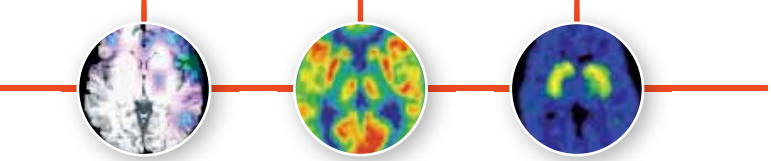
NIMH Chemical Synthesis and Drug Supply Program

Compound Catalog

October 2012

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

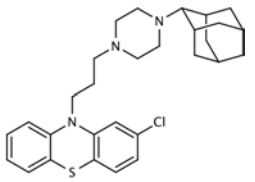
logP - Calculated Ghose-Crippen octanol-water partition coefficient (Viswanadhan, V.N., Ghose, A.K., Revankar, G.R. & Robins, R.K. *J. Chem. Inf. Comput. Sci.*, **1989**, *29*, 163-172.)

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



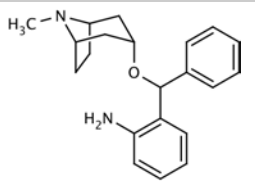
Mol. Formula : $C_{29}H_{38}Cl_3N_3S$ **FW :** 494.13 **HBA:** 3 **HBD:** 0 **RotB:** 5

PubChem ID : 62872 **CASRN :** 57942-72-0 **logP:** 6.56 **TPSA:** 10.9

Activity: Dopamine receptor antagonist.

NIMH Code : A-503

Compound name : Aminobenztropine



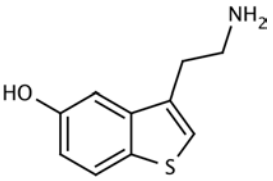
Mol. Formula : $C_{21}H_{26}N_2O$ **FW :** 322.44 **HBA:** 3 **HBD:** 1 **RotB:** 4

PubChem ID : 2143 **CASRN :** 88097-86-3 **logP:** 3.36 **TPSA:** 39.7

Activity: Muscarinic M_1 receptor ligand.

NIMH Code : A-504

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



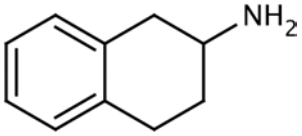
Mol. Formula : $C_{10}H_{11}NOS$ **FW :** 193.27 **HBA:** 2 **HBD:** 2 **RotB:** 2

PubChem ID : 25600 **CASRN :** 13012-93-6 **logP:** 1.29 **TPSA:** 47.9

Activity: Serotonin 5-HT_{1E} ligand.

NIMH Code : A-505

Compound name : 2-Aminotetralin hydrochloride



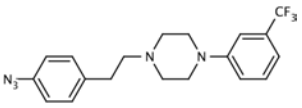
Mol. Formula : $C_{10}H_{14}ClN$ **FW :** 183.68 **HBA:** 1 **HBD:** 1 **RotB:** 0

PubChem ID : 34677 **CASRN :** 2954-50-9 **logP:** 1.93 **TPSA:** 27.6

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

NIMH Code : A-506

Compound name : p-Azido-PE-TFMPP hydrochloride



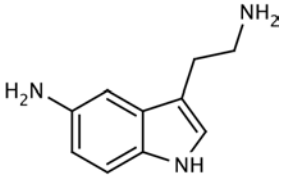
Mol. Formula : $C_{19}H_{21}ClF_3N_5$ **FW :** 411.85 **HBA:** 5 **HBD:** 0 **RotB:** 6

PubChem ID : 128737 **CASRN :** 105025-90-9 **logP:** 3.09 **TPSA:** 37.1

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

NIMH Code : A-507

Compound name : 5-Aminotryptamine dipicrate



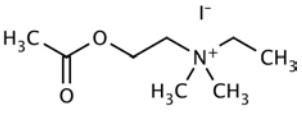
Mol. Formula : $C_{22}H_{19}N_9O_{14}$ **FW :** 633.44 **HBA:** 3 **HBD:** 2 **RotB:** 2

PubChem ID : 3083677 **CASRN :** 1078-00-8 **logP:** 0.66 **TPSA:** 69.5

Activity: Serotonin 5-HT_{1A} receptor agonist.

NIMH Code : A-508

Compound name : Acetoxyethyldimethylethylammonium iodide

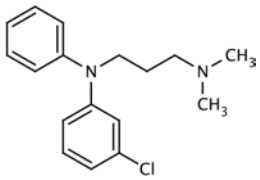


Mol. Formula : $C_8H_{18}INO_2$ **FW :** 287.14 **HBA:** 3 **HBD:** 0 **RotB:** 5

PubChem ID : - **CASRN :** - **logP:** -3.86 **TPSA:** 26.3

NIMH Code : A-509

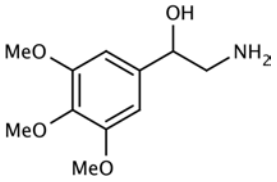
Compound name : *N*-(3-Chlorophenyl)-*N*-(γ-*N',N'*-dimethylaminopropyl)aniline hydrochloride



Mol. Formula :	$C_{17}H_{22}Cl_2N_2$	**FW :**	325.28	**HBA:**	2	**HBD:**	0	**RotB:**	6
PubChem ID :	-	**CASRN :**	82735-00-0			**logP:**	4.32	**TPSA:**	7.7

NIMH Code : A-510

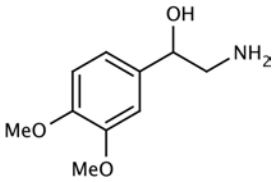
Compound name : 2-Amino-1-(3,4,5-trimethoxyphenyl)ethanol



Mol. Formula :	$C_{11}H_{17}NO_4$	**FW :**	227.26	**HBA:**	5	**HBD:**	2	**RotB:**	5
PubChem ID :	28894	**CASRN :**	18111-13-2			**logP:**	-0.00	**TPSA:**	75.6

NIMH Code : A-511

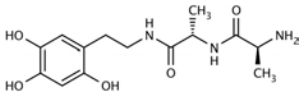
Compound name : 2-Amino-1-(3,4-dimethoxyphenyl)ethanol hydrochloride (DME)



Mol. Formula :	$C_{10}H_{16}ClNO_3$	**FW :**	233.69	**HBA:**	4	**HBD:**	2	**RotB:**	4
PubChem ID :	3863978	**CASRN :**	6924-15-8			**logP:**	0.15	**TPSA:**	66.3

NIMH Code : A-512

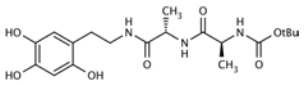
Compound name : Alanylalanyl-6-hydroxydopamine hydrochloride



Mol. Formula :	$C_{14}H_{22}ClN_3O_6$	**FW :**	347.79	**HBA:**	8	**HBD:**	6	**RotB:**	6
PubChem ID :	-	**CASRN :**	-			**logP:**	-0.82	**TPSA:**	146.5

NIMH Code : A-513

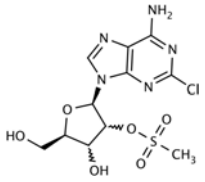
Compound name : *N*-(*t*-Butoxycarbonyl)-L-alanyl-*N*-[2-(2,4,5-trihydroxyphenyl)ethyl]-L-alaninamide



Mol. Formula :	$C_{19}H_{29}N_3O_7$	**FW :**	411.45	**HBA:**	10	**HBD:**	6	**RotB:**	9
PubChem ID :	-	**CASRN :**	-			**logP:**	0.90	**TPSA:**	157.2

NIMH Code : A-514

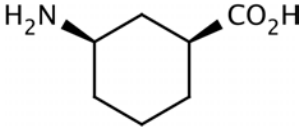
Compound name : 6-Amino-2-chloro-9-(2'-*O*-methylsulfonyl-β-D-xylofuranosyl)-9*H*-purine



Mol. Formula :	$C_{11}H_{14}ClN_5O_6S$	**FW :**	379.78	**HBA:**	11	**HBD:**	3	**RotB:**	4
PubChem ID :	254973	**CASRN :**	858675-99-7			**logP:**	-1.25	**TPSA:**	162.7

NIMH Code : A-701

Compound name : *cis*-3-Aminocyclohexanecarboxylic acid

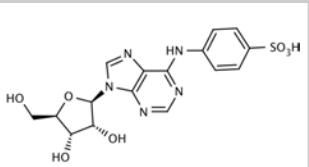


Mol. Formula :	$C_7H_{13}NO_2$	**FW :**	143.18	**HBA:**	3	**HBD:**	2	**RotB:**	1
PubChem ID :	544887	**CASRN :**	38541-66-1			**logP:**	-1.87	**TPSA:**	67.8

Activity: Neuronal GABA uptake inhibitor.

NIMH Code : A-702

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



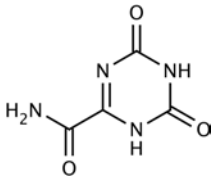
Mol. Formula : $C_{22}H_{32}N_6O_7S$ **FW :** 423.40 **HBA:** 12 **HBD:** 5 **RotB:** 5

PubChem ID : 9866960 **CASRN :** **logP:** -2.98 **TPSA:** 182.8

Activity: Water-soluble adenosine A_1 agonist.

NIMH Code : A-703

Compound name : Allantoxanamide



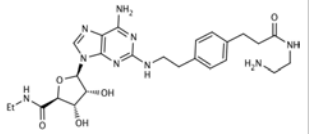
Mol. Formula : $C_4H_4N_4O_3$ **FW :** 156.10 **HBA:** 7 **HBD:** 1 **RotB:** 1

PubChem ID : 188244 **CASRN :** 69391-08-8 **logP:** -1.99 **TPSA:** 110.9

Activity: Uricase inhibitor.

NIMH Code : A-704

Compound name : APEC trifluoroacetate



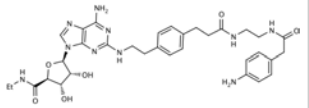
Mol. Formula : $C_{29}H_{37}F_6N_9O_9$ **FW :** 769.65 **HBA:** 14 **HBD:** 7 **RotB:** 12

PubChem ID : 3081741 **CASRN :** 126828-50-0 **logP:** -1.13 **TPSA:** 217.2

Activity: Adenosine A_2 receptor ligand.

NIMH Code : A-705

Compound name : p-Aminophenylacetyl-APEC



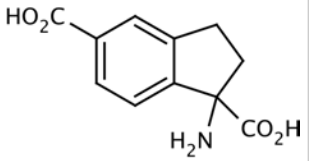
Mol. Formula : $C_{33}H_{42}N_{10}O_6$ **FW :** 674.75 **HBA:** 16 **HBD:** 8 **RotB:** 15

PubChem ID : 3081715 **CASRN :** 124190-27-8 **logP:** -0.31 **TPSA:** 244.7

Activity: Functionalized adenosine A_2 ligand.

NIMH Code : A-801

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



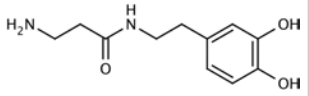
Mol. Formula : $C_{11}H_{11}NO_4$ **FW :** 221.21 **HBA:** 5 **HBD:** 3 **RotB:** 2

PubChem ID : 2071 **CASRN :** 168560-79-0 **logP:** -1.32 **TPSA:** 107.9

Activity: Metabotropic glutamate $mGluR_1$ antagonist.

NIMH Code : A-802

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



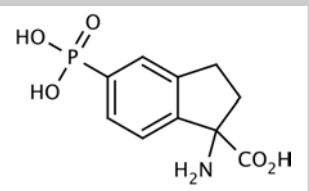
Mol. Formula : $C_{12}H_{18}N_2O_5$ **FW :** 270.28 **HBA:** 5 **HBD:** 4 **RotB:** 5

PubChem ID : 162755 **CASRN :** 54653-62-2 **logP:** -0.60 **TPSA:** 97.2

Activity: Sclerotin precursor.

NIMH Code : A-803

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



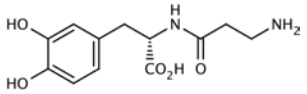
Mol. Formula : $C_{10}H_{12}NO_5P$ **FW :** 257.18 **HBA:** 6 **HBD:** 4 **RotB:** 2

PubChem ID : 4694355 **CASRN :** **logP:** -2.34 **TPSA:** 131.0

Activity: Metabotropic glutamate $mGluR_2$ ligand.

NIMH Code : A-804

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

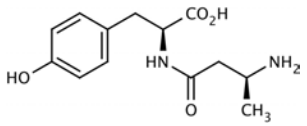


Mol. Formula : $C_{14}H_{17}F_3N_2O_7$ **FW :** 382.29 **HBA:** 7 **HBD:** 5 **RotB:** 6

PubChem ID : **CASRN :** **logP:** -2.66 **TPSA:** 137.3

NIMH Code : A-805

Compound name : Sarcophagine trifluoroacetate (Alanyltyrosine trifluoroacetate)

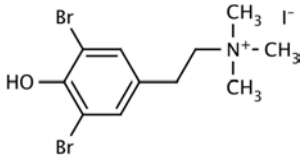


Mol. Formula : $C_{14}H_{17}F_3N_2O_6$ **FW :** 380.32 **HBA:** 6 **HBD:** 4 **RotB:** 6

PubChem ID : 92946 **CASRN :** 3061-88-9 **logP:** -1.94 **TPSA:** 117.1

NIMH Code : A-806

Compound name : Autonomium iodide

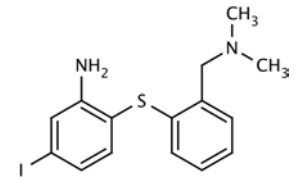


Mol. Formula : $C_{11}H_{16}Br_2INO$ **FW :** 464.96 **HBA:** 2 **HBD:** 1 **RotB:** 3

PubChem ID : **CASRN :** **logP:** -0.73 **TPSA:** 23.1

NIMH Code : A-807

Compound name : ADAM



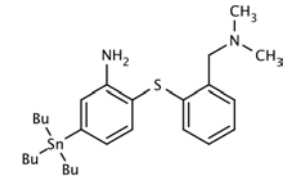
Mol. Formula : $C_{15}H_{17}IN_2S$ **FW :** 384.28 **HBA:** 2 **HBD:** 1 **RotB:** 4

PubChem ID : **CASRN :** **logP:** 4.20 **TPSA:** 30.5

Activity: Serotonin transporter ligand.

NIMH Code : A-808

Compound name : Tributylstannyl-ADAM



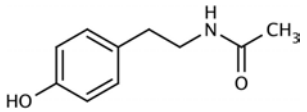
Mol. Formula : $C_{27}H_{44}N_2SSn$ **FW :** 547.43 **HBA:** 2 **HBD:** 1 **RotB:** 14

PubChem ID : **CASRN :** **logP:** 6.74 **TPSA:** 30.5

Activity: Radioiodinated ADAM precusor.

NIMH Code : A-901

Compound name : N-Acetyltyramine

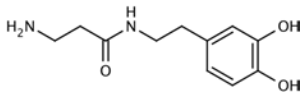


Mol. Formula : $C_{10}H_{13}NO_2$ **FW :** 179.22 **HBA:** 3 **HBD:** 2 **RotB:** 3

PubChem ID : 121051 **CASRN :** 1202-66-0 **logP:** 0.90 **TPSA:** 49.3

NIMH Code : A-902

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



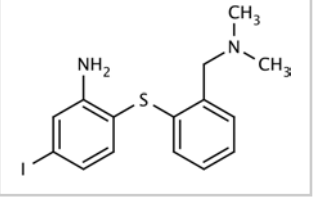
Mol. Formula : $C_{11}H_{17}ClN_2O_3$ **FW :** 260.72 **HBA:** 5 **HBD:** 4 **RotB:** 5

PubChem ID : 162755 **CASRN :** 54653-62-2 **logP:** -0.60 **TPSA:** 97.2

Activity: Sclerotin precursor.

NIMH Code : A-903

Compound name : ADAM dihydrochloride



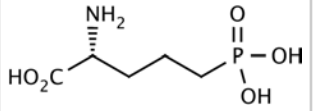
Mol. Formula : $C_{15}H_{19}Cl_2IN_2S$ **FW :** 457.20 **HBA:** 2 **HBD:** 1 **RotB:** 4

PubChem ID : **CASRN :** **logP:** 4.20 **TPSA:** 30.5

Activity: Serotonin transporter ligand.

NIMH Code : A-904

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



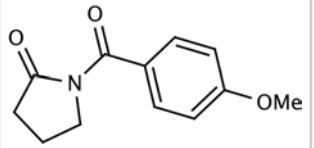
Mol. Formula : $C_5H_{12}NO_5P$ **FW :** 197.13 **HBA:** 6 **HBD:** 4 **RotB:** 5

PubChem ID : 135342 **CASRN :** 79088-68-8 **logP:** -3.23 **TPSA:** 128.1

Activity: NMDA receptor antagonist.

NIMH Code : A-905

Compound name : Aniracetam



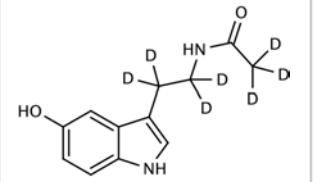
Mol. Formula : $C_{12}H_{13}NO_3$ **FW :** 219.24 **HBA:** 4 **HBD:** 0 **RotB:** 2

PubChem ID : 2196 **CASRN :** 72432-10-1 **logP:** 1.11 **TPSA:** 46.6

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

NIMH Code : A-906

Compound name : d_7-*N*-Acetylserotonin



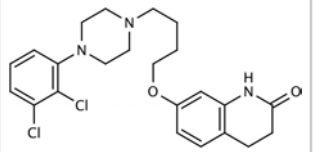
Mol. Formula : $C_{12}H_7D_7N_2O_2$. **FW :** 225.29 **HBA:** 4 **HBD:** 2 **RotB:** 3

PubChem ID : 903 **CASRN :** 1210-83-9 **logP:** 1.00 **TPSA:** 65.1

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

NIMH Code : A-907

Compound name : Aripiprazole



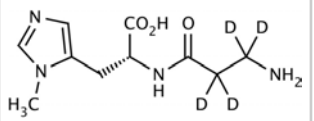
Mol. Formula : $C_{23}H_{27}Cl_2N_3O_2$ **FW :** 448.39 **HBA:** 5 **HBD:** 1 **RotB:** 7

PubChem ID : 60795 **CASRN :** 129722-12-9 **logP:** 4.90 **TPSA:** 46.0

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

NIMH Code : A-908

Compound name : Anserine-d_4



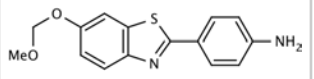
Mol. Formula : $C_{10}H_{12}D_4N_4O_3$ **FW :** 244.28 **HBA:** 7 **HBD:** 3 **RotB:** 6

PubChem ID : 11444 **CASRN :** 584-85-0 **logP:** -4.26 **TPSA:** 114.7

Activity: Stable isotope labeled anserine.

NIMH Code : A-909

Compound name : 6-MOMO-BTA-0



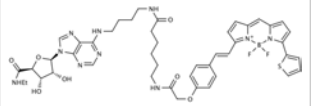
Mol. Formula : $C_{15}H_{14}N_2O_2S$ **FW :** 286.35 **HBA:** 4 **HBD:** 1 **RotB:** 4

PubChem ID : 11778756 **CASRN :** **logP:** 3.21 **TPSA:** 57.4

Activity: β-Amyloid plaque PET imaging agent precusor.

NIMH Code : A-910

Compound name : ABEA-X-BY630



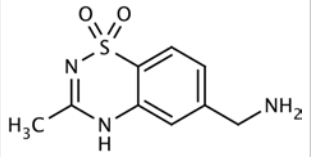
Mol. Formula : $C_{45}H_{51}BF_2N_{10}O_7S$ **FW :** 924.82 **HBA:** 17 **HBD:** 6 **RotB:** 21

PubChem ID : 16109359 **CASRN :** 21 **logP:** -2.13 **TPSA:** 209.8

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



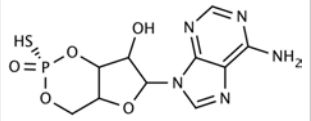
Mol. Formula : $C_9H_{12}ClN_3O_2S$ **FW :** 261.73 **HBA:** 5 **HBD:** 2 **RotB:** 1

PubChem ID : 121929 **CASRN :** 79987-38-5 **logP:** -0.48 **TPSA:** 86.2

Activity: Taurine antagonist.

NIMH Code : A-912

Compound name : (*S*p)-cAMPS triethylammonium salt



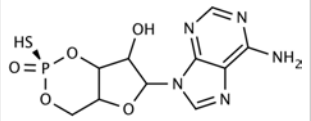
Mol. Formula : $C_{16}H_{27}N_6O_5PS$ **FW :** 446.46 **HBA:** 10 **HBD:** 2 **RotB:** 1

PubChem ID : 6858240 **CASRN :** 93602-66-5 **logP:** -3.10 **TPSA:** 134.6

Activity: Protein kinase A agonist.

NIMH Code : A-913

Compound name : (*R*p)-cAMPS triethylammonium salt



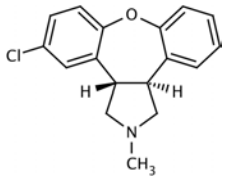
Mol. Formula : $C_{16}H_{27}N_6O_5PS$ **FW :** 446.46 **HBA:** 10 **HBD:** 2 **RotB:** 1

PubChem ID : 6858240 **CASRN :** **logP:** -3.10 **TPSA:** 134.6

Activity: Protein kinase A inhibitor.

NIMH Code : A-914

Compound name : Asenapine maleate



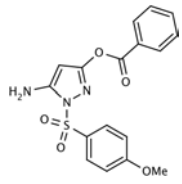
Mol. Formula : $C_{21}H_{20}ClNO_5$ **FW :** 401.84 **HBA:** 2 **HBD:** 0 **RotB:** 0

PubChem ID : 11954293 **CASRN :** 65576-45-6 **logP:** 3.72 **TPSA:** 12.5

Activity: Serotonergic, dopaminergic, & adrenergic receptor partial agonist.

NIMH Code : A-915

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



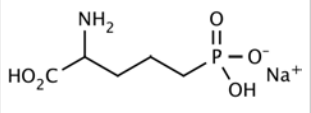
Mol. Formula : $C_{17}H_{15}N_3O_5S$ **FW :** 373.38 **HBA:** 8 **HBD:** 1 **RotB:** 5

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

Activity: NS3 West Nile virus protease inhibitor.

NIMH Code : A-916

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



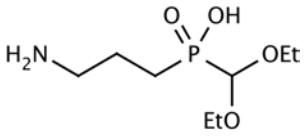
Mol. Formula : $C_5H_{11}NNaO_5P$ **FW :** 219.11 **HBA:** 6 **HBD:** 3 **RotB:** 5

PubChem ID : 1216 **CASRN :** **logP:** -3.23 **TPSA:** 128.1

Activity: NMDA glutamate receptor antagonist.

NIMH Code : A-917

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

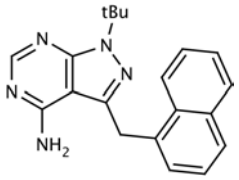


Mol. Formula :	$C_8H_{20}NO_4P$	**FW :**	225.22	**HBA:**	5	**HBD:**	2	**RotB:**	8
PubChem ID :	107699	**CASRN :**	123690-79-9			**logP:**	-1.29	**TPSA:**	86.2

Activity: $GABA_B$ receptor antagonist.

NIMH Code : A-918

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

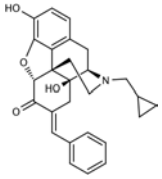


Mol. Formula :	$C_{20}H_{21}N_5$	**FW :**	331.41	**HBA:**	5	**HBD:**	1	**RotB:**	3
PubChem ID :	5154691	**CASRN :**	221244-14-0			**logP:**	3.64	**TPSA:**	69.6

Activity: CDK inhibitor.

NIMH Code : B-139

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

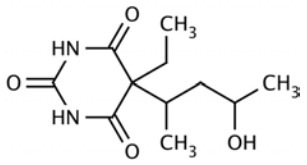


Mol. Formula :	$C_{27}H_{28}ClNO_4$	**FW :**	465.97	**HBA:**	5	**HBD:**	2	**RotB:**	3
PubChem ID :	5310988	**CASRN :**	5			**logP:**	3.41	**TPSA:**	71.2

Activity: Delta opioid δ1 receptor antagonist.

NIMH Code : B-501

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

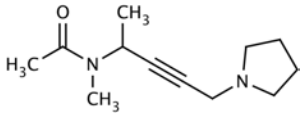


Mol. Formula :	$C_{11}H_{18}N_2O_4$	**FW :**	242.27	**HBA:**	6	**HBD:**	3	**RotB:**	4
PubChem ID :	94288	**CASRN :**	4241-40-1			**logP:**	0.43	**TPSA:**	95.5

Activity: Pentobarbitol metabolite.

NIMH Code : B-504

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

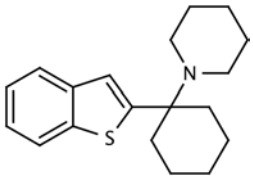


Mol. Formula :	$C_{14}H_{22}N_2O_5$	**FW :**	298.33	**HBA:**	3	**HBD:**	0	**RotB:**	4
PubChem ID :	55005	**CASRN :**	83481-69-0			**logP:**	0.73	**TPSA:**	24.8

Activity: Muscarinic receptor partial agonist (oxotremorine analog).

NIMH Code : B-701

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

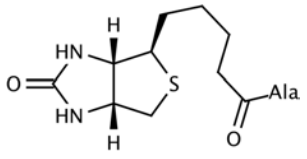


Mol. Formula :	$C_{19}H_{26}ClNS$	**FW :**	335.94	**HBA:**	1	**HBD:**	0	**RotB:**	2
PubChem ID :	123692	**CASRN :**	112726-66-6			**logP:**	5.50	**TPSA:**	4.4

Activity: Dopamine uptake inhibitor with little affinity for PCP sites.

NIMH Code : B-702

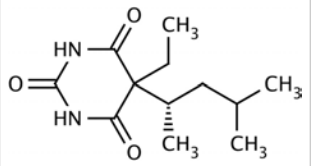
Compound name : Biotin-poly-DL-alanine



Mol. Formula :	-	**FW :**	299.39	**HBA:**	6	**HBD:**	3	**RotB:**	7
PubChem ID :	-	**CASRN :**	-			**logP:**	0.58	**TPSA:**	102.9

NIMH Code : B-704

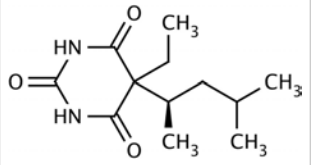
Compound name : (*S*)-(–)-5-(1,3-Dimethylbutyl)-5-ethylbarbituric acid (Diberal)



Mol. Formula :	$C_{12}H_{20}N_2O_3$	**FW :**	240.30	**HBA:**	5	**HBD:**	2	**RotB:**	4
PubChem ID :	18079	**CASRN :**	2964-06-9			**logP:**	2.18	**TPSA:**	75.3

NIMH Code : B-705

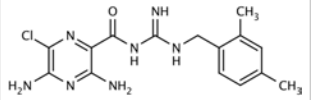
Compound name : (*R*)-(+)-5-(1,3-Dimethylbutyl)-5-ethylbarbituric acid (Diberal)



Mol. Formula :	$C_{12}H_{20}N_2O_3$	**FW :**	240.30	**HBA:**	5	**HBD:**	2	**RotB:**	4
PubChem ID :	18079	**CASRN :**	2964-06-9			**logP:**	2.18	**TPSA:**	75.3

NIMH Code : B-709

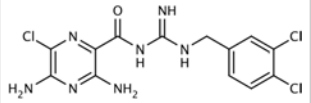
Compound name : 2',4'-Dimethylbenzamil hydrochloride



Mol. Formula :	$C_{15}H_{19}Cl_2N_7O$	**FW :**	384.26	**HBA:**	8	**HBD:**	5	**RotB:**	3
PubChem ID :	10247117	**CASRN :**				**logP:**	2.53	**TPSA:**	142.8
Activity:	Sodium/calcium exchanger inhibitor.								

NIMH Code : B-710

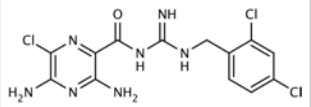
Compound name : 3',4'-Dichlorobenzamil hydrochloride



Mol. Formula :	$C_{13}H_{13}Cl_4N_7O$	**FW :**	425.10	**HBA:**	8	**HBD:**	5	**RotB:**	3
PubChem ID :	114771	**CASRN :**	1166-01-4			**logP:**	2.71	**TPSA:**	142.8
Activity:	Sodium/calcium exchanger inhibitor.								

NIMH Code : B-711

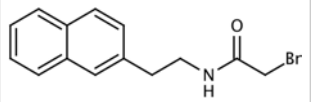
Compound name : 2',4'-Dichlorobenzamil hydrochloride



Mol. Formula :	$C_{13}H_{13}Cl_4N_7O$	**FW :**	425.10	**HBA:**	8	**HBD:**	5	**RotB:**	3
PubChem ID :	6610300	**CASRN :**				**logP:**	2.71	**TPSA:**	142.8
Activity:	Sodium/calcium exchanger inhibitor.								

NIMH Code : B-801

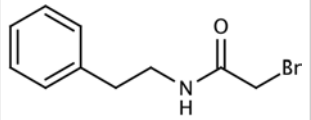
Compound name : N-Bromoacetylnapthalene-2-ethylamine



Mol. Formula :	$C_{14}H_{14}BrNO$	**FW :**	292.17	**HBA:**	2	**HBD:**	1	**RotB:**	4
PubChem ID :	23626931	**CASRN :**				**logP:**	2.92	**TPSA:**	29.1

NIMH Code : B-802

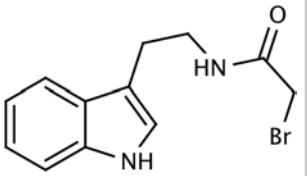
Compound name : N-Bromoacetyl-β-phenethylamine



Mol. Formula :	$C_{10}H_{12}BrNO$	**FW :**	242.11	**HBA:**	2	**HBD:**	1	**RotB:**	4
PubChem ID :	9881279	**CASRN :**				**logP:**	1.93	**TPSA:**	29.1

NIMH Code : B-803

Compound name : N-Bromoacetyltryptamine



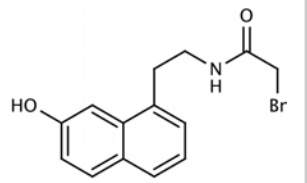
Mol. Formula : $C_{12}H_{13}BrN_2O$ **FW :** 281.15 **HBA:** 3 **HBD:** 1 **RotB:** 4

PubChem ID : 399698 **CASRN :** **logP:** 2.03 **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

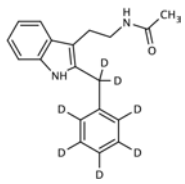


Mol. Formula : $C_{14}H_{14}BrNO_2$ **FW :** 308.17 **HBA:** 3 **HBD:** 2 **RotB:** 4

PubChem ID : **CASRN :** **logP:** 2.62 **TPSA:** 49.3

NIMH Code : B-805

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



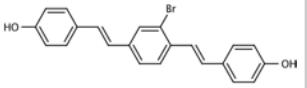
Mol. Formula : $C_{19}H_{13}D_7N_2O$ **FW :** 299.42 **HBA:** 3 **HBD:** 1 **RotB:** 5

PubChem ID : **CASRN :** **logP:** 3.16 **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

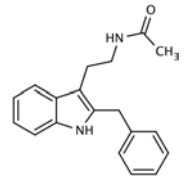


Mol. Formula : $C_{22}H_{17}BrO_2$ **FW :** 393.27 **HBA:** 2 **HBD:** 2 **RotB:** 4

PubChem ID : **CASRN :** **logP:** 6.81 **TPSA:** 40.5

NIMH Code : B-807

Compound name : Luzindole



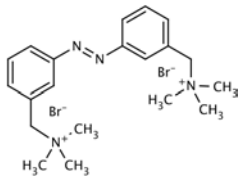
Mol. Formula : $C_{19}H_{20}N_2O$ **FW :** 292.37 **HBA:** 3 **HBD:** 1 **RotB:** 5

PubChem ID : 122162 **CASRN :** 117946-91-5 **logP:** 3.16 **TPSA:** 44.9

Activity: Melatonin receptor antagonist.

NIMH Code : B-901

Compound name : *trans*-Bis-Q



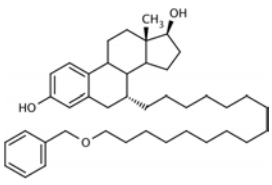
Mol. Formula : $C_{20}H_{30}Br_2N_4$ **FW :** 486.29 **HBA:** 4 **HBD:** 0 **RotB:** 6

PubChem ID : 133795 **CASRN :** 81931-05-7 **logP:** -4.06 **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

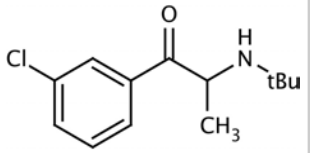


Mol. Formula : $C_{41}H_{62}O_3$ **FW :** 602.93 **HBA:** 3 **HBD:** 2 **RotB:** 19

PubChem ID : **CASRN :** **logP:** 11.63 **TPSA:** 49.7

NIMH Code : B-903

Compound name : Bupropion hydrochloride



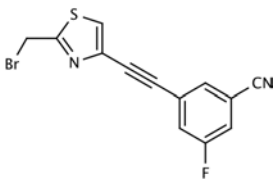
Mol. Formula : $C_{13}H_{19}Cl_2NO$ **FW :** 276.20 **HBA:** 2 **HBD:** 1 **RotB:** 4

PubChem ID : 62884 **CASRN :** 34841-36-6 **logP:** 3.27 **TPSA:** 33.7

Activity: Dopamine & norepinephrine reuptake inhibitor.

NIMH Code : B-904

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



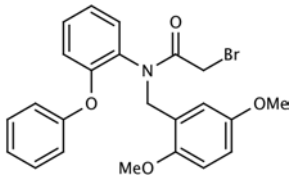
Mol. Formula : $C_{13}H_6BrFN_2S$ **FW :** 321.17 **HBA:** 2 **HBD:** 0 **RotB:** 3

PubChem ID : **CASRN :** **logP:** 3.98 **TPSA:** 36.7

Activity: Metabotropic glutamate $mGluR_5$ PET imaging ligand precursor.

NIMH Code : B-905

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



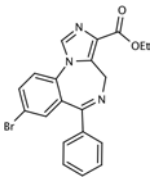
Mol. Formula : $C_{23}H_{22}BrNO_4$ **FW :** 456.33 **HBA:** 5 **HBD:** 0 **RotB:** 8

PubChem ID : **CASRN :** **logP:** 4.71 **TPSA:** 48.0

Activity: Brain peripheral benzodiazepine receptor (TSPO) ligand.

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

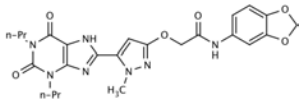


Mol. Formula : $C_{20}H_{16}BrN_3O_2$ **FW :** 410.26 **HBA:** 5 **HBD:** 0 **RotB:** 4

PubChem ID : 21930956 **CASRN :** **logP:** 3.48 **TPSA:** 56.5

NIMH Code : B-907

Compound name : MRE 2029-F20



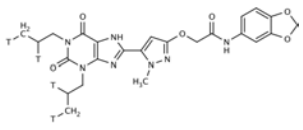
Mol. Formula : $C_{24}H_{27}N_7O_6$ **FW :** 509.51 **HBA:** 13 **HBD:** 1 **RotB:** 9

PubChem ID : **CASRN :** **logP:** 2.33 **TPSA:** 141.0

Activity: A_{2B} adenosine receptor antagonist.

NIMH Code : B-908

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



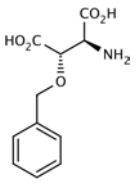
Mol. Formula : $C_{24}H_{27}N_7O_6$ **FW :** 517.55 **HBA:** 13 **HBD:** 1 **RotB:** 9

PubChem ID : **CASRN :** **logP:** 2.33 **TPSA:** 141.0

Activity: A_{2B} adenosine receptor radioligand.

NIMH Code : B-909

Compound name : DL-TBOA



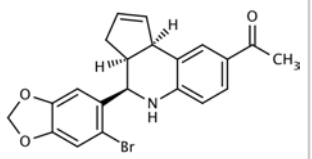
Mol. Formula : $C_{11}H_{13}NO_5$ **FW :** 239.22 **HBA:** 6 **HBD:** 3 **RotB:** 6

PubChem ID : 5311218 **CASRN :** **logP:** -2.08 **TPSA:** 117.1

Activity: Glutamate uptake inhibitor.

NIMH Code : B-910

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



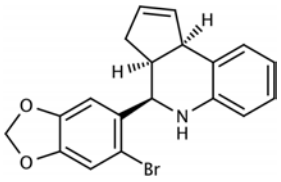
Mol. Formula : $C_{21}H_{18}BrNO_3$ **FW :** 412.28 **HBA:** 4 **HBD:** 1 **RotB:** 2

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

Activity: GPR30 agonist.

NIMH Code : B-911

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



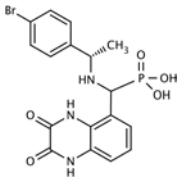
Mol. Formula : $C_{19}H_{16}BrNO_2$ **FW :** 370.24 **HBA:** 3 **HBD:** 1 **RotB:** 1

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

Activity: GPR30 antagonist.

NIMH Code : B-912

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)



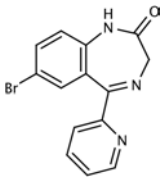
Mol. Formula : $C_{17}H_{18}BrClN_3O_5P$ **FW :** 490.67 **HBA:** 8 **HBD:** 3 **RotB:** 5

PubChem ID : 9868551 **CASRN :** 858131-65-4 **logP:** 0.82 **TPSA:** 130.6

Activity: NMDA receptor antagonist.

NIMH Code : B-913

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



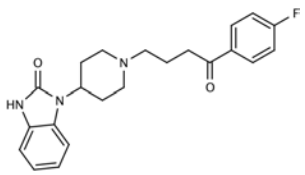
Mol. Formula : $C_{14}H_{10}BrN_3O$ **FW :** 316.15 **HBA:** 4 **HBD:** 1 **RotB:** 1

PubChem ID : 2441 **CASRN :** 1812-30-2 **logP:** 2.54 **TPSA:** 54.4

Activity: $GABA_A$ receptor allosteric modulator.

NIMH Code : B-914

Compound name : Benperidol



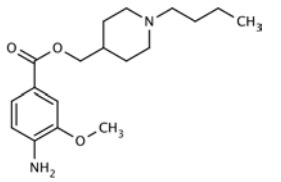
Mol. Formula : $C_{22}H_{24}FN_3O_2$ **FW :** 381.44 **HBA:** 5 **HBD:** 0 **RotB:** 6

PubChem ID : 16363 **CASRN :** 2062-84-2 **logP:** 3.12 **TPSA:** 52.7

Activity: Antipsychotic; Dopamine D2 receptor antagonist.

NIMH Code : B-915 new

Compound name : (1-Butylpiperidin-4-yl)methyl 4-Amino-3-methoxybenzoate



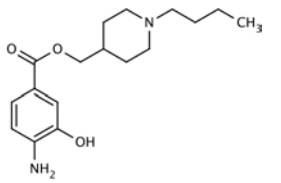
Mol. Formula : $C_{18}H_{28}N_2O_3$ **FW :** 320.43 **HBA:** 5 **HBD:** 1 **RotB:** 8

PubChem ID : 49783415 **CASRN :** - **logP:** 2.80 **TPSA:** 66.0

Activity: Serotonin 5-HT_4 receptor agonist.

NIMH Code : B-916 new

Compound name : (1-Butylpiperidin-4-yl)methyl 4-Amino-3-hydroxybenzoate

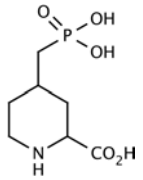


Mol. Formula : $C_{17}H_{26}N_2O_3$ **FW :** 306.40 **HBA:** 5 **HBD:** 2 **RotB:** 7

PubChem ID : 49780154 **CASRN :** **logP:** 2.06 **TPSA:** 77.0

NIMH Code : C-105

Compound name : CGS 19755 (Selfotel)

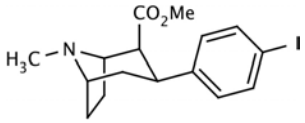


Mol. Formula :	$C_7H_{14}NO_5P$	**FW :**	223.16	**HBA:**	6	**HBD:**	4	**RotB:**	3
PubChem ID :	68736	**CASRN :**	110347-85-8			**logP:**	-3.28	**TPSA:**	117.1

Activity: Competitive NMDA antagonist.

NIMH Code : C-148

Compound name : RTI-55

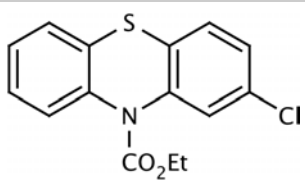


Mol. Formula :	$C_{20}H_{26}INO_8$	**FW :**	535.33	**HBA:**	3	**HBD:**	0	**RotB:**	3
PubChem ID :	108220	**CASRN :**	133647-95-7			**logP:**	3.44	**TPSA:**	30.7

Activity: Dopamine reuptake inhibitor.

NIMH Code : C-501

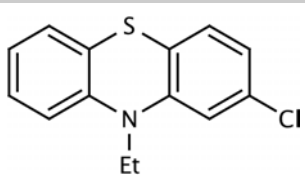
Compound name : 10-Carboethoxy-2-chlorophenothiazine



Mol. Formula :	$C_{15}H_{12}ClNO_2S$	**FW :**	305.78	**HBA:**	3	**HBD:**	0	**RotB:**	2
PubChem ID :		**CASRN :**				**logP:**	4.53	**TPSA:**	29.5

NIMH Code : C-502

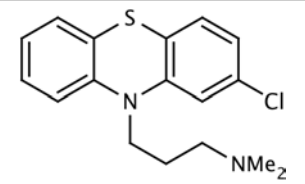
Compound name : N-Ethyl-2-chlorophenothiazine



Mol. Formula :	$C_{14}H_{12}ClNS$	**FW :**	261.77	**HBA:**	1	**HBD:**	0	**RotB:**	1
PubChem ID :		**CASRN :**	56301-63-4			**logP:**	4.81	**TPSA:**	3.2

NIMH Code : C-503

Compound name : Chlorpromazine hydrochloride

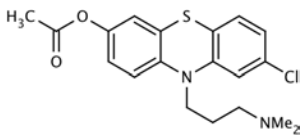


Mol. Formula :	$C_{17}H_{20}Cl_2N_2S$	**FW :**	355.33	**HBA:**	2	**HBD:**	0	**RotB:**	4
PubChem ID :	2726	**CASRN :**	69-09-0			**logP:**	4.54	**TPSA:**	7.7

Activity: Dopamine, 5-HT, histamine, adrenaline, & muscarinic receptor antagonist.

NIMH Code : C-504

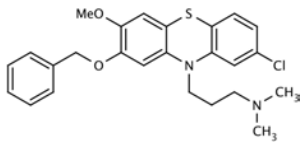
Compound name : 7-Acetoxychlorpromazine hydrogen maleate



Mol. Formula :	$C_{23}H_{25}ClN_2O_6S$	**FW :**	492.97	**HBA:**	4	**HBD:**	0	**RotB:**	6
PubChem ID :	547310	**CASRN :**				**logP:**	4.14	**TPSA:**	34.0

NIMH Code : C-505

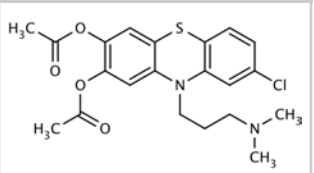
Compound name : 8-Benzyloxy-7-methoxychlorpromazine



Mol. Formula :	$C_{25}H_{27}ClN_2O_2S$	**FW :**	455.01	**HBA:**	4	**HBD:**	0	**RotB:**	8
PubChem ID :		**CASRN :**				**logP:**	5.94	**TPSA:**	26.1

NIMH Code : C-506

Compound name : 7,8-Diacetoxychlorpromazine hydrogen maleate

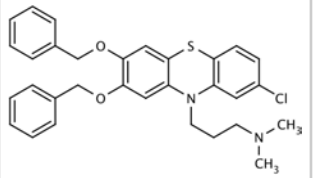


Mol. Formula : $C_{25}H_{27}ClN_2O_8S$ **FW :** 551.01 **HBA:** 6 **HBD:** 0 **RotB:** 8

PubChem ID : **CASRN :** **logP:** 3.75 **TPSA:** 60.3

NIMH Code : C-508

Compound name : 7,8-Dibenzyloxychlorpromazine

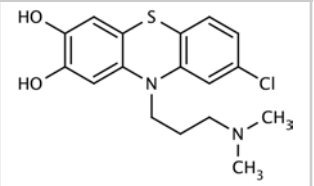


Mol. Formula : $C_{31}H_{31}ClN_2O_2S$ **FW :** 531.11 **HBA:** 4 **HBD:** 0 **RotB:** 10

PubChem ID : **CASRN :** **logP:** 7.67 **TPSA:** 26.1

NIMH Code : C-511

Compound name : 7,8-Dihydroxychlorpromazine hydrochloride



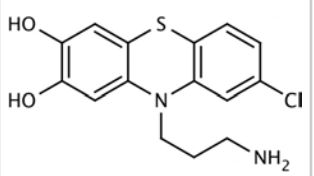
Mol. Formula : $C_{17}H_{20}Cl_2N_2O_2S$ **FW :** 387.32 **HBA:** 4 **HBD:** 2 **RotB:** 4

PubChem ID : 159916 **CASRN :** 21598-02-7 **logP:** 3.39 **TPSA:** 48.1

Activity: Chlorpromazine metabolite.

NIMH Code : C-512

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



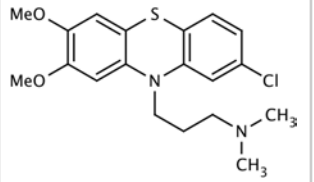
Mol. Formula : $C_{15}H_{16}C_2N_2O_2S$ **FW :** 359.27 **HBA:** 4 **HBD:** 3 **RotB:** 3

PubChem ID : 125358 **CASRN :** 95574-30-4 **logP:** 2.36 **TPSA:** 71.3

Activity: Chlorpromazine metabolite.

NIMH Code : C-513

Compound name : 7,8-Dimethoxychlorpromazine hydrochloride



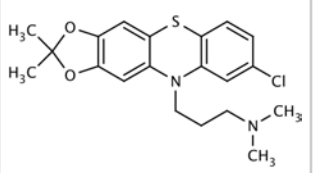
Mol. Formula : $C_{19}H_{24}Cl_2N_2O_2S$ **FW :** 415.38 **HBA:** 4 **HBD:** 0 **RotB:** 6

PubChem ID : 87327 **CASRN :** 17831-98-0 **logP:** 4.22 **TPSA:** 26.1

Activity: Chlorpromazine metabolite.

NIMH Code : C-514

Compound name : 7,8-(Dimethylmethylenedioxy)chlorpromazine



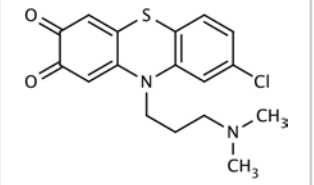
Mol. Formula : $C_{20}H_{23}ClN_2O_2S$ **FW :** 390.93 **HBA:** 4 **HBD:** 0 **RotB:** 4

PubChem ID : 114324 **CASRN :** 63834-02-6 **logP:** 4.64 **TPSA:** 26.1

Activity: Chlorpromazine metabolite.

NIMH Code : C-515

Compound name : 7,8-Dioxochlorpromazine hydrochloride



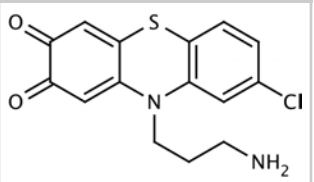
Mol. Formula : $C_{17}H_{18}Cl_2N_2O_2S$ **FW :** 385.31 **HBA:** 4 **HBD:** 0 **RotB:** 4

PubChem ID : 122845 **CASRN :** 52172-18-6 **logP:** 2.97 **TPSA:** 41.8

Activity: Chlorpromazine metabolite.

NIMH Code : C-516

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

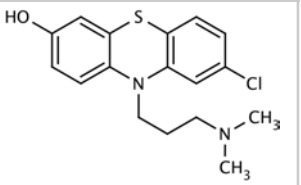


Mol. Formula : $C_{15}H_{14}Cl_2N_2O_2S$ **FW :** 357.26 **HBA:** 4 **HBD:** 1 **RotB:** 3

PubChem ID : 125595 **CASRN :** 95574-31-5 **logP:** 2.16 **TPSA:** 65.0

NIMH Code : C-518

Compound name : 7-Hydroxychlorpromazine hydrochloride



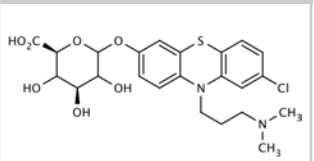
Mol. Formula : $C_{17}H_{20}Cl_2N_2OS$ **FW :** 371.33 **HBA:** 3 **HBD:** 1 **RotB:** 4

PubChem ID : 16414 **CASRN :** 2095-62-7 **logP:** 3.92 **TPSA:** 27.9

Activity: Dopamine receptor antagonist.

NIMH Code : C-519

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



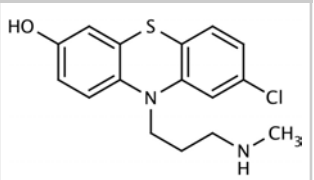
Mol. Formula : $C_{25}H_{28}ClF_3N_2O_9S$ **FW :** 625.01 **HBA:** 9 **HBD:** 4 **RotB:** 7

PubChem ID : **CASRN :** **logP:** -0.45 **TPSA:** 127.0

Activity: 7-Hydroxychlorpromazine metabolite.

NIMH Code : C-520

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



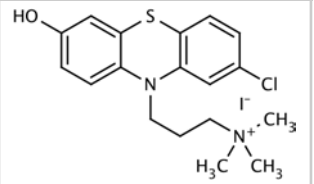
Mol. Formula : $C_{16}H_{18}Cl_2N_2OS$ **FW :** 357.30 **HBA:** 3 **HBD:** 2 **RotB:** 4

PubChem ID : 107410 **CASRN :** 3546-08-5 **logP:** 3.31 **TPSA:** 40.1

Activity: Chlorpromazine metabolite.

NIMH Code : C-521

Compound name : 7-Hydroxychlorpromazine methiodide



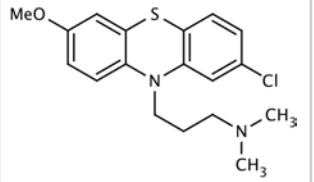
Mol. Formula : $C_{18}H_{22}ClIN_2OS$ **FW :** 476.80 **HBA:** 3 **HBD:** 1 **RotB:** 4

PubChem ID : **CASRN :** **logP:** 0.07 **TPSA:** 23.5

Activity: Dopamine receptor antagonist.

NIMH Code : C-523

Compound name : 7-Methoxychlorpromazine hydrochloride



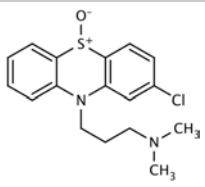
Mol. Formula : $C_{18}H_{22}Cl_2N_2OS$ **FW :** 385.35 **HBA:** 3 **HBD:** 0 **RotB:** 5

PubChem ID : 21115409 **CASRN :** 2752-11-6 **logP:** 4.38 **TPSA:** 16.9

Activity: Chlorpromazine metabolite.

NIMH Code : C-524

Compound name : Chlorpromazine sulfoxide hydrochloride



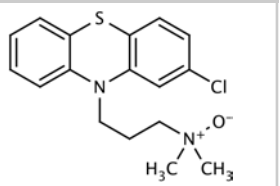
Mol. Formula : $C_{17}H_{20}Cl_2N_2OS$ **FW :** 371.33 **HBA:** 3 **HBD:** 0 **RotB:** 4

PubChem ID : 70413 **CASRN :** 969-99-30 **logP:** 3.16 **TPSA:** 24.8

Activity: Dopamine receptor antagonist.

NIMH Code : C-525

Compound name : Chlorpromazine-*N*-oxide



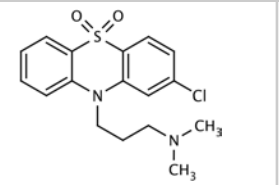
Mol. Formula : $C_{17}H_{19}ClN_2OS$ **FW :** 334.86 **HBA:** 3 **HBD:** 0 **RotB:** 4

PubChem ID : 443037 **CASRN :** 1672-76-0 **logP:** 3.41 **TPSA:** 30.1

Activity: Dopamine receptor antagonist.

NIMH Code : C-526

Compound name : Chlorpromazine sulfone hydrochloride

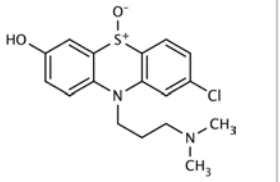


Mol. Formula : $C_{17}H_{20}Cl_2N_2O_2S$ **FW :** 387.32 **HBA:** 4 **HBD:** 0 **RotB:** 4

PubChem ID : 165214 **CASRN :** **logP:** 3.30 **TPSA:** 41.8

NIMH Code : C-528

Compound name : 7-Hydroxychlorpromazine sulfoxide

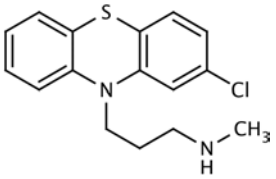


Mol. Formula : $C_{17}H_{19}ClN_2O_2S$ **FW :** 350.86 **HBA:** 4 **HBD:** 1 **RotB:** 4

PubChem ID : 21857538 **CASRN :** **logP:** 2.60 **TPSA:** 45.0

NIMH Code : C-529

Compound name : *nor*-1-Chlorpromazine hydrochloride



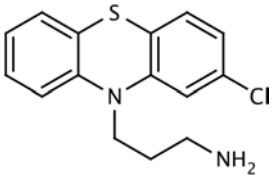
Mol. Formula : $C_{16}H_{18}Cl_2N_2S$ **FW :** 341.30 **HBA:** 2 **HBD:** 1 **RotB:** 4

PubChem ID : 520950 **CASRN :** 1225-64-5 **logP:** 4.15 **TPSA:** 19.9

Activity: Chlorpromazine metabolite.

NIMH Code : C-530

Compound name : *nor*-2-Chlorpromazine hydrochloride



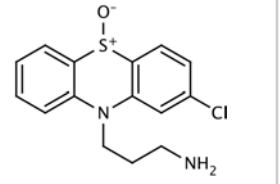
Mol. Formula : $C_{15}H_{16}Cl_2N_2S$ **FW :** 327.27 **HBA:** 2 **HBD:** 1 **RotB:** 3

PubChem ID : 197797 **CASRN :** 3763-80-2 **logP:** 3.72 **TPSA:** 30.9

Activity: Active metabolite of chlorpromazine.

NIMH Code : C-531

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



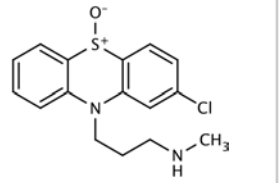
Mol. Formula : $C_{15}H_{16}Cl_2N_2OS$ **FW :** 343.27 **HBA:** 3 **HBD:** 1 **RotB:** 3

PubChem ID : 75220 **CASRN :** 2232-49-7 **logP:** 2.35 **TPSA:** 48.0

Activity: Chlorpromazine metabolite.

NIMH Code : C-532

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

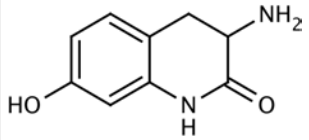


Mol. Formula : $C_{16}H_{18}Cl_2N_2OS$ **FW :** 357.30 **HBA:** 3 **HBD:** 1 **RotB:** 4

PubChem ID : 11723560 **CASRN :** **logP:** 2.78 **TPSA:** 36.9

NIMH Code : C-535

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

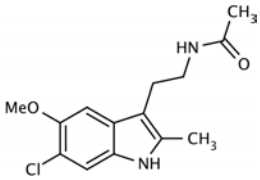


Mol. Formula : $C_9H_{10}N_2O_2$ **FW :** 178.19 **HBA:** 4 **HBD:** 3 **RotB:** 0

PubChem ID : **CASRN :** **logP:** -0.01 **TPSA:** 77.0

NIMH Code : C-536

Compound name : 6-Chloro-2-methylmelatonin

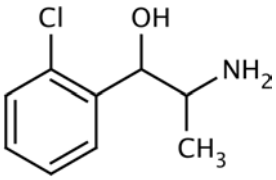


Mol. Formula : $C_{14}H_{17}ClN_2O_2$ **FW :** 280.75 **HBA:** 4 **HBD:** 1 **RotB:** 4

PubChem ID : **CASRN :** **logP:** 1.95 **TPSA:** 54.1

NIMH Code : C-537

Compound name : 2-Chloropropadrine hydrochloride

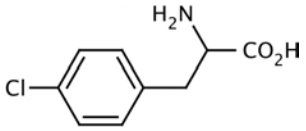


Mol. Formula : $C_9H_{13}Cl_2NO$ **FW :** 222.11 **HBA:** 2 **HBD:** 2 **RotB:** 2

PubChem ID : **CASRN :** **logP:** 1.49 **TPSA:** 47.9

NIMH Code : C-538

Compound name : (±)-p-Chlorophenylalanine (Fenclonine)



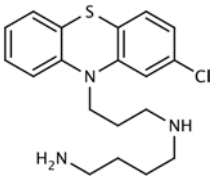
Mol. Formula : $C_9H_{10}ClNO_2$ **FW :** 199.63 **HBA:** 3 **HBD:** 2 **RotB:** 3

PubChem ID : 4652 **CASRN :** 7424-00-2 **logP:** -0.58 **TPSA:** 67.8

Activity: Serotonin receptor antagonist.

NIMH Code : C-701

Compound name : Chlorpromazine-10-spermidine dihydrochloride



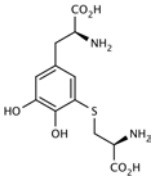
Mol. Formula : $C_{19}H_{26}Cl_3N_3S$ **FW :** 434.85 **HBA:** 3 **HBD:** 2 **RotB:** 8

PubChem ID : **CASRN :** **logP:** 3.93 **TPSA:** 47.5

Activity: Potential prodrug for polyamines.

NIMH Code : C-702

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



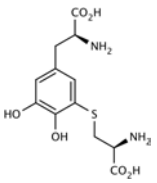
Mol. Formula : $C_{12}H_{16}N_2O_6S$ **FW :** 316.33 **HBA:** 8 **HBD:** 6 **RotB:** 7

PubChem ID : **CASRN :** **logP:** -4.79 **TPSA:** 176.0

Activity: Melanoma biomarker.

NIMH Code : C-702A

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



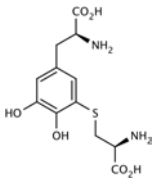
Mol. Formula : $C_{12}H_{18}Cl_2N_2O_6S$ **FW :** 389.25 **HBA:** 8 **HBD:** 6 **RotB:** 7

PubChem ID : **CASRN :** **logP:** -4.79 **TPSA:** 176.0

Activity: Melanoma biomarker.

NIMH Code : C-702B

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



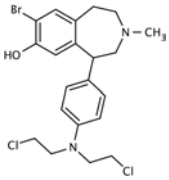
Mol. Formula : $C_{16}H_{18}F_6N_2O_{10}S$ **FW :** 544.38 **HBA:** 8 **HBD:** 6 **RotB:** 7

PubChem ID : **CASRN :** **logP:** -4.79 **TPSA:** 176.0

Activity: Melanoma biomarker.

NIMH Code : C-705

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



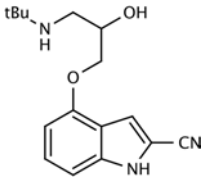
Mol. Formula : $C_{21}H_{26}BrCl_3N_2O$ **FW :** 508.71 **HBA:** 3 **HBD:** 1 **RotB:** 6

PubChem ID : **CASRN :** **logP:** 5.01 **TPSA:** 27.9

Activity: Dopamine D_1 receptor alkylating ligand.

NIMH Code : C-706

Compound name : Cyanopindolol fumarate



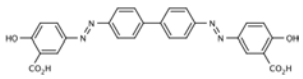
Mol. Formula : $C_{36}H_{46}N_6O_8$ **FW :** 690.79 **HBA:** 5 **HBD:** 2 **RotB:** 6

PubChem ID : 155346 **CASRN :** 69906-85-0 **logP:** 1.75 **TPSA:** 85.7

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

NIMH Code : C-707

Compound name : Chrysamine G



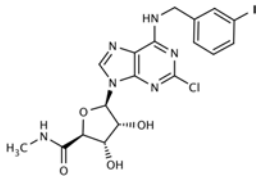
Mol. Formula : $C_{26}H_{18}N_4O_6$ **FW :** 482.44 **HBA:** 10 **HBD:** 4 **RotB:** 7

PubChem ID : 6506185 **CASRN :** 6472-91-9 **logP:** 8.44 **TPSA:** 170.2

Activity: β-Amyloid ligand.

NIMH Code : C-708

Compound name : Chloro-IB-MECA



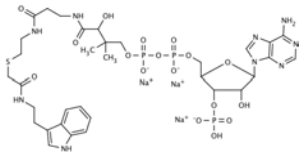
Mol. Formula : $C_{18}H_{18}ClIN_6O_4$ **FW :** 544.73 **HBA:** 10 **HBD:** 4 **RotB:** 5

PubChem ID : 393593 **CASRN :** 163042-96-4 **logP:** 1.51 **TPSA:** 134.4

Activity: A_3 adenosine receptor ligand.

NIMH Code : C-711

Compound name : Coenzyme A-*S*-acetyltryptamine



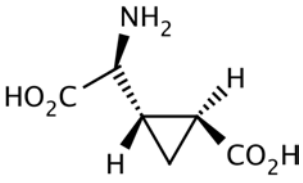
Mol. Formula : $C_{33}H_{45}N_9Na_3O_{17}P_3S$ **FW :** 1033.72 **HBA:** 26 **HBD:** 7 **RotB:** 24

PubChem ID : 2822 **CASRN :** **logP:** -5.73 **TPSA:** 402.8

Activity: Arylalkylamine N-acetyltransferase (AANAT) inhibitor.

NIMH Code : C-801

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



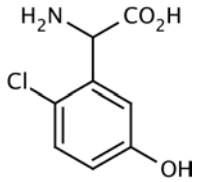
Mol. Formula : $C_6H_9NO_4$ **FW :** 159.14 **HBA:** 5 **HBD:** 3 **RotB:** 3

PubChem ID : 5310956 **CASRN :** 22255-17-0 **logP:** -3.25 **TPSA:** 107.9

Activity: Metabotropic glutamate $mGluR_2$ receptor agonist.

NIMH Code : C-802

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



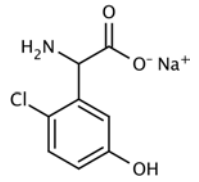
Mol. Formula : $C_8H_8ClNO_3$ **FW :** 201.61 **HBA:** 4 **HBD:** 3 **RotB:** 2

PubChem ID : 3645780 **CASRN :** **logP:** -1.17 **TPSA:** 88.0

Activity: Metabotropic glutamate $mGlu_5$ receptor agonist.

NIMH Code : C-802A

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



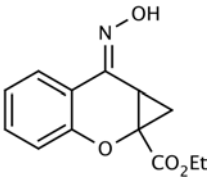
Mol. Formula : $C_8H_7ClNNaO_3$ **FW :** 223.59 **HBA:** 4 **HBD:** 2 **RotB:** 2

PubChem ID : 3645780 **CASRN :** **logP:** -1.17 **TPSA:** 88.0

Activity: Metabotropic glutamate $mGlu_5$ receptor agonist.

NIMH Code : C-803

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



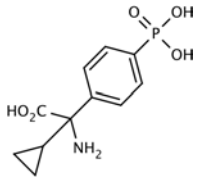
Mol. Formula : $C_{13}H_{13}NO_4$ **FW :** 247.25 **HBA:** 5 **HBD:** 1 **RotB:** 3

PubChem ID : 6278000 **CASRN :** 179067-99-3 **logP:** 1.66 **TPSA:** 71.0

Activity: Metabotropic glutamate $mGluR_1$ receptor antagonist.

NIMH Code : C-804

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



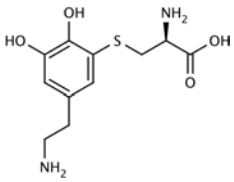
Mol. Formula : $C_{11}H_{14}NO_5P$ **FW :** 271.21 **HBA:** 6 **HBD:** 4 **RotB:** 4

PubChem ID : 2878 **CASRN :** **logP:** -1.97 **TPSA:** 131.0

Activity: Metabotropic glutamate $mGluR_3$ receptor antagonist.

NIMH Code : C-805A

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

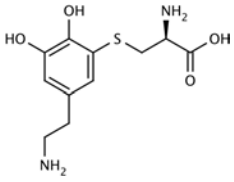


Mol. Formula : $C_{15}H_{18}F_6N_2O_8S$ **FW :** 500.37 **HBA:** 6 **HBD:** 5 **RotB:** 6

PubChem ID : 122084 **CASRN :** 99558-89-1 **logP:** -2.70 **TPSA:** 135.9

NIMH Code : C-805B

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

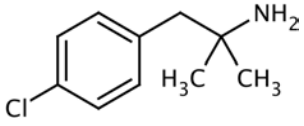


Mol. Formula : $C_{11}H_{18}Cl_2N_2O_4S$ **FW :** 345.24 **HBA:** 6 **HBD:** 5 **RotB:** 6

PubChem ID : 122084 **CASRN :** 99558-89-1 **logP:** -2.70 **TPSA:** 135.9

NIMH Code : C-806

Compound name : Chlorophentermine hydrochloride



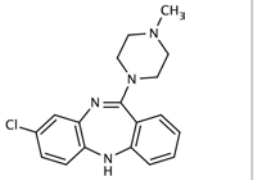
Mol. Formula : $C_{10}H_{15}Cl_2N$ **FW :** 220.14 **HBA:** 1 **HBD:** 1 **RotB:** 2

PubChem ID : 10007 **CASRN :** 151-06-4 **logP:** 2.69 **TPSA:** 27.6

Activity: Sympathomimetic.

NIMH Code : C-807

Compound name : Clozapine



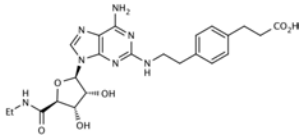
Mol. Formula : $C_{18}H_{19}ClN_4$ **FW :** 326.82 **HBA:** 4 **HBD:** 1 **RotB:** 0

PubChem ID : SID: 24277892 **CASRN :** 5786-21-0 **logP:** 3.40 **TPSA:** 30.9

Activity: Dopamine D_4 receptor antagonist.

NIMH Code : C-901

Compound name : CGS 21680 hydrochloride



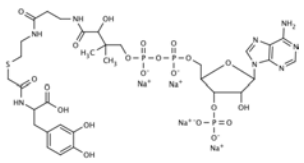
Mol. Formula : $C_{23}H_{30}ClN_7O_6$ **FW :** 535.98 **HBA:** 13 **HBD:** 6 **RotB:** 10

PubChem ID : 10256643 **CASRN :** 124182-57-6 **logP:** -0.87 **TPSA:** 200.6

Activity: Adenosine A_2 receptor agonist.

NIMH Code : C-902

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

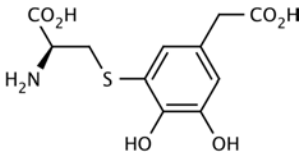


Mol. Formula : $C_{32}H_{43}N_8Na_4O_{21}P_3S$ **FW :** 1092.67 **HBA:** 29 **HBD:** 9 **RotB:** 25

PubChem ID : **CASRN :** **logP:** -5.70 **TPSA:** 467.6

NIMH Code : C-903

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

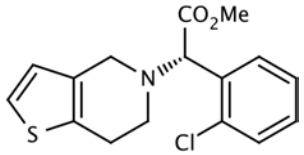


Mol. Formula : $C_{11}H_{14}ClNO_6S$ **FW :** 323.75 **HBA:** 7 **HBD:** 5 **RotB:** 6

PubChem ID : 128185 **CASRN :** 102986-13-0 **logP:** -2.09 **TPSA:** 148.4

NIMH Code : C-904

Compound name : Clopidogrel hydrogen sulfate



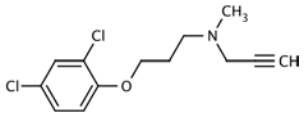
Mol. Formula : $C_{16}H_{18}ClNO_6S_2$ **FW :** 419.90 **HBA:** 3 **HBD:** 0 **RotB:** 4

PubChem ID : 115366 **CASRN :** 135046-48-9 **logP:** 4.03 **TPSA:** 29.5

Activity: Purinergic P_2Y_{12} receptor inhibitor.

NIMH Code : C-905

Compound name : Clorgyline hydrochloride



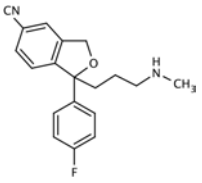
Mol. Formula : $C_{13}H_{16}Cl_3NO$ **FW :** 308.63 **HBA:** 2 **HBD:** 0 **RotB:** 6

PubChem ID : 28767 **CASRN :** 17780-75-5 **logP:** 3.33 **TPSA:** 13.7

Activity: Monoamine oxidase inhibitor.

NIMH Code : C-906

Compound name : N-Norcitalopram oxalate



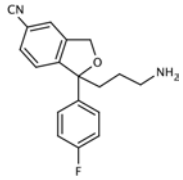
Mol. Formula : $C_{21}H_{21}FN_2O_5$ **FW :** 400.40 **HBA:** 3 **HBD:** 1 **RotB:** 5

PubChem ID : 162180 **CASRN :** 62498-67-3 **logP:** 3.38 **TPSA:** 49.6

Activity: Citalopram metabolite.

NIMH Code : C-907

Compound name : N,N-Dinorcitalopram oxalate



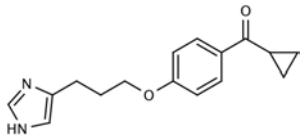
Mol. Formula : $C_{20}H_{19}FN_2O_5$ **FW :** 386.37 **HBA:** 3 **HBD:** 1 **RotB:** 4

PubChem ID : 162976 **CASRN :** 62498-69-5 **logP:** 2.95 **TPSA:** 60.7

Activity: Citalopram metabolite.

NIMH Code : C-908

Compound name : Ciproxifan



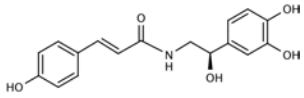
Mol. Formula : $C_{20}H_{22}N_2O_6$ **FW :** 270.33 **HBA:** 4 **HBD:** 0 **RotB:** 7

PubChem ID : 6422124 **CASRN :** 184025-19-2 **logP:** 2.37 **TPSA:** 55.0

Activity: Histamine H_3 receptor antagonist.

NIMH Code : C-909

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



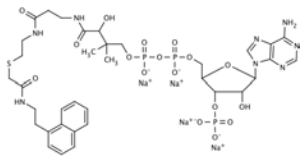
Mol. Formula : $C_{17}H_{17}NO_5$ **FW :** 315.32 **HBA:** 6 **HBD:** 5 **RotB:** 5

PubChem ID : **CASRN :** **logP:** 1.74 **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



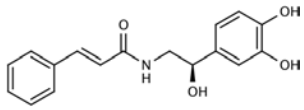
Mol. Formula : $C_{35}H_{45}N_8Na_4O_{17}P_3S$ **FW :** 1066.72 **HBA:** 25 **HBD:** 6 **RotB:** 24

PubChem ID : **CASRN :** **logP:** -4.84 **TPSA:** 387.0

Activity: Melatonin arylalkylamine-N-acetyltransferase rhythm enzyme ligand.

NIMH Code : C-911

Compound name : *N*-Cinnamoylnorepinephrine

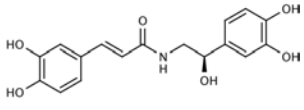


Mol. Formula : $C_{17}H_{17}NO_4$ **FW :** 299.32 **HBA:** 5 **HBD:** 4 **RotB:** 5

PubChem ID : **CASRN :** **logP:** 2.04 **TPSA:** 89.8

NIMH Code : C-912

Compound name : *N*-Caffeoylnorepinephrine

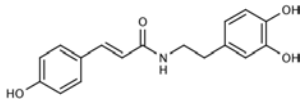


Mol. Formula : $C_{17}H_{17}NO_6$ **FW :** 331.32 **HBA:** 7 **HBD:** 6 **RotB:** 5

PubChem ID : **CASRN :** **logP:** 1.43 **TPSA:** 130.3

NIMH Code : C-913

Compound name : *N*-Coumaroyldopamine

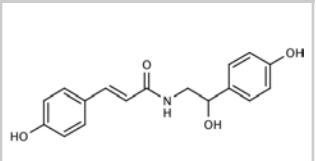


Mol. Formula : $C_{17}H_{17}NO_4$ **FW :** 299.32 **HBA:** 5 **HBD:** 4 **RotB:** 5

PubChem ID : 11630793 **CASRN :** **logP:** 2.66 **TPSA:** 89.8

NIMH Code : C-914

Compound name : *N*-Coumaroyloctopamine

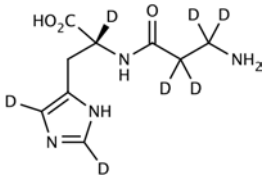


Mol. Formula : $C_{17}H_{17}NO_4$ **FW :** 299.32 **HBA:** 5 **HBD:** 4 **RotB:** 5

PubChem ID : 23874492 **CASRN :** **logP:** 2.04 **TPSA:** 89.8

NIMH Code : C-915

Compound name : Carnosine-d7



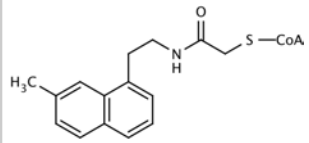
Mol. Formula : $C_9H_{14}N_4O_3$ **FW :** 233.28 **HBA:** 7 **HBD:** 3 **RotB:** 6

PubChem ID : 9369 **CASRN :** **logP:** -4.48 **TPSA:** 125.6

Activity: Stable isotope labeled carnosine.

NIMH Code : C-916

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



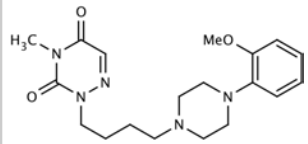
Mol. Formula : $C_{37}H_{49}N_8O_{17}P_3S_2$ **FW :** 1034.88 **HBA:** 25 **HBD:** 6 **RotB:** 25

PubChem ID : **CASRN :** **logP:** -3.71 **TPSA:** 387.0

Activity: Melatonin arylalkylamine-N-acetyltransferase rhythm enzyme ligand.

NIMH Code : C-917

Compound name : CUMI-101



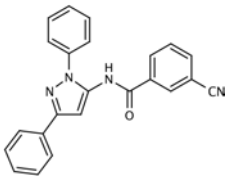
Mol. Formula : $C_{19}H_{27}N_5O_3$ **FW :** 373.45 **HBA:** 8 **HBD:** 0 **RotB:** 7

PubChem ID : 21830793 **CASRN :** **logP:** 1.79 **TPSA:** 69.9

Activity: Serotonin 5-HT_{1A} receptor agonist.

NIMH Code : C-918

Compound name : CDPPB



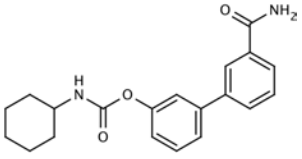
Mol. Formula : $C_{23}H_{16}N_4O$ **FW :** 364.40 **HBA:** 5 **HBD:** 1 **RotB:** 4

PubChem ID : 11245456 **CASRN :** 781652-57-1 **logP:** 5.13 **TPSA:** 70.7

Activity: Metabotropic glutamate $mGluR_5$ positive allosteric modulator.

NIMH Code : C-919

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



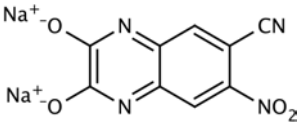
Mol. Formula : $C_{20}H_{22}N_2O_3$ **FW :** 338.40 **HBA:** 5 **HBD:** 2 **RotB:** 5

PubChem ID : 1383884 **CASRN :** 546141-08-6 **logP:** 3.77 **TPSA:** 81.4

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

NIMH Code : C-920

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



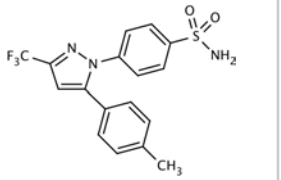
Mol. Formula : $C_9H_2N_4Na_2O_4$ **FW :** 276.12 **HBA:** 8 **HBD:** 0 **RotB:** 1

PubChem ID : 2821 **CASRN :** 115066-14-3 **logP:** 1.68 **TPSA:** 135.9

Activity: AMPA/kainate receptor antagonist.

NIMH Code : C-921

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



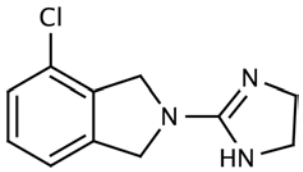
Mol. Formula : $C_{17}H_{14}F_3N_3O_2S$ **FW :** 381.37 **HBA:** 5 **HBD:** 1 **RotB:** 4

PubChem ID : 2662 **CASRN :** 169590-42-5 **logP:** 4.01 **TPSA:** 78.0

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)



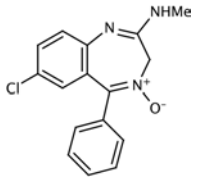
Mol. Formula : $C_{11}H_{13}ClIN_3$ **FW :** 349.60 **HBA:** 3 **HBD:** 1 **RotB:** 0

PubChem ID : 127951 **CASRN :** 170034-96-5 **logP:** 1.71 **TPSA:** 29.2

Activity: Selective I2 imidazoline receptor ligand.

NIMH Code : C-923 new

Compound name : Chlordiazepoxide (Librium)



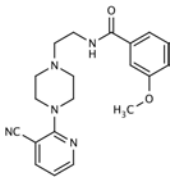
Mol. Formula : $C_{16}H_{14}ClN_3O$ **FW :** 299.76 **HBA:** 4 **HBD:** 1 **RotB:** 1

PubChem ID : 2712 **CASRN :** 58-25-3 **logP:** 3.05 **TPSA:** 53.1

Activity: Prototypical benzodiazepine anxiolytic; $GABA_A$ receptor allosteric modulator.

NIMH Code : C-924 new

Compound name : N-[2-[4-(3-Cyanopyridin-2-yl)piperazin-1-yl]ethyl]-3-methoxybenzamide (TA-2)



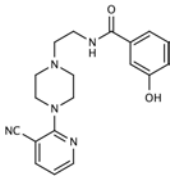
Mol. Formula : $C_{20}H_{23}N_5O_2$ **FW :** 365.43 **HBA:** 7 **HBD:** 1 **RotB:** 6

PubChem ID : - **CASRN :** 1252676-34-8 **logP:** 1.88 **TPSA:** 81.5

Activity: Dopamine D4 receptor ligand.

NIMH Code : C-925 new

Compound name : N-[2-[4-(3-Cyanopyridin-2-yl)piperazin-1-yl]ethyl]-3-hydroxybenzamide



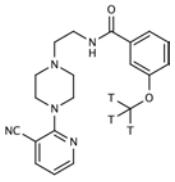
Mol. Formula : $C_{19}H_{21}N_5O_2$ **FW :** 351.40 **HBA:** 7 **HBD:** 2 **RotB:** 5

PubChem ID : - **CASRN :** 1252676-40-6 **logP:** 1.73 **TPSA:** 92.5

Activity: Dopamine D4 receptor ligand precursor.

NIMH Code : C-926 new

Compound name : *N*-[2-[4-(3-Cyanopyridin-2-yl)piperazin-1-yl]ethyl]-3-[^{3}H]methoxybenzamide ([^{3}H]TA-2)



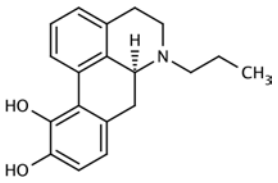
Mol. Formula : $C_{20}H_{23}N_5O_2$ **FW :** 371.45 **HBA:** 7 **HBD:** 1 **RotB:** 6

PubChem ID : - **CASRN :** - **logP:** 1.88 **TPSA:** 81.5

Activity: Dopamine D4 receptor radioligand.

NIMH Code : D-041

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



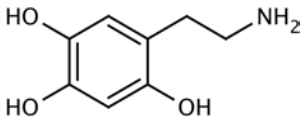
Mol. Formula : $C_{19}H_{22}ClNO_2$ **FW :** 331.84 **HBA:** 3 **HBD:** 2 **RotB:** 2

PubChem ID : 13533173 **CASRN :** 79703-31-4 **logP:** 3.67 **TPSA:** 47.7

Activity: Limbic-selective dopamine receptor antagonist.

NIMH Code : D-501

Compound name : 6-Hydroxydopamine hydrobromide (Oxidopamine)



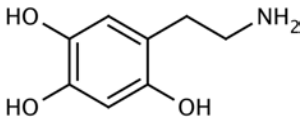
Mol. Formula : $C_8H_{12}BrNO_3$ **FW :** 250.09 **HBA:** 4 **HBD:** 4 **RotB:** 2

PubChem ID : 176170 **CASRN :** 636-00-0 **logP:** -0.15 **TPSA:** 88.3

Activity: Catecholaminergic neurotoxin.

NIMH Code : D-502

Compound name : 6-Hydroxydopamine hydrochloride (Oxidopamine)



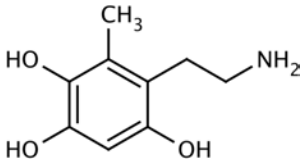
Mol. Formula : $C_8H_{12}ClNO_3$ **FW :** 205.64 **HBA:** 4 **HBD:** 4 **RotB:** 2

PubChem ID : 160157 **CASRN :** 28094-15-7 **logP:** -0.15 **TPSA:** 88.3

Activity: Catecholaminergic neurotoxin.

NIMH Code : D-503

Compound name : 2-Methyl-6-hydroxydopamine hydrobromide

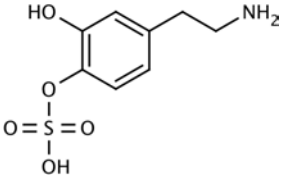


Mol. Formula : $C_9H_{14}BrNO_3$ **FW :** 264.12 **HBA:** 4 **HBD:** 4 **RotB:** 2

PubChem ID : **CASRN :** **logP:** 0.48 **TPSA:** 88.3

NIMH Code : D-504

Compound name : Dopamine-4-O-sulfate



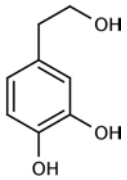
Mol. Formula : $C_8H_{11}NO_5S$ **FW :** 233.24 **HBA:** 6 **HBD:** 3 **RotB:** 4

PubChem ID : 123932 **CASRN :** 38339-02-5 **logP:** -0.05 **TPSA:** 114.3

Activity: Possible norepinephrine precursor.

NIMH Code : D-505

Compound name : Hydroxytyrosol



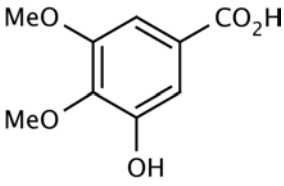
Mol. Formula : $C_{14}H_{22}N_2O_3$ **FW :** 154.16 **HBA:** 3 **HBD:** 3 **RotB:** 2

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

Activity: Platelet aggregation inhibitor.

NIMH Code : D-506

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



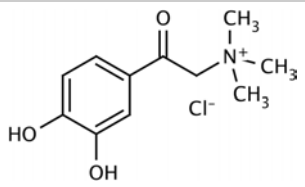
Mol. Formula : $C_9H_{10}O_5$ **FW :** 198.17 **HBA:** 5 **HBD:** 2 **RotB:** 3

PubChem ID : 74709 **CASRN :** 1916-08-1 **logP:** 1.01 **TPSA:** 78.8

Activity: Thiopurine methyltransferase inhibitor.

NIMH Code : D-507

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

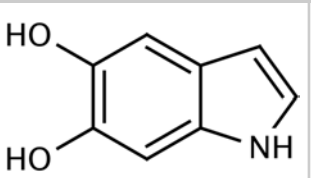


Mol. Formula : $C_{11}H_{16}ClNO_3$ **FW :** 245.70 **HBA:** 4 **HBD:** 2 **RotB:** 3

PubChem ID : 412800 **CASRN :** **logP:** -3.35 **TPSA:** 57.5

NIMH Code : D-509

Compound name : 5,6-Dihydroxyindole

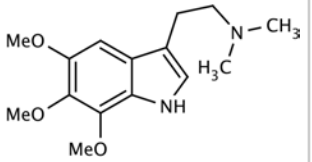


Mol. Formula :	$C_8H_7NO_2$	**FW :** 149.15	**HBA:** 3	**HBD:** 2	**RotB:** 0
PubChem ID :	114683	**CASRN :** 3131-52-0		**logP:** 1.46	**TPSA:** 56.3

Activity: Catechol O-methyltransferase (COMT) inhibitor.

NIMH Code : D-510

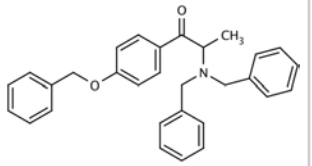
Compound name : 5,6,7-Trimethoxy-N,N-dimethyltryptamine



Mol. Formula :	$C_{15}H_{22}N_2O_3$	**FW :** 278.35	**HBA:** 5	**HBD:** 0	**RotB:** 6
PubChem ID :	12650292	**CASRN :** -		**logP:** 1.83	**TPSA:** 47.9

NIMH Code : D-511

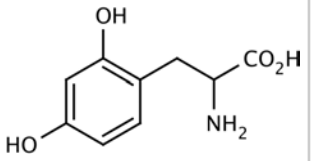
Compound name : 4'-Benzyloxy-2-dibenzylaminopropiophenone



Mol. Formula :	$C_{30}H_{29}NO_2$	**FW :** 435.56	**HBA:** 3	**HBD:** 0	**RotB:** 10
PubChem ID :	-	**CASRN :** -		**logP:** 7.01	**TPSA:** 29.5

NIMH Code : D-512

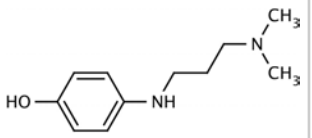
Compound name : (±)-2,4-Dihydroxyphenylalanine



Mol. Formula :	$C_9H_{11}NO_4$	**FW :** 197.19	**HBA:** 5	**HBD:** 4	**RotB:** 3
PubChem ID :	251462	**CASRN :** 582-34-3		**logP:** -1.79	**TPSA:** 108.2

NIMH Code : D-513

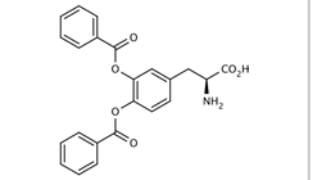
Compound name : 4-(γ-N,N-Dimethylaminopropylamino)phenol dimaleate



Mol. Formula :	$C_{19}H_{26}N_2O_9$	**FW :** 426.42	**HBA:** 3	**HBD:** 2	**RotB:** 5
PubChem ID :	20283862	**CASRN :** -		**logP:** 0.97	**TPSA:** 36.7

NIMH Code : D-514

Compound name : L-3,4-Dibenzoyloxyphenylalanine

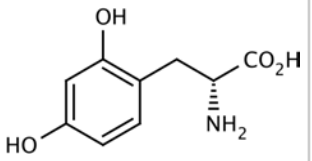


Mol. Formula :	$C_{23}H_{19}NO_6$	**FW :** 405.40	**HBA:** 7	**HBD:** 2	**RotB:** 9
PubChem ID :	149369	**CASRN :** 120382-00-5		**logP:** 2.14	**TPSA:** 120.4

Activity: Na-K-ATPase inhibitor.

NIMH Code : D-515

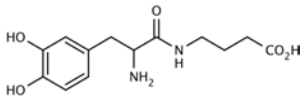
Compound name : (+)-2,4-Dihydroxyphenylalanine



Mol. Formula :	$C_9H_{11}NO_4$	**FW :** 197.19	**HBA:** 5	**HBD:** 4	**RotB:** 3
PubChem ID :	152670	**CASRN :** 24146-06-3		**logP:** -1.79	**TPSA:** 108.2

NIMH Code : D-516

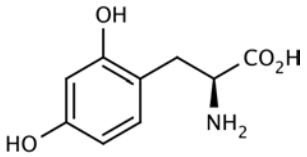
Compound name : (±)-3,4-Dihydroxyphenylalanyl-GABA



Mol. Formula :	$C_{13}H_{18}N_2O_5$	**FW :**	282.29	**HBA:**	7	**HBD:**	5	**RotB:**	7
PubChem ID :		**CASRN :**				**logP:**	-2.37	**TPSA:**	137.3

NIMH Code : D-517

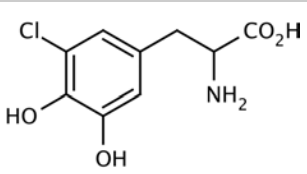
Compound name : (–)-2,4-Dihydroxyphenylalanine



Mol. Formula :	$C_9H_{11}NO_4$	**FW :**	197.19	**HBA:**	5	**HBD:**	4	**RotB:**	3
PubChem ID :	152670	**CASRN :**	24146-06-3			**logP:**	-1.79	**TPSA:**	108.2

NIMH Code : D-518

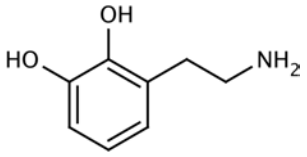
Compound name : (±)-3-Chloro-4,5-dihydroxyphenylalanine hydrobromide



Mol. Formula :	$C_9H_{11}BrClNO_4$	**FW :**	312.54	**HBA:**	5	**HBD:**	4	**RotB:**	3
PubChem ID :		**CASRN :**				**logP:**	-1.19	**TPSA:**	108.2

NIMH Code : D-519

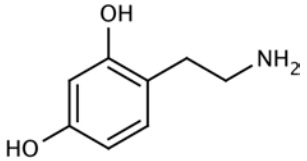
Compound name : 2,3-Dihydroxy-β-phenethylamine hydrobromide



Mol. Formula :	$C_8H_{12}BrNO_2$	**FW :**	234.09	**HBA:**	3	**HBD:**	3	**RotB:**	2
PubChem ID :		**CASRN :**				**logP:**	0.15	**TPSA:**	68.1

NIMH Code : D-520

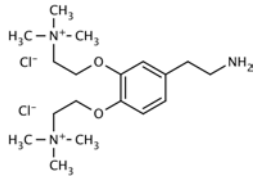
Compound name : 2,4-Dihydroxy-β-phenethylamine hydrochloride



Mol. Formula :	$C_8H_{12}ClNO_2$	**FW :**	189.64	**HBA:**	3	**HBD:**	3	**RotB:**	2
PubChem ID :	150962	**CASRN :**	2039-62-5			**logP:**	0.11	**TPSA:**	68.1

NIMH Code : D-521

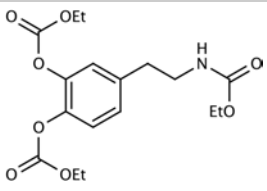
Compound name : 3,4-Di-(β-trimethylammoniumethoxy)-β-phenethylamine hydrochloride dichloride



Mol. Formula :	$C_{18}H_{36}Cl_3N_3O_2$	**FW :**	432.86	**HBA:**	5	**HBD:**	1	**RotB:**	10
PubChem ID :		**CASRN :**				**logP:**	-7.22	**TPSA:**	46.1

NIMH Code : D-522

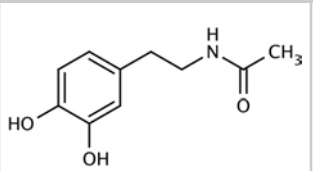
Compound name : 3,4-Diethylcarbonato-β-phenethylamine carbamate



Mol. Formula :	$C_{17}H_{23}NO_8$	**FW :**	369.37	**HBA:**	9	**HBD:**	1	**RotB:**	13
PubChem ID :		**CASRN :**				**logP:**	3.35	**TPSA:**	109.4

NIMH Code : D-523

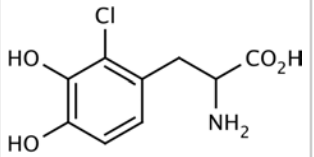
Compound name : N-Acetyl-3,4-dihydroxy-β-phenethylamine



Mol. Formula :	$C_{10}H_{13}NO_3$	**FW :**	195.22	**HBA:**	4	**HBD:**	3	**RotB:**	3
PubChem ID :	100526	**CASRN :**	2494-12-4			**logP:**	0.60	**TPSA:**	69.6

NIMH Code : D-524

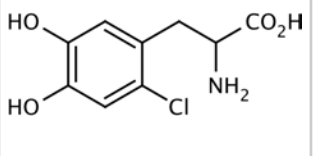
Compound name : (±)-2-Chloro-3,4-dihydroxyphenylalanine hydrobromide



Mol. Formula :	$C_9H_{11}BrClNO_4$	**FW :**	312.54	**HBA:**	5	**HBD:**	4	**RotB:**	3
PubChem ID :		**CASRN :**				**logP:**	-1.19	**TPSA:**	108.2

NIMH Code : D-525

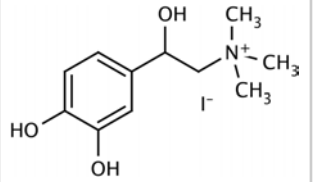
Compound name : (±)-6-Chloro-3,4-dihydroxyphenylalanine hydrobromide



Mol. Formula :	$C_9H_{11}BrClNO_4$	**FW :**	312.54	**HBA:**	5	**HBD:**	4	**RotB:**	3
PubChem ID :		**CASRN :**				**logP:**	-1.19	**TPSA:**	108.2

NIMH Code : D-528

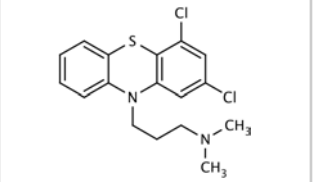
Compound name : (±)-(N,N-Dimethyl)ephedrine Iodide



Mol. Formula :	$C_{11}H_{18}INO_3$	**FW :**	339.17	**HBA:**	4	**HBD:**	3	**RotB:**	3
PubChem ID :	3082487	**CASRN :**	38522-73-5			**logP:**	-3.49	**TPSA:**	60.7

NIMH Code : D-529

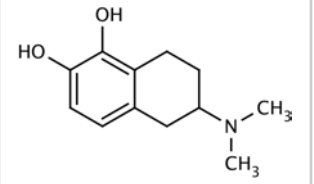
Compound name : 2,4-Dichloropromazine hydrochloride



Mol. Formula :	$C_{17}H_{19}Cl_3N_2S$	**FW :**	389.77	**HBA:**	2	**HBD:**	0	**RotB:**	4
PubChem ID :	77273	**CASRN :**	3689-36-9			**logP:**	5.14	**TPSA:**	7.7

NIMH Code : D-701

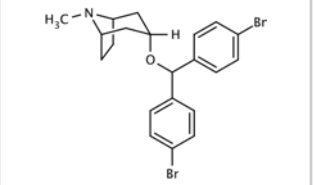
Compound name : (±)-5,6-Dihydroxy-2-(N,N-dimethyl)aminotetralin hydrobromide



Mol. Formula :	$C_{12}H_{18}BrNO_2$	**FW :**	288.18	**HBA:**	3	**HBD:**	2	**RotB:**	1
PubChem ID :	37032	**CASRN :**	39478-90-5			**logP:**	1.49	**TPSA:**	44.9

NIMH Code : D-702

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

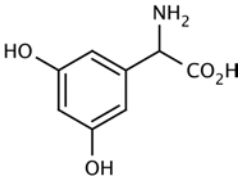


Mol. Formula :	$C_{21}H_{24}Br_2ClNO$	**FW :**	501.68	**HBA:**	2	**HBD:**	0	**RotB:**	4
PubChem ID :	10096017	**CASRN :**				**logP:**	5.72	**TPSA:**	13.7

Activity: Dopamine uptake inhibitor.

NIMH Code : D-801

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

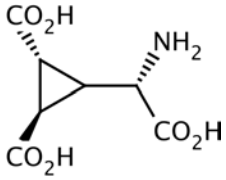


Mol. Formula :	$C_8H_9NO_4$	**FW :**	183.16	**HBA:**	5	**HBD:**	4	**RotB:**	2
PubChem ID :	108001	**CASRN :**	146255-66-5			**logP:**	-2.08	**TPSA:**	108.2

Activity: Metabotropic glutamate $mGluR_1$ & $mGluR_5$ 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

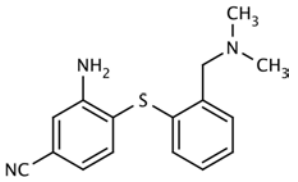


Mol. Formula :	$C_7H_9NO_6$	**FW :**	203.15	**HBA:**	7	**HBD:**	4	**RotB:**	4
PubChem ID :	5310979	**CASRN :**	147782-19-2			**logP:**	-4.08	**TPSA:**	148.0

Activity: Metabotropic glutamate $mGluR_2$ receptor agonist.

NIMH Code : D-803

Compound name : DASB hydrochloride

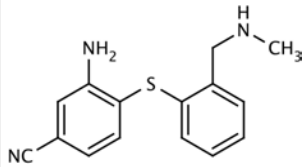


Mol. Formula :	$C_{16}H_{18}ClN_3S$	**FW :**	319.85	**HBA:**	3	**HBD:**	1	**RotB:**	4
PubChem ID :	10446567	**CASRN :**	627490-01-1			**logP:**	3.13	**TPSA:**	54.3

Activity: Serotonin transporter ligand.

NIMH Code : D-804

Compound name : Desmethyl-DASB

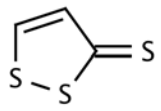


Mol. Formula :	$C_{15}H_{15}N_3S$	**FW :**	269.37	**HBA:**	3	**HBD:**	2	**RotB:**	4
PubChem ID :	10612056	**CASRN :**				**logP:**	2.75	**TPSA:**	66.4

Activity: DASB PET ligand precursor.

NIMH Code : D-805

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

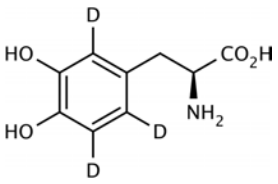


Mol. Formula :	$C_3H_2S_3$	**FW :**	134.24	**HBA:**	0	**HBD:**	0	**RotB:**	0
PubChem ID :	68296	**CASRN :**	534-25-8			**logP:**	2.07	**TPSA:**	0.0

Activity: Antineoplastic agent.

NIMH Code : D-901

Compound name : L-DOPA-ring-d_3

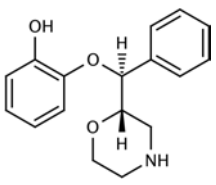


Mol. Formula :	$C_9H_8D_3NO_4$	**FW :**	200.21	**HBA:**	5	**HBD:**	4	**RotB:**	3
PubChem ID :	12297005	**CASRN :**	53587-29-4			**logP:**	-1.79	**TPSA:**	108.2

Activity: Stable isotope labeled L-DOPA.

NIMH Code : D-902

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

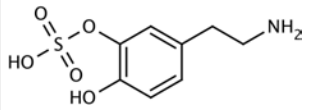


Mol. Formula :	$C_{17}H_{19}NO_3$	**FW :**	285.34	**HBA:**	4	**HBD:**	2	**RotB:**	4
PubChem ID :	10469169	**CASRN :**	-			**logP:**	2.77	**TPSA:**	55.3

Activity: Roboxetine PET ligand precusor.

NIMH Code : D-903

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



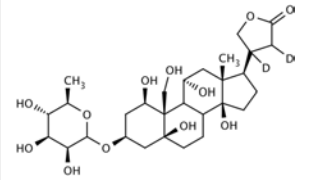
Mol. Formula : $C_8H_{11}NO_5S$ **FW :** 233.24 **HBA:** 6 **HBD:** 3 **RotB:** 4

PubChem ID : 122136 **CASRN :** 51317-41-0 **logP:** -0.05 **TPSA:** 114.3

Activity: L-DOPA metabolite.

NIMH Code : D-904

Compound name : d_2-Dihydroouabain



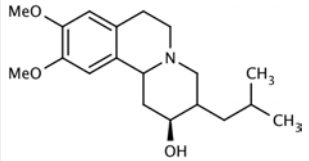
Mol. Formula : -3.0472586 **FW :** 588.68 **HBA:** 12 **HBD:** 8 **RotB:** 4

PubChem ID : 14450 **CASRN :** 588.6807 **logP:** -3.05 **TPSA:** 206.6

Activity: Stable isotope labeled ouabain ionotropic antagonist.

NIMH Code : D-905

Compound name : (–)-α-Dihydrotetrabenazine



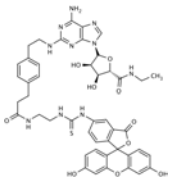
Mol. Formula : $C_{19}H_{29}NO_3$ **FW :** 319.44 **HBA:** 4 **HBD:** 1 **RotB:** 4

PubChem ID : 123836 **CASRN :** 3466-75-9 **logP:** 2.67 **TPSA:** 43.1

Activity: Optical isomer of putative tetrabenazine metabolite.

NIMH Code : D-906

Compound name : FITC-APEC



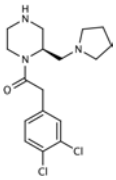
Mol. Formula : $C_{46}H_{46}N_{10}O_{10}S$ **FW :** 1159.03 **HBA:** 20 **HBD:** 10 **RotB:** 14

PubChem ID : - **CASRN :** - **logP:** 3.39 **TPSA:** 289.6

Activity: Fluorescent adenosine A_{2a} receptor ligand.

NIMH Code : D-907

Compound name : Descarboxymethyl GR103545 dihydrochloride



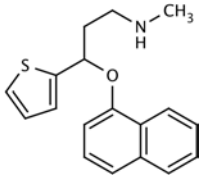
Mol. Formula : $C_{17}H_{23}Cl_2N_3O$ **FW :** 429.21 **HBA:** 4 **HBD:** 1 **RotB:** 4

PubChem ID : 9906680 **CASRN :** **logP:** 2.41 **TPSA:** 36.8

Activity: GR103545 PET ligand precursor.

NIMH Code : D-908

Compound name : Duloxetine hydrochloride



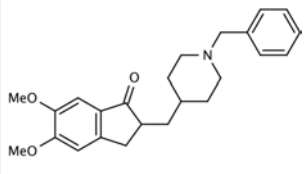
Mol. Formula : $C_{18}H_{19}NOS$ **FW :** 333.88 **HBA:** 2 **HBD:** 1 **RotB:** 6

PubChem ID : 60835 **CASRN :** 116539-59-4 **logP:** 4.20 **TPSA:** 25.8

Activity: Serotonin & norepinephrine reuptake inhibitor.

NIMH Code : D-909

Compound name : Donepezil



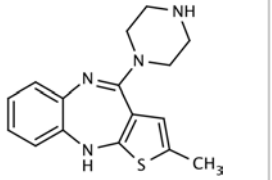
Mol. Formula : $C_{24}H_{29}NO_3$ **FW :** 379.49 **HBA:** 4 **HBD:** 0 **RotB:** 6

PubChem ID : 3152 **CASRN :** 120011-70-3 **logP:** 4.21 **TPSA:** 40.0

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)



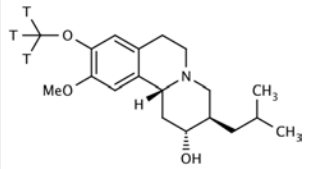
Mol. Formula : $C_{16}H_{18}N_4S$ **FW :** 298.41 **HBA:** 4 **HBD:** 2 **RotB:** 0

PubChem ID : **CASRN :** **logP:** 3.01 **TPSA:** 44.2

Activity: Olanzapine metabolite.

NIMH Code : D-911

Compound name : Tritium-labeled dihydrotetrabenazine



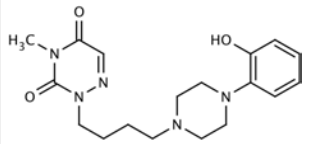
Mol. Formula : $C_{19}H_{29}NO_3$ **FW :** 325.46 **HBA:** 4 **HBD:** 1 **RotB:** 4

PubChem ID : **CASRN :** 1 **logP:** 2.67 **TPSA:** 43.1

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



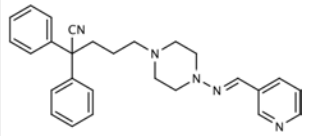
Mol. Formula : $C_{18}H_{25}N_5O_3$ **FW :** 359.42 **HBA:** 8 **HBD:** 1 **RotB:** 6

PubChem ID : **CASRN :** **logP:** 1.65 **TPSA:** 80.9

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

NIMH Code : D-913

Compound name : SC-26196



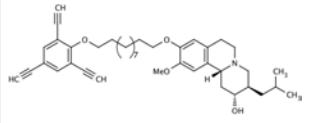
Mol. Formula : $C_{27}H_{29}N_5$ **FW :** 423.55 **HBA:** 5 **HBD:** 0 **RotB:** 8

PubChem ID : 9845201 **CASRN :** **logP:** 4.07 **TPSA:** 56.7

Activity: Δ6 Desaturase inhibitor.

NIMH Code : D-914

Compound name : Dihydrotetrabenazine derivative

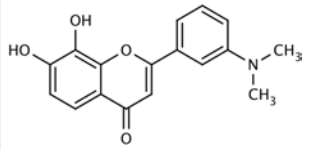


Mol. Formula : $C_{41}H_{53}NO_4$ **FW :** 623.86 **HBA:** 5 **HBD:** 1 **RotB:** 17

PubChem ID : **CASRN :** 17 **logP:** 8.46 **TPSA:** 52.4

NIMH Code : D-915

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

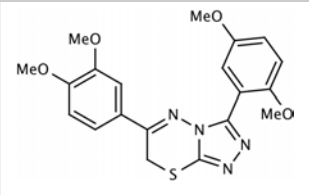


Mol. Formula : $C_{17}H_{15}NO_4$ **FW :** 297.31 **HBA:** 5 **HBD:** 2 **RotB:** 2

PubChem ID : **CASRN :** **logP:** 2.47 **TPSA:** 72.8

NIMH Code : D-916

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



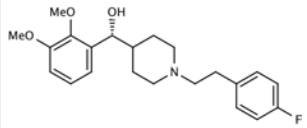
Mol. Formula : $C_{20}H_{20}N_4O_4S$ **FW :** 412.46 **HBA:** 8 **HBD:** 0 **RotB:** 6

PubChem ID : - **CASRN :** - **logP:** 2.31 **TPSA:** 80.0

Activity: Phosphodiesterase 4 (PDE4) inhibitor.

NIMH Code : D-917

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



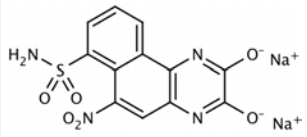
Mol. Formula : $C_{22}H_{28}NFO_3$ **FW :** 373.46 **HBA:** 4 **HBD:** 1 **RotB:** 7

PubChem ID : 60858 **CASRN :** 139290-65-6 **logP:** 3.59 **TPSA:** 43.1

Activity: Serotonin 5-HT_{2A} receptor antagonist.

NIMH Code : D-918

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



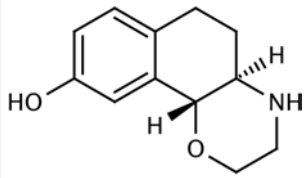
Mol. Formula : $C_{12}H_6N_4Na_2O_6S$ **FW :** 380.24 **HBA:** 10 **HBD:** 1 **RotB:** 2

PubChem ID : 10616800 **CASRN :** 118876-58-7 **logP:** 1.42 **TPSA:** 172.2

Activity: AMPA/kainate receptor antagonist.

NIMH Code : D-919 new

Compound name : (+)-(4a*R*,10b*R*)-3,4,4a,5,6,10b-Hexahydro-2*H*-naphtho[1,2-b]-1,4-oxazine-9-ol hydrochloride ((+)-N-Despropyl-PHNO hydrochloride)

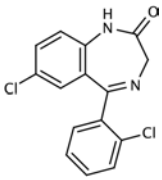


Mol. Formula : $C_{12}H_{16}ClNO_2$ **FW :** 241.71 **HBA:** 3 **HBD:** 2 **RotB:** 0

PubChem ID : 13435417 **CASRN :** - **logP:** 0.72 **TPSA:** 48.9

NIMH Code : D-920 new

Compound name : Delorazepam (Chlordesmethyldiazepam)



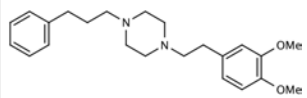
Mol. Formula : $C_{15}H_{10}Cl_2N_2O$ **FW :** 305.16 **HBA:** 3 **HBD:** 1 **RotB:** 1

PubChem ID : 16929 **CASRN :** 2894-67-9 **logP:** 3.82 **TPSA:** 41.5

Activity: $GABA_A$ receptor allosteric modulator.

NIMH Code : D-921 new

Compound name : 1-[2-(3,4-Dimethoxyphenyl)ethyl]-4-(3-phenylpropyl)piperazine dihydrochloride; (SA-4503 dihydrochloride)



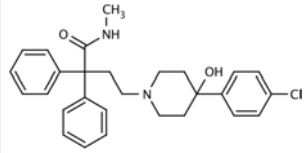
Mol. Formula : $C_{23}H_{34}Cl_2N_2O_2$ **FW :** 441.43 **HBA:** 4 **HBD:** 0 **RotB:** 9

PubChem ID : 9907323 **CASRN :** 165377-43-5 (base) **logP:** 4.19 **TPSA:** 26.1

Activity: Sigma receptor agonist.

NIMH Code : D-922 new

Compound name : 4-[4-(4-Chlorophenyl)-4-hydroxypiperidin-1-yl]-*N*-methyl-2,2-diphenylbutanamide hydrochloride (*N*-Desmethyl loperamide hydrochloride)

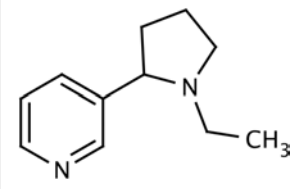


Mol. Formula : $C_{28}H_{32}Cl_2N_2O_2$ **FW :** 499.47 **HBA:** 4 **HBD:** 2 **RotB:** 7

PubChem ID : 9805944 **CASRN :** 66164-07-6 **logP:** 4.55 **TPSA:** 53.8

NIMH Code : E-701A

Compound name : N-Ethylnornicotine tartrate



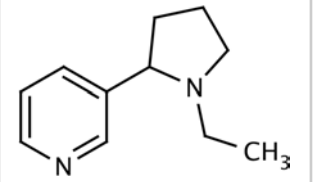
Mol. Formula : $C_{19}H_{28}N_2O_{12}$ **FW :** 326.34 **HBA:** 2 **HBD:** 0 **RotB:** 2

PubChem ID : **CASRN :** **logP:** 1.52 **TPSA:** 17.3

Activity: Nicotine analog.

NIMH Code : E-701B

Compound name : N-Ethylnornicotine



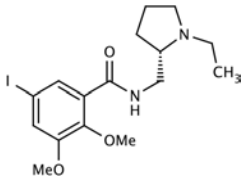
Mol. Formula : $C_{11}H_{16}N_2$ **FW :** 176.26 **HBA:** 2 **HBD:** 0 **RotB:** 2

PubChem ID : 201440 **CASRN :** 5979-92-0 **logP:** 1.52 **TPSA:** 17.3

Activity: Nicotine analog.

NIMH Code : E-703

Compound name : Epidepride



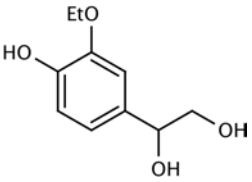
Mol. Formula : $C_{16}H_{23}IN_2O_3$ **FW :** 418.27 **HBA:** 5 **HBD:** 1 **RotB:** 6

PubChem ID : 86101 **CASRN :** 107188-87-4 **logP:** 2.50 **TPSA:** 52.0

Activity: Dopamine D_2 receptor antagonist.

NIMH Code : E-704

Compound name : EHPG piperazine salt



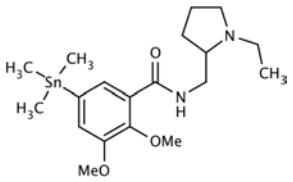
Mol. Formula : $C_{24}H_{38}N_2O_8$ **FW :** 482.59 **HBA:** 4 **HBD:** 3 **RotB:** 4

PubChem ID : 194138 **CASRN :** 62024-68-4 **logP:** 0.47 **TPSA:** 69.9

Activity: Catecholamine turnover biomarker.

NIMH Code : E-705

Compound name : 5-Trimethylstannylepidepride



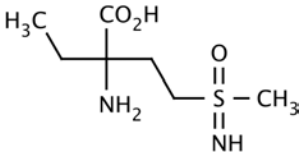
Mol. Formula : $C_{19}H_{32}N_2O_3Sn$ **FW :** 455.18 **HBA:** 5 **HBD:** 1 **RotB:** 7

PubChem ID : **CASRN :** **logP:** 0.94 **TPSA:** 52.0

Activity: Radioiodinated epidepride precusor.

NIMH Code : E-706

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



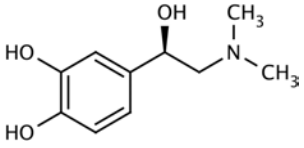
Mol. Formula : $C_7H_{16}N_2O_3S$ **FW :** 208.28 **HBA:** 5 **HBD:** 3 **RotB:** 5

PubChem ID : 128339 **CASRN :** 66735-68-0 **logP:** -3.49 **TPSA:** 108.7

Activity: Glutamate synthetase inhibitor.

NIMH Code : E-707

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

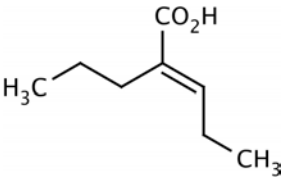


Mol. Formula : $C_{14}H_{21}NO_9$ **FW :** 347.32 **HBA:** 4 **HBD:** 3 **RotB:** 3

PubChem ID : 3054685 **CASRN :** 554-99-4 **logP:** 0.35 **TPSA:** 65.1

NIMH Code : E-708

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



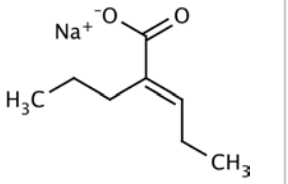
Mol. Formula : $C_8H_{14}O_2$ **FW :** 142.20 **HBA:** 2 **HBD:** 1 **RotB:** 4

PubChem ID : 6437068 **CASRN :** 60218-41-9 **logP:** 2.65 **TPSA:** 40.1

Activity: Anticonvulsant; valproic acid metabolite.

NIMH Code : E-709

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



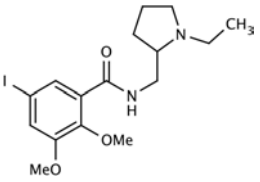
Mol. Formula : $C_8H_{13}O_2Na$ **FW :** 164.18 **HBA:** 2 **HBD:** 0 **RotB:** 4

PubChem ID : 23675457 **CASRN :** 69827-64-1 **logP:** 2.65 **TPSA:** 40.1

Activity: Valproic acid metabolite.

NIMH Code : E-901

Compound name : [^{125}I]Epidepride



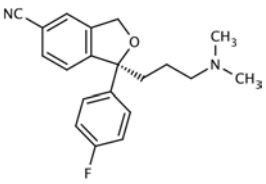
Mol. Formula : $C_{16}H_{23}IN_2O_3$ **FW :** 418.27 **HBA:** 5 **HBD:** 1 **RotB:** 6

PubChem ID : 449726 **CASRN :** 107188-87-4 **logP:** 2.50 **TPSA:** 52.0

Activity: Radioiodinated dopamine D_2 receptor antagonist.

NIMH Code : E-902

Compound name : Escitalopram oxalate



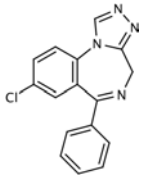
Mol. Formula : $C_{20}H_{21}FN_2O$ **FW :** 414.43 **HBA:** 3 **HBD:** 0 **RotB:** 5

PubChem ID : 146570 **CASRN :** 128196-01-0 **logP:** 3.76 **TPSA:** 37.5

Activity: Serotonin 5-HT reuptake inhibitor.

NIMH Code : E-903

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



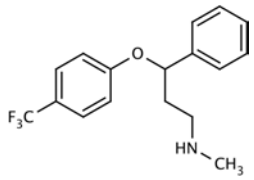
Mol. Formula : $C_{16}H_{11}ClN_4$ **FW :** 294.74 **HBA:** 4 **HBD:** 0 **RotB:** 1

PubChem ID : 3261 **CASRN :** 0 **logP:** 2.09 **TPSA:** 43.1

Activity: $GABA_A$ receptor allosteric modulator.

NIMH Code : F-132

Compound name : (±)-Fluoxetine hydrochloride



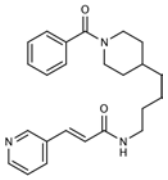
Mol. Formula : $C_{17}H_{19}ClF_3NO$ **FW :** 345.79 **HBA:** 2 **HBD:** 1 **RotB:** 7

PubChem ID : 3386 **CASRN :** 54910-89-3 **logP:** 4.17 **TPSA:** 25.8

Activity: Serotonin uptake inhibitor.

NIMH Code : F-901

Compound name : FK866



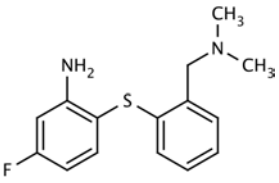
Mol. Formula : $C_{24}H_{29}N_3O_2$ **FW :** 391.51 **HBA:** 5 **HBD:** 1 **RotB:** 8

PubChem ID : 6914657 **CASRN :** 201034-75-5 **logP:** 3.16 **TPSA:** 62.3

Activity: Nicotinamide phosphoribosyltransferase inhibitor.

NIMH Code : F-902

Compound name : 4-Fluoro-ADAM



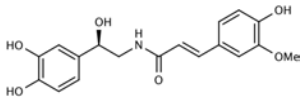
Mol. Formula : $C_{15}H_{17}FN_2S$ **FW :** 276.37 **HBA:** 2 **HBD:** 1 **RotB:** 4

PubChem ID : 10265481 **CASRN :** **logP:** 3.42 **TPSA:** 30.5

Activity: Serotonin transporter PET ligand reference standard.

NIMH Code : F-903

Compound name : *N*-Feruloylnorepinephrine

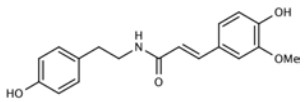


Mol. Formula : $C_{18}H_{19}NO_6$ **FW :** 345.35 **HBA:** 7 **HBD:** 5 **RotB:** 6

PubChem ID : **CASRN :** **logP:** 1.58 **TPSA:** 119.3

NIMH Code : F-904

Compound name : Feruloyltyramine



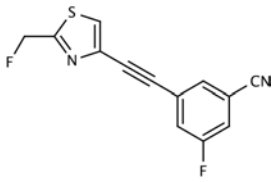
Mol. Formula : $C_{18}H_{19}NO_4$ **FW :** 313.35 **HBA:** 5 **HBD:** 3 **RotB:** 6

PubChem ID : 5280537 **CASRN :** 65646-26-6 **logP:** 2.80 **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



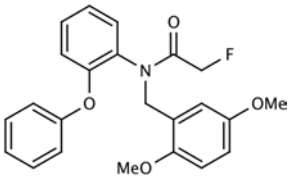
Mol. Formula : $C_{13}H_6F_2N_2S$ **FW :** 260.26 **HBA:** 2 **HBD:** 0 **RotB:** 3

PubChem ID : **CASRN :** **logP:** 3.33 **TPSA:** 36.7

Activity: Metabotropic glutamate $mGluR_5$ PET ligand reference standard.

NIMH Code : F-906

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



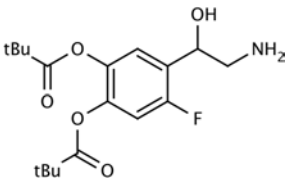
Mol. Formula : $C_{23}H_{22}FNO_4$ **FW :** 395.42 **HBA:** 5 **HBD:** 0 **RotB:** 8

PubChem ID : **CASRN :** **logP:** 4.06 **TPSA:** 48.0

Activity: Brain peripheral benzodiazepine receptor (TSPO) ligand.

NIMH Code : F-907

Compound name : 6-Fluoronorepinephrine dipivalate hydrochloride

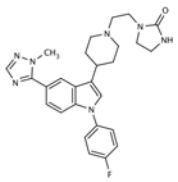


Mol. Formula : $C_{18}H_{27}ClFNO_5$ **FW :** 391.86 **HBA:** 6 **HBD:** 2 **RotB:** 8

PubChem ID : **CASRN :** **logP:** 3.42 **TPSA:** 100.5

NIMH Code : F-908

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

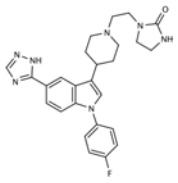


Mol. Formula : $C_{27}H_{30}FN_7O$ **FW :** 487.57 **HBA:** 8 **HBD:** 1 **RotB:** 6

PubChem ID : - **CASRN :** - **logP:** 2.92 **TPSA:** 72.4

NIMH Code : F-909

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

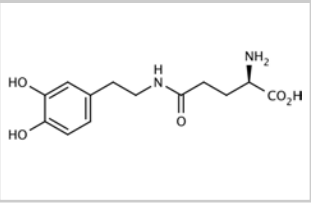


Mol. Formula : $C_{26}H_{28}FN_7O$ **FW :** 473.55 **HBA:** 8 **HBD:** 1 **RotB:** 6

PubChem ID : - **CASRN :** - **logP:** 2.11 **TPSA:** 83.3

NIMH Code : G-501

Compound name : γ-Glutamyldopamine

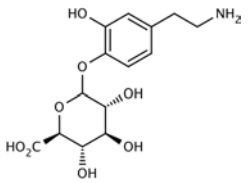


Mol. Formula : $C_{13}H_{18}N_2O_5$ **FW :** 282.29 **HBA:** 7 **HBD:** 5 **RotB:** 7

PubChem ID : 22806192 **CASRN :** **logP:** -2.37 **TPSA:** 137.3

NIMH Code : G-502

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



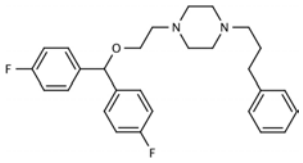
Mol. Formula : $C_{14}H_{19}NO_8$ **FW :** 329.30 **HBA:** 9 **HBD:** 6 **RotB:** 5

PubChem ID : 3082490 **CASRN :** 38632-24-5 **logP:** -3.43 **TPSA:** 167.2

Activity: Dopamine metabolite.

NIMH Code : G-801

Compound name : GBR-12909 dihydrochloride (Vanoxerine)



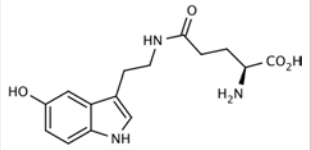
Mol. Formula : $C_{28}H_{34}Cl_2F_2N_2O$ **FW :** 523.49 **HBA:** 3 **HBD:** 0 **RotB:** 10

PubChem ID : 10238982 **CASRN :** 67469-78-7 **logP:** 6.24 **TPSA:** 16.9

Activity: Dopamine reuptake inhibitor.

NIMH Code : G-802

Compound name : γ-Glutamylserotonin

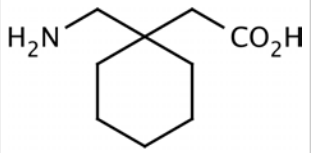


Mol. Formula : $C_{15}H_{19}N_3O_4$ **FW :** 305.33 **HBA:** 7 **HBD:** 4 **RotB:** 7

PubChem ID : 15234235 **CASRN :** **logP:** -1.97 **TPSA:** 132.9

NIMH Code : G-901

Compound name : Gabapentin



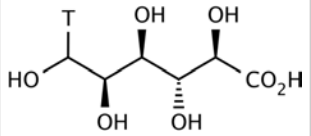
Mol. Formula : $C_9H_{17}NO_2$ **FW :** 171.24 **HBA:** 3 **HBD:** 2 **RotB:** 3

PubChem ID : 3446 **CASRN :** 60142-96-3 **logP:** -1.27 **TPSA:** 67.8

Activity: Gamma aminobutyric acid (GABA) analog.

NIMH Code : G-902

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

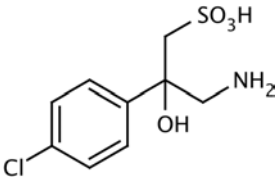


Mol. Formula : $C_6H_{12}O_7$ **FW :** 198.16 **HBA:** 7 **HBD:** 6 **RotB:** 5

PubChem ID : 604 **CASRN :** 13382-27-9 **logP:** -3.41 **TPSA:** 141.3

NIMH Code : H-113

Compound name : 2-Hydroxysaclofen



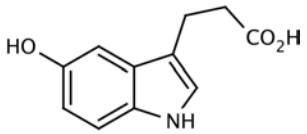
Mol. Formula : $C_9H_{12}ClNO_4S$ **FW :** 265.71 **HBA:** 5 **HBD:** 3 **RotB:** 4

PubChem ID : 1564 **CASRN :** 117354-64-0 **logP:** -0.99 **TPSA:** 105.1

Activity: γ-Aminobutyric acid $GABA_B$ antagonist.

NIMH Code : H-501

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

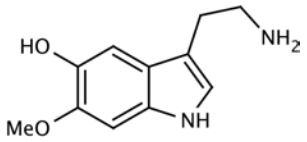


Mol. Formula :	$C_{11}H_{11}NO_3$	**FW :** 205.21	**HBA:** 4	**HBD:** 2	**RotB:** 3
PubChem ID :		**CASRN :**		**logP:** 1.85	**TPSA:** 76.2

Activity: GC/MS internal standard for catecholamine assay.

NIMH Code : H-502

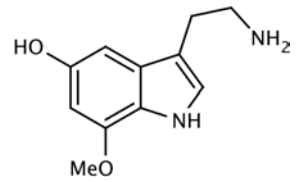
Compound name : 5-Hydroxy-6-methoxytryptamine creatinine sulfate



Mol. Formula :	$C_{15}H_{23}N_5O_7S$	**FW :** 206.24	**HBA:** 4	**HBD:** 2	**RotB:** 3
PubChem ID :		**CASRN :**		**logP:** 0.26	**TPSA:** 72.9

NIMH Code : H-503

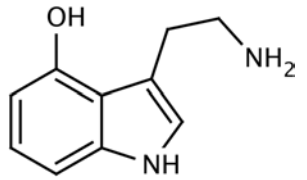
Compound name : 5-Hydroxy-7-methoxytryptamine creatinine sulfate



Mol. Formula :	$C_{15}H_{23}N_5O_7S$	**FW :** 206.24	**HBA:** 4	**HBD:** 2	**RotB:** 3
PubChem ID :		**CASRN :**		**logP:** 0.11	**TPSA:** 72.9

NIMH Code : H-504

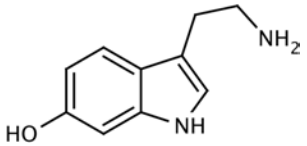
Compound name : 4-Hydroxytryptamine creatinine sulfate



Mol. Formula :	$C_{14}H_{21}N_5O_6S$	**FW :** 176.22	**HBA:** 3	**HBD:** 2	**RotB:** 2
PubChem ID :		**CASRN :**		**logP:** 0.33	**TPSA:** 63.7

NIMH Code : H-505

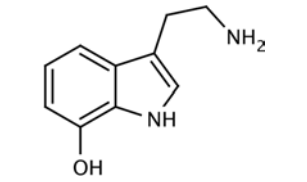
Compound name : 6-Hydroxytryptamine creatinine sulfate



Mol. Formula :	$C_{14}H_{21}N_5O_6S$	**FW :** 176.22	**HBA:** 3	**HBD:** 2	**RotB:** 2
PubChem ID :		**CASRN :**		**logP:** 0.47	**TPSA:** 63.7

NIMH Code : H-506

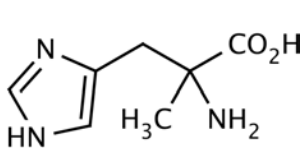
Compound name : 7-Hydroxytryptamine creatinine sulfate



Mol. Formula :	$C_{14}H_{21}N_5O_6S$	**FW :** 176.22	**HBA:** 3	**HBD:** 2	**RotB:** 2
PubChem ID :		**CASRN :**		**logP:** 0.51	**TPSA:** 63.7

NIMH Code : H-507

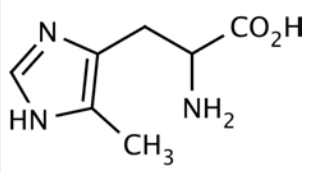
Compound name : α-Methylhistidine hydrochloride



Mol. Formula :	$C_7H_{12}ClN_3O_2$	**FW :** 205.64	**HBA:** 5	**HBD:** 2	**RotB:** 3
PubChem ID :	16219696	**CASRN :** 32381-18-3		**logP:** -2.85	**TPSA:** 96.5

NIMH Code : H-509

Compound name : 4-Methylhistidine hydrochloride

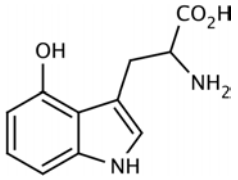


Mol. Formula : $C_7H_{12}ClN_3O_2$ **FW :** 205.64 **HBA:** 5 **HBD:** 2 **RotB:** 3

PubChem ID : 10773449 **CASRN :** **logP:** -3.09 **TPSA:** 96.5

NIMH Code : H-510

Compound name : 4-Hydroxytryptophan acetate

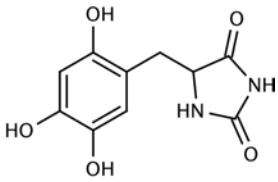


Mol. Formula : $C_{13}H_{16}N_2O_5$ **FW :** 280.28 **HBA:** 5 **HBD:** 3 **RotB:** 3

PubChem ID : 589768 **CASRN :** **logP:** -1.39 **TPSA:** 103.8

NIMH Code : H-511

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

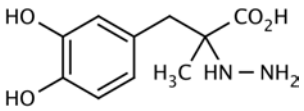


Mol. Formula : $C_{10}H_{10}N_2O_5$ **FW :** 238.20 **HBA:** 7 **HBD:** 5 **RotB:** 2

PubChem ID : **CASRN :** **logP:** -0.14 **TPSA:** 116.1

NIMH Code : H-512

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



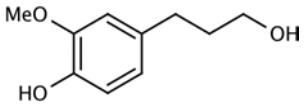
Mol. Formula : $C_{10}H_{14}N_2O_4$ **FW :** 226.23 **HBA:** 6 **HBD:** 5 **RotB:** 4

PubChem ID : 2563 **CASRN :** 38821-49-7 **logP:** -1.19 **TPSA:** 118.6

Activity: Aromatic-L-amino-acid decarboxylase inhibitor.

NIMH Code : H-513

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

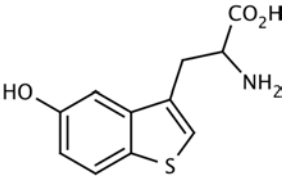


Mol. Formula : $C_{10}H_{14}O_3$ **FW :** 182.22 **HBA:** 3 **HBD:** 2 **RotB:** 4

PubChem ID : 16822 **CASRN :** 2305-13-7 **logP:** 1.48 **TPSA:** 49.7

NIMH Code : H-515

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

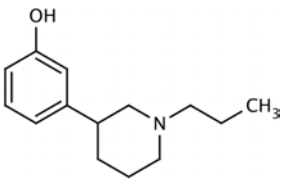


Mol. Formula : $C_{11}H_{11}NO_3S$ **FW :** 237.28 **HBA:** 4 **HBD:** 3 **RotB:** 3

PubChem ID : 32334 **CASRN :** 24358-04-1 **logP:** -0.61 **TPSA:** 88.0

NIMH Code : H-516

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



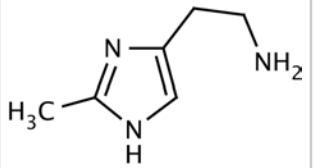
Mol. Formula : $C_{14}H_{22}BrNO$ **FW :** 300.23 **HBA:** 2 **HBD:** 1 **RotB:** 3

PubChem ID : 23045647 **CASRN :** 75240-91-4 **logP:** 2.67 **TPSA:** 24.7

Activity: Antiparkinson agent; dopaminergic agent.

NIMH Code : H-517

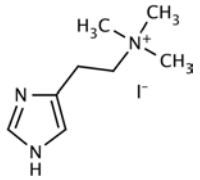
Compound name : 2-Methylhistamine dipicrate



Mol. Formula :	$C_{18}H_{17}N_9O_{14}$	**FW :**	583.38	**HBA:**	3	**HBD:**	1	**RotB:**	2
PubChem ID :	91613	**CASRN :**	34392-54-6			**logP:**	-0.58	**TPSA:**	56.3

NIMH Code : H-518

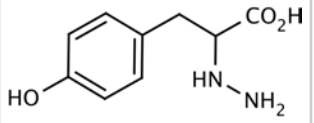
Compound name : N,N-Dimethylhistamine methiodide



Mol. Formula :	$C_8H_{16}N_3I$	**FW :**	281.14	**HBA:**	3	**HBD:**	0	**RotB:**	3
PubChem ID :		**CASRN :**				**logP:**	-4.05	**TPSA:**	28.7

NIMH Code : H-520

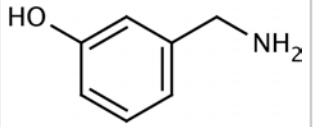
Compound name : (±)-2-Hydrazino-3-(4-hydroxyphenyl)propionic acid



Mol. Formula :	$C_9H_{12}N_2O_3$	**FW :**	196.20	**HBA:**	5	**HBD:**	4	**RotB:**	4
PubChem ID :	151250	**CASRN :**	5060-36-6			**logP:**	-1.06	**TPSA:**	98.4
Activity:	Fungal tyrosinase inhibitor.								

NIMH Code : H-521

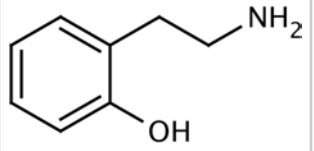
Compound name : 3-Hydroxybenzylamine



Mol. Formula :	C_7H_9NO	**FW :**	123.15	**HBA:**	2	**HBD:**	2	**RotB:**	1
PubChem ID :	735894	**CASRN :**				**logP:**	0.27	**TPSA:**	47.9

NIMH Code : H-522

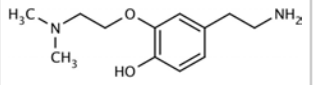
Compound name : 2-Hydroxy-β-phenethylamine hydrochloride



Mol. Formula :	$C_8H_{12}ClNO$	**FW :**	173.64	**HBA:**	2	**HBD:**	2	**RotB:**	2
PubChem ID :	199864	**CASRN :**	5136-97-0			**logP:**	0.78	**TPSA:**	47.9

NIMH Code : H-523

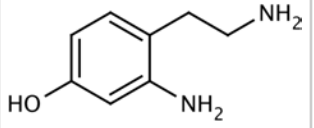
Compound name : 4(3)-Hydroxy-3(4)-(β-dimethylaminoethoxy)-β-phenethylamine dihydrochloride



Mol. Formula :	$C_{12}H_{22}Cl_2N_2O_2$	**FW :**	297.22	**HBA:**	4	**HBD:**	2	**RotB:**	6
PubChem ID :		**CASRN :**				**logP:**	0.52	**TPSA:**	61.5

NIMH Code : H-525

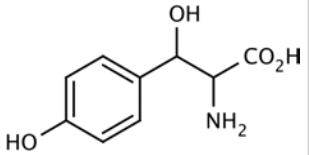
Compound name : 2-Amino-4-hydroxy-β-phenethylamine dihydrobromide



Mol. Formula :	$C_8H_{14}Br_2N_2O$	**FW :**	314.02	**HBA:**	3	**HBD:**	3	**RotB:**	2
PubChem ID :	9877425	**CASRN :**				**logP:**	-0.24	**TPSA:**	73.9

NIMH Code : H-526

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

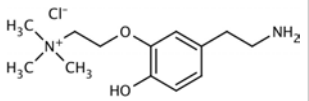


Mol. Formula : $C_9H_{11}NO_4$ **FW :** 197.19 **HBA:** 5 **HBD:** 4 **RotB:** 3

PubChem ID : 94134 **CASRN :** 1078-17-7 **logP:** -2.41 **TPSA:** 108.2

NIMH Code : H-527

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

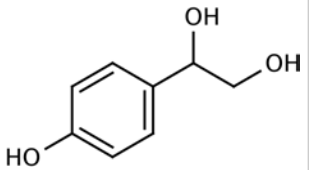


Mol. Formula : $C_{13}H_{24}Cl_2N_2O_2$ **FW :** 311.25 **HBA:** 4 **HBD:** 2 **RotB:** 6

PubChem ID : **CASRN :** **logP:** -1.74 **TPSA:** 57.1

NIMH Code : H-528

Compound name : 4-Hydroxyphenylglycol



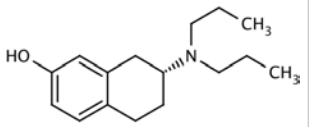
Mol. Formula : $C_8H_{10}O_3$ **FW :** 154.16 **HBA:** 3 **HBD:** 3 **RotB:** 2

PubChem ID : 3081980 **CASRN :** 2380-75-8 **logP:** 0.27 **TPSA:** 60.7

Activity: Octopamine metabolite.

NIMH Code : H-701

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



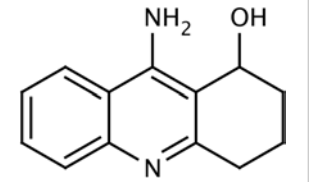
Mol. Formula : $C_{16}H_{26}BrNO$ **FW :** 328.29 **HBA:** 2 **HBD:** 1 **RotB:** 5

PubChem ID : 11957566 **CASRN :** 159795-63-8 **logP:** 3.28 **TPSA:** 24.7

Activity: Dopamine D_3 agonist.

NIMH Code : H-703

Compound name : Velnacrine maleate



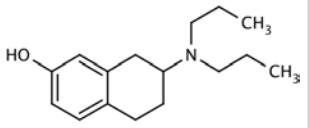
Mol. Formula : $C_{17}H_{18}N_2O_5$ **FW :** 330.34 **HBA:** 3 **HBD:** 2 **RotB:** 0

PubChem ID : 6364836 **CASRN :** 104675-29-8 **logP:** 1.40 **TPSA:** 60.4

Activity: Cholinesterase Inhibitor.

NIMH Code : H-704

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



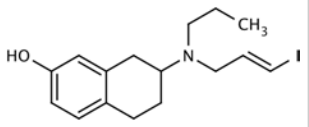
Mol. Formula : $C_{16}H_{26}BrNO$ **FW :** 328.29 **HBA:** 2 **HBD:** 1 **RotB:** 5

PubChem ID : 11957554 **CASRN :** 82730-72-1 **logP:** 3.28 **TPSA:** 24.7

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



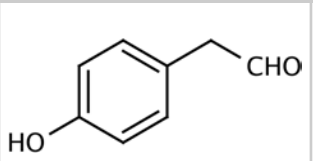
Mol. Formula : $C_{16}H_{23}ClINO$ **FW :** 407.72 **HBA:** 2 **HBD:** 1 **RotB:** 5

PubChem ID : 6305587 **CASRN :** 148258-46-2 **logP:** 4.62 **TPSA:** 24.7

Activity: Dopamine D_3 receptor agonist.

NIMH Code : H-901

Compound name : 4-Hydroxyphenylacetaldehyde



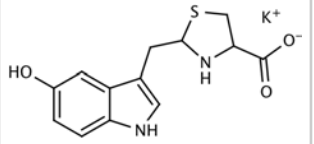
Mol. Formula : $C_8H_8O_2$ **FW :** 136.15 **HBA:** 2 **HBD:** 1 **RotB:** 2

PubChem ID : 440113 **CASRN :** 7339-87-9 **logP:** 1.15 **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

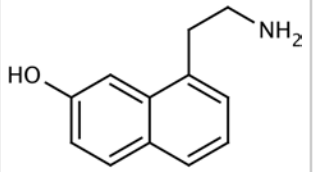


Mol. Formula : $C_{13}H_{13}KN_2O_3S$ **FW :** 316.42 **HBA:** 5 **HBD:** 2 **RotB:** 3

PubChem ID : **CASRN :** **logP:** -0.84 **TPSA:** 92.8

NIMH Code : H-903

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



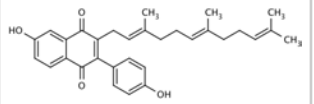
Mol. Formula : $C_{12}H_{14}ClNO$ **FW :** 223.70 **HBA:** 2 **HBD:** 2 **RotB:** 2

PubChem ID : 10058277 **CASRN :** **logP:** 1.50 **TPSA:** 47.9

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

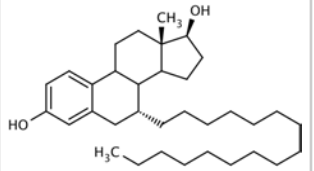


Mol. Formula : $C_{31}H_{34}O_4$ **FW :** 470.60 **HBA:** 4 **HBD:** 2 **RotB:** 9

PubChem ID : **CASRN :** **logP:** 7.49 **TPSA:** 77.4

NIMH Code : H-905

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

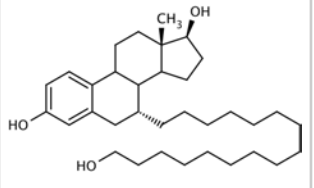


Mol. Formula : $C_{34}H_{56}O_2$ **FW :** 496.81 **HBA:** 2 **HBD:** 2 **RotB:** 15

PubChem ID : **CASRN :** **logP:** 10.70 **TPSA:** 40.5

NIMH Code : H-906

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

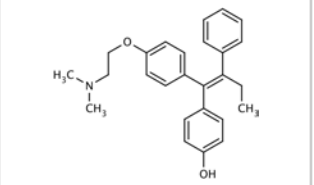


Mol. Formula : $C_{34}H_{56}O_3$ **FW :** 512.81 **HBA:** 3 **HBD:** 3 **RotB:** 16

PubChem ID : **CASRN :** **logP:** 9.26 **TPSA:** 60.7

NIMH Code : H-907

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



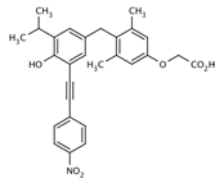
Mol. Formula : $C_{26}H_{29}NO_2$ **FW :** 387.51 **HBA:** 3 **HBD:** 1 **RotB:** 8

PubChem ID : 449459 **CASRN :** 68392-35-8 **logP:** 5.69 **TPSA:** 33.9

Activity: Estrogen receptor modulator.

NIMH Code : H-908

Compound name : NH-3

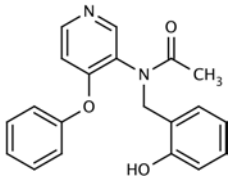


Mol. Formula :	$C_{28}H_{27}NO_6$	**FW :** 473.52	**HBA:** 7	**HBD:** 2	**RotB:** 9
PubChem ID :	10027822	**CASRN :**		**logP:** 7.41	**TPSA:** 115.4

Activity: β-Subtype thyroid hormone receptor antagonist.

NIMH Code : H-909

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

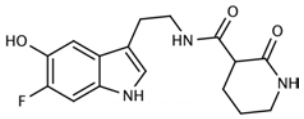


Mol. Formula :	$C_{20}H_{18}N_2O_3$	**FW :** 334.37	**HBA:** 5	**HBD:** 1	**RotB:** 5
PubChem ID :	24754521	**CASRN :**		**logP:** 2.78	**TPSA:** 62.7

Activity: Brain peripheral benzodiazepine receptor (TSPO) ligand.

NIMH Code : H-910 new

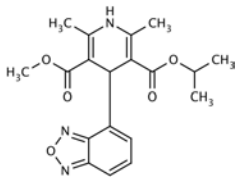
Compound name : *N*-[2-(5-Hydroxy-6-fluoro-1*H*-indol-3-yl)ethyl]-2-oxopiperidine-3-carboxamide (6-Fluoro-HIOC)



Mol. Formula :	$C_{16}H_{18}FN_3O_3$	**FW :** 319.33	**HBA:** 6	**HBD:** 3	**RotB:** 4
PubPubChem ID :	-	**CASRN :** -		**logP:** 0.97	**TPSA:** 94.2

NIMH Code : I-124

Compound name : Isradipine

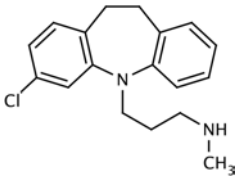


Mol. Formula :	$C_{19}H_{21}N_3O_5$	**FW :** 371.39	**HBA:** 8	**HBD:** 1	**RotB:** 6
PubChem ID :	3784	**CASRN :** 75695-93-1		**logP:** 2.00	**TPSA:** 103.6

Activity: Calcium channel blocker.

NIMH Code : I-501

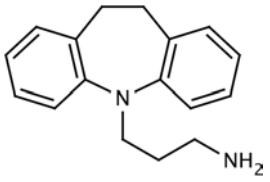
Compound name : 3-Chloro-*N*-desmethylimipramine hydrochloride



Mol. Formula :	$C_{18}H_{22}Cl_2N_2$	**FW :** 337.29	**HBA:** 2	**HBD:** 1	**RotB:** 4
PubChem ID :	16219718	**CASRN :** 303-48-0		**logP:** 4.50	**TPSA:** 19.9

NIMH Code : I-502

Compound name : N,N-Didesmethylimipramine hydrochloride

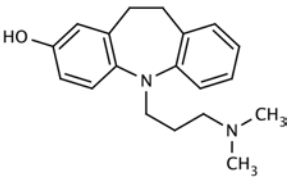


Mol. Formula :	$C_{17}H_{21}ClN_2$	**FW :** 288.82	**HBA:** 2	**HBD:** 1	**RotB:** 3
PubChem ID :	13358128	**CASRN :** 2095-95-6		**logP:** 3.46	**TPSA:** 30.9

Activity: Imipramine metabolite.

NIMH Code : I-503

Compound name : 2-Hydroxyimipramine

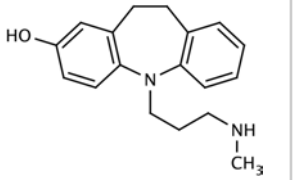


Mol. Formula :	$C_{19}H_{24}N_2O$	**FW :** 296.41	**HBA:** 3	**HBD:** 1	**RotB:** 4
PubChem ID :	108051	**CASRN :** 303-70-8		**logP:** 3.80	**TPSA:** 27.9

Activity: Imipramine metabolite.

NIMH Code : I-504

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



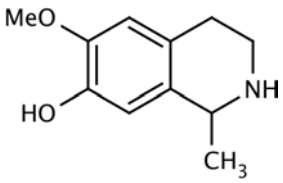
Mol. Formula : $C_{18}H_{22}N_2O$ **FW :** 282.38 **HBA:** 3 **HBD:** 2 **RotB:** 4

PubChem ID : 121249 **CASRN :** 1977-15-7 **logP:** 3.17 **TPSA:** 40.1

Activity: Tricyclic antidepressive agent; Imipramine metabolite.

NIMH Code : I-505

Compound name : (±)-Isosalsoline hydrochloride

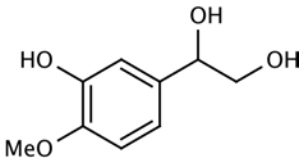


Mol. Formula : $C_{11}H_{16}ClNO_2$ **FW :** 229.70 **HBA:** 3 **HBD:** 2 **RotB:** 1

PubChem ID : 46697 **CASRN :** 4593-97-9 **logP:** 1.24 **TPSA:** 46.1

NIMH Code : I-701

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

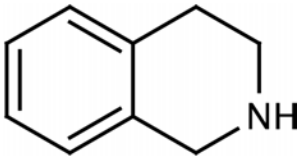


Mol. Formula : $C_9H_{12}O_4$ **FW :** 184.19 **HBA:** 4 **HBD:** 3 **RotB:** 3

PubChem ID : 170451 **CASRN :** 40979-91-7 **logP:** 0.11 **TPSA:** 69.9

NIMH Code : I-702

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



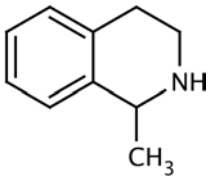
Mol. Formula : $C_9H_{12}ClN$ **FW :** 169.65 **HBA:** 1 **HBD:** 1 **RotB:** 0

PubChem ID : 7046 **CASRN :** 91-21-4 **logP:** 1.57 **TPSA:** 16.6

Activity: Potential dopaminergic neurotoxin.

NIMH Code : I-703

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



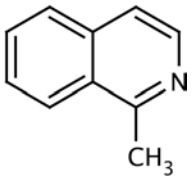
Mol. Formula : $C_{10}H_{14}ClN$ **FW :** 183.68 **HBA:** 1 **HBD:** 1 **RotB:** 0

PubChem ID : 9812950 **CASRN :** 4965-09-7 **logP:** 1.99 **TPSA:** 16.6

Activity: Potential dopaminergic neurotoxin.

NIMH Code : I-704

Compound name : 1-Methylisoquinoline hydrochloride



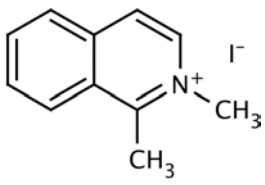
Mol. Formula : $C_{10}H_{10}ClN$ **FW :** 179.65 **HBA:** 1 **HBD:** 0 **RotB:** 0

PubChem ID : 12236795 **CASRN :** 1721-93-3 **logP:** 1.88 **TPSA:** 12.9

Activity: Potential dopaminergic neurotoxin.

NIMH Code : I-705

Compound name : 1,2-Dimethylisoquinolinium iodide

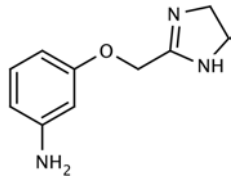


Mol. Formula : $C_{11}H_{12}IN$ **FW :** 285.12 **HBA:** 1 **HBD:** 0 **RotB:** 0

PubChem ID : 12236796 **CASRN :** 51843-14-2 **logP:** -2.53 **TPSA:** 3.9

NIMH Code : I-706

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



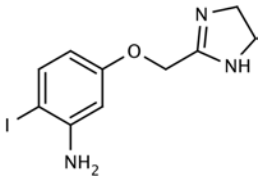
Mol. Formula : $C_{10}H_{15}Cl_2N_3O$ **FW :** 264.15 **HBA:** 4 **HBD:** 2 **RotB:** 3

PubChem ID : 10352540 **CASRN :** **logP:** 0.06 **TPSA:** 61.3

Activity: Imidazoline-guaninidine binding site (IGRS) ligand.

NIMH Code : I-707

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



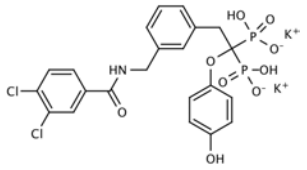
Mol. Formula : $C_{10}H_{14}Cl_2IN_3O$ **FW :** 390.05 **HBA:** 4 **HBD:** 2 **RotB:** 3

PubChem ID : **CASRN :** **logP:** 0.99 **TPSA:** 61.3

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



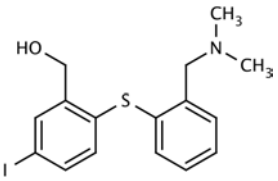
Mol. Formula : $C_{22}H_{19}Cl_2K_2NP_2O_9$ **FW :** 652.44 **HBA:** 10 **HBD:** 4 **RotB:** 9

PubChem ID : 21736614 **CASRN :** 142523-37-3 **logP:** 3.32 **TPSA:** 179.3

Activity: Non-hydrolysable inhibitor of myo-inositol monophosphatase.

NIMH Code : I-801

Compound name : IDAM hydrochloride



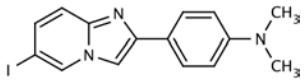
Mol. Formula : $C_{16}H_{19}ClINOS$ **FW :** 435.75 **HBA:** 2 **HBD:** 1 **RotB:** 5

PubChem ID : 9865652 **CASRN :** **logP:** 4.26 **TPSA:** 24.7

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



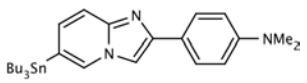
Mol. Formula : $C_{15}H_{14}IN_3$ **FW :** 363.20 **HBA:** 3 **HBD:** 0 **RotB:** 2

PubChem ID : 10133297 **CASRN :** **logP:** 3.83 **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



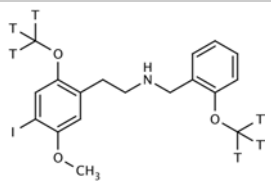
Mol. Formula : $C_{27}H_{41}N_3Sn$ **FW :** 526.34 **HBA:** 3 **HBD:** 0 **RotB:** 12

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

Activity: Radio-iodinated IMPY precursor.

NIMH Code : I-903

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



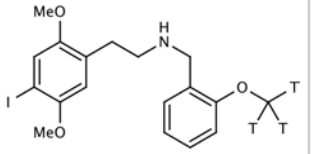
Mol. Formula : $C_{18}H_{22}INO_3$ **FW :** 439.33 **HBA:** 4 **HBD:** 1 **RotB:** 8

PubChem ID : 10251906 **CASRN :** **logP:** 4.00 **TPSA:** 44.3

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



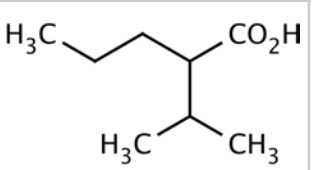
Mol. Formula : $C_{18}H_{22}INO_3$ **FW :** 433.30 **HBA:** 4 **HBD:** 1 **RotB:** 8

PubChem ID : 10251906 **CASRN :** **logP:** 4.00 **TPSA:** 44.3

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

NIMH Code : I-905

Compound name : 2-Isopropylpentanoic acid (PIA)



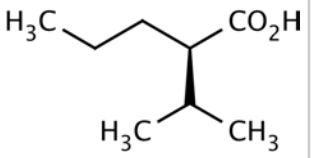
Mol. Formula : $C_8H_{16}O_2$ **FW :** 144.21 **HBA:** 2 **HBD:** 1 **RotB:** 4

PubChem ID : 147513 **CASRN :** 62391-99-5 **logP:** 2.64 **TPSA:** 40.1

Activity: Anticonvulsant.

NIMH Code : I-906

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



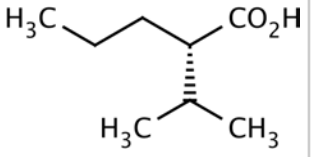
Mol. Formula : $C_8H_{16}O_2$ **FW :** 144.21 **HBA:** 2 **HBD:** 1 **RotB:** 4

PubChem ID : 10197756 **CASRN :** **logP:** 2.64 **TPSA:** 40.1

Activity: Anticonvulsant.

NIMH Code : I-907

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



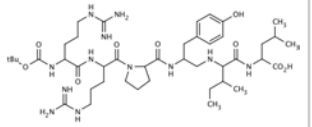
Mol. Formula : $C_8H_{16}O_2$ **FW :** 144.21 **HBA:** 2 **HBD:** 1 **RotB:** 4

PubChem ID : 10176197 **CASRN :** **logP:** 2.64 **TPSA:** 40.1

Activity: Anticonvulsant.

NIMH Code : J-901

Compound name : JMV-431



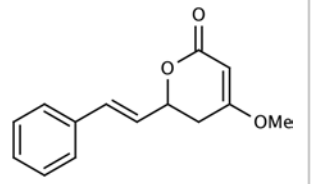
Mol. Formula : $C_{47}H_{82}N_{12}O_{13}$ **FW :** 1023.23 **HBA:** 21 **HBD:** 13 **RotB:** 28

PubChem ID : **CASRN :** **logP:** -2.56 **TPSA:** 350.2

Activity: Neurotensin receptor subtype 2 agonist.

NIMH Code : K-501

Compound name : Kawain



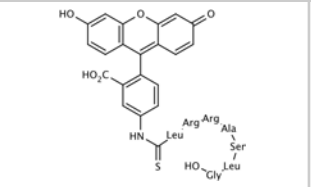
Mol. Formula : $C_{14}H_{14}O_3$ **FW :** 230.26 **HBA:** 3 **HBD:** 0 **RotB:** 3

PubChem ID : 5369129 **CASRN :** 1635-33-2 **logP:** 2.43 **TPSA:** 35.5

Activity: Anticonvulsant; axiolytic.

NIMH Code : K-701

Compound name : Kemptide fluorescein



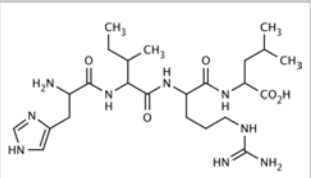
Mol. Formula : $C_{53}H_{72}N_{14}O_{14}S$ **FW :** 1161.29 **HBA:** 28 **HBD:** 18 **RotB:** 30

PubChem ID : **CASRN :** **logP:** -4.75 **TPSA:** 473.0

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

NIMH Code : L-901

Compound name : β-Lactotensin



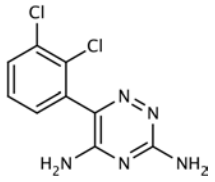
Mol. Formula : $C_{30}H_{46}F_9N_9O_{11}$ **FW :** 879.73 **HBA:** 14 **HBD:** 8 **RotB:** 17

PubChem ID : **CASRN :** **logP:** -2.60 **TPSA:** 247.4

Activity: Neurotensin receptor subtype 2 agonist.

NIMH Code : L-902

Compound name : Lamotrigine



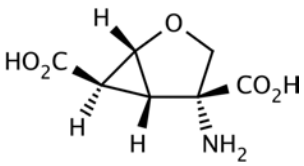
Mol. Formula : $C_9H_7Cl_2N_5$ **FW :** 256.09 **HBA:** 5 **HBD:** 2 **RotB:** 1

PubChem ID : 3878 **CASRN :** 84057-84-1 **logP:** 1.93 **TPSA:** 90.7

Activity: Voltage-sensitive sodium channel inhibitor.

NIMH Code : L-903

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



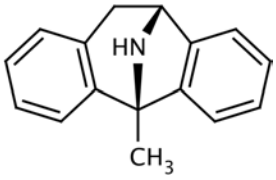
Mol. Formula : $C_7H_9NO_5$ **FW :** 187.15 **HBA:** 6 **HBD:** 3 **RotB:** 2

PubChem ID : 10197984 **CASRN :** 191471-52-0 **logP:** -3.90 **TPSA:** 117.1

Activity: Group II mGlu receptor agonist.

NIMH Code : M-107

Compound name : (+)-MK-801



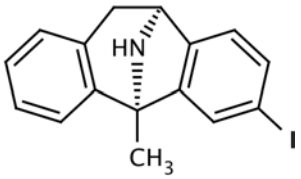
Mol. Formula : $C_{20}H_{19}NO_4$ **FW :** 337.37 **HBA:** 1 **HBD:** 1 **RotB:** 0

PubChem ID : 180081 **CASRN :** 77086-22-7 **logP:** 3.31 **TPSA:** 16.6

Activity: Non-competitive NMDA antagonist.

NIMH Code : M-141

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



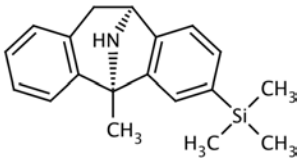
Mol. Formula : $C_{16}H_{15}ClIN$ **FW :** 383.65 **HBA:** 1 **HBD:** 1 **RotB:** 0

PubChem ID : 449735 **CASRN :** **logP:** 4.24 **TPSA:** 16.6

Activity: NMDA antagonist MK-801 analog.

NIMH Code : M-143

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



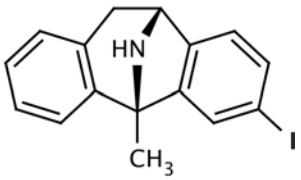
Mol. Formula : $C_{19}H_{24}ClNSi$ **FW :** 329.94 **HBA:** 1 **HBD:** 1 **RotB:** 1

PubChem ID : **CASRN :** **logP:** 4.88 **TPSA:** 16.6

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

NIMH Code : M-144

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



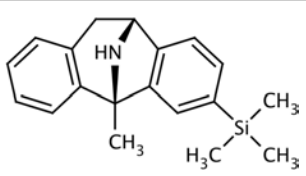
Mol. Formula : $C_{16}H_{15}ClIN$ **FW :** 383.65 **HBA:** 1 **HBD:** 1 **RotB:** 0

PubChem ID : 449735 **CASRN :** **logP:** 4.24 **TPSA:** 16.6

Activity: NMDA antagonist MK-801 analog.

NIMH Code : M-145

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



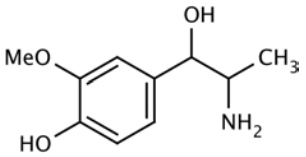
Mol. Formula : $C_{19}H_{24}ClNSi` **FW :** 329.94 **HBA:** 1 **HBD:** 1 **RotB:** 1

PubChem ID : **CASRN :** **logP:** 4.88 **TPSA:** 16.6

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

NIMH Code : M-501

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

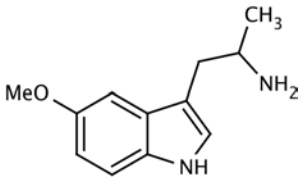


Mol. Formula : $C_{12}H_{17}NO_7` **FW :** 287.27 **HBA:** 4 **HBD:** 3 **RotB:** 3

PubChem ID : **CASRN :** **logP:** -0.00 **TPSA:** 77.3

NIMH Code : M-502

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

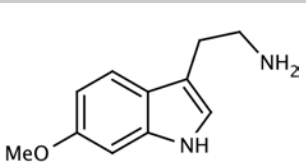


Mol. Formula : $C_{12}H_{17}ClN_2O` **FW :** 240.73 **HBA:** 3 **HBD:** 1 **RotB:** 3

PubChem ID : 36906 **CASRN :** 1137-04-8 **logP:** 1.75 **TPSA:** 52.7

NIMH Code : M-503

Compound name : 6-Methoxytryptamine creatinine sulfate

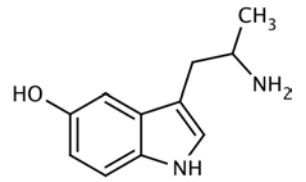


Mol. Formula : $C_{15}H_{23}N_5O_6S` **FW :** 514.56 **HBA:** 7 **HBD:** 3 **RotB:** 3

PubChem ID : 17654 **CASRN :** 3610-36-4 **logP:** 1.33 **TPSA:** 52.7

NIMH Code : M-504

Compound name : α-Methylserotonin hydrogen oxalate



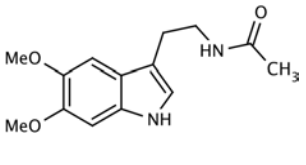
Mol. Formula : $C_{13}H_{16}N_2O_5` **FW :** 280.28 **HBA:** 3 **HBD:** 2 **RotB:** 2

PubChem ID : 2107 **CASRN :** **logP:** 0.84 **TPSA:** 63.7

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

NIMH Code : M-506

Compound name : 6-Methoxymelatonin



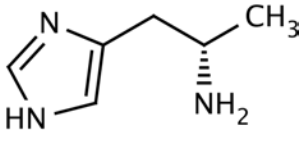
Mol. Formula : $C_{14}H_{18}N_2O_3` **FW :** 262.30 **HBA:** 5 **HBD:** 1 **RotB:** 5

PubChem ID : 189748 **CASRN :** 69845-43-8 **logP:** 0.99 **TPSA:** 63.4

Activity: 6-Hydroxymelatonin metabolite.

NIMH Code : M-507

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



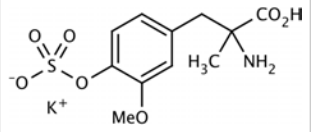
Mol. Formula : $C_9H_{14}N_3O_6` **FW :** 215.21 **HBA:** 3 **HBD:** 1 **RotB:** 2

PubChem ID : 6603865 **CASRN :** **logP:** -0.28 **TPSA:** 56.3

Activity: Histamine H_3 agonist.

NIMH Code : M-508

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

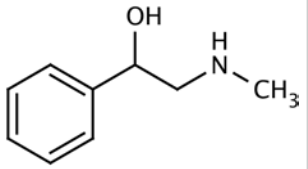


Mol. Formula : $C_{11}H_{14}KNO_7S$ **FW :** 343.40 **HBA:** 8 **HBD:** 2 **RotB:** 6

PubChem ID : **CASRN :** **logP:** -0.46 **TPSA:** 143.4

NIMH Code : M-509

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



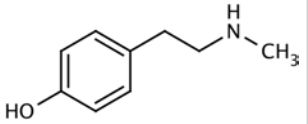
Mol. Formula : $C_9H_{13}NO$ **FW :** 151.21 **HBA:** 2 **HBD:** 2 **RotB:** 3

PubChem ID : 913 **CASRN :** 6589-55-5 **logP:** 0.90 **TPSA:** 36.8

Activity: Monoamine oxidase A/B substrate.

NIMH Code : M-510

Compound name : N-Methyltyramine hydrobromide

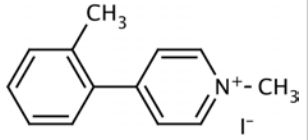


Mol. Formula : $C_9H_{14}BrNO$ **FW :** 232.12 **HBA:** 2 **HBD:** 2 **RotB:** 3

PubChem ID : 22324146 **CASRN :** 370-98-9 **logP:** 0.96 **TPSA:** 36.8

NIMH Code : M-701

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



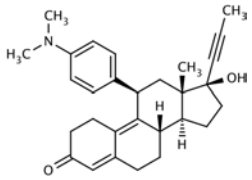
Mol. Formula : $C_{13}H_{14}NI$ **FW :** 311.16 **HBA:** 1 **HBD:** 0 **RotB:** 1

PubChem ID : 163849 **CASRN :** 111342-39-3 **logP:** -1.03 **TPSA:** 3.9

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

NIMH Code : M-703

Compound name : Mifepristone



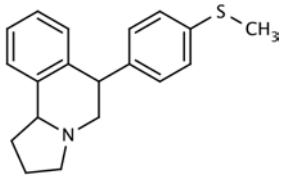
Mol. Formula : $C_{29}H_{35}NO_2$ **FW :** 429.59 **HBA:** 3 **HBD:** 1 **RotB:** 3

PubChem ID : 6712024 **CASRN :** 84371-65-3 **logP:** 5.13 **TPSA:** 40.5

Activity: Progesterone receptor antagonist.

NIMH Code : M-704

Compound name : (±)-McN-5652



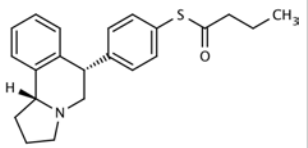
Mol. Formula : $C_{19}H_{22}ClNO_4S$ **FW :** 395.90 **HBA:** 1 **HBD:** 0 **RotB:** 2

PubChem ID : 9994677 **CASRN :** **logP:** 4.55 **TPSA:** 4.4

Activity: Serotonin transporter inhibitor.

NIMH Code : M-706

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



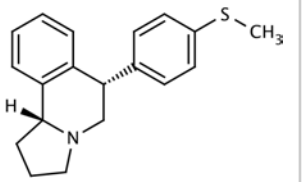
Mol. Formula : $C_{22}H_{25}NOS$ **FW :** 351.51 **HBA:** 2 **HBD:** 0 **RotB:** 5

PubChem ID : **CASRN :** 167548-65-4 **logP:** 5.15 **TPSA:** 21.5

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

NIMH Code : M-707

Compound name : (+)-McN-5652



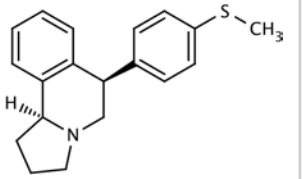
Mol. Formula : $C_{19}H_{22}ClNO_4S$ **FW :** 395.90 **HBA:** 1 **HBD:** 0 **RotB:** 2

PubChem ID : 146919 **CASRN :** 103729-16-4 **logP:** 4.55 **TPSA:** 4.4

Activity: Serotonin transporter inhibitor (active enantiomer).

NIMH Code : M-708

Compound name : (–)-McN-5652



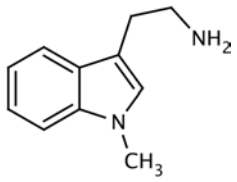
Mol. Formula : $C_{19}H_{22}ClNO_4S$ **FW :** 395.90 **HBA:** 1 **HBD:** 0 **RotB:** 2

PubChem ID : 6336338 **CASRN :** **logP:** 4.55 **TPSA:** 4.4

Activity: Serotonin transporter inhibitor (inactive enantiomer).

NIMH Code : M-709

Compound name : 1-Methyltryptamine hydrochloride

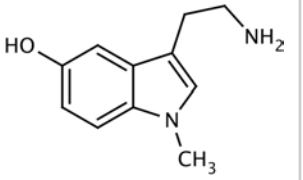


Mol. Formula : $C_{11}H_{15}ClN_2$ **FW :** 210.70 **HBA:** 2 **HBD:** 1 **RotB:** 2

PubChem ID : 23492 **CASRN :** 7518-21-0 **logP:** 1.71 **TPSA:** 32.6

NIMH Code : M-710

Compound name : 1-Methylserotonin hydrogen maleate



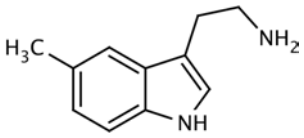
Mol. Formula : $C_{15}H_{18}N_2O_5$ **FW :** 306.31 **HBA:** 3 **HBD:** 2 **RotB:** 2

PubChem ID : 440945 **CASRN :** **logP:** 0.70 **TPSA:** 52.8

Activity: Serotonin analog.

NIMH Code : M-711

Compound name : 5-Methyltryptamine hydrogen maleate



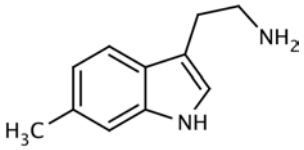
Mol. Formula : $C_{15}H_{18}N_2O_4$ **FW :** 290.31 **HBA:** 2 **HBD:** 1 **RotB:** 2

PubChem ID : 15760 **CASRN :** 1821-47-2 **logP:** 2.00 **TPSA:** 43.4

Activity: Serotonin analog.

NIMH Code : M-712

Compound name : 6-Methyltryptamine hydrogen maleate



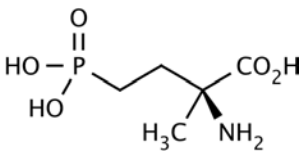
Mol. Formula : $C_{15}H_{18}N_2O_4$ **FW :** 290.31 **HBA:** 2 **HBD:** 1 **RotB:** 2

PubChem ID : 190006 **CASRN :** 62500-90-7 **logP:** 2.00 **TPSA:** 43.4

Activity: Serotonin analog.

NIMH Code : M-801

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



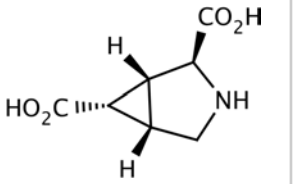
Mol. Formula : $C_5H_{12}NO_5P$ **FW :** 197.13 **HBA:** 6 **HBD:** 4 **RotB:** 4

PubChem ID : 1795543 **CASRN :** 157381-42-5 **logP:** -3.44 **TPSA:** 128.1

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

NIMH Code : M-802

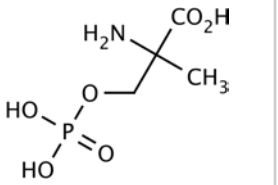
Compound name : (1*R*,2*S*,5*S*,6*S*)-3-Azabicyclo[3.1.0]hexane-2,6-dicarboxylic acid



Mol. Formula :	$C_7H_9NO_4$	**FW :** 171.15	**HBA:** 5	**HBD:** 3	**RotB:** 2
PubChem ID :	10329748	**CASRN :**		**logP:** -3.57	**TPSA:** 96.9
Activity:	Inhibitor of the Na-dependent, high-affinity synaptosomal Glu transporter.				

NIMH Code : M-803

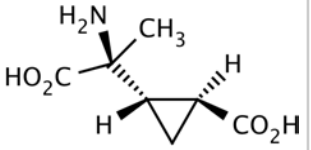
Compound name : (±)-α-Methylserine-*O*-phosphate



Mol. Formula :	$C_4H_{10}NO_6P$	**FW :** 199.10	**HBA:** 7	**HBD:** 4	**RotB:** 4
PubChem ID :	3964633	**CASRN :** 66515-29-5		**logP:** -2.73	**TPSA:** 140.2
Activity:	Metabotropic glutamate mGluR antagonist.				

NIMH Code : M-804

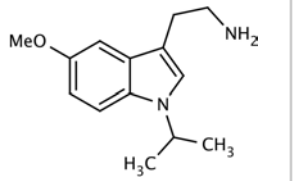
Compound name : (2*S*,3*S*,4*S*)-2-Methyl-2-(carboxycyclopropyl)glycine



Mol. Formula :	$C_7H_{11}NO_4$	**FW :** 173.17	**HBA:** 5	**HBD:** 3	**RotB:** 3
PubChem ID :	6536817	**CASRN :** 157141-16-7		**logP:** -2.81	**TPSA:** 107.9
Activity:	Metabotropic glutamate $mGluR_2$ antagonist.				

NIMH Code : M-805

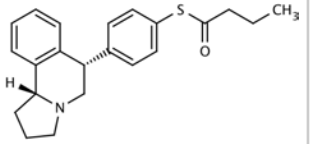
Compound name : 5-Methoxy-1-isopropyltryptamine



Mol. Formula :	$C_{14}H_{20}N_2O$	**FW :** 232.32	**HBA:** 3	**HBD:** 1	**RotB:** 4
PubChem ID :	24820144	**CASRN :** 109921-55-3		**logP:** 2.33	**TPSA:** 41.8
Activity:	Serotonin analog.				

NIMH Code : M-901

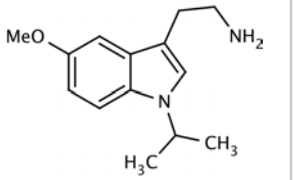
Compound name : (+)-McN-5652 *S*-Desmethyl-*S*-butyryl ester tartrate



Mol. Formula :	$C_{26}H_{31}NO_7S$	**FW :** 501.59	**HBA:** 2	**HBD:** 0	**RotB:** 5
PubChem ID :		**CASRN :** 167548-65-4		**logP:** 5.15	**TPSA:** 21.5
Activity:	(+)-McN-5652 PET ligand precursor.				

NIMH Code : M-902

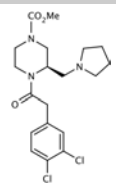
Compound name : 5-Methoxy-1-isopropyltryptamine oxalate



Mol. Formula :	$C_{16}H_{22}N_2O_5$	**FW :** 322.36	**HBA:** 3	**HBD:** 1	**RotB:** 4
PubChem ID :	24820144	**CASRN :**		**logP:** 2.33	**TPSA:** 41.8
Activity:	Serotonin analog.				

NIMH Code : M-903

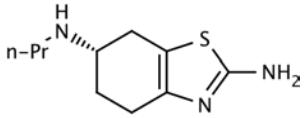
Compound name : GR103545



Mol. Formula :	$C_{19}H_{25}Cl_2N_3O_3$	**FW :** 530.40	**HBA:** 6	**HBD:** 0	**RotB:** 5
PubChem ID :	6603856	**CASRN :**		**logP:** 2.64	**TPSA:** 54.3
Activity:	Opioid receptor agonist.				

NIMH Code : M-904

Compound name : Mirapex (Pramipexole)

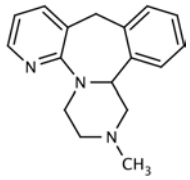


Mol. Formula :	$C_{10}H_{17}N_3S$	**FW :** 211.33	**HBA:** 3	**HBD:** 2	**RotB:** 3
PubChem ID :	119570	**CASRN :** 104632-26-0		**logP:** 1.76	**TPSA:** 55.5

Activity: Dopamine D_3 agonist.

NIMH Code : M-905

Compound name : Mirtazapine

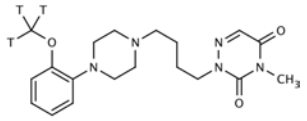


Mol. Formula :	$C_{17}H_{19}N_3$	**FW :** 265.35	**HBA:** 3	**HBD:** 0	**RotB:** 0
PubChem ID :	4205	**CASRN :** 0		**logP:** 3.21	**TPSA:** 19.4

Activity: Serotonin & noradrenergic antagonist.

NIMH Code : M-906

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

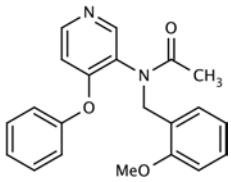


Mol. Formula :	$C_{19}H_{27}N_5O_3$	**FW :** 379.47	**HBA:** 8	**HBD:** 0	**RotB:** 7
PubChem ID :	21830793	**CASRN :**		**logP:** 1.79	**TPSA:** 69.9

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

NIMH Code : M-907

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

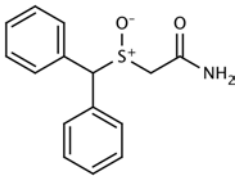


Mol. Formula :	$C_{21}H_{20}N_2O_3$	**FW :** 348.40	**HBA:** 5	**HBD:** 0	**RotB:** 6
PubChem ID :	9841240	**CASRN :**		**logP:** 2.92	**TPSA:** 51.7

Activity: Brain peripheral benzodiazepine receptor (TSPO) ligand.

NIMH Code : M-908

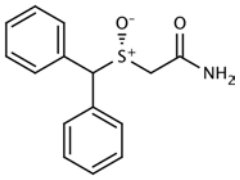
Compound name : (±)-Modafinil



Mol. Formula :	$C_{15}H_{15}NO_2S$	**FW :** 273.35	**HBA:** 3	**HBD:** 1	**RotB:** 5
PubChem ID :	4236	**CASRN :** 68693-11-8		**logP:** 1.53	**TPSA:** 60.2

NIMH Code : M-909

Compound name : (*R*)-(–)-Modafinil

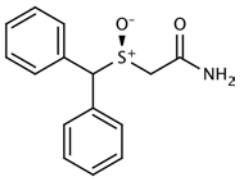


Mol. Formula :	$C_{15}H_{15}NO_2S$	**FW :** 273.35	**HBA:** 3	**HBD:** 1	**RotB:** 5
PubChem ID :	9690109	**CASRN :** 112111-43-0		**logP:** 1.53	**TPSA:** 60.2

Activity: Dopamine D_2 partial agonist.

NIMH Code : M-910

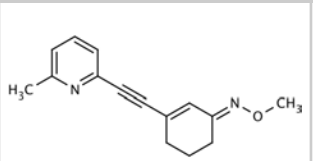
Compound name : (*S*)-(+)-Modafinil



Mol. Formula :	$C_{15}H_{15}NO_2S$	**FW :** 273.35	**HBA:** 3	**HBD:** 1	**RotB:** 5
PubChem ID :		**CASRN :**		**logP:** 1.53	**TPSA:** 60.2

NIMH Code : M-911

Compound name : ABP688

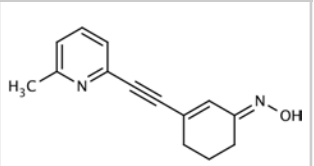


Mol. Formula :	$C_{15}H_{16}N_2O$	**FW :**	240.30	**HBA:**	3	**HBD:**	0	**RotB:**	3
PubChem ID :	11481862	**CASRN :**				**logP:**	3.02	**TPSA:**	34.5

Activity: Metabotropic glutamate mGluR5 antagonist.

NIMH Code : M-912

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

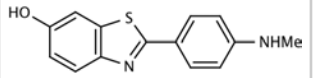


Mol. Formula :	$C_{14}H_{14}N_2O$	**FW :**	226.27	**HBA:**	3	**HBD:**	1	**RotB:**	2
PubChem ID :		**CASRN :**				**logP:**	2.65	**TPSA:**	45.5

Activity: ABP688 PET ligand precursor.

NIMH Code : M-913

Compound name : 6-OH-BTA-1

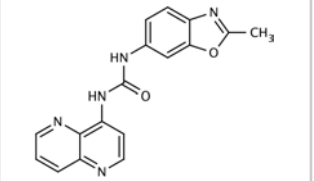


Mol. Formula :	$C_{14}H_{12}N_2OS$	**FW :**	256.32	**HBA:**	3	**HBD:**	2	**RotB:**	2
PubChem ID :	10171487	**CASRN :**	566169-93-5			**logP:**	3.31	**TPSA:**	45.2

Activity: Aggregated amyloid protein ligand; Thioflavin-T analog.

NIMH Code : M-914

Compound name : SB-334867

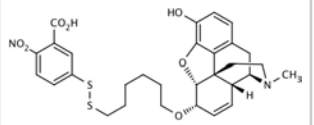


Mol. Formula :	$C_{17}H_{13}N_5O_2$	**FW :**	319.32	**HBA:**	7	**HBD:**	2	**RotB:**	2
PubChem ID :	6604926	**CASRN :**	249889-64-3			**logP:**	1.91	**TPSA:**	92.9

Activity: Orexin subtype 1 antagonist.

NIMH Code : M-915

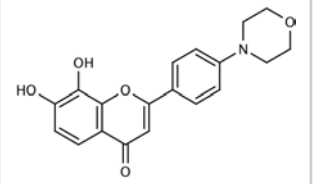
Compound name : Morphine-SH-DTNB derivative



Mol. Formula :	$C_{30}H_{34}N_2O_7S_2$	**FW :**	598.73	**HBA:**	9	**HBD:**	2	**RotB:**	12
PubChem ID :		**CASRN :**	9			**logP:**	2.94	**TPSA:**	129.1

NIMH Code : M-916

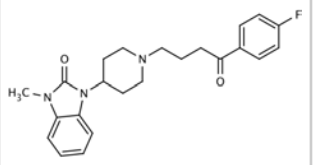
Compound name : 2-(4-Morphin-4-ylphenyl)-7,8-dihydroxy-4H-chromen-4-one



Mol. Formula :	$C_{19}H_{17}NO_5$	**FW :**	339.34	**HBA:**	6	**HBD:**	2	**RotB:**	2
PubChem ID :		**CASRN :**				**logP:**	2.25	**TPSA:**	82.1

NIMH Code : M-917 new

Compound name : *N*-Methylbenperidol

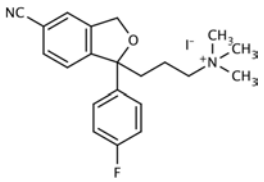


Mol. Formula :	$C_{23}H_{26}FN_3O_2$	**FW :**	395.47	**HBA:**	5	**HBD:**	0	**RotB:**	6
PubChem ID :	131585	**CASRN :**	133066-70-3			**logP:**	3.16	**TPSA:**	43.9

Activity: Dopamine D2 receptor ligand.

NIMH Code : M-918 new

Compound name : (*RS*)-1-[3-(Trimethylamino)propyl]-1-(4-fluorophenyl)-1,3-dihydroisobenofuran-5-carbonitrile iodide (*N*-Methyl-citalopram)



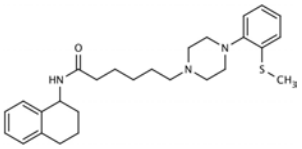
Mol. Formula : $C_{21}H_{24}IFN_2O$ **FW :** 466.33 **HBA:** 3 **HBD:** 0 **RotB:** 5

PubChem ID : - **CASRN :** 960496-06-4 **logP:** -0.40 **TPSA:** 33.0

Activity: Selective serotonin reuptake inhibitor.

NIMH Code : M-919 new

Compound name : 4-[2-(Methylthio)phenyl]-*N*-(1,2,3,4-tetrahydronaphthalen-1-yl)-1-piperazinehexanamide hydrochloride (LP-44)



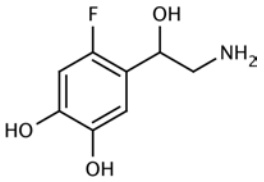
Mol. Formula : $C_{27}H_{37}N_3OS \cdot 1.8\ HCl$ **FW :** 524.59 **HBA:** 4 **HBD:** 1 **RotB:** 9

PubChem ID : 11224758 **CASRN :** 824958-12-5 **logP:** 5.58 **TPSA:** 36.8

Activity: Serotonin 5-HT_7 receptor agonist.

NIMH Code : N-502

Compound name : 6-Fluoronorepinephrine oxalate



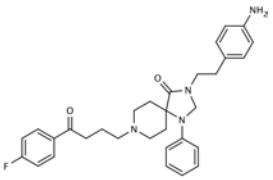
Mol. Formula : $C_{18}H_{22}F_2N_2O_{10}$ **FW :** 464.37 **HBA:** 4 **HBD:** 4 **RotB:** 2

PubChem ID : 1862 **CASRN :** 86820-21-5 **logP:** -0.78 **TPSA:** 88.3

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

NIMH Code : N-701

Compound name : p-Aminophenethylspiperone



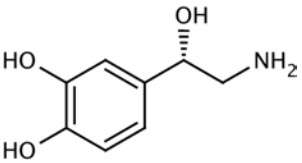
Mol. Formula : $C_{31}H_{35}FN_4O_2$ **FW :** 514.63 **HBA:** 6 **HBD:** 1 **RotB:** 9

PubChem ID : 125085 **CASRN :** 93801-18-4 **logP:** 4.48 **TPSA:** 71.1

Activity: Dopamine D_2 antagonist.

NIMH Code : N-702

Compound name : (+)-Norepinephrine tartrate



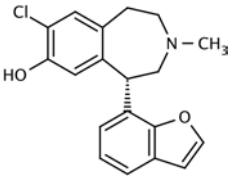
Mol. Formula : $C_{12}H_{17}NO_9$ **FW :** 319.26 **HBA:** 4 **HBD:** 4 **RotB:** 2

PubChem ID : 5814 **CASRN :** 636-88-4 **logP:** -0.68 **TPSA:** 88.3

Activity: Unnatural enantiomer of norepinephrine.

NIMH Code : N-703

Compound name : (+)-NNC 01-0112



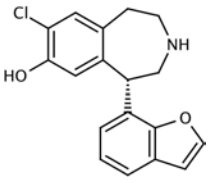
Mol. Formula : $C_{19}H_{18}ClNO_2$ **FW :** 327.81 **HBA:** 3 **HBD:** 1 **RotB:** 1

PubChem ID : 130424 **CASRN :** 125341-24-4 **logP:** 3.33 **TPSA:** 37.8

Activity: Dopamine D_1 receptor ligand.

NIMH Code : N-704

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



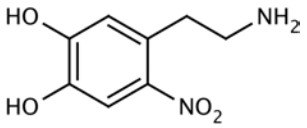
Mol. Formula : $C_{18}H_{17}Cl_2NO_2$ **FW :** 350.24 **HBA:** 3 **HBD:** 2 **RotB:** 1

PubChem ID : 20135382 **CASRN :** **logP:** 2.68 **TPSA:** 50.0

Activity: NNC-01-0112 PET ligand precusor.

NIMH Code : N-705

Compound name : 6-Nitrodopamine



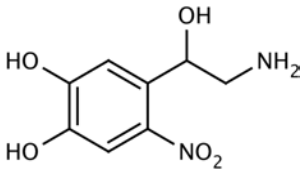
Mol. Formula : $C_8H_{10}N_2O_{14}$ **FW :** 198.18 **HBA:** 6 **HBD:** 3 **RotB:** 3

PubChem ID : 10932412 **CASRN :** **logP:** -0.17 **TPSA:** 116.8

Activity: Nitrated catecholamine.

NIMH Code : N-706

Compound name : 6-Nitronorepinephrine



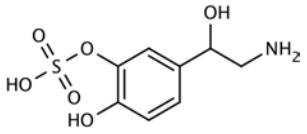
Mol. Formula : $C_8H_{10}N_2O_5$ **FW :** 214.18 **HBA:** 7 **HBD:** 4 **RotB:** 3

PubChem ID : **CASRN :** **logP:** -1.06 **TPSA:** 137.0

Activity: Nitrated catecholamine.

NIMH Code : N-707

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



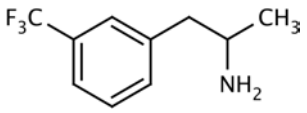
Mol. Formula : $C_8H_{11}NO_6S$ **FW :** 249.24 **HBA:** 7 **HBD:** 4 **RotB:** 4

PubChem ID : 10083394 **CASRN :** **logP:** -0.97 **TPSA:** 134.5

Activity: Catechol O-methyltransferase inhibitor.

NIMH Code : N-801

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



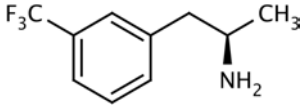
Mol. Formula : $C_{10}H_{13}ClF_3N$ **FW :** 239.67 **HBA:** 1 **HBD:** 1 **RotB:** 3

PubChem ID : 120765 **CASRN :** 673-18-7 **logP:** 2.68 **TPSA:** 27.6

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

NIMH Code : N-802

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



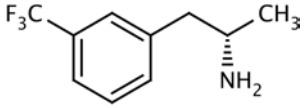
Mol. Formula : $C_{10}H_{13}ClF_3N$ **FW :** 239.67 **HBA:** 1 **HBD:** 1 **RotB:** 3

PubChem ID : 12895728 **CASRN :** **logP:** 2.68 **TPSA:** 27.6

Activity: Serotonin uptake inhibitor.

NIMH Code : N-803

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



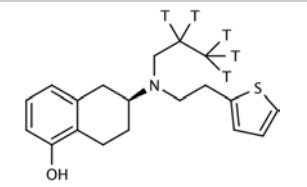
Mol. Formula : $C_{10}H_{13}ClF_3N$ **FW :** 239.67 **HBA:** 1 **HBD:** 1 **RotB:** 3

PubChem ID : 9815618 **CASRN :** **logP:** 2.68 **TPSA:** 27.6

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



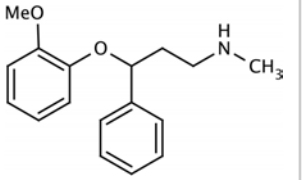
Mol. Formula : $C_{19}H_{26}ClNOS$ **FW :** 361.97 **HBA:** 2 **HBD:** 1 **RotB:** 6

PubChem ID : 6917969 **CASRN :** 92206-54-7 **logP:** 4.34 **TPSA:** 24.7

Activity: Radiolabeled dopamine receptor agonist.

NIMH Code : N-901

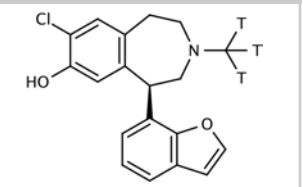
Compound name : (±)-Nisoxetine hydrochloride



Mol. Formula :	$C_{17}H_{22}ClNO_2$	**FW :** 307.82	**HBA:** 3	**HBD:** 1	**RotB:** 7
PubChem ID :	134453	**CASRN :** 57754-86-6		**logP:** 3.14	**TPSA:** 35.1
Activity:	Norepinephrine uptake inhibitor.				

NIMH Code : N-902

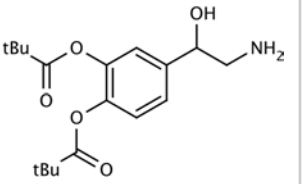
Compound name : (+)-8-Chloro-5-(7-benzofuranyl)-7-hydroxy-3-methyl-2,3,4,5-tetrahydro-1*H*-3-benzazepine, [^{3}H]NNC-01-0112



Mol. Formula :	$C_{19}H_{19}ClNO_2$	**FW :** 333.83	**HBA:** 3	**HBD:** 1	**RotB:** 1
PubChem ID :	130424	**CASRN :**		**logP:** 3.33	**TPSA:** 37.8
Activity:	Radiolabeled dopamine D_1 receptor ligand.				

NIMH Code : N-903

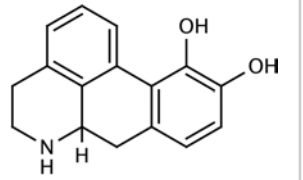
Compound name : Norepinephrine dipivalate hydrochloride



Mol. Formula :	$C_{18}H_{28}ClNO_5$	**FW :** 373.87	**HBA:** 6	**HBD:** 2	**RotB:** 8
PubChem ID :		**CASRN :**		**logP:** 3.28	**TPSA:** 100.5

NIMH Code : N-904

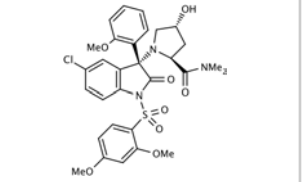
Compound name : *(R)*-(–)-Norapomorphine hydrobromide



Mol. Formula :	$C_{16}H_{16}BrNO_2$	**FW :** 334.21	**HBA:** 3	**HBD:** 3	**RotB:** 0
PubChem ID :	30133	**CASRN :** 20382-69-8		**logP:** 1.83	**TPSA:** 57.1
Activity:	Dopamine D_3 receptor ligand.				

NIMH Code : N-905 new

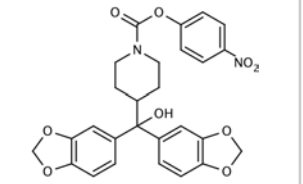
Compound name : Nelivaptan



Mol. Formula :	$C_{30}H_{32}ClN_3O_8S$	**FW :** 630.11	**HBA:** 11	**HBD:** 1	**RotB:** 7
PubChem ID :	9895468	**CASRN :** 439687-69-1		**logP:** 2.69	**TPSA:** 125.9
Activity:	Selective, orally-active non-peptide vasopressin V1b receptor antagonist.				

NIMH Code : N-906 new

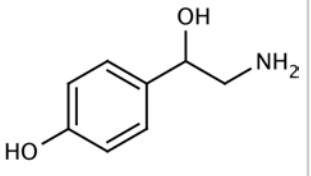
Compound name : 4-Nitrophenyl-4-[bis(1,3-benzodioxol-5-yl)(hydroxy)methyl]piperidine-1-carboxylate (JZL 184)



Mol. Formula :	$C_{27}H_{24}N_2O_9$	**FW :** 520.49	**HBA:** 11	**HBD:** 1	**RotB:** 6
PubChem ID :	25021165	**CASRN :** 1101854-58-3		**logP:** 3.95	**TPSA:** 132.5
Activity:	Potent and selective monoacylglycerol lipase (MAGL) inhibitor.				

NIMH Code : O-501

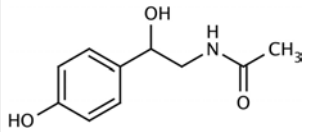
Compound name : (–)-Octopamine



Mol. Formula :	$C_8H_{11}NO_2$	**FW :** 153.18	**HBA:** 3	**HBD:** 3	**RotB:** 2
PubChem ID :	4581	**CASRN :** 104-14-3		**logP:** -0.32	**TPSA:** 68.1
Activity:	Biogenic amine formed by β-hydroxylation of tyramine.				

NIMH Code : O-502

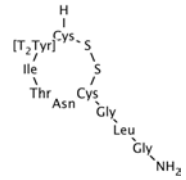
Compound name : N-Acetyl-(±)-octopamine



Mol. Formula :	$C_{10}H_{13}NO_3$	**FW :**	195.22	**HBA:**	4	**HBD:**	3	**RotB:**	3
PubChem ID :	193691	**CASRN :**	33141-15-0			**logP:**	-0.02	**TPSA:**	69.6

NIMH Code : O-801

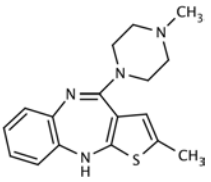
Compound name : [^{3}H][Thr^4,Gly^7]Oxytocin



Mol. Formula :	$C_{39}H_{61}N_{11}O_{12}S_2$	**FW :**	944.11	**HBA:**	23	**HBD:**	13	**RotB:**	17
PubChem ID :	3080871	**CASRN :**	60786-59-6			**logP:**	-3.89	**TPSA:**	387.1
Activity:	Radiolabeled oxytocin analog.								

NIMH Code : O-901

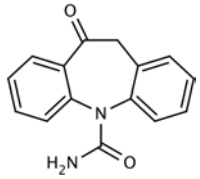
Compound name : Olanzapine



Mol. Formula :	$C_{17}H_{20}N_4S$	**FW :**	312.43	**HBA:**	4	**HBD:**	1	**RotB:**	0
PubChem ID :	4585	**CASRN :**	132539-06-1			**logP:**	3.39	**TPSA:**	30.9
Activity:	Serotonin uptake inhibitor.								

NIMH Code : O-902

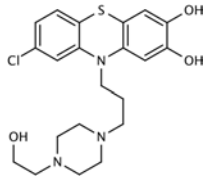
Compound name : Oxcarbazepine



Mol. Formula :	$C_{15}H_{12}N_2O_2$	**FW :**	252.27	**HBA:**	4	**HBD:**	1	**RotB:**	0
PubChem ID :	34312	**CASRN :**	28721-07-5			**logP:**	1.82	**TPSA:**	63.4
Activity:	Sodium channel inhibitor.								

NIMH Code : P-501

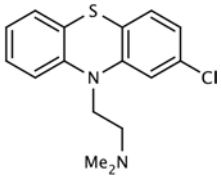
Compound name : 7,8-Dihydroxyperphenazine dihydrochloride



Mol. Formula :	$C_{21}H_{28}Cl_3N_3O_3S$	**FW :**	508.89	**HBA:**	6	**HBD:**	3	**RotB:**	6
PubChem ID :		**CASRN :**				**logP:**	2.88	**TPSA:**	71.6

NIMH Code : P-503

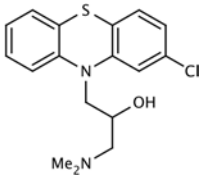
Compound name : 2-Chloro-10-(2-dimethylaminoethyl)phenothiazine hydrochloride



Mol. Formula :	$C_{16}H_{18}Cl_2N_2S$	**FW :**	341.30	**HBA:**	2	**HBD:**	0	**RotB:**	3
PubChem ID :	168055	**CASRN :**	2095-24-1			**logP:**	4.48	**TPSA:**	7.7

NIMH Code : P-504

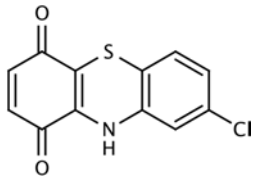
Compound name : (±)-2-Chloro-10-(3-dimethylamino-2-hydroxypropyl)phenothiazine hydrogen maleate



Mol. Formula :	$C_{21}H_{23}ClN_2O_5S$	**FW :**	450.94	**HBA:**	3	**HBD:**	1	**RotB:**	4
PubChem ID :		**CASRN :**				**logP:**	3.84	**TPSA:**	27.9

NIMH Code : P-505

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

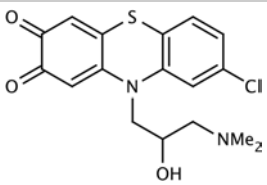


Mol. Formula : $C_{12}H_6ClNO_2S$ **FW :** 263.70 **HBA:** 3 **HBD:** 0 **RotB:** 0

PubChem ID : **CASRN :** **logP:** 2.41 **TPSA:** 46.2

NIMH Code : P-506

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

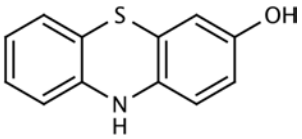


Mol. Formula : $C_{17}H_{18}Cl_2N_2O_3S$ **FW :** 401.31 **HBA:** 5 **HBD:** 1 **RotB:** 4

PubChem ID : **CASRN :** **logP:** 2.28 **TPSA:** 62.1

NIMH Code : P-508

Compound name : 3-Hydroxyphenothiazine

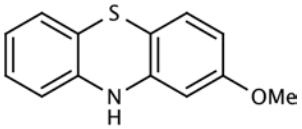


Mol. Formula : $C_{12}H_9NOS$ **FW :** 215.27 **HBA:** 2 **HBD:** 2 **RotB:** 0

PubChem ID : 74725 **CASRN :** 1927-44-2 **logP:** 3.33 **TPSA:** 32.3

NIMH Code : P-509

Compound name : 2-Methoxyphenothiazine

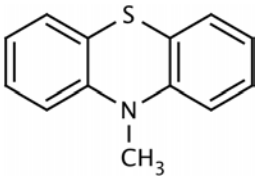


Mol. Formula : $C_{13}H_{11}NOS$ **FW :** 229.30 **HBA:** 2 **HBD:** 1 **RotB:** 1

PubChem ID : 74490 **CASRN :** 1771-18-2 **logP:** 3.47 **TPSA:** 21.3

NIMH Code : P-510

Compound name : N-Methylphenothiazine

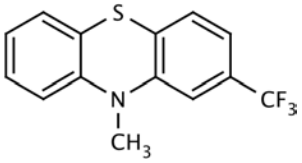


Mol. Formula : $C_{13}H_{11}NS$ **FW :** 213.30 **HBA:** 1 **HBD:** 0 **RotB:** 0

PubChem ID : 71015 **CASRN :** 1207-72-3 **logP:** 3.85 **TPSA:** 3.2

NIMH Code : P-511

Compound name : N-Methyl-2-(trifluoromethyl)phenothiazine

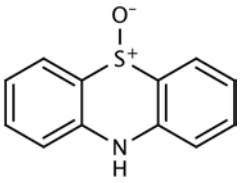


Mol. Formula : $C_{14}H_{10}F_3NS$ **FW :** 281.30 **HBA:** 1 **HBD:** 0 **RotB:** 1

PubChem ID : **CASRN :** **logP:** 4.73 **TPSA:** 3.2

NIMH Code : P-512

Compound name : Phenothiazine-5-oxide

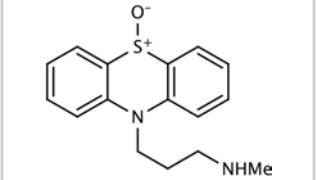


Mol. Formula : $C_{12}H_9NOS$ **FW :** 215.27 **HBA:** 2 **HBD:** 1 **RotB:** 0

PubChem ID : 71014 **CASRN :** 1207-71-2 **logP:** 2.25 **TPSA:** 29.1

NIMH Code : P-513

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

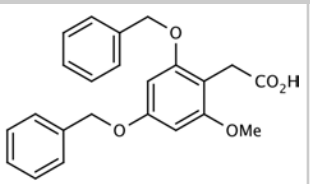


Mol. Formula : $C_{16}H_{19}ClN_2OS$ **FW :** 322.85 **HBA:** 3 **HBD:** 1 **RotB:** 4

PubChem ID : 23275476 **CASRN :** **logP:** 2.17 **TPSA:** 36.9

NIMH Code : P-514

Compound name : 2,4-Dibenzyloxy-5-methoxyphenylacetic acid

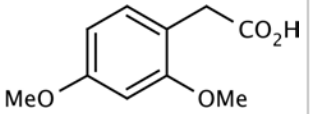


Mol. Formula : $C_{23}H_{22}O_5$ **FW :** 378.42 **HBA:** 5 **HBD:** 1 **RotB:** 9

PubChem ID : **CASRN :** **logP:** 4.59 **TPSA:** 67.8

NIMH Code : P-515

Compound name : 2,4-Dimethoxyphenylacetic acid

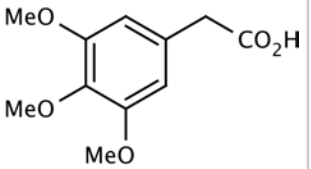


Mol. Formula : $C_{10}H_{12}O_4$ **FW :** 196.20 **HBA:** 4 **HBD:** 1 **RotB:** 4

PubChem ID : 350555 **CASRN :** 6496-89-5 **logP:** 1.30 **TPSA:** 58.6

NIMH Code : P-516

Compound name : 3,4,5-Trimethoxyphenylacetic acid



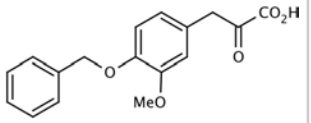
Mol. Formula : $C_{11}H_{14}O_5$ **FW :** 226.23 **HBA:** 5 **HBD:** 1 **RotB:** 5

PubChem ID : 70372 **CASRN :** 951-82-6 **logP:** 1.14 **TPSA:** 67.8

Activity: Mescaline metabolite.

NIMH Code : P-517

Compound name : 4-Benzyloxyphenyl-3-methoxypyruvic acid

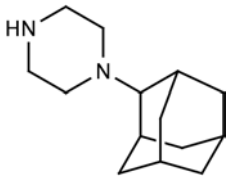


Mol. Formula : $C_{17}H_{16}O_5$ **FW :** 300.31 **HBA:** 5 **HBD:** 1 **RotB:** 7

PubChem ID : **CASRN :** **logP:** 3.31 **TPSA:** 75.7

NIMH Code : P-518

Compound name : N-(2-Adamantyl)piperazine dihydrochloride

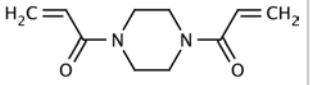


Mol. Formula : $C_{14}H_{26}Cl_2N_2$ **FW :** 293.28 **HBA:** 2 **HBD:** 1 **RotB:** 1

PubChem ID : 4599242 **CASRN :** **logP:** 1.83 **TPSA:** 16.5

NIMH Code : P-519

Compound name : 1,4-Diacryloylpiperazine



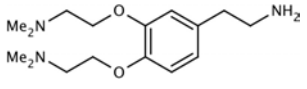
Mol. Formula : $C_{10}H_{14}N_2O_2$ **FW :** 194.23 **HBA:** 4 **HBD:** 0 **RotB:** 2

PubChem ID : 193422 **CASRN :** 6342-17-2 **logP:** 0.00 **TPSA:** 40.6

Activity: Cross-linking monomer for development of polyacrylamide gels.

NIMH Code : P-520

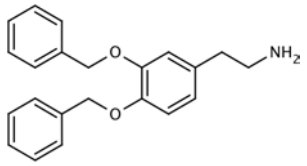
Compound name : 3,4-Di(β-dimethylaminoethoxy)-β-phenethylamine trihydrochloride



Mol. Formula :	$C_{16}H_{32}Cl_3N_3O_2$	**FW :**	404.80	**HBA:**	5	**HBD:**	1	**RotB:**	10
PubChem ID :		**CASRN :**				**logP:**	1.11	**TPSA:**	55.0

NIMH Code : P-521

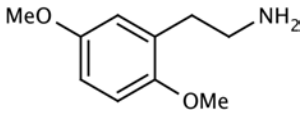
Compound name : 3,4-Dibenzyloxy-β-phenethylamine hydrochloride



Mol. Formula :	$C_{22}H_{24}ClNO_2$	**FW :**	369.88	**HBA:**	3	**HBD:**	1	**RotB:**	8
PubChem ID :	423869	**CASRN :**	1699-56-5			**logP:**	4.52	**TPSA:**	46.1

NIMH Code : P-522

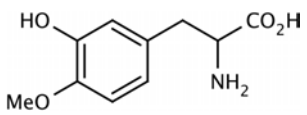
Compound name : 2,5-Dimethoxy-β-phenethylamine hydrochloride



Mol. Formula :	$C_{10}H_{16}ClNO_2$	**FW :**	217.69	**HBA:**	3	**HBD:**	1	**RotB:**	4
PubChem ID :	24187012	**CASRN :**	3166-74-3			**logP:**	1.07	**TPSA:**	46.1

NIMH Code : P-526

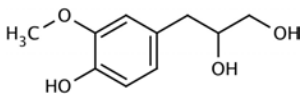
Compound name : 3-Hydroxy-4-methoxy-(±)-phenylalanine



Mol. Formula :	$C_{10}H_{13}NO_4$	**FW :**	211.21	**HBA:**	5	**HBD:**	3	**RotB:**	4
PubChem ID :	586369	**CASRN :**	4368-01-8			**logP:**	-1.65	**TPSA:**	97.2

NIMH Code : P-528

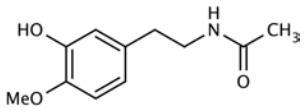
Compound name : Vanillyl glycol



Mol. Formula :	$C_{16}H_{26}N_2O_4$	**FW :**	198.22	**HBA:**	4	**HBD:**	3	**RotB:**	4
PubChem ID :	161566	**CASRN :**	27391-18-0			**logP:**	0.40	**TPSA:**	69.9
Activity:	Lignin model compound.								

NIMH Code : P-701

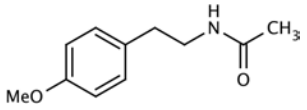
Compound name : N-Acetyl-3-hydroxy-4-methoxy-β-phenethylamine



Mol. Formula :	$C_{11}H_{15}NO_3$	**FW :**	209.24	**HBA:**	4	**HBD:**	2	**RotB:**	4
PubChem ID :	591256	**CASRN :**				**logP:**	0.75	**TPSA:**	58.6

NIMH Code : P-703

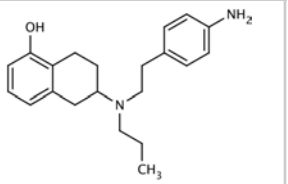
Compound name : N-Acetyl-4-methoxy-β-phenethylamine



Mol. Formula :	$C_{11}H_{15}NO_2$	**FW :**	193.24	**HBA:**	3	**HBD:**	1	**RotB:**	4
PubChem ID :	584258	**CASRN :**				**logP:**	1.05	**TPSA:**	38.3

NIMH Code : P-706

Compound name : (±)-2-[*N*-(4'-Aminophenylethyl)-*N*-propyl]amino-5-hydroxytetralin dihydrochloride

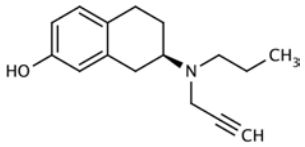


Mol. Formula : $C_{21}H_{30}Cl_2N_2O$ **FW :** 397.38 **HBA:** 3 **HBD:** 2 **RotB:** 6

PubChem ID : **CASRN :** **logP:** 3.54 **TPSA:** 50.7

NIMH Code : P-707

Compound name : (*R*)-(+)-2-(*N*-Propargyl-*N*-propyl)amino-7-hydroxytetralin hydrochloride



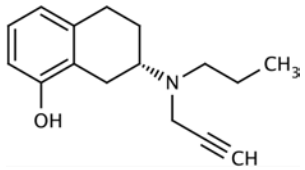
Mol. Formula : $C_{16}H_{22}ClNO$ **FW :** 279.81 **HBA:** 2 **HBD:** 1 **RotB:** 4

PubChem ID : 9992020 **CASRN :** **logP:** 3.31 **TPSA:** 24.7

Activity: Radiolabeling (*R*)-(+)-7-hydroxy-DPAT precursor.

NIMH Code : P-708

Compound name : (*R*)-(–)-2-(*N*-Propargyl-*N*-propyl)amino-8-hydroxytetralin hydrochloride



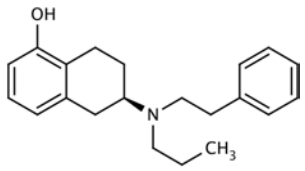
Mol. Formula : $C_{16}H_{22}ClNO$ **FW :** 279.81 **HBA:** 2 **HBD:** 1 **RotB:** 4

PubChem ID : **CASRN :** **logP:** 3.34 **TPSA:** 24.7

Activity: Radiolabeling (*R*)-(+)-8-hydroxy-DPAT precursor.

NIMH Code : P-709

Compound name : (*S*)-(–)-2-(*N*-Phenylethyl-*N*-propyl)amino-5-hydroxytetralin hydrochloride

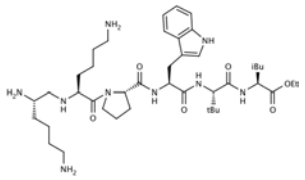


Mol. Formula : $C_{21}H_{28}ClNO$ **FW :** 345.91 **HBA:** 2 **HBD:** 1 **RotB:** 6

PubChem ID : **CASRN :** **logP:** 4.40 **TPSA:** 24.7

NIMH Code : P-710

Compound name : PD149163



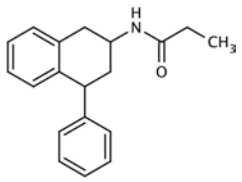
Mol. Formula : $C_{52}H_{76}F_{15}N_9O_{16}$ **FW :** 1368.19 **HBA:** 15 **HBD:** 7 **RotB:** 26

PubChem ID : **CASRN :** **logP:** 2.11 **TPSA:** 244.7

Activity: Neurotensin agonist.

NIMH Code : P-801

Compound name : (±)-4-Phenyl-2-(propioamido)tetraline



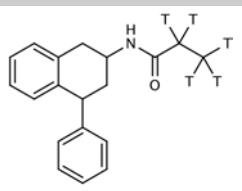
Mol. Formula : $C_{19}H_{21}NO$ **FW :** 279.38 **HBA:** 2 **HBD:** 1 **RotB:** 3

PubChem ID : 3976006 **CASRN :** 0 **logP:** 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



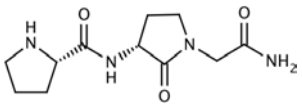
Mol. Formula : $C_{19}H_{21}NO$ **FW :** 289.42 **HBA:** 2 **HBD:** 1 **RotB:** 3

PubChem ID : 10708579 **CASRN :** **logP:** 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



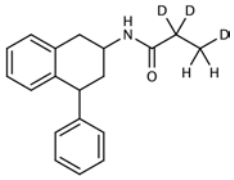
Mol. Formula : $C_{11}H_{18}N_4O_3$ **FW :** 254.29 **HBA:** 7 **HBD:** 3 **RotB:** 4

PubChem ID : 129409 **CASRN :** 106732-52-9 **logP:** -2.79 **TPSA:** 109.1

Activity: MSH release-inhibiting hormone antagonist.

NIMH Code : P-804

Compound name : (±)-4-Phenyl-2-[2',2',3'-^{2}H]-(propioamido)tetralin



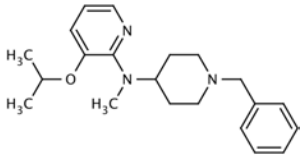
Mol. Formula : $C_{19}H_{18}D_3NO$ **FW :** 282.39 **HBA:** 2 **HBD:** 1 **RotB:** 3

PubChem ID : 3976006 **CASRN :** 134865-74-0 **logP:** 3.87 **TPSA:** 29.1

Activity: Deuterated melatonin receptor antagonist.

NIMH Code : P-805

Compound name : PNU-101,958



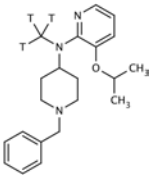
Mol. Formula : $C_{21}H_{31}Cl_2N_3O$ **FW :** 412.40 **HBA:** 4 **HBD:** 0 **RotB:** 6

PubChem ID : 5615 **CASRN :** 170856-57-2 **logP:** 3.83 **TPSA:** 29.8

Activity: Dopamine D_4 antagonist.

NIMH Code : P-901

Compound name : [^{3}H]PNU-101,958



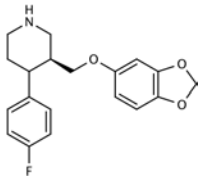
Mol. Formula : $C_{21}H_{29}N_3O$ **FW :** 345.50 **HBA:** 4 **HBD:** 0 **RotB:** 6

PubChem ID : **CASRN :** **logP:** 3.83 **TPSA:** 29.8

Activity: Radiolabeled D_4 receptor antagonist.

NIMH Code : P-902

Compound name : Paroxetine hydrochloride



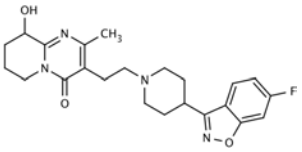
Mol. Formula : $C_{19}H_{21}ClFNO_3$ **FW :** 365.83 **HBA:** 4 **HBD:** 1 **RotB:** 4

PubChem ID : 62878 **CASRN :** 61869-08-7 **logP:** 3.15 **TPSA:** 44.3

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)



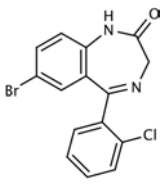
Mol. Formula : $C_{23}H_{27}FN_4O_3$ **FW :** 426.48 **HBA:** 7 **HBD:** 1 **RotB:** 4

PubChem ID : 115237 **CASRN :** 144598-75-4 **logP:** 1.76 **TPSA:** 83.4

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)



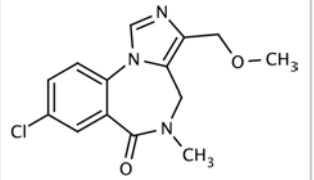
Mol. Formula : $C_{15}H_{10}BrClN_2O$ **FW :** 349.61 **HBA:** 3 **HBD:** 1 **RotB:** 1

PubChem ID : 40113 **CASRN :** 51753-57-2 **logP:** 3.98 **TPSA:** 41.5

Activity: $GABA_A$ receptor allosteric modulator.

NIMH Code : P-905

Compound name : PWZ-029

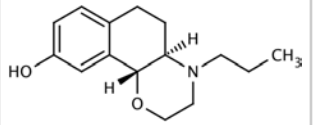


Mol. Formula :	$C_{14}H_{14}ClN_3O_2$	**FW :**	291.73	**HBA:**	5	**HBD:**	0	**RotB:**	2
PubChem ID :	9971547	**CASRN :**	164025-33-6			**logP:**	0.31	**TPSA:**	47.4

Activity: $GABA_A$ inverse agonist.

NIMH Code : P-906 new

Compound name : (+)-(4a*R*,10b*R*)-3,4,4a,5,6,10b-Hexahydro-4-propyl-2*H*-naphth[1,2-b]-1,4-oxazin-9-ol hydrochloride ((+)-PHNO hydrochloride; Naxagolide)

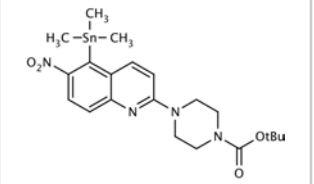


Mol. Formula :	$C_{15}H_{22}ClNO_2$	**FW :**	283.79	**HBA:**	3	**HBD:**	1	**RotB:**	2
PubChem ID :	57533	**CASRN :**	99705-65-4			**logP:**	2.88	**TPSA:**	36.7

Activity: Dopamine D2 receptor agonist.

NIMH Code : Q-707

Compound name : N-(*tert*-Butyloxycarbonyl)-6-nitro-5-(trimethylstannyl)quipazine

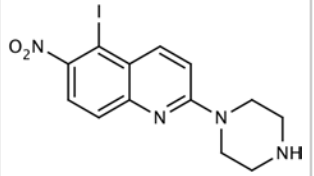


Mol. Formula :	$C_{21}H_{30}N_4O_4Sn$	**FW :**	521.20	**HBA:**	8	**HBD:**	0	**RotB:**	5
PubChem ID :		**CASRN :**				**logP:**	3.40	**TPSA:**	91.5

Activity: Serotonin uptake inhibitor radioiodination precursor.

NIMH Code : Q-708

Compound name : 5-Iodo-6-nitroquipazine

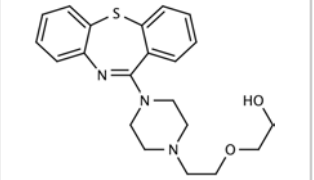


Mol. Formula :	$C_{13}H_{13}IN_4O_2$	**FW :**	384.17	**HBA:**	6	**HBD:**	1	**RotB:**	2
PubChem ID :	10091399	**CASRN :**	139593-11-6			**logP:**	3.17	**TPSA:**	78.6

Activity: Serotonin uptake inhibitor.

NIMH Code : Q-901

Compound name : Quetiapine

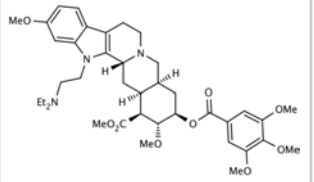


Mol. Formula :	$C_{21}H_{25}N_3O_2S$	**FW :**	499.58	**HBA:**	5	**HBD:**	1	**RotB:**	5
PubChem ID :	5002	**CASRN :**	111974-69 -7			**logP:**	2.81	**TPSA:**	48.3

Activity: Dopamine, serotonin, & adrenergic antagonist; antihistaminic.

NIMH Code : R-501

Compound name : 1-(β-Diethylamino)ethylreserpine dipicrate

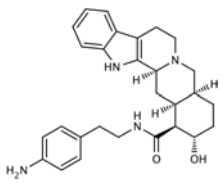


Mol. Formula :	12	**FW :**	1166.06	**HBA:**	12	**HBD:**	0	**RotB:**	15
PubChem ID :	65518	**CASRN :**	229.1039			**logP:**	4.49	**TPSA:**	112.6

Activity: Hypotensive agent.

NIMH Code : R-701

Compound name : 17α-Hydroxy-20α-yohimban-16β-(N-4-aminophenylethyl)carboxamide dihydrochloride

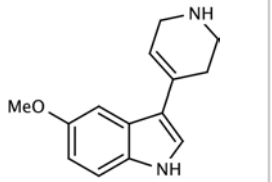


Mol. Formula :	$C_{28}H_{36}Cl_2N_4O_2$	**FW :**	531.52	**HBA:**	6	**HBD:**	3	**RotB:**	4
PubChem ID :		**CASRN :**	4			**logP:**	2.55	**TPSA:**	94.4

Activity: Adrenergic α2 ligand radioiodination precursor.

NIMH Code : R-702

Compound name : RU-24969



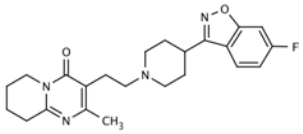
Mol. Formula : $C_{16}H_{19}N_2O_3$ **FW :** 574.67 **HBA:** 3 **HBD:** 1 **RotB:** 2

PubChem ID : 108029 **CASRN :** 107008-28-6 **logP:** 1.91 **TPSA:** 41.6

Activity: Serotonin 5-$HT_{1A/1B}$ agonist.

NIMH Code : R-901

Compound name : Risperidone



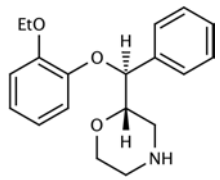
Mol. Formula : $C_{23}H_{27}FN_4O_2$ **FW :** 410.48 **HBA:** 6 **HBD:** 0 **RotB:** 4

PubChem ID : 5073 **CASRN :** 106266-06-2 **logP:** 2.63 **TPSA:** 63.1

Activity: Serotonin & dopamine antagonist.

NIMH Code : R-902

Compound name : (±)-Reboxetine mesylate



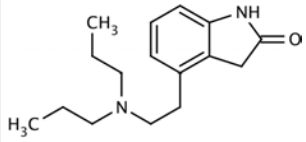
Mol. Formula : $C_{20}H_{27}NO_6S$ **FW :** 409.50 **HBA:** 4 **HBD:** 1 **RotB:** 6

PubChem ID : 5311403 **CASRN :** 98769-81-4 **logP:** 3.28 **TPSA:** 44.3

Activity: Norepinephrine reuptake inhibitor.

NIMH Code : R-903

Compound name : Ropinirole hydrochloride



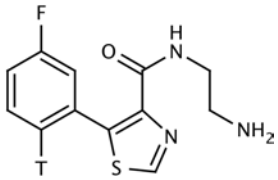
Mol. Formula : $C_{16}H_{24}N_2O$ **FW :** 296.84 **HBA:** 3 **HBD:** 1 **RotB:** 7

PubChem ID : 68727 **CASRN :** 91374-21-9 **logP:** 3.06 **TPSA:** 33.5

Activity: Dopamine D_2, D_3 & D_4 receptor agonist.

NIMH Code : R-904

Compound name : [^{3}H]Ro 41-1049



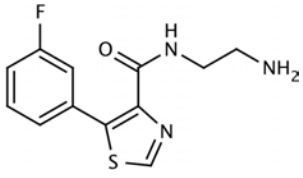
Mol. Formula : $C_{12}H_{12}FN_3OS$ **FW :** 267.32 **HBA:** 4 **HBD:** 2 **RotB:** 4

PubChem ID : **CASRN :** **logP:** 1.08 **TPSA:** 69.6

Activity: Radiolabeled MAO inhibitor.

NIMH Code : R-905

Compound name : Ro 41-1049 hydrochloride



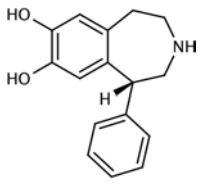
Mol. Formula : $C_{12}H_{13}ClFN_3OS$ **FW :** 301.77 **HBA:** 4 **HBD:** 2 **RotB:** 4

PubChem ID : 5311308 **CASRN :** 127500-84-9 **logP:** 1.08 **TPSA:** 69.6

Activity: MAO inhibitor.

NIMH Code : S-101

Compound name : (*R*)-(+)-SKF-38393 hydrochloride



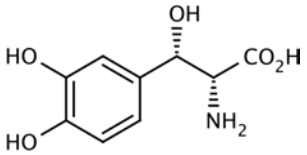
Mol. Formula : $C_{16}H_{18}ClNO_2$ **FW :** 291.77 **HBA:** 3 **HBD:** 3 **RotB:** 1

PubChem ID : 6852375 **CASRN :** 62751-59-1 **logP:** 1.88 **TPSA:** 57.1

Activity: Dopamine D_1 receptor agonist; active enantiomer of (±)-SKF-38393.

NIMH Code : S-501

Compound name : (+)-*threo*-3-(3,4-Dihydroxyphenyl)serine

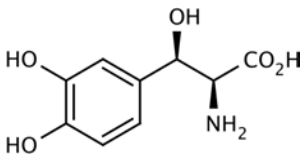


Mol. Formula : $C_9H_{11}NO_5$ **FW :** 213.19 **HBA:** 6 **HBD:** 5 **RotB:** 3

PubChem ID : 443940 **CASRN :** 23651-95-8 **logP:** -2.71 **TPSA:** 128.5

NIMH Code : S-502

Compound name : (–)-*threo*-3-(3,4-Dihydroxyphenyl)serine

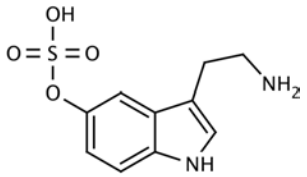


Mol. Formula : $C_9H_{11}NO_5$ **FW :** 213.19 **HBA:** 6 **HBD:** 5 **RotB:** 3

PubChem ID : 164631 **CASRN :** 13147-26-7 **logP:** -2.71 **TPSA:** 128.5

NIMH Code : S-503

Compound name : Serotonin-*O*-sulfate

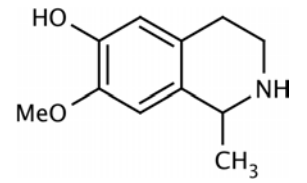


Mol. Formula : $C_{10}H_{12}N_2O_4S$ **FW :** 256.28 **HBA:** 6 **HBD:** 2 **RotB:** 4

PubChem ID : 152151 **CASRN :** 16310-20-6 **logP:** -0.30 **TPSA:** 109.9

NIMH Code : S-504

Compound name : (±)-Salsoline hydrochloride



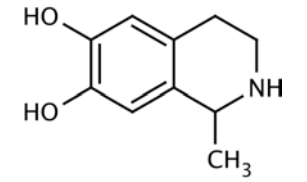
Mol. Formula : $C_{11}H_{16}ClNO_2$ **FW :** 229.70 **HBA:** 3 **HBD:** 2 **RotB:** 1

PubChem ID : 46695 **CASRN :** 89-31-6 **logP:** 1.14 **TPSA:** 46.1

Activity: Salsolinol metabolite; endogenous neurotoxin.

NIMH Code : S-505

Compound name : (±)-Salsolinol hydrochloride



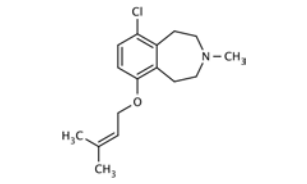
Mol. Formula : $C_{10}H_{14}ClNO_2$ **FW :** 215.68 **HBA:** 3 **HBD:** 3 **RotB:** 0

PubChem ID : 54456 **CASRN :** 525-72-4 **logP:** 0.96 **TPSA:** 57.1

Activity: Dopamine neurotoxic derivative.

NIMH Code : S-701

Compound name : SKF-104078



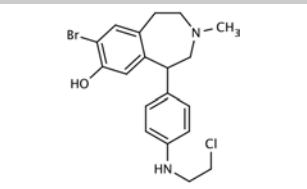
Mol. Formula : $C_{20}H_{26}ClNO_5$ **FW :** 395.88 **HBA:** 2 **HBD:** 0 **RotB:** 3

PubChem ID : 122295 **CASRN :** 110857-22-2 **logP:** 4.05 **TPSA:** 13.7

Activity: Adrenergic α2 antagonist.

NIMH Code : S-703

Compound name : (±)-4'-(2-Chloroethylamino)-SKF-83566 dihydrobromide



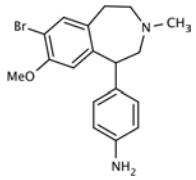
Mol. Formula : $C_{19}H_{24}Br_3ClN_2O$ **FW :** 571.57 **HBA:** 3 **HBD:** 2 **RotB:** 4

PubChem ID : **CASRN :** **logP:** 3.70 **TPSA:** 36.7

Activity: Dopamine D_1 receptor alkylating ligand.

NIMH Code : S-704

Compound name : (±)-4'-Amino-8-*O*-methyl-SKF-83566



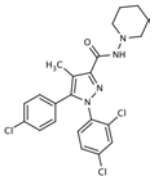
Mol. Formula : $C_{18}H_{21}BrN_2O$ **FW :** 361.28 **HBA:** 3 **HBD:** 1 **RotB:** 2

PubChem ID : **CASRN :** **logP:** 3.52 **TPSA:** 39.7

Activity: Dopamine D1 receptor precursor alkylating ligand (antagonist).

NIMH Code : S-705

Compound name : SR 141716



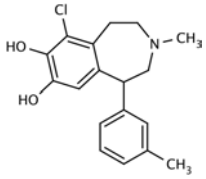
Mol. Formula : $C_{22}H_{21}Cl_3N_4O$ **FW :** 463.79 **HBA:** 5 **HBD:** 1 **RotB:** 4

PubChem ID : 104850 **CASRN :** 158681-13-1 **logP:** 5.91 **TPSA:** 50.2

Activity: Cannabinoid CB_1 receptor inverse agonist.

NIMH Code : S-706

Compound name : SKF-83959 hydrobromide



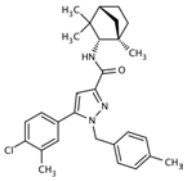
Mol. Formula : $C_{18}H_{21}BrClNO_2$ **FW :** 398.72 **HBA:** 3 **HBD:** 2 **RotB:** 1

PubChem ID : 133538 **CASRN :** 80751-85-5 **logP:** 3.46 **TPSA:** 44.9

Activity: Dopamine D_1 receptor agonist.

NIMH Code : S-801

Compound name : SR 144528



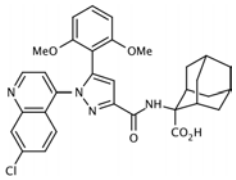
Mol. Formula : $C_{29}H_{34}ClN_3O$ **FW :** 476.05 **HBA:** 4 **HBD:** 1 **RotB:** 5

PubChem ID : 3081355 **CASRN :** 192703-06 -3 **logP:** 7.45 **TPSA:** 46.9

Activity: Cannabinoid CB_2 receptor antagonist.

NIMH Code : S-802

Compound name : SR 48692



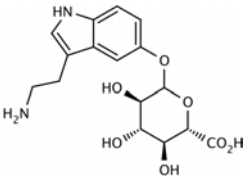
Mol. Formula : $C_{32}H_{31}ClN_4O_5$ **FW :** 587.07 **HBA:** 9 **HBD:** 2 **RotB:** 6

PubChem ID : 119192 **CASRN :** 146362-70-1 **logP:** 3.85 **TPSA:** 118.4

Activity: Neurotensin NT_1 antagonist.

NIMH Code : S-803

Compound name : Serotonin-*O*-β-D-glucuronide

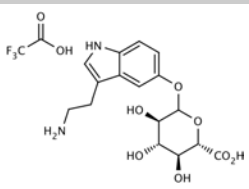


Mol. Formula : $C_{16}H_{20}N_2O_7$ **FW :** 352.34 **HBA:** 9 **HBD:** 5 **RotB:** 5

PubChem ID : **CASRN :** **logP:** -3.03 **TPSA:** 162.7

NIMH Code : S-803A

Compound name : Serotonin-*O*-β-D-glucuronide trifluoroacetate

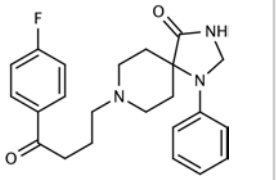


Mol. Formula : $C_{18}H_{21}F_3N_2O_9$ **FW :** 580.39 **HBA:** 11 **HBD:** 6 **RotB:** 6

PubChem ID : **CASRN :** **logP:** -3.03 **TPSA:** 162.7

NIMH Code : S-901

Compound name : Spiperone



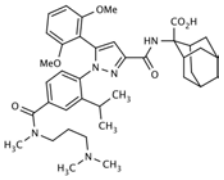
Mol. Formula : $C_{23}H_{26}FN_3O_2$ **FW :** 395.47 **HBA:** 5 **HBD:** 1 **RotB:** 6

PubChem ID : 5265 **CASRN :** 749-02-0 **logP:** 3.07 **TPSA:** 53.9

Activity: Serotonin 5-HT_{1A}, 5-HT_{2A}, 5-HT_7, & dopamine D_2 antagonist.

NIMH Code : S-902

Compound name : SR 142948



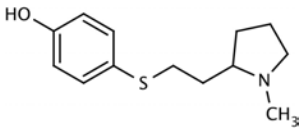
Mol. Formula : $C_{39}H_{52}ClN_5O_6$ **FW :** 722.31 **HBA:** 11 **HBD:** 2 **RotB:** 12

PubChem ID : 5311451 **CASRN :** 184162-64-9 **logP:** 2.54 **TPSA:** 130.3

Activity: Neurotensin receptor antagonist.

NIMH Code : S-903

Compound name : SIB-1553A



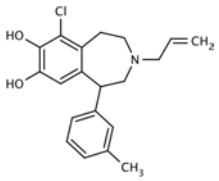
Mol. Formula : $C_{13}H_{20}ClNOS$ **FW :** 273.82 **HBA:** 2 **HBD:** 1 **RotB:** 4

PubChem ID : 9881989 **CASRN :** **logP:** 1.93 **TPSA:** 24.7

Activity: Nicotinic acetylcholine receptor agonist; possible cognitive enhancer.

NIMH Code : S-904

Compound name : SKF-83822 hydrobromide



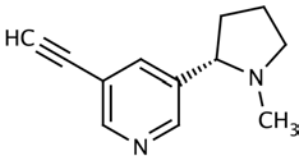
Mol. Formula : $C_{20}H_{23}BrClNO_2$ **FW :** 424.76 **HBA:** 3 **HBD:** 2 **RotB:** 3

PubChem ID : 10020353 **CASRN :** 74115-08-5 **logP:** 4.45 **TPSA:** 47.7

Activity: Dopamine D_1 receptor agonist.

NIMH Code : S-905

Compound name : SIB-1508Y



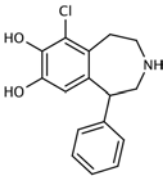
Mol. Formula : $C_{16}H_{18}N_2O_4$ **FW :** 302.33 **HBA:** 2 **HBD:** 0 **RotB:** 1

PubChem ID : 10968648 **CASRN :** 192231-16 -6 **logP:** 1.31 **TPSA:** 17.3

Activity: Neuronal nicotinic acetylcholine receptor agonist.

NIMH Code : S-906

Compound name : SKF-81297 hydrobromide



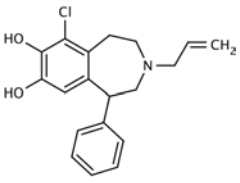
Mol. Formula : $C_{16}H_{17}BrClNO_2$ **FW :** 370.67 **HBA:** 3 **HBD:** 3 **RotB:** 1

PubChem ID : 11957706 **CASRN :** 71636-61-8 **logP:** 2.26 **TPSA:** 57.1

Activity: Dopamine D_1 receptor agonist.

NIMH Code : S-907

Compound name : SKF-82958 hydrobromide



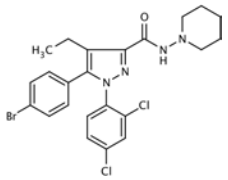
Mol. Formula : $C_{19}H_{21}BrClNO_2$ **FW :** 410.73 **HBA:** 3 **HBD:** 2 **RotB:** 3

PubChem ID : 9909521 **CASRN :** 80751-65-1 **logP:** 3.93 **TPSA:** 47.7

Activity: Dopamine D_1 receptor agonist.

NIMH Code : S-908

Compound name : SR 147778



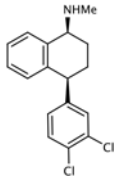
Mol. Formula : $C_{23}H_{22}BrCl_2N_4O$ **FW :** 522.27 **HBA:** 5 **HBD:** 1 **RotB:** 5

PubChem ID : 9849616 **CASRN :** 288104-79-0 **logP:** 6.52 **TPSA:** 50.2

Activity: Cannaboid CB_1 receptor antagonist.

NIMH Code : S-909

Compound name : Sertraline hydrochloride



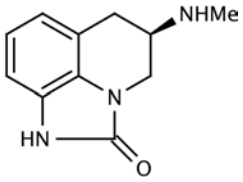
Mol. Formula : $C_{17}H_{18}Cl_3N$ **FW :** 342.69 **HBA:** 1 **HBD:** 1 **RotB:** 2

PubChem ID : 63009 **CASRN :** 79617-96-2 **logP:** 5.15 **TPSA:** 16.6

Activity: Serotonin reuptake inhibitor; used to treat depression and OCD.

NIMH Code : S-910

Compound name : Sumanirole maleate



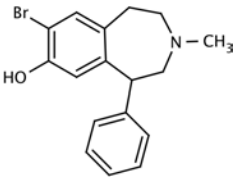
Mol. Formula : $C_{15}H_{17}N_3O_5$ **FW :** 319.31 **HBA:** 4 **HBD:** 1 **RotB:** 1

PubChem ID : 177343 **CASRN :** 179386-43 -7 **logP:** 0.93 **TPSA:** 49.0

Activity: Dopamine D2 receptor ligand.

NIMH Code : S-911

Compound name : SKF-83566 HBr



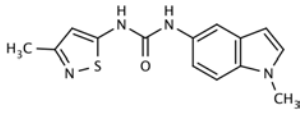
Mol. Formula : $C_{17}H_{19}Br_2NO$ **FW :** 413.15 **HBA:** 2 **HBD:** 1 **RotB:** 1

PubChem ID : 1243 **CASRN :** 99295-33-7 **logP:** 3.60 **TPSA:** 24.7

Activity: Dopamine D2 receptor antagonist.

NIMH Code : S-912

Compound name : *N*-(1-Methyl-1*H*-indol-5-yl)-N'-(3-methylisothiazol-5-yl)urea (SB 204741)



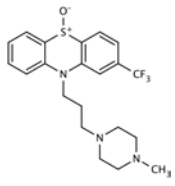
Mol. Formula : $C_{14}H_{14}N_4OS$ **FW :** 286.35 **HBA:** 5 **HBD:** 2 **RotB:** 2

PubChem ID : 3277600 **CASRN :** 152239-46-8 **logP:** 2.71 **TPSA:** 59.0

Activity: 5-HT_{2B} receptor antagonist.

NIMH Code : T-501

Compound name : Trifluoperazine-5-oxide

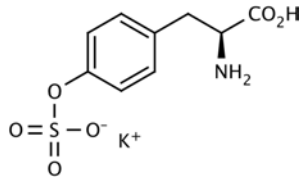


Mol. Formula : $C_{21}H_{24}F_3N_3OS$ **FW :** 423.50 **HBA:** 4 **HBD:** 0 **RotB:** 5

PubChem ID : 159622 **CASRN :** 1549-88-8 **logP:** 3.28 **TPSA:** 28.0

NIMH Code : T-502

Compound name : (–)-Tyrosine-*O*-sulfate potassium salt

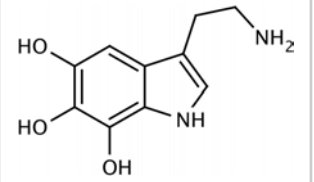


Mol. Formula : $C_9H_{10}NO_6SK$ **FW :** 299.34 **HBA:** 7 **HBD:** 2 **RotB:** 5

PubChem ID : 514186 **CASRN :** **logP:** -0.74 **TPSA:** 134.2

NIMH Code : T-503

Compound name : 5,6,7-Trihydroxytryptamine creatinine sulfate

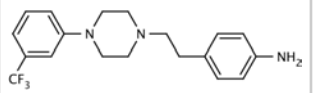


Mol. Formula : $C_{14}H_{21}N_5O_8S$ **FW :** 321.33 **HBA:** 9 **HBD:** 6 **RotB:** 2

PubChem ID : **CASRN :** **logP:** -0.31 **TPSA:** 104.1

NIMH Code : T-504

Compound name : 1-[2-(4-Aminophenyl)ethyl]-4-(3-trifluoromethylphenyl)piperazine dihydrochloride



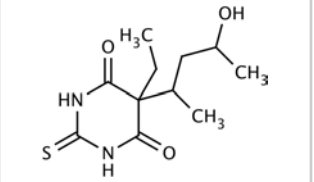
Mol. Formula : $C_{19}H_{24}Cl_2F_3N_3$ **FW :** 422.32 **HBA:** 3 **HBD:** 1 **RotB:** 5

PubChem ID : 121930 **CASRN :** 1814-64-8 **logP:** 3.99 **TPSA:** 33.7

Activity: Serotonin 5-HT_{1A} receptor agonist.

NIMH Code : T-506

Compound name : 5-Ethyl-5-(1'-methyl-3'-hydroxybutyl)-2-thiobarbituric acid



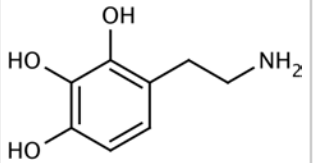
Mol. Formula : $C_{11}H_{18}N_2O_3S$ **FW :** 258.34 **HBA:** 5 **HBD:** 3 **RotB:** 4

PubChem ID : **CASRN :** **logP:** 1.32 **TPSA:** 75.6

Activity: Thiopental metabolite.

NIMH Code : T-507

Compound name : 2,3,4-Trihydroxy-β-phenethylamine hydrochloride



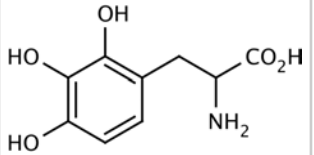
Mol. Formula : $C_8H_{12}ClNO_3$ **FW :** 205.64 **HBA:** 4 **HBD:** 4 **RotB:** 2

PubChem ID : 193386 **CASRN :** 4228-71-1 **logP:** -0.25 **TPSA:** 88.3

Activity: Arylsulfatase inhibitor; potential neurotoxin.

NIMH Code : T-508

Compound name : 2,3,4-Trihydroxy-(±)-phenylalanine



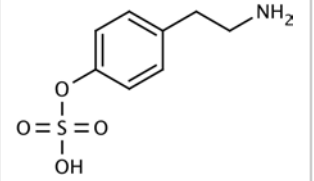
Mol. Formula : $C_9H_{11}NO_5$ **FW :** 213.19 **HBA:** 6 **HBD:** 5 **RotB:** 3

PubChem ID : 22326275 **CASRN :** **logP:** -2.10 **TPSA:** 128.5

Activity: Neurotoxic DOPA metabolite.

NIMH Code : T-509

Compound name : Tyramine-*O*-sulfate

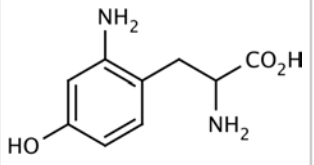


Mol. Formula : $C_8H_{11}NO_4S$ **FW :** 217.24 **HBA:** 5 **HBD:** 2 **RotB:** 4

PubChem ID : 153005 **CASRN :** 30223-92-8 **logP:** -0.40 **TPSA:** 94.1

NIMH Code : T-510

Compound name : 2-Amino-(±)-Tyrosine

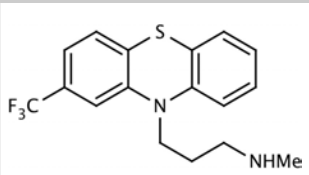


Mol. Formula : $C_9H_{12}N_2O_3$ **FW :** 196.20 **HBA:** 5 **HBD:** 4 **RotB:** 3

PubChem ID : 5134354 **CASRN :** **logP:** -2.32 **TPSA:** 114.0

NIMH Code : T-511

Compound name : N-Desmethyltriflupromazine hydrochloride

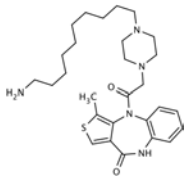


Mol. Formula : $C_{17}H_{18}ClF_3N_2S$ **FW :** 374.85 **HBA:** 2 **HBD:** 1 **RotB:** 5

PubChem ID : 10337209 **CASRN :** **logP:** 4.43 **TPSA:** 19.9

NIMH Code : T-701

Compound name : Telenzepine Amine Congener (TAC) dihydrobromide



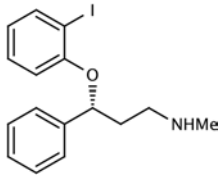
Mol. Formula : $C_{28}H_{43}Br_2N_5O_2S$ **FW :** 673.55 **HBA:** 7 **HBD:** 2 **RotB:** 12

PubChem ID : 9892600 **CASRN :** **logP:** 3.82 **TPSA:** 84.7

Activity: Muscarinic M_1 antagonist analog.

NIMH Code : T-702

Compound name : (*R*)-(–)-*N*-Methyl-3-(2-iodophenoxy)-3-phenylpropanamine hydrochloride



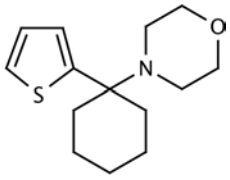
Mol. Formula : $C_{16}H_{19}ClINO$ **FW :** 403.69 **HBA:** 2 **HBD:** 1 **RotB:** 6

PubChem ID : 10021849 **CASRN :** **logP:** 4.22 **TPSA:** 25.8

Activity: Norepinephrine transport inhibitor.

NIMH Code : T-703

Compound name : 1-[1-(2-Thienyl)cyclohexyl]morpholine



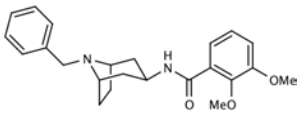
Mol. Formula : $C_{14}H_{21}NOS$ **FW :** 251.39 **HBA:** 2 **HBD:** 0 **RotB:** 2

PubChem ID : 210739 **CASRN :** 21602-66-4 **logP:** 3.33 **TPSA:** 13.7

Activity: PCP analog.

NIMH Code : T-704

Compound name : Tropapride hydrochloride



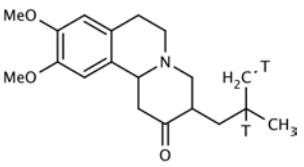
Mol. Formula : $C_{23}H_{29}ClN_2O_3$ **FW :** 416.94 **HBA:** 5 **HBD:** 1 **RotB:** 6

PubChem ID : 3065827 **CASRN :** 109021-66-1 **logP:** 3.01 **TPSA:** 52.0

Activity: Dopamine D_2 receptor antagonist.

NIMH Code : T-801

Compound name : [^{3}H]Tetrabenazine



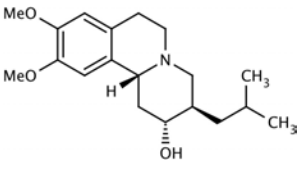
Mol. Formula : $C_{19}H_{27}NO_3$ **FW :** 321.44 **HBA:** 4 **HBD:** 0 **RotB:** 4

PubChem ID : 6018 **CASRN :** 0 **logP:** 3.40 **TPSA:** 40.0

Activity: Radiolabeled adrenergic uptake inhibitor.

NIMH Code : T-802

Compound name : (+)-α-Dihydrotetrabenazine



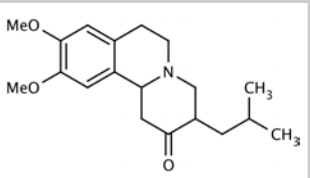
Mol. Formula : $C_{19}H_{29}NO_3$ **FW :** 319.44 **HBA:** 4 **HBD:** 1 **RotB:** 4

PubChem ID : 123836 **CASRN :** 4 **logP:** 2.67 **TPSA:** 43.1

Activity: Active metabolite of tetrabenazine.

NIMH Code : T-901

Compound name : (±)-Tetrabenazine



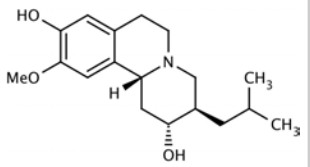
Mol. Formula : $C_{19}H_{27}NO_3$ **FW :** 317.42 **HBA:** 4 **HBD:** 0 **RotB:** 4

PubChem ID : 6018 **CASRN :** 58-46-8 **logP:** 3.40 **TPSA:** 40.0

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



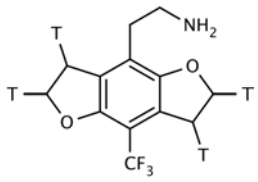
Mol. Formula : $C_{18}H_{27}NO_3$ **FW :** 305.41 **HBA:** 4 **HBD:** 2 **RotB:** 3

PubChem ID : **CASRN :** 4 **logP:** 2.41 **TPSA:** 57.0

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

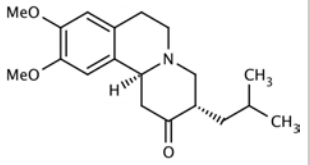


Mol. Formula : $C_{13}H_{14}F_3NO_2$ **FW :** 281.28 **HBA:** 3 **HBD:** 1 **RotB:** 3

PubChem ID : **CASRN :** **logP:** 2.03 **TPSA:** 46.1

NIMH Code : T-904

Compound name : (–)-Tetrabenazine



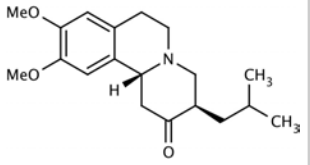
Mol. Formula : $C_{19}H_{27}NO_3$ **FW :** 317.42 **HBA:** 4 **HBD:** 0 **RotB:** 4

PubChem ID : 667453 **CASRN :** 0 **logP:** 3.40 **TPSA:** 40.0

Activity: Dopamine depleting agent; optical isomer of tetrabenazine.

NIMH Code : T-905

Compound name : (+)-Tetrabenazine



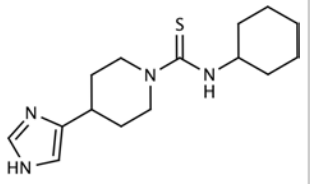
Mol. Formula : $C_{19}H_{27}NO_3$ **FW :** 317.42 **HBA:** 4 **HBD:** 0 **RotB:** 4

PubChem ID : 11634155 **CASRN :** 0 **logP:** 3.40 **TPSA:** 40.0

Activity: Dopamine depleting agent; optical isomer of tetrabenazine.

NIMH Code : T-906

Compound name : Thioperamide maleate



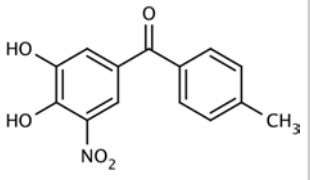
Mol. Formula : $C_{15}H_{24}N_4S$ **FW :** 408.52 **HBA:** 4 **HBD:** 1 **RotB:** 2

PubChem ID : 3035905 **CASRN :** 106243-16-7 **logP:** 2.28 **TPSA:** 44.0

Activity: Histamine H_3 antagonist; anticonvulsant.

NIMH Code : T-907

Compound name : Tolcapone



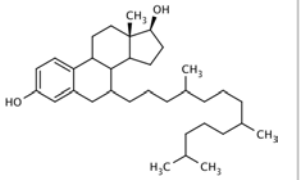
Mol. Formula : $C_{14}H_{11}NO_5$ **FW :** 273.24 **HBA:** 6 **HBD:** 2 **RotB:** 3

PubChem ID : 4659569 **CASRN :** 134308-13-7 **logP:** 3.28 **TPSA:** 106.2

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

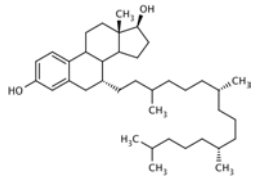


Mol. Formula : $C_{34}H_{56}O_2$ **FW :** 496.81 **HBA:** 2 **HBD:** 2 **RotB:** 12

PubChem ID : **CASRN :** **logP:** 10.23 **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

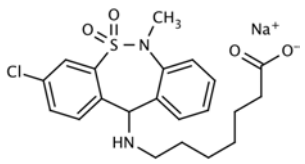


Mol. Formula : $C_{38}H_{64}O_2$ **FW :** 552.91 **HBA:** 2 **HBD:** 2 **RotB:** 15

PubChem ID : **CASRN :** 15 **logP:** 11.85 **TPSA:** 40.5

NIMH Code : T-910

Compound name : Tianeptine, sodium salt



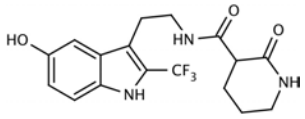
Mol. Formula : $C_{21}H_{24}ClN_2NaO_4S$ **FW :** 458.93 **HBA:** 6 **HBD:** 1 **RotB:** 8

PubChem ID : 23663953 **CASRN :** 30123-17-2 **logP:** 1.53 **TPSA:** 94.1

Activity: Serotonin reuptake enhancer.

NIMH Code : T-911 new

Compound name : *N*-[2-(2-Trifluoromethyl-5-hydroxy-1*H*-indol-3-yl)ethyl]-2-oxopiperidine-3-carboxamide (2-Trifluoromethyl-HIOC)

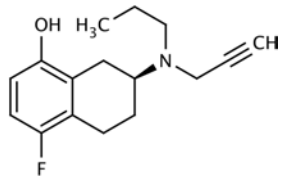


Mol. Formula : $C_{17}H_{18}F_3N_3O_3$ **FW :** 369.34 **HBA:** 6 **HBD:** 3 **RotB:** 5

PubChem ID : - **CASRN :** - **logP:** 1.62 **TPSA:** 94.2

NIMH Code : U-703

Compound name : (*S*)-(–)-*N*-Propargyl-UH-301 hydrochloride



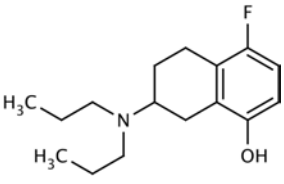
Mol. Formula : $C_{16}H_{21}ClFNO$ **FW :** 297.80 **HBA:** 2 **HBD:** 1 **RotB:** 4

PubChem ID : **CASRN :** **logP:** 3.39 **TPSA:** 24.7

Activity: Serotonin receptor antagonist radiolabel precursor.

NIMH Code : U-801

Compound name : Tritiated UH-301



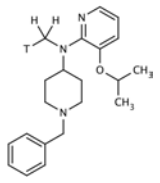
Mol. Formula : $C_{16}H_{24}FNO$ **FW :** 265.37 **HBA:** 2 **HBD:** 1 **RotB:** 5

PubChem ID : 5122 **CASRN :** 127126-21-0 **logP:** 3.38 **TPSA:** 24.7

Activity: Radiolabeled serotonin 5-HT_{1A} receptor antagonist.

NIMH Code : U-802

Compound name : Tritiated U-101,958 [N-methyl-^{3}H]

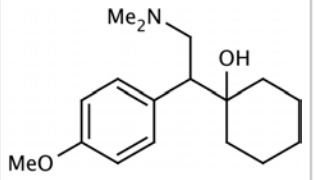


Mol. Formula : $C_{21}H_{29}N_3O$ **FW :** 341.48 **HBA:** 4 **HBD:** 0 **RotB:** 6

PubChem ID : - **CASRN :** - **logP:** 3.83 **TPSA:** 29.8

NIMH Code : V-901

Compound name : Venlafaxine

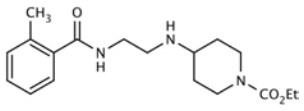


Mol. Formula :	$C_{17}H_{27}NO_2$	**FW :**	277.40	**HBA:**	3	**HBD:**	1	**RotB:**	5
PubChem ID :	5656	**CASRN :**	99300-78-4			**logP:**	2.74	**TPSA:**	33.9

Activity: Serotonin and norepinephrine reuptake inhibitor; antidepressant.

NIMH Code : V-902

Compound name : VU0357017 hydrochloride

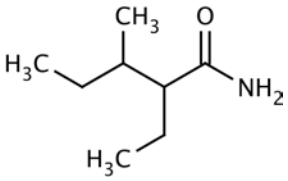


Mol. Formula :	$C_{18}H_{28}ClN_3O_3$	**FW :**	369.89	**HBA:**	6	**HBD:**	2	**RotB:**	7
PubChem ID :	25010775	**CASRN :**				**logP:**	1.43	**TPSA:**	75.3

Activity: Muscarinic M_1 receptor allosteric modulator.

NIMH Code : V-903 new

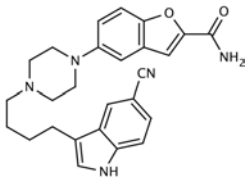
Compound name : 2-Ethyl-3-methylvaleramide (Valnoctamide)



Mol. Formula :	$C_8H_{17}NO$	**FW :**	143.23	**HBA:**	2	**HBD:**	1	**RotB:**	4
PubChem ID :	20140	**CASRN :**	4171-13-5			**logP:**	1.83	**TPSA:**	43.1

NIMH Code : V-904 new

Compound name : 5-{4-[4-(5-Cyano-1*H*-indol-3-yl)butyl]piperazin-1-yl}-1-benzofuran-2-carboxamide dihydrochloride (Vilazodone dihydrochloride)

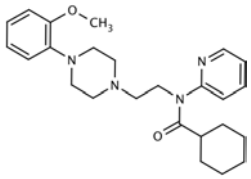


Mol. Formula :	$C_{26}H_{29}Cl_2N_5O_2$	**FW :**	514.45	**HBA:**	7	**HBD:**	1	**RotB:**	7
PubChem ID :	6918314	**CASRN :**	163521-12-8			**logP:**	3.72	**TPSA:**	103.5

Activity: Selective serotonin reuptake inhibitor & 5-HT_{1A} receptor partial agonist.

NIMH Code : W-108

Compound name : WAY-100635 maleate

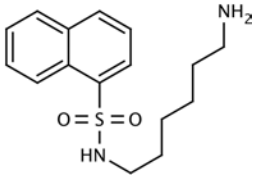


Mol. Formula :	$C_{29}H_{38}N_4O_6$	**FW :**	538.64	**HBA:**	6	**HBD:**	0	**RotB:**	7
PubChem ID :	5684	**CASRN :**	634908-75-1			**logP:**	4.16	**TPSA:**	48.9

Activity: Serotonin 5-HT_{1A} receptor antagonist.

NIMH Code : W-501

Compound name : N-(6-Aminohexyl)-1-napthalenesulfonamide hydrochloride

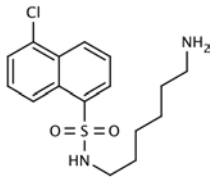


Mol. Formula :	$C_{16}H_{23}ClN_2O_2S$	**FW :**	342.88	**HBA:**	4	**HBD:**	2	**RotB:**	7
PubChem ID :	4314	**CASRN :**	79458-81-4			**logP:**	1.85	**TPSA:**	73.8

Activity: Calmodulin antagonist.

NIMH Code : W-502

Compound name : N-(6-Aminohexyl)-5-chloro-1-napthalenesulfonamide hydrochloride

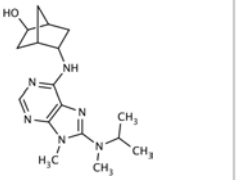


Mol. Formula :	$C_{16}H_{22}Cl_2N_2O_2S$	**FW :**	377.33	**HBA:**	4	**HBD:**	2	**RotB:**	7
PubChem ID :	5681	**CASRN :**	65595-90-6			**logP:**	2.45	**TPSA:**	73.8

Activity: Calmodulin antagonist.

NIMH Code : W-801

Compound name : WRC-0571



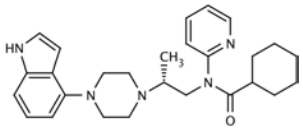
Mol. Formula : $C_{17}H_{26}N_6O$ **FW :** 330.43 **HBA:** 7 **HBD:** 2 **RotB:** 4

PubChem ID : 9902054 **CASRN :** **logP:** 1.79 **TPSA:** 79.1

Activity: Adenosine A_1 receptor antagonist.

NIMH Code : W-901

Compound name : WAY 405



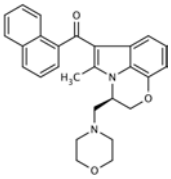
Mol. Formula : $C_{27}H_{37}Cl_2N_5O$ **FW :** 518.52 **HBA:** 6 **HBD:** 0 **RotB:** 6

PubChem ID : **CASRN :** **logP:** 4.84 **TPSA:** 55.5

Activity: Serotonin 5-HT_{1A} receptor antagonist.

NIMH Code : W-902

Compound name : WIN 55212-2 mesylate



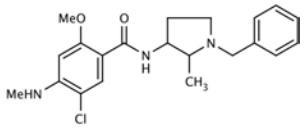
Mol. Formula : $C_{28}H_{30}N_2O_6S$ **FW :** 522.61 **HBA:** 5 **HBD:** 0 **RotB:** 4

PubChem ID : 5689 **CASRN :** 131543-23-2 **logP:** 4.47 **TPSA:** 43.7

Activity: Calcium channel blocker.

NIMH Code : Y-701

Compound name : (±)-YM-09151-2 (Nemonapride)



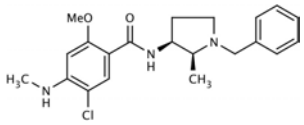
Mol. Formula : $C_{21}H_{26}ClN_3O_2$ **FW :** 387.90 **HBA:** 5 **HBD:** 2 **RotB:** 6

PubChem ID : 4452 **CASRN :** 75272-39-8 **logP:** 3.07 **TPSA:** 54.8

Activity: Dopamine D_2 receptor antagonist; antipsychotic.

NIMH Code : Y-702

Compound name : (–)-YM-09151-2



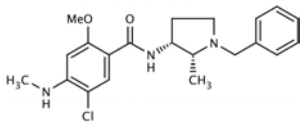
Mol. Formula : $C_{21}H_{26}ClN_3O_2$ **FW :** 387.90 **HBA:** 5 **HBD:** 2 **RotB:** 6

PubChem ID : 156333 **CASRN :** 70325-83-6 **logP:** 3.07 **TPSA:** 54.8

Activity: Inactive stereoisomer of YM-09151-2.

NIMH Code : Y-703

Compound name : (+)-YM-09151-2



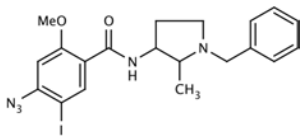
Mol. Formula : $C_{21}H_{26}ClN_3O_2$ **FW :** 387.90 **HBA:** 5 **HBD:** 2 **RotB:** 6

PubChem ID : 9952220 **CASRN :** 70325-83-6 **logP:** 3.07 **TPSA:** 54.8

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



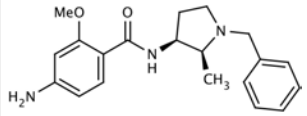
Mol. Formula : $C_{20}H_{23}ClIN_5O_2$ **FW :** 527.79 **HBA:** 7 **HBD:** 1 **RotB:** 6

PubChem ID : **CASRN :** **logP:** 2.04 **TPSA:** 72.2

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



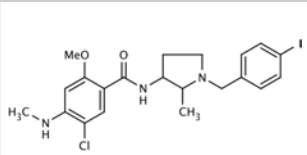
Mol. Formula : $C_{20}H_{25}N_3O_2$ **FW :** 339.43 **HBA:** 5 **HBD:** 2 **RotB:** 5

PubChem ID : **CASRN :** **logP:** 2.17 **TPSA:** 68.8

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



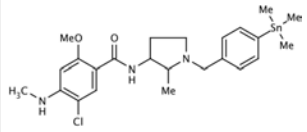
Mol. Formula : $C_{21}H_{25}ClIN_3O_2$ **FW :** 513.80 **HBA:** 5 **HBD:** 2 **RotB:** 6

PubChem ID : **CASRN :** **logP:** 4.00 **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



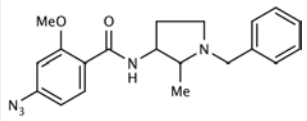
Mol. Formula : $C_{24}H_{34}ClN_3O_2Sn$ **FW :** 550.71 **HBA:** 5 **HBD:** 2 **RotB:** 7

PubChem ID : **CASRN :** **logP:** 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



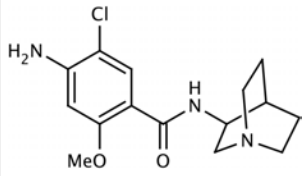
Mol. Formula : $C_{20}H_{24}ClN_5O_2$ **FW :** 401.89 **HBA:** 7 **HBD:** 1 **RotB:** 6

PubChem ID : **CASRN :** **logP:** 1.08 **TPSA:** 72.2

Activity: Reference standard for YM-09151-2 analogs.

NIMH Code : Z-901

Compound name : (±)-Zacopride hydrochloride



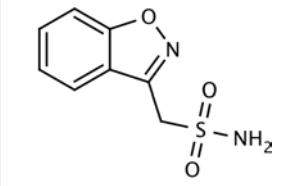
Mol. Formula : $C_{15}H_{21}Cl_2N_3O_2$ **FW :** 346.25 **HBA:** 5 **HBD:** 2 **RotB:** 3

PubChem ID : 108182 **CASRN :** 90182-92-6 **logP:** 1.04 **TPSA:** 68.8

Activity: Serotonin 5-HT_3 receptor antagonist; 5-HT_4 receptor agonist.

NIMH Code : Z-902

Compound name : Zonisamide



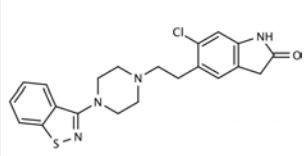
Mol. Formula : $C_8H_8N_2O_3S$ **FW :** 212.23 **HBA:** 5 **HBD:** 1 **RotB:** 2

PubChem ID : 5734 **CASRN :** 68291-97-4 **logP:** 0.11 **TPSA:** 86.2

Activity: Anticonvulsant; antioxidant.

NIMH Code : Z-903

Compound name : Ziprasidone hydrochloride



Mol. Formula : $C_{21}H_{22}Cl_2N_4OS$ **FW :** 449.40 **HBA:** 5 **HBD:** 1 **RotB:** 4

PubChem ID : 219099 **CASRN :** 122883-93-6 **logP:** 4.30 **TPSA:** 48.5

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).

RTI International

RTI International, located in Research Triangle Park, North Carolina, is an independent nonprofit contract research organization dedicated to conducting research and development that improves the human condition by turning knowledge into practice. RTI International provides innovative research and technical solutions to governments and businesses worldwide in the areas of health and pharmaceuticals, education and training, surveys and statistics, advanced technology, democratic governance, economic and social development, advanced technology, energy, and the environment. For additional information about RTI International, please visit www.rti.org.

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.

Contact Informaton

Jamie Driscoll, B.S.
NIMH Project Officer
Chief of Research Services, MCGNRB, DNBBS, NIMH
6001 Executive Boulevard, Room 7187 (MSC 9641)
Bethesda, MD 20892-9641
Rockville, MD 20852 (overnight, courier)

Voice: (301) 443-3636
Fax: (301) 402-4740
Email: jdrisco1@mail.nih.gov

Linda S. Brady, Ph.D.
NIMH Alternate Project Officer
Chief, MCGNRB, DNBBS, NIMH
6001 Executive Boulevard, Room 7185 (MSC 9641)
Bethesda, MD 20892-9641
Rockville, MD 20852 (overnight, courier)

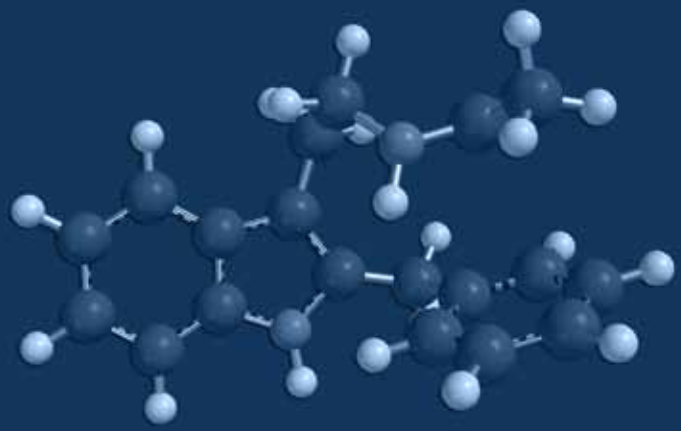
Voice: (301) 443-5288
Fax: (301) 402-4740
Email: lbrady@mail.nih.gov

Ken Rehder, Ph.D.
RTI Principal Investigator
RTI International
PO Box 12194
Research Triangle Park, NC 27709-2194

Voice: (919) 541-6681
Fax: (919) 541-8868
Email: krehder@rti.org

Anita H. Lewin, Ph.D.
Senior Research Chemist
RTI International
PO Box 12194
Research Triangle Park, NC 27709-2194

Voice: (919) 541-6691
Fax: (919) 541-8868
Email: ahl@rti.org



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