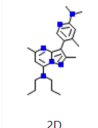
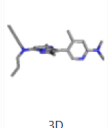


COMPOUND

R121919

PubChem CID	9821250
Structure	2D 3D
Molecular Formula	C ₂₂ H ₃₂ N ₆
Synonyms	R121919 R-121919 R 121919 3-(6-dimethylamino-4-methylpyridin-3-yl)-2,5-dimethyl-N,N-dipropylpyrazolo(5,1-b)pyrimidin-7-amine 3-(6-dimethylamino-4-methylpyridin-3-yl)-2,5-dimethyl-N,N-dipropylpyrazolo[5,1-b]pyrimidin-7-amine View More...
Molecular Weight	380.5 g/mol <i>Computed by PubChem 2.2 (PubChem release 2025.09.15)</i>
Dates	Create: 2006-10-25 Modify: 2026-05-23

Cite

Download

CONTENTS

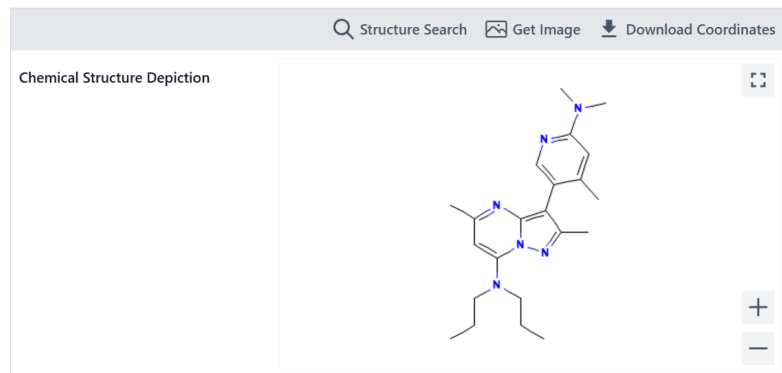
Title and Summary

- 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

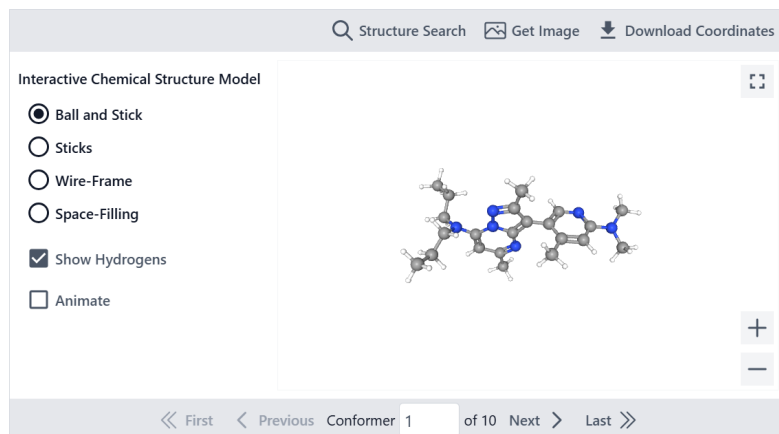
1 Structures



1.1 2D Structure



1.2 3D Conformer



PubChem

2 Names and Identifiers



2.1 Computed Descriptors



2.1.1 IUPAC Name



3-[6-(dimethylamino)-4-methyl-3-pyridinyl]-2,5-dimethyl-*N,N*-dipropylpyrazolo[1,5-*a*]pyrimidin-7-amine
Computed by Lexichem TK 2.9.3 (PubChem release 2025.09.15)

PubChem

2.1.2 InChI



InChI=1S/C22H32N6/c1-8-10-27(11-9-2)20-13-16(4)24-22-21(17(5)25-28(20)22)18-14-23-19(26(6)7)12-15(18)3/h12-14H,8-11H2,1-7H3
Computed by InChI 1.07.4 (PubChem release 2025.09.15)

PubChem

2.1.3 InChIKey



ANNRUWYFVIGKHA-UHFFFAOYSA-N
Computed by InChI 1.07.4 (PubChem release 2025.09.15)

PubChem

2.1.4 SMILES



CCCN(CCC)C1=CC(=NC2=C(C(=NN12)C)C3=CN=C(C=C3C)N(C)C)C
Computed by OEChem 4.2.0 (PubChem release 2025.09.15)

PubChem

2.2 Molecular Formula



C₂₂H₃₂N₆
Computed by PubChem 2.2 (PubChem release 2025.09.15)

PubChem

2.3 Other Identifiers



2.3.1 CAS



195055-03-9

► ChemIDplus; EPA DSSTox; FDA Global Substance Registration System (GSRS)

2.3.2 Deprecated CAS



292073-75-7

► ChemIDplus

2.3.3 UNII



G82N555U1N

► FDA Global Substance Registration System (GSRS)

2.3.4 ChEMBL ID



CHEMBL309138

► ChEMBL

2.3.5 DSSTox Substance ID



DTXSID00173162

► EPA DSSTox

2.3.6 HMDB ID



HMDB0244848

► Human Metabolome Database (HMDB)

2.3.7 Nikkaji Number



J1.775.143C

► Japan Chemical Substance Dictionary (Nikkaji)

2.3.8 Pharos Ligand ID



46P5BXHLK5CU

► Pharos

2.3.9 Wikidata



Q27088503

► Wikidata

2.4 Synonyms



2.4.1 MeSH Entry Terms



R 121919
R-121919
R121919

► Medical Subject Headings (MeSH)

2.4.2 Depositor-Supplied Synonyms

R121919	CHEMBL3
R-121919	3-[6-(dim
R 121919	3-[6-(dim
3-(6-dimethylamino-4-methylpyridin-3-yl)-2,5-dimethyl-N,N-dipropylpyrazolo[5,1-b]pyrimidin-7-amine	G82N555
3-(6-dimethylamino-4-methylpyridin-3-yl)-2,5-dimethyl-N,N-dipropylpyrazolo[5,1-b]pyrimidin-7-amine	R-121,919
RefChem:164905	Pyrazolo(
195055-03-9	UNII-G82
3-(6-(Dimethylamino)-4-methylpyridin-3-yl)-2,5-dimethyl-N,N-dipropylpyrazolo[1,5-a]pyrimidin-7-amine	ANNRUW
NBI-30775	GTPL3520
NBI 30775	orb170674

PubChem

3 Chemical and Physical Properties

3.1 Computed Properties

Property Name	Property Value	Reference
Molecular Weight	380.5 g/mol	Computed by PubChem 2.2 (PubChem release 2025.09.15)
XLogP3-AA	4.7	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	5	Computed by Cactvs 3.4.8.24 (PubChem release 2025.09.15)
Rotatable Bond Count	7	Computed by Cactvs 3.4.8.24 (PubChem release 2025.09.15)
Exact Mass	380.26884505 Da	Computed by PubChem 2.2 (PubChem release 2025.09.15)
Monoisotopic Mass	380.26884505 Da	Computed by PubChem 2.2 (PubChem release 2025.09.15)
Topological Polar Surface Area	49.6 Å²	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	480	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 2025.04.14)

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 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



500808323

► PubChem

4.3.2 Related Substances



All Count	162
Same Count	97
Mixture Count	65

► PubChem

4.3.3 Substances by Category



6 categories

 Download

Chemical Vendors (44)

BenchChem

PubChem SID: 445915035

External ID: B1676987

A2B Chem

PubChem SID: 444216749

External ID: AE80889

MolCore

PubChem SID: 446150283

External ID: DY100512

PubChem SID: 335962911

External ID: MC100512

BOC Sciences

PubChem SID: 341108510

External ID: 195055-03-9

Starshine Chemical

PubChem SID: 476004699

External ID: 2023-03-08C118

Pharmacore Co., Limited

PubChem SID: 522761528

External ID: 201310037

eNovation Chemicals

PubChem SID: 482821679

External ID: Y1325813

Key Organics/BIONET

PubChem SID: 480468257

External ID: MS-26233

LGC Standards

PubChem SID: 485269493

External ID: TRC-D461680

PubChem SID: 496017649

External ID: TRC-D461680-100MG

Biorbyt

PubChem SID: 516458752

External ID: orb1706740

MedChemexpress MCE

PubChem SID: 335988874

External ID: HY-14127

10X CHEM

PubChem SID: 491577466	External ID: TX00ACD9
Molport	
PubChem SID: 123393545	External ID: MolPort-009-200-030
Accel Scientific	
PubChem SID: 507638793	External ID: EC00ADDD
Angel Pharmatech Ltd.	
PubChem SID: 485719068	External ID: AG220351
Finetech Industry Limited	
PubChem SID: 347846178	External ID: FT-0767007
CymitQuimica	
PubChem SID: 470466746	External ID: CQ_195055-03-9
Biosynce Pharmatech	
PubChem SID: 500186357	External ID: BW11452
AChemBlock	
PubChem SID: 523383878	External ID: L22226
Alfa Chemistry	
PubChem SID: 486466314	External ID: ACM195055039
AA BLOCKS	
PubChem SID: 381971950	External ID: AA00AB4T
CATO Research Chemicals Inc. (Chemical Vendors, Research and Development)	
PubChem SID: 517903124	External ID: CP124716
AbaChemScene	
PubChem SID: 335988626	External ID: CS-6231
Ambinter	
PubChem SID: 373278671	External ID: Amb21864539
Synblock Inc	
PubChem SID: 170512574	External ID: AB21702
Smolecule	
PubChem SID: 438486479	External ID: S536784
TargetMol	
PubChem SID: 443843774	External ID: T16713
Mcule	
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AKos Consulting & Solutions	
PubChem SID: 163841125	External ID: AKOS016002213
001Chemical	
PubChem SID: 375782261	External ID: DY100512
Debye Scientific Co., Ltd	
PubChem SID: 387018230	External ID: DB-065875
eMolecules	
PubChem SID: 490798713	External ID: 300736013
Chem-Space.com Database	
PubChem SID: 434730011	External ID: CSSB00020617902
MuseChem	
PubChem SID: 355036611	External ID: R022288
RR Scientific	
PubChem SID: 472462227	External ID: R641850
Cooke Chemical Co., Ltd	
PubChem SID: 482347861	External ID: M5290135
SynHet - Synthetic Heterocycles	
PubChem SID: 506096184	External ID: CAS-195055-03-9
Angene Chemical	
PubChem SID: 521799799	External ID: AG00AB7L
Glxxx Labs Inc	
PubChem SID: 508633400	External ID: GLXC-07156
DC Chemicals	
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ChemoSapiens	
PubChem SID: 517673864	External ID: 463781
Excenen Pharmatech	
PubChem SID: 497399674	External ID: EX-A9425
Curation Efforts (12)	
BindingDB (Curation Efforts, Research and Development)	
PubChem SID: 104009905	External ID: 50116105
ChEMBL (Curation Efforts, Research and Development)	
PubChem SID: 103261565	External ID: ChEMBL309138
ChemIDplus (Curation Efforts, Governmental Organizations, Research and Development)	
PubChem SID: 163641963	External ID: 0195055039
Comparative Toxicogenomics Database (CTD) (Curation Efforts, Research and Development)	
PubChem SID: 53786946	External ID: C412383
Egon Willighagen, Department of Bioinformatics - BiGCaT, Maastricht University	
PubChem SID: 385652400	External ID: Q27088503
EPA DSSTox (Curation Efforts, Governmental Organizations, Research and Development)	
PubChem SID: 315733572	External ID: DTXSID00173162
FDA Global Substance Registration System (GSRS) (Curation Efforts, Governmental Organizations)	
PubChem SID: 198989082	External ID: G82N555U1N
Human Metabolome Database (HMDB) (Curation Efforts, Research and Development)	
PubChem SID: 447219388	External ID: HMDB0244848
IUPHAR/BPS Guide to PHARMACOLOGY (Curation Efforts, Research and Development)	
PubChem SID: 53801047	External ID: 3520
SureChEMBL (Curation Efforts, Research and Development)	
PubChem SID: 514292020	External ID: SCHEMBL29482251
PubChem SID: 231411451	External ID: SCHEMBL5600844
Wikidata	
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Governmental Organizations (6)	
ChemIDplus (Curation Efforts, Governmental Organizations, Research and Development)	
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EPA DSSTox (Curation Efforts, Governmental Organizations, Research and Development)	
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FDA Global Substance Registration System (GSRS) (Curation Efforts, Governmental Organizations)	
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Japan Chemical Substance Dictionary (Nikkaji)	
PubChem SID: 275641588	External ID: J1.775.143C
PATENTSCOPE (WIPO)	
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PubChem Reference Collection	
PubChem SID: 500808323	External ID: 164905
Journal Publishers (1)	
Springer Nature	
PubChem SID: 341724528	External ID: 28051527-460869447

Research and Development (16)	
BindingDB (Curation Efforts, Research and Development)	
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ChemIDplus (Curation Efforts, Governmental Organizations, Research and Development)	
PubChem SID: 163641963	External ID: 0195055039
Comparative Toxicogenomics Database (CTD) (Curation Efforts, Research and Development)	
PubChem SID: 53786946	External ID: C412383
EPA DSSTox (Curation Efforts, Governmental Organizations, Research and Development)	
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IBM	
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ICCB-Longwood Screening Facility, Harvard Medical School	
PubChem SID: 385154886	External ID: HMS3746007
IUPHAR/BPS Guide to PHARMACOLOGY (Curation Efforts, Research and Development)	
PubChem SID: 53801047	External ID: 3520
MolGenie	
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Novartis Institutes for BioMedical Research	
PubChem SID: 406841242	External ID: MOABOX:1368
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Legacy Depositors (31)	
3WAY PHARM INC (Chemical Vendors)	
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Adooq BioScience (Chemical Vendors)	
PubChem SID: 383545647	External ID: A13535
AK Scientific, Inc. (AKSCI) (Chemical Vendors)	
PubChem SID: 252458474	External ID: 0092AB
Amadis Chemical (Chemical Vendors)	
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Anward (Chemical Vendors)	
PubChem SID: 160826912	External ID: ANW-59414
Aurora Fine Chemicals LLC (Chemical Vendors)	
PubChem SID: 297447390	External ID: A13.107.232
BePharm Ltd. (Chemical Vendors)	
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Bic Biotech (Chemical Vendors)	
PubChem SID: 383452840	External ID: NSZB-A261838
BioChemPartner (Chemical Vendors)	
PubChem SID: 375568221	External ID: BCP23964
ChangChem (Chemical Vendors)	
PubChem SID: 249727181	External ID: CD-1823
Chemieliva Pharmaceutical Co., Ltd (Chemical Vendors)	
PubChem SID: 348873953	External ID: PBCM0392104
ChemSpider (Research and Development)	
PubChem SID: 44857210	External ID: 7996999

ChemTik (Chemical Vendors)	
PubChem SID: 163093065	External ID: CTK888151
Collaborative Drug Discovery, Inc. (Subscription Services)	
PubChem SID: 180387880	External ID: 1376671
Davey Lab, Department of Microbiology, NEIDL, Boston University (Research and Development)	
PubChem SID: 441298587	External ID: BRD-K00004717
DiscoveryGate (Subscription Services)	
PubChem SID: 24124712	External ID: 9821250
Founder Pharma (Chemical Vendors)	
PubChem SID: 250193094	External ID: FD08533
Hefei Hirisun Pharmatech Co., Ltd (Chemical Vendors)	
PubChem SID: 319437071	External ID: HR130240
iChemical Technology USA Inc (Chemical Vendors)	
PubChem SID: 354308350	External ID: EBD260575
King Scientific (Chemical Vendors)	
PubChem SID: 346403411	External ID: KS-000006AG
LabNetwork, a WuXi AppTec Company (Chemical Vendors)	
PubChem SID: 346691994	External ID: LN00191830
Lan Pharmatech (Chemical Vendors)	
PubChem SID: 433840555	External ID: LAN-B45904
NextBio (Subscription Services)	
PubChem SID: 78286784	External ID: 9821250
NextMove Software (Curation Efforts, Research and Development)	
PubChem SID: 223815564	External ID: ANNRUWYFVIGKHA-UHFFFAOYSA-N
OXCHEM CORPORATION (Chemical Vendors)	
PubChem SID: 255414332	External ID: AX8150177
SCRIPDB (Research and Development)	
PubChem SID: 141141919	External ID: US20100249138A1-20100930-C00016_1
THE BioTek (Chemical Vendors)	
PubChem SID: 434301419	External ID: bt-276593
Thomson Pharma (Journal Publishers, Subscription Services)	
PubChem SID: 14780138	External ID: 00003247
ToxPlanet (Subscription Services)	
PubChem SID: 319339429	External ID: ToxPlanet-MTK1MDU1LTAzLTk5ODIxMjUw
Tractus (Chemical Vendors)	
PubChem SID: 204405561	External ID: TC-148159
ZINC (Chemical Vendors)	
PubChem SID: 255791805	External ID: ZINC602283

► PubChem

4.4 Entrez Crosslinks



PubMed Count	8
Taxonomy Count	1
Gene Count	5

► PubChem

5 Chemical Vendors



42 vendors

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BenchChem

PubChem SID: 445915035

Purchasable Chemical: B1676987

A2B Chem

PubChem SID: 444216749

Purchasable Chemical: AE80889

MolCore

PubChem SID: 446150283

Purchasable Chemical: DY100512

PubChem SID: 335962911

Purchasable Chemical: MC100512

BOC Sciences

PubChem SID: 341108510

Purchasable Chemical: 195055-03-9

Starshine Chemical

PubChem SID: 476004699

Purchasable Chemical: 2023-03-08C118

Pharmacore Co., Limited

PubChem SID: 522761528

Purchasable Chemical: 201310037

eNovation Chemicals

PubChem SID: 482821679

Purchasable Chemical: Y1325813

Key Organics/BIONET

PubChem SID: 480468257

Purchasable Chemical: MS-26233

LGC Standards

PubChem SID: 485269493

Purchasable Chemical: TRC-D461680

PubChem SID: 496017649

Purchasable Chemical: TRC-D461680-100MG

Biorbyt

PubChem SID: 516458752

Purchasable Chemical: orb1706740

MedChemexpress MCE

PubChem SID: 335988874

Purchasable Chemical: HY-14127

10X CHEM

PubChem SID: 491577466

Purchasable Chemical: TX00ACD9

Molport

PubChem SID: 123393545

Purchasable Chemical: MolPort-009-200-030

Accel Scientific

PubChem SID: 507638793

Purchasable Chemical: EC00ADDD

Angel Pharmatech Ltd.

PubChem SID: 485719068

Purchasable Chemical: AG220351

Finetech Industry Limited

PubChem SID: 347846178

Purchasable Chemical: FT-0767007

CymitQuimica

PubChem SID: 470466746

Purchasable Chemical: CQ_195055-03-9

Biosynce Pharmatech

PubChem SID: 500186357

Purchasable Chemical: BW11452

ACheckBlock

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Purchasable Chemical: L22226

Alfa Chemistry

PubChem SID: 486466314

Purchasable Chemical: ACM195055039

AA BLOCKS

PubChem SID: 381971950

Purchasable Chemical: AA00AB4T

CATO Research Chemicals Inc. (Chemical Vendors, Research and Development)

PubChem SID: 517903124

Purchasable Chemical: CP124716

AbaChemScene

PubChem SID: 335988626

Purchasable Chemical: CS-6231

Ambinter

PubChem SID: 373278671

Purchasable Chemical: Amb21864539

Synblock Inc

PubChem SID: 170512574

Purchasable Chemical: AB21702

Smolecule

PubChem SID: 438486479

Purchasable Chemical: S536784

TargetMol	PubChem SID: 443843774	Purchasable Chemical: T16713
Mcule	PubChem SID: 492627638	Purchasable Chemical: MCULE-4600444159
AKos Consulting & Solutions	PubChem SID: 163841125	Purchasable Chemical: AKOS016002213
001Chemical	PubChem SID: 375782261	Purchasable Chemical: DY100512
Debye Scientific Co., Ltd	PubChem SID: 387018230	Purchasable Chemical: DB-065875
eMolecules	PubChem SID: 490798713	Purchasable Chemical: 300736013
Chem-Space.com Database	PubChem SID: 434730011	Purchasable Chemical: CSSB00020617902
MuseChem	PubChem SID: 355036611	Purchasable Chemical: R022288
RR Scientific	PubChem SID: 472462227	Purchasable Chemical: R641850
Cooke Chemical Co., Ltd	PubChem SID: 482347861	Purchasable Chemical: M5290135
SynHet - Synthetic Heterocycles	PubChem SID: 506096184	Purchasable Chemical: CAS-195055-03-9
Angene Chemical	PubChem SID: 521799799	Purchasable Chemical: AG00AB7L
Glix Labs Inc	PubChem SID: 508633400	Purchasable Chemical: GLXC-07156
DC Chemicals	PubChem SID: 341138560	Purchasable Chemical: DC10401
ChemoSapiens	PubChem SID: 517673864	Purchasable Chemical: 463781
Excenen Pharmatech	PubChem SID: 497399674	Purchasable Chemical: EX-A9425

► PubChem

6 Associated Disorders and Diseases



2 items Download		
Source Disease	Evidence ⓘ	Data Source
Chemical and Drug Induced Liver Injury	PMID:21618986	Comparative Toxicogenomics Database (CTD)
Depressive Disorder	PMID:21618986	Comparative Toxicogenomics Database (CTD)

► Comparative Toxicogenomics Database (CTD)

7 Literature



7.1 Consolidated References



25 items	Download
Search SORT BY Publication Date - Most Recent	
Blocking CRH receptors in adults mitigates age-related memory impairments provoked by early-life adversity Publication Name: Neuropsychopharmacology : official publication of the American College of Neuropsychopharmacology Publication Date: 2019-11-07 PMCID: PMC6969076 PMID: 31698409 DOI: 10.1038/s41386-019-0562-x	
Generating the Blood Exposome Database Using a Comprehensive Text Mining and Database Fusion Approach Publication Name: Environmental Health Perspectives Publication Date: 2019-09 PMCID: PMC6794490 PMID: 31557052 DOI: 10.1289/ehp4713	
Discovery of 4-chloro-2-(2,4-dichloro-6-methylphenoxy)-1-methyl-7-(pentan-3-yl)-1H-benzimidazole, a novel CRF1 receptor antagonist Publication Name: Bioorganic & Medicinal Chemistry Publication Date: 2017-03-01 PMID: 28174066 DOI: 10.1016/j.bmc.2016.11.011	
Design and Synthesis of Benzimidazoles As Novel Corticotropin-Releasing Factor 1 Receptor Antagonists Publication Name: Journal of Medicinal Chemistry Publication Date: 2016-03-07 PMID: 26901666 DOI: 10.1021/acs.jmedchem.5b01715	
Synthesis, binding affinity, radiolabeling, and microPET evaluation of 4-(2-substituted-4-substituted)-8-(dialkylamino)-6-methyl-1-substituted-3,4-dihydropyrido[2,3-b]pyrazin-2(1H)-ones as ligands for brain corticotropin-releasing factor type-1 (CRF1) receptors Publication Name: Bioorganic & Medicinal Chemistry Letters Publication Date: 2015-11-15 PMCID: PMC4628894 PMID: 26456805 DOI: 10.1016/j.bmcl.2015.10.010	
<< First < Previous Page 1 of 5 Next > Last >>	

► PubChem

7.2 NLM Curated PubMed Citations



All NLM Curated PubMed Citations	Download
► Medical Subject Headings (MeSH)	

7.3 Springer Nature References

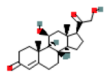
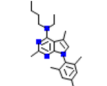


2 items	Download
 Identification of molecules potentially involved in mediating the in vivo actions of the corticotropin-releasing hormone receptor 1 antagonist, NBI30775 (R121919) PMID: 15682302 Publication Date: 2005 Publication Name: Psychopharmacology	
Blocking CRH receptors in adults mitigates age-related memory impairments provoked by early-life adversity PMID: 31698409 Publication Date: 2019 Publication Name: Neuropsychopharmacology	

► Springer Nature

7.4 Chemical Co-Occurrences in Literature



Showing 3 of 100 View More Co-Occurrence and Evidence Data ↗		Download
Chemical	Selected evidence	
 Corticotropin CID 16186200	32 articles View All ↗	
	Effects of the high-affinity corticotropin-releasing hormone receptor 1 antagonist R121919 in major depression: the first 20 patients treated PMID 10867111; DOI 10.1016/s0022-3956(00)00016-9; Journal of Psychiatric Research 2000-05-01	
	Consequences of chronic social stress on behaviour and vasopressin gene expression in the PVN of DBA/2OlaHsd mice--influence of treatment with the CRHR1-antagonist R121919/NBI 30775 PMID 18515457; DOI 10.1177/0269881108089813; Journal of psychopharmacology (Oxford, England) 2008-05-30	
 Corticosterone CID 5753	19 articles View All ↗	
	The Corticotropin-Releasing Factor1 Receptor Antagonist R121919 Attenuates the Behavioral and Endocrine Responses to Stress PMID 12538845; DOI 10.1124/jpet.102.042788; The Journal of Pharmacology and Experimental Therapeutics 2003-02-01 Name matches: corticosterone <i>r121919</i>	
	Persistent anxiolytic affects after chronic administration of the CRF1 receptor antagonist R121919 in rats PMID 20951149; DOI 10.1016/j.neuropharm.2010.10.004; Neuropharmacology 2011-06-01 Name matches: corticosterone <i>r121919</i>	
 CP-154526 CID 5311055	9 articles View All ↗	
	The effects of CRF antagonists, antalarmin, CP154,526, LWH234, and R121919, in the forced swim test and on swim-induced increases in adrenocorticotropin in rats PMID 15696320; DOI 10.1007/s00213-005-2164-z; Psychopharmacology 2005-02-05 Name matches: cp154,526 <i>r121919</i>	
	3-(4-Chloro-2-Morpholin-4-yl-Thiazol-5-yl)-8-(1-Ethylpropyl)-2,6-Dimethyl-Imidazo[1,2-b]Pyridazine: A Novel Brain-Penetrant, Orally Available Corticotropin-Releasing Factor Receptor 1 Antagonist with Efficacy in Animal Models of Alcoholism PMID 17344409; DOI 10.1523/jneurosci.4985-06.2007; The Journal of neuroscience : the official journal of the Society for Neuroscience 2007-03-07 Name matches: cp154526 <i>r121919</i>	
	Recent Advances in Small Molecule Antagonists of the Corticotropin- Releasing Factor Type-1 Receptor-Focus on Pharmacology and Pharmacokinetics PMID 16712469; DOI 10.2174/092986706776873014; Current Medicinal Chemistry 2006-05-01 (Review Article) Name matches: cp-154,526 <i>r121919</i>	

► PubChem

7.5 Chemical-Gene Co-Occurrences in Literature

Showing 3 of 88 View More Co-Occurrence and Evidence Data		Download
Gene/Protein/Enzyme	Selected evidence	
corticotropin releasing hormone receptor 1	63 articles	View All
	Consequences of chronic social stress on behaviour and vasopressin gene expression in the PVN of DBA/2OlaHsd mice--influence of treatment with the CRHR1-antagonist R121919/NBI 30775 PMID 18515457; DOI 10.1177/0269881108089813; Journal of psychopharmacology (Oxford, England) 2008-05-30 Name matches: <i>crhr1</i> <i>r121919</i> Persistent anxiolytic affects after chronic administration of the CRF1 receptor antagonist R121919 in rats PMID 20951149; DOI 10.1016/j.neuropharm.2010.10.004; Neuropharmacology 2011-06-01 Identification of molecules potentially involved in mediating the in vivo actions of the corticotropin-releasing hormone receptor 1 antagonist, NBI30775 (R121919) PMID 15682302; DOI 10.1007/s00213-004-2134-x; Psychopharmacology 2005-01-29	
	67 articles	View All
corticotropin releasing hormone	The anxiolytic effect of the CRH1 receptor antagonist R121919 depends on innate emotionality in rats PMID 11168542; DOI 10.1046/j.0953-816x.2000.01383.x; The European journal of neuroscience 2001-01-01 The effects of CRF antagonists, antalarmin, CP154,526, LWH234, and R121919, in the forced swim test and on swim-induced increases in adrenocorticotropin in rats PMID 15696320; DOI 10.1007/s00213-005-2164-z; Psychopharmacology 2005-02-05 Treatment with the CRH1-receptor-antagonist R121919 improves sleep-EEG in patients with depression PMID 14757326; DOI 10.1016/s0022-3956(03)00076-1; Journal of Psychiatric Research 2004-03-01 Name matches: <i>crh</i> <i>r121919</i>	
	13 articles	View All
proopiomelanocortin	The High-affinity Non-peptide CRH1Receptor Antagonist R121919 Attenuates Stress-induced Alterations in Plasma Oxytocin, Prolactin, and Testosterone Secretion in Rats PMID 12649771; DOI 10.1055/s-2003-38092; Pharmacopsychiatry 2003-01-01 The effects of CRF antagonists, antalarmin, CP154,526, LWH234, and R121919, in the forced swim test and on swim-induced increases in adrenocorticotropin in rats PMID 15696320; DOI 10.1007/s00213-005-2164-z; Psychopharmacology 2005-02-05 The anxiolytic effect of the CRH1 receptor antagonist R121919 depends on innate emotionality in rats PMID 11168542; DOI 10.1046/j.0953-816x.2000.01383.x; The European journal of neuroscience 2001-01-01	

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7.6 Chemical-Disease Co-Occurrences in Literature

Showing 3 of 50 View More Co-Occurrence and Evidence Data		Download
Disease	Selected evidence	
Anxiety Disorders	31 articlesView All	
	The CRH1 receptor antagonist R121919 attenuates stress-elicited sleep disturbances in rats, particularly in those with high innate anxiety PMID 12191624; DOI 10.1016/s0022-3956(02)00009-2; Journal of Psychiatric Research 2002-07-01 Name matches: anxiety <i>r121919</i> The High-affinity Non-peptide CRH1Receptor Antagonist R121919 Attenuates Stress-induced Alterations in Plasma Oxytocin, Prolactin, and Testosterone Secretion in Rats PMID 12649771; DOI 10.1055/s-2003-38092; Pharmacopsychiatry 2003-01-01 Name matches: anxiety <i>r121919</i> CRF-CRF1 Receptor System in the Central and Basolateral Nuclei of the Amygdala Differentially Mediates Excessive Eating of Palatable Food PMID 23748225; DOI 10.1038/npp.2013.147; Neuropsychopharmacology : official publication of the American College of Neuropsychopharmacology 2013-06-10 Name matches: anxiety <i>r121919</i>	
Depressive Disorder	20 articlesView All	
	Corticotropin-releasing hormone modulators and depression PMID 12625028; Current opinion in investigational drugs (London, England : 2000) 2003-01-01 (Review Article) Name matches: depression; depressive; depressives <i>r-121919</i> Treatment with the CRH1-receptor-antagonist R121919 improves sleep-EEG in patients with depression PMID 14757326; DOI 10.1016/s0022-3956(03)00076-1; Journal of Psychiatric Research 2004-03-01 Name matches: depression <i>r121919</i> Treatment of depression with the CRH-1-receptor antagonist R121919: endocrine changes and side effects PMID 14563384; DOI 10.1016/s0022-3956(03)00070-0; Journal of Psychiatric Research 2003-11-01 Name matches: depression <i>r121919</i>	
Striae Distensae	8 articlesView All	
	CRF-CRF1 Receptor System in the Central and Basolateral Nuclei of the Amygdala Differentially Mediates Excessive Eating of Palatable Food PMID 23748225; DOI 10.1038/npp.2013.147; Neuropsychopharmacology : official publication of the American College of Neuropsychopharmacology 2013-06-10 Name matches: stria <i>r121919</i> Chronic Stress Induces Maladaptive Behaviors by Activating Corticotropin-Releasing Hormone Signaling in the Mouse Oval Bed Nucleus of the Stria Terminalis PMID 32054675; DOI 10.1523/jneurosci.2410-19.2020; The Journal of neuroscience : the official journal of the Society for Neuroscience 2020-02-13 Name matches: stria <i>r121919</i> Protracted Withdrawal from Alcohol and Drugs of Abuse Impairs Long-Term Potentiation of Intrinsic Excitability in the Juxtacapsular Bed Nucleus of the Stria Terminalis PMID 19403807; DOI 10.1523/jneurosci.5129-08.2009; The Journal of neuroscience : the official journal of the Society for Neuroscience 2009-04-29 Name matches: stria <i>r121919</i>	

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7.7 Chemical-Organism Co-Occurrences in Literature

Showing 3 of 15 View More Co-Occurrence and Evidence Data Download

Organism	Selected evidence
rattus sp. (rats)	45 articlesView All Behavioral effects of the CRF1 receptor antagonist R121919 in rats selectively bred for high and low activity in the swim test PMID 18676086; DOI 10.1016/j.psyneuen.2008.05.003; Psychoneuroendocrinology 2008-09-01 Name matches: rats r121919 The CRH1 receptor antagonist R121919 attenuates stress-elicited sleep disturbances in rats, particularly in those with high innate anxiety PMID 12191624; DOI 10.1016/s0022-3956(02)00009-2; Journal of Psychiatric Research 2002-07-01 Name matches: rat; rats r121919 The anxiolytic effect of the CRH1 receptor antagonist R121919 depends on innate emotionality in rats PMID 11168542; DOI 10.1046/j.0953-816x.2000.01383.x; The European journal of neuroscience 2001-01-01 Name matches: rat; rats r121919
metazoa (animals)	25 articlesView All Persistent anxiolytic affects after chronic administration of the CRF1 receptor antagonist R121919 in rats PMID 20951149; DOI 10.1016/j.neuropharm.2010.10.004; Neuropharmacology 2011-06-01 Name matches: animals r121919 Corticotrophin releasing factor receptor 1 antagonists prevent chronic stress-induced behavioral changes and synapse loss in aged rats PMID 29477954; DOI 10.1016/j.psyneuen.2018.02.013; Psychoneuroendocrinology 2018-04-01 Name matches: animal; animals r121919 PRECLINICAL STUDY: Corticotropin-releasing factor-1 receptor antagonists decrease heroin self-administration in long- but not short-access rats PMID 19291009; DOI 10.1111/j.1369-1600.2008.00142.x; Addiction Biology 2009-03-05 Name matches: animals r121919
mus sp. (mice)	19 articlesView All Consequences of chronic social stress on behaviour and vasopressin gene expression in the PVN of DBA/2OlaHsd mice--influence of treatment with the CRHR1-antagonist R121919/NBI 30775 PMID 18515457; DOI 10.1177/0269881108089813; Journal of psychopharmacology (Oxford, England) 2008-05-30 Name matches: mice r121919 Evidence for independent actions of the CRF and ghrelin systems in binge-like alcohol drinking in mice PMID 40139339; DOI 10.1016/j.pnpbp.2025.111341; Progress in Neuro-Psychopharmacology and Biological Psychiatry 2025-04-02 Name matches: mice r121919 Increased Tau Phosphorylation and Aggregation in the Hippocampus of Mice Overexpressing Corticotropin-Releasing Factor PMID 25125464; DOI 10.3233/jad-141281; Journal of Alzheimer's disease : JAD 2014-12-02 Name matches: mice r121919

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8 Patents

8.1 Depositor-Supplied Patent Identifiers



157 items Download	
Search	SORT BY Priority Date - Most Recent
Mc2r modulator compounds	
Publication Number: WO-2024175925-A1	
Priority Date: 2023-02-23	
Mc2r modulator compounds	
Publication Number: WO-2024175928-A1	
Priority Date: 2023-02-23	
Mc2r modulator compounds	
Publication Number: WO-2024175927-A1	
Priority Date: 2023-02-23	
Treatment of congenital adrenal hyperplasia and polycystic ovary syndrome	
Publication Number: WO-2023163945-A1	
Priority Date: 2022-02-23	
Antagonist composition and application thereof in preparation of drug for treatment of sleep disorders with co-morbid psychiatric disorders	
Publication Number: WO-2023125112-A1	
Priority Date: 2021-12-29	
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[Link to all deposited patent identifiers](#)

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8.2 WIPO PATENTSCOPE



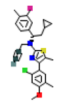
Patents are available for this chemical structure:

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

► PATENTSCOPE (WIPO)

8.3 Chemical Co-Occurrences in Patents

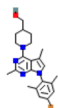


Showing 3 of 100 View More Co-Occurrence and Evidence Data Download	
Chemical	Selected evidence
 4-(2-Chloro-4-methoxy-5-methylphenyl)-N-((1S)-2-cyclopropyl-1-(3-fluoro-4-methylphenyl)ethyl)-5-methyl-N-2-propyn-1-yl-2-thiazolamine CID 5282340	11 patents from 6 patent families View All Treatment and prevention of tauopathies and amyloid beta amyloidosis by modulating CRF receptor signaling EP-2522351-B1; Grant Date: 2017-09-06 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
	7 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

3-(4-methoxy-2-methylphenyl)-2,5-dimethyl-N-pentan-3-ylpyrazolo[1,5-a]pyrimidin-7-amine
CID 9884878

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-11730739-B2; Grant Date: 2023-08-22



4-Piperidinemethanol, 1-(7-(4-bromo-2,6-dimethylphenyl)-2,5-dimethyl-7H-pyrrolo(2,3-d)pyrimidin-4-yl)-
CID 10478567

6 patents from 2 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-10837062-B2; Grant Date: 2020-11-17

Treatment of congenital adrenal hyperplasia
US-11730739-B2; Grant Date: 2023-08-22

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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	
Tauopathies	1 patent from 1 patent family Treatment and prevention of tauopathies and amyloid beta amyloidosis by modulating CRF receptor signaling EP-2522351-B1; Grant Date: 2017-09-06	View All
Amyloidosis	1 patent from 1 patent family Treatment and prevention of tauopathies and amyloid beta amyloidosis by modulating CRF receptor signaling EP-2522351-B1; Grant Date: 2017-09-06	View All
Pantothenate Kinase-Associated Neurodegeneration	1 patent from 1 patent family Treatment and prevention of tauopathies and amyloid beta amyloidosis by modulating CRF receptor signaling EP-2522351-B1; Grant Date: 2017-09-06	View All

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8.5 Chemical-Gene Co-Occurrences in Patents



Showing 3 of 34 View More Co-Occurrence and Evidence Data ↗		Download
Gene	Selected evidence	
avpr1b	5 patents from 2 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-10837062-B2; Grant Date: 2020-11-17 V1B receptor antagonist for use in the treatment of patients having elevated AVP levels and / or elevated copeptin levels JP-6309511-B2; Grant Date: 2018-04-11	
crhr1	6 patents from 3 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-10837062-B2; Grant Date: 2020-11-17 Treatment and prevention of tauopathies and amyloid beta amyloidosis by modulating CRF receptor signaling EP-2522351-B1; Grant Date: 2017-09-06 V1B receptor antagonist for use in the treatment of patients having elevated AVP levels and / or elevated copeptin levels JP-6309511-B2; Grant Date: 2018-04-11	
crhr2	4 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 V1B receptor antagonist for use in the treatment of patients having elevated AVP levels and / or elevated copeptin levels JP-6309511-B2; Grant Date: 2018-04-11	

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8.6 Chemical-Organism Co-Occurrences in Patents



Showing 3 of 35 View More Co-Occurrence and Evidence Data ↗		Download
Organism	Selected evidence	
rodentia (rodents)	3 patents from 2 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-10837062-B2; Grant Date: 2020-11-17 Treatment and prevention of tauopathies and amyloid beta amyloidosis by modulating CRF receptor signaling EP-2522351-B1; Grant Date: 2017-09-06	
salvia officinalis (garden sage)	2 patents from 1 patent family 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-10837062-B2; Grant Date: 2020-11-17	
entandrophragma utile	1 patent from 1 patent family 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-10837062-B2; Grant Date: 2020-11-17	

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9 Interactions and Pathways



9.1 Chemical-Target Interactions



8 items Download					
Search			SORT BY Data Source - A to Z		
Protein	Gene	Taxonomy	Action	Evidence	Data Source
	POMC	Rattus norvegicus (Norway rat)	R 121919 inhibits the reaction [lipopolysaccharides results in decreased secretion of POMC protein alternative form] r 121919 inhibits the reaction [ethanol results in decreased secretion of POMC protein alternative form]	PMID:12746300	Comparative Toxicogenomics Database (CTD)
	CRHR1	Rattus norvegicus (Norway rat)	R 121919 binds to and results in decreased activity of CRHR1 protein	PMID:21220416	Comparative Toxicogenomics Database (CTD)
	TNF	Rattus norvegicus (Norway rat)	R 121919 promotes the reaction [lipopolysaccharides results in increased secretion of TNF protein]	PMID:12746300	Comparative Toxicogenomics Database (CTD)
	ALAS2	Homo sapiens (human)	Inhibitor		Drug Gene Interaction database (DGIdb)
Corticotropin-releasing factor receptor 1	CRHR1	Homo sapiens (human)	Antagonist	PMID:10867111	IUPHAR/BPS Guide to PHARMACOLOGY

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

10 Biological Test Results



10.1 BioAssay Results



74 items Download	
Search	
SORT BY Activity Value - Increasing	
Binding affinity to recombinant human CRF1 receptor expressed in CHO cells Activity Outcome: Active Activity Type: Kd Activity Value: 0.000303 µM BioAssay AID: 622092 Target Name: LINC02210-CRHR1 - LINC02210-CRHR1 readthrough (human) Substance SID: 103261565 Compound CID: 9821250	
Binding affinity to recombinant human CRF1 receptor expressed in CHO cells Activity Outcome: Active Activity Type: Kd Activity Value: 0.000303 µM BioAssay AID: 622092 Target Name: CRHR1 - corticotropin releasing hormone receptor 1 (human) Substance SID: 103261565 Compound CID: 9821250	
Displacement of [125I]-Tyr0-sauvagine from human CRF1 receptor expressed in HEK293T cells after 2 hrs by scintillation counting Activity Outcome: Active Activity Type: Ki Activity Value: 0.002600 µM BioAssay AID: 1253854 Target Name: CRHR1 - corticotropin releasing hormone receptor 1 (human) Substance SID: 103261565 Compound CID: 9821250	
Displacement of [125I]-Tyr0-sauvagine from human CRF1 receptor expressed in HEK293T cells after 2 hrs by scintillation counting Activity Outcome: Active Activity Type: Ki Activity Value: 0.002600 µM BioAssay AID: 1253854	

Target Name: LINC02210-CRHR1 - LINC02210-CRHR1 readthrough (human)

Substance SID: [103261565](#) Compound CID: [9821250](#)

Displacement of [¹²⁵I]sauvagine from human CRF1 receptor expressed in IMR32 cells

Activity Outcome: [Active](#) Activity Type: Ki Activity Value: 0.003000 µM

BioAssay AID: [362068](#)

Target Name: LINC02210-CRHR1 - LINC02210-CRHR1 readthrough (human)

Substance SID: [103261565](#) Compound CID: [9821250](#)

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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 > Pyrimidines

[R 121919](#)

MeSH Concept: [M0368498](#)

MeSH Descriptor: [C412383](#)

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

11.2 ChemIDplus



9 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 (NCSU).

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

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► [ChemIDplus](#)

11.3 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. CRF₁ and CRF₂ receptors are activated non-selectively by CRH and UCN. CRF₂ receptors are selectively activated by UCN2 and UCN3. Binding to CRF receptors can be conducted using radioligands [¹²⁵I]Tyr⁰-CRF or [¹²⁵I]Tyr⁰-sauvagine with K_d values of 0.1-0.4 nM. CRF₁ and CRF₂ receptors are non-selectively antagonized by α-helical CRF, D-Phe-CRF-(12-41) and astressin. CRF₁ receptors are selectively antagonized by small molecules NBI27914, R121919, antalarmin, CP 154,526, CP 376,395. CRF₂ receptors are selectively antagonized by antisauvagine and astressin 2B. Although selective small molecule CRF₁ 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 CRF₁ receptor antagonists effectively reduce adrenocortical androgens and precursors in congenital adrenal hyperplasia.

► [IUPHAR/BPS Guide to PHARMACOLOGY](#)

11.4 ChEMBL Target Tree



2 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](#)

11.5 EPA DSSTox Classification



3 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](#)

[FDAUNII0421] LIST: FDA UNII List April 12th 2021 Download

Short_Description: FDA's Global Substance Registration System Unique Ingredient Identifiers (UNII)s file: April 12th 2021 download subset of chemicals with CASRN and/or structure SMILES

► [EPA DSSTox](#)

11.6 MolGenie Organic Chemistry Ontology



14 items	View in Classification Browser
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 > PubChemLite chemical entities > calculated properties	
drug like compounds	
Using a Fragment Based Druglikeness from OpenChemLib > -1	
MolGenie Organic Chemistry Ontology > PubChemLite chemical entities > substructural concepts > scaffolds > ring systems > plain ring systems > 3-membered ring systems > ring size 5,6,9	
pyrazolo[1,5-a]pyrimidines	
MolGenie Organic Chemistry Ontology > ChEMBL chemical entities > substructural concepts > scaffolds > ring systems > plain ring systems > 1-membered ring systems > ring size 6	
pyridines	
MolGenie Organic Chemistry Ontology > ChEMBL chemical entities > substructural concepts > scaffolds > simple organic compound scaffolds	
biaryls	
◀ First < Previous Page 1 of 3 Next > Last ▶	

► MolGenie

12 Information Sources



FILTER BY SOURCE

ALL SOURCES

1. ChEMBL

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<http://www.ebi.ac.uk/Information/termsofuse.html>

CHEMBL309138

<https://www.ebi.ac.uk/chembl/explore/compound/CHEMBL309138>

ChEMBL Protein Target Tree

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

2. ChemIDplus

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