H_{11}BrClNO_4$ **FW :** 312.55 **HBA:** 6 **HBD:** 4 **RotB:** 3

PubChem ID : **CASRN :** **AlogP:** -1.20 **TPSA:** 103.8

Catalog number : D-519

Drug name : 2,3-Dihydroxy-β-phenethylamine hydrobromide

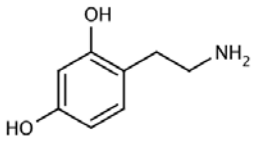


Mol. Formula : $C_8H_{12}BrNO_2$ **FW :** 234.09 **HBA:** 3 **HBD:** 3 **RotB:** 2

PubChem ID : **CASRN :** **AlogP:** 0.18 **TPSA:** 66.5

Catalog number : D-520

Drug name : 2,4-Dihydroxy-β-phenethylamine hydrochloride

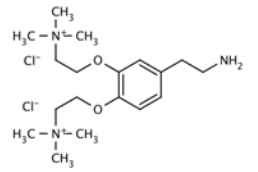


Mol. Formula : $C_8H_{12}ClNO_2$ **FW :** 189.64 **HBA:** 3 **HBD:** 3 **RotB:** 2

PubChem ID : 150962 **CASRN :** 2039-62-5 **AlogP:** 0.01 **TPSA:** 66.5

Catalog number : D-521

Drug name : 3,4-Di-(β-trimethylammoniumethoxy)-β-phenethylamine hydrochloride dichloride

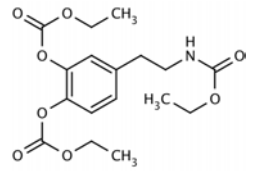


Mol. Formula : $C_{18}H_{36}Cl_3N_3O_2$ **FW :** 432.86 **HBA:** 3 **HBD:** 1 **RotB:** 10

PubChem ID : **CASRN :** **AlogP:** -8.28 **TPSA:** 44.5

Catalog number : D-522

Drug name : 3,4-Diethylcarbonato-β-phenethylamine carbamate

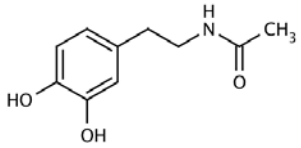


Mol. Formula : $C_{17}H_{23}NO_8$ **FW :** 369.37 **HBA:** 6 **HBD:** 1 **RotB:** 13

PubChem ID : **CASRN :** **AlogP:** 3.14 **TPSA:** 109.4

Catalog number : D-523

Drug name : N-Acetyl-3,4-dihydroxy-β-phenethylamine

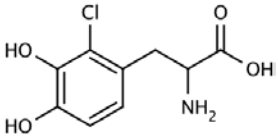


Mol. Formula : $C_{10}H_{13}NO_3$ **FW :** 195.22 **HBA:** 3 **HBD:** 3 **RotB:** 3

PubChem ID : 100526 **CASRN :** 2494-12-4 **AlogP:** 0.67 **TPSA:** 69.6

Catalog number : D-524

Drug name : (±)-2-Chloro-3,4-dihydroxyphenylalanine hydrobromide

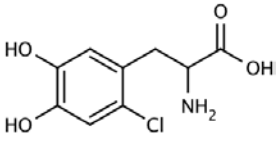


Mol. Formula : $C_9H_{11}BrClNO_4$ **FW :** 312.55 **HBA:** 6 **HBD:** 4 **RotB:** 3

PubChem ID : **CASRN :** **AlogP:** -1.20 **TPSA:** 103.8

Catalog number : D-525

Drug name : (±)-6-Chloro-3,4-dihydroxyphenylalanine hydrobromide

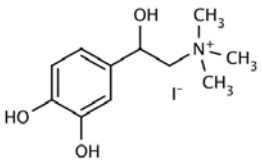


Mol. Formula : $C_9H_{11}BrClNO_4$ **FW :** 312.55 **HBA:** 6 **HBD:** 4 **RotB:** 3

PubChem ID : **CASRN :** **AlogP:** -1.20 **TPSA:** 103.8

Catalog number : D-528

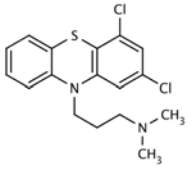
Drug name : (±)-(N,N-Dimethyl)ephedrine Iodide



Mol. Formula :	$C_{11}H_{18}INO_3$	**FW :**	339.17	**HBA:**	3	**HBD:**	3	**RotB:**	3
PubChem ID :	3082487	**CASRN :**	38522-73-5			**AlogP:**	-3.88	**TPSA:**	60.7

Catalog number : D-529

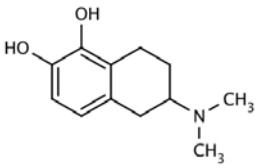
Drug name : 2,4-Dichloropromazine hydrochloride



Mol. Formula :	$C_{17}H_{19}Cl_3N_2S$	**FW :**	389.77	**HBA:**	5	**HBD:**	0	**RotB:**	4
PubChem ID :	77273	**CASRN :**	3689-36-9			**AlogP:**	5.07	**TPSA:**	31.8

Catalog number : D-701

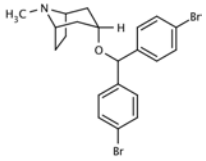
Drug name : (±)-5,6-Dihydroxy-2-(N,N-dimethyl)aminotetralin hydrobromide



Mol. Formula :	$C_{12}H_{18}BrNO_2$	**FW :**	288.19	**HBA:**	3	**HBD:**	2	**RotB:**	1
PubChem ID :	37032	**CASRN :**	39478-90-5			**AlogP:**	1.39	**TPSA:**	43.7

Catalog number : D-702

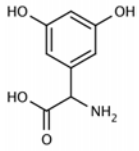
Drug name : 3-(4',4''-Dibromobenzhydryloxy)tropane hydrochloride



Mol. Formula :	$C_{21}H_{24}Br_2ClNO$	**FW :**	501.69	**HBA:**	2	**HBD:**	0	**RotB:**	4
PubChem ID :	10096017	**CASRN :**				**AlogP:**	5.66	**TPSA:**	12.5
Activity:	Dopamine uptake inhibitor								

Catalog number : D-801

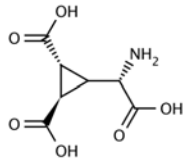
Drug name : (±)-3,5-Dihydroxyphenylglycine



Mol. Formula :	$C_8H_9NO_4$	**FW :**	183.16	**HBA:**	5	**HBD:**	4	**RotB:**	2
PubChem ID :	108001	**CASRN :**	146255-66-5			**AlogP:**	-1.96	**TPSA:**	103.8
Activity:	mGlu1 and mGlu5 receptor agonist								

Catalog number : D-802

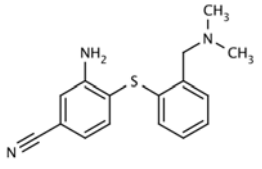
Drug name : (1*R*,2*R*)-3-[(1*S*)-1-Amino-2-hydroxy-2-oxo-ethyl]cyclopropane-1,2-di carboxylic acid



Mol. Formula :	$C_7H_9NO_6$	**FW :**	203.15	**HBA:**	7	**HBD:**	4	**RotB:**	4
PubChem ID :	5310979	**CASRN :**	147782-19-2			**AlogP:**	-3.84	**TPSA:**	137.9
Activity:	mGluR2 agonist								

Catalog number : D-803

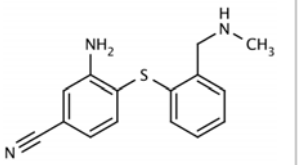
Drug name : DASB hydrochloride



Mol. Formula :	$C_{16}H_{18}ClN_3S$	**FW :**	319.85	**HBA:**	4	**HBD:**	1	**RotB:**	5
PubChem ID :	10446567	**CASRN :**	627490-01-1			**AlogP:**	3.47	**TPSA:**	78.4
Activity:	Serotonin 5-HT transporter ligand								

Catalog number : D-804

Drug name : Desmethyl-DASB



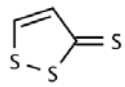
Mol. Formula : $C_{15}H_{15}N_3S$ **FW :** 269.37 **HBA:** 4 **HBD:** 2 **RotB:** 5

PubChem ID : 10612056 **CASRN :** **AlogP:** 3.11 **TPSA:** 87.1

Activity: DASB PET ligand precursor

Catalog number : D-805

Drug name : 1,2-Dithiole-3-thione



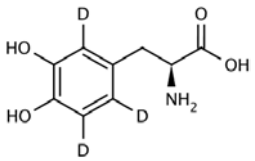
Mol. Formula : $C_3H_2S_3$ **FW :** 134.24 **HBA:** 3 **HBD:** 0 **RotB:** 0

PubChem ID : 68296 **CASRN :** 534-25-8 **AlogP:** 2.22 **TPSA:** 82.7

Activity: Antineoplastic agent

Catalog number : D-901

Drug name : L-DOPA-ring-d_3



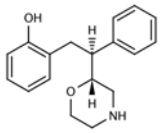
Mol. Formula : $C_9H_8D_3NO_4$ **FW :** 200.21 **HBA:** 5 **HBD:** 4 **RotB:** 3

PubChem ID : 12297005 **CASRN :** 53587-29-4 **AlogP:** -1.71 **TPSA:** 103.8

Activity: Stable isotope labeled L-DOPA

Catalog number : D-902

Drug name : (±)-*O*-Desethylreboxetine



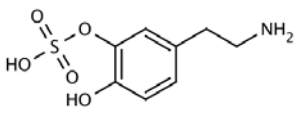
Mol. Formula : $C_{17}H_{19}NO_3$ **FW :** 285.34 **HBA:** 3 **HBD:** 2 **RotB:** 4

PubChem ID : **CASRN :** **AlogP:** 3.17 **TPSA:** 41.5

Activity: Roboxetine PET ligand precusor

Catalog number : D-903

Drug name : Dopamine-3-*O*-sulfate



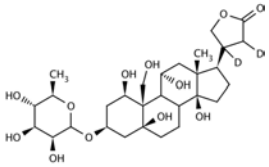
Mol. Formula : $C_8H_{11}NO_5S$ **FW :** 233.24 **HBA:** 5 **HBD:** 3 **RotB:** 4

PubChem ID : 122136 **CASRN :** 51317-41-0 **AlogP:** -1.20 **TPSA:** 118.2

Activity: L-DOPA metabolite

Catalog number : D-904

Drug name : d_2-Dihydroouabain



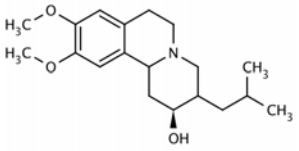
Mol. Formula : $C_{29}H_{44}D_2O_{12}$ **FW :** 588.68 **HBA:** 11 **HBD:** 8 **RotB:** 4

PubChem ID : 14450 **CASRN :** 1183-35-3 **AlogP:** -3.88 **TPSA:** 206.6

Activity: Stable isotope labeled ouabain inotropic action antagonist

Catalog number : D-905

Drug name : (–)-α-Dihydrotetrabenazine



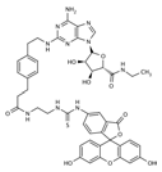
Mol. Formula : $C_{19}H_{29}NO_3$ **FW :** 319.45 **HBA:** 4 **HBD:** 1 **RotB:** 4

PubChem ID : 123836 **CASRN :** 3466-75-9 **AlogP:** 2.36 **TPSA:** 41.9

Activity: Optical isomer of putative tetrabenazine metabolite

Catalog number : D-906

Drug name : FITC-APEC



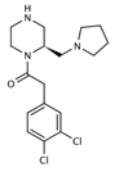
Mol. Formula : $C_{46}H_{46}N_{10}O_{10}S$ **FW :** 930.98 **HBA:** 14 **HBD:** 10 **RotB:** 14

PubChem ID : **CASRN :** **AlogP:** 2.86 **TPSA:** 321.7

Activity: Fluorescent adenosine A_{2a} receptor ligand

Catalog number : D-907

Drug name : Descarboxymethyl GR103545 dihydrochloride



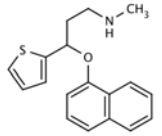
Mol. Formula : $C_{17}H_{23}Cl_2N_3O$ **FW :** 356.29 **HBA:** 5 **HBD:** 1 **RotB:** 4

PubChem ID : 9906680 **CASRN :** **AlogP:** 2.16 **TPSA:** 35.6

Activity: GR103545 PET ligand precursor

Catalog number : D-908

Drug name : Duloxetine hydrochloride



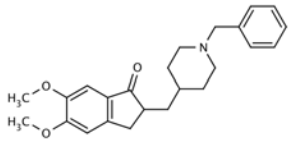
Mol. Formula : $C_{18}H_{19}NOS$ **FW :** 297.42 **HBA:** 3 **HBD:** 1 **RotB:** 6

PubChem ID : 60835 **CASRN :** 116539-59-4 **AlogP:** 4.14 **TPSA:** 49.5

Activity: Serotonin and norepinephrine reuptake inhibitor; antidepressant

Catalog number : D-909

Drug name : Donepezil



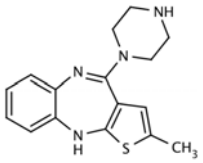
Mol. Formula : $C_{24}H_{29}NO_3$ **FW :** 379.49 **HBA:** 4 **HBD:** 0 **RotB:** 6

PubChem ID : 3152 **CASRN :** 120011-70-3 **AlogP:** 3.69 **TPSA:** 38.8

Activity: Reversible acetylcholinesterase inhibitor; Alzheimer's disease therapeutic

Catalog number : D-910

Drug name : 2-Methyl-4-(1-piperazinyl)-10H-thieno-[2,3-b][1,5]benzodiazepine; N-Desmethylolanzapine



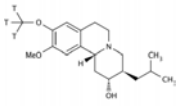
Mol. Formula : $C_{16}H_{18}N_4S$ **FW :** 298.41 **HBA:** 5 **HBD:** 2 **RotB:** 0

PubChem ID : **CASRN :** **AlogP:** 2.72 **TPSA:** 67.9

Activity: Olanzapine metabolite

Catalog number : D-911

Drug name : Tritium-labeled dihydrotetrabenazine



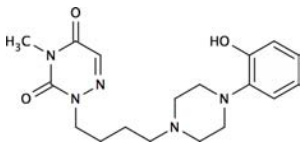
Mol. Formula : $C_{19}H_{29}NO_3$ **FW :** 319.44 **HBA:** 4 **HBD:** 1 **RotB:** 4

PubChem ID : **CASRN :** **AlogP:** 3.10 **TPSA:** 41.9

Activity: Radiolabeled dopamine uptake inhibitor

Catalog number : D-912

Drug name : 2-{4-[4-(2-Hydroxyphenyl)piperazin-1-yl]butyl}-4-methyl-1,2,4-triazine-3,5-(2*H*,4*H*)-dione



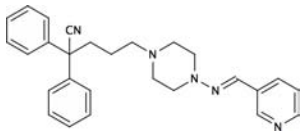
Mol. Formula : $C_{18}H_{25}N_5O_3$ **FW :** 359.42 **HBA:** 6 **HBD:** 1 **RotB:** 6

PubChem ID : **CASRN :** **AlogP:** 1.65 **TPSA:** 79.7

Activity: Serotonin 5-HT_{1A} receptor ligand

Catalog number : D-913

Drug name : SC-26196



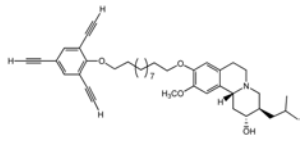
Mol. Formula : $C_{27}H_{29}N_5$ **FW :** 423.55 **HBA:** 5 **HBD:** 0 **RotB:** 8

PubChem ID : 9845201 **CASRN :** **AlogP:** 4.07 **TPSA:** 55.5

Activity: Δ6 Desaturase inhibitor, anti-inflammatory

Catalog number : D-914 new

Drug name : Dihydrotetrabenazine derivative

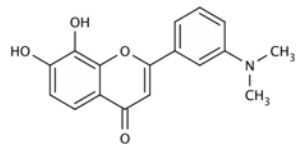


Mol. Formula : $C_{41}H_{53}NO_4$ **FW :** 623.86 **HBA:** **HBD:** **RotB:**

PubChem ID : **CASRN :** **AlogP:** **TPSA:**

Catalog number : D-915 new

Drug name : 2-(3-Dimethylaminophenyl)-7,8-dihydroxy-4H-chromen-4-one

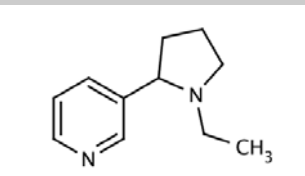


Mol. Formula : $C_{17}H_{15}NO_4$ **FW :** 297.30 **HBA:** **HBD:** **RotB:**

PubChem ID : **CASRN :** **AlogP:** **TPSA:**

Catalog number : E-701A

Drug name : N-Ethylnornicotine tartrate



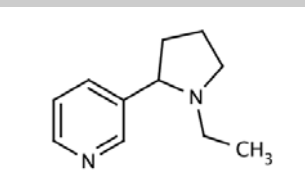
Mol. Formula : $C_{19}H_{28}N_2O_{12}$ **FW :** 476.44 **HBA:** 2 **HBD:** 0 **RotB:** 2

PubChem ID : **CASRN :** **AlogP:** 1.36 **TPSA:** 16.1

Activity: Nicotine analog

Catalog number : E-701B

Drug name : N-Ethylnornicotine



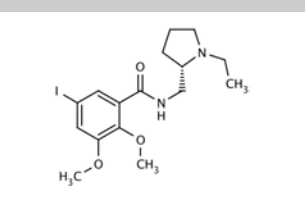
Mol. Formula : $C_{11}H_{16}N_2$ **FW :** 176.26 **HBA:** 2 **HBD:** 0 **RotB:** 2

PubChem ID : 201440 **CASRN :** 5979-92-0 **AlogP:** 1.36 **TPSA:** 16.1

Activity: Nicotine analog

Catalog number : E-703

Drug name : Epidepride



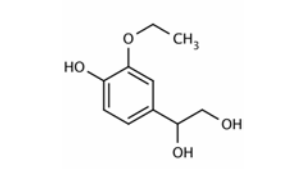
Mol. Formula : $C_{16}H_{23}IN_2O_3$ **FW :** 418.26 **HBA:** 4 **HBD:** 1 **RotB:** 6

PubChem ID : 86101 **CASRN :** 107188-87-4 **AlogP:** 2.15 **TPSA:** 50.8

Activity: Dopamine D_2 receptor antagonist

Catalog number : E-704

Drug name : EHPG piperazine salt



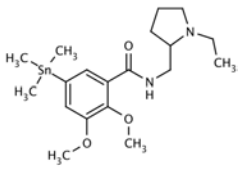
Mol. Formula : $C_{24}H_{38}N_2O_8$ **FW :** 482.57 **HBA:** 4 **HBD:** 3 **RotB:** 4

PubChem ID : 194138 **CASRN :** 62024-68-4 **AlogP:** 0.34 **TPSA:** 69.9

Activity: Catecholamine turnover biomarker

Catalog number : E-705

Drug name : 5-Trimethylstannylepidepride



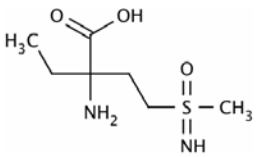
Mol. Formula : $C_{19}H_{32}N_2O_3Sn$ **FW :** 455.18 **HBA:** 4 **HBD:** 1 **RotB:** 7

PubChem ID : **CASRN :** **AlogP:** 0.94 **TPSA:** 50.8

Activity: Radioiodinated epidepride precusor

Catalog number : E-706

Drug name : (±)-α-Ethylmethionine-(*S*,*R*)-sulfoximine



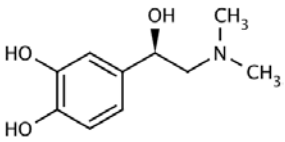
Mol. Formula : $C_7H_{16}N_2O_3S$ **FW :** 208.27 **HBA:** 3 **HBD:** 2 **RotB:** 4

PubChem ID : 128339 **CASRN :** 66735-68-0 **AlogP:** -1.08 **TPSA:** 75.3

Activity: Glutamate synthetase inhibitor

Catalog number : E-707

Drug name : (–)-*N*-Methylepinephrine tartrate

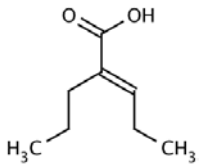


Mol. Formula : $C_{14}H_{21}NO_9$ **FW :** 347.32 **HBA:** 4 **HBD:** 3 **RotB:** 3

PubChem ID : 3054685 **CASRN :** 554-99-4 **AlogP:** 0.36 **TPSA:** 63.9

Catalog number : E-708

Drug name : (*E*)-2-Enevalproic acid



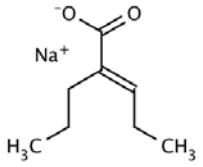
Mol. Formula : $C_8H_{14}O_2$ **FW :** 142.20 **HBA:** 2 **HBD:** 1 **RotB:** 4

PubChem ID : 6437068 **CASRN :** 60218-41-9 **AlogP:** 2.40 **TPSA:** 37.3

Activity: Anticonvulsant; valproic acid metabolite

Catalog number : E-709

Drug name : (*E*)-2-Enevalproate, sodium salt



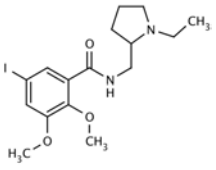
Mol. Formula : $C_8H_{13}O_2Na$ **FW :** 164.18 **HBA:** 2 **HBD:** 0 **RotB:** 4

PubChem ID : 23675457 **CASRN :** 69827-64-1 **AlogP:** 2.40 **TPSA:** 40.1

Activity: Valproic acid metabolite

Catalog number : E-901

Drug name : [^{125}I]Epidepride



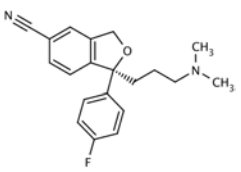
Mol. Formula : $C_{16}H_{23}IN_2O_3$ **FW :** 418.26 **HBA:** 4 **HBD:** 1 **RotB:** 6

PubChem ID : 449726 **CASRN :** 107188-87-4 **AlogP:** 2.15 **TPSA:** 50.8

Activity: Radioiodinated dopamine D_2 receptor antagonist

Catalog number : E-902

Drug name : Escitalopram oxalate



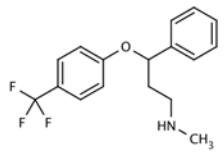
Mol. Formula : $C_{20}H_{21}FN_2O$ **FW :** 324.39 **HBA:** 4 **HBD:** 0 **RotB:** 6

PubChem ID : 146570 **CASRN :** 128196-01-0 **AlogP:** 3.56 **TPSA:** 36.3

Activity: Serotonin 5-HT reuptake inhibitor; antidepressant; anxiolytic

Catalog number : F-132

Drug name : (±)-Fluoxetine hydrochloride



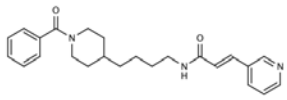
Mol. Formula : $C_{17}H_{19}ClF_3NO$ **FW :** 345.79 **HBA:** 5 **HBD:** 1 **RotB:** 7

PubChem ID : 3386 **CASRN :** 54910-89-3 **AlogP:** 4.19 **TPSA:** 21.3

Activity: Serotonin uptake inhibitor; antidepressant

Catalog number : F-901

Drug name : FK866



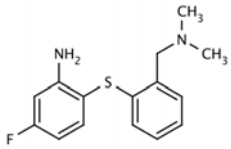
Mol. Formula : $C_{24}H_{29}N_3O_2$ **FW :** 391.51 **HBA:** 3 **HBD:** 1 **RotB:** 8

PubChem ID : 6914657 **CASRN :** 201034-75-5 **AlogP:** 3.02 **TPSA:** 62.3

Activity: Nicotinamide phosphoribosyltransferase inhibitor

Catalog number : F-902

Drug name : 4-Fluoro-ADAM



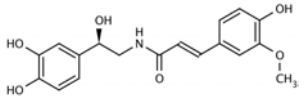
Mol. Formula : $C_{15}H_{17}FN_2S$ **FW :** 276.38 **HBA:** 4 **HBD:** 1 **RotB:** 4

PubChem ID : 10265481 **CASRN :** **AlogP:** 3.80 **TPSA:** 54.6

Activity: Serotonin 5-HT-selective PET imaging ligand reference standard

Catalog number : F-903

Drug name : *N*-Feruloylnorepinephrine

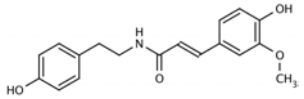


Mol. Formula : $C_{18}H_{19}NO_6$ **FW :** 345.35 **HBA:** 6 **HBD:** 5 **RotB:** 6

PubChem ID : **CASRN :** **AlogP:** 1.78 **TPSA:** 119.3

Catalog number : F-904

Drug name : Feruloyltyramine



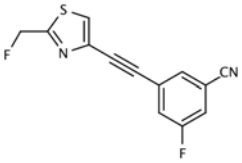
Mol. Formula : $C_{18}H_{19}NO_4$ **FW :** 313.35 **HBA:** 4 **HBD:** 3 **RotB:** 6

PubChem ID : 5280537 **CASRN :** 65646-26-6 **AlogP:** 2.99 **TPSA:** 78.8

Activity: Cannabis natural product; Induces hypothermia and motor incoordination.

Catalog number : F-905

Drug name : 3-Fluoro-5-{2-[2-(fluoromethyl)thiazol-4-yl]ethynyl}benzonitrile



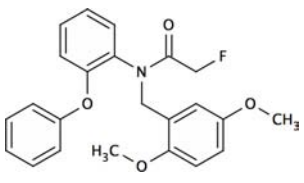
Mol. Formula : $C_{13}H_6F_2N_2S$ **FW :** 260.26 **HBA:** 5 **HBD:** 0 **RotB:** 4

PubChem ID : **CASRN :** **AlogP:** 3.07 **TPSA:** 64.9

Activity: mGluR5 PET imaging ligand

Catalog number : F-906

Drug name : *N*-[(2,5-Dimethoxyphenyl)methyl]-2-fluoro-*N*-(2-phenoxyphenyl)acetamide



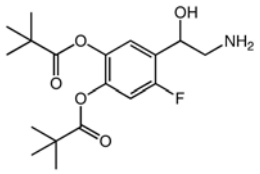
Mol. Formula : $C_{23}H_{22}FNO_4$ **FW :** 395.43 **HBA:** 5 **HBD:** 0 **RotB:** 8

PubChem ID : **CASRN :** **AlogP:** 2.84 **TPSA:** 60.9

Activity: Brain peripheral benzodiazepine receptor (TSPO) ligand

Catalog number : F-907 new

Drug name : 6-Fluoronorepinephrine dipivalate hydrochloride

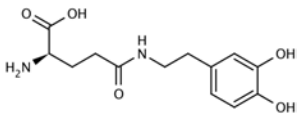


Mol. Formula : $C_{18}H_{27}ClFNO_5$ **FW :** 391.86 **HBA:** **HBD:** **RotB:**

PubChem ID : **CASRN :** **AlogP:** **TPSA:**

Catalog number : G-501

Drug name : γ-Glutamyldopamine

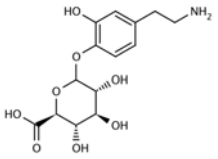


Mol. Formula : $C_{13}H_{18}N_2O_5$ **FW :** 282.30 **HBA:** 6 **HBD:** 5 **RotB:** 7

PubChem ID : 22806192 **CASRN :** **AlogP:** -2.36 **TPSA:** 132.9

Catalog number : G-502

Drug name : Dopamine-4-*O*-β-D-glucuronide



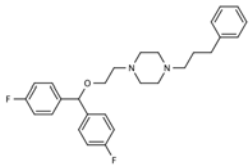
Mol. Formula : $C_{14}H_{19}NO_8$ **FW :** 329.31 **HBA:** 9 **HBD:** 6 **RotB:** 5

PubChem ID : 3082490 **CASRN :** 38632-24-5 **AlogP:** -7.40 **TPSA:** 162.7

Activity: Dopamine metabolite

Catalog number : G-801

Drug name : GBR-12909 dihydrochloride; Vanoxerine



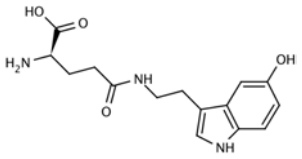
Mol. Formula : $C_{28}H_{34}Cl_2F_2N_2O$ **FW :** 523.50 **HBA:** 5 **HBD:** 0 **RotB:** 10

PubChem ID : 10238982 **CASRN :** 67469-78-7 **AlogP:** 6.12 **TPSA:** 15.7

Activity: Dopamine reuptake inhibitor; behavioral effects similar to cocaine

Catalog number : G-802

Drug name : γ-Glutamylserotonin

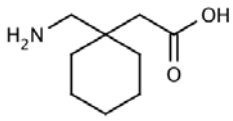


Mol. Formula : $C_{15}H_{19}N_3O_4$ **FW :** 305.35 **HBA:** 5 **HBD:** 5 **RotB:** 7

PubChem ID : 15234235 **CASRN :** **AlogP:** -1.97 **TPSA:** 128.4

Catalog number : G-901

Drug name : Gabapentin



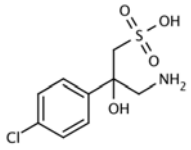
Mol. Formula : $C_9H_{17}NO_2$ **FW :** 171.24 **HBA:** 3 **HBD:** 2 **RotB:** 3

PubChem ID : 3446 **CASRN :** 60142-96-3 **AlogP:** -1.44 **TPSA:** 63.3

Activity: Anticonvulsant used to treat epilepsy and neuropathic pain.

Catalog number : H-113

Drug name : 2-Hydroxysaclofen



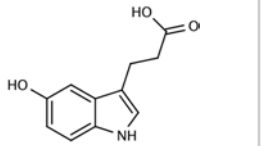
Mol. Formula : $C_9H_{12}ClNO_4S$ **FW :** 265.71 **HBA:** 6 **HBD:** 3 **RotB:** 4

PubChem ID : 1564 **CASRN :** 117354-64-0 **AlogP:** -1.49 **TPSA:** 109.0

Activity: $GABA_B$ receptor antagonist

Catalog number : H-501

Drug name : 5-Hydroxyindole-3-β-propionic acid



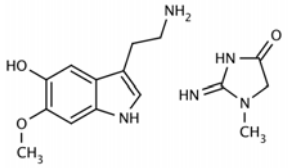
Mol. Formula : $C_{11}H_{11}NO_3$ **FW :** 205.21 **HBA:** 3 **HBD:** 3 **RotB:** 3

PubChem ID : **CASRN :** **AlogP:** 1.89 **TPSA:** 73.3

Activity: GC/MS internal standard for catecholamine assay

Catalog number : H-502

Drug name : 5-Hydroxy-6-methoxytryptamine creatinine sulfate

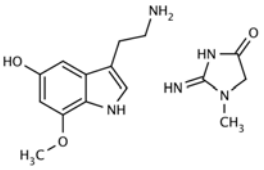


Mol. Formula : $C_{15}H_{23}N_5O_7S$ **FW :** 417.44 **HBA:** 3 **HBD:** 3 **RotB:** 3

PubChem ID : **CASRN :** **AlogP:** 0.09 **TPSA:** 71.3

Catalog number : H-503

Drug name : 5-Hydroxy-7-methoxytryptamine creatinine sulfate

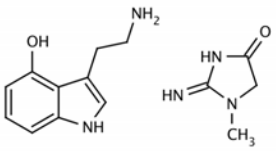


Mol. Formula : $C_{15}H_{23}N_5O_7S$ **FW :** 417.44 **HBA:** 3 **HBD:** 3 **RotB:** 3

PubChem ID : **CASRN :** **AlogP:** -0.40 **TPSA:** 71.3

Catalog number : H-504

Drug name : 4-Hydroxytryptamine creatinine sulfate

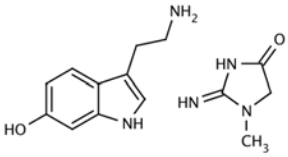


Mol. Formula : $C_{14}H_{21}N_5O_6S$ **FW :** 387.42 **HBA:** 2 **HBD:** 3 **RotB:** 2

PubChem ID : **CASRN :** **AlogP:** 0.24 **TPSA:** 62.0

Catalog number : H-505

Drug name : 6-Hydroxytryptamine creatinine sulfate

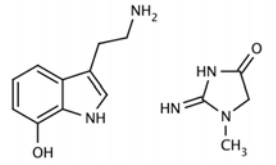


Mol. Formula : $C_{14}H_{21}N_5O_6S$ **FW :** 387.42 **HBA:** 2 **HBD:** 3 **RotB:** 2

PubChem ID : **CASRN :** **AlogP:** 0.44 **TPSA:** 62.0

Catalog number : H-506

Drug name : 7-Hydroxytryptamine creatinine sulfate

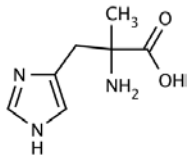


Mol. Formula : $C_{14}H_{21}N_5O_6S$ **FW :** 387.42 **HBA:** 2 **HBD:** 3 **RotB:** 2

PubChem ID : **CASRN :** **AlogP:** 0.48 **TPSA:** 62.0

Catalog number : H-507

Drug name : α-Methylhistidine hydrochloride

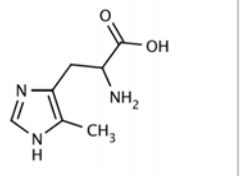


Mol. Formula : $C_7H_{12}ClN_3O_2$ **FW :** 205.63 **HBA:** 4 **HBD:** 3 **RotB:** 3

PubChem ID : 16219696 **CASRN :** 32381-18-3 **AlogP:** -3.17 **TPSA:** 92.0

Catalog number : H-509

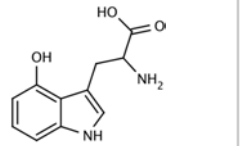
Drug name : 4-Methylhistidine hydrochloride



Mol. Formula :	$C_7H_{12}ClN_3O_2$	**FW :**	205.63	**HBA:**	4	**HBD:**	3	**RotB:**	3
PubChem ID :	10773449	**CASRN :**				**AlogP:**	-3.38	**TPSA:**	92.0

Catalog number : H-510

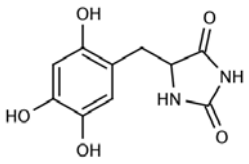
Drug name : 4-Hydroxytryptophan acetate



Mol. Formula :	$C_{13}H_{16}N_2O_5$	**FW :**	280.28	**HBA:**	4	**HBD:**	4	**RotB:**	3
PubChem ID :	589768	**CASRN :**				**AlogP:**	-1.33	**TPSA:**	99.3

Catalog number : H-511

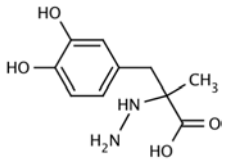
Drug name : 5-(2,4,5-Trihydroxybenzyl)hydantoin



Mol. Formula :	$C_{10}H_{10}N_2O_5$	**FW :**	238.20	**HBA:**	5	**HBD:**	5	**RotB:**	2
PubChem ID :		**CASRN :**				**AlogP:**	0.02	**TPSA:**	118.9

Catalog number : H-512

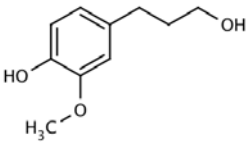
Drug name : (±)-2-(3,4-Dihydroxybenzyl)-2-hydrazinopropionic acid; Carbidopa



Mol. Formula :	$C_{10}H_{14}N_2O_4$	**FW :**	226.23	**HBA:**	6	**HBD:**	5	**RotB:**	4
PubChem ID :	2563	**CASRN :**	38821-49-7			**AlogP:**	-0.97	**TPSA:**	115.8
Activity:	Antiparkinson agent; dopaminergic agent								

Catalog number : H-513

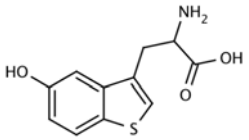
Drug name : 3-(4-Hydroxy-3-methoxyphenyl)-1-propanol; Dihydroconiferyl alcohol



Mol. Formula :	$C_{10}H_{14}O_3$	**FW :**	182.22	**HBA:**	3	**HBD:**	2	**RotB:**	4
PubChem ID :	16822	**CASRN :**	2305-13-7			**AlogP:**	1.32	**TPSA:**	49.7

Catalog number : H-515

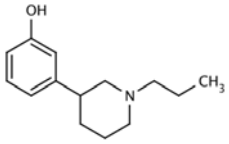
Drug name : β-(5-Hydroxy-3-benzo[b]thienyl)-α-aminopropionic acid



Mol. Formula :	$C_{11}H_{11}NO_3S$	**FW :**	237.28	**HBA:**	5	**HBD:**	3	**RotB:**	3
PubChem ID :	32334	**CASRN :**	24358-04-1			**AlogP:**	-0.68	**TPSA:**	111.8

Catalog number : H-516

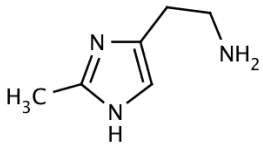
Drug name : 3-(3-Hydroxyphenyl)-*N*-(n-propyl)piperidine hydrobromide; Preclamol



Mol. Formula :	$C_{14}H_{22}BrNO$	**FW :**	300.24	**HBA:**	2	**HBD:**	1	**RotB:**	3
PubChem ID :	23045647	**CASRN :**	75240-91-4			**AlogP:**	2.57	**TPSA:**	23.5
Activity:	Antiparkinson agent; dopaminergic agent								

Catalog number : H-517

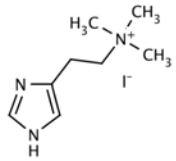
Drug name : 2-Methylhistamine dipicrate



Mol. Formula :	$C_{18}H_{17}N_9O_{14}$	**FW :**	583.38	**HBA:**	2	**HBD:**	2	**RotB:**	2
PubChem ID :	91613	**CASRN :**	34392-54-6			**AlogP:**	-0.52	**TPSA:**	54.7

Catalog number : H-518

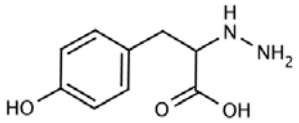
Drug name : N,N-Dimethylhistamine methiodide



Mol. Formula :	$C_8H_{16}N_3I$	**FW :**	281.14	**HBA:**	1	**HBD:**	1	**RotB:**	3
PubChem ID :		**CASRN :**				**AlogP:**	-4.60	**TPSA:**	28.7

Catalog number : H-520

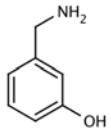
Drug name : (±)-2-Hydrazino-3-(4-hydroxyphenyl)propionic acid



Mol. Formula :	$C_9H_{12}N_2O_3$	**FW :**	196.21	**HBA:**	5	**HBD:**	4	**RotB:**	4
PubChem ID :	151250	**CASRN :**	5060-36-6			**AlogP:**	-0.61	**TPSA:**	95.6
Activity:	Fungal tyrosinase inhibitor								

Catalog number : H-521

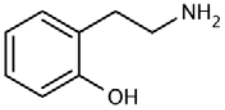
Drug name : 3-Hydroxybenzylamine



Mol. Formula :	C_7H_9NO	**FW :**	123.16	**HBA:**	2	**HBD:**	2	**RotB:**	1
PubChem ID :	735894	**CASRN :**				**AlogP:**	0.32	**TPSA:**	46.3

Catalog number : H-522

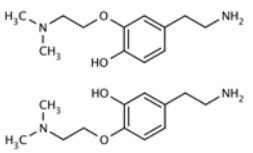
Drug name : 2-Hydroxy-β-phenethylamine hydrochloride



Mol. Formula :	$C_8H_{12}ClNO$	**FW :**	173.64	**HBA:**	2	**HBD:**	2	**RotB:**	2
PubChem ID :	199864	**CASRN :**	5136-97-0			**AlogP:**	0.82	**TPSA:**	46.3

Catalog number : H-523

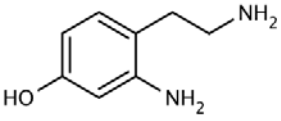
Drug name : 4(3)-Hydroxy-3(4)-(β-dimethylaminoethoxy)-β-phenethylamine dihydrochloride



Mol. Formula :	$C_{12}H_{22}Cl_2N_2O_2$	**FW :**	297.23	**HBA:**	4	**HBD:**	2	**RotB:**	6
PubChem ID :		**CASRN :**				**AlogP:**	0.32	**TPSA:**	58.7

Catalog number : H-525

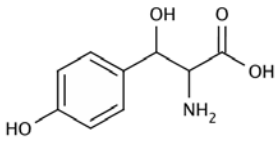
Drug name : 2-Amino-4-hydroxy-β-phenethylamine dihydrobromide



Mol. Formula :	$C_8H_{14}Br_2N_2O$	**FW :**	314.02	**HBA:**	3	**HBD:**	3	**RotB:**	2
PubChem ID :	9877425	**CASRN :**				**AlogP:**	-0.18	**TPSA:**	72.3

Catalog number : H-526

Drug name : *threo*-β-(4-Hydroxyphenyl)serine

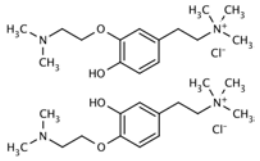


Mol. Formula : $C_9H_{11}NO_4$ **FW :** 197.19 **HBA:** 4 **HBD:** 3 **RotB:** 3

PubChem ID : 94134 **CASRN :** 1078-17-7 **AlogP:** -2.07 **TPSA:** 83.6

Catalog number : H-527

Drug name : 4(3)-Hydroxy-3(4)-(β-trimethylammoniumethoxy)-β-phenethylamine hydrochloride chloride

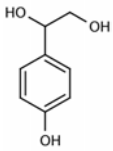


Mol. Formula : $C_{13}H_{24}Cl_2N_2O_2$ **FW :** 311.25 **HBA:** 3 **HBD:** 2 **RotB:** 6

PubChem ID : **CASRN :** **AlogP:** -2.73 **TPSA:** 55.5

Catalog number : H-528

Drug name : 4-Hydroxyphenylglycol



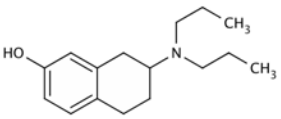
Mol. Formula : $C_8H_{10}O_3$ **FW :** 154.17 **HBA:** 3 **HBD:** 3 **RotB:** 2

PubChem ID : 3081980 **CASRN :** 2380-75-8 **AlogP:** 0.25 **TPSA:** 60.7

Activity: Octopamine metabolite

Catalog number : H-701

Drug name : (±)-7-Hydroxy-2-(*di-n*-propylamino)tetralin hydrobromide



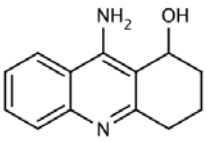
Mol. Formula : $C_{16}H_{26}BrNO$ **FW :** 328.29 **HBA:** 2 **HBD:** 1 **RotB:** 5

PubChem ID : 11957566 **CASRN :** 159795-63-8 **AlogP:** 3.00 **TPSA:** 23.5

Activity: Dopamine D_3 agonist

Catalog number : H-703

Drug name : Velnacrine maleate



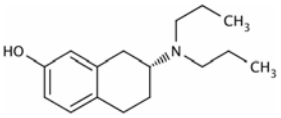
Mol. Formula : $C_{17}H_{18}N_2O_5$ **FW :** 330.34 **HBA:** 3 **HBD:** 2 **RotB:** 0

PubChem ID : 6364836 **CASRN :** 104675-29-8 **AlogP:** 1.30 **TPSA:** 59.1

Activity: Cholinesterase Inhibitor

Catalog number : H-704

Drug name : (*R*)-(+)-7-Hydroxy-2-(*di-n*-propylamino)tetralin hydrobromide



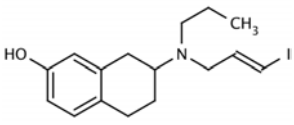
Mol. Formula : $C_{16}H_{26}BrNO$ **FW :** 328.29 **HBA:** 2 **HBD:** 1 **RotB:** 5

PubChem ID : 11957554 **CASRN :** 82730-72-1 **AlogP:** 3.00 **TPSA:** 23.5

Activity: Dopamine D3 receptor agonist

Catalog number : H-705

Drug name : (±)-*trans*-7-Hydroxy-2-[*N*-(*n*-propyl)-N-(3'-iodo-2'-propenyl)amino]tetralin hydrochloride



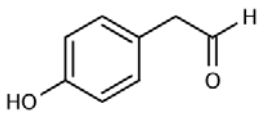
Mol. Formula : $C_{16}H_{23}ClINO$ **FW :** 407.72 **HBA:** 2 **HBD:** 1 **RotB:** 5

PubChem ID : 6305587 **CASRN :** 148258-46-2 **AlogP:** 4.74 **TPSA:** 23.5

Activity: Dopamine D_3 receptor agonist

Catalog number : H-901

Drug name : 4-Hydroxyphenylacetaldehyde



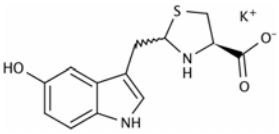
Mol. Formula : $C_8H_8O_2$ **FW :** 136.15 **HBA:** 2 **HBD:** 1 **RotB:** 2

PubChem ID : 440113 **CASRN :** 7339-87-9 **AlogP:** 0.98 **TPSA:** 37.3

Activity: Tyrosine metabolite

Catalog number : H-902

Drug name : 2-(5-Hydroxy-1H-indol-3-ylmethyl)thiazolidine-4-carboxylic acid potassium salt

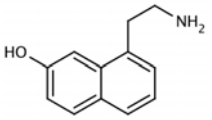


Mol. Formula : $C_{13}H_{13}KN_2O_3S$ **FW :** 316.42 **HBA:** 5 **HBD:** 3 **RotB:** 3

PubChem ID : **CASRN :** **AlogP:** -0.75 **TPSA:** 113.5

Catalog number : H-903

Drug name : N-[2-(7-hydroxy-1-naphthyl)ethyl]amine hydrochloride



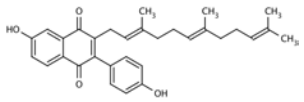
Mol. Formula : $C_{12}H_{14}ClNO$ **FW :** 223.70 **HBA:** 2 **HBD:** 2 **RotB:** 2

PubChem ID : 10058277 **CASRN :** **AlogP:** 1.51 **TPSA:** 46.3

Activity: Serotonin N-acetyltransferase inhibitor

Catalog number : H-904

Drug name : 6-Hydroxy-2-(4-hydroxyphenyl)-3-[(2E, 6E)-3,7,11-trimethyl-dodeca-2,6,10-trienyl]-[1,4]-naphthoquinone

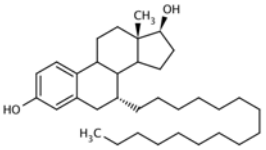


Mol. Formula : $C_{31}H_{34}O_4$ **FW :** 470.60 **HBA:** 4 **HBD:** 2 **RotB:** 9

PubChem ID : **CASRN :** **AlogP:** 6.70 **TPSA:** 74.6

Catalog number : H-905

Drug name : 7α-Hexadecylestra-1,3,5-trien-3,17β-diol

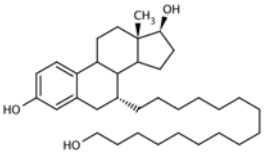


Mol. Formula : $C_{34}H_{56}O_2$ **FW :** 496.81 **HBA:** 2 **HBD:** 2 **RotB:** 15

PubChem ID : **CASRN :** **AlogP:** 9.98 **TPSA:** 40.5

Catalog number : H-906

Drug name : 7α-(16-Hydroxyhexadecyl)estra-1,3,5-trien-3,17β-diol

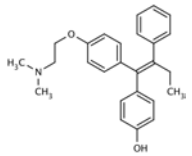


Mol. Formula : $C_{34}H_{56}O_3$ **FW :** 512.81 **HBA:** 3 **HBD:** 3 **RotB:** 16

PubChem ID : **CASRN :** **AlogP:** 8.54 **TPSA:** 60.7

Catalog number : H-907

Drug name : (*Z*)-4-Hydroxytamoxifen; Afimoxifene



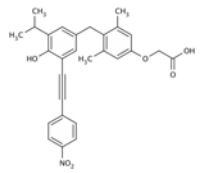
Mol. Formula : $C_{26}H_{29}NO_2$ **FW :** 387.51 **HBA:** 3 **HBD:** 1 **RotB:** 8

PubChem ID : 449459 **CASRN :** 68392-35-8 **AlogP:** 6.10 **TPSA:** 32.7

Activity: Estrogen receptor modulator

Catalog number : H-908

Drug name : NH-3; Thyromimetic 5b



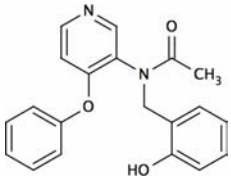
Mol. Formula : $C_{28}H_{27}NO_6$ **FW :** 473.52 **HBA:** 6 **HBD:** 2 **RotB:** 9

PubChem ID : 10027822 **CASRN :** **AlogP:** 7.20 **TPSA:** 112.6

Activity: β-Subtype thyroid hormone receptor antagonist

Catalog number : H-909

Drug name : *N*-(2-Hydroxybenzyl)-*N*-(4-phenoxypyridin-3-yl)acetamide



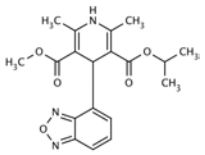
Mol. Formula : $C_{20}H_{18}N_2O_3$ **FW :** 334.38 **HBA:** 3 **HBD:** 1 **RotB:** 5

PubChem ID : 24754521 **CASRN :** **AlogP:** 2.78 **TPSA:** 62.7

Activity: Brain peripheral benzodiazepine receptor (TSPO) ligand

Catalog number : I-124

Drug name : Isradipine



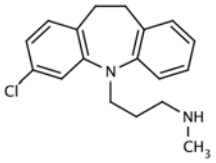
Mol. Formula : $C_{19}H_{21}N_3O_5$ **FW :** 371.39 **HBA:** 5 **HBD:** 1 **RotB:** 6

PubChem ID : 3784 **CASRN :** 75695-93-1 **AlogP:** 2.07 **TPSA:** 103.6

Activity: Antihypertensive Agent; calcium channel blocker; vasodilator

Catalog number : I-501

Drug name : 3-Chloro-*N*-desmethylimipramine hydrochloride

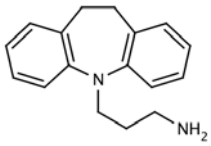


Mol. Formula : $C_{18}H_{22}Cl_2N_2$ **FW :** 337.29 **HBA:** 3 **HBD:** 1 **RotB:** 4

PubChem ID : 16219718 **CASRN :** 303-48-0 **AlogP:** 4.16 **TPSA:** 15.3

Catalog number : I-502

Drug name : N,N-Didesmethylimipramine hydrochloride



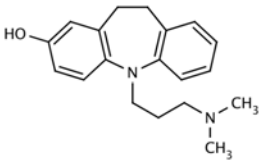
Mol. Formula : $C_{17}H_{21}ClN_2$ **FW :** 288.82 **HBA:** 2 **HBD:** 1 **RotB:** 3

PubChem ID : 13358128 **CASRN :** 2095-95-6 **AlogP:** 3.24 **TPSA:** 29.3

Activity: Imipramine metabolite

Catalog number : I-503

Drug name : 2-Hydroxyimipramine



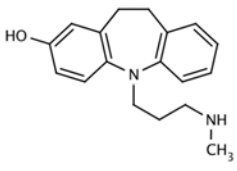
Mol. Formula : $C_{19}H_{24}N_2O$ **FW :** 296.31 **HBA:** 3 **HBD:** 1 **RotB:** 4

PubChem ID : 108051 **CASRN :** 303-70-8 **AlogP:** 3.54 **TPSA:** 26.7

Activity: Imipramine metabolite

Catalog number : I-504

Drug name : 2-Hydroxy-*N*-desmethylimipramine



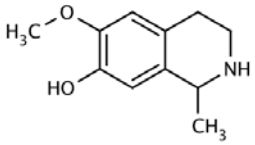
Mol. Formula : $C_{18}H_{22}N_2O$ **FW :** 282.38 **HBA:** 3 **HBD:** 2 **RotB:** 4

PubChem ID : 121249 **CASRN :** 1977-15-7 **AlogP:** 2.93 **TPSA:** 35.5

Activity: Tricyclic antidepressive agent; Imipramine metabolite

Catalog number : I-505

Drug name : (±)-Isosalsoline hydrochloride

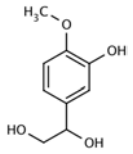


Mol. Formula : $C_{11}H_{16}ClNO_2$ **FW :** 229.71 **HBA:** 3 **HBD:** 2 **RotB:** 1

PubChem ID : 46697 **CASRN :** 4593-97-9 **AlogP:** 1.14 **TPSA:** 41.5

Catalog number : I-701

Drug name : (±)-4-Methoxy-3-hydroxyphenylethyleneglycol

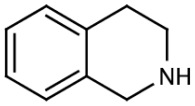


Mol. Formula : $C_9H_{12}O_4$ **FW :** 184.19 **HBA:** 4 **HBD:** 3 **RotB:** 3

PubChem ID : 170451 **CASRN :** 40979-91-7 **AlogP:** 0.00 **TPSA:** 69.9

Catalog number : I-702

Drug name : 1,2,3,4-Tetrahydroisoquinoline hydrochloride



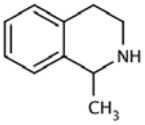
Mol. Formula : $C_9H_{12}ClN$ **FW :** 169.66 **HBA:** 1 **HBD:** 1 **RotB:** 0

PubChem ID : 7046 **CASRN :** 91-21-4 **AlogP:** 1.55 **TPSA:** 12.0

Activity: Potential dopaminergic neurotoxin

Catalog number : I-703

Drug name : (±)-1-Methyl-1,2,3,4-tetrahydroisoquinoline hydrochloride



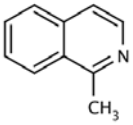
Mol. Formula : $C_{10}H_{14}ClN$ **FW :** 183.68 **HBA:** 1 **HBD:** 1 **RotB:** 0

PubChem ID : 9812950 **CASRN :** 4965-09-7 **AlogP:** 1.97 **TPSA:** 12.0

Activity: Potential dopaminergic neurotoxin

Catalog number : I-704

Drug name : 1-Methylisoquinoline hydrochloride



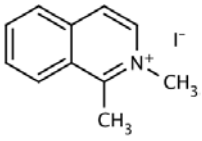
Mol. Formula : $C_{10}H_{10}ClN$ **FW :** 179.65 **HBA:** 1 **HBD:** 0 **RotB:** 0

PubChem ID : 12236795 **CASRN :** 1721-93-3 **AlogP:** 1.91 **TPSA:** 12.9

Activity: Potential dopaminergic neurotoxin

Catalog number : I-705

Drug name : 1,2-Dimethylisoquinolinium iodide

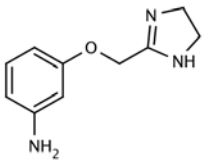


Mol. Formula : $C_{11}H_{12}IN$ **FW :** 285.13 **HBA:** 0 **HBD:** 0 **RotB:** 0

PubChem ID : 12236796 **CASRN :** 51843-14-2 **AlogP:** -2.34 **TPSA:** 3.9

Catalog number : I-706

Drug name : 2-(3-Aminophenoxy)methylimidazoline dihydrochloride



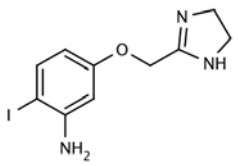
Mol. Formula : $C_{10}H_{15}Cl_2N_3O$ **FW :** 264.16 **HBA:** 4 **HBD:** 2 **RotB:** 3

PubChem ID : 10352540 **CASRN :** **AlogP:** 0.51 **TPSA:** 59.6

Activity: Imidazoline-guaninidine binding site (IGRS) ligand

Catalog number : I-707

Drug name : 2-(3-Amino-4-iodophenoxy)methylimidazoline dihydrochloride



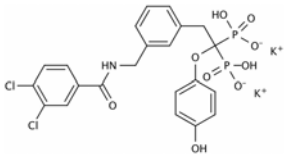
Mol. Formula : $C_{10}H_{14}Cl_2IN_3O$ **FW :** 390.05 **HBA:** 4 **HBD:** 2 **RotB:** 3

PubChem ID : **CASRN :** **AlogP:** 1.50 **TPSA:** 59.6

Activity: Imidazoline-guaninidine binding site (IGRS) ligand

Catalog number : I-709

Drug name : [2-[3-[[(3,4-Dichlorobenzoyl)amino]methyl]phenyl]-1-(4-hydroxyphenoxy) ethylidene]bisphosphonic acid, dipotassium salt



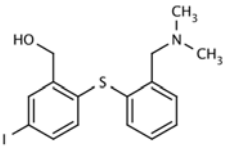
Mol. Formula : $C_{22}H_{19}Cl_2K_2NP_2O_9$ **FW :** 652.45 **HBA:** 11 **HBD:** 4 **RotB:** 9

PubChem ID : 21736614 **CASRN :** 142523-37-3 **AlogP:** 2.75 **TPSA:** 198.9

Activity: Non-hydrolysable inhibitor of myo-inositol monophosphatase

Catalog number : I-801

Drug name : IDAM hydrochloride



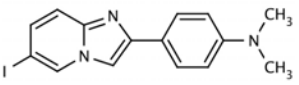
Mol. Formula : $C_{16}H_{19}ClINOS$ **FW :** 435.76 **HBA:** 3 **HBD:** 1 **RotB:** 5

PubChem ID : 9865652 **CASRN :** **AlogP:** 4.60 **TPSA:** 48.8

Activity: Serotonin transporter SPECT imaging agent; reference standard

Catalog number : I-901

Drug name : 2-(4'-N,N-Dimethylaminophenyl)-6-iodoimidazo[1,2-a]pyridine



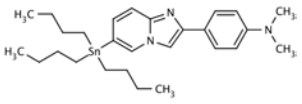
Mol. Formula : $C_{15}H_{14}IN_3$ **FW :** 363.20 **HBA:** 3 **HBD:** 0 **RotB:** 2

PubChem ID : 10133297 **CASRN :** **AlogP:** 4.38 **TPSA:** 20.5

Activity: Beta-amyloid aggregate-specific ligand

Catalog number : I-902

Drug name : 2-(4'-N,N-Dimethylaminophenyl)-6-(tributylstannyl)imidazo[1,2-a]pyridine



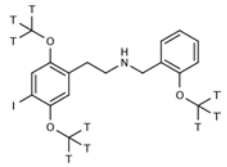
Mol. Formula : $C_{27}H_{41}N_3Sn$ **FW :** 526.34 **HBA:** 3 **HBD:** 0 **RotB:** 12

PubChem ID : 10994990 **CASRN :** **AlogP:** 6.47 **TPSA:** 20.5

Activity: Radio-iodinated IMPY precursor

Catalog number : I-903

Drug name : [^{3}H]I-NBMeO



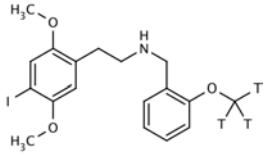
Mol. Formula : $C_{18}H_{22}INO_3$ **FW :** 427.28 **HBA:** 4 **HBD:** 1 **RotB:** 8

PubChem ID : 10251906 **CASRN :** **AlogP:** 3.83 **TPSA:** 39.7

Activity: Radiolabeled serotonin 5-HT_{2A} agonist

Catalog number : I-904

Drug name : 2-[C^3H_3]I-NBMeO N-[2-C^3H_3O]benzyl-2',5'-dimethoxy-4'-iodophenethylamine



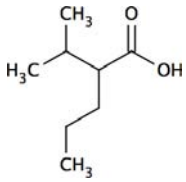
Mol. Formula : $C_{18}H_{22}INO_3$ **FW :** 427.28 **HBA:** 4 **HBD:** 1 **RotB:** 8

PubChem ID : 10251906 **CASRN :** **AlogP:** 3.83 **TPSA:** 39.7

Activity: Radiolabeled serotonin 5$HT_{2A/2C}$ agonist

Catalog number : I-905

Drug name : 2-Isopropylpentanoic acid; PIA



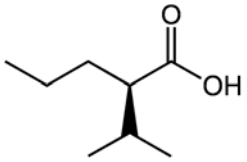
Mol. Formula : $C_8H_{16}O_2$ **FW :** 144.21 **HBA:** 2 **HBD:** 1 **RotB:** 4

PubChem ID : 147513 **CASRN :** 62391-99-5 **AlogP:** 2.64 **TPSA:** 37.3

Activity: Anticonvulsant

Catalog number : I-906 new

Drug name : (*R*)-2-Isopropylpentanoic acid



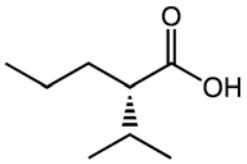
Mol. Formula : $C_8H_{16}O_2$ **FW :** 144.20 **HBA:** 2 **HBD:** 1 **RotB:** 4

PubChem ID : 10197756 **CASRN :** **AlogP:** 2.42 **TPSA:** 37.3

Activity: Anticonvulsant.

Catalog number : I-907 new

Drug name : (*S*)-2-Isopropylpentanoic acid



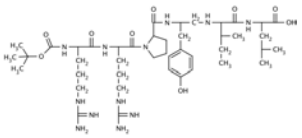
Mol. Formula : $C_8H_{16}O_2$ **FW :** 144.20 **HBA:** 2 **HBD:** 1 **RotB:** 4

PubChem ID : 10176197 **CASRN :** **AlogP:** 2.42 **TPSA:** 37.3

Activity: Anticonvulsant.

Catalog number : J-901

Drug name : JMV-431



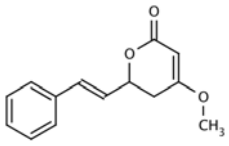
Mol. Formula : $C_{47}H_{82}N_{12}O_{13}$ **FW :** 1023.23 **HBA:** 16 **HBD:** 13 **RotB:** 28

PubChem ID : **CASRN :** **AlogP:** -5.09 **TPSA:** 339.3

Activity: Neurotensin receptor subtype 2 agonist

Catalog number : K-501

Drug name : Kawain



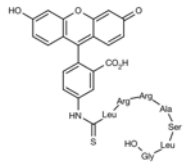
Mol. Formula : $C_{14}H_{14}O_3$ **FW :** 230.27 **HBA:** 2 **HBD:** 0 **RotB:** 3

PubChem ID : 5369129 **CASRN :** 1635-33-2 **AlogP:** 2.52 **TPSA:** 35.5

Activity: Anticonvulsant; axiolytic

Catalog number : K-701

Drug name : Kemptide fluorescein



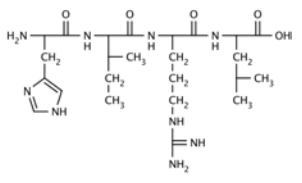
Mol. Formula : $C_{53}H_{72}N_{14}O_{14}S$ **FW :** 1161.29 **HBA:** 22 **HBD:** 18 **RotB:** 30

PubChem ID : **CASRN :** **AlogP:** -8.20 **TPSA:** 495.9

Activity: Fluorescently-labeled marker for protein kinase A (PKA)

Catalog number : L-901

Drug name : β-Lactotensin



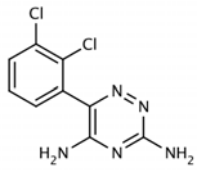
Mol. Formula : $C_{30}H_{46}F_9N_9O_{11}$ **FW :** 879.73 **HBA:** 10 **HBD:** 9 **RotB:** 17

PubChem ID : **CASRN :** **AlogP:** -5.03 **TPSA:** 241.2

Activity: Neurotensin receptor subtype 2 agonist

Catalog number : L-902

Drug name : Lamotrigine

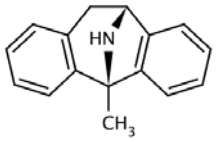


Mol. Formula :	$C_9H_7Cl_2N_5$	**FW :** 256.09	**HBA:** 2	**HBD:** 7	**RotB:** 1
PubChem ID :	3878	**CASRN :** 84057-84-1		**AlogP:** 1.51	**TPSA:** 90.7

Activity: Anticonvulsant; bipolar disorder therapeutic

Catalog number : M-107

Drug name : (+)-MK-801

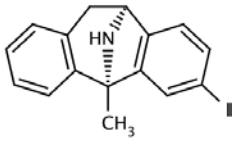


Mol. Formula :	$C_{20}H_{19}NO_4$	**FW :** 337.37	**HBA:** 1	**HBD:** 1	**RotB:** 0
PubChem ID :	180081	**CASRN :** 77086-22-7		**AlogP:** 3.30	**TPSA:** 12.0

Activity: Non-competitive NMDA glutamate receptor antagonist

Catalog number : M-141

Drug name : (–)-3-Iodo-MK-801 hydrochloride

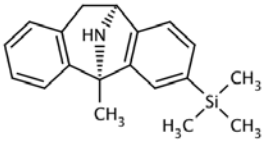


Mol. Formula :	$C_{16}H_{15}ClIN$	**FW :** 383.66	**HBA:** 1	**HBD:** 1	**RotB:** 0
PubChem ID :	449735	**CASRN :**		**AlogP:** 4.29	**TPSA:** 12.0

Activity: NMDA antagonist MK-801 analog

Catalog number : M-143

Drug name : (–)-3-Trimethylsilyl-MK-801 hydrochloride

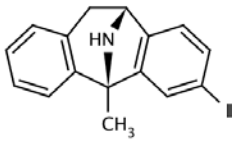


Mol. Formula :	$C_{19}H_{24}ClNSi$	**FW :** 329.95	**HBA:** 1	**HBD:** 1	**RotB:** 1
PubChem ID :		**CASRN :**		**AlogP:** 4.88	**TPSA:** 12.0

Activity: Radioiodinated (–)-3-iodo-MK-801 precursor

Catalog number : M-144

Drug name : (+)-3-Iodo-MK-801 hydrochloride

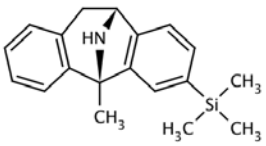


Mol. Formula :	$C_{16}H_{15}ClIN$	**FW :** 383.66	**HBA:** 1	**HBD:** 1	**RotB:** 0
PubChem ID :	449735	**CASRN :**		**AlogP:** 4.29	**TPSA:** 12.0

Activity: NMDA antagonist MK-801 analog

Catalog number : M-145

Drug name : (+)-3-Trimethylsilyl-MK-801 hydrochloride

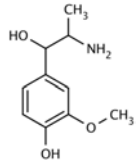


Mol. Formula :	$C_{19}H_{24}ClNSi$	**FW :** 329.95	**HBA:** 1	**HBD:** 1	**RotB:** 1
PubChem ID :		**CASRN :**		**AlogP:** 4.88	**TPSA:** 12.0

Activity: Radioiodinated (+)-3-iodo-MK-801 precursor

Catalog number : M-501

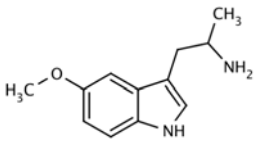
Drug name : 1-(3-Methoxy-4-hydroxyphenyl)-1-hydroxy-2-aminopropane hydrogen oxalate



Mol. Formula :	$C_{12}H_{17}NO_7$	**FW :** 287.27	**HBA:** 4	**HBD:** 3	**RotB:** 3
PubChem ID :		**CASRN :**		**AlogP:** -0.08	**TPSA:** 75.7

Catalog number : M-502

Drug name : (±)-3-(2-Aminopropyl)-5-methoxyindole hydrochloride

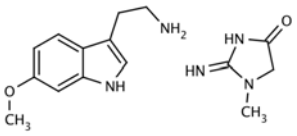


Mol. Formula : $C_{12}H_{17}ClN_2O$ **FW :** 240.73 **HBA:** 2 **HBD:** 2 **RotB:** 3

PubChem ID : 36906 **CASRN :** 1137-04-8 **AlogP:** 1.68 **TPSA:** 51.0

Catalog number : M-503

Drug name : 6-Methoxytryptamine creatinine sulfate

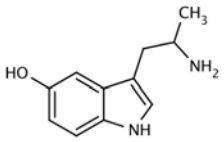


Mol. Formula : $C_{15}H_{23}N_5O_6S$ **FW :** 401.45 **HBA:** 2 **HBD:** 2 **RotB:** 3

PubChem ID : 17654 **CASRN :** 3610-36-4 **AlogP:** 1.26 **TPSA:** 51.0

Catalog number : M-504

Drug name : α-Methylserotonin hydrogen oxalate



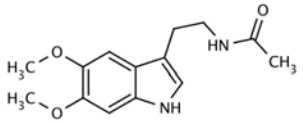
Mol. Formula : $C_{13}H_{16}N_2O_5$ **FW :** 280.28 **HBA:** 2 **HBD:** 3 **RotB:** 2

PubChem ID : 2107 **CASRN :** **AlogP:** 0.77 **TPSA:** 62.0

Activity: Serotonin 5-HT_{2B} receptor agonist

Catalog number : M-506

Drug name : 6-Methoxymelatonin



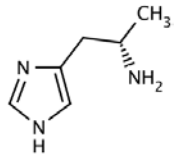
Mol. Formula : $C_{14}H_{18}N_2O_3$ **FW :** 262.31 **HBA:** 3 **HBD:** 2 **RotB:** 5

PubChem ID : 189748 **CASRN :** 69845-43-8 **AlogP:** 0.84 **TPSA:** 63.4

Activity: 6-Hydroxymelatonin metabolite

Catalog number : M-507

Drug name : (*R*)-(–)-α-Methylhistamine oxalate



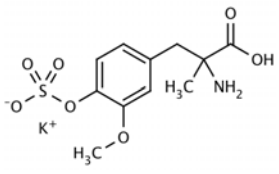
Mol. Formula : $C_9H_{14}N_3O_6$ **FW :** 260.23 **HBA:** 2 **HBD:** 2 **RotB:** 2

PubChem ID : 6603865 **CASRN :** **AlogP:** -0.39 **TPSA:** 54.7

Activity: Histamine H_3 agonist

Catalog number : M-508

Drug name : (±)-3-Methoxy-α-methyldopa-4-*O*-sulfate potassium salt

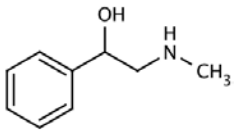


Mol. Formula : $C_{11}H_{14}KNO_7S$ **FW :** 343.40 **HBA:** 7 **HBD:** 2 **RotB:** 6

PubChem ID : **CASRN :** **AlogP:** -2.45 **TPSA:** 147.4

Catalog number : M-509

Drug name : (±)-2-Methylamino-1-phenylethanol



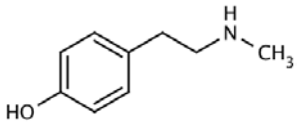
Mol. Formula : $C_9H_{13}NO$ **FW :** 151.21 **HBA:** 2 **HBD:** 2 **RotB:** 3

PubChem ID : 913 **CASRN :** 6589-55-5 **AlogP:** 0.90 **TPSA:** 32.3

Activity: Monoamine oxidase A/B substrate

Catalog number : M-510

Drug name : N-Methyltyramine hydrobromide

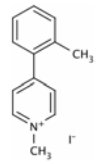


Mol. Formula : $C_9H_{14}BrNO$ **FW :** 232.12 **HBA:** 2 **HBD:** 2 **RotB:** 3

PubChem ID : 22324146 **CASRN :** 370-98-9 **AlogP:** 0.96 **TPSA:** 32.3

Catalog number : M-701

Drug name : 1-Methyl-4-(2'-methylphenyl)pyridinium iodide; 2'-MMPP$^+$



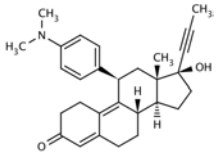
Mol. Formula : $C_{13}H_{14}NI$ **FW :** 311.17 **HBA:** 0 **HBD:** 0 **RotB:** 1

PubChem ID : 163849 **CASRN :** 111342-39-3 **AlogP:** -0.73 **TPSA:** 3.9

Activity: Neurotoxin with greater potency than MPP$^+$ in mice

Catalog number : M-703

Drug name : Mifepristone



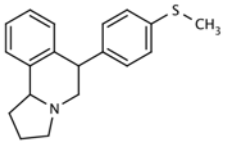
Mol. Formula : $C_{29}H_{35}NO_2$ **FW :** 429.59 **HBA:** 3 **HBD:** 1 **RotB:** 3

PubChem ID : 6712024 **CASRN :** 84371-65-3 **AlogP:** 4.90 **TPSA:** 40.5

Activity: Progesterone receptor antagonist; stimulates prolactin secretion

Catalog number : M-704

Drug name : (±)-McN-5652



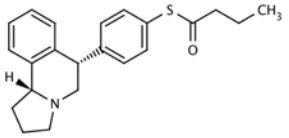
Mol. Formula : $C_{19}H_{22}ClNO_4S$ **FW :** 395.91 **HBA:** 2 **HBD:** 0 **RotB:** 2

PubChem ID : 9994677 **CASRN :** **AlogP:** 4.59 **TPSA:** 28.5

Activity: Serotonin transporter inhibitor

Catalog number : M-706

Drug name : (+)-McN-5652 *S*-Desmethyl-*S*-butyryl ester



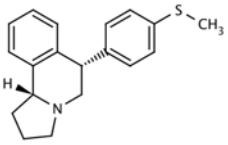
Mol. Formula : $C_{22}H_{25}NOS$ **FW :** 351.51 **HBA:** 3 **HBD:** 0 **RotB:** 5

PubChem ID : **CASRN :** 167548-65-4 **AlogP:** 5.04 **TPSA:** 45.6

Activity: (+)-McN-5652 PET ligand precursor

Catalog number : M-707

Drug name : (+)-McN-5652



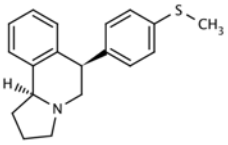
Mol. Formula : $C_{19}H_{22}ClNO_4S$ **FW :** 395.91 **HBA:** 2 **HBD:** 0 **RotB:** 2

PubChem ID : 146919 **CASRN :** 103729-16-4 **AlogP:** 4.59 **TPSA:** 28.5

Activity: Serotonin transporter inhibitor (active enantiomer)

Catalog number : M-708

Drug name : (–)-McN-5652



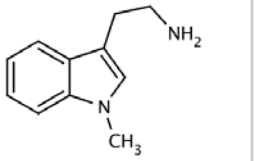
Mol. Formula : $C_{19}H_{22}ClNO_4S$ **FW :** 395.91 **HBA:** 2 **HBD:** 0 **RotB:** 2

PubChem ID : 6336338 **CASRN :** **AlogP:** 4.59 **TPSA:** 28.5

Activity: Serotonin transporter inhibitor (inactive enantiomer)

Catalog number : M-709

Drug name : 1-Methyltryptamine hydrochloride

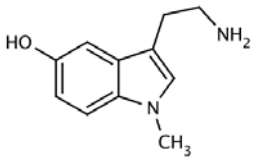


Mol. Formula : $C_{11}H_{15}ClN_2$ **FW :** 210.71 **HBA:** 1 **HBD:** 1 **RotB:** 2

PubChem ID : 23492 **CASRN :** 7518-21-0 **AlogP:** 1.76 **TPSA:** 31.0

Catalog number : M-710

Drug name : 1-Methylserotonin hydrogen maleate



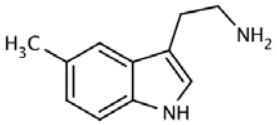
Mol. Formula : $C_{15}H_{18}N_2O_5$ **FW :** 306.32 **HBA:** 2 **HBD:** 2 **RotB:** 2

PubChem ID : 440945 **CASRN :** **AlogP:** 0.70 **TPSA:** 51.2

Activity: Serotonin analog

Catalog number : M-711

Drug name : 5-Methyltryptamine hydrogen maleate



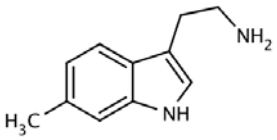
Mol. Formula : $C_{15}H_{18}N_2O_4$ **FW :** 290.32 **HBA:** 1 **HBD:** 2 **RotB:** 2

PubChem ID : 15760 **CASRN :** 1821-47-2 **AlogP:** 1.98 **TPSA:** 41.8

Activity: Serotonin analog

Catalog number : M-712

Drug name : 6-Methyltryptamine hydrogen maleate



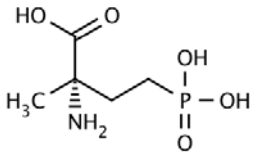
Mol. Formula : $C_{15}H_{18}N_2O_4$ **FW :** 290.32 **HBA:** 1 **HBD:** 2 **RotB:** 2

PubChem ID : 190006 **CASRN :** 62500-90-7 **AlogP:** 1.98 **TPSA:** 41.8

Activity: Serotonin analog

Catalog number : M-801

Drug name : (*S*)-2-Amino-2-methyl-4-phosphonobutanoic acid



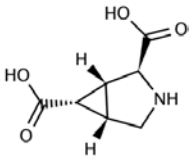
Mol. Formula : $C_5H_{12}NO_5P$ **FW :** 197.13 **HBA:** 6 **HBD:** 4 **RotB:** 4

PubChem ID : 1795543 **CASRN :** 157381-42-5 **AlogP:** -3.58 **TPSA:** 130.7

Activity: mGluR2/3 agonist

Catalog number : M-802

Drug name : (1*R*,2*S*,5*S*,6*S*)-3-Azabicyclo[3.1.0]hexane-2,6-dicarboxylic acid



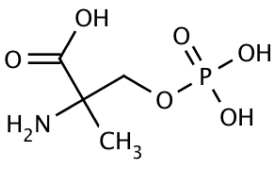
Mol. Formula : $C_7H_9NO_4$ **FW :** 171.15 **HBA:** 5 **HBD:** 3 **RotB:** 2

PubChem ID : 10329748 **CASRN :** **AlogP:** -3.41 **TPSA:** 86.6

Activity: Inhibitor of the Na-dependent, high-affinity synaptosomal Glu transporter

Catalog number : M-803

Drug name : (±)-α-Methylserine-*O*-phosphate



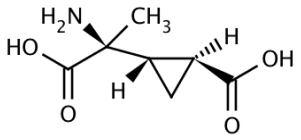
Mol. Formula : $C_4H_{10}NO_6P$ **FW :** 199.10 **HBA:** 6 **HBD:** 4 **RotB:** 4

PubChem ID : 3964633 **CASRN :** 66515-29-5 **AlogP:** -3.23 **TPSA:** 139.9

Activity: mGLuR antagonist

Catalog number : M-804

Drug name : (2*S*,3*S*,4*S*)-2-Methyl-2-(carboxycyclopropyl)glycine



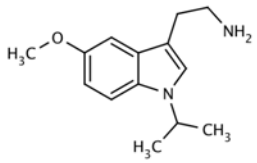
Mol. Formula : $C_7H_{11}NO_4$ **FW :** 173.17 **HBA:** 5 **HBD:** 3 **RotB:** 3

PubChem ID : 6536817 **CASRN :** 157141-16-7 **AlogP:** -2.98 **TPSA:** 100.6

Activity: mGluR2 antagonist

Catalog number : M-805

Drug name : 5-Methoxy-1-isopropyltryptamine



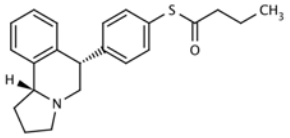
Mol. Formula : $C_{14}H_{20}N_2O$ **FW :** 232.33 **HBA:** 2 **HBD:** 1 **RotB:** 4

PubChem ID : 24820144 **CASRN :** 109921-55-3 **AlogP:** 2.27 **TPSA:** 40.2

Activity: Serotonin analog

Catalog number : M-901

Drug name : (+)-McN-5652 *S*-Desmethyl-*S*-butyryl ester tartrate



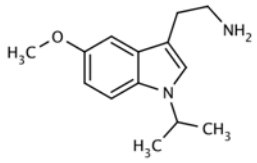
Mol. Formula : $C_{26}H_{31}NO_7S$ **FW :** 501.60 **HBA:** 3 **HBD:** 0 **RotB:** 5

PubChem ID : **CASRN :** 167548-65-4 **AlogP:** 5.04 **TPSA:** 45.6

Activity: (+)-McN-5652 PET ligand precursor

Catalog number : M-902

Drug name : 5-Methoxy-1-isopropyltryptamine oxalate



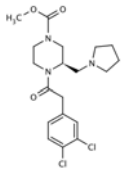
Mol. Formula : $C_{16}H_{22}N_2O_5$ **FW :** 322.36 **HBA:** 2 **HBD:** 1 **RotB:** 4

PubChem ID : 24820144 **CASRN :** **AlogP:** 2.27 **TPSA:** 40.2

Activity: Serotonin analog

Catalog number : M-903

Drug name : GR103545



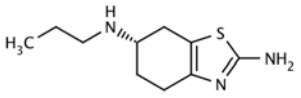
Mol. Formula : $C_{19}H_{25}Cl_2N_3O_3$ **FW :** 414.33 **HBA:** 6 **HBD:** 0 **RotB:** 5

PubChem ID : 6603856 **CASRN :** **AlogP:** 2.45 **TPSA:** 53.1

Activity: Opioid receptor agonist

Catalog number : M-904

Drug name : Mirapex; Pramipexole



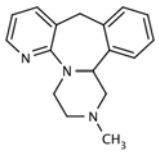
Mol. Formula : $C_{10}H_{17}N_3S$ **FW :** 211.33 **HBA:** 4 **HBD:** 2 **RotB:** 3

PubChem ID : 119570 **CASRN :** 104632-26-0 **AlogP:** 1.65 **TPSA:** 79.2

Activity: Dopamine D_3 agonist

Catalog number : M-905

Drug name : Mirtazapine



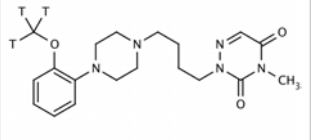
Mol. Formula : $C_{17}H_{19}N_3$ **FW :** 265.35 **HBA:** 3 **HBD:** 0 **RotB:** 0

PubChem ID : 4205 **CASRN :** 85650-52-8 **AlogP:** 3.38 **TPSA:** 19.4

Activity: Serotonin 5-HT antagonist; Tetracyclic antidepressant

Catalog number : M-906

Drug name : 2-{4-[4-C^3H_3]-2-Methoxyphenyl)piperazin-1-yl]butyl}-4-methyl-1,2,4-triazine-3,5-(2*H*,4*H*)dione; [^{3}H]CUMI-101



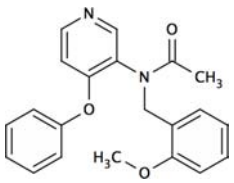
Mol. Formula : $C_{19}H_{27}N_5O_3$ **FW :** 373.46 **HBA:** 0 **HBD:** 6 **RotB:** 7

PubChem ID : 21830793 **CASRN :** **AlogP:** 2.07 **TPSA:** 68.7

Activity: Radiolabeled serotonin 5-HT_{1A} agonist

Catalog number : M-907

Drug name : *N*-[(2-Methoxyphenyl)methyl]-*N*-(4-phenoxypyridin-3-yl)acetamide



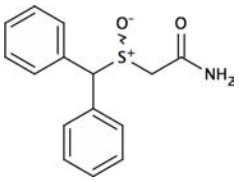
Mol. Formula : $C_{21}H_{20}N_2O_3$ **FW :** 348.40 **HBA:** 3 **HBD:** 0 **RotB:** 6

PubChem ID : 9841240 **CASRN :** **AlogP:** 2.92 **TPSA:** 51.7

Activity: Brain peripheral benzodiazepine receptor (TSPO) ligand

Catalog number : M-908

Drug name : (±)-Modafinil



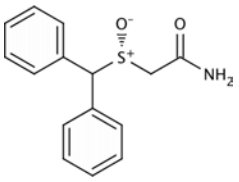
Mol. Formula : $C_{15}H_{15}NO_2S$ **FW :** 273.35 **HBA:** 2 **HBD:** 1 **RotB:** 5

PubChem ID : 4236 **CASRN :** 68693-11-8 **AlogP:** 1.53 **TPSA:** 79.4

Activity: Stimulant

Catalog number : M-909

Drug name : (*R*)-(–)-Modafinil



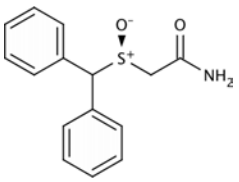
Mol. Formula : $C_{15}H_{15}NO_2S$ **FW :** 273.35 **HBA:** 2 **HBD:** 1 **RotB:** 5

PubChem ID : 9690109 **CASRN :** 112111-43-0 **AlogP:** 1.53 **TPSA:** 79.4

Activity: Stimulant

Catalog number : M-910

Drug name : (*S*)-(+)-Modafinil



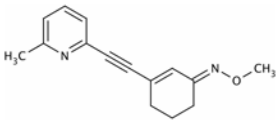
Mol. Formula : $C_{15}H_{15}NO_2S$ **FW :** 273.35 **HBA:** 2 **HBD:** 1 **RotB:** 5

PubChem ID : **CASRN :** **AlogP:** 1.53 **TPSA:** 79.4

Activity: Stimulant

Catalog number : M-911

Drug name : ABP688



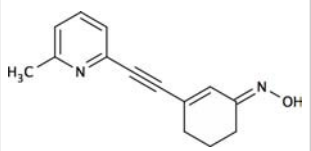
Mol. Formula : $C_{15}H_{16}N_2O$ **FW :** 240.31 **HBA:** 3 **HBD:** 0 **RotB:** 3

PubChem ID : 11481862 **CASRN :** **AlogP:** 3.02 **TPSA:** 34.5

Activity: Metabotropic glutamate mGluR5 antagonist

Catalog number : M-912

Drug name : 3-(6-Methyl-pyridin-2-ylethynyl)-cyclohex-2-enone oxime; Desmethyl ABP688



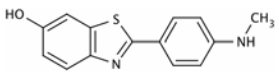
Mol. Formula : $C_{14}H_{14}N_2O$ **FW :** 226.27 **HBA:** 3 **HBD:** 1 **RotB:** 2

PubChem ID : **CASRN :** **AlogP:** 2.65 **TPSA:** 45.5

Activity: ABP688 PET ligand precursor

Catalog number : M-913

Drug name : 6-OH-BTA-1



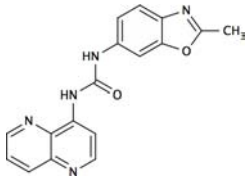
Mol. Formula : $C_{14}H_{12}N_2OS$ **FW :** 256.33 **HBA:** 4 **HBD:** 2 **RotB:** 2

PubChem ID : 10171487 **CASRN :** 566169-93-5 **AlogP:** 3.22 **TPSA:** 73.4

Activity: Aggregated amyloid protein ligand; Thioflavin-T analog

Catalog number : M-914

Drug name : SB-334867



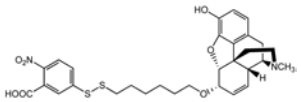
Mol. Formula : $C_{17}H_{13}N_5O_2$ **FW :** 319.32 **HBA:** 4 **HBD:** 2 **RotB:** 2

PubChem ID : 6604926 **CASRN :** 249889-64-3 **AlogP:** 1.91 **TPSA:** 92.9

Activity: Orexin receptor subtype 1 antagonist

Catalog number : M-915 new

Drug name : Morphine-SH-DTNB derivative

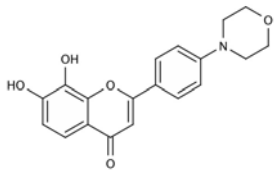


Mol. Formula : $C_{30}H_{34}N_2O_7S_2$ **FW :** 598.83 **HBA:** **HBD:** **RotB:**

PubChem ID : **CASRN :** **AlogP:** **TPSA:**

Catalog number : M-916 new

Drug name : 2-(4-Morphin-4-ylphenyl)-7,8-dihydroxy-4H-chromen-4-one

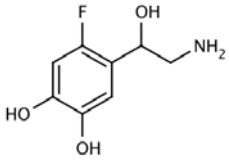


Mol. Formula : $C_{19}H_{17}NO_5$ **FW :** 339.34 **HBA:** **HBD:** **RotB:**

PubChem ID : **CASRN :** **AlogP:** **TPSA:**

Catalog number : N-502

Drug name : 6-Fluoronorepinephrine oxalate



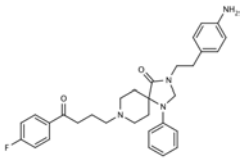
Mol. Formula : $C_{18}H_{22}F_2N_2O_{10}$ **FW :** 464.38 **HBA:** 5 **HBD:** 4 **RotB:** 2

PubChem ID : 1862 **CASRN :** 86820-21-5 **AlogP:** -0.90 **TPSA:** 86.7

Activity: α- & β-Adrenergic-sensitive cyclic AMP-generating systems activator

Catalog number : N-701

Drug name : p-Aminophenethylspiperone



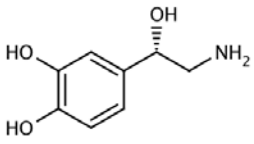
Mol. Formula : $C_{31}H_{35}FN_4O_2$ **FW :** 514.65 **HBA:** 6 **HBD:** 1 **RotB:** 9

PubChem ID : 125085 **CASRN :** 93801-18-4 **AlogP:** 4.51 **TPSA:** 69.9

Activity: Dopamine D_2 receptor antagonist; intermediate for photoaffinity agents

Catalog number : N-702

Drug name : (+)-Norepinephrine tartrate



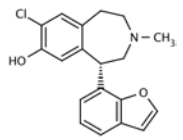
Mol. Formula : $C_{12}H_{17}NO_9$ **FW :** 319.27 **HBA:** 4 **HBD:** 4 **RotB:** 2

PubChem ID : 5814 **CASRN :** 636-88-4 **AlogP:** -0.67 **TPSA:** 86.7

Activity: Unnatural enantiomer of norepinephrine

Catalog number : N-703

Drug name : (+)-NNC 01-0112

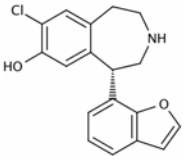


Mol. Formula :	$C_{19}H_{18}ClNO_2$	**FW :**	327.80	**HBA:**	3	**HBD:**	1	**RotB:**	1
PubChem ID :	130424	**CASRN :**	125341-24-4			**AlogP:**	3.37	**TPSA:**	36.6

Activity: Dopamine D_1 receptor ligand

Catalog number : N-704

Drug name : (+)-*N*-Desmethyl-NNC 01-0112 hydrochloride

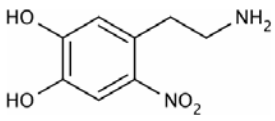


Mol. Formula :	$C_{18}H_{17}Cl_2NO_2$	**FW :**	350.23	**HBA:**	3	**HBD:**	2	**RotB:**	1
PubChem ID :	20135382	**CASRN :**				**AlogP:**	2.13	**TPSA:**	45.4

Activity: NNC-01-0112 PET ligand precusor

Catalog number : N-705

Drug name : 6-Nitrodopamine

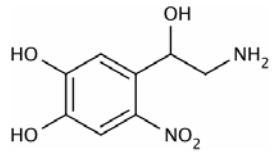


Mol. Formula :	$C_8H_{10}N_2O_{14}$	**FW :**	198.17	**HBA:**	5	**HBD:**	3	**RotB:**	3
PubChem ID :	10932412	**CASRN :**				**AlogP:**	-1.09	**TPSA:**	112.3

Activity: Nitrated catecholamine

Catalog number : N-706

Drug name : 6-Nitronorepinephrine

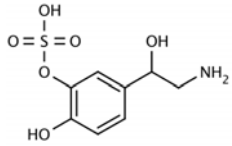


Mol. Formula :	$C_8H_{10}N_2O_5$	**FW :**	214.98	**HBA:**	6	**HBD:**	4	**RotB:**	3
PubChem ID :		**CASRN :**				**AlogP:**	-1.87	**TPSA:**	132.5

Activity: Nitrated catecholamine

Catalog number : N-707

Drug name : Norepinephrine-3-*O*-sulfate

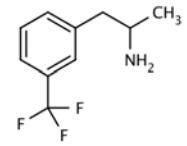


Mol. Formula :	$C_8H_{11}NO_6S$	**FW :**	249.24	**HBA:**	6	**HBD:**	4	**RotB:**	4
PubChem ID :	10083394	**CASRN :**				**AlogP:**	-2.13	**TPSA:**	138.5

Activity: Catechol O-methyltransferase inhibitor

Catalog number : N-801

Drug name : (±)-*N*-Norfenfluramine hydrochloride

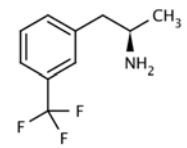


Mol. Formula :	$C_{10}H_{13}ClF_3N$	**FW :**	239.67	**HBA:**	4	**HBD:**	1	**RotB:**	3
PubChem ID :	120765	**CASRN :**	673-18-7			**AlogP:**	2.71	**TPSA:**	26.0

Activity: Serotonin uptake inhibitor

Catalog number : N-802

Drug name : (*R*)-(–)-*N*-Norfenfluramine hydrochloride

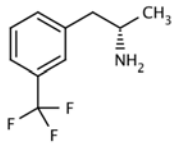


Mol. Formula :	$C_{10}H_{13}ClF_3N$	**FW :**	239.67	**HBA:**	4	**HBD:**	1	**RotB:**	3
PubChem ID :	12895728	**CASRN :**				**AlogP:**	2.71	**TPSA:**	26.0

Activity: Serotonin uptake inhibitor

Catalog number : N-803

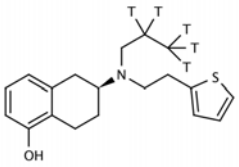
Drug name : (*S*)-(+)-*N*-Norfenfluramine hydrochloride



Mol. Formula :	$C_{10}H_{13}ClF_3N$	**FW :**	239.67	**HBA:**	4	**HBD:**	1	**RotB:**	3
PubChem ID :	9815618	**CASRN :**				**AlogP:**	2.71	**TPSA:**	26.0
Activity:	Serotonin uptake inhibitor								

Catalog number : N-804

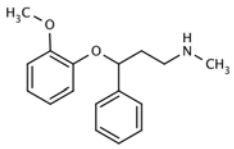
Drug name : [^{3}H]-(–)-2-(*N*-[2,3(n)^{3}H]Propyl-N-(2-thiofuranyl)-2'-ethylamino)-5-hydroxy -1,2,3,4-tetrahydronaphthalene hydrochloride



Mol. Formula :	$C_{19}H_{26}ClNOS$	**FW :**	351.94	**HBA:**	3	**HBD:**	1	**RotB:**	6
PubChem ID :	6917969	**CASRN :**	92206-54-7			**AlogP:**	4.06	**TPSA:**	51.7
Activity:	Radiolabeled dopamine receptor agonist								

Catalog number : N-901

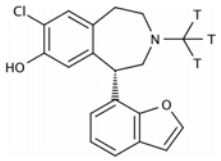
Drug name : (±)-Nisoxetine hydrochloride



Mol. Formula :	$C_{17}H_{22}ClNO_2$	**FW :**	307.82	**HBA:**	3	**HBD:**	1	**RotB:**	7
PubChem ID :	134453	**CASRN :**	57754-86-6			**AlogP:**	3.06	**TPSA:**	30.5
Activity:	Norepinephrine uptake inhibitor								

Catalog number : N-902

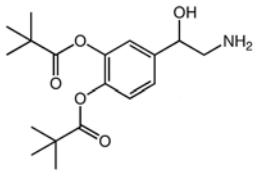
Drug name : (+)-8-Chloro-5-(7-benzofuranyl)-7-hydroxy-3-methyl-2,3,4,5-tetrahydro-1H-3-benzazepine, [^{3}H]NNC-01-0112



Mol. Formula :	$C_{19}H_{19}ClNO_2$	**FW :**	328.82	**HBA:**	3	**HBD:**	1	**RotB:**	1
PubChem ID :	130424	**CASRN :**				**AlogP:**	3.37	**TPSA:**	36.6
Activity:	Radiolabeled dopamine D_1 receptor ligand								

Catalog number : N-903 new

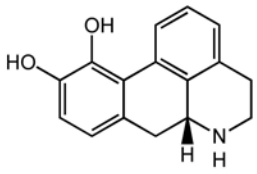
Drug name : Norepinephrine dipivalate hydrochloride



Mol. Formula :	$C_{18}H_{28}ClNO_5$	**FW :**	373.87	**HBA:**		**HBD:**		**RotB:**	
PubChem ID :		**CASRN :**				**AlogP:**		**TPSA:**	

Catalog number : N-904 new

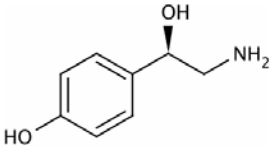
Drug name : *(R)*-(–)-Norapomorphine hydrobromide



Mol. Formula :	$C_{16}H_{16}BrNO_2$	**FW :**	334.21	**HBA:**	3	**HBD:**	3	**RotB:**	0
PubChem ID :	30133	**CASRN :**	20382-69-8			**AlogP:**	2.15	**TPSA:**	21.7
Activity:	Dopamine D3 receptor ligand.								

Catalog number : O-501

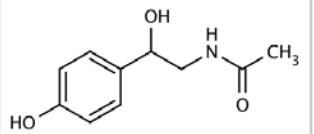
Drug name : (–)-Octopamine



Mol. Formula :	$C_8H_{11}NO_2$	**FW :**	153.18	**HBA:**	3	**HBD:**	3	**RotB:**	2
PubChem ID :	4581	**CASRN :**	104-14-3			**AlogP:**	-0.30	**TPSA:**	66.5
Activity:	Biogenic amine formed by β-hydroxylation of tyramine; adrenergic								

Catalog number : O-502

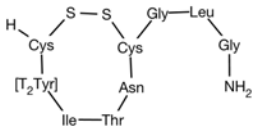
Drug name : N-Acetyl-(±)-octopamine



Mol. Formula :	$C_{10}H_{13}NO_3$	**FW :**	195.22	**HBA:**	3	**HBD:**	3	**RotB:**	3
PubChem ID :	193691	**CASRN :**	33141-15-0			**AlogP:**	0.03	**TPSA:**	69.6

Catalog number : O-801

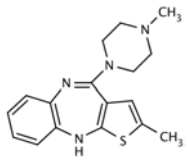
Drug name : [^{3}H][Thr^4,Gly^7]Oxytocin



Mol. Formula :	$C_{39}H_{61}N_{11}O_{12}S_2$	**FW :**	940.11	**HBA:**	17	**HBD:**	13	**RotB:**	17
PubChem ID :	3080871	**CASRN :**	60786-59-6			**AlogP:**	-3.52	**TPSA:**	436.1
Activity:	Radiolabeled oxytocin analog								

Catalog number : O-901

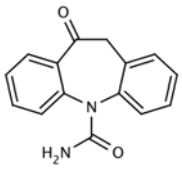
Drug name : Olanzapine



Mol. Formula :	$C_{17}H_{20}N_4S$	**FW :**	312.43	**HBA:**	5	**HBD:**	1	**RotB:**	0
PubChem ID :	4585	**CASRN :**	132539-06-1			**AlogP:**	3.09	**TPSA:**	59.1
Activity:	Serotonin 5-HT uptake inhibitor								

Catalog number : O-902

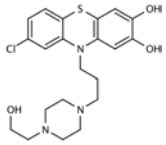
Drug name : Oxcarbazepine



Mol. Formula :	$C_{15}H_{12}N_2O_2$	**FW :**	252.27	**HBA:**	2	**HBD:**	1	**RotB:**	0
PubChem ID :	34312	**CASRN :**	28721-07-5			**AlogP:**	1.66	**TPSA:**	63.4
Activity:	Anticonvulsant								

Catalog number : P-501

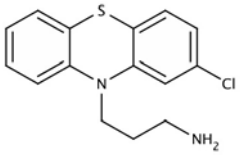
Drug name : 7,8-Dihydroxyperphenazine dihydrochloride



Mol. Formula :	$C_{21}H_{28}Cl_3N_3O_3S$	**FW :**	508.90	**HBA:**	8	**HBD:**	3	**RotB:**	6
PubChem ID :		**CASRN :**				**AlogP:**	2.84	**TPSA:**	95.7

Catalog number : P-502

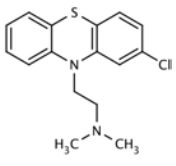
Drug name : 2-Chloro-10-(3-aminopropyl)phenothiazine hydrochloride



Mol. Formula :	$C_{15}H_{16}Cl_2N_2S$	**FW :**	327.28	**HBA:**	3	**HBD:**	1	**RotB:**	3
PubChem ID :		**CASRN :**	3763-80-2			**AlogP:**	4.47	**TPSA:**	

Catalog number : P-503

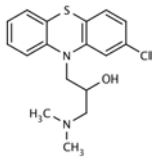
Drug name : 2-Chloro-10-(2-dimethylaminoethyl)phenothiazine hydrochloride



Mol. Formula :	$C_{16}H_{18}Cl_2N_2S$	**FW :**	341.30	**HBA:**	4	**HBD:**	0	**RotB:**	3
PubChem ID :	168055	**CASRN :**	2095-24-1			**AlogP:**	4.50	**TPSA:**	31.8

Catalog number : P-504

Drug name : (±)-2-Chloro-10-(3-dimethylamino-2-hydroxypropyl)phenothiazine hydrogen maleate

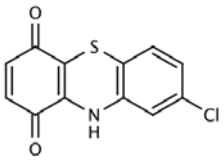


Mol. Formula : $C_{21}H_{23}ClN_2O_5S$ **FW :** 450.94 **HBA:** 5 **HBD:** 1 **RotB:** 4

PubChem ID : **CASRN :** **AlogP:** 3.83 **TPSA:** 52.0

Catalog number : P-505

Drug name : 2-Chloro-6,9-dioxophenothiazine

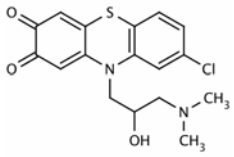


Mol. Formula : $C_{12}H_6ClNO_2S$ **FW :** 263.70 **HBA:** 5 **HBD:** 1 **RotB:** 0

PubChem ID : **CASRN :** **AlogP:** 2.26 **TPSA:** 71.5

Catalog number : P-506

Drug name : (±)-2-Chloro-7,8-dioxo-10-(3-dimethylamino-2-hydroxypropyl)phenothiazine hydrochloride

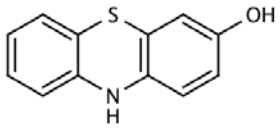


Mol. Formula : $C_{17}H_{18}Cl_2N_2O_3S$ **FW :** 401.31 **HBA:** 7 **HBD:** 1 **RotB:** 4

PubChem ID : **CASRN :** **AlogP:** 1.81 **TPSA:** 86.2

Catalog number : P-508

Drug name : 3-Hydroxyphenothiazine

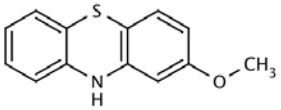


Mol. Formula : $C_{12}H_9NOS$ **FW :** 215.27 **HBA:** 3 **HBD:** 2 **RotB:** 0

PubChem ID : 74725 **CASRN :** 1927-44-2 **AlogP:** 3.48 **TPSA:** 57.6

Catalog number : P-509

Drug name : 2-Methoxyphenothiazine

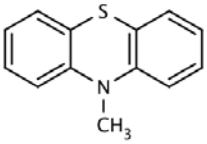


Mol. Formula : $C_{13}H_{11}NOS$ **FW :** 229.30 **HBA:** 3 **HBD:** 1 **RotB:** 1

PubChem ID : 74490 **CASRN :** 1771-18-2 **AlogP:** 3.51 **TPSA:** 46.6

Catalog number : P-510

Drug name : N-Methylphenothiazine

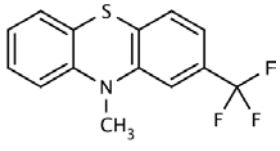


Mol. Formula : $C_{13}H_{11}NS$ **FW :** 213.30 **HBA:** 2 **HBD:** 0 **RotB:** 0

PubChem ID : 71015 **CASRN :** 1207-72-3 **AlogP:** 4.01 **TPSA:** 28.5

Catalog number : P-511

Drug name : N-Methyl-2-(trifluoromethyl)phenothiazine

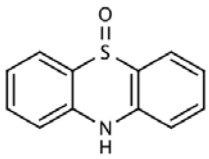


Mol. Formula : $C_{14}H_{10}F_3NS$ **FW :** 281.30 **HBA:** 5 **HBD:** 0 **RotB:** 1

PubChem ID : **CASRN :** **AlogP:** 4.89 **TPSA:** 28.5

Catalog number : P-512

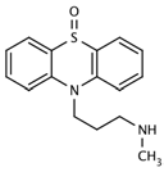
Drug name : Phenothiazine-5-oxide



Mol. Formula :	$C_{12}H_9NOS$	**FW :**	215.27	**HBA:**	2	**HBD:**	1	**RotB:**	0
PubChem ID :	71014	**CASRN :**	1207-71-2			**AlogP:**	1.79	**TPSA:**	48.3

Catalog number : P-513

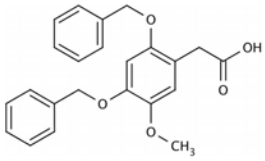
Drug name : *nor*-1-Promazine sulfoxide hydrochloride



Mol. Formula :	$C_{16}H_{19}ClN_2OS$	**FW :**	322.86	**HBA:**	3	**HBD:**	1	**RotB:**	4
PubChem ID :	23275476	**CASRN :**				**AlogP:**	1.70	**TPSA:**	51.6

Catalog number : P-514

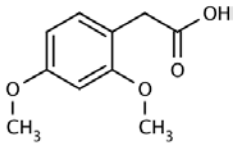
Drug name : 2,4-Dibenzyloxy-5-methoxyphenylacetic acid



Mol. Formula :	$C_{23}H_{22}O_5$	**FW :**	378.42	**HBA:**	5	**HBD:**	1	**RotB:**	9
PubChem ID :		**CASRN :**				**AlogP:**	4.47	**TPSA:**	65.0

Catalog number : P-515

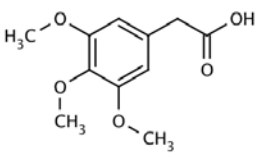
Drug name : 2,4-Dimethoxyphenylacetic acid



Mol. Formula :	$C_{10}H_{12}O_4$	**FW :**	196.20	**HBA:**	4	**HBD:**	1	**RotB:**	4
PubChem ID :	350555	**CASRN :**	6496-89-5			**AlogP:**	1.17	**TPSA:**	55.8

Catalog number : P-516

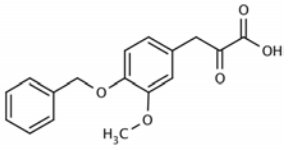
Drug name : 3,4,5-Trimethoxyphenylacetic acid



Mol. Formula :	$C_{11}H_{14}O_5$	**FW :**	226.23	**HBA:**	5	**HBD:**	1	**RotB:**	5
PubChem ID :	70372	**CASRN :**	951-82-6			**AlogP:**	0.92	**TPSA:**	65.0
Activity:	Mescaline metabolite								

Catalog number : P-517

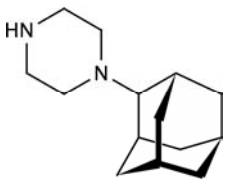
Drug name : 4-Benzyloxyphenyl-3-methoxypyruvic acid



Mol. Formula :	$C_{17}H_{16}O_5$	**FW :**	300.31	**HBA:**	5	**HBD:**	1	**RotB:**	7
PubChem ID :		**CASRN :**				**AlogP:**	3.42	**TPSA:**	72.8

Catalog number : P-518

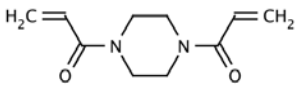
Drug name : N-(2-Adamantyl)piperazine dihydrochloride



Mol. Formula :	$C_{14}H_{26}Cl_2N_2$	**FW :**	293.28	**HBA:**	2	**HBD:**	1	**RotB:**	1
PubChem ID :	4599242	**CASRN :**				**AlogP:**	1.64	**TPSA:**	15.3

Catalog number : P-519

Drug name : 1,4-Diacryloylpiperazine

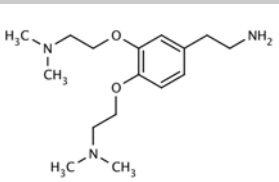


Mol. Formula :	$C_{10}H_{14}N_2O_2$	**FW :**	194.23	**HBA:**	2	**HBD:**	0	**RotB:**	2
PubChem ID :	193422	**CASRN :**	6342-17-2			**AlogP:**	0.07	**TPSA:**	40.6

Activity: Cross-linking monomer for development of polyacrylamide gels

Catalog number : P-520

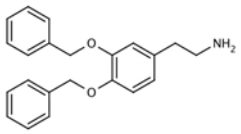
Drug name : 3,4-Di(β-dimethylaminoethoxy)-β-phenethylamine trihydrochloride



Mol. Formula :	$C_{16}H_{32}Cl_3N_3O_2$	**FW :**	404.81	**HBA:**	5	**HBD:**	1	**RotB:**	10
PubChem ID :		**CASRN :**				**AlogP:**	0.87	**TPSA:**	51.0

Catalog number : P-521

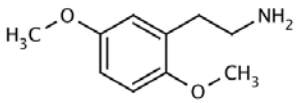
Drug name : 3,4-Dibenzyloxy-β-phenethylamine hydrochloride



Mol. Formula :	$C_{22}H_{24}ClNO_2$	**FW :**	369.89	**HBA:**	3	**HBD:**	1	**RotB:**	8
PubChem ID :	423869	**CASRN :**	1699-56-5			**AlogP:**	4.46	**TPSA:**	44.5

Catalog number : P-522

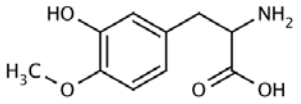
Drug name : 2,5-Dimethoxy-β-phenethylamine hydrochloride



Mol. Formula :	$C_{10}H_{16}ClNO_2$	**FW :**	217.70	**HBA:**	3	**HBD:**	1	**RotB:**	4
PubChem ID :	24187012	**CASRN :**	3166-74-3			**AlogP:**	0.91	**TPSA:**	44.5

Catalog number : P-526

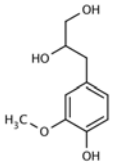
Drug name : 3-Hydroxy-4-methoxy-(±)-phenylalanine



Mol. Formula :	$C_{10}H_{13}NO_4$	**FW :**	211.22	**HBA:**	5	**HBD:**	3	**RotB:**	4
PubChem ID :	586369	**CASRN :**	4368-01-8			**AlogP:**	-1.68	**TPSA:**	92.8

Catalog number : P-528

Drug name : Vanillyl glycol

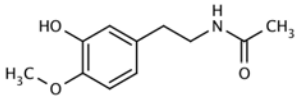


Mol. Formula :	$C_{16}H_{26}N_2O_4$	**FW :**	310.39	**HBA:**	4	**HBD:**	3	**RotB:**	4
PubChem ID :	161566	**CASRN :**	27391-18-0			**AlogP:**	0.25	**TPSA:**	69.9

Activity: Lignin model compound

Catalog number : P-701

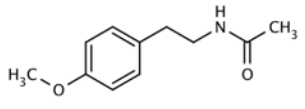
Drug name : N-Acetyl-3-hydroxy-4-methoxy-β-phenethylamine



Mol. Formula :	$C_{11}H_{15}NO_3$	**FW :**	209.25	**HBA:**	3	**HBD:**	2	**RotB:**	4
PubChem ID :	591256	**CASRN :**				**AlogP:**	0.71	**TPSA:**	58.6

Catalog number : P-703

Drug name : N-Acetyl-4-methoxy-β-phenethylamine

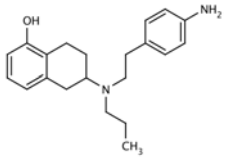


Mol. Formula : $C_{11}H_{15}NO_2$ **FW :** 193.25 **HBA:** 2 **HBD:** 1 **RotB:** 4

PubChem ID : 584258 **CASRN :** **AlogP:** 0.99 **TPSA:** 38.3

Catalog number : P-706

Drug name : (±)-2-[*N*-(4'-Aminophenylethyl)-*N*-propyl]amino-5-hydroxytetralin dihydrochloride

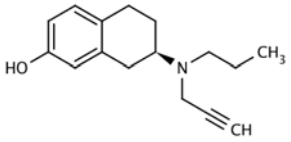


Mol. Formula : $C_{21}H_{30}Cl_2N_2O$ **FW :** 397.39 **HBA:** 3 **HBD:** 2 **RotB:** 6

PubChem ID : **CASRN :** **AlogP:** 3.37 **TPSA:** 49.5

Catalog number : P-707

Drug name : (*R*)-(+)-2-(*N*-Propargyl-*N*-propyl)amino-7-hydroxytetralin hydrochloride



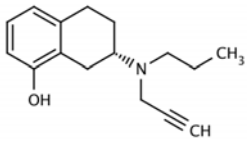
Mol. Formula : $C_{16}H_{22}ClNO$ **FW :** 279.81 **HBA:** 2 **HBD:** 1 **RotB:** 5

PubChem ID : 9992020 **CASRN :** **AlogP:** 3.43 **TPSA:** 23.5

Activity: Radiolabeling (*R*)-(+)-7-hydroxy-DPAT precursor

Catalog number : P-708

Drug name : (*R*)-(–)-2-(*N*-Propargyl-*N*-propyl)amino-8-hydroxytetralin hydrochloride



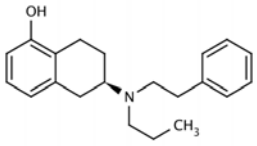
Mol. Formula : $C_{16}H_{22}ClNO$ **FW :** 279.81 **HBA:** 2 **HBD:** 1 **RotB:** 5

PubChem ID : **CASRN :** **AlogP:** 3.43 **TPSA:** 23.5

Activity: Radiolabeling (*R*)-(+)-8-hydroxy-DPAT precursor

Catalog number : P-709

Drug name : (*S*)-(–)-2-(*N*-Phenylethyl-*N*-propyl)amino-5-hydroxytetralin hydrochloride

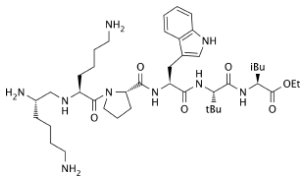


Mol. Formula : $C_{21}H_{28}ClNO$ **FW :** 345.91 **HBA:** 2 **HBD:** 1 **RotB:** 6

PubChem ID : **CASRN :** **AlogP:** 4.20 **TPSA:** 23.5

Catalog number : P-710

Drug name : PD149163



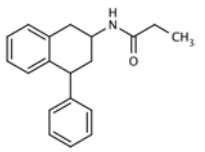
Mol. Formula : $C_{52}H_{76}F_{15}N_9O_{16}$ **FW :** 1368.20 **HBA:** 9 **HBD:** 8 **RotB:** 26

PubChem ID : **CASRN :** **AlogP:** 1.52 **TPSA:** 256.9

Activity: Neurotensin agonist

Catalog number : P-801

Drug name : (±)-4-Phenyl-2-(propioamido)tetraline



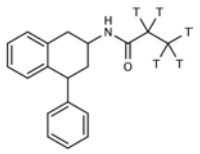
Mol. Formula : $C_{19}H_{21}NO$ **FW :** 279.38 **HBA:** 1 **HBD:** 1 **RotB:** 3

PubChem ID : 3976006 **CASRN :** 0 **AlogP:** 3.87 **TPSA:** 29.1

Activity: Melatonin receptor antagonist

Catalog number : P-802

Drug name : 4-Phenyl-2-[(2',3'(n)-^{3}H)propioamido]tetraline



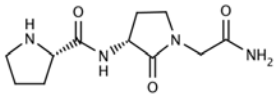
Mol. Formula : $C_{19}H_{21}NO$ **FW :** 279.38 **HBA:** 1 **HBD:** 1 **RotB:** 3

PubChem ID : 10708579 **CASRN :** **AlogP:** 3.87 **TPSA:** 29.1

Activity: Radiolabeled melatonin receptor antagonist

Catalog number : P-803

Drug name : 3-(*R*)-[2-(*S*)-(Pyrrolidinylcarbonyl)amino]-2-oxo-1-pyrrolidineacetamide



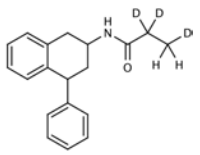
Mol. Formula : $C_{11}H_{18}N_4O_3$ **FW :** 254.28 **HBA:** 4 **HBD:** 3 **RotB:** 4

PubChem ID : 129409 **CASRN :** 106732-52-9 **AlogP:** -2.84 **TPSA:** 104.5

Activity: MSH release-inhibiting hormone antagonist

Catalog number : P-804

Drug name : (±)-4-Phenyl-2-[2',2',3'-^{2}H]-(propioamido)tetralin



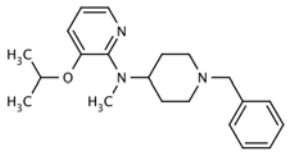
Mol. Formula : $C_{19}H_{18}D_3NO$ **FW :** 282.40 **HBA:** 1 **HBD:** 1 **RotB:** 3

PubChem ID : 3976006 **CASRN :** 134865-74-0 **AlogP:** 3.87 **TPSA:** 29.1

Activity: Deuterated melatonin receptor antagonist

Catalog number : P-805

Drug name : PNU-101,958



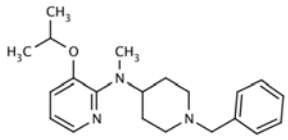
Mol. Formula : $C_{21}H_{31}Cl_2N_3O$ **FW :** 412.41 **HBA:** 4 **HBD:** 0 **RotB:** 6

PubChem ID : 5615 **CASRN :** 170856-57-2 **AlogP:** 3.95 **TPSA:** 28.6

Activity: Dopamine D_4 antagonist

Catalog number : P-901

Drug name : [^{3}H]PNU-101,958



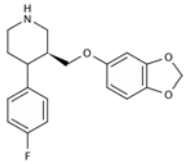
Mol. Formula : $C_{21}H_{29}N_3O$ **FW :** 339.47 **HBA:** 4 **HBD:** 0 **RotB:** 6

PubChem ID : **CASRN :** **AlogP:** 3.95 **TPSA:** 28.6

Activity: Radiolabeled D_4 receptor antagonist

Catalog number : P-902

Drug name : Paroxetine hydrochloride



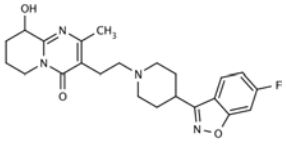
Mol. Formula : $C_{19}H_{21}ClFNO_3$ **FW :** 365.83 **HBA:** 4 **HBD:** 1 **RotB:** 4

PubChem ID : 62878 **CASRN :** 61869-08-7 **AlogP:** 3.58 **TPSA:** 39.7

Activity: Serotonin reuptake inhibitor; antidepressant

Catalog number : P-903

Drug name : 3-{2-[4-(6-Fluorobenzo[d]isoxazol-3-yl)-1-piperidyl]ethyl}-7-hydoxy-4-methyl -1,5-diazabicyclo[4.4.0]deca-3,5-dien-2-one; Paliperidone



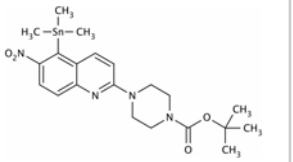
Mol. Formula : $C_{23}H_{27}FN_4O_3$ **FW :** 426.48 **HBA:** 6 **HBD:** 1 **RotB:** 4

PubChem ID : 115237 **CASRN :** 144598-75-4 **AlogP:** 2.02 **TPSA:** 82.2

Activity: Resperidone metabolite; antischizophrenic

Catalog number : Q-707

Drug name : N-(*tert*-Butyloxycarbonyl)-6-nitro-5-(trimethylstannyl)quipazine



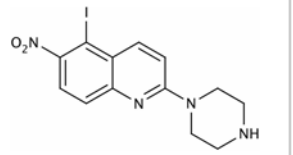
Mol. Formula : $C_{21}H_{30}N_4O_4Sn$ **FW :** 521.21 **HBA:** 6 **HBD:** 0 **RotB:** 5

PubChem ID : **CASRN :** **AlogP:** 3.40 **TPSA:** 91.5

Activity: Serotonin 5-HT uptake inhibitor radioiodination precursor

Catalog number : Q-708

Drug name : 5-Iodo-6-nitroquipazine



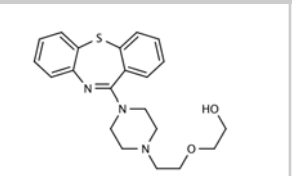
Mol. Formula : $C_{13}H_{13}IN_4O_2$ **FW :** 384.18 **HBA:** 5 **HBD:** 1 **RotB:** 2

PubChem ID : 10091399 **CASRN :** 139593-11-6 **AlogP:** 3.48 **TPSA:** 74.0

Activity: Serotonin 5-HT uptake inhibitor

Catalog number : Q-901

Drug name : Quetiapine



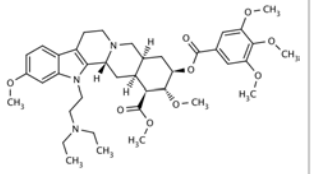
Mol. Formula : $C_{21}H_{25}N_3O_2S$ **FW :** 383.51 **HBA:** 6 **HBD:** 1 **RotB:** 5

PubChem ID : 5002 **CASRN :** 111974-69 -7 **AlogP:** 3.22 **TPSA:** 73.6

Activity: Antipsychotic agent

Catalog number : R-501

Drug name : 1-(β-Diethylamino)ethylreserpine dipicrate



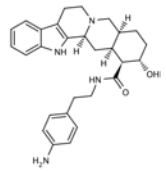
Mol. Formula : $C_{51}H_{59}N_9O_{23}$ **FW :** 1166.07 **HBA:** 9 **HBD:** 0 **RotB:** 15

PubChem ID : 65518 **CASRN :** 53-18-9 **AlogP:** 3.91 **TPSA:** 110.2

Activity: Hypotensive agent

Catalog number : R-701

Drug name : 17α-Hydroxy-20α-yohimban-16β-(N-4-aminophenylethyl)carboxamide dihydrochloride



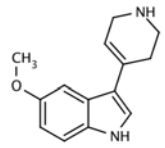
Mol. Formula : $C_{28}H_{36}Cl_2N_4O_2$ **FW :** 531.51 **HBA:** 4 **HBD:** 4 **RotB:** 4

PubChem ID : **CASRN :** **AlogP:** 2.34 **TPSA:** 94.4

Activity: Adrenergic α2 ligand radioiodination precursor

Catalog number : R-702

Drug name : RU-24969



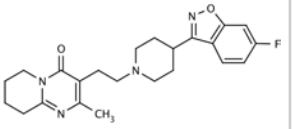
Mol. Formula : $C_{16}H_{19}N_2O_3$ **FW :** 287.34 **HBA:** 2 **HBD:** 2 **RotB:** 2

PubChem ID : 108029 **CASRN :** 107008-28-6 **AlogP:** 2.04 **TPSA:** 37.1

Activity: Serotonin 5-HT1A/1B agonist

Catalog number : R-901

Drug name : Risperidone



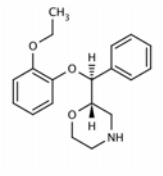
Mol. Formula : $C_{23}H_{27}FN_4O_2$ **FW :** 410.48 **HBA:** 5 **HBD:** 0 **RotB:** 4

PubChem ID : 5073 **CASRN :** 106266-06-2 **AlogP:** 2.89 **TPSA:** 61.9

Activity: Serotonin 5-HT and dopamine antagonist; antipsychotic agent

Catalog number : R-902

Drug name : (±)-Reboxetine mesylate



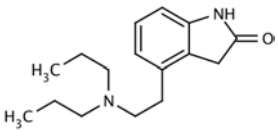
Mol. Formula : $C_{20}H_{27}NO_6S$ **FW :** 409.50 **HBA:** 4 **HBD:** 1 **RotB:** 6

PubChem ID : 5311403 **CASRN :** 98769-81-4 **AlogP:** 3.08 **TPSA:** 39.7

Activity: Adrenergic uptake inhibitor; antidepressant

Catalog number : R-903

Drug name : Ropinirole hydrochloride



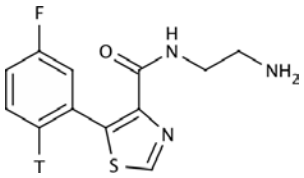
Mol. Formula : $C_{16}H_{24}N_2O$ **FW :** 260.37 **HBA:** 2 **HBD:** 1 **RotB:** 7

PubChem ID : 68727 **CASRN :** 91374-21-9 **AlogP:** 2.93 **TPSA:** 32.3

Activity: Non-ergoline dopamine agonist; used to treat Parkinson's disease

Catalog number : R-904

Drug name : [^{3}H]Ro 41-1049



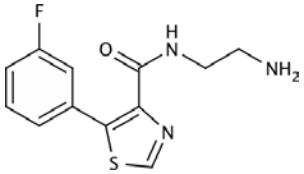
Mol. Formula : $C_{12}H_{12}FN_3OS$ **FW :** 265.31 **HBA:** 5 **HBD:** 2 **RotB:** 4

PubChem ID : **CASRN :** **AlogP:** 1.08 **TPSA:** 96.3

Activity: Radiolabeled MAO inhibitor

Catalog number : R-905

Drug name : Ro 41-1049 hydrochloride



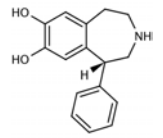
Mol. Formula : $C_{12}H_{13}ClFN_3OS$ **FW :** 301.77 **HBA:** 5 **HBD:** 2 **RotB:** 4

PubChem ID : 5311308 **CASRN :** 127500-84-9 **AlogP:** 1.08 **TPSA:** 96.3

Activity: MAO inhibitor

Catalog number : S-101

Drug name : (*R*)-(+)-SKF-38393 hydrochloride



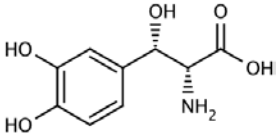
Mol. Formula : $C_{16}H_{18}ClNO_2$ **FW :** 291.78 **HBA:** 3 **HBD:** 3 **RotB:** 1

PubChem ID : 6852375 **CASRN :** 62751-59-1 **AlogP:** 1.86 **TPSA:** 52.5

Activity: Dopamine D_1 receptor agonist; active enantiomer of (±)-SKF-38393

Catalog number : S-501

Drug name : (+)-*threo*-3-(3,4-Dihydroxyphenyl)serine

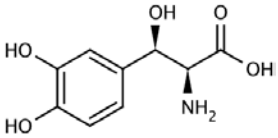


Mol. Formula : $C_9H_{11}NO_5$ **FW :** 213.19 **HBA:** 6 **HBD:** 5 **RotB:** 3

PubChem ID : 443940 **CASRN :** 23651-95-8 **AlogP:** -2.64 **TPSA:** 124.0

Catalog number : S-502

Drug name : (–)-*threo*-3-(3,4-Dihydroxyphenyl)serine

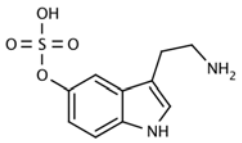


Mol. Formula : $C_9H_{11}NO_5$ **FW :** 213.19 **HBA:** 6 **HBD:** 5 **RotB:** 3

PubChem ID : 164631 **CASRN :** 13147-26-7 **AlogP:** -2.64 **TPSA:** 124.0

Catalog number : S-503

Drug name : Serotonin-*O*-sulfate

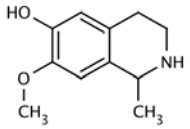


Mol. Formula : $C_{10}H_{12}N_2O_4S$ **FW :** 256.28 **HBA:** 4 **HBD:** 3 **RotB:** 4

PubChem ID : 152151 **CASRN :** 16310-20-6 **AlogP:** -2.01 **TPSA:** 113.8

Catalog number : S-504

Drug name : (±)-Salsoline hydrochloride



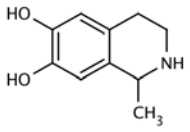
Mol. Formula : $C_{11}H_{16}ClNO_2$ **FW :** 229.71 **HBA:** 3 **HBD:** 2 **RotB:** 1

PubChem ID : 46695 **CASRN :** 89-31-6 **AlogP:** 1.03 **TPSA:** 41.5

Activity: Salsolinol metabolite; endogenous neurotoxin

Catalog number : S-505

Drug name : (±)-Salsolinol hydrochloride



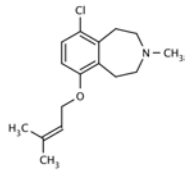
Mol. Formula : $C_{10}H_{14}ClNO_2$ **FW :** 215.69 **HBA:** 3 **HBD:** 3 **RotB:** 0

PubChem ID : 54456 **CASRN :** 525-72-4 **AlogP:** 0.96 **TPSA:** 52.5

Activity: Dopamine neurotoxic derivative

Catalog number : S-701

Drug name : SKF-104078



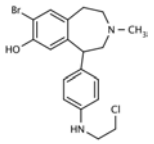
Mol. Formula : $C_{20}H_{26}ClNO_5$ **FW :** 395.88 **HBA:** 3 **HBD:** 0 **RotB:** 3

PubChem ID : 122295 **CASRN :** 110857-22-2 **AlogP:** 3.68 **TPSA:** 12.5

Activity: Adrenergic α2 antagonist

Catalog number : S-703

Drug name : (±)-4'-(2-Chloroethylamino)-SKF-83566 dihydrobromide



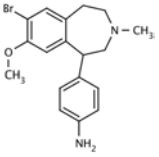
Mol. Formula : $C_{19}H_{24}Br_3ClN_2O$ **FW :** 571.57 **HBA:** 4 **HBD:** 2 **RotB:** 4

PubChem ID : **CASRN :** **AlogP:** 3.90 **TPSA:** 35.5

Activity: Dopamine D_1 receptor alkylating ligand

Catalog number : S-704

Drug name : (±)-4'-Amino-8-*O*-methyl-SKF-83566



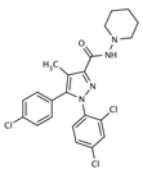
Mol. Formula : $C_{18}H_{21}BrN_2O$ **FW :** 361.08 **HBA:** 3 **HBD:** 1 **RotB:** 2

PubChem ID : **CASRN :** **AlogP:** 3.54 **TPSA:** 38.5

Activity: Dopamine D1 receptor precursor alkylating ligand (antagonist)

Catalog number : S-705

Drug name : SR 141716



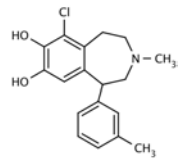
Mol. Formula : $C_{22}H_{21}Cl_3N_4O$ **FW :** 463.80 **HBA:** 6 **HBD:** 1 **RotB:** 4

PubChem ID : 104850 **CASRN :** 158681-13-1 **AlogP:** 5.36 **TPSA:** 50.2

Activity: Cannabinoid CB1 receptor antagonist

Catalog number : S-706

Drug name : SKF-83959 hydrobromide



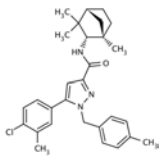
Mol. Formula : $C_{18}H_{21}BrClNO_2$ **FW :** 398.73 **HBA:** 4 **HBD:** 2 **RotB:** 1

PubChem ID : 133538 **CASRN :** 80751-85-5 **AlogP:** 3.36 **TPSA:** 43.7

Activity: Dopamine D_1 receptor agonist

Catalog number : S-801

Drug name : SR 144528



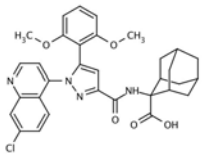
Mol. Formula : $C_{29}H_{34}ClN_3O$ **FW :** 476.06 **HBA:** 3 **HBD:** 1 **RotB:** 5

PubChem ID : 3081355 **CASRN :** 192703-06 -3 **AlogP:** 7.13 **TPSA:** 46.9

Activity: Cannabinoid CB2 receptor antagonist

Catalog number : S-802

Drug name : SR 48692



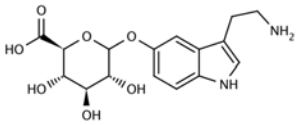
Mol. Formula : $C_{32}H_{31}ClN_4O_5$ **FW :** 587.08 **HBA:** 8 **HBD:** 2 **RotB:** 6

PubChem ID : 119192 **CASRN :** 146362-70-1 **AlogP:** 1.31 **TPSA:** 115.6

Activity: Neurotensin receptor antagonist

Catalog number : S-803

Drug name : Serotonin-*O*-β-D-glucuronide

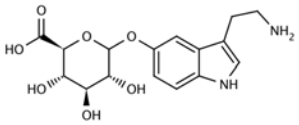


Mol. Formula : $C_{16}H_{20}N_2O_7$ **FW :** 352.34 **HBA:** 8 **HBD:** 6 **RotB:** 5

PubChem ID : **CASRN :** **AlogP:** -6.92 **TPSA:** 158.3

Catalog number : S-803A

Drug name : Serotonin-*O*-β-D-glucuronide trifluoroacetate

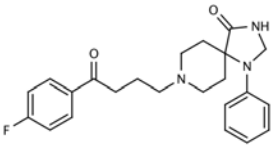


Mol. Formula : $C_{18}H_{21}F_3N_2O_9$ **FW :** 466.36 **HBA:** 8 **HBD:** 6 **RotB:** 5

PubChem ID : **CASRN :** **AlogP:** -6.92 **TPSA:** 158.3

Catalog number : S-901

Drug name : Spiperone



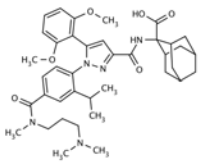
Mol. Formula : $C_{23}H_{26}FN_3O_2$ **FW :** 395.48 **HBA:** 5 **HBD:** 1 **RotB:** 6

PubChem ID : 5265 **CASRN :** 749-02-0 **AlogP:** 3.02 **TPSA:** 52.7

Activity: Dopamine D_2 receptor antagonist; antipsychotic

Catalog number : S-902

Drug name : SR 142948



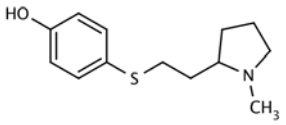
Mol. Formula : $C_{39}H_{52}ClN_5O_6$ **FW :** 722.33 **HBA:** 8 **HBD:** 2 **RotB:** 12

PubChem ID : 5311451 **CASRN :** 184162-64-9 **AlogP:** -2.31 **TPSA:** 126.2

Activity: Neurotensin receptor antagonist

Catalog number : S-903

Drug name : SIB-1553A



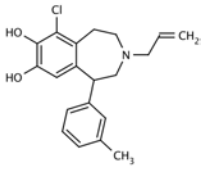
Mol. Formula : $C_{13}H_{20}ClNOS$ **FW :** 273.83 **HBA:** 3 **HBD:** 1 **RotB:** 4

PubChem ID : 9881989 **CASRN :** **AlogP:** 2.29 **TPSA:** 48.8

Activity: Nicotinic acetylcholine receptor agonist; possible cognitive enhancer

Catalog number : S-904

Drug name : SKF-83822 hydrobromide



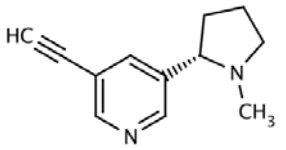
Mol. Formula : $C_{20}H_{23}BrClNO_2$ **FW :** 424.77 **HBA:** 4 **HBD:** 2 **RotB:** 3

PubChem ID : 10020353 **CASRN :** 74115-08-5 **AlogP:** 4.39 **TPSA:** 43.7

Activity: Dopamine D_1 agonist that stimulate adenylyl cyclase

Catalog number : S-905

Drug name : SIB-1508Y



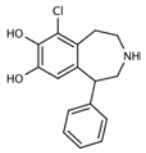
Mol. Formula : $C_{16}H_{18}N_2O_4$ **FW :** 302.33 **HBA:** 2 **HBD:** 0 **RotB:** 2

PubChem ID : 10968648 **CASRN :** 192231-16 -6 **AlogP:** 1.20 **TPSA:** 16.1

Activity: Neuronal nicotinic acetylcholine receptor agonist

Catalog number : S-906

Drug name : SKF-81297 hydrobromide



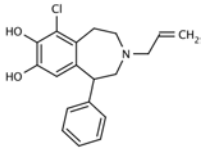
Mol. Formula : $C_{16}H_{17}BrClNO_2$ **FW :** 370.68 **HBA:** 4 **HBD:** 3 **RotB:** 1

PubChem ID : 11957706 **CASRN :** 71636-61-8 **AlogP:** 1.67 **TPSA:** 52.5

Activity: Dopamine D_1 agonist

Catalog number : S-907

Drug name : SKF-82958 hydrobromide



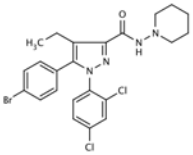
Mol. Formula : $C_{19}H_{21}BrClNO_2$ **FW :** 410.74 **HBA:** 4 **HBD:** 2 **RotB:** 3

PubChem ID : 9909521 **CASRN :** 80751-65-1 **AlogP:** 3.92 **TPSA:** 43.7

Activity: Dopamine D_1 agonist

Catalog number : S-908

Drug name : SR 147778



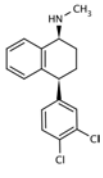
Mol. Formula : $C_{23}H_{22}BrCl_2N_4O$ **FW :** 522.26 **HBA:** 5 **HBD:** 1 **RotB:** 5

PubChem ID : 9849616 **CASRN :** 288104-79-0 **AlogP:** 6.03 **TPSA:** 50.2

Activity: Cannaboid CB_1 antagonist

Catalog number : S-909

Drug name : Sertraline hydrochloride



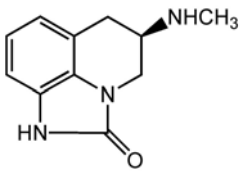
Mol. Formula : $C_{17}H_{18}Cl_3N$ **FW :** 342.69 **HBA:** 3 **HBD:** 1 **RotB:** 2

PubChem ID : 63009 **CASRN :** 79617-96-2 **AlogP:** 5.00 **TPSA:** 12.0

Activity: Serotonin reuptake inhibitor; used to treat depression and OCD

Catalog number : S-910 new

Drug name : Sumanirole maleate



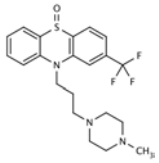
Mol. Formula : $C_{15}H_{17}N_3O_5$ **FW :** 319.30 **HBA:** 4 **HBD:** 2 **RotB:** 1

PubChem ID : 177343 **CASRN :** 179386-43 -7 **AlogP:** 1.08 **TPSA:** 44.4

Activity: Dopamine D2 receptor ligand.

Catalog number : T-501

Drug name : Trifluoperazine-5-oxide

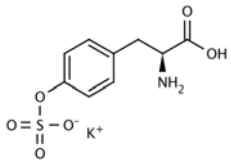


Mol. Formula : $C_{21}H_{24}F_3N_3OS$ **FW :** 423.50 **HBA:** 7 **HBD:** 0 **RotB:** 5

PubChem ID : 159622 **CASRN :** 1549-88-8 **AlogP:** 2.75 **TPSA:** 46.0

Catalog number : T-502

Drug name : (–)-Tyrosine-*O*-sulfate potassium salt

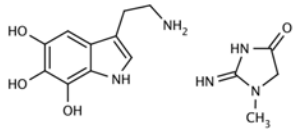


Mol. Formula : $C_9H_{10}NO_6SK$ **FW :** 299.26 **HBA:** 6 **HBD:** 2 **RotB:** 5

PubChem ID : 514186 **CASRN :** **AlogP:** -2.40 **TPSA:** 138.1

Catalog number : T-503

Drug name : 5,6,7-Trihydroxytryptamine creatinine sulfate

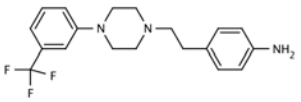


Mol. Formula : $C_{14}H_{21}N_5O_8S$ **FW :** 419.41 **HBA:** 4 **HBD:** 5 **RotB:** 2

PubChem ID : **CASRN :** **AlogP:** -1.19 **TPSA:** 102.5

Catalog number : T-504

Drug name : 1-[2-(4-Aminophenyl)ethyl]-4-(3-trifluoromethylphenyl)piperazine dihydrochloride



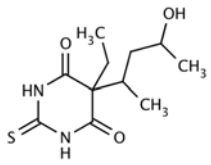
Mol. Formula : $C_{19}H_{24}Cl_2F_3N_3$ **FW :** 422.31 **HBA:** 6 **HBD:** 1 **RotB:** 5

PubChem ID : 121930 **CASRN :** 1814-64-8 **AlogP:** 4.24 **TPSA:** 32.5

Activity: Serotonin 5-HT agonist

Catalog number : T-506

Drug name : 5-Ethyl-5-(1'-methyl-3'-hydroxybutyl)-2-thiobarbituric acid



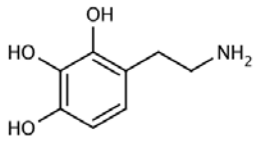
Mol. Formula : $C_{11}H_{18}N_2O_3S$ **FW :** 258.35 **HBA:** 4 **HBD:** 3 **RotB:** 4

PubChem ID : **CASRN :** **AlogP:** 1.17 **TPSA:** 110.5

Activity: Thiopental metabolite

Catalog number : T-507

Drug name : 2,3,4-Trihydroxy-β-phenethylamine hydrochloride



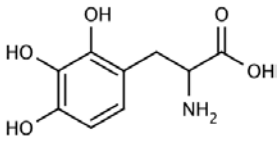
Mol. Formula : $C_8H_{12}ClNO_3$ **FW :** 205.64 **HBA:** 4 **HBD:** 4 **RotB:** 2

PubChem ID : 193386 **CASRN :** 4228-71-1 **AlogP:** -0.34 **TPSA:** 86.7

Activity: Arylsulfatase inhibitor; potential neurotoxin

Catalog number : T-508

Drug name : 2,3,4-Trihydroxy-(±)-phenylalanine



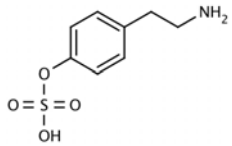
Mol. Formula : $C_9H_{11}NO_5$ **FW :** 213.19 **HBA:** 6 **HBD:** 5 **RotB:** 3

PubChem ID : 22326275 **CASRN :** **AlogP:** -2.00 **TPSA:** 124.0

Activity: Neurotoxic DOPA metabolite

Catalog number : T-509

Drug name : Tyramine-*O*-sulfate

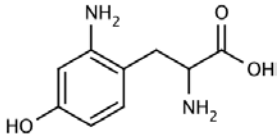


Mol. Formula : $C_8H_{11}NO_4S$ **FW :** 217.25 **HBA:** 4 **HBD:** 2 **RotB:** 4

PubChem ID : 153005 **CASRN :** 30223-92-8 **AlogP:** -2.11 **TPSA:** 98.0

Catalog number : T-510

Drug name : 2-Amino-(±)-Tyrosine

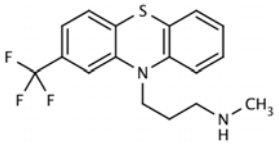


Mol. Formula : $C_9H_{12}N_2O_3$ **FW :** 196.21 **HBA:** 5 **HBD:** 4 **RotB:** 3

PubChem ID : 5134354 **CASRN :** **AlogP:** -2.21 **TPSA:** 109.6

Catalog number : T-511

Drug name : N-Desmethyltriflupromazine hydrochloride

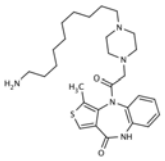


Mol. Formula : $C_{17}H_{18}ClF_3N_2S$ **FW :** 374.84 **HBA:** 6 **HBD:** 1 **RotB:** 5

PubChem ID : 10337209 **CASRN :** **AlogP:** 4.56 **TPSA:** 40.6

Catalog number : T-701

Drug name : Telenzepine Amine Congener (TAC) dihydrobromide



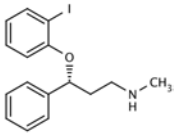
Mol. Formula : $C_{28}H_{43}Br_2N_5O_2S$ **FW :** 673.56 **HBA:** 6 **HBD:** 2 **RotB:** 12

PubChem ID : 9892600 **CASRN :** **AlogP:** 3.20 **TPSA:** 110.2

Activity: Muscarinic m_1 antagonist analog

Catalog number : T-702

Drug name : (*R*)-(–)-*N*-Methyl-3-(2-iodophenoxy)-3-phenylpropanamine hydrochloride



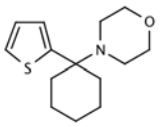
Mol. Formula : $C_{16}H_{19}ClINO$ **FW :** 403.69 **HBA:** 2 **HBD:** 1 **RotB:** 6

PubChem ID : 10021849 **CASRN :** **AlogP:** 4.30 **TPSA:** 21.3

Activity: Norepinephrine transport inhibitor

Catalog number : T-703

Drug name : 1-[1-(2-Thienyl)cyclohexyl]morpholine



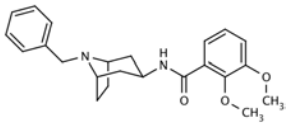
Mol. Formula : $C_{14}H_{21}NOS$ **FW :** 251.39 **HBA:** 3 **HBD:** 0 **RotB:** 2

PubChem ID : 210739 **CASRN :** 21602-66-4 **AlogP:** 2.73 **TPSA:** 40.7

Activity: PCP analog

Catalog number : T-704

Drug name : Tropapride hydrochloride



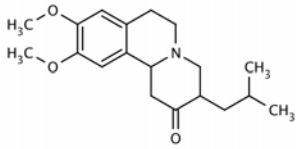
Mol. Formula : $C_{23}H_{29}ClN_2O_3$ **FW :** 416.95 **HBA:** 4 **HBD:** 1 **RotB:** 6

PubChem ID : 3065827 **CASRN :** 109021-66-1 **AlogP:** 2.66 **TPSA:** 50.8

Activity: Dopamine D_2 receptor antagonist

Catalog number : T-801

Drug name : [^{3}H]Tetrabenazine



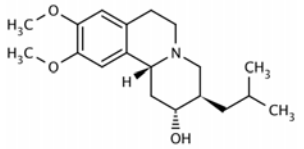
Mol. Formula : $C_{19}H_{27}NO_3$ **FW :** 317.42 **HBA:** 4 **HBD:** 0 **RotB:** 4

PubChem ID : 6018 **CASRN :** 58-46-8 **AlogP:** 3.33 **TPSA:** 38.8

Activity: Radiolabeled adrenergic uptake inhibitor

Catalog number : T-802

Drug name : (+)-α-Dihydrotetrabenazine



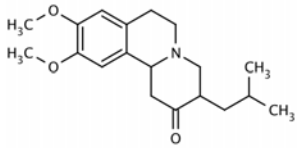
Mol. Formula : $C_{19}H_{29}NO_3$ **FW :** 319.45 **HBA:** 4 **HBD:** 1 **RotB:** 4

PubChem ID : 123836 **CASRN :** 3466-75-9 **AlogP:** 2.36 **TPSA:** 41.9

Activity: Active metabolite of tetrabenazine

Catalog number : T-901

Drug name : (±)-Tetrabenazine



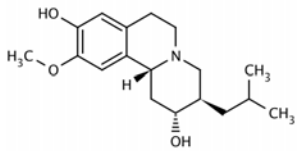
Mol. Formula : $C_{19}H_{27}NO_3$ **FW :** 317.43 **HBA:** 4 **HBD:** 0 **RotB:** 4

PubChem ID : 6018 **CASRN :** 58-46-8 **AlogP:** 3.33 **TPSA:** 38.8

Activity: Adrenergic uptake inhibitor; dopamine depleting agent; antipsychotic;

Catalog number : T-902

Drug name : (+)-(2*R*,3*R*,11b*R*)-9-*O*-Desmethyl-α-dihydrotetrabenazine



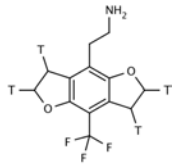
Mol. Formula : $C_{18}H_{27}NO_3$ **FW :** 305.42 **HBA:** 4 **HBD:** 2 **RotB:** 3

PubChem ID : **CASRN :** **AlogP:** 2.21 **TPSA:** 52.9

Activity: DTBZ PET precusor ligand

Catalog number : T-903

Drug name : [^{3}H]-1-(8-Trifluoromethyl-2,3,6,7-tetrahydrobenzo[1,2-b;4,5-b']difuran-4-yl)-2-aminoethane

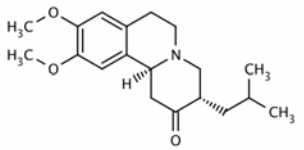


Mol. Formula : $C_{13}H_{14}F_3NO_2$ **FW :** 273.25 **HBA:** 6 **HBD:** 1 **RotB:** 3

PubChem ID : **CASRN :** **AlogP:** 1.76 **TPSA:** 44.5

Catalog number : T-904

Drug name : (–)-Tetrabenazine



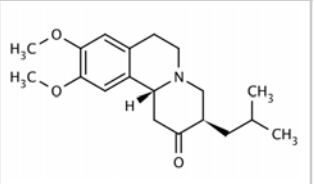
Mol. Formula : $C_{19}H_{27}NO_3$ **FW :** 317.44 **HBA:** 4 **HBD:** 0 **RotB:** 4

PubChem ID : 667453 **CASRN :** **AlogP:** 3.33 **TPSA:** 38.8

Activity: Dopamine depleting agent; optical isomer of tetrabenazine

Catalog number : T-905

Drug name : (+)-Tetrabenazine



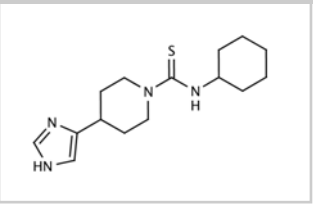
Mol. Formula : $C_{19}H_{27}NO_3$ **FW :** 317.44 **HBA:** 4 **HBD:** 0 **RotB:** 4

PubChem ID : 11634155 **CASRN :** **AlogP:** 3.33 **TPSA:** 38.8

Activity: Dopamine depleting agent; optical isomer of tetrabenazine

Catalog number : T-906

Drug name : Thioperamide maleate



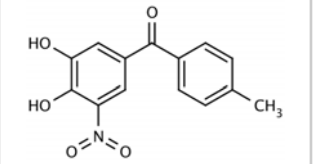
Mol. Formula : $C_{15}H_{24}N_4S$ **FW :** 292.44 **HBA:** 2 **HBD:** 2 **RotB:** 2

PubChem ID : 3035905 **CASRN :** 106243-16-7 **AlogP:** 1.90 **TPSA:** 76.0

Activity: Histamine H_3 antagonist; anticonvulsant

Catalog number : T-907

Drug name : Tolcapone



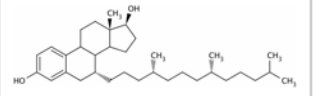
Mol. Formula : $C_{14}H_{11}NO_5$ **FW :** 273.24 **HBA:** 5 **HBD:** 2 **RotB:** 3

PubChem ID : 4659569 **CASRN :** 134308-13-7 **AlogP:** 3.12 **TPSA:** 103.4

Activity: Antiparkinson agent

Catalog number : T-908

Drug name : 7α-[(4*R*,8*R*)-4,8,12-Trimethyltridecyl]estra-1,3,5(10)-trien-3,17β-diol

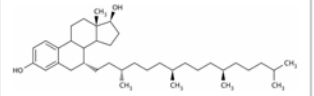


Mol. Formula : $C_{34}H_{56}O_2$ **FW :** 496.81 **HBA:** 2 **HBD:** 2 **RotB:** 12

PubChem ID : **CASRN :** **AlogP:** 9.79 **TPSA:** 40.5

Catalog number : T-909

Drug name : 7α-[(3*R*/*S*,7*R*,11*R*)-3,7,11,15-tetramethylhexadecyl]estra-1,3,5-trien-3,17β-diol

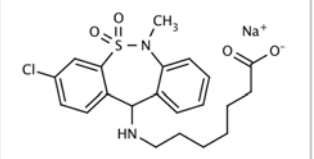


Mol. Formula : $C_{38}H_{64}O_2$ **FW :** 552.91 **HBA:** 2 **HBD:** 2 **RotB:** 15

PubChem ID : **CASRN :** **AlogP:** 11.30 **TPSA:** 40.5

Catalog number : T-910

Drug name : Tianeptine, sodium salt



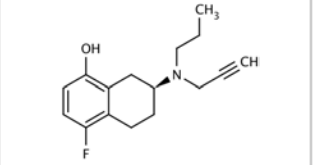
Mol. Formula : $C_{21}H_{24}ClN_2NaO_4S$ **FW :** 458.93 **HBA:** 6 **HBD:** 1 **RotB:** 8

PubChem ID : 23663953 **CASRN :** 30123-17-2 **AlogP:** 0.49 **TPSA:** 97.9

Activity: Serotonin reuptake enhancer

Catalog number : U-703

Drug name : (*S*)-(–)-*N*-Propargyl-UH-301 hydrochloride



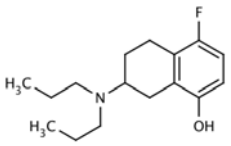
Mol. Formula : $C_{16}H_{21}ClFNO$ **FW :** 297.79 **HBA:** 3 **HBD:** 1 **RotB:** 5

PubChem ID : **CASRN :** **AlogP:** 3.57 **TPSA:** 23.5

Activity: Serotonin 5-HT antagonist radiolabel precursor

Catalog number : U-801

Drug name : Tritiated UH-301



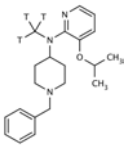
Mol. Formula : $C_{16}H_{24}FNO$ **FW :** 265.37 **HBA:** 3 **HBD:** 1 **RotB:** 5

PubChem ID : 5122 **CASRN :** 127126-21 -0 **AlogP:** 3.08 **TPSA:** 23.5

Activity: Radiolabeled serotonin 5-HT antagonist

Catalog number : U-802

Drug name : Tritiated U-101,958 [N-methyl-^{3}H]



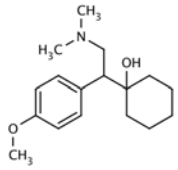
Mol. Formula : $C_{21}H_{29}N_3O$ **FW :** 339.47 **HBA:** 4 **HBD:** 0 **RotB:** 6

PubChem ID : 5615 **CASRN :** **AlogP:** 3.95 **TPSA:** 28.6

Activity: Radiolabled dopamine D_4 antagonist

Catalog number : V-901

Drug name : Venlafaxine



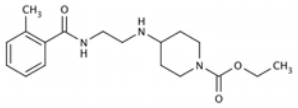
Mol. Formula : $C_{17}H_{27}NO_2$ **FW :** 277.41 **HBA:** 3 **HBD:** 1 **RotB:** 5

PubChem ID : 5656 **CASRN :** 99300-78-4 **AlogP:** 2.25 **TPSA:** 32.7

Activity: Serotonin and norepinephrine reuptake inhibitor; antidepressant

Catalog number : V-902 new

Drug name : VU0357017 hydrochloride



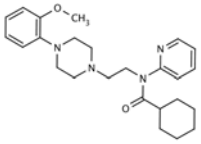
Mol. Formula : $C_{18}H_{28}ClN_3O_3$ **FW :** 369.89 **HBA:** 6 **HBD:** 2 **RotB:** 7

PubChem ID : 25010775 **CASRN :** **AlogP:** 1.61 **TPSA:** 70.7

Activity: Allosteric modulator of the M1 muscarinic receptor.

Catalog number : W-108

Drug name : WAY-100635 maleate



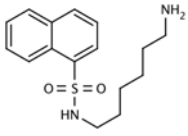
Mol. Formula : $C_{29}H_{38}N_4O_6$ **FW :** 538.65 **HBA:** 5 **HBD:** 0 **RotB:** 7

PubChem ID : 11957721 **CASRN :** 634908-75-1 **AlogP:** 4.09 **TPSA:** 48.9

Activity: Serotonin 5-HT receptor antagonist

Catalog number : W-501

Drug name : N-(6-Aminohexyl)-1-napthalenesulfonamide hydrochloride



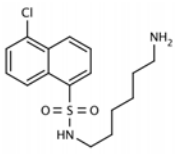
Mol. Formula : $C_{16}H_{23}ClN_2O_2S$ **FW :** 342.89 **HBA:** 3 **HBD:** 2 **RotB:** 7

PubChem ID : 4314 **CASRN :** 79458-81-4 **AlogP:** 1.55 **TPSA:** 80.6

Activity: Calmodulin antagonist

Catalog number : W-502

Drug name : N-(6-Aminohexyl)-5-chloro-1-napthalenesulfonamide hydrochloride



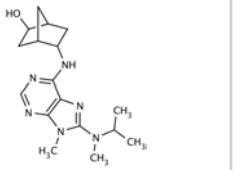
Mol. Formula : $C_{16}H_{22}Cl_2N_2O_2S$ **FW :** 377.33 **HBA:** 4 **HBD:** 2 **RotB:** 7

PubChem ID : 5681 **CASRN :** 65595-90-6 **AlogP:** 2.06 **TPSA:** 80.6

Activity: Calmodulin antagonist

Catalog number : W-801

Drug name : WRC-0571



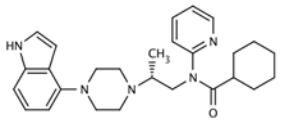
Mol. Formula : $C_{17}H_{26}N_6O$ **FW :** 330.44 **HBA:** 6 **HBD:** 2 **RotB:** 4

PubChem ID : 9902054 **CASRN :** **AlogP:** 2.12 **TPSA:** 79.1

Activity: Adenosine A_1 receptor antagonist

Catalog number : W-901

Drug name : WAY 405



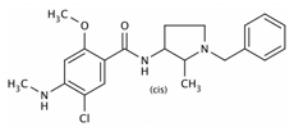
Mol. Formula : $C_{27}H_{37}Cl_2N_5O$ **FW :** 518.53 **HBA:** 4 **HBD:** 1 **RotB:** 6

PubChem ID : **CASRN :** **AlogP:** 4.85 **TPSA:** 55.5

Activity: Serotonin 5-HT_{1A} receptor antagonist

Catalog number : Y-701

Drug name : (±)-YM-09151-2; Nemonapride



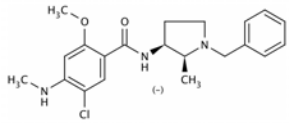
Mol. Formula : $C_{21}H_{26}ClN_3O_2$ **FW :** 387.91 **HBA:** 5 **HBD:** 2 **RotB:** 6

PubChem ID : 4452 **CASRN :** 75272-39-8 **AlogP:** 2.90 **TPSA:** 53.6

Activity: Dopamine D_2 receptor antagonist; antipsychotic

Catalog number : Y-702

Drug name : (–)-YM-09151-2



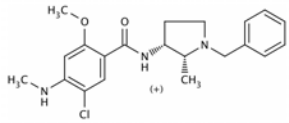
Mol. Formula : $C_{21}H_{26}ClN_3O_2$ **FW :** 387.91 **HBA:** 5 **HBD:** 2 **RotB:** 6

PubChem ID : 156333 **CASRN :** 70325-83-6 **AlogP:** 2.90 **TPSA:** 53.6

Activity: Inactive stereoisomer of YM-09151-2

Catalog number : Y-703

Drug name : (+)-YM-09151-2



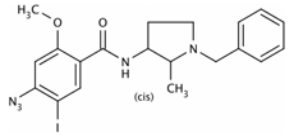
Mol. Formula : $C_{21}H_{26}ClN_3O_2$ **FW :** 387.91 **HBA:** 5 **HBD:** 2 **RotB:** 6

PubChem ID : 9952220 **CASRN :** 70325-83-6 **AlogP:** 2.90 **TPSA:** 53.6

Activity: Dopamine D_2 receptor agonist; active stereoisomer of YM-09151-2

Catalog number : Y-704

Drug name : (±)-*cis*-*N*-(1-Benzyl-2-methylpyrrolidin-3-yl)-4-azido-5-iodo-2-methoxybenzamide hydrochloride



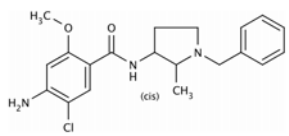
Mol. Formula : $C_{20}H_{23}ClIN_5O_2$ **FW :** 527.79 **HBA:** 5 **HBD:** 1 **RotB:** 6

PubChem ID : **CASRN :** **AlogP:** -0.54 **TPSA:** 71.0

Activity: Dopamine D_2 receptor photoaffinity ligand

Catalog number : Y-705

Drug name : (±)-*cis*-*N*-(1-Benzyl-2-methylpyrrolidin-3-yl)-4-amino-2-methoxybenzamide



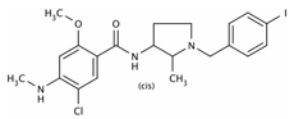
Mol. Formula : $C_{20}H_{25}N_3O_2$ **FW :** 339.44 **HBA:** 4 **HBD:** 2 **RotB:** 5

PubChem ID : **CASRN :** **AlogP:** 2.02 **TPSA:** 67.6

Activity: Dopamine D_2 receptor photoaffinity ligand precursor

Catalog number : Y-706

Drug name : (±)-*cis*-*N*-[1-(4'-Iodobenzyl)-2-methylpyrrolidin-3-yl]-5-chloro-2-methoxy-4-(methylamino)benzamide



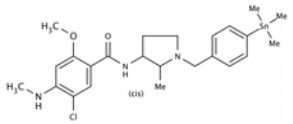
Mol. Formula : $C_{21}H_{25}ClIN_3O_2$ **FW :** 513.81 **HBA:** 5 **HBD:** 2 **RotB:** 6

PubChem ID : **CASRN :** **AlogP:** 3.89 **TPSA:** 53.6

Activity: Potential high affinity probe for dopamine D_2 receptors

Catalog number : Y-707

Drug name : (±)-*cis*-*N*-[1-(4'-Trimethylstannylbenzyl)-2-methylpyrrolidin-3-yl]-5-chloro-2-methoxy-4-(methylamino)benzamide



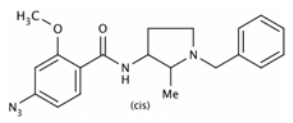
Mol. Formula : $C_{24}H_{34}ClN_3O_2Sn$ **FW :** 550.72 **HBA:** 5 **HBD:** 2 **RotB:** 7

PubChem ID : **CASRN :** **AlogP:** 2.68 **TPSA:** 53.6

Activity: 4'-Iodo-YM-09151-02 radioiodination precursor

Catalog number : Y-708

Drug name : (±)-*cis*-*N*-(1-Benzyl-2-methylpyrrolidin-3-yl)-4-azido-2-methoxybenzamide hydrochloride



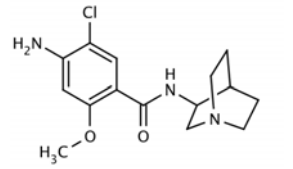
Mol. Formula : $C_{20}H_{24}ClN_5O_2$ **FW :** 401.90 **HBA:** 5 **HBD:** 1 **RotB:** 6

PubChem ID : **CASRN :** **AlogP:** -1.55 **TPSA:** 71.0

Activity: Reference standard for YM-09151-2 analogs

Catalog number : Z-901

Drug name : (±)-Zacopride hydrochloride



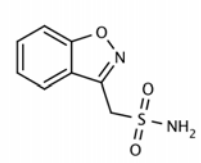
Mol. Formula : $C_{15}H_{21}Cl_2N_3O_2$ **FW :** 346.26 **HBA:** 5 **HBD:** 2 **RotB:** 3

PubChem ID : 108182 **CASRN :** 90182-92-6 **AlogP:** 0.72 **TPSA:** 67.6

Activity: Serotonin 5-HT_3 receptor antagonist; 5-HT_4 receptor agonist

Catalog number : Z-902

Drug name : Zonisamide



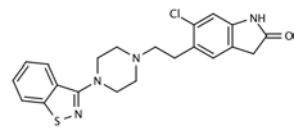
Mol. Formula : $C_8H_8N_2O_3S$ **FW :** 212.23 **HBA:** 3 **HBD:** 1 **RotB:** 2

PubChem ID : 5734 **CASRN :** 68291-97-4 **AlogP:** 0.52 **TPSA:** 94.6

Activity: Anticonvulsant; antioxidant

Catalog number : Z-903

Drug name : Ziprasidone hydrochloride



Mol. Formula : $C_{21}H_{22}Cl_2N_4OS$ **FW :** 449.40 **HBA:** 6 **HBD:** 1 **RotB:** 4

PubChem ID : 219099 **CASRN :** 122883-93-6 **AlogP:** 4.19 **TPSA:** 76.7

Activity: Atypical antipsychotic

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Visit the NIMH CSDSP website at www.nimh-repository.rti.org to obtain a complete description of the terms and conditions associated with receiving compounds from the NIMH CSDSP.

Publications

The NIMH would like to be apprised of publications resulting from the use of the compounds supplied through the NIMH CSDSP. If you have used compounds from the program in your research, indicate that the compounds were obtained from the NIMH CSDSP in the Materials and Methods section of your publication and send reprints to Jamie Driscoll (NIMH).

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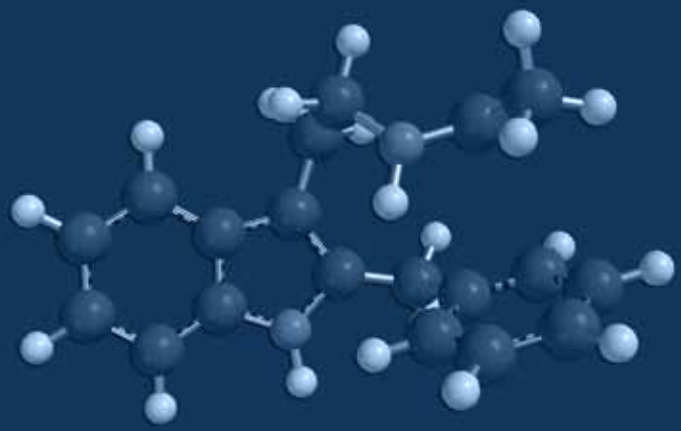

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