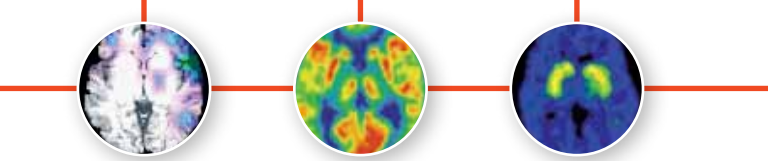
NIMH Chemical Synthesis and Drug Supply Program

Compound Catalog

October 2011

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

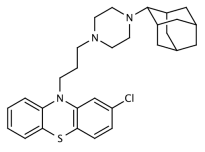
AlogP - Ghose-Crippen octanol-water partition coefficient
(Viswanadhan, V.N., Ghose, A.K., Revankar, G.R. & Robins, R.K. *J. Chem. Inf. Comput. Sci.*, **1989**, *29*, 163-172.)

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.

NIMH Code : A-502A

Compound name : Adapiprazine dihydrochloride



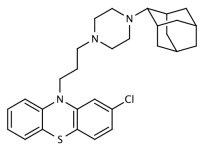
Mol. Formula : $C_{29}H_{38}Cl_3N_3S$ **FW :** 567.07 **HBA:** 5 **HBD:** 0 **RotB:** 5

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

Activity: Dopamine antagonist

NIMH Code : A-502B

Compound name : Adapiprazine



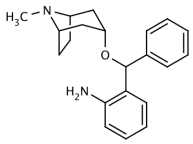
Mol. Formula : $C_{29}H_{36}ClN_3S$ **FW :** 494.13 **HBA:** 5 **HBD:** 0 **RotB:** 5

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

Activity: Dopamine antagonist

NIMH Code : A-503

Compound name : Aminobenztropine



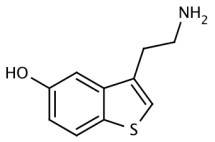
Mol. Formula : $C_{21}H_{26}N_2O$ **FW :** 322.45 **HBA:** 3 **HBD:** 1 **RotB:** 4

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

Activity: Muscarinic m_1 ligand

NIMH Code : A-504

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



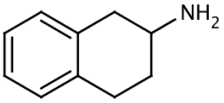
Mol. Formula : $C_{10}H_{11}NOS$ **FW :** 193.27 **HBA:** 3 **HBD:** 2 **RotB:** 2

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

Activity: Serotonin 5-HT_{1E} ligand

NIMH Code : A-505

Compound name : 2-Aminotetralin hydrochloride



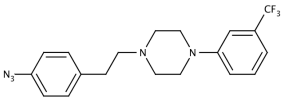
Mol. Formula : $C_{10}H_{14}ClN$ **FW :** 183.68 **HBA:** 1 **HBD:** 1 **RotB:** 0

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

Activity: Serotonin 5-HT_1 ligand

NIMH Code : A-506

Compound name : p-Azido-PE-TFMPP hydrochloride



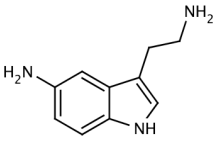
Mol. Formula : $C_{19}H_{21}ClF_3N_5$ **FW :** 411.86 **HBA:** 7 **HBD:** 0 **RotB:** 6

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

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

NIMH Code : A-507

Compound name : 5-Aminotryptamine dipicrate



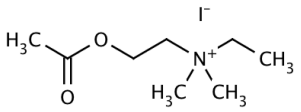
Mol. Formula : $C_{22}H_{19}N_9O_{14}$ **FW :** 633.44 **HBA:** 2 **HBD:** 3 **RotB:** 2

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

Activity: Serotonin 5-HT agonist

NIMH Code : A-508

Compound name : Acetoxyethyldimethylethylammonium iodide

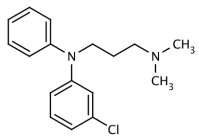


Mol. Formula : $C_8H_{18}INO_2$ **FW :** 287.14 **HBA:** 1 **HBD:** 0 **RotB:** 5

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

NIMH Code : A-509

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

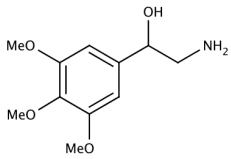


Mol. Formula : $C_{17}H_{22}Cl_2N_2$ **FW :** 325.28 **HBA:** 3 **HBD:** 0 **RotB:** 6

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

NIMH Code : A-510

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

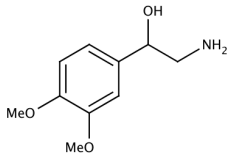


Mol. Formula : $C_{11}H_{17}NO_4$ **FW :** 227.26 **HBA:** 5 **HBD:** 2 **RotB:** 5

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

NIMH Code : A-511

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

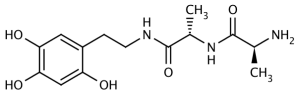


Mol. Formula : $C_{10}H_{16}ClNO_3$ **FW :** 233.70 **HBA:** 4 **HBD:** 2 **RotB:** 4

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

NIMH Code : A-512

Compound name : Alanylalanyl-6-hydroxydopamine hydrochloride

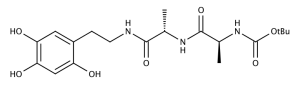


Mol. Formula : $C_{14}H_{22}ClN_3O_6$ **FW :** 347.80 **HBA:** 6 **HBD:** 6 **RotB:** 6

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

NIMH Code : A-513

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

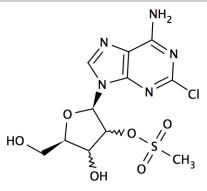


Mol. Formula : $C_{19}H_{29}N_3O_7$ **FW :** 411.46 **HBA:** 7 **HBD:** 6 **RotB:** 9

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

NIMH Code : A-514

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

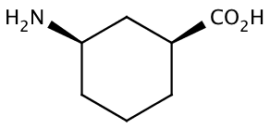


Mol. Formula : $C_{11}H_{14}ClN_5O_6S$ **FW :** 379.78 **HBA:** 10 **HBD:** 3 **RotB:** 4

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

NIMH Code : A-701

Compound name : *cis*-3-Aminocyclohexanecarboxylic acid



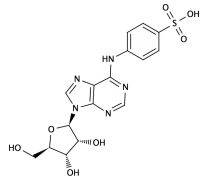
Mol. Formula : $C_7H_{13}NO_2$ **FW :** 143.19 **HBA:** 3 **HBD:** 2 **RotB:** 1

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

Activity: Neuronal GABA uptake inhibitor

NIMH Code : A-702

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



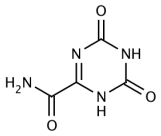
Mol. Formula : $C_{22}H_{32}N_6O_7S$ **FW :** 524.60 **HBA:** 11 **HBD:** 5 **RotB:** 5

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

Activity: Water-soluble Adenosine A_1 agonist

NIMH Code : A-703

Compound name : Allantoxanamide



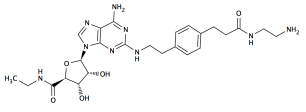
Mol. Formula : $C_4H_4N_4O_3$ **FW :** 156.10 **HBA:** 4 **HBD:** 3 **RotB:** 1

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

Activity: Uricase inhibitor

NIMH Code : A-704

Compound name : APEC trifluoroacetate



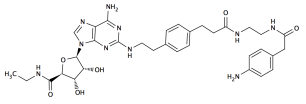
Mol. Formula : $C_{29}H_{37}F_6N_9O_9$ **FW :** 769.66 **HBA:** 11 **HBD:** 7 **RotB:** 12

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

Activity: Adenosine A_2 receptor ligand

NIMH Code : A-705

Compound name : p-Aminophenylacetyl-APEC



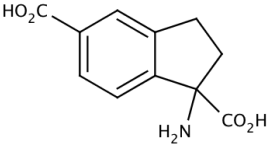
Mol. Formula : $C_{33}H_{42}N_{10}O_6$ **FW :** 674.76 **HBA:** 12 **HBD:** 8 **RotB:** 15

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

Activity: Functionalized adenosine A_2 ligand

NIMH Code : A-801

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



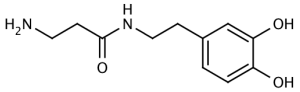
Mol. Formula : $C_{11}H_{11}NO_4$ **FW :** 221.21 **HBA:** 5 **HBD:** 3 **RotB:** 2

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

Activity: Metabotropic glutamate $mGluR_1$ antagonist

NIMH Code : A-802

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



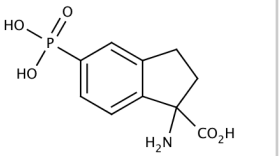
Mol. Formula : $C_{12}H_{18}N_2O_5$ **FW :** 270.29 **HBA:** 4 **HBD:** 4 **RotB:** 5

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

Activity: Sclerotin precursor

NIMH Code : A-803

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



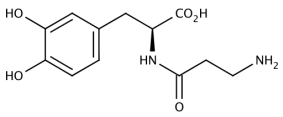
Mol. Formula : $C_{10}H_{12}NO_5P$ **FW :** 257.18 **HBA:** 6 **HBD:** 4 **RotB:** 2

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

Activity: Metabotropic glutamate $mGluR_2$ ligand

NIMH Code : A-804

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

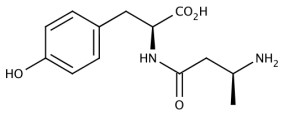


Mol. Formula : $C_{14}H_{17}F_3N_2O_7$ **FW :** 382.29 **HBA:** 6 **HBD:** 5 **RotB:** 6

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

NIMH Code : A-805

Compound name : Sarcophagine trifluoroacetate; Alanyltyrosine trifluoroacetate

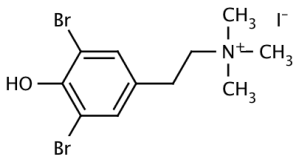


Mol. Formula : $C_{14}H_{17}F_3N_2O_6$ **FW :** 366.29 **HBA:** 5 **HBD:** 4 **RotB:** 6

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

NIMH Code : A-806

Compound name : Autonomium iodide

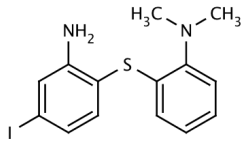


Mol. Formula : $C_{11}H_{16}Br_2INO$ **FW :** 464.97 **HBA:** 1 **HBD:** 1 **RotB:** 3

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

NIMH Code : A-807

Compound name : ADAM



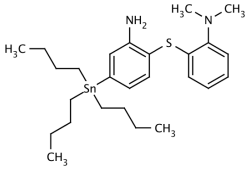
Mol. Formula : $C_{15}H_{17}IN_2S$ **FW :** 384.28 **HBA:** 3 **HBD:** 1 **RotB:** 3

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

Activity: Serotonin 5-HT transporter ligand

NIMH Code : A-808

Compound name : Tributylstannyl-ADAM



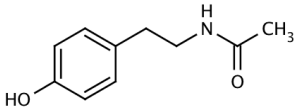
Mol. Formula : $C_{27}H_{44}N_2SSn$ **FW :** 547.42 **HBA:** 3 **HBD:** 1 **RotB:** 13

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

Activity: Radioiodinated ADAM precusor

NIMH Code : A-901

Compound name : N-Acetyltyramine

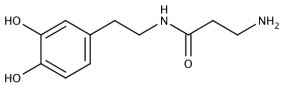


Mol. Formula : $C_{10}H_{13}NO_2$ **FW :** 179.22 **HBA:** 2 **HBD:** 2 **RotB:** 3

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

NIMH Code : A-902

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



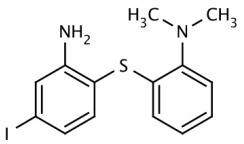
Mol. Formula : $C_{11}H_{17}ClN_2O_3$ **FW :** 260.72 **HBA:** 4 **HBD:** 4 **RotB:** 5

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

Activity: Sclerotin precursor

NIMH Code : A-903

Compound name : ADAM dihydrochloride



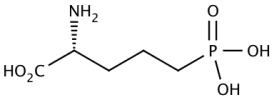
Mol. Formula : $C_{15}H_{19}Cl_2IN_2S$ **FW :** 457.20 **HBA:** 3 **HBD:** 1 **RotB:** 3

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

Activity: Serotonin 5-HT transporter ligand

NIMH Code : A-904

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



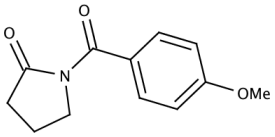
Mol. Formula : $C_5H_{12}NO_5P$ **FW :** 197.13 **HBA:** 6 **HBD:** 4 **RotB:** 5

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

Activity: NMDA antagonist

NIMH Code : A-905

Compound name : Aniracetam



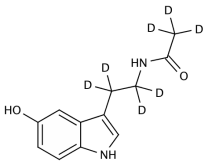
Mol. Formula : $C_{12}H_{13}NO_3$ **FW :** 219.24 **HBA:** 3 **HBD:** 0 **RotB:** 2

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

Activity: D_2/D_3, nACh, & 5-HT_{2A} ligand

NIMH Code : A-906

Compound name : d_7-*N*-Acetylserotonin



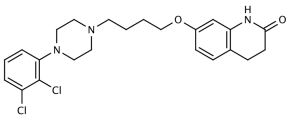
Mol. Formula : $C_{12}H_7D_7N_2O_2$. **FW :** 225.29 **HBA:** 2 **HBD:** 3 **RotB:** 3

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

Activity: Stable isotope labeled melatonin MT_1, MT_2, and MT_3 agonist

NIMH Code : A-907

Compound name : Aripiprazole



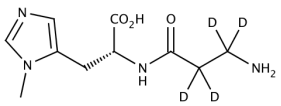
Mol. Formula : $C_{23}H_{27}Cl_2N_3O_2$ **FW :** 448.39 **HBA:** 6 **HBD:** 1 **RotB:** 7

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

Activity: Dopamine D_2 & serotonin 5HT_{1A} partial agonist

NIMH Code : A-908

Compound name : Anserine-d_4



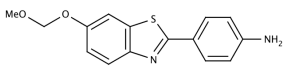
Mol. Formula : $C_{10}H_{12}D_4N_4O_3$ **FW :** 244.28 **HBA:** 5 **HBD:** 3 **RotB:** 6

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

Activity: Stable isotope labeled anserine

NIMH Code : A-909

Compound name : 6-MOMO-BTA-0



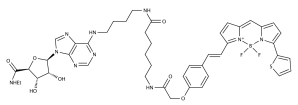
Mol. Formula : $C_{15}H_{14}N_2O_2S$ **FW :** 286.35 **HBA:** 5 **HBD:** 1 **RotB:** 4

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

Activity: β-Amyloid plaque PET imaging agent precusor

NIMH Code : A-910

Compound name : ABEA-X-BY630



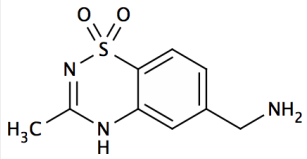
Mol. Formula : $C_{45}H_{51}BF_2N_{10}O_7S$ **FW :** 924.82 **HBA:** 14 **HBD:** 6 **RotB:** 21

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

Activity: Fluorescent adenosine A_3 agonist

NIMH Code : A-911

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



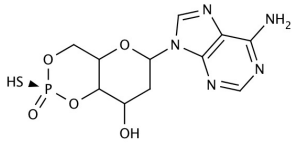
Mol. Formula : $C_9H_{12}ClN_3O_2S$ **FW :** 261.73 **HBA:** 5 **HBD:** 2 **RotB:** 1

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

Activity: Taurine antagonist

NIMH Code : A-912

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



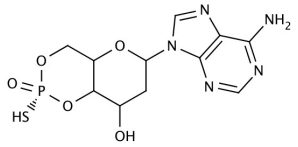
Mol. Formula : $C_{16}H_{27}N_6O_5PS$ **FW :** 446.46 **HBA:** 11 **HBD:** 3 **RotB:** 5

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

Activity: Protein kinase A agonist

NIMH Code : A-913

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



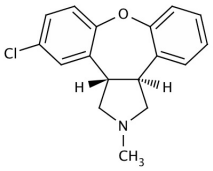
Mol. Formula : $C_{16}H_{27}N_6O_5PS$ **FW :** 446.46 **HBA:** 11 **HBD:** 3 **RotB:** 5

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

Activity: Protein kinase A inhibitor

NIMH Code : A-914

Compound name : Asenapine maleate



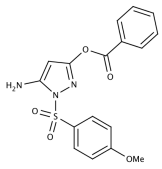
Mol. Formula : $C_{21}H_{20}ClNO_5$ **FW :** 401.84 **HBA:** 2 **HBD:** 0 **RotB:** 0

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

Activity: Serotonergic, dopaminergic, & adrenergic partial agonist

NIMH Code : A-915 new

Compound name : [5-Amino-1-(4-methoxyphenyl)sulfonylpyrazol-3-yl]benzoate



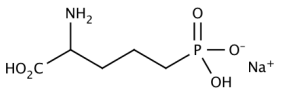
Mol. Formula : $C_{17}H_{15}N_3O_5S$ **FW :** 373.38 **HBA:** 6 **HBD:** 1 **RotB:** 5

PubChem ID : **CASRN :** **AlogP:** 2.57 **TPSA:** 113.5

Activity: NS3 West Nile virus protease inhibitor

NIMH Code : A-916 new

Compound name : (±)-2-Amino-5-phosphonopentanoic acid sodium salt

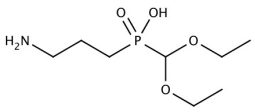


Mol. Formula : $C_5H_{11}NNaO_5P$ **FW :** **HBA:** 6 **HBD:** 4 **RotB:** 5

PubChem ID : **CASRN :** **AlogP:** -3.23 **TPSA:** 120.9

NIMH Code : A-917 new

Compound name : (3-Aminopropyl)(diethoxymethyl)phosphinic acid; CGP 35348



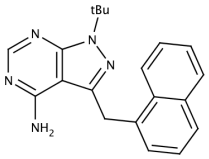
Mol. Formula : $C_8H_{20}NO_4P$ **FW :** 225.22 **HBA:** 5 **HBD:** 2 **RotB:** 8

PubChem ID : 107699 **CASRN :** 123690-79-9 **AlogP:** -1.29 **TPSA:** 81.8

Activity: $GABA_B$ receptor antagonist

NIMH Code : A-918 new

Compound name : 4-Amino-1-tert-butyl-3-(1'-naphthylmethyl)pyrazolo[3,4-d]pyrimidine; 1-NM-PP1



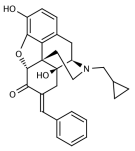
Mol. Formula : $C_{20}H_{21}N_5$ **FW :** 331.41 **HBA:** 4 **HBD:** 1 **RotB:** 3

PubChem ID : **CASRN :** 221244-14-0 **AlogP:** 3.64 **TPSA:** 69.6

Activity: CDK inhibitor

NIMH Code : B-139

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



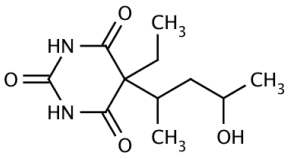
Mol. Formula : $C_{27}H_{28}ClNO_4$ **FW :** 465.97 **HBA:** 5 **HBD:** 2 **RotB:** 3

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

Activity: Delta opioid δ1 antagonist

NIMH Code : B-501

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



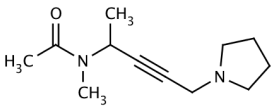
Mol. Formula : $C_{11}H_{18}N_2O_4$ **FW :** 242.28 **HBA:** 4 **HBD:** 3 **RotB:** 4

PubChem ID : 94288 **CASRN :** 4241-40-1 **AlogP:** 0.43 **TPSA:** 95.5

Activity: Pentobarbitol metabolite

NIMH Code : B-504

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



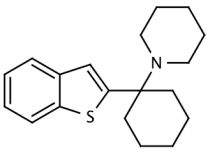
Mol. Formula : $C_{14}H_{22}N_2O_5$ **FW :** 298.33 **HBA:** 2 **HBD:** 0 **RotB:** 4

PubChem ID : 55005 **CASRN :** 83481-69-0 **AlogP:** 0.48 **TPSA:** 23.6

Activity: Muscarinic partial agonist (oxotremorine analog)

NIMH Code : B-701

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



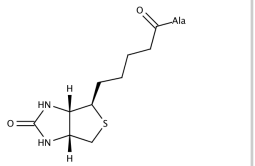
Mol. Formula : $C_{19}H_{26}ClNS$ **FW :** 335.94 **HBA:** 2 **HBD:** 0 **RotB:** 2

PubChem ID : 123692 **CASRN :** 112726-66-6 **AlogP:** 4.88 **TPSA:** 31.5

Activity: Dopamine uptake inhibitor with little affinity for PCP sites

NIMH Code : B-702

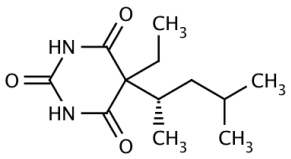
Compound name : Biotin-poly-DL-alanine



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

NIMH Code : B-704

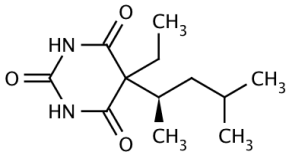
Compound name : (*S*)-(–)-5-(1,3-Dimethylbutyl)-5-ethylbarbituric acid; Diberal



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	

NIMH Code : B-705

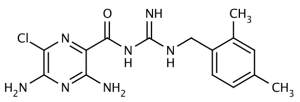
Compound name : (*R*)-(+)-5-(1,3-Dimethylbutyl)-5-ethylbarbituric acid; Diberal



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	

NIMH Code : B-709

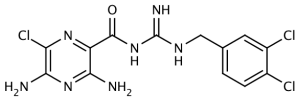
Compound name : 2',4'-Dimethylbenzamil hydrochloride



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 inhibitor					

NIMH Code : B-710

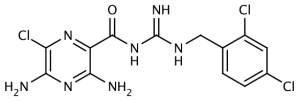
Compound name : 3',4'-Dichlorobenzamil hydrochloride



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					

NIMH Code : B-711

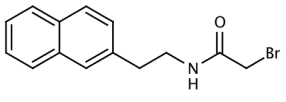
Compound name : 2',4'-Dichlorobenzamil hydrochloride



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					

NIMH Code : B-801

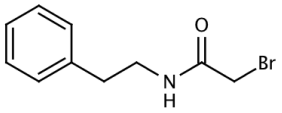
Compound name : N-Bromoacetylnapthalene-2-ethylamine



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	

NIMH Code : B-802

Compound name : N-Bromoacetyl-β-phenethylamine

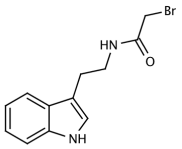


Mol. Formula : $C_{10}H_{12}BrNO$ **FW :** 242.12 **HBA:** 1 **HBD:** 1 **RotB:** 4

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

NIMH Code : B-803

Compound name : N-Bromoacetyltryptamine



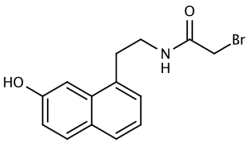
Mol. Formula : $C_{12}H_{13}BrN_2O$ **FW :** 281.16 **HBA:** 1 **HBD:** 2 **RotB:** 4

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

Activity: Reversible inhibitor of melatonin secretion in the pineal gland

NIMH Code : B-804

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

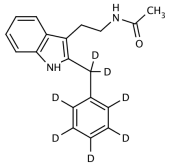


Mol. Formula : $C_{14}H_{14}BrNO_2$ **FW :** 308.18 **HBA:** 2 **HBD:** 2 **RotB:** 4

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

NIMH Code : B-805

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



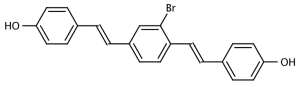
Mol. Formula : $C_{19}H_{13}D_7N_2O$ **FW :** 299.42 **HBA:** 1 **HBD:** 2 **RotB:** 5

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

Activity: Stable isotope labeled melatonin receptor antagonist luzindole

NIMH Code : B-806

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

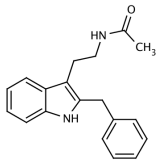


Mol. Formula : $C_{22}H_{17}BrO_2$ **FW :** 393.28 **HBA:** 2 **HBD:** 2 **RotB:** 4

PubChem ID : **CASRN :** **AlogP:** 7.70 **TPSA:** 40.5

NIMH Code : B-807

Compound name : Luzindole



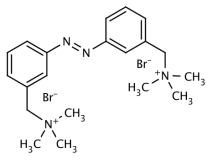
Mol. Formula : $C_{19}H_{20}N_2O$ **FW :** 292.38 **HBA:** 1 **HBD:** 2 **RotB:** 5

PubChem ID : 122162 **CASRN :** 117946-91-5 **AlogP:** 3.04 **TPSA:** 44.9

Activity: Melatonin receptor antagonist

NIMH Code : B-901

Compound name : *trans*-Bis-Q



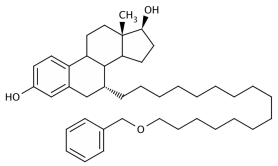
Mol. Formula : $C_{20}H_{30}Br_2N_4$ **FW :** 486.29 **HBA:** 2 **HBD:** 0 **RotB:** 6

PubChem ID : 133795 **CASRN :** 81931-05-7 **AlogP:** -5.03 **TPSA:** 24.7

Activity: Photochromic acetylcholine receptor activator

NIMH Code : B-902

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

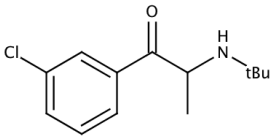


Mol. Formula : $C_{41}H_{62}O_3$ **FW :** 602.94 **HBA:** 3 **HBD:** 2 **RotB:** 21

PubChem ID : **CASRN :** **AlogP:** 11.68 **TPSA:** 49.7

NIMH Code : B-903

Compound name : Bupropion hydrochloride



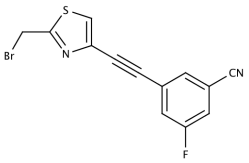
Mol. Formula : $C_{13}H_{19}Cl_2NO$ **FW :** 276.21 **HBA:** 3 **HBD:** 1 **RotB:** 4

PubChem ID : 62884 **CASRN :** 34841-36-6 **AlogP:** 2.75 **TPSA:** 29.1

Activity: Dopamine & norepinephrine reuptake inhibitor

NIMH Code : B-904

Compound 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: Metabotropic gluatamate $mGluR_5$ PET imaging ligand precursor

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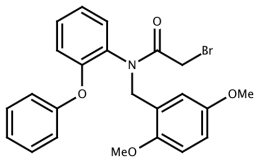
NIMH Code : B-905

Compound 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

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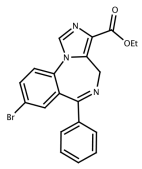
NIMH Code : B-906

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

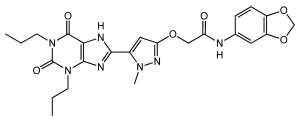


Mol. Formula : $C_{20}H_{16}BrN_3O_2$ **FW :** 410.26 **HBA:** 3 **HBD:** 0 **RotB:** 4

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

NIMH Code : B-907

Compound name : MRE 2029-F20



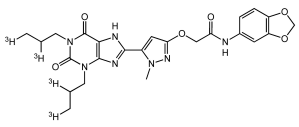
Mol. Formula : $C_{24}H_{27}N_7O_6$ **FW :** 509.52 **HBA:** 8 **HBD:** 2 **RotB:** 9

PubChem ID : **CASRN :** **AlogP:** 2.33 **TPSA:** 143.9

Activity: A_{2B} adenosine receptor antagonist

NIMH Code : B-908

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



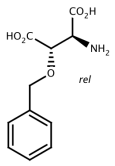
Mol. Formula : $C_{24}H_{27}N_7O_6$ **FW :** 509.51 **HBA:** 8 **HBD:** 2 **RotB:** 9

PubChem ID : **CASRN :** **AlogP:** 2.33 **TPSA:** 143.9

Activity: A_{2B} adenosine receptor radioligand

NIMH Code : B-909

Compound name : DL-TBOA



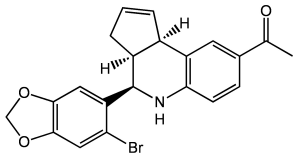
Mol. Formula : $C_{11}H_{13}NO_5$ **FW :** 239.23 **HBA:** 6 **HBD:** 4 **RotB:** 7

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

Activity: Glutamate uptake inhibitor.

NIMH Code : B-910 new

Compound name : 1-[4-(6-Bromo-benzo[1,3]dioxol-5-yl)-3a,4,5,9b-tetrahydro-3*H*-cyclopenta[c] quinolin-8-yl]-ethanone



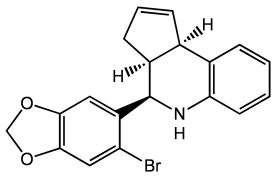
Mol. Formula : $C_{21}H_{18}BrNO_3$ **FW :** 412.28 **HBA:** 4 **HBD:** 1 **RotB:** 2

PubChem ID : **CASRN :** **AlogP:** 3.94 **TPSA:** 47.6

Activity: GPR30 agonist

NIMH Code : B-911 new

Compound name : 4-(6-Bromo-benzo[1,3]dioxol-5-yl)-3a,4,5,9b-tetrahydro-3*H*-cyclopenta[c] quinoline



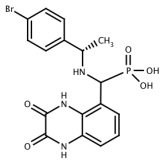
Mol. Formula : $C_{19}H_{16}BrNO_2$ **FW :** 370.24 **HBA:** 3 **HBD:** 1 **RotB:** 1

PubChem ID : **CASRN :** **AlogP:** 4.38 **TPSA:** 30.5

Activity: GPR30 antagonist

NIMH Code : B-912 new

Compound name : {(*R,S*)-[(*S*)-1-(4-Bromophenyl)ethylamino](2,3-dioxo-1,2,3,4-tetrahydroquinoxalin-5-yl)methyl}phosphonic acid HCl (PEAQX HCl)



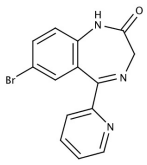
Mol. Formula : $C_{17}H_{18}BrClN_3O_5P$ **FW :** 490.67 **HBA:** 8 **HBD:** 5 **RotB:** 5

PubChem ID : - **CASRN :** 858131-65-4 **AlogP:** 0.80 **TPSA:** 138.0

Activity: NMDA receptor antagonist

NIMH Code : B-913 new

Compound name : 7-Bromo-5-(pyridin-2-yl)-1,3-dihydro-2H-1,4-benzodiazepin-2-one (bromazepam)



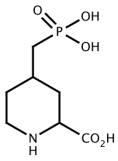
Mol. Formula : $C_{14}H_{10}BrN_3O$ **FW :** 316.15 **HBA:** 3 **HBD:** 1 **RotB:** 1

PubChem ID : 2441 **CASRN :** 1812-30-2 **AlogP:** 1.70 **TPSA:** 54.4

Activity: $GABA_A$ receptor allosteric modulator

NIMH Code : C-105

Compound name : CGS 19755; Selfotel



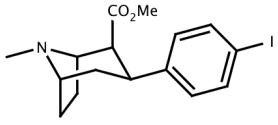
Mol. Formula : $C_7H_{14}NO_5P$ **FW :** 223.17 **HBA:** 6 **HBD:** 4 **RotB:** 3

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

Activity: Competitive NMDA antagonist

NIMH Code : C-148

Compound name : RTI-55



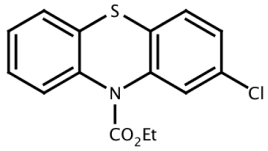
Mol. Formula : $C_{20}H_{26}INO_8$ **FW :** 535.32 **HBA:** 2 **HBD:** 0 **RotB:** 3

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

Activity: Dopamine reuptake inhibitor

NIMH Code : C-501

Compound name : 10-Carboethoxy-2-chlorophenothiazine

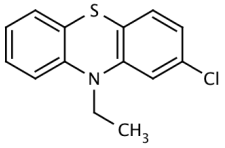


Mol. Formula : $C_{15}H_{12}ClNO_2S$ **FW :** 305.79 **HBA:** 5 **HBD:** 0 **RotB:** 2

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

NIMH Code : C-502

Compound name : N-Ethyl-2-chlorophenothiazine

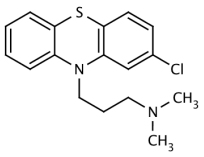


Mol. Formula : $C_{14}H_{12}ClNS$ **FW :** 261.78 **HBA:** 3 **HBD:** 0 **RotB:** 1

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

NIMH Code : C-503

Compound name : Chlorpromazine hydrochloride



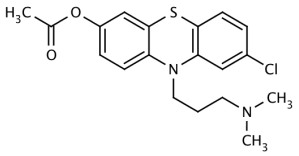
Mol. Formula : $C_{17}H_{20}Cl_2N_2S$ **FW :** 355.33 **HBA:** 4 **HBD:** 0 **RotB:** 4

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

Activity: Dopamine, serotonin, histamine, adrenaline, and muscarinic receptor

NIMH Code : C-504

Compound name : 7-Acetoxychlorpromazine hydrogen maleate

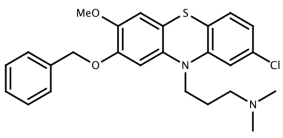


Mol. Formula : $C_{23}H_{25}ClN_2O_6S$ **FW :** 429.98 **HBA:** 5 **HBD:** 0 **RotB:** 6

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

NIMH Code : C-505

Compound name : 8-Benzyloxy-7-methoxychlorpromazine

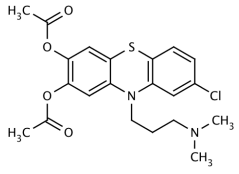


Mol. Formula : $C_{25}H_{27}ClN_2O_2S$ **FW :** 455.02 **HBA:** 6 **HBD:** 1 **RotB:** 7

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

NIMH Code : C-506

Compound name : 7,8-Diacetoxychlorpromazine hydrogen maleate

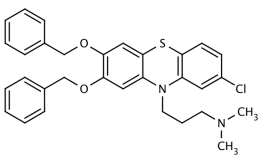


Mol. Formula : $C_{25}H_{27}ClN_2O_8S$ **FW :** 551.02 **HBA:** 6 **HBD:** 0 **RotB:** 8

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

NIMH Code : C-508

Compound name : 7,8-Dibenzyloxychlorpromazine

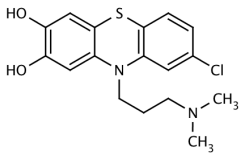


Mol. Formula : $C_{31}H_{31}ClN_2O_2S$ **FW :** 531.12 **HBA:** 6 **HBD:** 0 **RotB:** 10

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

NIMH Code : C-511

Compound name : 7,8-Dihydroxychlorpromazine hydrochloride



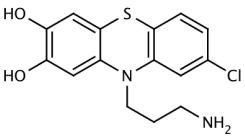
Mol. Formula : $C_{17}H_{20}Cl_2N_2O_2S$ **FW :** 387.33 **HBA:** 6 **HBD:** 2 **RotB:** 4

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

Activity: Chlorpromazine metabolite

NIMH Code : C-512

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



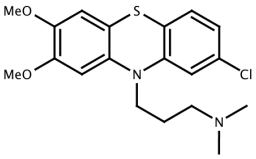
Mol. Formula : $C_{15}H_{16}C_2N_2O_2S$ **FW :** 359.29 **HBA:** 6 **HBD:** 3 **RotB:** 3

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

Activity: Chlorpromazine metabolite

NIMH Code : C-513

Compound name : 7,8-Dimethoxychlorpromazine hydrochloride



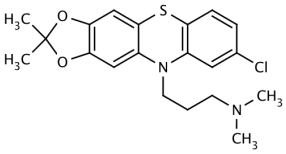
Mol. Formula : $C_{19}H_{24}Cl_2N_2O_2S$ **FW :** 415.39 **HBA:** 6 **HBD:** 0 **RotB:** 6

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

Activity: Chlorpromazine metabolite

NIMH Code : C-514

Compound name : 7,8-(Dimethylmethylenedioxy)chlorpromazine



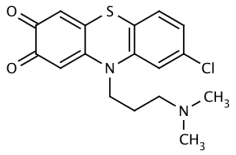
Mol. Formula : $C_{20}H_{23}ClN_2O_2S$ **FW :** 390.93 **HBA:** 6 **HBD:** 0 **RotB:** 4

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

Activity: Chlorpromazine metabolite

NIMH Code : C-515

Compound name : 7,8-Dioxochlorpromazine hydrochloride



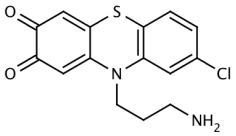
Mol. Formula : $C_{17}H_{18}Cl_2N_2O_2S$ **FW :** 385.31 **HBA:** 6 **HBD:** 0 **RotB:** 4

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

Activity: Chlorpromazine metabolite

NIMH Code : C-516

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

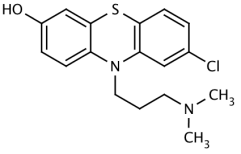


Mol. Formula : $C_{15}H_{14}Cl_2N_2O_2S$ **FW :** 357.26 **HBA:** 6 **HBD:** 1 **RotB:** 3

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

NIMH Code : C-518

Compound name : 7-Hydroxychlorpromazine hydrochloride



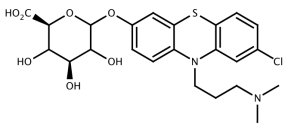
Mol. Formula : $C_{17}H_{20}Cl_2N_2OS$ **FW :** 371.33 **HBA:** 5 **HBD:** 1 **RotB:** 4

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

Activity: Dopamine antagonist

NIMH Code : C-519

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



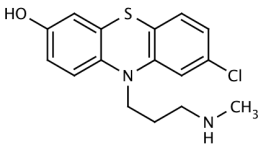
Mol. Formula : $C_{25}H_{28}ClF_3N_2O_9S$ **FW :** 625.02 **HBA:** 11 **HBD:** 4 **RotB:** 7

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

Activity: 7-Hydroxychlorpromazine metabolite

NIMH Code : C-520

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



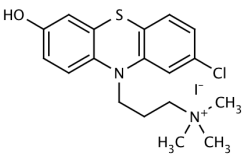
Mol. Formula : $C_{16}H_{18}Cl_2N_2OS$ **FW :** 357.31 **HBA:** 5 **HBD:** 2 **RotB:** 4

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

Activity: Chlorpromazine metabolite

NIMH Code : C-521

Compound name : 7-Hydroxychlorpromazine methiodide



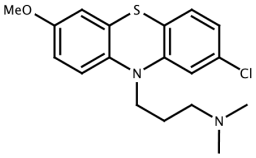
Mol. Formula : $C_{18}H_{22}ClIN_2OS$ **FW :** 476.81 **HBA:** 4 **HBD:** 1 **RotB:** 4

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

Activity: Dopamine antagonist

NIMH Code : C-523

Compound name : 7-Methoxychlorpromazine hydrochloride



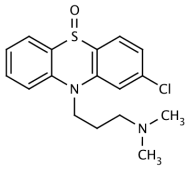
Mol. Formula : $C_{18}H_{22}Cl_2N_2OS$ **FW :** 385.36 **HBA:** 5 **HBD:** 0 **RotB:** 5

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

Activity: Chlorpromazine metabolite

NIMH Code : C-524

Compound name : Chlorpromazine sulfoxide hydrochloride



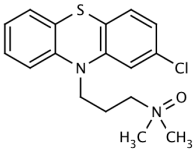
Mol. Formula : $C_{17}H_{20}Cl_2N_2OS$ **FW :** 371.33 **HBA:** 4 **HBD:** 0 **RotB:** 4

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

Activity: Dopamine antagonist

NIMH Code : C-525

Compound name : Chlorpromazine-*N*-oxide



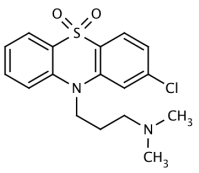
Mol. Formula : $C_{17}H_{19}ClN_2OS$ **FW :** 334.87 **HBA:** 0 **HBD:** 0 **RotB:** 4

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

Activity: Dopamine antagonist

NIMH Code : C-526

Compound name : Chlorpromazine sulfone hydrochloride

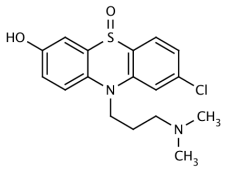


Mol. Formula : $C_{17}H_{20}Cl_2N_2O_2S$ **FW :** 387.33 **HBA:** 5 **HBD:** 0 **RotB:** 4

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

NIMH Code : C-528

Compound name : 7-Hydroxychlorpromazine sulfoxide

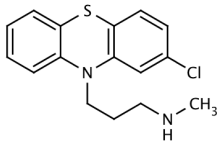


Mol. Formula : $C_{17}H_{19}ClN_2O_2S$ **FW :** 350.87 **HBA:** 5 **HBD:** 1 **RotB:** 4

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

NIMH Code : C-529

Compound name : *nor*-1-Chlorpromazine hydrochloride



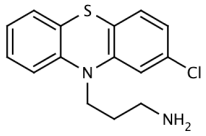
Mol. Formula : $C_{16}H_{18}Cl_2N_2S$ **FW :** 341.30 **HBA:** 4 **HBD:** 1 **RotB:** 4

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

Activity: Chlorpromazine metabolite

NIMH Code : C-530

Compound name : *nor*-2-Chlorpromazine hydrochloride



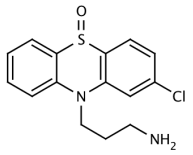
Mol. Formula : $C_{15}H_{16}Cl_2N_2S$ **FW :** 327.27 **HBA:** 4 **HBD:** 1 **RotB:** 3

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

Activity: Active metabolite of chlorpromazine.

NIMH Code : C-531

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



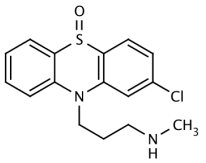
Mol. Formula : $C_{15}H_{16}Cl_2N_2OS$ **FW :** 343.27 **HBA:** 4 **HBD:** 1 **RotB:** 3

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

Activity: Chlorpromazine metabolite

NIMH Code : C-532

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

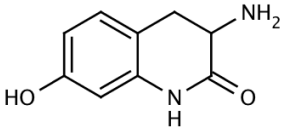


Mol. Formula : $C_{16}H_{18}Cl_2N_2OS$ **FW :** 357.30 **HBA:** 4 **HBD:** 1 **RotB:** 4

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

NIMH Code : C-535

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

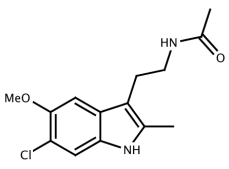


Mol. Formula : $C_9H_{10}N_2O_2$ **FW :** 178.19 **HBA:** 3 **HBD:** 3 **RotB:** 0

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

NIMH Code : C-536

Compound name : 6-Chloro-2-methylmelatonin



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

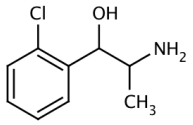
PubChem ID : **CASRN :** **AlogP:** 1.62 **TPSA:** 54.1

NIMH Code : C-537

Compound 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



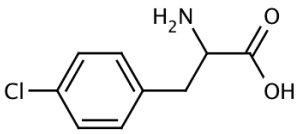
NIMH Code : C-538

Compound 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



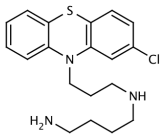
NIMH Code : C-701

Compound 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



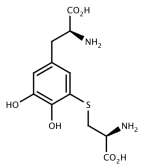
NIMH Code : C-702

Compound 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



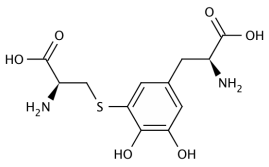
NIMH Code : C-702A

Compound 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



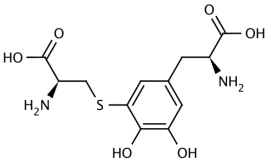
NIMH Code : C-702B

Compound 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



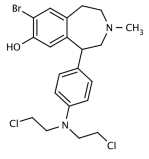
NIMH Code : C-705

Compound 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

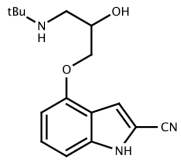
PubChem ID : **CASRN :** **AlogP:** 5.30 **TPSA:** 26.7

Activity: Dopamine D_1 receptor alkylating ligand



NIMH Code : C-706

Compound name : Cyanopindolol fumarate



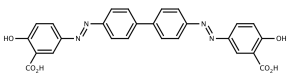
Mol. Formula : $C_{36}H_{46}N_6O_8$ **FW :** 690.80 **HBA:** 4 **HBD:** 3 **RotB:** 7

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

Activity: Adrenergic β1 antagonist; 5-HT_{1A} receptor antagonist

NIMH Code : C-707

Compound name : Chrysamine G



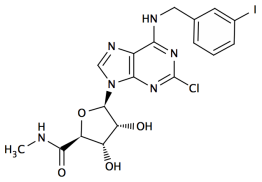
Mol. Formula : $C_{26}H_{18}N_4O_6$ **FW :** 482.46 **HBA:** 10 **HBD:** 4 **RotB:** 7

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

Activity: β-Amyloid ligand

NIMH Code : C-708

Compound name : Chloro-IB-MECA



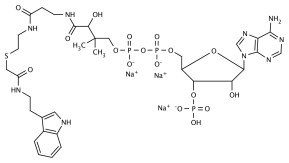
Mol. Formula : $C_{18}H_{18}ClIN_6O_4$ **FW :** 544.74 **HBA:** 9 **HBD:** 4 **RotB:** 5

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

Activity: A_3 adenosine receptor ligand

NIMH Code : C-711A

Compound name : Coenzyme A-*S*-acetyltryptamine



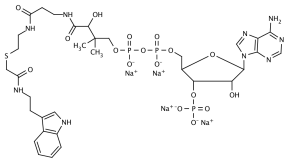
Mol. Formula : $C_{33}H_{45}N_9Na_3O_{17}P_3S$ **FW :** 1033.73 **HBA:** 18 **HBD:** 8 **RotB:** 24

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

Activity: Arylalkylamine N-acetyltransferase (AANAT) inhibitor

NIMH Code : C-711B

Compound name : Coenzyme A-*S*-acetyltryptamine



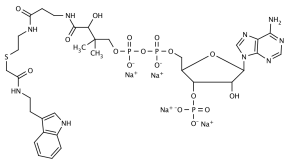
Mol. Formula : $C_{33}H_{44}N_9Na_4O_{17}P_3S$ **FW :** 1055.71 **HBA:** 18 **HBD:** 7 **RotB:** 24

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

Activity: Arylalkylamine N-acetyltransferase (AANAT) inhibitor

NIMH Code : C-711C

Compound name : Coenzyme A-*S*-acetyltryptamine



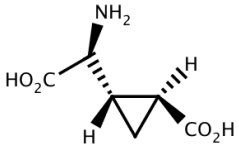
Mol. Formula : $C_{33}H_{44}N_9Na_4O_{17}P_3S$ **FW :** 1055.70 **HBA:** 18 **HBD:** 7 **RotB:** 24

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

Activity: Arylalkylamine N-acetyltransferase (AANAT) inhibitor

NIMH Code : C-801

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



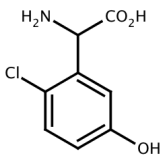
Mol. Formula : $C_6H_9NO_4$ **FW :** 159.14 **HBA:** 5 **HBD:** 3 **RotB:** 3

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

Activity: Metabotropic glutamate $mGluR_2$ agonist

NIMH Code : C-802

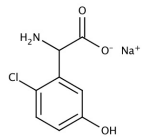
Compound name : (*RS*)-2-Chloro-5-hydroxyphenylglycine



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:	Metabotropic glutamate $mGlu_5$ agonist				

NIMH Code : C-802A new

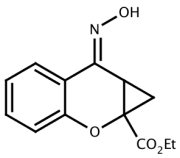
Compound name : (*RS*)-2-Chloro-5-hydroxyphenylglycine, sodium salt



Mol. Formula :	$C_8H_7ClNNaO_3$	**FW :** 223.59	**HBA:** 5	**HBD:** 3	**RotB:** 2
PubChem ID :	3645780	**CASRN :**		**AlogP:** -1.16	**TPSA:** 83.6
Activity:	Metabotropic glutamate $mGlu_5$ agonist				

NIMH Code : C-803

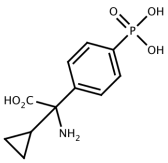
Compound name : 7-(Hydroxyimino)cyclopropa[*b*]chromen-1a-carboxylate ethyl ester



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:	Metabotropic glutamate $mGluR_1$ antagonist				

NIMH Code : C-804

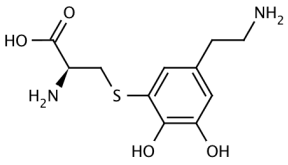
Compound name : (*RS*)-α-Cyclopropyl-4-phosphonophenylglycine



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:	Metabotropic glutamate $mGluR_3$ antagonist				

NIMH Code : C-805A

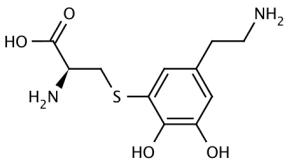
Compound name : 5-(*S*)-Cysteinyldopamine trifluoroacetate



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

NIMH Code : C-805B

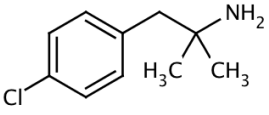
Compound name : 5-(*S*)-Cysteinyldopamine dihydrochloride



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

NIMH Code : C-806

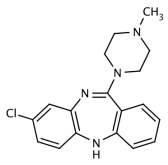
Compound name : Chlorophentermine hydrochloride



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				

NIMH Code : C-807

Compound name : Clozapine



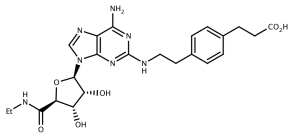
Mol. Formula : $C_{18}H_{19}ClN_4$ **FW :** 326.83 **HBA:** 5 **HBD:** 1 **RotB:** 0

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

Activity: Dopamine D_4 antagonist

NIMH Code : C-901

Compound name : CGS 21680 hydrochloride



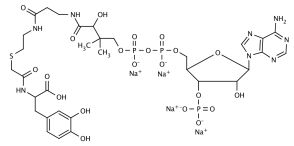
Mol. Formula : $C_{23}H_{30}ClN_7O_6$ **FW :** 535.99 **HBA:** 11 **HBD:** 6 **RotB:** 10

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

Activity: Adenosine A_2 agonist

NIMH Code : C-902

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

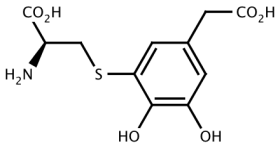


Mol. Formula : $C_{32}H_{43}N_8Na_4O_{21}P_3S$ **FW :** 1092.68 **HBA:** 22 **HBD:** 9 **RotB:** 25

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

NIMH Code : C-903

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

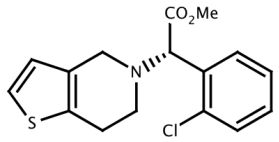


Mol. Formula : $C_{11}H_{14}ClNO_6S$ **FW :** 323.75 **HBA:** 8 **HBD:** 5 **RotB:** 6

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

NIMH Code : C-904

Compound name : Clopidogrel hydrogen sulfate



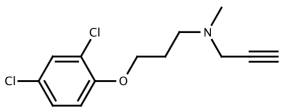
Mol. Formula : $C_{16}H_{18}ClNO_6S_2$ **FW :** 419.90 **HBA:** 4 **HBD:** 0 **RotB:** 4

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

Activity: Purinergic P_2Y_{12} inhibitor

NIMH Code : C-905

Compound name : Clorgyline hydrochloride



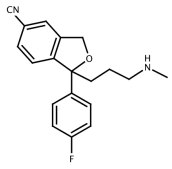
Mol. Formula : $C_{13}H_{16}Cl_3NO$ **FW :** 308.64 **HBA:** 4 **HBD:** 0 **RotB:** 7

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

Activity: Monoamine oxidase inhibitor

NIMH Code : C-906

Compound name : N-Norcitalopram oxalate



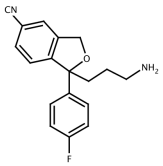
Mol. Formula : $C_{21}H_{21}FN_2O_5$ **FW :** 400.41 **HBA:** 4 **HBD:** 1 **RotB:** 6

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

Activity: Citalopram metabolite

NIMH Code : C-907

Compound name : N,N-Dinorcitalopram oxalate



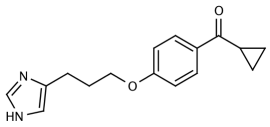
Mol. Formula : $C_{20}H_{19}FN_2O_5$ **FW :** 386.38 **HBA:** 4 **HBD:** 1 **RotB:** 5

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

Activity: Citalopram metabolite

NIMH Code : C-908

Compound name : Ciproxifan



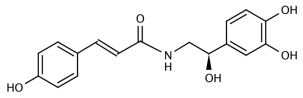
Mol. Formula : $C_{20}H_{22}N_2O_6$ **FW :** 386.40 **HBA:** 3 **HBD:** 1 **RotB:** 7

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

Activity: Histamine H_3 antagonist

NIMH Code : C-909

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



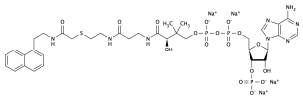
Mol. Formula : $C_{17}H_{17}NO_5$ **FW :** 315.32 **HBA:** 5 **HBD:** 5 **RotB:** 5

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

Activity: Plant metabolite implicated in tomato defense against pathogens

NIMH Code : C-910

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



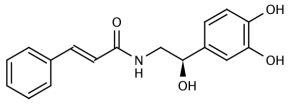
Mol. Formula : $C_{35}H_{45}N_8Na_4O_{17}P_3S$ **FW :** 1066.72 **HBA:** 18 **HBD:** 6 **RotB:** 24

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

Activity: Melatonin arylalkylamine-N-acetyltransferase rhythm enzyme ligand

NIMH Code : C-911

Compound name : *N*-Cinnamoylnorepinephrine

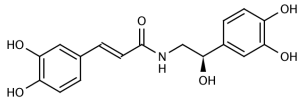


Mol. Formula : $C_{17}H_{17}NO_4$ **FW :** 299.32 **HBA:** 4 **HBD:** 4 **RotB:** 5

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

NIMH Code : C-912

Compound name : *N*-Caffeoylnorepinephrine

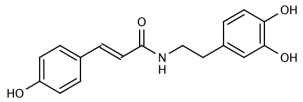


Mol. Formula : $C_{17}H_{17}NO_6$ **FW :** 331.32 **HBA:** 6 **HBD:** 6 **RotB:** 5

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

NIMH Code : C-913

Compound name : *N*-Coumaroyldopamine

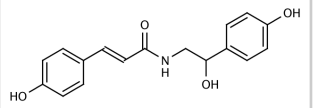


Mol. Formula : $C_{17}H_{17}NO_4$ **FW :** 299.32 **HBA:** 4 **HBD:** 4 **RotB:** 5

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

NIMH Code : C-914

Compound name : *N*-Coumaroyloctopamine

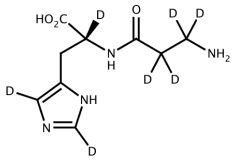


Mol. Formula : $C_{17}H_{17}NO_4$ **FW :** 299.32 **HBA:** 4 **HBD:** 4 **RotB:** 5

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

NIMH Code : C-915

Compound name : Carnosine-d7



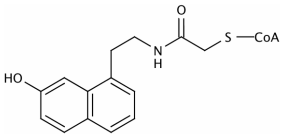
Mol. Formula : $C_9H_{14}N_4O_3$ **FW :** 226.23 **HBA:** 5 **HBD:** 4 **RotB:** 6

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

Activity: Stable isotope labeled carnosine

NIMH Code : C-916

Compound 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

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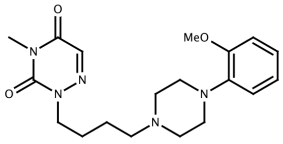
NIMH Code : C-917

Compound name : CUMI-101



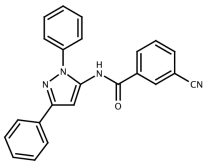
Mol. Formula : $C_{19}H_{27}N_5O_3$ **FW :** 373.45 **HBA:** 6 **HBD:** 0 **RotB:** 7

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

Activity: Serotonin 5-HT_{1A} agonist

NIMH Code : C-918

Compound 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: Metabotropic gluatamate $mGluR_5$ positive allosteric modulator

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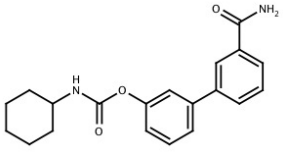
NIMH Code : C-919 new

Compound name : Cyclohexylcarbamic acid 3'-carbamoylphenyl-3-yl ester (URB597)



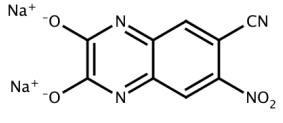
Mol. Formula : $C_{20}H_{22}N_2O_3$ **FW :** 338.40 **HBA:** 3 **HBD:** 2 **RotB:** 5

PubChem ID : 1383884 **CASRN :** 546141-08-6 **AlogP:** 3.80 **TPSA:** 81.4

Activity: Fatty-acid amide hydrolase (FAAH) inhibitor.

NIMH Code : C-920 new

Compound name : 6-Cyano-7-nitroquinoxaline-2,3-dione disodium salt (CNQX disodium salt)

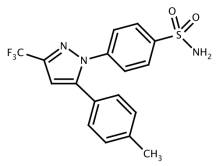


Mol. Formula : $C_9H_2N_4Na_2O_4$ **FW :** 276.12 **HBA:** 7 **HBD:** 0 **RotB:** 0

PubChem ID : 2821 **CASRN :** 115066-14-3 **AlogP:** 1.68 **TPSA:** 142.0

NIMH Code : C-921 new

Compound name : 4-[5-(4-Methylphenyl)-3-trifluoromethyl)-1*H*-pyrazol-1-yl]benzenesulfonamide (celecoxib)



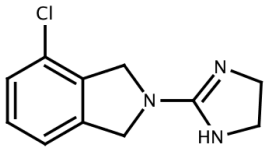
Mol. Formula : $C_{17}H_{14}F_3N_3O_2S$ **FW :** 381.37 **HBA:** 7 **HBD:** 1 **RotB:** 3

PubChem ID : 2662 **CASRN :** 169590-42-5 **AlogP:** 3.40 **TPSA:** 86.4

Activity: Cyclooxygenase 2 inhibitor

NIMH Code : C-922

Compound name : 4-Chloro-2-(4,5-dihydro-1H-imidazol-2-yl)-2,3-dihydro-1H-isoindole hydroiodide; RS 45041-190 hydroiodide



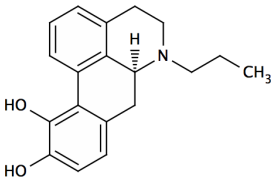
Mol. Formula : $C_{11}H_{13}ClIN_3$ **FW :** 349.60 **HBA:** 3 **HBD:** 1 **RotB:** 1

PubChem ID : 127951 **CASRN :** 170034-96-5 **AlogP:** 1.71 **TPSA:** 27.6

Activity: Selective I2 imidazoline receptor ligand.

NIMH Code : D-041

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



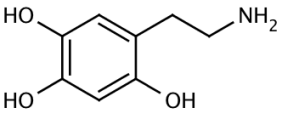
Mol. Formula : $C_{19}H_{22}ClNO_2$ **FW :** 331.84 **HBA:** 3 **HBD:** 2 **RotB:** 2

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

Activity: Limbic-selective dopamine antagonist

NIMH Code : D-501

Compound name : 6-Hydroxydopamine hydrobromide; Oxidopamine



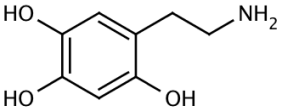
Mol. Formula : $C_8H_{12}BrNO_3$ **FW :** 250.09 **HBA:** 4 **HBD:** 4 **RotB:** 2

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

Activity: Catecholaminergic neurotoxin

NIMH Code : D-502

Compound name : 6-Hydroxydopamine hydrochloride; Oxidopamine



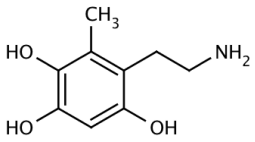
Mol. Formula : $C_8H_{12}ClNO_3$ **FW :** 205.64 **HBA:** 4 **HBD:** 4 **RotB:** 2

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

Activity: Catecholaminergic neurotoxin

NIMH Code : D-503

Compound name : 2-Methyl-6-hydroxydopamine hydrobromide

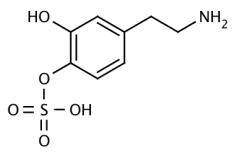


Mol. Formula : $C_9H_{14}BrNO_3$ **FW :** 264.12 **HBA:** 4 **HBD:** 4 **RotB:** 2

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

NIMH Code : D-504

Compound name : Dopamine-4-O-sulfate



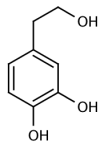
Mol. Formula : $C_8H_{11}NO_5S$ **FW :** 233.24 **HBA:** 5 **HBD:** 3 **RotB:** 4

PubChem ID : 123932 **CASRN :** 38339-02-5 **AlogP:** -1.75 **TPSA:** 118.2

Activity: Possible norepinephrine precursor

NIMH Code : D-505

Compound name : Hydroxytyrosol



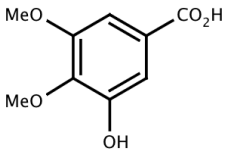
Mol. Formula : $C_{14}H_{22}N_2O_3$ **FW :** 266.34 **HBA:** 3 **HBD:** 3 **RotB:** 2

PubChem ID : 82755 **CASRN :** 10597-60-1 **AlogP:** 0.89 **TPSA:** 60.7

Activity: Platelet aggregation inhibitor

NIMH Code : D-506

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



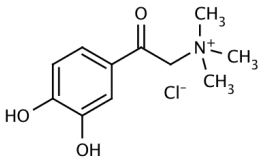
Mol. Formula : $C_9H_{10}O_5$ **FW :** 198.18 **HBA:** 5 **HBD:** 2 **RotB:** 3

PubChem ID : 74709 **CASRN :** 1916-08-1 **AlogP:** 0.77 **TPSA:** 76.0

Activity: Thiopurine methyltransferase inhibitor

NIMH Code : D-507

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

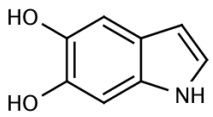


Mol. Formula : $C_{11}H_{16}ClNO_3$ **FW :** 245.71 **HBA:** 3 **HBD:** 2 **RotB:** 3

PubChem ID : 412800 **CASRN :** **AlogP:** -3.92 **TPSA:** 57.5

NIMH Code : D-509

Compound name : 5,6-Dihydroxyindole



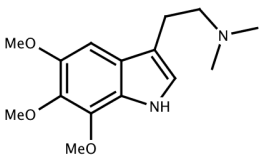
Mol. Formula : $C_8H_7NO_2$ **FW :** 149.15 **HBA:** 2 **HBD:** 3 **RotB:** 0

PubChem ID : 114683 **CASRN :** 3131-52-0 **AlogP:** 1.58 **TPSA:** 56.3

Activity: Catechol O-methyltransferase (COMT) inhibitor

NIMH Code : D-510

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

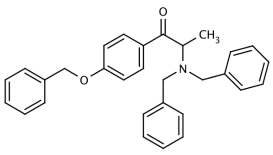


Mol. Formula : $C_{15}H_{22}N_2O_3$ **FW :** 278.35 **HBA:** 4 **HBD:** 1 **RotB:** 6

PubChem ID : **CASRN :** **AlogP:** 1.53 **TPSA:** 46.7

NIMH Code : D-511

Compound name : 4'-Benzyloxy-2-dibenzylaminopropiophenone

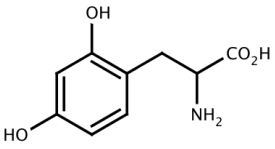


Mol. Formula : $C_{30}H_{29}NO_2$ **FW :** 435.59 **HBA:** 3 **HBD:** 0 **RotB:** 10

PubChem ID : **CASRN :** **AlogP:** 6.84 **TPSA:** 29.5

NIMH Code : D-512

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

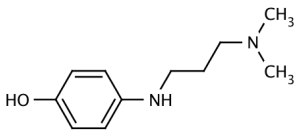


Mol. Formula : $C_9H_{11}NO_4$ **FW :** 197.19 **HBA:** 5 **HBD:** 4 **RotB:** 3

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

NIMH Code : D-513

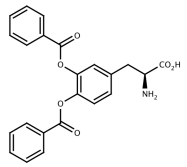
Compound name : 4-(γ-N,N-Dimethylaminopropylamino)phenol dimaleate



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

NIMH Code : D-514

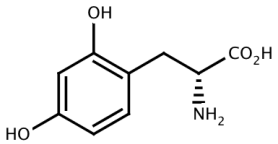
Compound name : L-3,4-Dibenzoyloxyphenylalanine



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				

NIMH Code : D-515

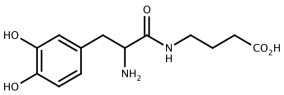
Compound name : (+)-2,4-Dihydroxyphenylalanine



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

NIMH Code : D-516

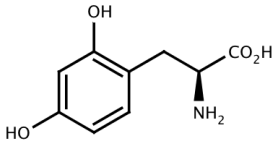
Compound name : (±)-3,4-Dihydroxyphenylalanyl-GABA



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

NIMH Code : D-517

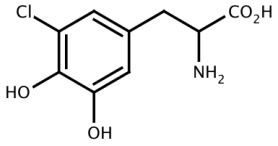
Compound name : (–)-2,4-Dihydroxyphenylalanine



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

NIMH Code : D-518

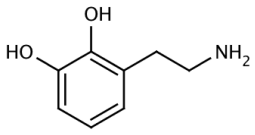
Compound name : (±)-3-Chloro-4,5-dihydroxyphenylalanine hydrobromide



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

NIMH Code : D-519

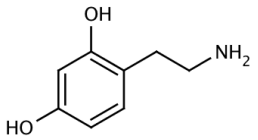
Compound name : 2,3-Dihydroxy-β-phenethylamine hydrobromide



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

NIMH Code : D-520

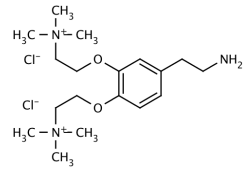
Compound name : 2,4-Dihydroxy-β-phenethylamine hydrochloride



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

NIMH Code : D-521

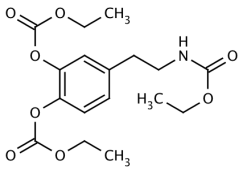
Compound name : 3,4-Di-(β-trimethylammoniumethoxy)-β-phenethylamine hydrochloride dichloride



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

NIMH Code : D-522

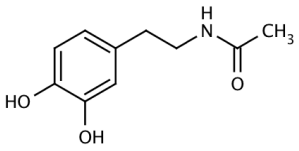
Compound name : 3,4-Diethylcarbonato-β-phenethylamine carbamate



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

NIMH Code : D-523

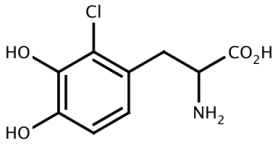
Compound name : N-Acetyl-3,4-dihydroxy-β-phenethylamine



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

NIMH Code : D-524

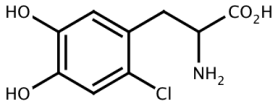
Compound name : (±)-2-Chloro-3,4-dihydroxyphenylalanine hydrobromide



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

NIMH Code : D-525

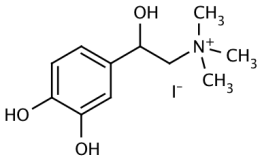
Compound name : (±)-6-Chloro-3,4-dihydroxyphenylalanine hydrobromide



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

NIMH Code : D-528

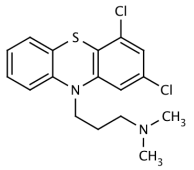
Compound name : (±)-(N,N-Dimethyl)ephedrine Iodide



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

NIMH Code : D-529

Compound name : 2,4-Dichloropromazine hydrochloride

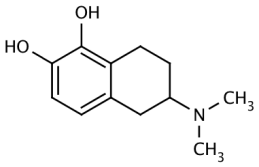


Mol. Formula : $C_{17}H_{19}Cl_3N_2S$ **FW :** 389.77 **HBA:** 5 **HBD:** 0 **RotB:** 4

PubChem ID : 77273 **CASRN :** 3689-36-9 **AlogP:** 5.07 **TPSA:** 31.8

NIMH Code : D-701

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

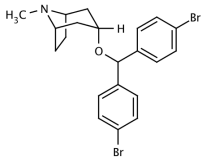


Mol. Formula : $C_{12}H_{18}BrNO_2$ **FW :** 288.19 **HBA:** 3 **HBD:** 2 **RotB:** 1

PubChem ID : 37032 **CASRN :** 39478-90-5 **AlogP:** 1.39 **TPSA:** 43.7

NIMH Code : D-702

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



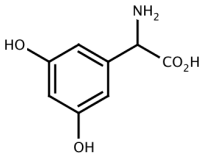
Mol. Formula : $C_{21}H_{24}Br_2ClNO$ **FW :** 501.69 **HBA:** 2 **HBD:** 0 **RotB:** 4

PubChem ID : 10096017 **CASRN :** **AlogP:** 5.66 **TPSA:** 12.5

Activity: Dopamine uptake inhibitor

NIMH Code : D-801

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



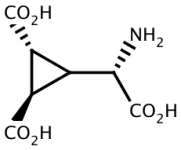
Mol. Formula : $C_8H_9NO_4$ **FW :** 183.16 **HBA:** 5 **HBD:** 4 **RotB:** 2

PubChem ID : 108001 **CASRN :** 146255-66-5 **AlogP:** -1.96 **TPSA:** 103.8

Activity: Metabotropic gluatamate $mGluR_1$ and $mGluR_5$ agonist

NIMH Code : D-802

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



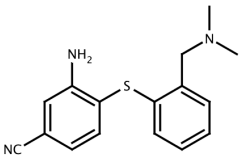
Mol. Formula : $C_7H_9NO_6$ **FW :** 203.15 **HBA:** 7 **HBD:** 4 **RotB:** 4

PubChem ID : 5310979 **CASRN :** 147782-19-2 **AlogP:** -3.84 **TPSA:** 137.9

Activity: Metabotropic gluatamate $mGluR_2$ agonist

NIMH Code : D-803

Compound name : DASB hydrochloride



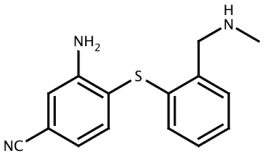
Mol. Formula : $C_{16}H_{18}ClN_3S$ **FW :** 319.85 **HBA:** 4 **HBD:** 1 **RotB:** 5

PubChem ID : 10446567 **CASRN :** 627490-01-1 **AlogP:** 3.47 **TPSA:** 78.4

Activity: Serotonin 5-HT transporter ligand

NIMH Code : D-804

Compound name : Desmethyl-DASB



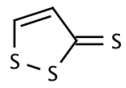
Mol. Formula : $C_{15}H_{15}N_3S$ **FW :** 269.37 **HBA:** 4 **HBD:** 2 **RotB:** 5

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

Activity: DASB PET ligand precursor

NIMH Code : D-805

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

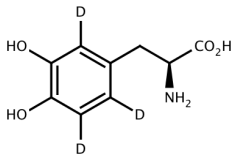


Mol. Formula :	$C_3H_2S_3$	**FW :**	134.24	**HBA:**	3	**HBD:**	0	**RotB:**	0
PubChem ID :	68296	**CASRN :**	534-25-8			**AlogP:**	2.22	**TPSA:**	82.7

Activity: Antineoplastic agent

NIMH Code : D-901

Compound name : L-DOPA-ring-d_3

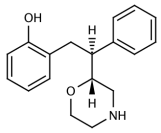


Mol. Formula :	$C_9H_8D_3NO_4$	**FW :**	200.21	**HBA:**	5	**HBD:**	4	**RotB:**	3
PubChem ID :	12297005	**CASRN :**	53587-29-4			**AlogP:**	-1.71	**TPSA:**	103.8

Activity: Stable isotope labeled L-DOPA

NIMH Code : D-902

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

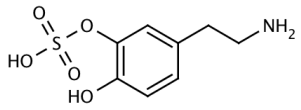


Mol. Formula :	$C_{17}H_{19}NO_3$	**FW :**	285.34	**HBA:**	3	**HBD:**	2	**RotB:**	4
PubChem ID :		**CASRN :**				**AlogP:**	3.17	**TPSA:**	41.5

Activity: Roboxetine PET ligand precusor

NIMH Code : D-903

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

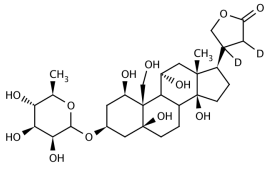


Mol. Formula :	$C_8H_{11}NO_5S$	**FW :**	233.24	**HBA:**	5	**HBD:**	3	**RotB:**	4
PubChem ID :	122136	**CASRN :**	51317-41-0			**AlogP:**	-1.20	**TPSA:**	118.2

Activity: L-DOPA metabolite

NIMH Code : D-904

Compound name : d_2-Dihydroouabain

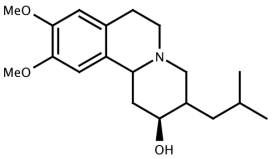


Mol. Formula :	$C_{29}H_{44}D_2O_{12}$	**FW :**	588.68	**HBA:**	11	**HBD:**	8	**RotB:**	4
PubChem ID :	14450	**CASRN :**	1183-35-3			**AlogP:**	-3.88	**TPSA:**	206.6

Activity: Stable isotope labeled ouabain inotropic action antagonist

NIMH Code : D-905

Compound name : (–)-α-Dihydrotetrabenazine

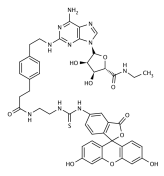


Mol. Formula :	$C_{19}H_{29}NO_3$	**FW :**	319.45	**HBA:**	4	**HBD:**	1	**RotB:**	4
PubChem ID :	123836	**CASRN :**	3466-75-9			**AlogP:**	2.36	**TPSA:**	41.9

Activity: Optical isomer of putative tetrabenazine metabolite

NIMH Code : D-906

Compound name : FITC-APEC

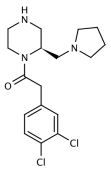


Mol. Formula :	$C_{46}H_{46}N_{10}O_{10}S$	**FW :**	930.98	**HBA:**	14	**HBD:**	10	**RotB:**	14
PubChem ID :		**CASRN :**				**AlogP:**	2.86	**TPSA:**	321.7

Activity: Fluorescent adenosine A_{2a} ligand

NIMH Code : D-907

Compound name : Descarboxymethyl GR103545 dihydrochloride



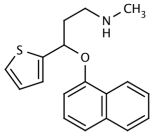
Mol. Formula : $C_{17}H_{23}Cl_2N_3O$ **FW :** 356.29 **HBA:** 5 **HBD:** 1 **RotB:** 4

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

Activity: GR103545 PET ligand precursor

NIMH Code : D-908

Compound name : Duloxetine hydrochloride



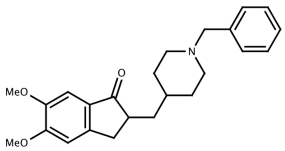
Mol. Formula : $C_{18}H_{19}NOS$ **FW :** 297.42 **HBA:** 3 **HBD:** 1 **RotB:** 6

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

Activity: Serotonin & norepinephrine reuptake inhibitor

NIMH Code : D-909

Compound name : Donepezil



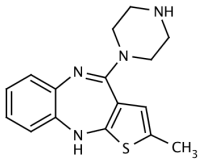
Mol. Formula : $C_{24}H_{29}NO_3$ **FW :** 379.49 **HBA:** 4 **HBD:** 0 **RotB:** 6

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

Activity: Reversible acetylcholinesterase inhibitor

NIMH Code : D-910

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



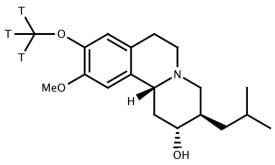
Mol. Formula : $C_{16}H_{18}N_4S$ **FW :** 298.41 **HBA:** 5 **HBD:** 2 **RotB:** 0

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

Activity: Olanzapine metabolite

NIMH Code : D-911

Compound name : Tritium-labeled dihydrotetrabenazine



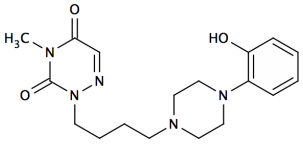
Mol. Formula : $C_{19}H_{29}NO_3$ **FW :** 319.44 **HBA:** 4 **HBD:** 1 **RotB:** 4

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

Activity: Radiolabeled dopamine uptake inhibitor

NIMH Code : D-912

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



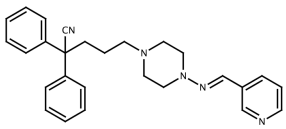
Mol. Formula : $C_{18}H_{25}N_5O_3$ **FW :** 359.42 **HBA:** 6 **HBD:** 1 **RotB:** 6

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

Activity: Serotonin 5-HT_{1A} ligand

NIMH Code : D-913

Compound name : SC-26196



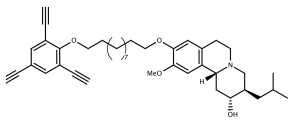
Mol. Formula : $C_{27}H_{29}N_5$ **FW :** 423.55 **HBA:** 5 **HBD:** 0 **RotB:** 8

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

Activity: Δ6 Desaturase inhibitor

NIMH Code : D-914

Compound name : Dihydrotetrabenazine derivative

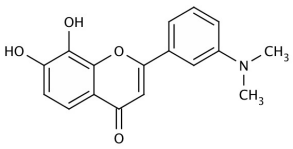


Mol. Formula : $C_{41}H_{53}NO_4$ **FW :** 623.86 **HBA:** 5 **HBD:** 1 **RotB:** 17

PubChem ID : **CASRN :** **AlogP:** 8.46 **TPSA:** 51.2

NIMH Code : D-915

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

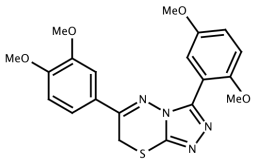


Mol. Formula : $C_{17}H_{15}NO_4$ **FW :** 297.30 **HBA:** 5 **HBD:** 2 **RotB:** 2

PubChem ID : **CASRN :** **AlogP:** 2.47 **TPSA:** 70.0

NIMH Code : D-916 new

Compound name : 3-(2,5-Dimethoxyphenyl)-6-(3,4-dimethoxy¬phenyl)-7*H*-[1,2,4]triazolo[3,4-b][1,3,4]thiadiazine



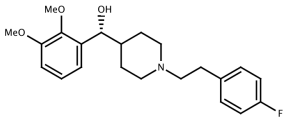
Mol. Formula : $C_{20}H_{20}N_4O_4S$ **FW :** 412.46 **HBA:** 7 **HBD:** 0 **RotB:** 6

PubChem ID : **CASRN :** **AlogP:** 2.31 **TPSA:** 80.0

Activity: Phosphodiesterase 4 (PDE4) inhibitor

NIMH Code : D-917 new

Compound name : (*R*)-(+)-α-(2,3-Dimethoxyphenyl)-1-[2-(4-fluorophenyl)ethyl]-4-piperidinemethanol (volinanserin)



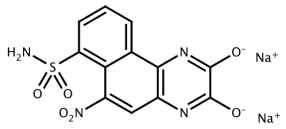
Mol. Formula : $C_{22}H_{28}NFO_3$ **FW :** 373.46 **HBA:** 5 **HBD:** 1 **RotB:** 7

PubChem ID : 60858 **CASRN :** 139290-65-6 **AlogP:** 3.90 **TPSA:** 41.9

Activity: 5-HT_{2A} antagonist

NIMH Code : D-918 new

Compound name : 2,3-Dioxo-6-nitro-1,2,3,4-tetrahydrobenzo[f]quinoxaline-7-sulfonamide disodium salt; NBQX disodium salt

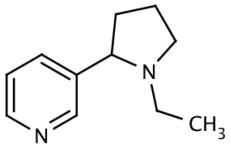


Mol. Formula : $C_{12}H_6N_4Na_2O_6S$ **FW :** 380.24 **HBA:** 8 **HBD:** 3 **RotB:** 2

PubChem ID : **CASRN :** 118876-58-7 **AlogP:** 1.42 **TPSA:** 172.2

NIMH Code : E-701A

Compound name : N-Ethylnornicotine tartrate



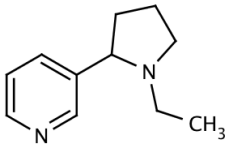
Mol. Formula : $C_{19}H_{28}N_2O_{12}$ **FW :** 476.44 **HBA:** 2 **HBD:** 0 **RotB:** 2

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

Activity: Nicotine analog

NIMH Code : E-701B

Compound name : N-Ethylnornicotine



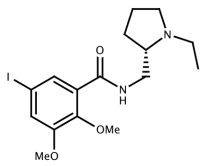
Mol. Formula : $C_{11}H_{16}N_2$ **FW :** 176.26 **HBA:** 2 **HBD:** 0 **RotB:** 2

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

Activity: Nicotine analog

NIMH Code : E-703

Compound name : Epidepride



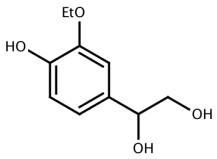
Mol. Formula : $C_{16}H_{23}IN_2O_3$ **FW :** 418.26 **HBA:** 4 **HBD:** 1 **RotB:** 6

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

Activity: Dopamine D_2 receptor antagonist

NIMH Code : E-704

Compound name : EHPG piperazine salt



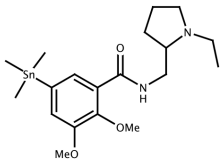
Mol. Formula : $C_{24}H_{38}N_2O_8$ **FW :** 482.57 **HBA:** 4 **HBD:** 3 **RotB:** 4

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

Activity: Catecholamine turnover biomarker

NIMH Code : E-705

Compound name : 5-Trimethylstannylepidepride



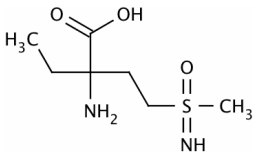
Mol. Formula : $C_{19}H_{32}N_2O_3Sn$ **FW :** 455.18 **HBA:** 4 **HBD:** 1 **RotB:** 7

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

Activity: Radioiodinated epidepride precusor

NIMH Code : E-706

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



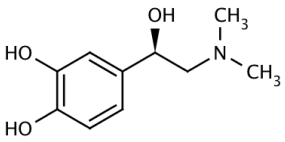
Mol. Formula : $C_7H_{16}N_2O_3S$ **FW :** 208.27 **HBA:** 3 **HBD:** 2 **RotB:** 4

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

Activity: Glutamate synthetase inhibitor

NIMH Code : E-707

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

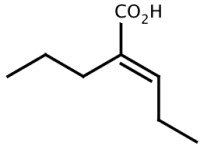


Mol. Formula : $C_{14}H_{21}NO_9$ **FW :** 347.32 **HBA:** 4 **HBD:** 3 **RotB:** 3

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

NIMH Code : E-708

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



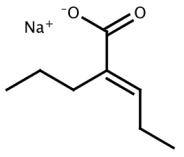
Mol. Formula : $C_8H_{14}O_2$ **FW :** 142.20 **HBA:** 2 **HBD:** 1 **RotB:** 4

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

Activity: Anticonvulsant; valproic acid metabolite

NIMH Code : E-709

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



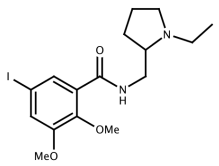
Mol. Formula : $C_8H_{13}O_2Na$ **FW :** 164.18 **HBA:** 2 **HBD:** 0 **RotB:** 4

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

Activity: Valproic acid metabolite

NIMH Code : E-901

Compound name : [^{125}I]Epidepride



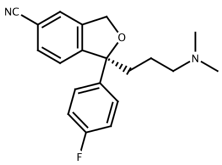
Mol. Formula : $C_{16}H_{23}IN_2O_3` **FW :** 418.26 **HBA:** 4 **HBD:** 1 **RotB:** 6

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

Activity: Radioiodinated dopamine D_2 antagonist

NIMH Code : E-902

Compound name : Escitalopram oxalate



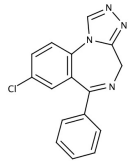
Mol. Formula : $C_{20}H_{21}FN_2O$ **FW :** 324.39 **HBA:** 4 **HBD:** 0 **RotB:** 6

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

Activity: Serotonin 5-HT reuptake inhibitor

NIMH Code : E-903 new

Compound name : 8-Chloro-6-phenyl-4H-[1,2,4]triazolo[4,3-a][1,4]benzodiazepine (estazolam)



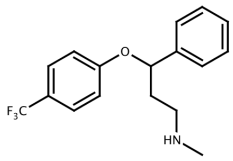
Mol. Formula : $C_{16}H_{11}ClN_4$ **FW :** 294.74 **HBA:** 3 **HBD:** 0 **RotB:** 1

PubChem ID : 3261 **CASRN :** 29975-16-4 **AlogP:** 2.09 **TPSA:** 43.1

Activity: $GABA_A$ receptor allosteric modulator

NIMH Code : F-132

Compound name : (±)-Fluoxetine hydrochloride



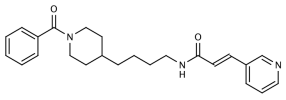
Mol. Formula : $C_{17}H_{19}ClF_3NO$ **FW :** 345.79 **HBA:** 5 **HBD:** 1 **RotB:** 7

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

Activity: Serotonin uptake inhibitor

NIMH Code : F-901

Compound name : FK866



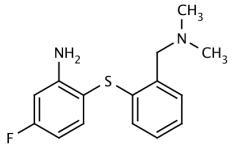
Mol. Formula : $C_{24}H_{29}N_3O_2$ **FW :** 391.51 **HBA:** 3 **HBD:** 1 **RotB:** 8

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

Activity: Nicotinamide phosphoribosyltransferase inhibitor

NIMH Code : F-902

Compound name : 4-Fluoro-ADAM



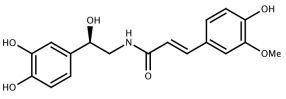
Mol. Formula : $C_{15}H_{17}FN_2S$ **FW :** 276.38 **HBA:** 4 **HBD:** 1 **RotB:** 4

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

Activity: Serotonin 5HT selective PET ligand reference standard

NIMH Code : F-903

Compound name : *N*-Feruloylnorepinephrine

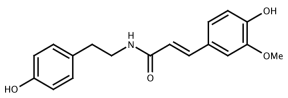


Mol. Formula : $C_{18}H_{19}NO_6$ **FW :** 345.35 **HBA:** 6 **HBD:** 5 **RotB:** 6

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

NIMH Code : F-904

Compound name : Feruloyltyramine



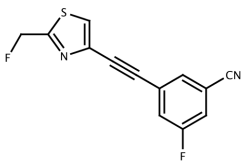
Mol. Formula : $C_{18}H_{19}NO_4$ **FW :** 313.35 **HBA:** 4 **HBD:** 3 **RotB:** 6

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

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

NIMH Code : F-905

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



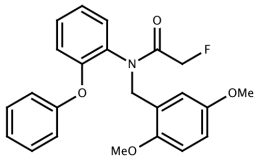
Mol. Formula : $C_{13}H_6F_2N_2S$ **FW :** 260.26 **HBA:** 5 **HBD:** 0 **RotB:** 4

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

Activity: Metabotropic gluatamate $mGluR_5$ PET ligand reference standard

NIMH Code : F-906

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



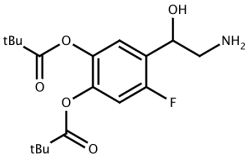
Mol. Formula : $C_{23}H_{22}FNO_4$ **FW :** 395.43 **HBA:** 5 **HBD:** 0 **RotB:** 8

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

Activity: Brain peripheral benzodiazepine receptor (TSPO) ligand

NIMH Code : F-907

Compound name : 6-Fluoronorepinephrine dipivalate hydrochloride

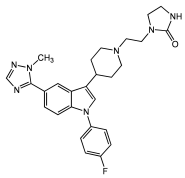


Mol. Formula : $C_{18}H_{27}ClFNO_5$ **FW :** 391.86 **HBA:** 4 **HBD:** 2 **RotB:** 8

PubChem ID : **CASRN :** **AlogP:** 3.42 **TPSA:** 98.9

NIMH Code : F-908 new

Compound name : 1-(2-(4-(1-(4-Fluorophenyl)-5-(1-methyl-1*H*-1,2,4-triazol-5-yl)-1*H*-indol-3-yl)-1-piperidinyl)ethyl)imidazolidin-2-one

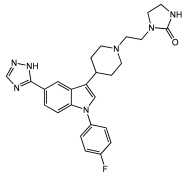


Mol. Formula : $C_{27}H_{30}FN_7O$ **FW :** 487.57 **HBA:** 4 **HBD:** 1 **RotB:** 6

PubChem ID : - **CASRN :** - **AlogP:** 2.92 **TPSA:** 71.2

NIMH Code : F-909 new

Compound name : 1-(2-(4-(1-(4-Fluorophenyl)-5-(1*H*-1,2,4-triazol-5-yl)-1*H*-indol-5-yl)-1-piperidinyl) ethyl)imidazolidin-2-one

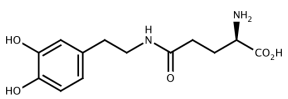


Mol. Formula : $C_{26}H_{28}FN_7O$ **FW :** 473.54 **HBA:** 4 **HBD:** 2 **RotB:** 6

PubChem ID : - **CASRN :** - **AlogP:** 2.11 **TPSA:** 82.1

NIMH Code : G-501

Compound name : γ-Glutamyldopamine

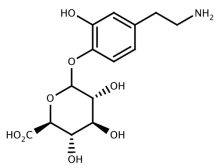


Mol. Formula : $C_{13}H_{18}N_2O_5$ **FW :** 282.30 **HBA:** 6 **HBD:** 5 **RotB:** 7

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

NIMH Code : G-502

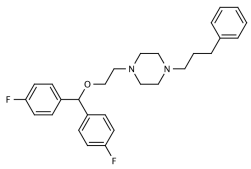
Compound name : Dopamine-4-*O*-β-D-glucuronide



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								

NIMH Code : G-801

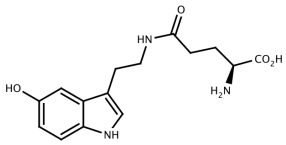
Compound name : GBR-12909 dihydrochloride; Vanoxerine



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								

NIMH Code : G-802

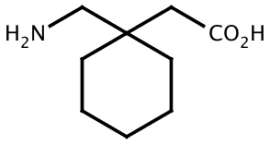
Compound name : γ-Glutamylserotonin



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

NIMH Code : G-901

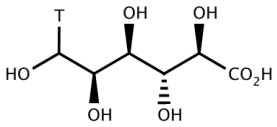
Compound name : Gabapentin



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:	Gamma aminobutyric acid (GABA) analog								

NIMH Code : G-902 new

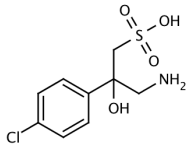
Compound name : [^{3}H]D-Galactonic acid



Mol. Formula :	$C_6H_{12}O_7$	**FW :**	196.16	**HBA:**	7	**HBD:**	6	**RotB:**	5
PubChem ID :	604	**CASRN :**	13382-27-9			**AlogP:**	-3.40	**TPSA:**	138.0

NIMH Code : H-113

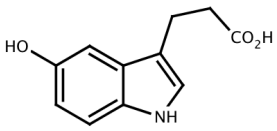
Compound name : 2-Hydroxysaclofen



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:	γ-Aminobutyric acid $GABA_B$ antagonist								

NIMH Code : H-501

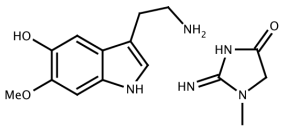
Compound name : 5-Hydroxyindole-3-β-propionic acid



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								

NIMH Code : H-502

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

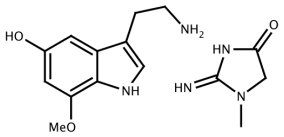


Mol. Formula : $C_{15}H_{23}N_5O_7S$ **FW :** 417.44 **HBA:** 3 **HBD:** 3 **RotB:** 3

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

NIMH Code : H-503

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

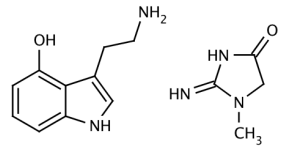


Mol. Formula : $C_{15}H_{23}N_5O_7S$ **FW :** 417.44 **HBA:** 3 **HBD:** 3 **RotB:** 3

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

NIMH Code : H-504

Compound name : 4-Hydroxytryptamine creatinine sulfate

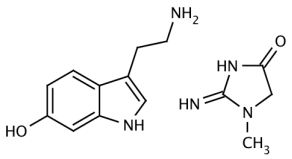


Mol. Formula : $C_{14}H_{21}N_5O_6S$ **FW :** 387.42 **HBA:** 2 **HBD:** 3 **RotB:** 2

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

NIMH Code : H-505

Compound name : 6-Hydroxytryptamine creatinine sulfate

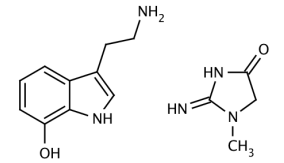


Mol. Formula : $C_{14}H_{21}N_5O_6S$ **FW :** 387.42 **HBA:** 2 **HBD:** 3 **RotB:** 2

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

NIMH Code : H-506

Compound name : 7-Hydroxytryptamine creatinine sulfate

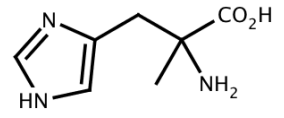


Mol. Formula : $C_{14}H_{21}N_5O_6S$ **FW :** 387.42 **HBA:** 2 **HBD:** 3 **RotB:** 2

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

NIMH Code : H-507

Compound name : α-Methylhistidine hydrochloride

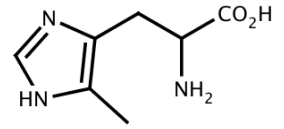


Mol. Formula : $C_7H_{12}ClN_3O_2$ **FW :** 205.63 **HBA:** 4 **HBD:** 3 **RotB:** 3

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

NIMH Code : H-509

Compound name : 4-Methylhistidine hydrochloride

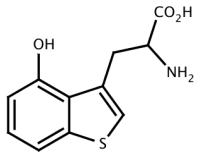


Mol. Formula : $C_7H_{12}ClN_3O_2$ **FW :** 205.63 **HBA:** 4 **HBD:** 3 **RotB:** 3

PubChem ID : 10773449 **CASRN :** **AlogP:** -3.38 **TPSA:** 92.0

NIMH Code : H-510

Compound name : 4-Hydroxytryptophan acetate

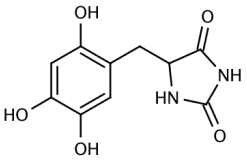


Mol. Formula : $C_{13}H_{16}N_2O_5$ **FW :** 280.28 **HBA:** 4 **HBD:** 4 **RotB:** 3

PubChem ID : 589768 **CASRN :** **AlogP:** -1.33 **TPSA:** 99.3

NIMH Code : H-511

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

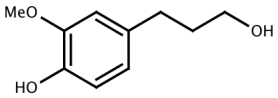


Mol. Formula : $C_{10}H_{10}N_2O_5$ **FW :** 238.20 **HBA:** 5 **HBD:** 5 **RotB:** 2

PubChem ID : **CASRN :** **AlogP:** 0.02 **TPSA:** 118.9

NIMH Code : H-512

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



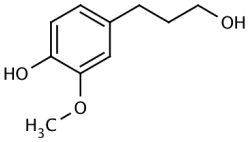
Mol. Formula : $C_{10}H_{14}N_2O_4$ **FW :** 226.23 **HBA:** 6 **HBD:** 5 **RotB:** 4

PubChem ID : 2563 **CASRN :** 38821-49-7 **AlogP:** -0.97 **TPSA:** 115.8

Activity: Aromatic-L-amino-acid decarboxylase inhibitor

NIMH Code : H-513

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

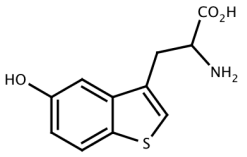


Mol. Formula : $C_{10}H_{14}O_3$ **FW :** 182.22 **HBA:** 3 **HBD:** 2 **RotB:** 4

PubChem ID : 16822 **CASRN :** 2305-13-7 **AlogP:** 1.32 **TPSA:** 49.7

NIMH Code : H-515

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

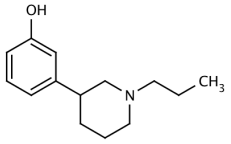


Mol. Formula : $C_{11}H_{11}NO_3S$ **FW :** 237.28 **HBA:** 5 **HBD:** 3 **RotB:** 3

PubChem ID : 32334 **CASRN :** 24358-04-1 **AlogP:** -0.68 **TPSA:** 111.8

NIMH Code : H-516

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



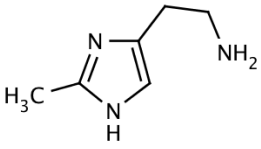
Mol. Formula : $C_{14}H_{22}BrNO$ **FW :** 300.24 **HBA:** 2 **HBD:** 1 **RotB:** 3

PubChem ID : 23045647 **CASRN :** 75240-91-4 **AlogP:** 2.57 **TPSA:** 23.5

Activity: Antiparkinson agent; dopaminergic agent

NIMH Code : H-517

Compound name : 2-Methylhistamine dipicrate

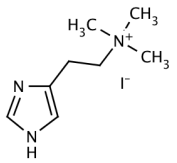


Mol. Formula : $C_{18}H_{17}N_9O_{14}$ **FW :** 583.38 **HBA:** 2 **HBD:** 2 **RotB:** 2

PubChem ID : 91613 **CASRN :** 34392-54-6 **AlogP:** -0.52 **TPSA:** 54.7

NIMH Code : H-518

Compound name : N,N-Dimethylhistamine methiodide

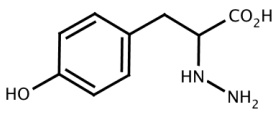


Mol. Formula : $C_8H_{16}N_3I$ **FW :** 281.14 **HBA:** 1 **HBD:** 1 **RotB:** 3

PubChem ID : **CASRN :** **AlogP:** -4.60 **TPSA:** 28.7

NIMH Code : H-520

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



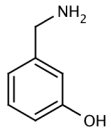
Mol. Formula : $C_9H_{12}N_2O_3$ **FW :** 196.21 **HBA:** 5 **HBD:** 4 **RotB:** 4

PubChem ID : 151250 **CASRN :** 5060-36-6 **AlogP:** -0.61 **TPSA:** 95.6

Activity: Fungal tyrosinase inhibitor

NIMH Code : H-521

Compound name : 3-Hydroxybenzylamine

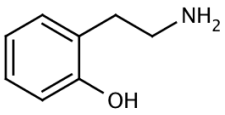


Mol. Formula : C_7H_9NO **FW :** 123.16 **HBA:** 2 **HBD:** 2 **RotB:** 1

PubChem ID : 735894 **CASRN :** **AlogP:** 0.32 **TPSA:** 46.3

NIMH Code : H-522

Compound name : 2-Hydroxy-β-phenethylamine hydrochloride

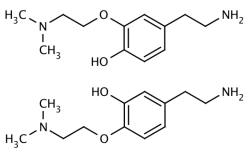


Mol. Formula : $C_8H_{12}ClNO$ **FW :** 173.64 **HBA:** 2 **HBD:** 2 **RotB:** 2

PubChem ID : 199864 **CASRN :** 5136-97-0 **AlogP:** 0.82 **TPSA:** 46.3

NIMH Code : H-523

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

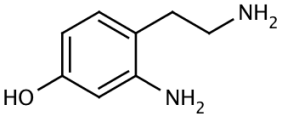


Mol. Formula : $C_{12}H_{22}Cl_2N_2O_2$ **FW :** 297.23 **HBA:** 4 **HBD:** 2 **RotB:** 6

PubChem ID : **CASRN :** **AlogP:** 0.32 **TPSA:** 58.7

NIMH Code : H-525

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

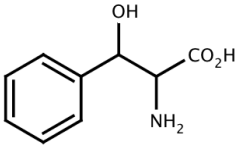


Mol. Formula : $C_8H_{14}Br_2N_2O$ **FW :** 314.02 **HBA:** 3 **HBD:** 3 **RotB:** 2

PubChem ID : 9877425 **CASRN :** **AlogP:** -0.18 **TPSA:** 72.3

NIMH Code : H-526

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



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

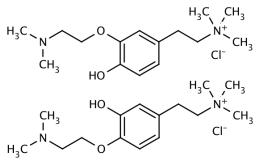
PubChem ID : 94134 **CASRN :** 1078-17-7 **AlogP:** -2.07 **TPSA:** 83.6

NIMH Code : H-527

Compound 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



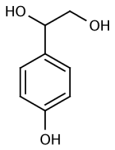
NIMH Code : H-528

Compound 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



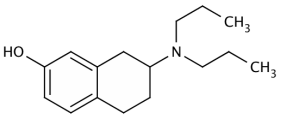
NIMH Code : H-701

Compound 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



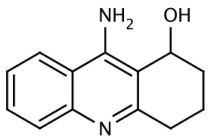
NIMH Code : H-703

Compound 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



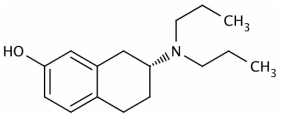
NIMH Code : H-704

Compound 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



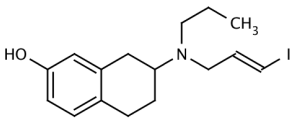
NIMH Code : H-705

Compound 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



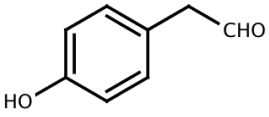
NIMH Code : H-901

Compound name : 4-Hydroxyphenylacetaldehyde

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

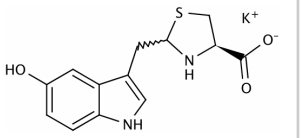
PubChem ID : 440113 **CASRN :** 7339-87-9 **AlogP:** 0.98 **TPSA:** 37.3

Activity: Tyrosine metabolite



NIMH Code : H-902

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

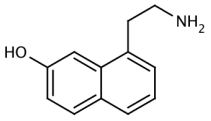


Mol. Formula : $C_{13}H_{13}KN_2O_3S$ **FW :** 316.42 **HBA:** 5 **HBD:** 3 **RotB:** 3

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

NIMH Code : H-903

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



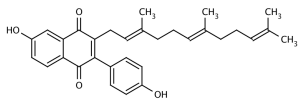
Mol. Formula : $C_{12}H_{14}ClNO$ **FW :** 223.70 **HBA:** 2 **HBD:** 2 **RotB:** 2

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

Activity: Serotonin N-acetyltransferase inhibitor

NIMH Code : H-904

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

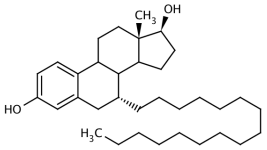


Mol. Formula : $C_{31}H_{34}O_4$ **FW :** 470.60 **HBA:** 4 **HBD:** 2 **RotB:** 9

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

NIMH Code : H-905

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

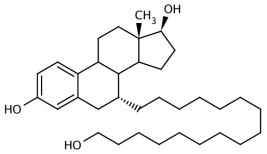


Mol. Formula : $C_{34}H_{56}O_2$ **FW :** 496.81 **HBA:** 2 **HBD:** 2 **RotB:** 15

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

NIMH Code : H-906

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

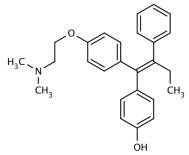


Mol. Formula : $C_{34}H_{56}O_3$ **FW :** 512.81 **HBA:** 3 **HBD:** 3 **RotB:** 16

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

NIMH Code : H-907

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



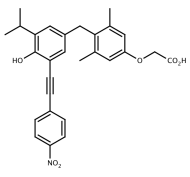
Mol. Formula : $C_{26}H_{29}NO_2$ **FW :** 387.51 **HBA:** 3 **HBD:** 1 **RotB:** 8

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

Activity: Estrogen receptor modulator

NIMH Code : H-908

Compound name : NH-3; Thyromimetic 5b



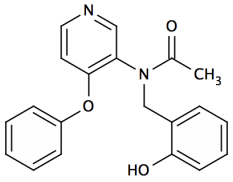
Mol. Formula : $C_{28}H_{27}NO_6$ **FW :** 473.52 **HBA:** 6 **HBD:** 2 **RotB:** 9

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

Activity: β-Subtype thyroid hormone receptor antagonist

NIMH Code : H-909

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



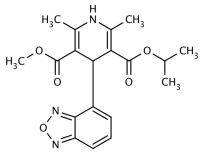
Mol. Formula : $C_{20}H_{18}N_2O_3$ **FW :** 334.38 **HBA:** 3 **HBD:** 1 **RotB:** 5

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

Activity: Brain peripheral benzodiazepine receptor (TSPO) ligand

NIMH Code : I-124

Compound name : Isradipine



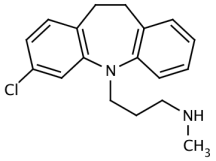
Mol. Formula : $C_{19}H_{21}N_3O_5$ **FW :** 371.39 **HBA:** 5 **HBD:** 1 **RotB:** 6

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

Activity: Calcium channel blocker

NIMH Code : I-501

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

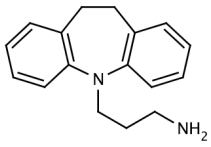


Mol. Formula : $C_{18}H_{22}Cl_2N_2$ **FW :** 337.29 **HBA:** 3 **HBD:** 1 **RotB:** 4

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

NIMH Code : I-502

Compound name : N,N-Didesmethylimipramine hydrochloride



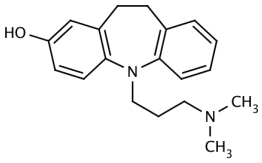
Mol. Formula : $C_{17}H_{21}ClN_2$ **FW :** 288.82 **HBA:** 2 **HBD:** 1 **RotB:** 3

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

Activity: Imipramine metabolite

NIMH Code : I-503

Compound name : 2-Hydroxyimipramine



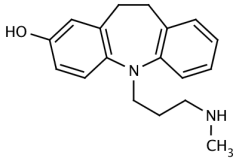
Mol. Formula : $C_{19}H_{24}N_2O$ **FW :** 296.31 **HBA:** 3 **HBD:** 1 **RotB:** 4

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

Activity: Imipramine metabolite

NIMH Code : I-504

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



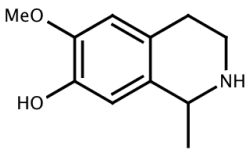
Mol. Formula : $C_{18}H_{22}N_2O$ **FW :** 282.38 **HBA:** 3 **HBD:** 2 **RotB:** 4

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

Activity: Tricyclic antidepressive agent; Imipramine metabolite

NIMH Code : I-505

Compound name : (±)-Isosalsoline hydrochloride

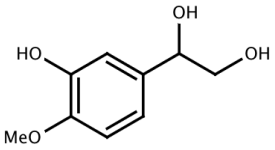


Mol. Formula : $C_{11}H_{16}ClNO_2$ **FW :** 229.71 **HBA:** 3 **HBD:** 2 **RotB:** 1

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

NIMH Code : I-701

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

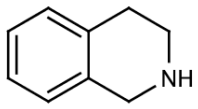


Mol. Formula : $C_9H_{12}O_4$ **FW :** 184.19 **HBA:** 4 **HBD:** 3 **RotB:** 3

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

NIMH Code : I-702

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



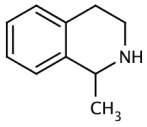
Mol. Formula : $C_9H_{12}ClN$ **FW :** 169.66 **HBA:** 1 **HBD:** 1 **RotB:** 0

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

Activity: Potential dopaminergic neurotoxin

NIMH Code : I-703

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



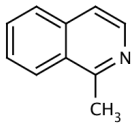
Mol. Formula : $C_{10}H_{14}ClN$ **FW :** 183.68 **HBA:** 1 **HBD:** 1 **RotB:** 0

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

Activity: Potential dopaminergic neurotoxin

NIMH Code : I-704

Compound name : 1-Methylisoquinoline hydrochloride



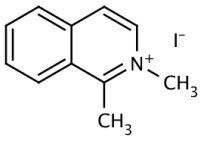
Mol. Formula : $C_{10}H_{10}ClN$ **FW :** 179.65 **HBA:** 1 **HBD:** 0 **RotB:** 0

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

Activity: Potential dopaminergic neurotoxin

NIMH Code : I-705

Compound name : 1,2-Dimethylisoquinolinium iodide

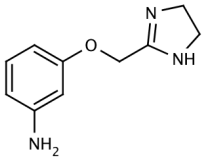


Mol. Formula : $C_{11}H_{12}IN$ **FW :** 285.13 **HBA:** 0 **HBD:** 0 **RotB:** 0

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

NIMH Code : I-706

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



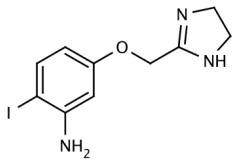
Mol. Formula : $C_{10}H_{15}Cl_2N_3O$ **FW :** 264.16 **HBA:** 4 **HBD:** 2 **RotB:** 3

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

Activity: Imidazoline-guaninidine binding site (IGRS) ligand

NIMH Code : I-707

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



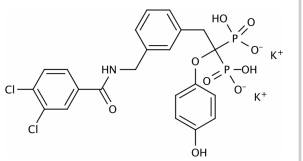
Mol. Formula : $C_{10}H_{14}Cl_2IN_3O$ **FW :** 390.05 **HBA:** 4 **HBD:** 2 **RotB:** 3

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

Activity: Imidazoline-guaninidine binding site (IGRS) ligand

NIMH Code : I-709

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



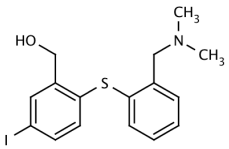
Mol. Formula : $C_{22}H_{19}Cl_2K_2NP_2O_9$ **FW :** 652.45 **HBA:** 11 **HBD:** 4 **RotB:** 9

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

Activity: Non-hydrolysable inhibitor of myo-inositol monophosphatase

NIMH Code : I-801

Compound name : IDAM hydrochloride



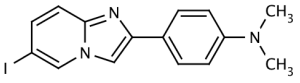
Mol. Formula : $C_{16}H_{19}ClINOS$ **FW :** 435.76 **HBA:** 3 **HBD:** 1 **RotB:** 5

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

Activity: Serotonin transporter SPECT imaging agent; reference standard

NIMH Code : I-901

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



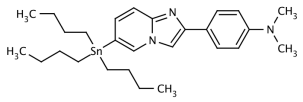
Mol. Formula : $C_{15}H_{14}IN_3$ **FW :** 363.20 **HBA:** 3 **HBD:** 0 **RotB:** 2

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

Activity: Beta-amyloid aggregate-specific ligand

NIMH Code : I-902

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



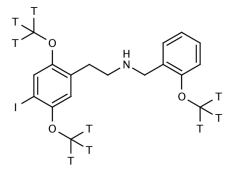
Mol. Formula : $C_{27}H_{41}N_3Sn$ **FW :** 526.34 **HBA:** 3 **HBD:** 0 **RotB:** 12

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

Activity: Radio-iodinated IMPY precursor

NIMH Code : I-903

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



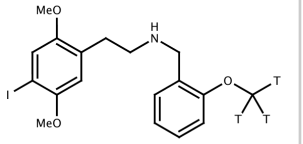
Mol. Formula : $C_{18}H_{22}INO_3$ **FW :** 427.28 **HBA:** 4 **HBD:** 1 **RotB:** 8

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

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

NIMH Code : I-904

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



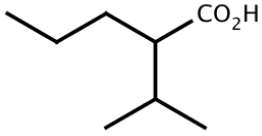
Mol. Formula : $C_{18}H_{22}INO_3$ **FW :** 427.28 **HBA:** 4 **HBD:** 1 **RotB:** 8

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

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

NIMH Code : I-905

Compound name : 2-Isopropylpentanoic acid; PIA



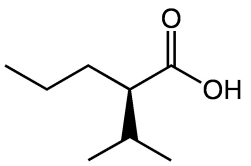
Mol. Formula : $C_8H_{16}O_2$ **FW :** 144.21 **HBA:** 2 **HBD:** 1 **RotB:** 4

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

Activity: Anticonvulsant

NIMH Code : I-906 new

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



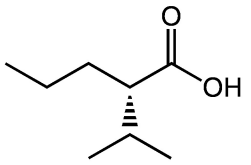
Mol. Formula : $C_8H_{16}O_2$ **FW :** 144.20 **HBA:** 2 **HBD:** 1 **RotB:** 4

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

Activity: Anticonvulsant.

NIMH Code : I-907 new

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



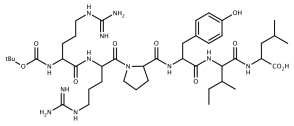
Mol. Formula : $C_8H_{16}O_2$ **FW :** 144.20 **HBA:** 2 **HBD:** 1 **RotB:** 4

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

Activity: Anticonvulsant.

NIMH Code : J-901

Compound name : JMV-431



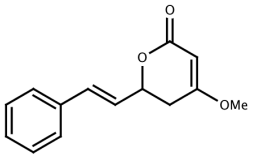
Mol. Formula : $C_{47}H_{82}N_{12}O_{13}$ **FW :** 1023.23 **HBA:** 16 **HBD:** 13 **RotB:** 28

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

Activity: Neurotensin receptor subtype 2 agonist

NIMH Code : K-501

Compound name : Kawain



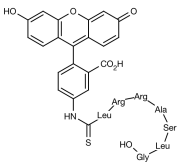
Mol. Formula : $C_{14}H_{14}O_3$ **FW :** 230.27 **HBA:** 2 **HBD:** 0 **RotB:** 3

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

Activity: Anticonvulsant; axiolytic

NIMH Code : K-701

Compound name : Kemptide fluorescein



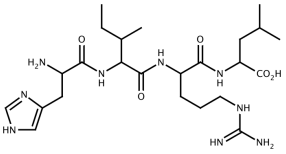
Mol. Formula : $C_{53}H_{72}N_{14}O_{14}S$ **FW :** 1161.29 **HBA:** 22 **HBD:** 18 **RotB:** 30

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

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

NIMH Code : L-901

Compound name : β-Lactotensin



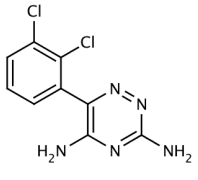
Mol. Formula : $C_{30}H_{46}F_9N_9O_{11}$ **FW :** 879.73 **HBA:** 10 **HBD:** 9 **RotB:** 17

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

Activity: Neurotensin receptor subtype 2 agonist

NIMH Code : L-902

Compound name : Lamotrigine



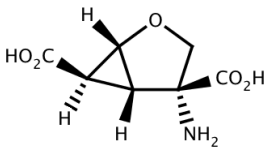
Mol. Formula : $C_9H_7Cl_2N_5$ **FW :** 256.09 **HBA:** 2 **HBD:** 7 **RotB:** 1

PubChem ID : 3878 **CASRN :** 84057-84-1 **AlogP:** 1.51 **TPSA:** 90.7

Activity: Voltage-sensitive sodium channel inhibitor

NIMH Code : L-903 new

Compound name : (1*R*,4*R*,5*S*,6*R*)-4-Amino-2-oxabicyclo[3.1.0]hexane-4,6-dicarboxylic acid (LY379268)



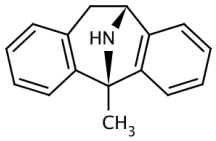
Mol. Formula : $C_7H_9NO_5$ **FW :** 187.15 **HBA:** 6 **HBD:** 3 **RotB:** 2

PubChem ID : 10197984 **CASRN :** 191471-52-0 **AlogP:** -3.90 **TPSA:** 109.9

Activity: Group II mGlu receptor agonist.

NIMH Code : M-107

Compound name : (+)-MK-801



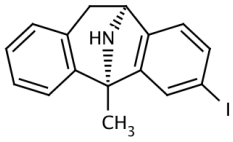
Mol. Formula : $C_{20}H_{19}NO_4$ **FW :** 337.37 **HBA:** 1 **HBD:** 1 **RotB:** 0

PubChem ID : 180081 **CASRN :** 77086-22-7 **AlogP:** 3.30 **TPSA:** 12.0

Activity: Non-competitive NMDA antagonist

NIMH Code : M-141

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



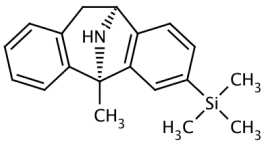
Mol. Formula : $C_{16}H_{15}ClIN$ **FW :** 383.66 **HBA:** 1 **HBD:** 1 **RotB:** 0

PubChem ID : 449735 **CASRN :** **AlogP:** 4.29 **TPSA:** 12.0

Activity: NMDA antagonist MK-801 analog

NIMH Code : M-143

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



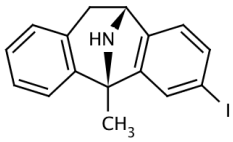
Mol. Formula : $C_{19}H_{24}ClNSi$ **FW :** 329.95 **HBA:** 1 **HBD:** 1 **RotB:** 1

PubChem ID : **CASRN :** **AlogP:** 4.88 **TPSA:** 12.0

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

NIMH Code : M-144

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



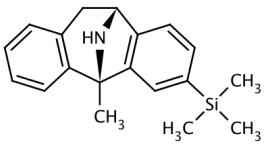
Mol. Formula : $C_{16}H_{15}ClIN$ **FW :** 383.66 **HBA:** 1 **HBD:** 1 **RotB:** 0

PubChem ID : 449735 **CASRN :** **AlogP:** 4.29 **TPSA:** 12.0

Activity: NMDA antagonist MK-801 analog

NIMH Code : M-145

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



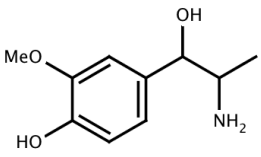
Mol. Formula : $C_{19}H_{24}ClNSi$ **FW :** 329.95 **HBA:** 1 **HBD:** 1 **RotB:** 1

PubChem ID : **CASRN :** **AlogP:** 4.88 **TPSA:** 12.0

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

NIMH Code : M-501

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

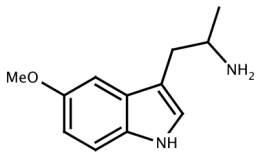


Mol. Formula : $C_{12}H_{17}NO_7$ **FW :** 287.27 **HBA:** 4 **HBD:** 3 **RotB:** 3

PubChem ID : **CASRN :** **AlogP:** -0.08 **TPSA:** 75.7

NIMH Code : M-502

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

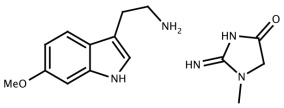


Mol. Formula : $C_{12}H_{17}ClN_2O$ **FW :** 240.73 **HBA:** 2 **HBD:** 2 **RotB:** 3

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

NIMH Code : M-503

Compound name : 6-Methoxytryptamine creatinine sulfate

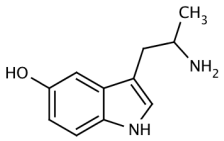


Mol. Formula : $C_{15}H_{23}N_5O_6S$ **FW :** 401.45 **HBA:** 2 **HBD:** 2 **RotB:** 3

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

NIMH Code : M-504

Compound name : α-Methylserotonin hydrogen oxalate



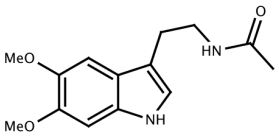
Mol. Formula : $C_{13}H_{16}N_2O_5$ **FW :** 280.28 **HBA:** 2 **HBD:** 3 **RotB:** 2

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

Activity: Serotonin 5-HT_{2B} agonist

NIMH Code : M-506

Compound name : 6-Methoxymelatonin



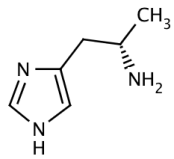
Mol. Formula : $C_{14}H_{18}N_2O_3$ **FW :** 262.31 **HBA:** 3 **HBD:** 2 **RotB:** 5

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

Activity: 6-Hydroxymelatonin metabolite

NIMH Code : M-507

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



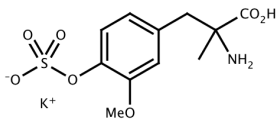
Mol. Formula : $C_9H_{14}N_3O_6$ **FW :** 260.23 **HBA:** 2 **HBD:** 2 **RotB:** 2

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

Activity: Histamine H_3 agonist

NIMH Code : M-508

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

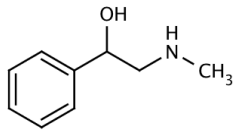


Mol. Formula : $C_{11}H_{14}KNO_7S$ **FW :** 343.40 **HBA:** 7 **HBD:** 2 **RotB:** 6

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

NIMH Code : M-509

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



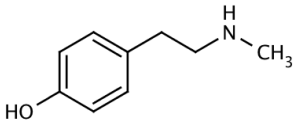
Mol. Formula : $C_9H_{13}NO$ **FW :** 151.21 **HBA:** 2 **HBD:** 2 **RotB:** 3

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

Activity: Monoamine oxidase A/B substrate

NIMH Code : M-510

Compound name : N-Methyltyramine hydrobromide

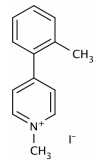


Mol. Formula : $C_9H_{14}BrNO$ **FW :** 232.12 **HBA:** 2 **HBD:** 2 **RotB:** 3

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

NIMH Code : M-701

Compound 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

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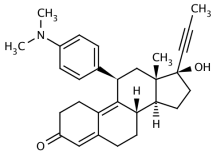
NIMH Code : M-703

Compound name : Mifepristone



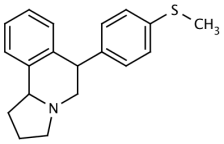
Mol. Formula : $C_{29}H_{35}NO_2$ **FW :** 429.59 **HBA:** 3 **HBD:** 1 **RotB:** 3

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

Activity: Progesterone receptor antagonist

NIMH Code : M-704

Compound name : (±)-McN-5652



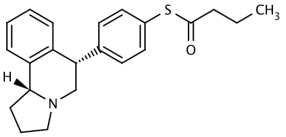
Mol. Formula : $C_{19}H_{22}ClNO_4S$ **FW :** 395.91 **HBA:** 2 **HBD:** 0 **RotB:** 2

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

Activity: Serotonin transporter inhibitor

NIMH Code : M-706

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



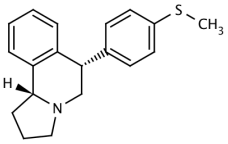
Mol. Formula : $C_{22}H_{25}NOS$ **FW :** 351.51 **HBA:** 3 **HBD:** 0 **RotB:** 5

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

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

NIMH Code : M-707

Compound name : (+)-McN-5652



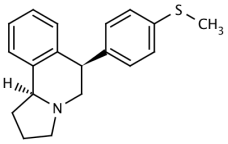
Mol. Formula : $C_{19}H_{22}ClNO_4S$ **FW :** 395.91 **HBA:** 2 **HBD:** 0 **RotB:** 2

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

Activity: Serotonin transporter inhibitor (active enantiomer)

NIMH Code : M-708

Compound name : (–)-McN-5652



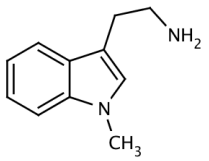
Mol. Formula : $C_{19}H_{22}ClNO_4S$ **FW :** 395.91 **HBA:** 2 **HBD:** 0 **RotB:** 2

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

Activity: Serotonin transporter inhibitor (inactive enantiomer)

NIMH Code : M-709

Compound name : 1-Methyltryptamine hydrochloride

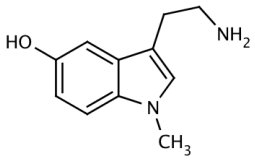


Mol. Formula : $C_{11}H_{15}ClN_2$ **FW :** 210.71 **HBA:** 1 **HBD:** 1 **RotB:** 2

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

NIMH Code : M-710

Compound name : 1-Methylserotonin hydrogen maleate



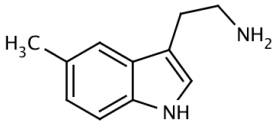
Mol. Formula : $C_{15}H_{18}N_2O_5$ **FW :** 306.32 **HBA:** 2 **HBD:** 2 **RotB:** 2

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

Activity: Serotonin analog

NIMH Code : M-711

Compound name : 5-Methyltryptamine hydrogen maleate



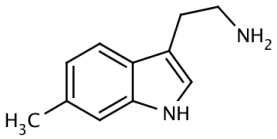
Mol. Formula : $C_{15}H_{18}N_2O_4$ **FW :** 290.32 **HBA:** 1 **HBD:** 2 **RotB:** 2

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

Activity: Serotonin analog

NIMH Code : M-712

Compound name : 6-Methyltryptamine hydrogen maleate



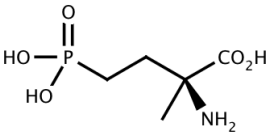
Mol. Formula : $C_{15}H_{18}N_2O_4$ **FW :** 290.32 **HBA:** 1 **HBD:** 2 **RotB:** 2

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

Activity: Serotonin analog

NIMH Code : M-801

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



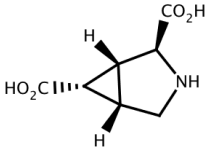
Mol. Formula : $C_5H_{12}NO_5P$ **FW :** 197.13 **HBA:** 6 **HBD:** 4 **RotB:** 4

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

Activity: Metabotropic glutamate $mGluR_{2/3}$ agonist

NIMH Code : M-802

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



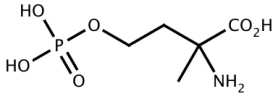
Mol. Formula : $C_7H_9NO_4$ **FW :** 171.15 **HBA:** 5 **HBD:** 3 **RotB:** 2

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

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

NIMH Code : M-803

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



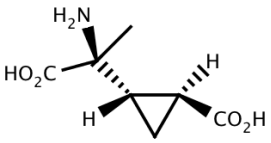
Mol. Formula : $C_4H_{10}NO_6P$ **FW :** 199.10 **HBA:** 6 **HBD:** 4 **RotB:** 4

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

Activity: Metabotropic glutamate mGluR antagonist

NIMH Code : M-804

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



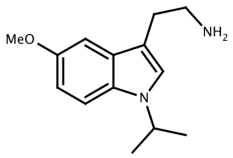
Mol. Formula : $C_7H_{11}NO_4$ **FW :** 173.17 **HBA:** 5 **HBD:** 3 **RotB:** 3

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

Activity: Metabotropic glutamate $mGluR_2$ antagonist

NIMH Code : M-805

Compound name : 5-Methoxy-1-isopropyltryptamine



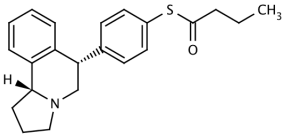
Mol. Formula : $C_{14}H_{20}N_2O$ **FW :** 232.33 **HBA:** 2 **HBD:** 1 **RotB:** 4

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

Activity: Serotonin analog

NIMH Code : M-901

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



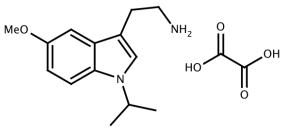
Mol. Formula : $C_{26}H_{31}NO_7S$ **FW :** 501.60 **HBA:** 3 **HBD:** 0 **RotB:** 5

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

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

NIMH Code : M-902

Compound name : 5-Methoxy-1-isopropyltryptamine oxalate



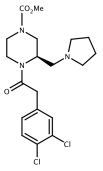
Mol. Formula : $C_{16}H_{22}N_2O_5$ **FW :** 322.36 **HBA:** 2 **HBD:** 1 **RotB:** 4

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

Activity: Serotonin analog

NIMH Code : M-903

Compound name : GR103545



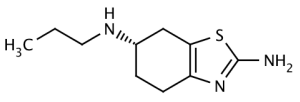
Mol. Formula : $C_{19}H_{25}Cl_2N_3O_3$ **FW :** 414.33 **HBA:** 6 **HBD:** 0 **RotB:** 5

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

Activity: Opioid receptor agonist

NIMH Code : M-904

Compound name : Mirapex; Pramipexole



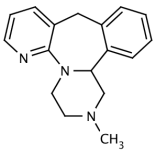
Mol. Formula : $C_{10}H_{17}N_3S$ **FW :** 211.33 **HBA:** 4 **HBD:** 2 **RotB:** 3

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

Activity: Dopamine D_3 agonist

NIMH Code : M-905

Compound name : Mirtazapine



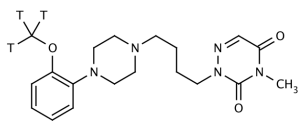
Mol. Formula : $C_{17}H_{19}N_3$ **FW :** 265.35 **HBA:** 3 **HBD:** 0 **RotB:** 0

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

Activity: Serotonin & noradrenergic antagonist

NIMH Code : M-906

Compound name : 2-{4-[4-C^{3}H$_3$]-2-Methoxyphenyl)piperazin-1-yl]butyl}-4-methyl-1,2,4-triazine-3,5-(2*H*,4*H*)dione; [^{3}H]CUMI-101



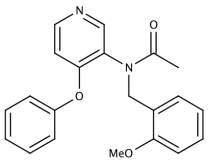
Mol. Formula : $C_{19}H_{27}N_5O_3$ **FW :** 373.46 **HBA:** 0 **HBD:** 6 **RotB:** 7

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

Activity: Radiolabeled serotonin 5-HT$_{1A}$ agonist

NIMH Code : M-907

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



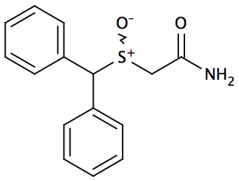
Mol. Formula : $C_{21}H_{20}N_2O_3$ **FW :** 348.40 **HBA:** 3 **HBD:** 0 **RotB:** 6

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

Activity: Brain peripheral benzodiazepine receptor (TSPO) ligand

NIMH Code : M-908

Compound name : (±)-Modafinil

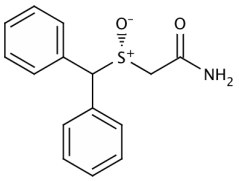


Mol. Formula : $C_{15}H_{15}NO_2S$ **FW :** 273.35 **HBA:** 2 **HBD:** 1 **RotB:** 5

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

NIMH Code : M-909

Compound name : (*R*)-(–)-Modafinil



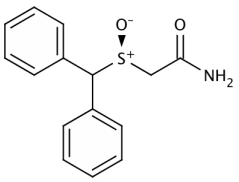
Mol. Formula : $C_{15}H_{15}NO_2S$ **FW :** 273.35 **HBA:** 2 **HBD:** 1 **RotB:** 5

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

Activity: Dopamine D$_2$ partial agonist

NIMH Code : M-910

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

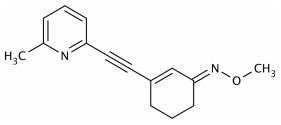


Mol. Formula : $C_{15}H_{15}NO_2S$ **FW :** 273.35 **HBA:** 2 **HBD:** 1 **RotB:** 5

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

NIMH Code : M-911

Compound name : ABP688



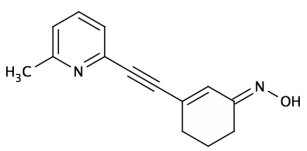
Mol. Formula : $C_{15}H_{16}N_2O$ **FW :** 240.31 **HBA:** 3 **HBD:** 0 **RotB:** 3

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

Activity: Metabotropic glutamate mGluR5 antagonist

NIMH Code : M-912

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



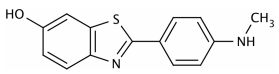
Mol. Formula : $C_{14}H_{14}N_2O$ **FW :** 226.27 **HBA:** 3 **HBD:** 1 **RotB:** 2

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

Activity: ABP688 PET ligand precursor

NIMH Code : M-913

Compound name : 6-OH-BTA-1



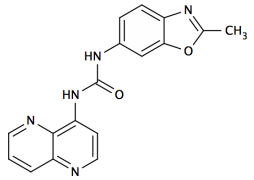
Mol. Formula : $C_{14}H_{12}N_2OS$ **FW :** 256.33 **HBA:** 4 **HBD:** 2 **RotB:** 2

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

Activity: Aggregated amyloid protein ligand; Thioflavin-T analog

NIMH Code : M-914

Compound name : SB-334867



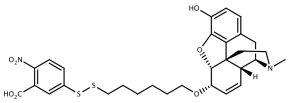
Mol. Formula : $C_{17}H_{13}N_5O_2$ **FW :** 319.32 **HBA:** 4 **HBD:** 2 **RotB:** 2

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

Activity: Orexin subtype 1 antagonist

NIMH Code : M-915

Compound name : Morphine-SH-DTNB derivative

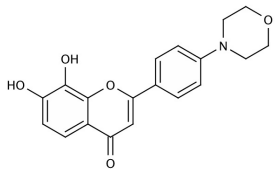


Mol. Formula : $C_{30}H_{34}N_2O_7S_2$ **FW :** 598.83 **HBA:** 8 **HBD:** 2 **RotB:** 12

PubChem ID : **CASRN :** **AlogP:** 2.94 **TPSA:** 125.1

NIMH Code : M-916

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

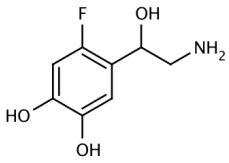


Mol. Formula : $C_{19}H_{17}NO_5$ **FW :** 339.34 **HBA:** 6 **HBD:** 2 **RotB:** 2

PubChem ID : **CASRN :** **AlogP:** 2.25 **TPSA:** 79.2

NIMH Code : N-502

Compound name : 6-Fluoronorepinephrine oxalate



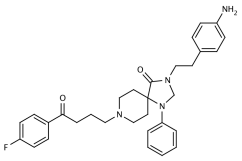
Mol. Formula : $C_{18}H_{22}F_2N_2O_{10}$ **FW :** 464.38 **HBA:** 5 **HBD:** 4 **RotB:** 2

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

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

NIMH Code : N-701

Compound name : p-Aminophenethylspiperone



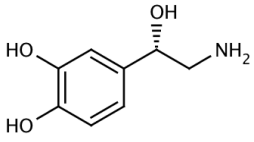
Mol. Formula : $C_{31}H_{35}FN_4O_2$ **FW :** 514.65 **HBA:** 6 **HBD:** 1 **RotB:** 9

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

Activity: Dopamine D_2 antagonist

NIMH Code : N-702

Compound name : (+)-Norepinephrine tartrate



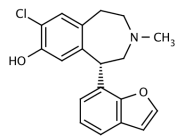
Mol. Formula : $C_{12}H_{17}NO_9$ **FW :** 319.27 **HBA:** 4 **HBD:** 4 **RotB:** 2

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

Activity: Unnatural enantiomer of norepinephrine

NIMH Code : N-703

Compound name : (+)-NNC 01-0112



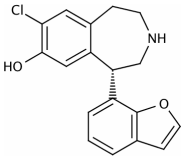
Mol. Formula : $C_{19}H_{18}ClNO_2$ **FW :** 327.80 **HBA:** 3 **HBD:** 1 **RotB:** 1

PubChem ID : 130424 **CASRN :** 125341-24-4 **AlogP:** 3.37 **TPSA:** 36.6

Activity: Dopamine D_1 receptor ligand

NIMH Code : N-704

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



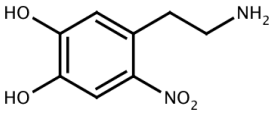
Mol. Formula : $C_{18}H_{17}Cl_2NO_2$ **FW :** 350.23 **HBA:** 3 **HBD:** 2 **RotB:** 1

PubChem ID : 20135382 **CASRN :** **AlogP:** 2.13 **TPSA:** 45.4

Activity: NNC-01-0112 PET ligand precusor

NIMH Code : N-705

Compound name : 6-Nitrodopamine



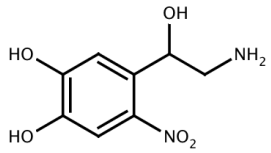
Mol. Formula : $C_8H_{10}N_2O_{14}$ **FW :** 198.17 **HBA:** 5 **HBD:** 3 **RotB:** 3

PubChem ID : 10932412 **CASRN :** **AlogP:** -1.09 **TPSA:** 112.3

Activity: Nitrated catecholamine

NIMH Code : N-706

Compound name : 6-Nitronorepinephrine



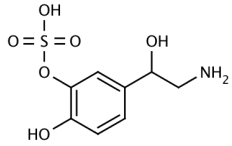
Mol. Formula : $C_8H_{10}N_2O_5$ **FW :** 214.98 **HBA:** 6 **HBD:** 4 **RotB:** 3

PubChem ID : **CASRN :** **AlogP:** -1.87 **TPSA:** 132.5

Activity: Nitrated catecholamine

NIMH Code : N-707

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



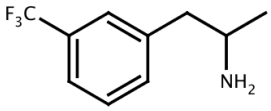
Mol. Formula : $C_8H_{11}NO_6S$ **FW :** 249.24 **HBA:** 6 **HBD:** 4 **RotB:** 4

PubChem ID : 10083394 **CASRN :** **AlogP:** -2.13 **TPSA:** 138.5

Activity: Catechol O-methyltransferase inhibitor

NIMH Code : N-801

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



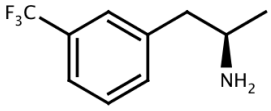
Mol. Formula : $C_{10}H_{13}ClF_3N$ **FW :** 239.67 **HBA:** 4 **HBD:** 1 **RotB:** 3

PubChem ID : 120765 **CASRN :** 673-18-7 **AlogP:** 2.71 **TPSA:** 26.0

Activity: Serotonin releaser & $5HT_{2B}$ agonist

NIMH Code : N-802

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



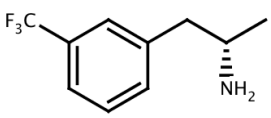
Mol. Formula : $C_{10}H_{13}ClF_3N$ **FW :** 239.67 **HBA:** 4 **HBD:** 1 **RotB:** 3

PubChem ID : 12895728 **CASRN :** **AlogP:** 2.71 **TPSA:** 26.0

Activity: Serotonin uptake inhibitor

NIMH Code : N-803

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



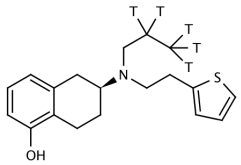
Mol. Formula : $C_{10}H_{13}ClF_3N$ **FW :** 239.67 **HBA:** 4 **HBD:** 1 **RotB:** 3

PubChem ID : 9815618 **CASRN :** **AlogP:** 2.71 **TPSA:** 26.0

Activity: Serotonin uptake inhibitor

NIMH Code : N-804

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



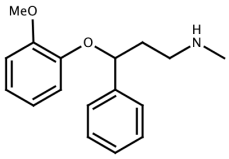
Mol. Formula : $C_{19}H_{26}ClNOS$ **FW :** 351.94 **HBA:** 3 **HBD:** 1 **RotB:** 6

PubChem ID : 6917969 **CASRN :** 92206-54-7 **AlogP:** 4.06 **TPSA:** 51.7

Activity: Radiolabeled dopamine receptor agonist

NIMH Code : N-901

Compound name : (±)-Nisoxetine hydrochloride



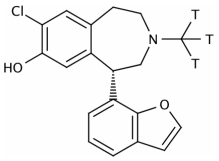
Mol. Formula : $C_{17}H_{22}ClNO_2$ **FW :** 307.82 **HBA:** 3 **HBD:** 1 **RotB:** 7

PubChem ID : 134453 **CASRN :** 57754-86-6 **AlogP:** 3.06 **TPSA:** 30.5

Activity: Norepinephrine uptake inhibitor

NIMH Code : N-902

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



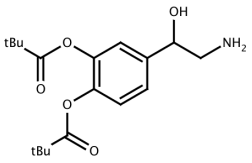
Mol. Formula : $C_{19}H_{19}ClNO_2$ **FW :** 328.82 **HBA:** 3 **HBD:** 1 **RotB:** 1

PubChem ID : 130424 **CASRN :** **AlogP:** 3.37 **TPSA:** 36.6

Activity: Radiolabeled dopamine D_1 receptor ligand

NIMH Code : N-903

Compound name : Norepinephrine dipivalate hydrochloride

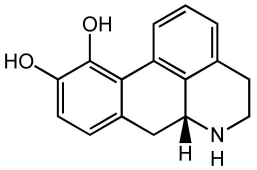


Mol. Formula : $C_{18}H_{28}ClNO_5$ **FW :** 373.87 **HBA:** 4 **HBD:** 2 **RotB:** 8

PubChem ID : **CASRN :** **AlogP:** 3.28 **TPSA:** 98.9

NIMH Code : N-904

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



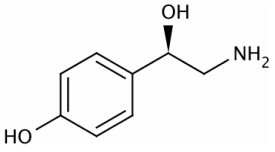
Mol. Formula : $C_{16}H_{16}BrNO_2$ **FW :** 334.21 **HBA:** 3 **HBD:** 3 **RotB:** 0

PubChem ID : 30133 **CASRN :** 20382-69-8 **AlogP:** 2.15 **TPSA:** 21.7

Activity: Dopamine D3 receptor ligand.

NIMH Code : O-501

Compound name : (–)-Octopamine



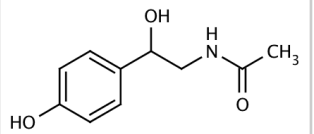
Mol. Formula : $C_8H_{11}NO_2$ **FW :** 153.18 **HBA:** 3 **HBD:** 3 **RotB:** 2

PubChem ID : 4581 **CASRN :** 104-14-3 **AlogP:** -0.30 **TPSA:** 66.5

Activity: Biogenic amine formed by β-hydroxylation of tyramine

NIMH Code : O-502

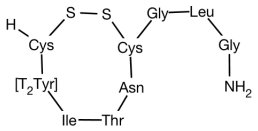
Compound name : N-Acetyl-(±)-octopamine



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

NIMH Code : O-801

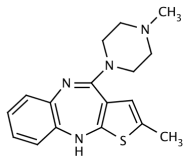
Compound name : [^{3}H][Thr^4,Gly^7]Oxytocin



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								

NIMH Code : O-901

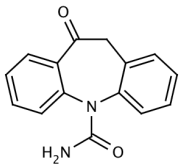
Compound name : Olanzapine



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								

NIMH Code : O-902

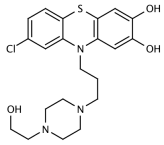
Compound name : Oxcarbazepine



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:	Sodium channel inhibitor								

NIMH Code : P-501

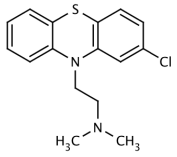
Compound name : 7,8-Dihydroxyperphenazine dihydrochloride



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

NIMH Code : P-503

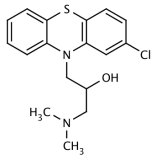
Compound name : 2-Chloro-10-(2-dimethylaminoethyl)phenothiazine hydrochloride



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

NIMH Code : P-504

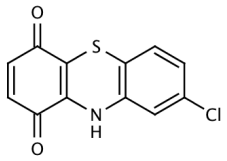
Compound name : (±)-2-Chloro-10-(3-dimethylamino-2-hydroxypropyl)phenothiazine hydrogen maleate



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

NIMH Code : P-505

Compound name : 2-Chloro-6,9-dioxophenothiazine

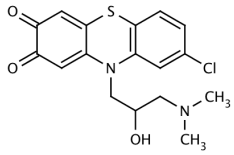


Mol. Formula : $C_{12}H_6ClNO_2S$ **FW :** 263.70 **HBA:** 5 **HBD:** 1 **RotB:** 0

PubChem ID : **CASRN :** **AlogP:** 2.26 **TPSA:** 71.5

NIMH Code : P-506

Compound name : (±)-2-Chloro-7,8-dioxo-10-(3-dimethylamino-2-hydroxypropyl)phenothiazine hydrochloride

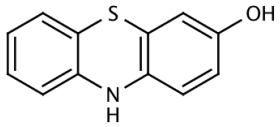


Mol. Formula : $C_{17}H_{18}Cl_2N_2O_3S$ **FW :** 401.31 **HBA:** 7 **HBD:** 1 **RotB:** 4

PubChem ID : **CASRN :** **AlogP:** 1.81 **TPSA:** 86.2

NIMH Code : P-508

Compound name : 3-Hydroxyphenothiazine

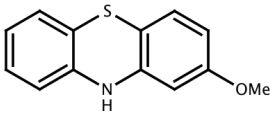


Mol. Formula : $C_{12}H_9NOS$ **FW :** 215.27 **HBA:** 3 **HBD:** 2 **RotB:** 0

PubChem ID : 74725 **CASRN :** 1927-44-2 **AlogP:** 3.48 **TPSA:** 57.6

NIMH Code : P-509

Compound name : 2-Methoxyphenothiazine

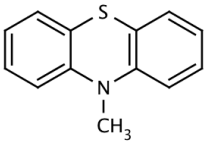


Mol. Formula : $C_{13}H_{11}NOS$ **FW :** 229.30 **HBA:** 3 **HBD:** 1 **RotB:** 1

PubChem ID : 74490 **CASRN :** 1771-18-2 **AlogP:** 3.51 **TPSA:** 46.6

NIMH Code : P-510

Compound name : N-Methylphenothiazine

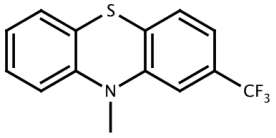


Mol. Formula : $C_{13}H_{11}NS$ **FW :** 213.30 **HBA:** 2 **HBD:** 0 **RotB:** 0

PubChem ID : 71015 **CASRN :** 1207-72-3 **AlogP:** 4.01 **TPSA:** 28.5

NIMH Code : P-511

Compound name : N-Methyl-2-(trifluoromethyl)phenothiazine

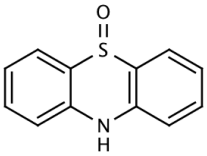


Mol. Formula : $C_{14}H_{10}F_3NS$ **FW :** 281.30 **HBA:** 5 **HBD:** 0 **RotB:** 1

PubChem ID : **CASRN :** **AlogP:** 4.89 **TPSA:** 28.5

NIMH Code : P-512

Compound name : Phenothiazine-5-oxide

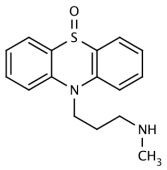


Mol. Formula : $C_{12}H_9NOS$ **FW :** 215.27 **HBA:** 2 **HBD:** 1 **RotB:** 0

PubChem ID : 71014 **CASRN :** 1207-71-2 **AlogP:** 1.79 **TPSA:** 48.3

NIMH Code : P-513

Compound name : *nor*-1-Promazine sulfoxide hydrochloride

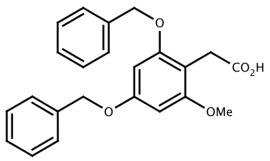


Mol. Formula : $C_{16}H_{19}ClN_2OS$ **FW :** 322.86 **HBA:** 3 **HBD:** 1 **RotB:** 4

PubChem ID : 23275476 **CASRN :** **AlogP:** 1.70 **TPSA:** 51.6

NIMH Code : P-514

Compound name : 2,4-Dibenzyloxy-5-methoxyphenylacetic acid

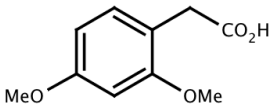


Mol. Formula : $C_{23}H_{22}O_5$ **FW :** 378.42 **HBA:** 5 **HBD:** 1 **RotB:** 9

PubChem ID : **CASRN :** **AlogP:** 4.47 **TPSA:** 65.0

NIMH Code : P-515

Compound name : 2,4-Dimethoxyphenylacetic acid

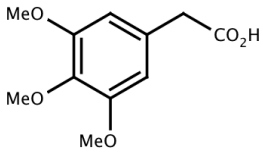


Mol. Formula : $C_{10}H_{12}O_4$ **FW :** 196.20 **HBA:** 4 **HBD:** 1 **RotB:** 4

PubChem ID : 350555 **CASRN :** 6496-89-5 **AlogP:** 1.17 **TPSA:** 55.8

NIMH Code : P-516

Compound name : 3,4,5-Trimethoxyphenylacetic acid



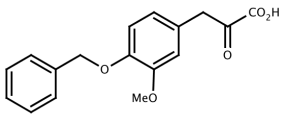
Mol. Formula : $C_{11}H_{14}O_5$ **FW :** 226.23 **HBA:** 5 **HBD:** 1 **RotB:** 5

PubChem ID : 70372 **CASRN :** 951-82-6 **AlogP:** 0.92 **TPSA:** 65.0

Activity: Mescaline metabolite

NIMH Code : P-517

Compound name : 4-Benzyloxyphenyl-3-methoxypyruvic acid

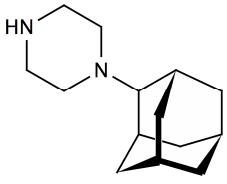


Mol. Formula : $C_{17}H_{16}O_5$ **FW :** 300.31 **HBA:** 5 **HBD:** 1 **RotB:** 7

PubChem ID : **CASRN :** **AlogP:** 3.42 **TPSA:** 72.8

NIMH Code : P-518

Compound name : N-(2-Adamantyl)piperazine dihydrochloride

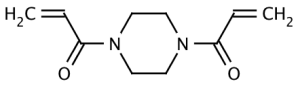


Mol. Formula : $C_{14}H_{26}Cl_2N_2$ **FW :** 293.28 **HBA:** 2 **HBD:** 1 **RotB:** 1

PubChem ID : 4599242 **CASRN :** **AlogP:** 1.64 **TPSA:** 15.3

NIMH Code : P-519

Compound name : 1,4-Diacryloylpiperazine



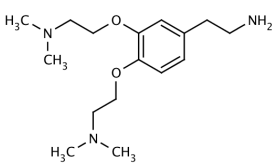
Mol. Formula : $C_{10}H_{14}N_2O_2$ **FW :** 194.23 **HBA:** 2 **HBD:** 0 **RotB:** 2

PubChem ID : 193422 **CASRN :** 6342-17-2 **AlogP:** 0.07 **TPSA:** 40.6

Activity: Cross-linking monomer for development of polyacrylamide gels

NIMH Code : P-520

Compound name : 3,4-Di(β-dimethylaminoethoxy)-β-phenethylamine trihydrochloride

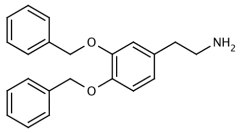


Mol. Formula : $C_{16}H_{32}Cl_3N_3O_2$ **FW :** 404.81 **HBA:** 5 **HBD:** 1 **RotB:** 10

PubChem ID : **CASRN :** **AlogP:** 0.87 **TPSA:** 51.0

NIMH Code : P-521

Compound name : 3,4-Dibenzyloxy-β-phenethylamine hydrochloride

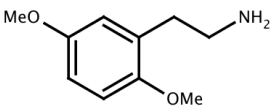


Mol. Formula : $C_{22}H_{24}ClNO_2$ **FW :** 369.89 **HBA:** 3 **HBD:** 1 **RotB:** 8

PubChem ID : 423869 **CASRN :** 1699-56-5 **AlogP:** 4.46 **TPSA:** 44.5

NIMH Code : P-522

Compound name : 2,5-Dimethoxy-β-phenethylamine hydrochloride

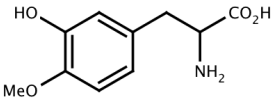


Mol. Formula : $C_{10}H_{16}ClNO_2$ **FW :** 217.70 **HBA:** 3 **HBD:** 1 **RotB:** 4

PubChem ID : 24187012 **CASRN :** 3166-74-3 **AlogP:** 0.91 **TPSA:** 44.5

NIMH Code : P-526

Compound name : 3-Hydroxy-4-methoxy-(±)-phenylalanine

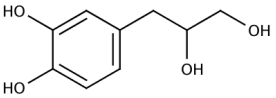


Mol. Formula : $C_{10}H_{13}NO_4$ **FW :** 211.22 **HBA:** 5 **HBD:** 3 **RotB:** 4

PubChem ID : 586369 **CASRN :** 4368-01-8 **AlogP:** -1.68 **TPSA:** 92.8

NIMH Code : P-528

Compound name : Vanillyl glycol



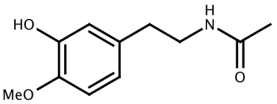
Mol. Formula : $C_{16}H_{26}N_2O_4$ **FW :** 310.39 **HBA:** 4 **HBD:** 3 **RotB:** 4

PubChem ID : 161566 **CASRN :** 27391-18-0 **AlogP:** 0.25 **TPSA:** 69.9

Activity: Lignin model compound

NIMH Code : P-701

Compound name : N-Acetyl-3-hydroxy-4-methoxy-β-phenethylamine

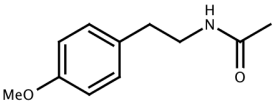


Mol. Formula : $C_{11}H_{15}NO_3$ **FW :** 209.25 **HBA:** 3 **HBD:** 2 **RotB:** 4

PubChem ID : 591256 **CASRN :** **AlogP:** 0.71 **TPSA:** 58.6

NIMH Code : P-703

Compound name : N-Acetyl-4-methoxy-β-phenethylamine

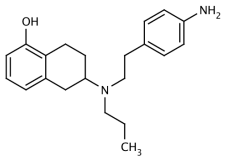


Mol. Formula : $C_{11}H_{15}NO_2$ **FW :** 193.25 **HBA:** 2 **HBD:** 1 **RotB:** 4

PubChem ID : 584258 **CASRN :** **AlogP:** 0.99 **TPSA:** 38.3

NIMH Code : P-706

Compound name : (±)-2-[*N*-(4'-Aminophenylethyl)-*N*-propyl]amino-5-hydroxytetralin dihydrochloride

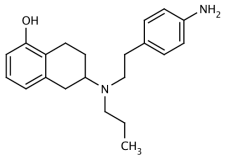


Mol. Formula : $C_{21}H_{30}Cl_2N_2O$ **FW :** 397.39 **HBA:** 3 **HBD:** 2 **RotB:** 6

PubChem ID : **CASRN :** **AlogP:** 3.37 **TPSA:** 49.5

NIMH Code : P-706A new

Compound name : (±)-2-[*N*-(4'-Aminophenylethyl)-*N*-propyl]amino-5-hydroxytetralin hydrochloride

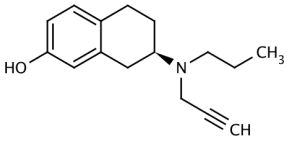


Mol. Formula : $C_{21}H_{29}ClN_2O$ **FW :** 360.92 **HBA:** 3 **HBD:** 2 **RotB:** 6

PubChem ID : **CASRN :** **AlogP:** 3.37 **TPSA:** 49.5

NIMH Code : P-707

Compound name : (*R*)-(+)-2-(*N*-Propargyl-*N*-propyl)amino-7-hydroxytetralin hydrochloride



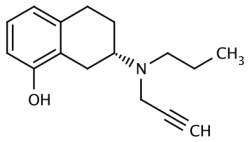
Mol. Formula : $C_{16}H_{22}ClNO$ **FW :** 279.81 **HBA:** 2 **HBD:** 1 **RotB:** 5

PubChem ID : 9992020 **CASRN :** **AlogP:** 3.43 **TPSA:** 23.5

Activity: Radiolabeling (*R*)-(+)-7-hydroxy-DPAT precursor

NIMH Code : P-708

Compound name : (*R*)-(–)-2-(*N*-Propargyl-*N*-propyl)amino-8-hydroxytetralin hydrochloride



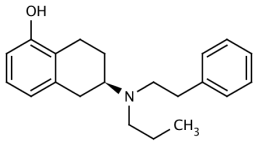
Mol. Formula : $C_{16}H_{22}ClNO$ **FW :** 279.81 **HBA:** 2 **HBD:** 1 **RotB:** 5

PubChem ID : **CASRN :** **AlogP:** 3.43 **TPSA:** 23.5

Activity: Radiolabeling (*R*)-(+)-8-hydroxy-DPAT precursor

NIMH Code : P-709

Compound name : (*S*)-(–)-2-(*N*-Phenylethyl-*N*-propyl)amino-5-hydroxytetralin hydrochloride

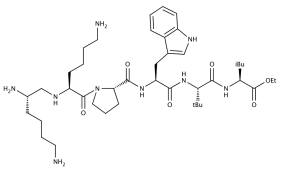


Mol. Formula : $C_{21}H_{28}ClNO$ **FW :** 345.91 **HBA:** 2 **HBD:** 1 **RotB:** 6

PubChem ID : **CASRN :** **AlogP:** 4.20 **TPSA:** 23.5

NIMH Code : P-710

Compound name : PD149163



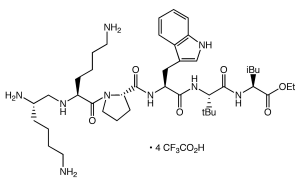
Mol. Formula : $C_{52}H_{76}F_{15}N_9O_{16}$ **FW :** 1368.20 **HBA:** 9 **HBD:** 8 **RotB:** 26

PubChem ID : **CASRN :** **AlogP:** 1.52 **TPSA:** 256.9

Activity: Neurotensin agonist

NIMH Code : P-710A

Compound name : PD149163



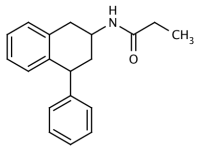
Mol. Formula : $C_{50}H_{75}F_{12}N_9O_{14}$ **FW :** 1254.16 **HBA:** 9 **HBD:** 8 **RotB:** 26

PubChem ID : **CASRN :** **AlogP:** 2.11 **TPSA:** 239.8

Activity: Neurotensin agonist

NIMH Code : P-801

Compound name : (±)-4-Phenyl-2-(propioamido)tetraline



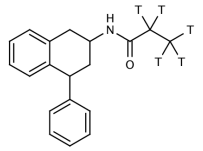
Mol. Formula : $C_{19}H_{21}NO$ **FW :** 279.38 **HBA:** 1 **HBD:** 1 **RotB:** 3

PubChem ID : 3976006 **CASRN :** 0 **AlogP:** 3.87 **TPSA:** 29.1

Activity: Melatonin receptor antagonist

NIMH Code : P-802

Compound name : 4-Phenyl-2-[(2',3'(n)-^{3}H)propioamido]tetraline



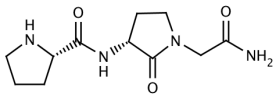
Mol. Formula : $C_{19}H_{21}NO$ **FW :** 279.38 **HBA:** 1 **HBD:** 1 **RotB:** 3

PubChem ID : 10708579 **CASRN :** **AlogP:** 3.87 **TPSA:** 29.1

Activity: Radiolabeled melatonin receptor antagonist

NIMH Code : P-803

Compound name : 3-(*R*)-[2-(*S*)-(Pyrrolidinylcarbonyl)amino]-2-oxo-1-pyrrolidineacetamide



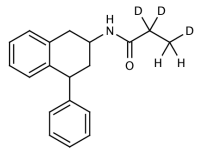
Mol. Formula : $C_{11}H_{18}N_4O_3$ **FW :** 254.28 **HBA:** 4 **HBD:** 3 **RotB:** 4

PubChem ID : 129409 **CASRN :** 106732-52-9 **AlogP:** -2.84 **TPSA:** 104.5

Activity: MSH release-inhibiting hormone antagonist

NIMH Code : P-804

Compound name : (±)-4-Phenyl-2-[2',2',3'-^{2}H]-(propioamido)tetralin



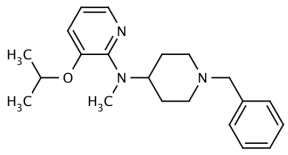
Mol. Formula : $C_{19}H_{18}D_3NO$ **FW :** 282.40 **HBA:** 1 **HBD:** 1 **RotB:** 3

PubChem ID : 3976006 **CASRN :** 134865-74-0 **AlogP:** 3.87 **TPSA:** 29.1

Activity: Deuterated melatonin receptor antagonist

NIMH Code : P-805

Compound name : PNU-101,958



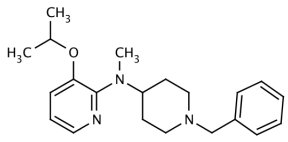
Mol. Formula : $C_{21}H_{31}Cl_2N_3O$ **FW :** 412.41 **HBA:** 4 **HBD:** 0 **RotB:** 6

PubChem ID : 5615 **CASRN :** 170856-57-2 **AlogP:** 3.95 **TPSA:** 28.6

Activity: Dopamine D_4 antagonist

NIMH Code : P-901

Compound name : [^{3}H]PNU-101,958



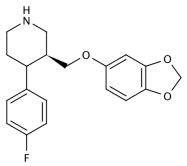
Mol. Formula : $C_{21}H_{29}N_3O$ **FW :** 339.47 **HBA:** 4 **HBD:** 0 **RotB:** 6

PubChem ID : **CASRN :** **AlogP:** 3.95 **TPSA:** 28.6

Activity: Radiolabeled D_4 receptor antagonist

NIMH Code : P-902

Compound name : Paroxetine hydrochloride



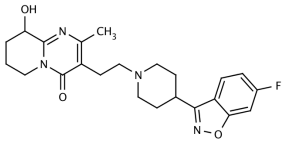
Mol. Formula : $C_{19}H_{21}ClFNO_3$ **FW :** 365.83 **HBA:** 4 **HBD:** 1 **RotB:** 4

PubChem ID : 62878 **CASRN :** 61869-08-7 **AlogP:** 3.58 **TPSA:** 39.7

Activity: Serotonin reuptake inhibitor

NIMH Code : P-903

Compound 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



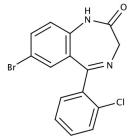
Mol. Formula : $C_{23}H_{27}FN_4O_3$ **FW :** 426.48 **HBA:** 6 **HBD:** 1 **RotB:** 4

PubChem ID : 115237 **CASRN :** 144598-75-4 **AlogP:** 2.02 **TPSA:** 82.2

Activity: Resperidone metabolite; antischizophrenic

NIMH Code : P-904 new

Compound name : 7-Bromo-5-(2-chlorophenyl)-1,3-dihydro-2H-1,4-benzodiazepin-2-one (phenazepam)



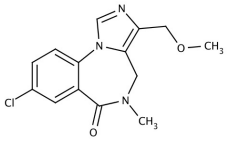
Mol. Formula : $C_{15}H_{10}BrClN_2O$ **FW :** 349.62 **HBA:** 2 **HBD:** 1 **RotB:** 1

PubChem ID : 40113 **CASRN :** 51753-57-2 **AlogP:** **TPSA:** 41.5

Activity: $GABA_A$ receptor allosteric modulator

NIMH Code : P-905 new

Compound name : PWZ-029



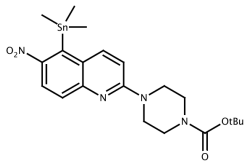
Mol. Formula : $C_{14}H_{14}ClN_3O_2$ **FW :** 291.73 **HBA:** 3 **HBD:** 0 **RotB:** 2

PubChem ID : 9971547 **CASRN :** 164025-33-6 **AlogP:** 0.31 **TPSA:** 47.4

Activity: $GABA_A$ inverse agonist

NIMH Code : Q-707

Compound 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

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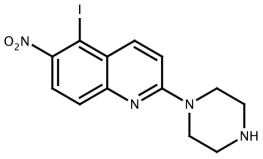
NIMH Code : Q-708

Compound name : 5-Iodo-6-nitroquipazine



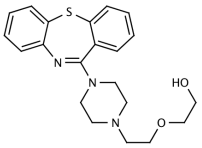
Mol. Formula : $C_{13}H_{13}IN_4O_2$ **FW :** 384.18 **HBA:** 5 **HBD:** 1 **RotB:** 2

PubChem ID : 10091399 **CASRN :** 139593-11-6 **AlogP:** 3.48 **TPSA:** 74.0

Activity: Serotonin 5-HT uptake inhibitor

NIMH Code : Q-901

Compound 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: Dopamine, serotonin, & adrenergic antagonist; antihistaminic

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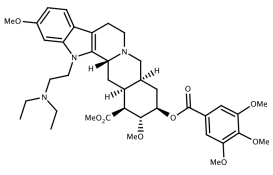
NIMH Code : R-501

Compound name : 1-(β-Diethylamino)ethylreserpine dipicrate



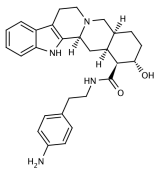
Mol. Formula : $C_{51}H_{59}N_9O_{23}$ **FW :** 1166.07 **HBA:** 9 **HBD:** 0 **RotB:** 15

PubChem ID : 65518 **CASRN :** 53-18-9 **AlogP:** 3.91 **TPSA:** 110.2

Activity: Hypotensive agent

NIMH Code : R-701

Compound name : 17α-Hydroxy-20α-yohimban-16β-(N-4-aminophenylethyl)carboxamide dihydrochloride



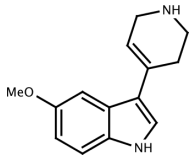
Mol. Formula : $C_{28}H_{36}Cl_2N_4O_2$ **FW :** 531.51 **HBA:** 4 **HBD:** 4 **RotB:** 4

PubChem ID : **CASRN :** **AlogP:** 2.34 **TPSA:** 94.4

Activity: Adrenergic α2 ligand radioiodination precursor

NIMH Code : R-702

Compound name : RU-24969



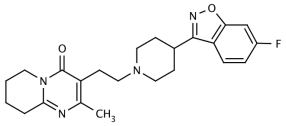
Mol. Formula : $C_{16}H_{19}N_2O_3$ **FW :** 287.34 **HBA:** 2 **HBD:** 2 **RotB:** 2

PubChem ID : 108029 **CASRN :** 107008-28-6 **AlogP:** 2.04 **TPSA:** 37.1

Activity: Serotonin 5-$HT_{1A/1B}$ agonist

NIMH Code : R-901

Compound name : Risperidone



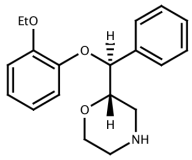
Mol. Formula : $C_{23}H_{27}FN_4O_2$ **FW :** 410.48 **HBA:** 5 **HBD:** 0 **RotB:** 4

PubChem ID : 5073 **CASRN :** 106266-06-2 **AlogP:** 2.89 **TPSA:** 61.9

Activity: Serotonin & dopamine antagonist

NIMH Code : R-902

Compound name : (±)-Reboxetine mesylate



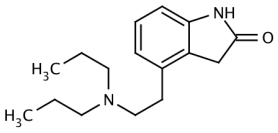
Mol. Formula : $C_{20}H_{27}NO_6S$ **FW :** 409.50 **HBA:** 4 **HBD:** 1 **RotB:** 6

PubChem ID : 5311403 **CASRN :** 98769-81-4 **AlogP:** 3.08 **TPSA:** 39.7

Activity: Norepinephrine reuptake inhibitor

NIMH Code : R-903

Compound name : Ropinirole hydrochloride



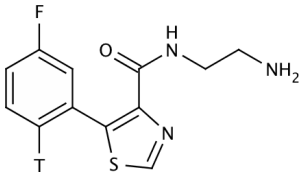
Mol. Formula : $C_{16}H_{24}N_2O$ **FW :** 260.37 **HBA:** 2 **HBD:** 1 **RotB:** 7

PubChem ID : 68727 **CASRN :** 91374-21-9 **AlogP:** 2.93 **TPSA:** 32.3

Activity: Dopamine D_2, D_3 & D_4 agonist

NIMH Code : R-904

Compound name : [^{3}H]Ro 41-1049



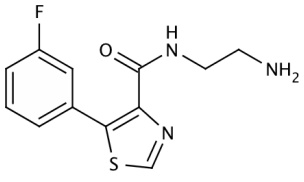
Mol. Formula : $C_{12}H_{12}FN_3OS$ **FW :** 265.31 **HBA:** 5 **HBD:** 2 **RotB:** 4

PubChem ID : **CASRN :** **AlogP:** 1.08 **TPSA:** 96.3

Activity: Radiolabeled MAO inhibitor

NIMH Code : R-905

Compound name : Ro 41-1049 hydrochloride



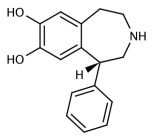
Mol. Formula : $C_{12}H_{13}ClFN_3OS$ **FW :** 301.77 **HBA:** 5 **HBD:** 2 **RotB:** 4

PubChem ID : 5311308 **CASRN :** 127500-84-9 **AlogP:** 1.08 **TPSA:** 96.3

Activity: MAO inhibitor

NIMH Code : S-101

Compound name : (*R*)-(+)-SKF-38393 hydrochloride



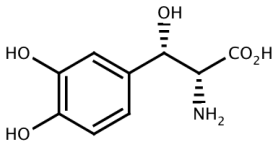
Mol. Formula : $C_{16}H_{18}ClNO_2$ **FW :** 291.78 **HBA:** 3 **HBD:** 3 **RotB:** 1

PubChem ID : 6852375 **CASRN :** 62751-59-1 **AlogP:** 1.86 **TPSA:** 52.5

Activity: Dopamine D_1 receptor agonist; active enantiomer of (±)-SKF-38393

NIMH Code : S-501

Compound name : (+)-*threo*-3-(3,4-Dihydroxyphenyl)serine

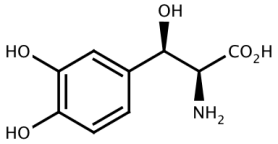


Mol. Formula : $C_9H_{11}NO_5$ **FW :** 213.19 **HBA:** 6 **HBD:** 5 **RotB:** 3

PubChem ID : 443940 **CASRN :** 23651-95-8 **AlogP:** -2.64 **TPSA:** 124.0

NIMH Code : S-502

Compound name : (–)-*threo*-3-(3,4-Dihydroxyphenyl)serine

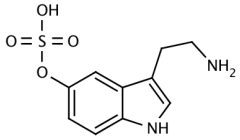


Mol. Formula : $C_9H_{11}NO_5$ **FW :** 213.19 **HBA:** 6 **HBD:** 5 **RotB:** 3

PubChem ID : 164631 **CASRN :** 13147-26-7 **AlogP:** -2.64 **TPSA:** 124.0

NIMH Code : S-503

Compound name : Serotonin-*O*-sulfate

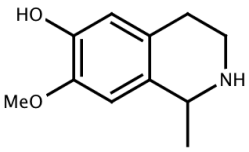


Mol. Formula : $C_{10}H_{12}N_2O_4S$ **FW :** 256.28 **HBA:** 4 **HBD:** 3 **RotB:** 4

PubChem ID : 152151 **CASRN :** 16310-20-6 **AlogP:** -2.01 **TPSA:** 113.8

NIMH Code : S-504

Compound name : (±)-Salsoline hydrochloride



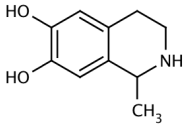
Mol. Formula : $C_{11}H_{16}ClNO_2$ **FW :** 229.71 **HBA:** 3 **HBD:** 2 **RotB:** 1

PubChem ID : 46695 **CASRN :** 89-31-6 **AlogP:** 1.03 **TPSA:** 41.5

Activity: Salsolinol metabolite; endogenous neurotoxin

NIMH Code : S-505

Compound name : (±)-Salsolinol hydrochloride



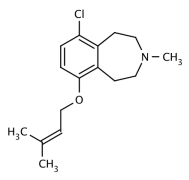
Mol. Formula : $C_{10}H_{14}ClNO_2$ **FW :** 215.69 **HBA:** 3 **HBD:** 3 **RotB:** 0

PubChem ID : 54456 **CASRN :** 525-72-4 **AlogP:** 0.96 **TPSA:** 52.5

Activity: Dopamine neurotoxic derivative

NIMH Code : S-701

Compound name : SKF-104078



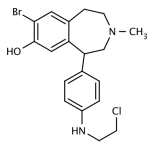
Mol. Formula : $C_{20}H_{26}ClNO_5$ **FW :** 395.88 **HBA:** 3 **HBD:** 0 **RotB:** 3

PubChem ID : 122295 **CASRN :** 110857-22-2 **AlogP:** 3.68 **TPSA:** 12.5

Activity: Adrenergic α2 antagonist

NIMH Code : S-703

Compound name : (±)-4'-(2-Chloroethylamino)-SKF-83566 dihydrobromide



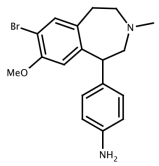
Mol. Formula : $C_{19}H_{24}Br_3ClN_2O$ **FW :** 571.57 **HBA:** 4 **HBD:** 2 **RotB:** 4

PubChem ID : **CASRN :** **AlogP:** 3.90 **TPSA:** 35.5

Activity: Dopamine D_1 receptor alkylating ligand

NIMH Code : S-704

Compound name : (±)-4'-Amino-8-*O*-methyl-SKF-83566



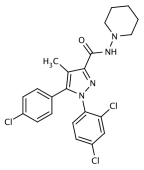
Mol. Formula : $C_{18}H_{21}BrN_2O$ **FW :** 361.08 **HBA:** 3 **HBD:** 1 **RotB:** 2

PubChem ID : **CASRN :** **AlogP:** 3.54 **TPSA:** 38.5

Activity: Dopamine D1 receptor precursor alkylating ligand (antagonist)

NIMH Code : S-705

Compound name : SR 141716



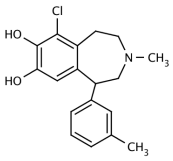
Mol. Formula : $C_{22}H_{21}Cl_3N_4O$ **FW :** 463.80 **HBA:** 6 **HBD:** 1 **RotB:** 4

PubChem ID : 104850 **CASRN :** 158681-13-1 **AlogP:** 5.36 **TPSA:** 50.2

Activity: Cannabinoid CB_1 inverse agonist

NIMH Code : S-706

Compound name : SKF-83959 hydrobromide



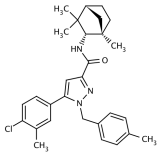
Mol. Formula : $C_{18}H_{21}BrClNO_2$ **FW :** 398.73 **HBA:** 4 **HBD:** 2 **RotB:** 1

PubChem ID : 133538 **CASRN :** 80751-85-5 **AlogP:** 3.36 **TPSA:** 43.7

Activity: Dopamine D_1 receptor agonist

NIMH Code : S-801

Compound name : SR 144528



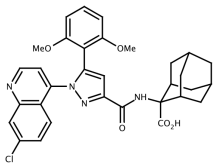
Mol. Formula : $C_{29}H_{34}ClN_3O$ **FW :** 476.06 **HBA:** 3 **HBD:** 1 **RotB:** 5

PubChem ID : 3081355 **CASRN :** 192703-06 -3 **AlogP:** 7.13 **TPSA:** 46.9

Activity: Cannabinoid CB_2 receptor antagonist

NIMH Code : S-802

Compound name : SR 48692



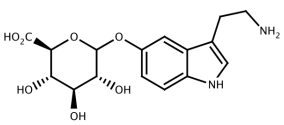
Mol. Formula : $C_{32}H_{31}ClN_4O_5$ **FW :** 587.08 **HBA:** 8 **HBD:** 2 **RotB:** 6

PubChem ID : 119192 **CASRN :** 146362-70-1 **AlogP:** 1.31 **TPSA:** 115.6

Activity: Neurotensin NT_1 antagonist

NIMH Code : S-803

Compound name : Serotonin-*O*-β-D-glucuronide

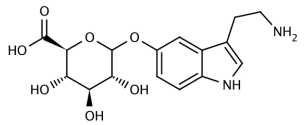


Mol. Formula : $C_{16}H_{20}N_2O_7$ **FW :** 352.34 **HBA:** 8 **HBD:** 6 **RotB:** 5

PubChem ID : **CASRN :** **AlogP:** -6.92 **TPSA:** 158.3

NIMH Code : S-803A

Compound name : Serotonin-*O*-β-D-glucuronide trifluoroacetate

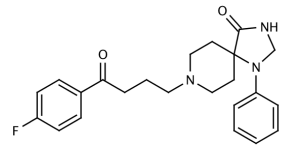


Mol. Formula : $C_{18}H_{21}F_3N_2O_9$ **FW :** 466.36 **HBA:** 8 **HBD:** 6 **RotB:** 5

PubChem ID : **CASRN :** **AlogP:** -6.92 **TPSA:** 158.3

NIMH Code : S-901

Compound name : Spiperone



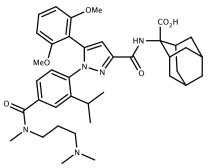
Mol. Formula : $C_{23}H_{26}FN_3O_2$ **FW :** 395.48 **HBA:** 5 **HBD:** 1 **RotB:** 6

PubChem ID : 5265 **CASRN :** 749-02-0 **AlogP:** 3.02 **TPSA:** 52.7

Activity: Serotonin $5HT_{1A}$, $5HT_{2A}$, $5HT_7$, & dopamine D_2 antagonist

NIMH Code : S-902

Compound name : SR 142948



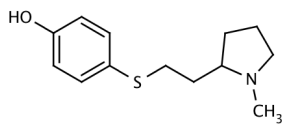
Mol. Formula : $C_{39}H_{52}ClN_5O_6$ **FW :** 722.33 **HBA:** 8 **HBD:** 2 **RotB:** 12

PubChem ID : 5311451 **CASRN :** 184162-64-9 **AlogP:** -2.31 **TPSA:** 126.2

Activity: Neurotensin receptor antagonist

NIMH Code : S-903

Compound name : SIB-1553A



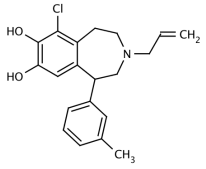
Mol. Formula : $C_{13}H_{20}ClNOS$ **FW :** 273.83 **HBA:** 3 **HBD:** 1 **RotB:** 4

PubChem ID : 9881989 **CASRN :** **AlogP:** 2.29 **TPSA:** 48.8

Activity: Nicotinic acetylcholine receptor agonist; possible cognitive enhancer

NIMH Code : S-904

Compound name : SKF-83822 hydrobromide



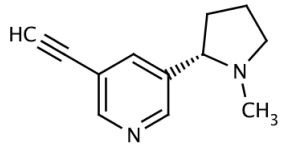
Mol. Formula : $C_{20}H_{23}BrClNO_2$ **FW :** 424.77 **HBA:** 4 **HBD:** 2 **RotB:** 3

PubChem ID : 10020353 **CASRN :** 74115-08-5 **AlogP:** 4.39 **TPSA:** 43.7

Activity: Dopamine D_1 agonist that stimulate adenylyl cyclase

NIMH Code : S-905

Compound name : SIB-1508Y



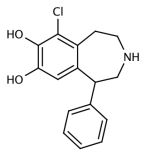
Mol. Formula : $C_{16}H_{18}N_2O_4$ **FW :** 302.33 **HBA:** 2 **HBD:** 0 **RotB:** 2

PubChem ID : 10968648 **CASRN :** 192231-16 -6 **AlogP:** 1.20 **TPSA:** 16.1

Activity: Neuronal nicotinic acetylcholine receptor agonist

NIMH Code : S-906

Compound name : SKF-81297 hydrobromide



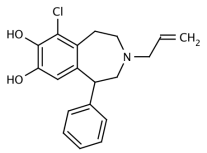
Mol. Formula : $C_{16}H_{17}BrClNO_2$ **FW :** 370.68 **HBA:** 4 **HBD:** 3 **RotB:** 1

PubChem ID : 11957706 **CASRN :** 71636-61-8 **AlogP:** 1.67 **TPSA:** 52.5

Activity: Dopamine D_1 agonist

NIMH Code : S-907

Compound name : SKF-82958 hydrobromide



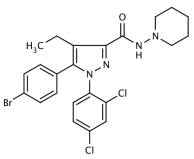
Mol. Formula : $C_{19}H_{21}BrClNO_2$ **FW :** 410.74 **HBA:** 4 **HBD:** 2 **RotB:** 3

PubChem ID : 9909521 **CASRN :** 80751-65-1 **AlogP:** 3.92 **TPSA:** 43.7

Activity: Dopamine D_1 agonist

NIMH Code : S-908

Compound name : SR 147778



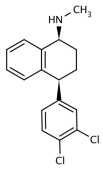
Mol. Formula : $C_{23}H_{22}BrCl_2N_4O$ **FW :** 522.26 **HBA:** 5 **HBD:** 1 **RotB:** 5

PubChem ID : 9849616 **CASRN :** 288104-79-0 **AlogP:** 6.03 **TPSA:** 50.2

Activity: Cannaboid CB_1 antagonist

NIMH Code : S-909

Compound name : Sertraline hydrochloride



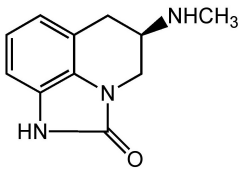
Mol. Formula : $C_{17}H_{18}Cl_3N$ **FW :** 342.69 **HBA:** 3 **HBD:** 1 **RotB:** 2

PubChem ID : 63009 **CASRN :** 79617-96-2 **AlogP:** 5.00 **TPSA:** 12.0

Activity: Serotonin reuptake inhibitor; used to treat depression and OCD

NIMH Code : S-910

Compound name : Sumanirole maleate



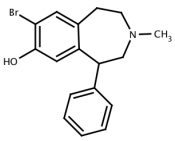
Mol. Formula : $C_{15}H_{17}N_3O_5$ **FW :** 319.30 **HBA:** 4 **HBD:** 2 **RotB:** 1

PubChem ID : 177343 **CASRN :** 179386-43 -7 **AlogP:** 1.08 **TPSA:** 44.4

Activity: Dopamine D2 receptor ligand.

NIMH Code : S-911 new

Compound name : SKF-83566 HBr



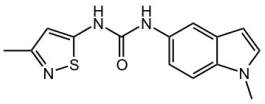
Mol. Formula : $C_{17}H_{19}Br_2NO$ **FW :** 413.15 **HBA:** 2 **HBD:** 1 **RotB:** 1

PubChem ID : 1243 **CASRN :** 99295-33-7 **AlogP:** 4.00 **TPSA:**

Activity: Dopamine D2 receptor antagonist

NIMH Code : S-912 new

Compound name : *N*-(1-Methyl-1*H*-indol-5-yl)-N'-(3-methylisothiazol-5-yl)urea (SB 204741)



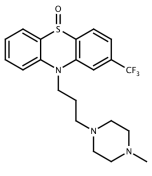
Mol. Formula : $C_{14}H_{14}N_4OS$ **FW :** 286.35 **HBA:** 2 **HBD:** 2 **RotB:** 2

PubChem ID : 3277600 **CASRN :** 152239-46-8 **AlogP:** 2.40 **TPSA:** 87.2

Activity: 5-HT_{2B} receptor antagonist

NIMH Code : T-501

Compound name : Trifluoperazine-5-oxide

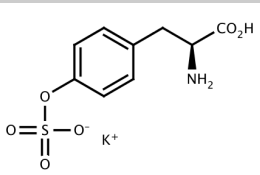


Mol. Formula : $C_{21}H_{24}F_3N_3OS$ **FW :** 423.50 **HBA:** 7 **HBD:** 0 **RotB:** 5

PubChem ID : 159622 **CASRN :** 1549-88-8 **AlogP:** 2.75 **TPSA:** 46.0

NIMH Code : T-502

Compound name : (–)-Tyrosine-*O*-sulfate potassium salt

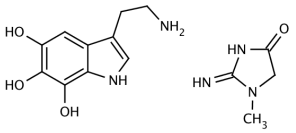


Mol. Formula : $C_9H_{10}NO_6SK$ **FW :** 299.26 **HBA:** 6 **HBD:** 2 **RotB:** 5

PubChem ID : 514186 **CASRN :** **AlogP:** -2.40 **TPSA:** 138.1

NIMH Code : T-503

Compound name : 5,6,7-Trihydroxytryptamine creatinine sulfate

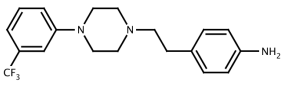


Mol. Formula : $C_{14}H_{21}N_5O_8S$ **FW :** 419.41 **HBA:** 4 **HBD:** 5 **RotB:** 2

PubChem ID : **CASRN :** **AlogP:** -1.19 **TPSA:** 102.5

NIMH Code : T-504

Compound name : 1-[2-(4-Aminophenyl)ethyl]-4-(3-trifluoromethylphenyl)piperazine dihydrochloride



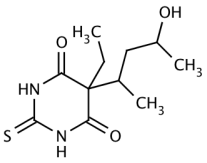
Mol. Formula : $C_{19}H_{24}Cl_2F_3N_3$ **FW :** 422.31 **HBA:** 6 **HBD:** 1 **RotB:** 5

PubChem ID : 121930 **CASRN :** 1814-64-8 **AlogP:** 4.24 **TPSA:** 32.5

Activity: Serotonin 5-HT agonist

NIMH Code : T-506

Compound name : 5-Ethyl-5-(1'-methyl-3'-hydroxybutyl)-2-thiobarbituric acid



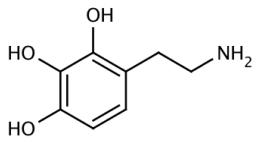
Mol. Formula : $C_{11}H_{18}N_2O_3S$ **FW :** 258.35 **HBA:** 4 **HBD:** 3 **RotB:** 4

PubChem ID : **CASRN :** **AlogP:** 1.17 **TPSA:** 110.5

Activity: Thiopental metabolite

NIMH Code : T-507

Compound name : 2,3,4-Trihydroxy-β-phenethylamine hydrochloride



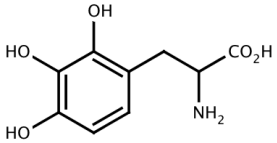
Mol. Formula : $C_8H_{12}ClNO_3$ **FW :** 205.64 **HBA:** 4 **HBD:** 4 **RotB:** 2

PubChem ID : 193386 **CASRN :** 4228-71-1 **AlogP:** -0.34 **TPSA:** 86.7

Activity: Arylsulfatase inhibitor; potential neurotoxin

NIMH Code : T-508

Compound name : 2,3,4-Trihydroxy-(±)-phenylalanine



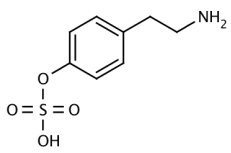
Mol. Formula : $C_9H_{11}NO_5$ **FW :** 213.19 **HBA:** 6 **HBD:** 5 **RotB:** 3

PubChem ID : 22326275 **CASRN :** **AlogP:** -2.00 **TPSA:** 124.0

Activity: Neurotoxic DOPA metabolite

NIMH Code : T-509

Compound name : Tyramine-*O*-sulfate

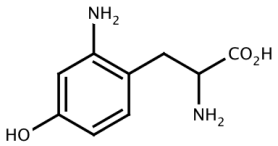


Mol. Formula : $C_8H_{11}NO_4S$ **FW :** 217.25 **HBA:** 4 **HBD:** 2 **RotB:** 4

PubChem ID : 153005 **CASRN :** 30223-92-8 **AlogP:** -2.11 **TPSA:** 98.0

NIMH Code : T-510

Compound name : 2-Amino-(±)-Tyrosine

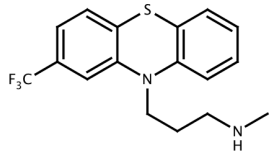


Mol. Formula : $C_9H_{12}N_2O_3$ **FW :** 196.21 **HBA:** 5 **HBD:** 4 **RotB:** 3

PubChem ID : 5134354 **CASRN :** **AlogP:** -2.21 **TPSA:** 109.6

NIMH Code : T-511

Compound name : N-Desmethyltriflupromazine hydrochloride

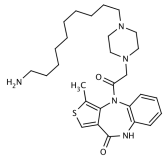


Mol. Formula : $C_{17}H_{18}ClF_3N_2S$ **FW :** 374.84 **HBA:** 6 **HBD:** 1 **RotB:** 5

PubChem ID : 10337209 **CASRN :** **AlogP:** 4.56 **TPSA:** 40.6

NIMH Code : T-701

Compound name : Telenzepine Amine Congener (TAC) dihydrobromide



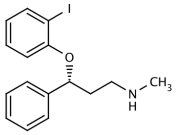
Mol. Formula : $C_{28}H_{43}Br_2N_5O_2S$ **FW :** 673.56 **HBA:** 6 **HBD:** 2 **RotB:** 12

PubChem ID : 9892600 **CASRN :** **AlogP:** 3.20 **TPSA:** 110.2

Activity: Muscarinic m_1 antagonist analog

NIMH Code : T-702

Compound name : (*R*)-(–)-*N*-Methyl-3-(2-iodophenoxy)-3-phenylpropanamine hydrochloride



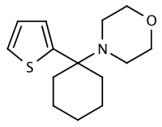
Mol. Formula : $C_{16}H_{19}ClINO$ **FW :** 403.69 **HBA:** 2 **HBD:** 1 **RotB:** 6

PubChem ID : 10021849 **CASRN :** **AlogP:** 4.30 **TPSA:** 21.3

Activity: Norepinephrine transport inhibitor

NIMH Code : T-703

Compound name : 1-[1-(2-Thienyl)cyclohexyl]morpholine



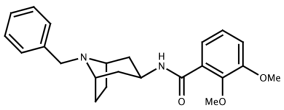
Mol. Formula : $C_{14}H_{21}NOS$ **FW :** 251.39 **HBA:** 3 **HBD:** 0 **RotB:** 2

PubChem ID : 210739 **CASRN :** 21602-66-4 **AlogP:** 2.73 **TPSA:** 40.7

Activity: PCP analog

NIMH Code : T-704

Compound name : Tropapride hydrochloride



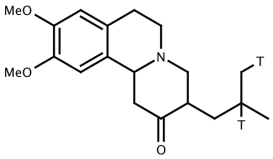
Mol. Formula : $C_{23}H_{29}ClN_2O_3$ **FW :** 416.95 **HBA:** 4 **HBD:** 1 **RotB:** 6

PubChem ID : 3065827 **CASRN :** 109021-66-1 **AlogP:** 2.66 **TPSA:** 50.8

Activity: Dopamine D_2 receptor antagonist

NIMH Code : T-801

Compound name : [^{3}H]Tetrabenazine



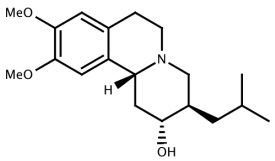
Mol. Formula : $C_{19}H_{27}NO_3$ **FW :** 317.42 **HBA:** 4 **HBD:** 0 **RotB:** 4

PubChem ID : 6018 **CASRN :** 58-46-8 **AlogP:** 3.33 **TPSA:** 38.8

Activity: Radiolabeled adrenergic uptake inhibitor

NIMH Code : T-802

Compound name : (+)-α-Dihydrotetrabenazine



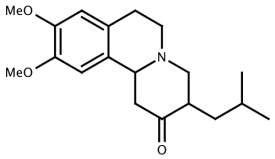
Mol. Formula : $C_{19}H_{29}NO_3$ **FW :** 319.45 **HBA:** 4 **HBD:** 1 **RotB:** 4

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

Activity: Active metabolite of tetrabenazine

NIMH Code : T-901

Compound name : (±)-Tetrabenazine



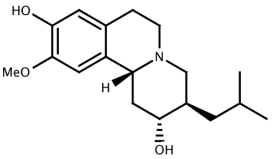
Mol. Formula : $C_{19}H_{27}NO_3$ **FW :** 317.43 **HBA:** 4 **HBD:** 0 **RotB:** 4

PubChem ID : 6018 **CASRN :** 58-46-8 **AlogP:** 3.33 **TPSA:** 38.8

Activity: Adrenergic uptake inhibitor; dopamine depleting agent; antipsychotic;

NIMH Code : T-902

Compound name : (+)-(2*R*,3*R*,11b*R*)-9-*O*-Desmethyl-α-dihydrotetrabenazine



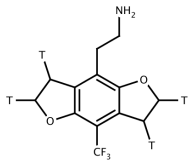
Mol. Formula : $C_{18}H_{27}NO_3$ **FW :** 305.42 **HBA:** 4 **HBD:** 2 **RotB:** 3

PubChem ID : **CASRN :** **AlogP:** 2.21 **TPSA:** 52.9

Activity: DTBZ PET precusor ligand

NIMH Code : T-903

Compound name : [^{3}H]-1-(8-Trifluoromethyl-2,3,6,7-tetrahydrobenzo[1,2-b;4,5-b']difuran-4-yl)-2-aminoethane

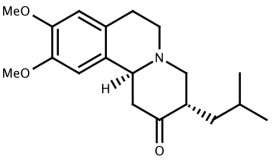


Mol. Formula : $C_{13}H_{14}F_3NO_2$ **FW :** 273.25 **HBA:** 6 **HBD:** 1 **RotB:** 3

PubChem ID : **CASRN :** **AlogP:** 1.76 **TPSA:** 44.5

NIMH Code : T-904

Compound name : (–)-Tetrabenazine



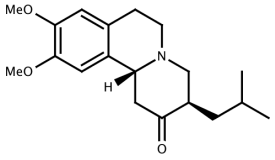
Mol. Formula : $C_{19}H_{27}NO_3$ **FW :** 317.44 **HBA:** 4 **HBD:** 0 **RotB:** 4

PubChem ID : 667453 **CASRN :** **AlogP:** 3.33 **TPSA:** 38.8

Activity: Dopamine depleting agent; optical isomer of tetrabenazine

NIMH Code : T-905

Compound name : (+)-Tetrabenazine



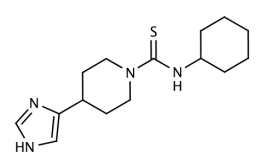
Mol. Formula : $C_{19}H_{27}NO_3$ **FW :** 317.44 **HBA:** 4 **HBD:** 0 **RotB:** 4

PubChem ID : 11634155 **CASRN :** **AlogP:** 3.33 **TPSA:** 38.8

Activity: Dopamine depleting agent; optical isomer of tetrabenazine

NIMH Code : T-906

Compound name : Thioperamide maleate



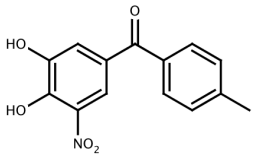
Mol. Formula : $C_{15}H_{24}N_4S$ **FW :** 292.44 **HBA:** 2 **HBD:** 2 **RotB:** 2

PubChem ID : 3035905 **CASRN :** 106243-16-7 **AlogP:** 1.90 **TPSA:** 76.0

Activity: Histamine H_3 antagonist; anticonvulsant

NIMH Code : T-907

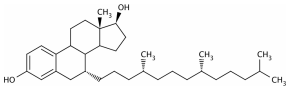
Compound name : Tolcapone



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								

NIMH Code : T-908

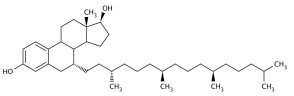
Compound name : 7α-[(4*R*,8*R*)-4,8,12-Trimethyltridecyl]estra-1,3,5(10)-trien-3,17β-diol



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

NIMH Code : T-909

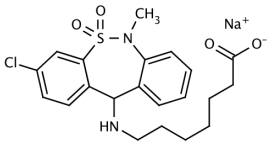
Compound name : 7α-[(3*R*/*S*,7*R*,11*R*)-3,7,11,15-tetramethylhexadecyl]estra-1,3,5-trien-3,17β-diol



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

NIMH Code : T-910

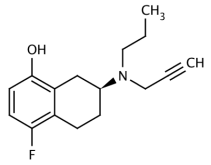
Compound name : Tianeptine, sodium salt



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								

NIMH Code : U-703

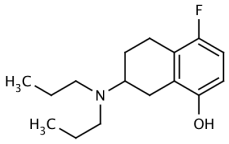
Compound name : (*S*)-(–)-*N*-Propargyl-UH-301 hydrochloride



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								

NIMH Code : U-801

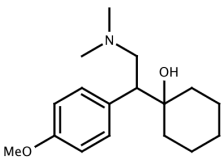
Compound name : Tritiated UH-301



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								

NIMH Code : V-901

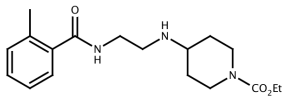
Compound name : Venlafaxine



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								

NIMH Code : V-902

Compound name : VU0357017 hydrochloride



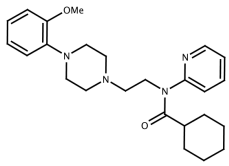
Mol. Formula : $C_{18}H_{28}ClN_3O_3$ **FW :** 369.89 **HBA:** 6 **HBD:** 2 **RotB:** 7

PubChem ID : 25010775 **CASRN :** **AlogP:** 1.61 **TPSA:** 70.7

Activity: Allosteric modulator of the M1 muscarinic receptor.

NIMH Code : W-108

Compound name : WAY-100635 maleate



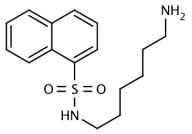
Mol. Formula : $C_{29}H_{38}N_4O_6$ **FW :** 538.65 **HBA:** 5 **HBD:** 0 **RotB:** 7

PubChem ID : 11957721 **CASRN :** 634908-75-1 **AlogP:** 4.09 **TPSA:** 48.9

Activity: Serotonin 5-HT receptor antagonist

NIMH Code : W-501

Compound name : N-(6-Aminohexyl)-1-napthalenesulfonamide hydrochloride



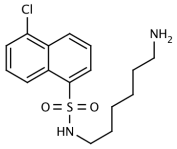
Mol. Formula : $C_{16}H_{23}ClN_2O_2S$ **FW :** 342.89 **HBA:** 3 **HBD:** 2 **RotB:** 7

PubChem ID : 4314 **CASRN :** 79458-81-4 **AlogP:** 1.55 **TPSA:** 80.6

Activity: Calmodulin antagonist

NIMH Code : W-502

Compound name : N-(6-Aminohexyl)-5-chloro-1-napthalenesulfonamide hydrochloride



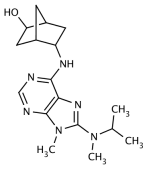
Mol. Formula : $C_{16}H_{22}Cl_2N_2O_2S$ **FW :** 377.33 **HBA:** 4 **HBD:** 2 **RotB:** 7

PubChem ID : 5681 **CASRN :** 65595-90-6 **AlogP:** 2.06 **TPSA:** 80.6

Activity: Calmodulin antagonist

NIMH Code : W-801

Compound name : WRC-0571



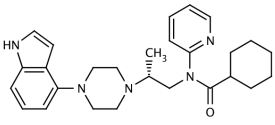
Mol. Formula : $C_{17}H_{26}N_6O$ **FW :** 330.44 **HBA:** 6 **HBD:** 2 **RotB:** 4

PubChem ID : 9902054 **CASRN :** **AlogP:** 2.12 **TPSA:** 79.1

Activity: Adenosine A_1 receptor antagonist

NIMH Code : W-901

Compound name : WAY 405



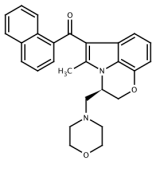
Mol. Formula : $C_{27}H_{37}Cl_2N_5O$ **FW :** 518.53 **HBA:** 4 **HBD:** 1 **RotB:** 6

PubChem ID : **CASRN :** **AlogP:** 4.85 **TPSA:** 55.5

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

NIMH Code : W-902 new

Compound name : WIN 55212-2 mesylate



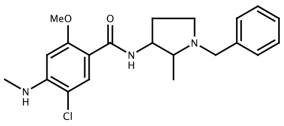
Mol. Formula : $C_{28}H_{30}N_2O_6S$ **FW :** 522.61 **HBA:** 4 **HBD:** 0 **RotB:** 4

PubChem ID : 5689 **CASRN :** 131543-23-2 **AlogP:** 4.40 **TPSA:** 43.7

Activity: Calcium channel blocker

NIMH Code : Y-701

Compound name : (±)-YM-09151-2; Nemonapride



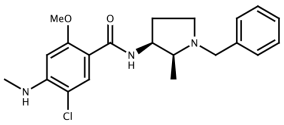
Mol. Formula : $C_{21}H_{26}ClN_3O_2$ **FW :** 387.91 **HBA:** 5 **HBD:** 2 **RotB:** 6

PubChem ID : 4452 **CASRN :** 75272-39-8 **AlogP:** 2.90 **TPSA:** 53.6

Activity: Dopamine D_2 receptor antagonist; antipsychotic

NIMH Code : Y-702

Compound name : (–)-YM-09151-2



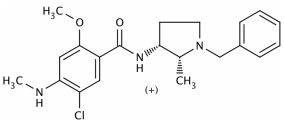
Mol. Formula : $C_{21}H_{26}ClN_3O_2$ **FW :** 387.91 **HBA:** 5 **HBD:** 2 **RotB:** 6

PubChem ID : 156333 **CASRN :** 70325-83-6 **AlogP:** 2.90 **TPSA:** 53.6

Activity: Inactive stereoisomer of YM-09151-2

NIMH Code : Y-703

Compound name : (+)-YM-09151-2



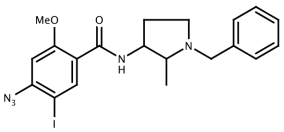
Mol. Formula : $C_{21}H_{26}ClN_3O_2$ **FW :** 387.91 **HBA:** 5 **HBD:** 2 **RotB:** 6

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

NIMH Code : Y-704

Compound name : (±)-*cis*-*N*-(1-Benzyl-2-methylpyrrolidin-3-yl)-4-azido-5-iodo-2-methoxybenzamide hydrochloride



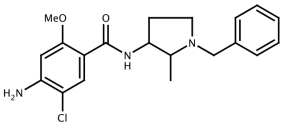
Mol. Formula : $C_{20}H_{23}ClIN_5O_2$ **FW :** 527.79 **HBA:** 5 **HBD:** 1 **RotB:** 6

PubChem ID : **CASRN :** **AlogP:** -0.54 **TPSA:** 71.0

Activity: Dopamine D_2 receptor photoaffinity ligand

NIMH Code : Y-705

Compound name : (±)-*cis*-*N*-(1-Benzyl-2-methylpyrrolidin-3-yl)-4-amino-2-methoxybenzamide



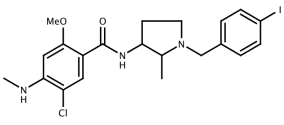
Mol. Formula : $C_{20}H_{25}N_3O_2$ **FW :** 339.44 **HBA:** 4 **HBD:** 2 **RotB:** 5

PubChem ID : **CASRN :** **AlogP:** 2.02 **TPSA:** 67.6

Activity: Dopamine D_2 receptor photoaffinity ligand precursor

NIMH Code : Y-706

Compound name : (±)-*cis*-*N*-[1-(4'-Iodobenzyl)-2-methylpyrrolidin-3-yl]-5-chloro-2-methoxy-4-(methylamino)benzamide



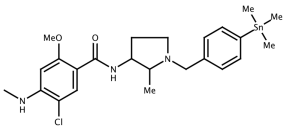
Mol. Formula : $C_{21}H_{25}ClIN_3O_2$ **FW :** 513.81 **HBA:** 5 **HBD:** 2 **RotB:** 6

PubChem ID : **CASRN :** **AlogP:** 3.89 **TPSA:** 53.6

Activity: Potential high affinity probe for dopamine D_2 receptors

NIMH Code : Y-707

Compound name : (±)-*cis*-*N*-[1-(4'-Trimethylstannylbenzyl)-2-methylpyrrolidin-3-yl]-5-chloro-2-methoxy-4-(methylamino)benzamide



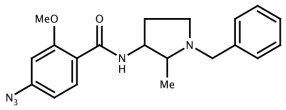
Mol. Formula : $C_{24}H_{34}ClN_3O_2Sn$ **FW :** 550.72 **HBA:** 5 **HBD:** 2 **RotB:** 7

PubChem ID : **CASRN :** **AlogP:** 2.68 **TPSA:** 53.6

Activity: 4'-Iodo-YM-09151-02 radioiodination precursor

NIMH Code : Y-708

Compound name : (±)-*cis*-*N*-(1-Benzyl-2-methylpyrrolidin-3-yl)-4-azido-2-methoxybenzamide hydrochloride



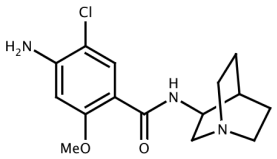
Mol. Formula : $C_{20}H_{24}ClN_5O_2$ **FW :** 401.90 **HBA:** 5 **HBD:** 1 **RotB:** 6

PubChem ID : **CASRN :** **AlogP:** -1.55 **TPSA:** 71.0

Activity: Reference standard for YM-09151-2 analogs

NIMH Code : Z-901

Compound name : (±)-Zacopride hydrochloride



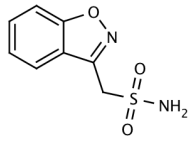
Mol. Formula : $C_{15}H_{21}Cl_2N_3O_2$ **FW :** 346.26 **HBA:** 5 **HBD:** 2 **RotB:** 3

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

NIMH Code : Z-902

Compound name : Zonisamide



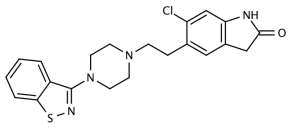
Mol. Formula : $C_8H_8N_2O_3S$ **FW :** 212.23 **HBA:** 3 **HBD:** 1 **RotB:** 2

PubChem ID : 5734 **CASRN :** 68291-97-4 **AlogP:** 0.52 **TPSA:** 94.6

Activity: Anticonvulsant; antioxidant

NIMH Code : Z-903

Compound 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

Terms and Conditions

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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RTI International is honored to have been selected to operate the NIMH CSDSP. RTI International scientists look forward to working with investigators in the neuroscience area to meet their research needs and to receiving suggestions for additional compounds to include in the NIMH CSDSP.

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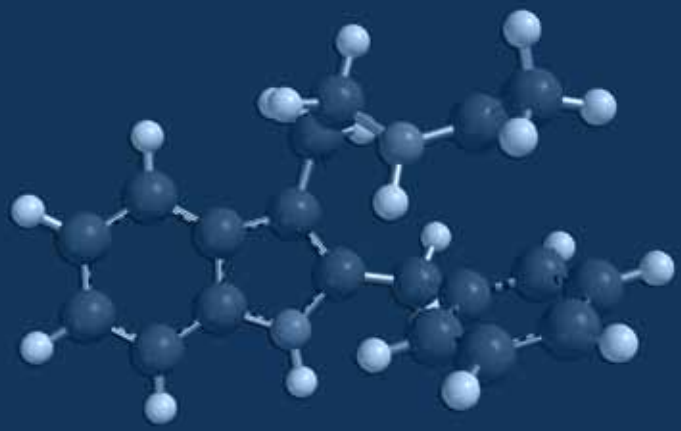

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