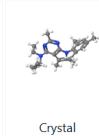
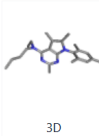
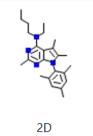


COMPOUND

Antalarmin

PubChem CID	177990
Structure	 2D3DCrystal
Molecular Formula	C ₂₄ H ₃₄ N ₄
Synonyms	Antalarmin 157284-96-3 G3DNT7X7YL 7H-Pyrrolo(2,3-d)pyrimidin-4-amine, N-butyl-N-ethyl-2,5,6-trimethyl-7-(2,4,6-trimethylphenyl)- CHEBI:139557 View More...
Molecular Weight	378.6 g/mol <i>Computed by PubChem 2.2 (PubChem release 2025.09.15)</i>
Dates	Create: 2005-03-26 Modify: 2026-05-23
Description	Antalarmin is a pyrrolopyrimidine that is 7H-pyrrolo[2,3-d]pyrimidin-4-amine which is substituted by methyl groups at positions 2, 5, and 6, by a mesityl group at position 7, and in which the amino substituent at position 4 has been substituted by ethyl and butyl groups. It is an antagonist of corticotropin-releasing factor 1 (CRF-1) receptors (<i>K_i</i> = 1 nM). It has a role as a corticotropin-releasing factor receptor antagonist. It is a pyrrolopyrimidine and a tertiary amino compound. ► ChEBI

Cite

Download

CONTENTS

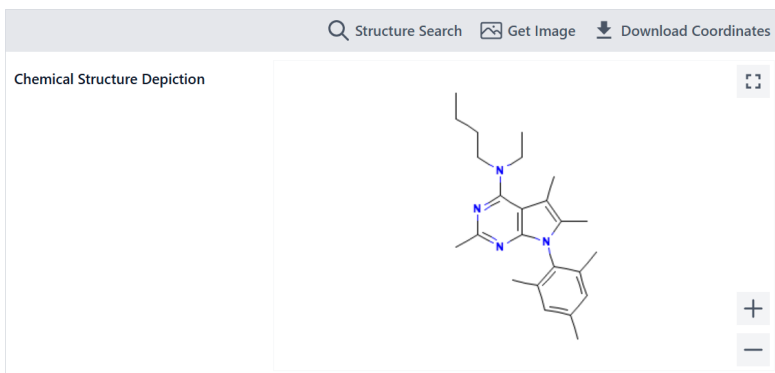
Title and Summary

- 1 Structures
- 2 Names and Identifiers
- 3 Chemical and Physical Properties
- 4 Related Records
- 5 Chemical Vendors
- 6 Associated Disorders and Diseases
- 7 Literature
- 8 Patents
- 9 Interactions and Pathways
- 10 Biological Test Results
- 11 Classification
- 12 Information Sources

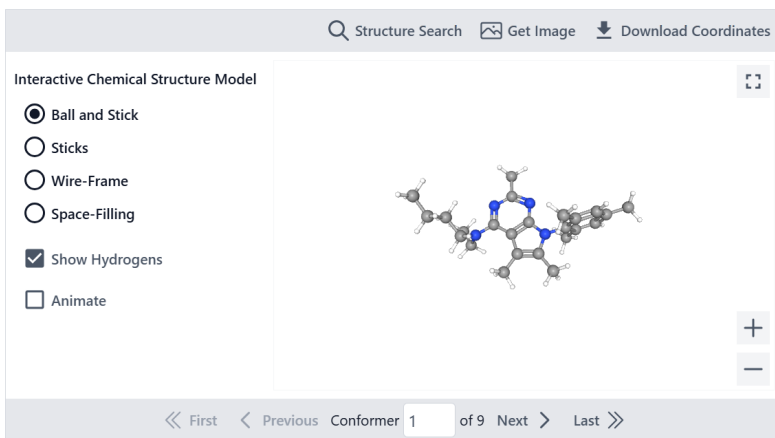
1 Structures



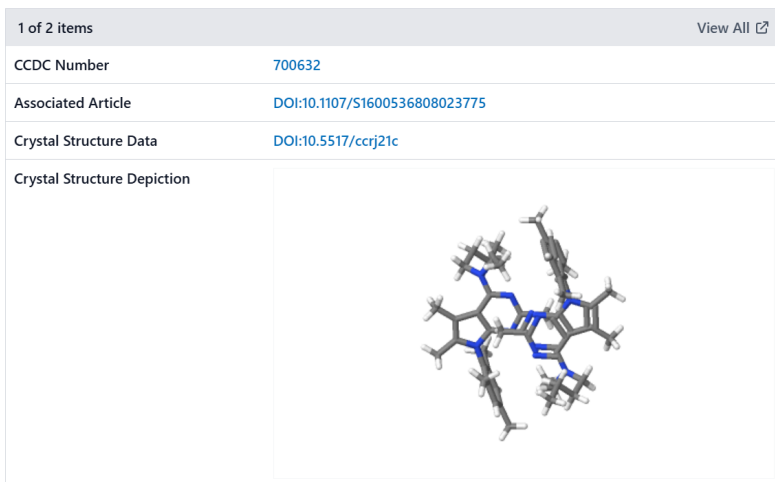
1.1 2D Structure



1.2 3D Conformer



1.3 Crystal Structures



2 Names and Identifiers



2.1 Computed Descriptors



2.1.1 IUPAC Name



N-butyl-*N*-ethyl-2,5,6-trimethyl-7-(2,4,6-trimethylphenyl)pyrrolo[2,3-*d*]pyrimidin-4-amine

Computed by Lexichem TK 2.9.3 (PubChem release 2025.09.15)

► [PubChem](#)

2.1.2 InChI



InChI=1S/C₂₄H₃₄N₄/c1-9-11-12-27(10-2)23-21-18(6)19(7)28(24(21)26-20(8)25-23)22-16(4)13-15(3)14-17(22)5/h13-14H,9-12H2,1-8H3

Computed by InChI 1.07.4 (PubChem release 2025.09.15)

► [PubChem](#)

2.1.3 InChIKey



IXPROWGEHNVJOY-UHFFFAOYSA-N

Computed by InChI 1.07.4 (PubChem release 2025.09.15)

► [PubChem](#)

2.1.4 SMILES



CCCCN(CC)C1=NC(=NC2=C1C(=C(N2C3=C(C=C(C3C)C)C)C)C

Computed by OEChem 4.2.0 (PubChem release 2025.09.15)

► [PubChem](#)

2.2 Molecular Formula



C₂₄H₃₄N₄

Computed by PubChem 2.2 (PubChem release 2025.09.15)

► [PubChem](#)

2.3 Other Identifiers



2.3.1 CAS



157284-96-3

► [CAS Common Chemistry](#); [ChemIDplus](#); [DTP/NCI](#); [EPA DSSTox](#); [FDA Global Substance Registration System \(GSRS\)](#)

2.3.2 UNII



G3DNT7X7YL

► [FDA Global Substance Registration System \(GSRS\)](#)

2.3.3 ChEBI ID



[CHEBI:139557](#)

► [ChEBI](#)

2.3.4 ChEMBL ID



[ChEMBL296641](#)

► [ChEMBL](#); [Open Targets](#)

2.3.5 DSSTox Substance ID

DTXSID50166241

▶ EPA DSSTox

2.3.6 HMDB ID

HMDB0248455

▶ Human Metabolome Database (HMDB)

2.3.7 Nikkaji Number

J1.099.376H

▶ Japan Chemical Substance Dictionary (Nikkaji)

2.3.8 NSC Number

NSC715590

▶ DTP/NCI

2.3.9 Pharos Ligand ID

VF5RBRNC2F35

▶ Pharos

2.3.10 Wikidata

Q4770927

▶ Wikidata

2.3.11 Wikipedia

Antalarmin

▶ Wikipedia

2.4 Synonyms

2.4.1 MeSH Entry Terms

antalarmin
N-butyl-N-ethyl-(2,5,6-trimethyl-7-(2,4,6-trimethylphenyl)-7H-pyrrolo(2,3-d)pyrimidin-4-yl)amine

▶ Medical Subject Headings (MeSH)

2.4.2 Depositor-Supplied Synonyms

Antalarmin	DTXCID7088732
157284-96-3	N-butyl-N-ethyl-(2
G3DNT7X7YL	N-butyl-N-ethyl-7-
7H-Pyrrolo(2,3-d)pyrimidin-4-amine, N-butyl-N-ethyl-2,5,6-trimethyl-7-(2,4,6-trimethylphenyl)-	N-butyl-N-ethyl-2,
CHEBI:139557	CHEMBL296641
DTXSID50166241	Butyl-ethyl-[2,5,6-t
7H-Pyrrolo[2,3-d]pyrimidin-4-amine, N-butyl-N-ethyl-2,5,6-trimethyl-7-(2,4,6-trimethylphenyl)-	N-BUTYL-N-ETHYL
N-butyl-N-ethyl-2,5,6-trimethyl-7-(2,4,6-trimethylphenyl)pyrrolo(3,2-e)pyrimidin-4-amine	UNII-G3DNT7X7YL
N-butyl-N-ethyl-2,5,6-trimethyl-7-(2,4,6-trimethylphenyl)pyrrolo[3,2-e]pyrimidin-4-amine	SCHEMBL466243
RefChem:112939	GTPL3489

► PubChem

3 Chemical and Physical Properties

3.1 Computed Properties

Property Name	Property Value	Reference
Molecular Weight	378.6 g/mol	Computed by PubChem 2.2 (PubChem release 2025.09.15)
XLogP3-AA	6.6	Computed by XLogP3 3.0 (PubChem release 2025.09.15)
Hydrogen Bond Donor Count	0	Computed by Cactvs 3.4.8.24 (PubChem release 2025.09.15)
Hydrogen Bond Acceptor Count	3	Computed by Cactvs 3.4.8.24 (PubChem release 2025.09.15)
Rotatable Bond Count	6	Computed by Cactvs 3.4.8.24 (PubChem release 2025.09.15)
Exact Mass	378.27834710 Da	Computed by PubChem 2.2 (PubChem release 2025.09.15)
Monoisotopic Mass	378.27834710 Da	Computed by PubChem 2.2 (PubChem release 2025.09.15)
Topological Polar Surface Area	34 Å ²	Computed by Cactvs 3.4.8.24 (PubChem release 2025.09.15)
Heavy Atom Count	28	Computed by PubChem
Formal Charge	0	Computed by PubChem
Complexity	485	Computed by Cactvs 3.4.8.24 (PubChem release 2025.09.15)
Isotope Atom Count	0	Computed by PubChem
Defined Atom Stereocenter Count	0	Computed by PubChem
Undefined Atom Stereocenter Count	0	Computed by PubChem
Defined Bond Stereocenter Count	0	Computed by PubChem
Undefined Bond Stereocenter Count	0	Computed by PubChem
Covalently-Bonded Unit Count	1	Computed by PubChem
Compound Is Canonicalized	Yes	Computed by PubChem (release 2025.09.15)

► PubChem

4 Related Records

4.1 Related Compounds with Annotation

Follow these links to [do a live 2D search](#) or [do a live 3D search](#) for this compound, sorted by annotation score. This section is deprecated (see [the neighbor discontinuation help page](#) for details), but these live search links provide equivalent functionality to the table that was previously shown here.

► PubChem

4.2 Related Compounds



Same Connectivity Count	3
Same Parent, Connectivity Count	5
Same Parent, Exact Count	3
Mixtures, Components, and Neutralized Forms Count	7
Similar Compounds (2D)	View in PubChem Search
Similar Conformers (3D)	View in PubChem Search

► [PubChem](#)

4.3 Substances



4.3.1 PubChem Reference Collection SID



500756357

► [PubChem](#)

4.3.2 Related Substances



All Count	167
Same Count	80
Mixture Count	87

► [PubChem](#)

4.3.3 Substances by Category



7 categories		Download
Chemical Vendors (31)		
CymitQuimica		
PubChem SID: 470397800	External ID: CQ_157284-96-3	
AstaTech, Inc.		
PubChem SID: 508542249	External ID: H42650	
Smolecule		
PubChem SID: 438448765	External ID: S518988	
ChemoSapiens		
PubChem SID: 517487120	External ID: 527306	
Mcule		
PubChem SID: 492811751	External ID: MCULE-8035034088	
Angene Chemical		
PubChem SID: 521726595	External ID: AG001PCX	
Excenen Pharmatech		
PubChem SID: 521587976	External ID: EX-A6937A	
EvitaChem		
PubChem SID: 485958822	External ID: evt-259218	
AA BLOCKS		
PubChem SID: 479913091	External ID: AA001PA5	
RR Scientific		
PubChem SID: 481278552	External ID: R616310	
Molport		
PubChem SID: 89094831	External ID: MolPort-002-051-899	
AiFChem, an XtalPi Company		
PubChem SID: 508293054	External ID: ACVAKW987	

MedChemexpress MCE	
PubChem SID: 476263408	External ID: HY-124475
Biosynth	
PubChem SID: 505209984	External ID: FA183627
J&H Chemical Co.,Ltd	
PubChem SID: 469509290	External ID: JH640073
PubChem SID: 469509293	External ID: JH640076
Debye Scientific Co., Ltd	
PubChem SID: 496714924	External ID: DA-50491
A2B Chem	
PubChem SID: 480587795	External ID: AA79321
Ambeed	
PubChem SID: 523658674	External ID: A528921
TargetMol	
PubChem SID: 494462829	External ID: T70433
BLD Pharm	
PubChem SID: 405011920	External ID: BD672982
Biorbyt	
PubChem SID: 516465571	External ID: orb1739047
eNovation Chemicals	
PubChem SID: 523135815	External ID: Y4255269
BenchChem	
PubChem SID: 445818674	External ID: B1665562
Alfa Chemistry	
PubChem SID: 527962356	External ID: PI157284963
AbaChemScene	
PubChem SID: 476270415	External ID: CS-0086611
10X CHEM	
PubChem SID: 497658657	External ID: TX001QIL
eMolecules	
PubChem SID: 490789859	External ID: 300104277
ChemShuttle	
PubChem SID: 528216224	External ID: 205308
Starshine Chemical	
PubChem SID: 468447320	External ID: starbld0195858
Ambinter	
PubChem SID: 369172286	External ID: Amb23594568
Curation Efforts (14)	
BindingDB (Curation Efforts, Research and Development)	
PubChem SID: 103967718	External ID: 50074501
ChEBI (Curation Efforts, Research and Development)	
PubChem SID: 85339243	External ID: CHEBI:139557
ChEMBL (Curation Efforts, Research and Development)	
PubChem SID: 103224906	External ID: CHEMBL296641
ChemIDplus (Curation Efforts, Governmental Organizations, Research and Development)	
PubChem SID: 135154868	External ID: 0157284963
Comparative Toxicogenomics Database (CTD) (Curation Efforts, Research and Development)	
PubChem SID: 53790815	External ID: C103016
Egon Willighagen, Department of Bioinformatics - BiGCaT, Maastricht University	
PubChem SID: 385786426	External ID: Q4770927
EPA DSSTox (Curation Efforts, Governmental Organizations, Research and Development)	
PubChem SID: 315726677	External ID: DTXSID50166241
FDA Global Substance Registration System (GSRS) (Curation Efforts, Governmental Organizations)	
PubChem SID: 474492549	External ID: G3DNT7X7YL
Human Metabolome Database (HMDB) (Curation Efforts, Research and Development)	
PubChem SID: 447222657	External ID: HMDB0248455
IUPHAR/BPS Guide to PHARMACOLOGY (Curation Efforts, Research and Development)	
PubChem SID: 178100478	External ID: 3489

SureChEMBL (Curation Efforts, Research and Development)	
PubChem SID: 514635617	External ID: SCHEMBL29832078
PubChem SID: 226784410	External ID: SCHEMBL466243
Therapeutic Target Database (TTD) (Curation Efforts, Research and Development)	
PubChem SID: 349977748	External ID: D03KJS
Wikidata	
PubChem SID: 386623422	External ID: Q4770927
Governmental Organizations (8)	
ChEMIDplus (Curation Efforts, Governmental Organizations, Research and Development)	
PubChem SID: 135154868	External ID: 0157284963
DTP/NCI	
PubChem SID: 533085	External ID: 715590
EPA DSSTox (Curation Efforts, Governmental Organizations, Research and Development)	
PubChem SID: 315726677	External ID: DTXSID50166241
FDA Global Substance Registration System (GSRS) (Curation Efforts, Governmental Organizations)	
PubChem SID: 474492549	External ID: G3DNT7X7YL
Japan Chemical Substance Dictionary (Nikkaji)	
PubChem SID: 272809127	External ID: J1.099.376H
National Center for Advancing Translational Sciences (NCATS) (Governmental Organizations, NIH Initiatives)	
PubChem SID: 29217488	External ID: NCGC00165732-01
PATENTSCOPE (WIPO)	
PubChem SID: 403651209	External ID: IXPROWGEHNVJOY-UHFFFAOYSA-N
PubChem Reference Collection	
PubChem SID: 500756357	External ID: 112939
Journal Publishers (2)	
Springer Nature	
PubChem SID: 341724598	External ID: 28051594-15223796
Wiley	
PubChem SID: 386242998	External ID: 67815
NIH Initiatives (1)	
National Center for Advancing Translational Sciences (NCATS) (Governmental Organizations, NIH Initiatives)	
PubChem SID: 29217488	External ID: NCGC00165732-01
Research and Development (19)	
Ace Therapeutics	
PubChem SID: 491486406	External ID: SMD063
BindingDB (Curation Efforts, Research and Development)	
PubChem SID: 103967718	External ID: 50074501
ChEBI (Curation Efforts, Research and Development)	
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ChEMBL (Curation Efforts, Research and Development)	
PubChem SID: 103224906	External ID: CHEMBL296641
ChEMIDplus (Curation Efforts, Governmental Organizations, Research and Development)	
PubChem SID: 135154868	External ID: 0157284963
Comparative Toxicogenomics Database (CTD) (Curation Efforts, Research and Development)	
PubChem SID: 53790815	External ID: C103016
Crystallography Open Database (COD)	
PubChem SID: 385895362	External ID: 2219134
EPA DSSTox (Curation Efforts, Governmental Organizations, Research and Development)	
PubChem SID: 315726677	External ID: DTXSID50166241
Google Patents	
PubChem SID: 419500351	External ID: 10632597
Human Metabolome Database (HMDB) (Curation Efforts, Research and Development)	
PubChem SID: 447222657	External ID: HMDB0248455
IBM	

PubChem SID: 128235206	External ID: F41397E083E975DB736D6C69C39AB015
IUPHAR/BPS Guide to PHARMACOLOGY (Curation Efforts, Research and Development)	
PubChem SID: 178100478	External ID: 3489
MolGenie	
PubChem SID: 500916902	External ID: 190000007425
Novartis Institutes for BioMedical Research	
PubChem SID: 406842893	External ID: MOABOX:5714
Probes & Drugs portal	
PubChem SID: 482179663	External ID: PD046976
Shanghai Titan Scientific	
PubChem SID: 513262681	External ID: Titan-29362
SureChEMBL (Curation Efforts, Research and Development)	
PubChem SID: 514635617	External ID: SCHEMBL29832078
PubChem SID: 226784410	External ID: SCHEMBL466243
Therapeutic Target Database (TTD) (Curation Efforts, Research and Development)	
PubChem SID: 349977748	External ID: D03KJS
Legacy Depositors (20)	
ABI Chem (Chemical Vendors)	
PubChem SID: 104426837	External ID: AC1L433C
Amadis Chemical (Chemical Vendors)	
PubChem SID: 497989838	External ID: A1245047
Aurora Fine Chemicals LLC (Chemical Vendors)	
PubChem SID: 300397614	External ID: A24.069.642
PubChem SID: 289681911	External ID: K02.128.888
ChemBank (Research and Development)	
PubChem SID: 11444292	External ID: NCI60_039940
ChemExper Chemical Directory (Chemical Vendors)	
PubChem SID: 3249268	External ID: jcoH@@@Xi[IEEEEbdlhlhXhkRUGCVDEQUMU@QDP@@
ChemSpider (Research and Development)	
PubChem SID: 33501322	External ID: 154945
Collaborative Drug Discovery, Inc. (Subscription Services)	
PubChem SID: 179294243	External ID: 42468
Davey Lab, Department of Microbiology, NEIDL, Boston University (Research and Development)	
PubChem SID: 441294748	External ID: BRD-K01363385
DiscoveryGate (Subscription Services)	
PubChem SID: 10258823	External ID: 177990
LeadScope (Subscription Services)	
PubChem SID: 50040462	External ID: LS-139513
NextBio (Subscription Services)	
PubChem SID: 50815298	External ID: 177990
NovoSeek (Chemical Vendors)	
PubChem SID: 57395584	External ID: 177990
Prous Science Drugs of the Future (Journal Publishers)	
PubChem SID: 12014909	External ID: 213577
SCRIPDB (Research and Development)	
PubChem SID: 141141924	External ID: US20100249138A1-20100930-C00017_1
THE BioTek (Chemical Vendors)	
PubChem SID: 434140597	External ID: bt-259218
Thomson Pharma (Journal Publishers, Subscription Services)	
PubChem SID: 14829248	External ID: 00001672
ToxPlanet (Subscription Services)	
PubChem SID: 319186255	External ID: ToxPlanet-MTU3Mjg0LTk2LTMTMxNzc5OTA=
xPharm: The Comprehensive Pharmacology Reference (Journal Publishers)	
PubChem SID: 7978712	External ID: 7880
ZINC (Chemical Vendors)	
PubChem SID: 256202830	External ID: ZINC1539136

► PubChem

4.4 Entrez Crosslinks



PubMed Count	198
Taxonomy Count	4
OMIM Count	1
Gene Count	9

► PubChem

5 Chemical Vendors



30 vendors		Download
CymitQuimica	PubChem SID: 470397800	Purchasable Chemical: CQ_157284-96-3
AstaTech, Inc.	PubChem SID: 508542249	Purchasable Chemical: H42650
Smolecule	PubChem SID: 438448765	Purchasable Chemical: S518988
ChemoSapiens	PubChem SID: 517487120	Purchasable Chemical: 527306
Mcule	PubChem SID: 492811751	Purchasable Chemical: MCULE-8035034088
Angene Chemical	PubChem SID: 521726595	Purchasable Chemical: AG001PCX
Excenen Pharmatech	PubChem SID: 521587976	Purchasable Chemical: EX-A6937A
EvitaChem	PubChem SID: 485958822	Purchasable Chemical: evt-259218
AA BLOCKS	PubChem SID: 479913091	Purchasable Chemical: AA001PA5
RR Scientific	PubChem SID: 481278552	Purchasable Chemical: R616310
Molport	PubChem SID: 89094831	Purchasable Chemical: MolPort-002-051-899
AiFCheM, an XtalPi Company	PubChem SID: 508293054	Purchasable Chemical: ACVAKW987
MedChemexpress MCE	PubChem SID: 476263408	Purchasable Chemical: HY-124475
Biosynth	PubChem SID: 505209984	Purchasable Chemical: FA183627
J&H Chemical Co.,Ltd	PubChem SID: 469509290	Purchasable Chemical: JH640073
	PubChem SID: 469509293	Purchasable Chemical: JH640076
Debye Scientific Co., Ltd	PubChem SID: 496714924	Purchasable Chemical: DA-50491
A2B Chem	PubChem SID: 480587795	Purchasable Chemical: AA79321
Ambeed	PubChem SID: 523658674	Purchasable Chemical: A528921
TargetMol	PubChem SID: 494462829	Purchasable Chemical: T70433
BLD Pharm	PubChem SID: 405011920	Purchasable Chemical: BD672982
Biorbyt	PubChem SID: 516465571	Purchasable Chemical: orb1739047
eNovation Chemicals		

PubChem SID: 523135815	Purchasable Chemical: Y4255269
BenchChem	
PubChem SID: 445818674	Purchasable Chemical: B1665562
Alfa Chemistry	
PubChem SID: 527962356	Purchasable Chemical: P1157284963
AbaChemScene	
PubChem SID: 476270415	Purchasable Chemical: CS-0086611
10X CHEM	
PubChem SID: 497658657	Purchasable Chemical: TX001QIL
eMolecules	
PubChem SID: 490789859	Purchasable Chemical: 300104277
ChemShuttle	
PubChem SID: 528216224	Purchasable Chemical: 205308
Starshine Chemical	
PubChem SID: 468447320	Purchasable Chemical: starbld0195858
Ambinter	
PubChem SID: 369172286	Purchasable Chemical: Amb23594568

► PubChem

6 Associated Disorders and Diseases



4 items Download		
Source Disease	Evidence ⓘ	Data Source
Anxiety Disorders	PMID:22231481	Comparative Toxicogenomics Database (CTD)
Bradycardia	PMID:16710322	Comparative Toxicogenomics Database (CTD)
Cocaine-Related Disorders	PMID:19339610	Comparative Toxicogenomics Database (CTD)
Hyperkinesia	PMID:19339610	Comparative Toxicogenomics Database (CTD)

► Comparative Toxicogenomics Database (CTD); Therapeutic Target Database (TTD)

7 Literature



7.1 Consolidated References



209 items Download	
Search	SORT BY Publication Date - Most Recent
Synthesis of 2-imino and 2-hydrazono thiazolo[4,5- d]pyrimidines as corticotropin releasing factor (CRF) antagonists Publication Name: European Journal of Medicinal Chemistry Publication Date: 2017-09-29 PMID: 28750312 DOI: 10.1016/j.ejmech.2017.07.016	
Sustained glucocorticoid exposure recruits cortico-limbic CRH signaling to modulate endocannabinoid function Publication Name: Psychoneuroendocrinology Publication Date: 2016-04 PMCID: PMC4788523 PMID: 26821211 DOI: 10.1016/j.psyneuen.2016.01.004	
Polymorphism in the corticotropin-releasing factor receptor 1 (CRF1-R) gene plays a role in shaping the high anxious phenotype of Marchigian Sardinian alcohol-preferring (msP) rats Publication Name: Psychopharmacology Publication Date: 2014-09-27 PMCID: PMC4339612 PMID: 25260340 DOI: 10.1007/s00213-014-3743-7	
Synthesis of substituted pyrimidines as corticotropin releasing factor (CRF) receptor ligands	

Publication Name: European Journal of Medicinal Chemistry

Publication Date: 2014-05-06

PMID: 24675175 DOI: 10.1016/j.ejmech.2014.03.040

Regulation of Estradiol and Progesterone Production by CRH-R1 and -R2 Is through Divergent Signaling Pathways in Cultured Human Placental Trophoblasts

Publication Name: Endocrinology

Publication Date: 2012-10-01

PMID: 22865371 DOI: 10.1210/en.2012-1453

« First < Previous Page 1 of 42 Next > Last »

► PubChem

7.2 NLM Curated PubMed Citations



All NLM Curated PubMed Citations

Download

► Medical Subject Headings (MeSH)

7.3 Springer Nature References



2 items

Download



The CRF1 receptor antagonist antalarmin attenuates yohimbine-induced increases in operant alcohol self-administration and reinstatement of alcohol seeking in rats

PMID: 17705061

Publication Date: 2007

Publication Name: Psychopharmacology



Polymorphism in the corticotropin-releasing factor receptor 1 (CRF1-R) gene plays a role in shaping the high anxious phenotype of Marchigian Sardinian alcohol-preferring (msP) rats

PMID: 25260340

Publication Date: 2014

Publication Name: Psychopharmacology

► Springer Nature

7.4 Wiley References



1 item

Download

Efficient Synthesis of Pyrrolo [2,3-d] Pyrimidines Containing 1,4-Disubstituted-1,2,3-Triazole Derivatives

DOI: 10.1002/jhet.2611

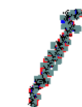
Publication Date: 2017

Publication Name: J. Heterocyclic Chem.

► Wiley

7.5 Chemical Co-Occurrences in Literature



Showing 3 of 100 View More Co-Occurrence and Evidence Data		Download
Chemical	Selected evidence	
 Corticorelin CID 16186200	117 articles	View All
	Corticotropin-releasing hormone stimulates NF-kappaB in human epidermal keratinocytes PMID 15171702; DOI 10.1677/joe.0.181r001; The Journal of endocrinology 2004-06-01	
	Corticotropin-releasing hormone attenuates vascular endothelial growth factor release from human HaCaT keratinocytes PMID 19852986; DOI 10.1016/j.regpep.2009.10.001; Regulatory Peptides 2010-02-25	
 Pyrrole CID 8027	112 articles	View All
	Glucocorticoid blockade reverses psychological stress-induced abnormalities in epidermal structure and function PMID 16857896; DOI 10.1152/ajpregu.00010.2006; American journal of physiology. Regulatory, integrative and comparative physiology 2006-12-01	
	Corticotropin-releasing hormone stimulates NF-kappaB in human epidermal keratinocytes PMID 15171702; DOI 10.1677/joe.0.181r001; The Journal of endocrinology 2004-06-01	
 Astressin 2B CID 90488758	25 articles	View All
	ORIGINAL ARTICLE: Urocortin Increases IL-4 and IL-10 Secretion and Reverses LPS-induced TNF-α Release from Human Trophoblast Primary Cells PMID 19703147; DOI 10.1111/j.1600-0897.2009.00729.x; American journal of reproductive immunology (New York, N.Y. : 1989) 2009-09-11	
	Urocortin 1 inhibits guinea pig gallbladder contractility in vitro via corticotropin-releasing factor receptor 2 PMID 22007876; DOI 10.1139/y11-076; Canadian journal of physiology and pharmacology 2011-11-01	
	Differential effects of acute morphine, and chronic morphine-withdrawal on obsessive-compulsive behavior: Inhibitory influence of CRF receptor antagonists on chronic morphine-withdrawal PMID 22863536; DOI 10.1016/j.npep.2012.06.002; Neuropeptides 2012-10-01	

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7.6 Chemical-Gene Co-Occurrences in Literature



Showing 3 of 100 View More Co-Occurrence and Evidence Data		 Download
Gene/Protein/Enzyme	Selected evidence	
corticotropin releasing hormone	171 articles	View All
Corticotropin-Releasing Hormone Skin Signaling is Receptor-Mediated and is Predominant in the Sebaceous Glands PMID 17326013; DOI 10.1055/s-2007-961811; Hormone and metabolic research = Hormon- und Stoffwechselforschung = Hormones et métabolisme 2007-02-01 Corticosterone implants to the amygdala and type 1 CRH receptor regulation: Effects on behavior and colonic sensitivity PMID 15904708; DOI 10.1016/j.bbr.2005.03.001; Behavioural Brain Research 2005-06-03 Divergent Roles of the CRH Receptors in the Control of Gonadotropin Secretion Induced by Acute Restraint Stress at Proestrus PMID 22893722; DOI 10.1210/en.2012-1333; Endocrinology 2012-10-01		
corticotropin releasing hormone receptor 1	109 articles	View All
Polymorphism in the corticotropin-releasing factor receptor 1 (CRF1-R) gene plays a role in shaping the high anxious phenotype of Marchigian Sardinian alcohol-preferring (msP) rats PMID 25260340; DOI 10.1007/s00213-014-3743-7; Psychopharmacology 2014-09-27 CRH Acts on CRH-R1 and -R2 to Differentially Modulate the Expression of Large-Conductance Calcium-Activated Potassium Channels in Human Pregnant Myometrium PMID 21878514; DOI 10.1210/en.2011-0262; Endocrinology 2011-08-30 Corticotropin-releasing hormone stimulates SGK-1 kinase expression in cultured hippocampal neurons via CRH-R1 PMID 18713960; DOI 10.1152/ajpendo.90462.2008; American journal of physiology. Endocrinology and metabolism 2008-10-01		
corticotropin releasing hormone receptor 2	49 articles	View All
Involvement of CRF2 receptor in the brain regions in restraint-induced anorexia PMID 21666520; DOI 10.1097/wnr.0b013e3283487467; NeuroReport 2011-07-13 Impaired CRH and Urocortin Expression and Function in Eutopic Endometrium of Women with Endometriosis PMID 21289256; DOI 10.1210/jc.2010-2263; The Journal of clinical endocrinology and metabolism 2011-04-01 Corticotropin-Releasing Hormone Receptor Type 1 and Type 2 Mediate Differential Effects on 15-Hydroxy Prostaglandin Dehydrogenase Expression in Cultured Human Chorion Trophoblasts PMID 17463062; DOI 10.1210/en.2006-1212; Endocrinology 2007-08-01		

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7.7 Chemical-Disease Co-Occurrences in Literature

Showing 3 of 100 View More Co-Occurrence and Evidence Data Download

Disease	Selected evidence
Anxiety Disorders	48 articles View All Corticotropin-Releasing Factor Modulation of Forebrain GABAergic Transmission has a Pivotal Role in the Expression of Anabolic Steroid-Induced Anxiety in the Female Mouse PMID 22298120; DOI 10.1038/npp.2011.334; Neuropsychopharmacology : official publication of the American College of Neuropsychopharmacology 2012-02-01 Antidepressant efficacy screening of novel targets in the chick anxiety-depression model PMID 19300238; DOI 10.1097/fbp.0b013e32832a8082; Behavioural Pharmacology 2009-03-01 Blockade of CRF1 and CCK2 receptors attenuated the elevated anxiety-like behavior induced by immobilization stress PMID 21295058; DOI 10.1016/j.pbb.2011.01.022; Pharmacology, biochemistry, and behavior 2011-05-01
Depressive Disorder	25 articles View All Antidepressant efficacy screening of novel targets in the chick anxiety-depression model PMID 19300238; DOI 10.1097/fbp.0b013e32832a8082; Behavioural Pharmacology 2009-03-01 Increased Depression-Like Behaviors in Corticotropin-Releasing Factor Receptor-2-Deficient Mice: Sexually Dichotomous Responses PMID 12832554; DOI 10.1523/jneurosci.23-12-05295.2003; The Journal of neuroscience : the official journal of the Society for Neuroscience 2003-06-15 Chronic Mild Stress (CMS) in Mice: Of Anhedonia, 'Anomalous Anxiolysis' and Activity PMID 19177164; DOI 10.1371/journal.pone.0004326; PLoS ONE 2009-01-29
Inflammation	19 articles View All Corticotropin releasing hormone (CRH) antagonist attenuates adjuvant induced arthritis: role of CRH in peripheral inflammation PMID 12064844; The Journal of rheumatology 2002-06-01 In vivo and in vitro characterization of antalarmin, a nonpeptide corticotropin-releasing hormone (CRH) receptor antagonist: suppression of pituitary ACTH release and peripheral inflammation. PMID 8940412; DOI 10.1210/en.137.12.5747; Endocrinology 1996-12-01 Corticotropin-releasing hormone antagonists possess anti-inflammatory effects in the mouse ileum PMID 12145804; DOI 10.1053/gast.2002.34783; Gastroenterology 2002-08-01

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7.8 Chemical-Organism Co-Occurrences in Literature

Showing 3 of 39 [View More Co-Occurrence and Evidence Data](#) [Download](#)

Organism	Selected evidence
rattus sp. (rats)	89 articles View All Peripheral injection of sauvagine prevents repeated colorectal distension-induced visceral pain in female rats PMID 15949637; DOI 10.1016/j.peptides.2005.02.004; Peptides 2005-07-01 The effect of chronic CRF1 receptor blockade on the central CCK systems of Fawn-Hooded rats PMID 14599712; DOI 10.1016/s0167-0115(03)00189-7; Regulatory Peptides 2003-11-15 Stress-Induced Intracellular Trafficking of Corticotropin-Releasing Factor Receptors in Rat Locus Coeruleus Neurons PMID 17947354; DOI 10.1210/en.2007-0705; Endocrinology 2007-10-18
mus sp. (mice)	39 articles View All Mechanisms involved in the anti-inflammatory action of inhaled tea tree oil in mice PMID 17327476; Experimental biology and medicine (Maywood, N.J.) 2007-03-01 Chronic Mild Stress (CMS) in Mice: Of Anhedonia, 'Anomalous Anxiolysis' and Activity PMID 19177164; DOI 10.1371/journal.pone.0004326; PLoS ONE 2009-01-29 Dependence-induced increases in ethanol self-administration in mice are blocked by the CRF1 receptor antagonist antalarmin and by CRF1 receptor knockout PMID 17482248; DOI 10.1016/j.pbb.2007.03.009; Pharmacology, biochemistry, and behavior 2007-04-01
metazoa (animals)	36 articles View All Endocrine and behavioral effects of neuromedin S PMID 17900576; DOI 10.1016/j.yhbeh.2007.08.002; Hormones and Behavior 2007-12-01 Polymorphism in the corticotropin-releasing factor receptor 1 (CRF1-R) gene plays a role in shaping the high anxious phenotype of Marchigian Sardinian alcohol-preferring (msP) rats PMID 25260340; DOI 10.1007/s00213-014-3743-7; Psychopharmacology 2014-09-27 Treatment with a CRH-R1 antagonist prevents stress-induced suppression of the central neural drive to the reproductive axis in female macaques PMID 20823449; DOI 10.1152/ajpendo.00224.2010; American journal of physiology. Endocrinology and metabolism 2011-01-01

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8 Patents [?](#) [↗](#)

8.1 Depositor-Supplied Patent Identifiers [?](#) [↗](#)

913 items	Download
Search	SORT BY Priority Date - Most Recent
Fatty acid conjugated cyclic peptides Publication Number: WO-2025128794-A1 Priority Date: 2023-12-15	
Compositions and methods for managing alcohol and drug addiction Publication Number: WO-2025088359-A1 Priority Date: 2023-10-24	
Crhr1 agonists for use in the treatment of social anxiety disorders Publication Number: WO-2025046136-A1 Priority Date: 2023-09-01	
Crhr1 agonists for use in the treatment of social anxiety disorders Publication Number: EP-4516309-A1 Priority Date: 2023-09-01	
Pde 7 modulator compounds Publication Number: WO-2025042956-A1 Priority Date: 2023-08-22	
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8.2 WIPO PATENTSCOPE



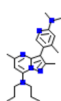
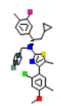
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<https://patentscope.wipo.int/search/en/result.jsf?inchikey=IXPROWGEHNVJOY-UHFFFAOYSA-N>

► PATENTSCOPE (WIPO)

8.3 Chemical Co-Occurrences in Patents



Showing 3 of 100	View More Co-Occurrence and Evidence Data	Download
Chemical	Selected evidence	
 R121919 CID 9821250	10 patents from 6 patent families View All Treatment and prevention of tauopathies and amyloid beta amyloidosis by modulating CRF receptor signaling EP-2522351-B1; Grant Date: 2017-09-06 Method for predicting a treatment response to a CRHR1 antagonist and/or a V1B antagonist in a patient with depressive and/or anxiety symptoms US-10837062-B2; Grant Date: 2020-11-17 Treatment of congenital adrenal hyperplasia US-10905690-B2; Grant Date: 2021-02-02	
 4-(2-Chloro-4-methoxy-5-methylphenyl)-N-((1S)-2-cyclopropyl-1-(3-fluoro-4-methylphenyl)ethyl)-5-methyl-N-2-propyn-1-yl-2-thiazolamine CID 5282340	8 patents from 4 patent families View All Treatment and prevention of tauopathies and amyloid beta amyloidosis by modulating CRF receptor signaling EP-2522351-B1; Grant Date: 2017-09-06 Treatment of congenital adrenal hyperplasia US-10905690-B2; Grant Date: 2021-02-02 Method for predicting a treatment response to a CRHR1 antagonist and/or a V1B antagonist in a patient with depressive and/or anxiety symptoms US-10837062-B2; Grant Date: 2020-11-17	



1 patent from 1 patent family [View All](#)

Genetic predictors of a response to treatment with crhr1 antagonists
EP-3277835-B1; Grant Date: 2019-01-09

2-[2-amino-1-[6-(dimethylamino)-4-methyl-3-pyridinyl]prop-1-enyl]-6-methyl-N,N-dipropylpyrimidin-4-amine
CID 158478226

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8.4 Chemical-Disease Co-Occurrences in Patents



Showing 3 of 100 View More Co-Occurrence and Evidence Data		Download
Disease	Selected evidence	
Ovarian Cysts	1 patent from 1 patent family View All	
	Compositions and methods for the treatment of endometriosis US-10729693-B2; Grant Date: 2020-08-04	
Tauopathies	2 patents from 2 patent families View All	
	Treatment and prevention of tauopathies and amyloid beta amyloidosis by modulating CRF receptor signaling EP-2522351-B1; Grant Date: 2017-09-06	
	Allosteric corticotropin-releasing factor receptor 1 (CRFR1) antagonists that decrease p-tau and improve cognition US-11077108-B2; Grant Date: 2021-08-03	
Amyloidosis	2 patents from 2 patent families View All	
	Treatment and prevention of tauopathies and amyloid beta amyloidosis by modulating CRF receptor signaling EP-2522351-B1; Grant Date: 2017-09-06	
	Allosteric corticotropin-releasing factor receptor 1 (CRFR1) antagonists that decrease p-tau and improve cognition US-11077108-B2; Grant Date: 2021-08-03	

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8.5 Chemical-Gene Co-Occurrences in Patents



Showing 3 of 100 View More Co-Occurrence and Evidence Data ↗		Download
Gene	Selected evidence	
crh	29 patents from 18 patent families View All ↗ Compositions and methods for the treatment of endometriosis US-10729693-B2; Grant Date: 2020-08-04 Treatment and prevention of tauopathies and amyloid beta amyloidosis by modulating CRF receptor signaling EP-2522351-B1; Grant Date: 2017-09-06 Method for predicting a treatment response to a CRHR1 antagonist and/or a V1B antagonist in a patient with depressive and/or anxiety symptoms US-10190168-B2; Grant Date: 2019-01-29	
crhr2	10 patents from 5 patent families View All ↗ Treatment and prevention of tauopathies and amyloid beta amyloidosis by modulating CRF receptor signaling EP-2522351-B1; Grant Date: 2017-09-06 Corticotropin releasing factor receptor 2 agonists EP-1465922-B1; Grant Date: 2008-01-09 CRFR2 selective ligands US-7141546-B1; Grant Date: 2006-11-28	
crhr1	12 patents from 9 patent families View All ↗ Method for predicting a treatment response to a CRHR1 antagonist and/or a V1B antagonist in a patient with depressive and/or anxiety symptoms US-10190168-B2; Grant Date: 2019-01-29 Compositions and methods for the treatment of endometriosis US-10729693-B2; Grant Date: 2020-08-04 Treatment and prevention of tauopathies and amyloid beta amyloidosis by modulating CRF receptor signaling EP-2522351-B1; Grant Date: 2017-09-06	

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8.6 Chemical-Organism Co-Occurrences in Patents



Showing 3 of 100 View More Co-Occurrence and Evidence Data ↗		Download
Organism	Selected evidence	
mammalia (mammals)	18 patents from 11 patent families View All ↗ Compositions and methods for the treatment of endometriosis US-10729693-B2; Grant Date: 2020-08-04 QT dispersion and heart rate variability improvement with CRF antagonists to prevent sudden death US-6384039-B1; Grant Date: 2002-05-07 Use of CRF antagonists and renin-angiotensin system inhibitors US-6387894-B1; Grant Date: 2002-05-14	
rodentia (rodents)	17 patents from 10 patent families View All ↗ Compositions and methods for the treatment of endometriosis US-10729693-B2; Grant Date: 2020-08-04 Treatment and prevention of tauopathies and amyloid beta amyloidosis by modulating CRF receptor signaling EP-2522351-B1; Grant Date: 2017-09-06 Method for predicting a treatment response to a CRHR1 antagonist and/or a V1B antagonist in a patient with depressive and/or anxiety symptoms US-10190168-B2; Grant Date: 2019-01-29	
rattus (rats)	21 patents from 12 patent families View All ↗ Compositions and methods for the treatment of endometriosis US-10729693-B2; Grant Date: 2020-08-04	

Treatment and prevention of tauopathies and amyloid beta amyloidosis by modulating CRF receptor signaling
EP-2522351-B1; Grant Date: 2017-09-06

CRFR2 selective ligands
US-7141546-B1; Grant Date: 2006-11-28

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9 Interactions and Pathways



9.1 Chemical-Target Interactions



12 items Download					
Search			SORT BY Data Source - A to Z		
Protein	Gene	Taxonomy	Action ⓘ	Evidence ⓘ	Data Source
	CYP11A1	Homo sapiens (human)	Antalarmin results in decreased expression of CYP11A1 mRNA	PMID:16014403	Comparative Toxicogenomics Database (CTD)
	STAR	Homo sapiens (human)	Antalarmin results in decreased expression of STAR mRNA	PMID:16014403	Comparative Toxicogenomics Database (CTD)
	CRHR1	Homo sapiens (human)	Antalarmin binds to and results in decreased activity of CRHR1 protein	PMID:16014403	Comparative Toxicogenomics Database (CTD)
	SULT2A1	Homo sapiens (human)	Antalarmin results in decreased expression of SULT2A1 mRNA	PMID:16014403	Comparative Toxicogenomics Database (CTD)
Corticotropin-releasing factor receptor 1	CRHR1	Homo sapiens (human)	Antagonist	PMID:8940412	IUPHAR/BPS Guide to PHARMACOLOGY
◀ First < Previous Page 1 of 3 Next > Last ▶					

► Comparative Toxicogenomics Database (CTD); Drug Gene Interaction database (DGIdb); IUPHAR/BPS Guide to ...

10 Biological Test Results



10.1 BioAssay Results



113 items Download	
Search SORT BY Activity Value - Increasing	
Binding affinity to recombinant human Corticotropin releasing factor receptor 1 (hCRF1) expressed in 293EBNA cells	
Activity Outcome: Active Activity Type: Ki Activity Value: 0.000840 μM	
BioAssay AID: 53968	
Target Name: CRHR1 - corticotropin releasing hormone receptor 1 (human)	
Substance SID: 103224906 Compound CID: 177990	
Binding affinity to recombinant human Corticotropin releasing factor receptor 1 (hCRF1) expressed in 293EBNA cells	
Activity Outcome: Active Activity Type: Ki Activity Value: 0.000840 μM	
BioAssay AID: 53968	
Target Name: LINC02210-CRHR1 - LINC02210-CRHR1 readthrough (human)	
Substance SID: 103224906 Compound CID: 177990	
Affinity for the Corticotropin releasing factor receptor 1 (CRHR1) was determined in rat brain	
Activity Outcome: Active Activity Type: Ki Activity Value: 0.001000 μM	
BioAssay AID: 53982	

Target Name: [Crhr1 - corticotropin releasing hormone receptor 1 \(Norway rat\)](#)

Substance SID: [103224906](#) Compound CID: [177990](#)

Compound was tested for the binding affinity to rat corticotropin releasing factor receptor

Activity Outcome: [Active](#) Activity Type: Ki Activity Value: 0.001000 μ M

BioAssay AID: [53819](#)

Target Name: [Crhr1 - corticotropin releasing hormone receptor 1 \(Norway rat\)](#)

Substance SID: [103224906](#) Compound CID: [177990](#)

Compound was tested for the binding affinity to rat corticotropin releasing factor receptor

Activity Outcome: [Active](#) Activity Type: Ki Activity Value: 0.001000 μ M

BioAssay AID: [53819](#)

Target Name: [Crhr2 - corticotropin releasing hormone receptor 2 \(Norway rat\)](#)

Substance SID: [103224906](#) Compound CID: [177990](#)

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11 Classification



11.1 MeSH Tree



1 item

[View in Classification Browser](#)

MeSH Tree > Chemicals and Drugs Category > Heterocyclic Compounds > Heterocyclic Compounds, 1-Ring > Azoles > Pyrroles

⌵ Show alternative paths

[antalarmin](#)

MeSH Concept: [M0269484](#)

MeSH Descriptor: [C103016](#)

► [Medical Subject Headings \(MeSH\)](#)

11.2 ChEBI Ontology



1 item

[View in Classification Browser](#)

ChEBI Ontology > chemical entity > molecular entity > main group molecular entity > p-block molecular entity > carbon group molecular entity > organic molecular entity > organic amino compound > tertiary amino compound

⌵ Show alternative paths

[antalarmin](#)

A pyrrolopyrimidine that is 7H-pyrrolo[2,3-d]pyrimidin-4-amine which is substituted by methyl groups at positions 2, 5, and 6, by a mesityl group at position 7, and in which the amino substituent at position 4 has been substituted by ethyl and butyl groups. It is an antagonist of corticotropin-releasing factor 1 (CRF-1) receptors (K_i = 1 nM).

► [ChEBI](#)

11.3 ChemIDplus



11 items	View in Classification Browser
ChemIDplus Chemical Information Classification > Other Resources (Internet Locators)	
CTD Comparative Toxicogenomics Database - CTD selects and organizes gene, sequence, chemical, reference, and taxonomic data about gene-chemical interactions. It is hosted at North Carolina State University (NCSSU).	
ChemIDplus Chemical Information Classification > NLM Resources (File Locators)	
DrugPortal Drug Information Portal - Portal to selected drug information from the U.S. National Library of Medicine and other key U.S. Government agencies	
ChemIDplus Chemical Information Classification > Other Resources (Internet Locators)	
EPA CompTox	
ChemIDplus Chemical Information Classification > NLM Resources (File Locators)	
MeSH Medical Subject Heading and Supplementary Concept Records - ChemIDplus includes only the chemical names and chemical MeSH headings from this file. This search retrieves information from both MeSH headings and Supplementary Concept Records	
ChemIDplus Chemical Information Classification > NLM Resources (File Locators)	
PubChem PubChem Substance Database - The PubChem Substance Database contains the chemical structures of small organic molecules and information on their biological activities	
« First < Previous Page 1 of 3 Next > Last »	

► ChemIDplus

11.4 IUPHAR / BPS Guide to PHARMACOLOGY Target Classification



1 item	View in Classification Browser
Guide to Pharmacology Target Classification > Receptors > G protein-coupled receptors	
Corticotropin-releasing factor receptors Corticotropin-releasing factor (CRF, nomenclature as agreed by the NC-IUPHAR subcommittee on Corticotropin-releasing Factor Receptors) receptors are activated by the endogenous peptides corticotrophin-releasing hormone, a 41 amino-acid peptide, urocortin 1, 40 amino-acids, urocortin 2, 38 amino-acids and urocortin 3, 38 amino-acids. CRF ₁ and CRF ₂ receptors are activated non-selectively by CRH and UCN. CRF ₂ receptors are selectively activated by UCN2 and UCN3. Binding to CRF receptors can be conducted using radioligands [¹²⁵ I]Tyr ⁰ -CRF or [¹²⁵ I]Tyr ⁰ -sauvagine with K _d values of 0.1-0.4 nM. CRF ₁ and CRF ₂ receptors are non-selectively antagonized by α-helical CRF, D-Phe-CRF-(12-41) and astressin. CRF ₁ receptors are selectively antagonized by small molecules NBI27914, R121919, antalarmin, CP 154,526, CP 376,395. CRF ₂ receptors are selectively antagonized by antisauvagine and astressin 2B. Although selective small molecule CRF ₁ receptor antagonists were not effective in treating major depressive disorder, posttraumatic stress disorder, or alcohol use disorder in clinical trials, recent phase 2 studies have found that CRF ₁ receptor antagonists effectively reduce adrenocortical androgens and precursors in congenital adrenal hyperplasia.	

► IUPHAR/BPS Guide to PHARMACOLOGY

11.5 ChEMBL Target Tree



3 items	View in Classification Browser
ChEMBL Protein Target Tree > Membrane receptor > Family B G protein-coupled receptor > Peptide receptor (family B GPCR) > Corticotropin releasing factor receptor	
Corticotropin releasing factor receptor Cell surface proteins that bind corticotropin-releasing hormone with high affinity and trigger intracellular changes which influence the behavior of cells. The corticotropin releasing-hormone receptors on anterior pituitary cells mediate the stimulation of corticotropin release by hypothalamic corticotropin releasing factor. The physiological consequence of activating corticotropin-releasing hormone receptors on central neurons is not well understood. [MESH:D018019]	
ChEMBL Protein Target Tree > Enzyme	
Transferase A group of enzymes that catalyze the transfer of a functional group from one molecule to another	
ChEMBL Protein Target Tree > Epigenetic regulator > Eraser > Histone deacetylase	
HDAC class IIb	

► ChEMBL

11.6 EPA DSSTox Classification



4 items	View in Classification Browser
CompTox Chemicals Dashboard Chemical Lists > LIST ⌵ Show alternative paths [BLOODEXPOSOME] LIST: BLOODEXPOSOME Chemicals identified as part of the blood exposome Short_Description: Chemicals identified as part of the blood exposome	
CompTox Chemicals Dashboard Chemical Lists > EPA ⌵ Show alternative paths [REFCHEMDB] EPA LIST: Article "Workflow for Defining Reference Chemicals for Assessing Performance of In Vitro Assays" Short_Description: List of chemicals associated with the article "Workflow for Defining Reference Chemicals for Assessing Performance of In Vitro Assays"	
CompTox Chemicals Dashboard Chemical Lists > LIST ⌵ Show alternative paths [WIKIPEDIA] LIST: Wikipedia Chemicals_0131_2026 Short_Description: Wikipedia includes data for thousands of chemicals. ChemBoxes and DrugBoxes includes data such as CAS Registry Numbers, SMILES and InChIs.	
CompTox Chemicals Dashboard Chemical Lists > MISCELLANEOUS ⌵ Show alternative paths [CTD] Comparative Toxicogenomics Database Short_Description: CTD is a robust, publicly available database that aims to advance understanding about how environmental exposures affect human health.	

► EPA DSSTox

11.7 MolGenie Organic Chemistry Ontology



24 items	View in Classification Browser
MolGenie Organic Chemistry Ontology > ChEBI chemical entities > calculated properties	
lipophilic compounds Using a Fragment Based LogP from OpenChemLib > 5.	
MolGenie Organic Chemistry Ontology > ChEBI chemical entities > substructural concepts > scaffolds > simple organic compound scaffolds > benzene derivatives > alkyl benzene derivatives > methylbenzenes > trimethylbenzenes	
mesitylenes A trimethylbenzene carrying methyl substituents at positions 1, 3 and 5. ChEBI: 34833 MeSH: C010219	
MolGenie Organic Chemistry Ontology > PubChemLite chemical entities > substructural concepts > functional groups > nitrogen containing functional groups > amines > tertiary amines	
alkyl aryl tertiary amines	
MolGenie Organic Chemistry Ontology > ChEBI chemical entities > substructural concepts > scaffolds > simple organic compound scaffolds > benzene derivatives	
anilines	
MolGenie Organic Chemistry Ontology > PubChemLite chemical entities > substructural concepts > scaffolds > simple organic compound scaffolds > benzene derivatives > alkyl benzene derivatives > methylbenzenes > xylenes	
m-xylene A xylene carrying methyl groups at positions 1 and 3. ChEBI: 28488 MeSH: C031285	
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► MolGenie

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Antalarmin

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Antalarmin

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<https://gsrs.ncats.nih.gov/ginas/app/beta/substances/G3DNT7X7YL>

6. ChEBI

Antalarmin

<https://www.ebi.ac.uk/chebi/searchId.do?chebiId=ChEBI:139557>

ChEBI Ontology

<https://www.ebi.ac.uk/chebi/>

7. ChEMBL

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ANTALARMIN

<https://www.ebi.ac.uk/chembl/explore/compound/CHEMBL296641>

ChEMBL Protein Target Tree

<https://www.ebi.ac.uk/chembl/g/#browse/targets>

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