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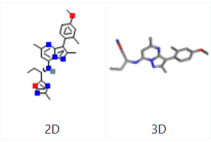
COMPOUND

Verucerfont

PubChem CID	11596613
Structure	 2D 3D
Primary Hazards	Irritant Health Hazard Laboratory Chemical Safety Summary (LCSS) Datasheet
Molecular Formula	$C_{22}H_{26}N_6O_2$
Synonyms	VERUCERFONT 885220-61-1 GSK561679 GSK561679A GSK-561679 View More...
Molecular Weight	406.5 g/mol *Computed by PubChem 2.2 (PubChem release 2025.04.14)*
Dates	Create: 2006-10-26 Modify: 2026-05-23
Description	Verucerfont has been used in trials studying the treatment of Congenital Adrenal Hyperplasia. DrugBank

Cite Download

CONTENTS

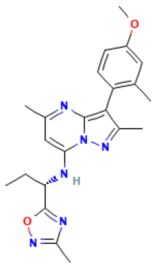
Title and Summary
1 Structures
2 Names and Identifiers
3 Chemical and Physical Properties
4 Related Records
5 Chemical Vendors
6 Drug and Medication Information
7 Safety and Hazards
8 Associated Disorders and Diseases
9 Literature
10 Patents
11 Interactions and Pathways
12 Biological Test Results
13 Classification
14 Information Sources

1 Structures

1.1 2D Structure

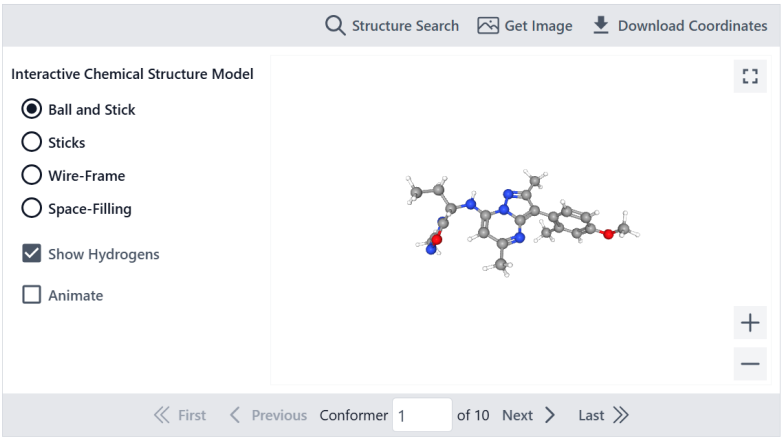
Structure Search Get Image Download Coordinates

Chemical Structure Depiction



PubChem

1.2 3D Conformer



PubChem

2 Names and Identifiers

2.1 Computed Descriptors

2.1.1 IUPAC Name

3-(4-methoxy-2-methylphenyl)-2,5-dimethyl-*N*-[(1*S*)-1-(3-methyl-1,2,4-oxadiazol-5-yl)propyl]pyrazolo[1,5-a]pyrimidin-7-amine

Computed by Lexichem TK 2.7.0 (PubChem release 2025.04.14)

PubChem

2.1.2 InChI

InChI=1S/C22H26N6O2/c1-7-18(22-24-15(5)27-30-22)25-19-11-13(3)23-21-20(14(4)26-28(19)21)17-9-8-16(29-6)10-12(17)2/h8-11,18,25H,7H2,1-6H3/t18-/m0/s1

Computed by InChI 1.07.2 (PubChem release 2025.04.14)

PubChem

2.1.3 InChIKey

VKHVAUKFLBBZFJ-SFHVURJKSA-N

Computed by InChI 1.07.2 (PubChem release 2025.04.14)

PubChem

2.1.4 SMILES

CC[C@@H](C1=NC(=NO1)C)NC2=CC(=NC3=C(C(=NN23)C)C4=C(C=C(C=C4)OC)C)C

Computed by OEChem 2.3.0 (PubChem release 2025.04.14)

PubChem

2.2 Molecular Formula

$C_{22}H_{26}N_6O_2$

Computed by PubChem 2.2 (PubChem release 2025.04.14)

PubChem

2.3 Other Identifiers

2.3.1 CAS

885220-61-1

- CAS Common Chemistry; ChemIDplus; DrugBank; EPA DSSTox; European Chemicals Agency (ECHA); FDA Globa···

2.3.2 European Community (EC) Number

629-872-6

- European Chemicals Agency (ECHA)

2.3.3 UNII

X60608B091

- FDA Global Substance Registration System (GSRS)

2.3.4 ChEMBL ID

CHEMBL1287935

- ChEMBL; Open Targets

2.3.5 DrugBank ID

DB12512

- DrugBank

2.3.6 DSSTox Substance ID

DTXSID501032013

- EPA DSSTox

2.3.7 International Nonproprietary Names (INN)

VERUCERFONT

- FDA Global Substance Registration System (GSRS)

2.3.8 KEGG ID

D09695

- KEGG

2.3.9 Metabolomics Workbench ID

153488

- Metabolomics Workbench

2.3.10 NCI Thesaurus Code

C152869

- NCI Thesaurus (NCIt)

2.3.11 Pharos Ligand ID

4W43ZXF751KD

Pharos

2.3.12 United States Adopted Name (USAN)

VERUCERFONT

FDA Global Substance Registration System (GSRS)

2.3.13 Wikidata

Q21098847

Wikidata

2.3.14 Wikipedia

Verucerfont

Wikipedia

2.4 Synonyms

2.4.1 Depositor-Supplied Synonyms

VERUCERFONT	GSK-561,679
885220-61-1	VERUCERFONT [WHO-DD]
GSK561679	3-(4-METHOXY-2-METHYLPHENYL)-2,5-DIMETHYL-N-[(1S)-1-(3-METHYL-1,2,4-OXADIAZOL YL)PROPYL]PYRAZOLO[1,5-A]PYRIMIDIN-7-AMINE
GSK561679A	
GSK-561679	X60608B091
NBI-77860	DTXSID501032013
Verucerfont [USAN]	Compound (S)-8d [PMID: 21074436]
Verucerfont [USAN:INN]	PYRAZOLO(1,5-A)PYRIMIDIN-7-AMINE, 3-(4-METHOXY-2-METHYLPHENYL)-2,5-DIMETHYL 1,2,4-OXADIAZOL-5-YL)PROPYL)-
GSK-561679A	
VERUCERFONT [INN]	Compound (S)-8d (PMID: 21074436)

PubChem

3 Chemical and Physical Properties

3.1 Computed Properties

Property Name	Property Value	Reference
Molecular Weight	406.5 g/mol	Computed by PubChem 2.2 (PubChem release 2025.04.14)
XLogP3-AA	4.5	Computed by XLogP3 3.0 (PubChem release 2025.04.14)
Hydrogen Bond Donor Count	1	Computed by Cactvs 3.4.8.18 (PubChem release 2025.04.14)
Hydrogen Bond Acceptor Count	7	Computed by Cactvs 3.4.8.18 (PubChem release 2025.04.14)
Rotatable Bond Count	6	Computed by Cactvs 3.4.8.18 (PubChem release 2025.04.14)
Exact Mass	406.21172409 Da	Computed by PubChem 2.2 (PubChem release 2025.04.14)
Monoisotopic Mass	406.21172409 Da	Computed by PubChem 2.2 (PubChem release 2025.04.14)
Topological Polar Surface Area	90.4 $Å^2$	Computed by Cactvs 3.4.8.18 (PubChem release 2025.04.14)
Heavy Atom Count	30	Computed by PubChem
Formal Charge	0	Computed by PubChem

Complexity	568	Computed by Cactvs 3.4.8.18 (PubChem release 2025.04.14)
Isotope Atom Count	0	Computed by PubChem
Defined Atom Stereocenter Count	1	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

3.2 Chemical Classes

3.2.1 Drugs

Pharmaceuticals -> Listed in ZINC15

S55 | ZINC15PHARMA | Pharmaceuticals from ZINC15 | DOI:10.5281/zenodo.3247749

NORMAN Suspect List Exchange

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	4
Same Stereo Count	2
Same Isotope Count	3
Same Parent, Connectivity Count	4
Same Parent, Stereo Count	2
Same Parent, Isotope Count	3
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

505897748

PubChem

4.3.2 Related Substances

Same Count	84

PubChem

4.3.3 Substances by Category

6 categories — Download

- Chemical Vendors (43) +
- Curation Efforts (14) +
- Governmental Organizations (5) +
- Journal Publishers (1) +
- Research and Development (18) +
- Legacy Depositors (17) +

PubChem

4.4 Entrez Crosslinks

PubMed Count	4
Gene Count	1

PubChem

5 Chemical Vendors

41 vendors — Download

TargetMol
PubChem SID: 443842567 — Purchasable Chemical: T7361

Accel Scientific
PubChem SID: 507673880 — Purchasable Chemical: EC00H530

Chem-Space.com Database
PubChem SID: 435910002 — Purchasable Chemical: CSSB00102563426

RR Scientific
PubChem SID: 472462229 — Purchasable Chemical: R781208

Mcule
PubChem SID: 493125912 — Purchasable Chemical: MCULE-5962496210
PubChem SID: 493112345 — Purchasable Chemical: MCULE-7710130017

10X CHEM
PubChem SID: 491613607 — Purchasable Chemical: TX00H42W

MuseChem
PubChem SID: 355035968 — Purchasable Chemical: I010023

A2B Chem
PubChem SID: 444220622 — Purchasable Chemical: AH96740

Key Organics/BIONET
PubChem SID: 480468993 — Purchasable Chemical: MS-26970

Combi-Blocks
PubChem SID: 482634779 — Purchasable Chemical: HB-8426

Debye Scientific Co., Ltd
PubChem SID: 496733002 — Purchasable Chemical: DA-68574

Smolecule
PubChem SID: 438492112 — Purchasable Chemical: S546717

AbMole Bioscience
PubChem SID: 387061193 — Purchasable Chemical: M6198

AA BLOCKS
PubChem SID: 381973416 — Purchasable Chemical: AA00H2UG

Angene Chemical
PubChem SID: 521838336 — Purchasable Chemical: AG00H2X8

001Chemical

PubChem SID: 375744257 Purchasable Chemical: DY445239

Alfa Chemistry
PubChem SID: 528047375 Purchasable Chemical: PR885220611

ChemShuttle
PubChem SID: 348269967 Purchasable Chemical: 182880

BenchChem
PubChem SID: 446489178 Purchasable Chemical: B1683048

Accela ChemBio Inc.
PubChem SID: 517749494 Purchasable Chemical: SY235580

AbaChemScene
PubChem SID: 348479975 Purchasable Chemical: CS-8099

Hangzhou APIChem Technology
PubChem SID: 374387154 Purchasable Chemical: AC-30339

eMolecules
PubChem SID: 490911654 Purchasable Chemical: 89940724

Excenen Pharmatech
PubChem SID: 363706825 Purchasable Chemical: EX-A1718

MedChemexpress MCE
PubChem SID: 350079950 Purchasable Chemical: HY-14875

CymitQuimica
PubChem SID: 470757926 Purchasable Chemical: CQ_885220-61-1

eNovation Chemicals
PubChem SID: 508698167 Purchasable Chemical: Y1299664

InvivoChem
PubChem SID: 500197673 Purchasable Chemical: V3636

DempoChem
PubChem SID: 523960283 Purchasable Chemical: 885220-61-1

Molport
PubChem SID: 383007523 Purchasable Chemical: MolPort-046-418-170

DC Chemicals
PubChem SID: 363538650 Purchasable Chemical: DC10766

Starshine Chemical
PubChem SID: 476036823 Purchasable Chemical: 2023-03-14B3189

Glixx Labs Inc
PubChem SID: 495944872 Purchasable Chemical: GLXC-15284

SynHet - Synthetic Heterocycles
PubChem SID: 506250589 Purchasable Chemical: CAS-885220-61-1

BOC Sciences
PubChem SID: 441157858 Purchasable Chemical: 885220-61-1
PubChem SID: 488427644 Purchasable Chemical: B0084-460213

AstaTech, Inc.
PubChem SID: 445663879 Purchasable Chemical: 43741

ChemoSapiens
PubChem SID: 517542691 Purchasable Chemical: 482878

BLD Pharm
PubChem SID: 375934943 Purchasable Chemical: BD00787381

Biorbyt
PubChem SID: 516423428 Purchasable Chemical: orb1299884

AChemBlock
PubChem SID: 523359272 Purchasable Chemical: Q65456

Ambinter
PubChem SID: 369108591 Purchasable Chemical: Amb24093379

▸ PubChem

6 Drug and Medication Information

6.1 Drug Indication

6 items Download

Search SORT BY MeSH Heading - A to Z

MeSH Heading	EFO Term	Max Phase
Adrenal Hyperplasia, Congenital	congenital adrenal hyperplasia	Phase 1
Alcoholism	alcohol dependence	Phase 2
Depressive Disorder, Major	major depressive disorder	Phase 2
Irritable Bowel Syndrome	irritable bowel syndrome	Phase 2
Phobia, Social	social anxiety disorder	Phase 1

First Previous Page 1 of 2 Next Last

ChEMBL

6.2 Clinical Trials

6.2.1 ClinicalTrials.gov

9 items Download

Search SORT BY Date - Most Recent

Analyzing Female Trauma Exposed Responses to a Medication
CTID: NCT01814332
Phase: Phase 2 **Status:** Completed
Date: 2021-06-25

A Study of the Effects of a New Antidepressant Treatment (GSK561679) in Females With Major Depressive Disorder
CTID: NCT00733980
Phase: Phase 2 **Status:** Completed
Date: 2017-11-17

To Investigate Effects GSK561679 on Part of the Body's System That Controls the Balance of Many of the Hormones.
CTID: NCT00426608
Phase: Phase 1 **Status:** Completed
Date: 2017-09-11

A Study To Compare The Putative Anxiolytic Effect Of 2 New Drugs In Subjects With Social Anxiety Disorder
CTID: NCT00555139
Phase: Phase 1 **Status:** Completed
Date: 2017-08-04

Evaluation of GSK561679 in Women With Post-Traumatic Stress Disorder
CTID: NCT01018992
Phase: Phase 2 **Status:** Completed
Date: 2017-03-07

First Previous Page 1 of 2 Next Last

ClinicalTrials.gov

6.2.2 EU Clinical Trials Register

2 items Download

A double-blind, randomised, placebo controlled, three-period crossover study to investigate the pharmacodynamic effect of two CRF-1 antagonists GSK561679 and GW876008 on meal induced cortisol responses in patients with IBS.

EudraCT: 2007-000929-22

Phase: Phase 2 **Status:** Prematurely Ended

Date: 2007-07-06

Estudio doble ciego, aleatorizado, controlado con placebo y alprazolam, de diseño cruzado con tres periodos y bloques incompletos, para comparar mediante Resonancia Magnética Funcional, las posibles propiedades ansiolíticas de GW876008 y GSK561679, tras la administración de una dosis única, en sujetos con trastorno de fobia social.

EudraCT: 2006-004212-48

Phase: Phase 2 **Status:** Completed

Date: 2007-01-24

▸ EU Clinical Trials Register

6.3 EMA Drug Information

1 item Download

Category/Dataset: Orphan designations

Active Substance: verucerfont

Status: Withdrawn

Therapeutic Use: Treatment of congenital adrenal hyperplasia

Publish Date: 2015-10-02 **Update Date:** 2016-02-10

▸ European Medicines Agency (EMA)

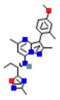
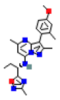
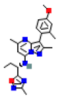
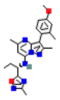
6.4 Drug Development Summary

Max Phase	Phase 2

▸ ChEMBL

6.5 Drug Targets

5 items Download

Structure	Gene	Protein	Open Targets Target ID
	CRHR1	corticotropin releasing hormone receptor 1	ENSG00000120088
	CRHR1	corticotropin releasing hormone receptor 1	ENSG00000120088
	CRHR1	corticotropin releasing hormone receptor 1	ENSG00000120088
	CRHR1	corticotropin releasing hormone receptor 1	ENSG00000120088

CRHR1	corticotropin releasing hormone receptor 1	ENSG00000120088

▸ Open Targets

7 Safety and Hazards

7.1 Hazards Identification

7.1.1 GHS Classification

Pictogram(s)	Irritant, Health Hazard
Signal	Warning
GHS Hazard Statements	H302 (100%): Harmful if swallowed [Warning Acute toxicity, oral] H361 (100%): Suspected of damaging fertility or the unborn child [Warning Reproductive toxicity]
Precautionary Statement Codes	P203, P264, P270, P280, P301+P317, P318, P330, P405, and P501
ECHA C&L Notifications Summary	*Aggregated GHS information provided per 2 reports by companies from 2 notifications to the ECHA C&L Inventory. Each notification may be associated with multiple companies.* *Information may vary between notifications depending on impurities, additives, and other factors. The percentage value in parenthesis indicates the notified classification ratio from companies that provide hazard codes. Only hazard codes with percentage values above 10% are shown. For more detailed information, please visit ECHA C&L website.*

▸ European Chemicals Agency (ECHA)

7.1.2 Hazard Classes and Categories

Acute Tox. 4 (100%)

Repr. 2 (100%)

▸ European Chemicals Agency (ECHA)

8 Associated Disorders and Diseases

6 items — Download

Search — SORT BY Source Disease - A to Z

Source Disease	Data Source
Adrenal Hyperplasia, Congenital	ChEMBL
Alcoholism	ChEMBL
Depressive Disorder, Major	ChEMBL
Irritable Bowel Syndrome	ChEMBL
Phobia, Social	ChEMBL

First Previous Page 1 of 2 Next Last

▸ Therapeutic Target Database (TTD)

9 Literature

9.1 Consolidated References

38 items Download

Search SORT BY Publication Date - Most Recent

BNST CRF receptor type 1 modulates mechanical hypersensitivity induced by adolescent alcohol exposure in adult female mice
Publication Name: Psychopharmacology
Publication Date: 2024-09-30
PMCID: PMC12884584 **PMID:** 39348004 **DOI:** 10.1007/s00213-024-06693-8

Genetic analyses point to alterations in immune-related pathways underpinning the association between psychiatric disorders and COVID-19
Publication Name: Molecular Psychiatry
Publication Date: 2024-07-03
PMID: 38956374 **DOI:** 10.1038/s41380-024-02643-0

A Neuroanatomic and Pathophysiologic Framework for Novel Pharmacological Approaches to the Treatment of Post-traumatic Stress Disorder
Publication Name: Drugs
Publication Date: 2024-02
PMID: 38413493 **DOI:** 10.1007/s40265-023-01983-5

Adrenal Insufficiency
Publication Name: Pediatric Endocrinology
Publication Date: 2024
DOI: 10.1007/978-3-031-66296-6_10

Endocrinological Treatment Targets for Depressive Disorder
Publication Name: Recent Advances and Challenges in the Treatment of Major Depressive Disorder
Publication Date: 2024
PMID: 39261421 **DOI:** 10.1007/978-981-97-4402-2_1

First Previous Page 1 of 8 Next Last

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9.2 Springer Nature References

32 items Download

Search SORT BY Publication Date - Oldest

Adrenal Insufficiency
Publication Date: 2024
Publication Name: Pediatric Endocrinology

The hormone trigger in PTSD
Publication Date: 2011
Publication Name: Science-Business eXchange

Depressing Times
Publication Date: 2002
Publication Name: Pharmaceutical Innovation

Effect of the CRF1-receptor antagonist pexacerfont on stress-induced eating and food craving
PMID: 27595147
Publication Date: 2016

Publication Name: Psychopharmacology

Evaluation of a corticotropin releasing hormone type 1 receptor antagonist in women with posttraumatic stress disorder: study protocol for a randomized controlled trial

PMID: 24950747

Publication Date: 2014

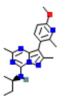
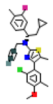
Publication Name: Trials

First Previous Page 1 of 7 Next Last

Springer Nature

9.3 Chemical Co-Occurrences in Literature

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

Chemical	Selected evidence
 Pexacerfont CID 9884366	9 articles View All Behavioral, biological, and chemical perspectives on targeting CRF(1) receptor antagonists to treat alcoholism PMID 23294766; DOI 10.1016/j.drugalcdep.2012.12.017; Drug and Alcohol Dependence 2013-03-01 (Review Article) The Role of fMRI in Drug Development: An Update PMID 36928856; DOI 10.1007/978-3-031-21054-9_13; Drug Development in Psychiatry 2023-01-01 Corticotropin releasing factor-binding protein (CRF-BP) as a potential new therapeutic target in Alzheimer's disease and stress disorders PMID 31641098; DOI 10.1038/s41398-019-0581-8; Translational Psychiatry 2019-10-22 (Review Article)
Oxadiazole CID 10197612	8 articles View All The CRH1 Antagonist GSK561679 Increases Human Fear But Not Anxiety as Assessed by Startle PMID 25430779; DOI 10.1038/npp.2014.316; Neuropsychopharmacology : official publication of the American College of Neuropsychopharmacology 2014-11-28 Evaluation of a corticotropin releasing hormone type 1 receptor antagonist in women with posttraumatic stress disorder: study protocol for a randomized controlled trial PMID 24950747; DOI 10.1186/1745-6215-15-240; Trials 2014-06-21 Corticotropin-Releasing Factor Receptor 1 Antagonism Is Ineffective for Women With Posttraumatic Stress Disorder PMID 28793974; DOI 10.1016/j.biopsych.2017.06.024; Biological Psychiatry 2017-12-15
 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	3 articles View All The CRF1 receptor antagonist SSR125543 prevents stress-induced cognitive deficit associated with hippocampal dysfunction: Comparison with paroxetine and d-cycloserine PMID 23407783; DOI 10.1007/s00213-013-3020-1; Psychopharmacology 2013-02-14 Behavioral, biological, and chemical perspectives on targeting CRF(1) receptor antagonists to treat alcoholism PMID 23294766; DOI 10.1016/j.drugalcdep.2012.12.017; Drug and Alcohol Dependence 2013-03-01 (Review Article) CRF1 receptor antagonists do not reverse pharmacological disruption of prepulse inhibition in rodents PMID 24186076; DOI 10.1007/s00213-013-3315-2; Psychopharmacology 2013-11-02

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9.4 Chemical-Gene Co-Occurrences in Literature

Showing 3 of 18 View More Co-Occurrence and Evidence Data | Download

Gene/Protein/Enzyme	Selected evidence
corticotropin releasing hormone receptor 1	16 articles View All DNA methylation levels are associated with CRF1 receptor antagonist treatment outcome in women with post-traumatic stress disorder PMID 30390684; DOI 10.1186/s13148-018-0569-x; Clinical Epigenetics 2018-11-03 Name matches: **crhr1** *gsk561679* Corticotropin-Releasing Factor Receptor 1 Antagonism Is Ineffective for Women With Posttraumatic Stress Disorder PMID 28793974; DOI 10.1016/j.biopsych.2017.06.024; Biological Psychiatry 2017-12-15 The CRH1 Antagonist GSK561679 Increases Human Fear But Not Anxiety as Assessed by Startle PMID 25430779; DOI 10.1038/npp.2014.316; Neuropsychopharmacology : official publication of the American College of Neuropsychopharmacology 2014-11-28
corticotropin releasing hormone	18 articles View All The CRH1 Antagonist GSK561679 Increases Human Fear But Not Anxiety as Assessed by Startle PMID 25430779; DOI 10.1038/npp.2014.316; Neuropsychopharmacology : official publication of the American College of Neuropsychopharmacology 2014-11-28 DNA methylation levels are associated with CRF1 receptor antagonist treatment outcome in women with post-traumatic stress disorder PMID 30390684; DOI 10.1186/s13148-018-0569-x; Clinical Epigenetics 2018-11-03 Psychophysiological treatment outcomes: Corticotropin-releasing factor type 1 receptor antagonist increases inhibition of fear-potentiated startle in PTSD patients PMID 30807663; DOI 10.1111/psyp.13356; Psychophysiology 2019-02-26
corticotropin releasing hormone binding protein	2 articles View All Behavioral, biological, and chemical perspectives on targeting CRF(1) receptor antagonists to treat alcoholism PMID 23294766; DOI 10.1016/j.drugalcdep.2012.12.017; Drug and Alcohol Dependence 2013-03-01 (Review Article) Name matches: **crhbp** *gsk561679* Corticotropin releasing factor-binding protein (CRF-BP) as a potential new therapeutic target in Alzheimer's disease and stress disorders PMID 31641098; DOI 10.1038/s41398-019-0581-8; Translational Psychiatry 2019-10-22 (Review Article)

▸ PubChem

9.5 Chemical-Disease Co-Occurrences in Literature

Showing 3 of 36 View More Co-Occurrence and Evidence Data | Download

Disease	Selected evidence
Stress Disorders, Post-Traumatic	8 articles View All Corticotropin-Releasing Factor Receptor 1 Antagonism Is Ineffective for Women With Posttraumatic Stress Disorder PMID 28793974; DOI 10.1016/j.biopsych.2017.06.024; Biological Psychiatry 2017-12-15 Name matches: **posttraumatic stress disorder**; **ptsd** *gsk561679* DNA methylation levels are associated with CRF1 receptor antagonist treatment outcome in women with post-traumatic stress disorder PMID 30390684; DOI 10.1186/s13148-018-0569-x; Clinical Epigenetics 2018-11-03 Name matches: **post-traumatic stress disorder**; **ptsd** *gsk561679* Evaluation of a corticotropin releasing hormone type 1 receptor antagonist in women with posttraumatic stress disorder: study protocol for a randomized controlled trial PMID 24950747; DOI 10.1186/1745-6215-15-240; Trials 2014-06-21 Name matches: **posttraumatic stress disorder**; **ptsd** *gsk561679*
Anxiety Disorders	7 articles View All The CRH1 Antagonist GSK561679 Increases Human Fear But Not Anxiety as Assessed by Startle PMID 25430779; DOI 10.1038/npp.2014.316; Neuropsychopharmacology : official publication of the American College of Neuropsychopharmacology 2014-11-28 Name matches: **anxiety** *gsk561679* Corticotropin-Releasing Factor Receptor 1 Antagonism Is Ineffective for Women With Posttraumatic Stress Disorder PMID 28793974; DOI 10.1016/j.biopsych.2017.06.024; Biological Psychiatry 2017-12-15 Name matches: **generalized anxiety disorder** *gsk561679* Discovery of NBI-77860/GSK561679, a potent corticotropin-releasing factor (CRF1) receptor antagonist with improved pharmacokinetic properties PMID 21074436; DOI 10.1016/j.bmcl.2010.10.095; Bioorganic & Medicinal Chemistry Letters 2010-12-15 Name matches: **anxiety** *gsk561679*
Alcoholism	5 articles View All Behavioral, biological, and chemical perspectives on targeting CRF(1) receptor antagonists to treat alcoholism PMID 23294766; DOI 10.1016/j.drugalcdep.2012.12.017; Drug and Alcohol Dependence 2013-03-01 (Review Article) Name matches: **alcohol addiction**; **alcohol dependence**; **alcohol use disorders**; **alcoholics**; **alcoholism** *gsk561679* Corticotropin-Releasing Factor (CRF) Neurocircuitry and Neuropharmacology in Alcohol Drinking PMID 29374836; DOI 10.1007/164_2017_86; Handbook of experimental pharmacology 2018-01-01 (Review Article) Noradrenergic tone mediates marble burying behavior after chronic stress and ethanol PMID 32588079; DOI 10.1007/s00213-020-05589-7; Psychopharmacology 2020-06-25

▸ PubChem

9.6 Chemical-Organism Co-Occurrences in Literature

Showing 3 of 6 View More Co-Occurrence and Evidence Data | Download

Organism	Selected evidence
homo sapiens (human)	12 articles View All **The CRH1 Antagonist GSK561679 Increases Human Fear But Not Anxiety as Assessed by Startle** PMID 25430779; DOI 10.1038/npp.2014.316; Neuropsychopharmacology : official publication of the American College of Neuropsychopharmacology 2014-11-28 Name matches: **human**; **humans** *gsk561679* **Evaluation of a corticotropin releasing hormone type 1 receptor antagonist in women with posttraumatic stress disorder: study protocol for a randomized controlled trial** PMID 24950747; DOI 10.1186/1745-6215-15-240; Trials 2014-06-21 Name matches: **human** *gsk561679* **Discovery of NBI-77860/GSK561679, a potent corticotropin-releasing factor (CRF1) receptor antagonist with improved pharmacokinetic properties** PMID 21074436; DOI 10.1016/j.bmcl.2010.10.095; Bioorganic & Medicinal Chemistry Letters 2010-12-15
metazoa (animals)	5 articles View All **The CRH1 Antagonist GSK561679 Increases Human Fear But Not Anxiety as Assessed by Startle** PMID 25430779; DOI 10.1038/npp.2014.316; Neuropsychopharmacology : official publication of the American College of Neuropsychopharmacology 2014-11-28 Name matches: **animal** *gsk561679* **Behavioral, biological, and chemical perspectives on targeting CRF(1) receptor antagonists to treat alcoholism** PMID 23294766; DOI 10.1016/j.drugalcdep.2012.12.017; Drug and Alcohol Dependence 2013-03-01 (Review Article) Name matches: **animal** *gsk561679* **Corticotropin-Releasing Factor (CRF) Neurocircuitry and Neuropharmacology in Alcohol Drinking** PMID 29374836; DOI 10.1007/164_2017_86; Handbook of experimental pharmacology 2018-01-01 (Review Article)
rodentia (rodents)	3 articles View All **The CRF1 Antagonist Verucerfont in Anxious Alcohol-Dependent Women: Translation of Neuroendocrine, But not of Anti-Craving Effects** PMID 27109623; DOI 10.1038/npp.2016.61; Neuropsychopharmacology : official publication of the American College of Neuropsychopharmacology 2016-04-25 **Effect of the CRF1-receptor antagonist pexacerfont on stress-induced eating and food craving** PMID 27595147; DOI 10.1007/s00213-016-4424-5; Psychopharmacology 2016-09-05 **CRF1 receptor antagonists do not reverse pharmacological disruption of prepulse inhibition in rodents** PMID 24186076; DOI 10.1007/s00213-013-3315-2; Psychopharmacology 2013-11-02

▸ PubChem

10 Patents

10.1 Depositor-Supplied Patent Identifiers

160 items Download

Search SORT BY Priority Date - Most Recent

A method for preparing 3,5-disubstituted 1,2,4-oxadiazole compounds
Publication Number: CN-118026946-A
Priority Date: 2024-02-07

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

First Previous Page 1 of 32 Next Last

PubChem

Link to all deposited patent identifiers

PubChem

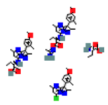
10.2 WIPO PATENTSCOPE

Patents are available for this chemical structure:
https://patentscope.wipo.int/search/en/result.jsf?inchikey=VKHVAUKFLBBZFJ-SFHVURJKSA-N

PATENTSCOPE (WIPO)

10.3 Chemical Co-Occurrences in Patents

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

Chemical	Selected evidence
3-(4-methoxy-2-methylphenyl)-2,5-dimethyl-N-[(1S)-1-(3-methyl-1,2,4,3-trioxazolidin-5-yl)propyl]pyrazolo[1,5-a]pyrimidin-7-amine CID 87078177	2 patents from 2 patent families View All Pyrazolo [1,5-alpha] pyrimidinyl derivatives useful as corticotropin-releasing factor (CRF) receptor antagonists US-8088779-B2; Grant Date: 2012-01-03 Pyrazolo[1, 5 -alpha]pyrimidinyl derivatives useful as corticotropin-releasing factor (CRF) receptor antagonists EP-1934222-B1; Grant Date: 2012-07-25
 (2S)-2-aminobutanoic acid; [(E)-1-aminoethylideneamino] (2S)-2-[[3-(4-methoxy-2-methylphenyl)-2,5-	1 patent from 1 patent family View All Pyrazolo [1,5-alpha] pyrimidinyl derivatives useful as corticotropin-releasing factor (CRF) receptor antagonists US-8088779-B2; Grant Date: 2012-01-03

dimethylpyrazolo[1,5-a]pyrimidin-7-yl]amino]butanoate;7-chloro-3-(4-methoxy-2-methylphenyl)-2,5-dimethylpyrazolo[1,5-a]pyrimidine;(2S)-2-[[3-(4-methoxy-2-methylphenyl)-2,5-dimethylpyrazolo[1,5-a]pyrimidin-7-yl]amino]butanoic acid

CID 172919508

7-Chloro-3-(4-methoxy-2-methylphenyl)-2,5-dimethylpyrazolo[1,5-a]pyrimidine

CID 59777389

3 patents from 2 patent families View All

Pyrazolo [1,5-alpha] pyrimidinyl derivatives useful as corticotropin-releasing factor (CRF) receptor antagonists
US-8088779-B2; Grant Date: 2012-01-03

Pyrazolo (1,5-alpha) pyrimidinyl derivatives useful as corticotropin-releasing factor (crf) receptor antagonists
EP-1802627-B1; Grant Date: 2012-08-29

PubChem

10.4 Chemical-Disease Co-Occurrences in Patents

Showing 3 of 36 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
Depressive Disorder	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-10190168-B2; Grant Date: 2019-01-29 Compositions and methods for the treatment of endometriosis US-10729693-B2; Grant Date: 2020-08-04
Endometriosis	1 patent from 1 patent family View All Compositions and methods for the treatment of endometriosis US-10729693-B2; Grant Date: 2020-08-04

PubChem

10.5 Chemical-Gene Co-Occurrences in Patents

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

Gene	Selected evidence
crh	3 patents from 2 patent families View All Compositions and methods for the treatment of endometriosis US-10729693-B2; Grant Date: 2020-08-04 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
crhr1	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-10190168-B2; Grant Date: 2019-01-29 Compositions and methods for the treatment of endometriosis US-10729693-B2; Grant Date: 2020-08-04
avpr1b	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-10190168-B2; Grant Date: 2019-01-29

PubChem

10.6 Chemical-Organism Co-Occurrences in Patents

Showing 3 of 12 View More Co-Occurrence and Evidence Data | Download

Organism	Selected evidence
mammalia (mammals)	1 patent from 1 patent family View All Compositions and methods for the treatment of endometriosis US-10729693-B2; Grant Date: 2020-08-04
rodentia (rodents)	3 patents from 2 patent families View All Compositions and methods for the treatment of endometriosis US-10729693-B2; Grant Date: 2020-08-04 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
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

PubChem

11 Interactions and Pathways

11.1 Chemical-Target Interactions

7 items | Download

Search | SORT BY Data Source - A to Z

Protein	Gene	Taxonomy	Action	Evidence	Data Source
Corticotropin-releasing factor receptor 1	CRHR1	Homo sapiens (human)	Antagonist	PMID:37713619	DrugBank
	CRHR1	Homo sapiens (human)	Inhibitor		Drug Gene Interaction database (DGIdb)
	CRHR1	Homo sapiens (human)	NBI 77860 binds to and results in decreased activity of CRHR1 protein	PMID:23294766	Comparative Toxicogenomics Database (CTD)
	ALAS2	Homo sapiens (human)	Inhibitor		Drug Gene Interaction database (DGIdb)
	CRHR1	Homo sapiens (human)			Drug Gene Interaction database (DGIdb)

First | Previous | Page 1 of 2 | Next | Last

ChEMBL; Comparative Toxicogenomics Database (CTD); Drug Gene Interaction database (DGIdb); DrugBank; IU...

12 Biological Test Results

12.1 BioAssay Results

11 items | Download

Search | SORT BY Activity Value - Increasing

Antagonist activity at human recombinant CRF1 receptor
Activity Outcome: Active Activity Type: Ki Activity Value: 0.006310 µM
BioAssay AID: 538004
Target Name: CRHR1 - corticotropin releasing hormone receptor 1 (human)
Substance SID: 123091511 Compound CID: 11596613

Antagonist activity at human recombinant CRF1 receptor
Activity Outcome: Active Activity Type: Ki Activity Value: 0.006310 µM
BioAssay AID: 538004
Target Name: LINC02210-CRHR1 - LINC02210-CRHR1 readthrough (human)
Substance SID: 123091511 Compound CID: 11596613

Antagonist activity at human recombinant CRF1 receptor
Activity Outcome: Active Activity Type: IC50 Activity Value: 0.100000 µM
BioAssay AID: 538004
Target Name: CRHR1 - corticotropin releasing hormone receptor 1 (human)
Substance SID: 123091511 Compound CID: 11596613

Antagonist activity at human recombinant CRF1 receptor
Activity Outcome: Active Activity Type: IC50 Activity Value: 0.100000 µM
BioAssay AID: 538004
Target Name: LINC02210-CRHR1 - LINC02210-CRHR1 readthrough (human)
Substance SID: 123091511 Compound CID: 11596613

AUC (0 to 24 hrs) in rat at 10 mg/kg, po
Activity Outcome: Probe
BioAssay AID: 538007

Target Name: Rattus norvegicus (Norway rat)

Substance SID: 123091511 Compound CID: 11596613

First Previous Page 1 of 3 Next Last

PubChem

13 Classification

13.1 NCI Thesaurus Tree

1 item View in Classification Browser

NCI Thesaurus > Drug, Food, Chemical or Biomedical Material > Pharmacologic Substance > Hormone Therapy Agent > Hormone Antagonist > Anti-Adrenal

Verucerfont

NCI Thesaurus (NCIt)

13.2 KEGG: Target-based Classification of Drugs

1 item View in Classification Browser

Target-based classification of drugs > G Protein-coupled receptors > Secretin receptor family > Corticotropin-releasing hormone > CRHR1 [HSA:1394] [KO:K04578]

Verucerfont (USAN/INN)

KEGG

13.3 ChemIDplus

10 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)

ClinicalTrials.gov

ClinicalTrials.gov - ClinicalTrials.gov offers up-to-date information for locating federally and privately supported clinical trials for a wide range of diseases and conditions

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 andSupplementary Concept Records

First Previous Page 1 of 2 Next Last

ChemIDplus

13.4 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 congentical adrenal hyperplasia.

▸ IUPHAR/BPS Guide to PHARMACOLOGY

13.5 ChEMBL Target Tree

1 item — 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

13.6 UN GHS Classification

15 items — View in Classification Browser

GHS Classification > Hazard Statement Codes > H300: Health Hazards

H302: Harmful if swallowed [Warning: Acute toxicity, oral]

GHS Classification > Hazard Statement Codes > H300: Health Hazards

H361: Suspected of damaging fertility or the unborn child [Warning: Reproductive toxicity]

GHS Classification > Hazard Classes > Health Hazards

Acute toxicity, oral

GHS Classification > Hazard Classes > Health Hazards

Reproductive toxicity

GHS Classification > Hazard Pictograms

GHS07

First Previous Page 1 of 3 Next Last

▸ GHS Classification (UNECE)

13.7 NORMAN Suspect List Exchange Classification

1 item — View in Classification Browser

NORMAN Suspect List Exchange Classification

S00 | SUSDAT | Merged NORMAN Suspect List: SusDat

A merged list of >100,000 structures from the NORMAN Network Suspect List Exchange, available from https://www.norman-network.com/nds/susdat/. Compiled by Reza Aalizadeh, University of Athens, including RTI and toxicity values, support by Nikiforos Alygizakis, EI. Hazard and Exposure values provided by Stellan Fischer, KEMI. Dataset DOI:10.5281/zenodo.2664077

▸ NORMAN Suspect List Exchange

13.8 EPA DSSTox Classification

9 items — View in Classification Browser

CompTox Chemicals Dashboard Chemical Lists > LIST

Show alternative paths

[CPDAT] Navigation Panel to CPDat Versioned Structure Lists

Short_Description: CPDat Structure lists are versioned iteratively and this panel navigates between the various versions

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 > LIST

Show alternative paths

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

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

CompTox Chemicals Dashboard Chemical Lists > MISCELLANEOUS

Show alternative paths

[LCSSPUBCHEM] Laboratory Chemical Safety Summary (LCSS) data subset from PubChem

Short_Description: The PubChem Laboratory Chemical Safety Summary (LCSS) provides pertinent chemical health and safety data for a given PubChem Compound record (Last updated 1/5/2026)

CompTox Chemicals Dashboard Chemical Lists > MISCELLANEOUS

Show alternative paths

[METABWKBEN] Metabolomics Workbench Metabolite Database

Short_Description: The Metabolomics Workbench Metabolite Database contains structures and annotations of biologically relevant metabolites.

First Previous Page 1 of 2 Next Last

▸ EPA DSSTox

13.9 MolGenie Organic Chemistry Ontology

20 items View in Classification Browser

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 > simple organic compound scaffolds > benzene derivatives > alkyl benzene derivatives > methylbenzenes

toluenes

Any member of the class of benzenes that is a substituted benzene in which the substituents include one (and only one) methyl group.
ChEBI: 27024
MeSH: D014050

MolGenie Organic Chemistry Ontology > ChEMBL chemical entities > substructural concepts > functional groups > oxygen containing functional groups > ethers

aryl alkyl ethers

MolGenie Organic Chemistry Ontology > ChEMBL chemical entities > substructural concepts > scaffolds > simple organic compound scaffolds

biaryls

First Previous Page 1 of 4 Next Last

▸ MolGenie

13.10 Chemicals in PubChem from Regulatory Sources

1 item View in Classification Browser

Chemicals in PubChem from Regulatory Sources > EU EMA

Orphan drugs and substances

Drug and substance information from orphan designations

▸ PubChem

13.11 Open Targets Classification

5 items View in Classification Browser

Disease Classification > gastrointestinal disease > intestinal disease

irritable bowel syndrome

Irritable bowel syndrome (IBS) is a chronic functional condition of the lower gastrointestinal (GI) tract characterized by abdominal pain or discomfort and disordered bowel habit (diarrhea, constipation, or fluctuation between the two).

Disease Classification > nervous system disease > central nervous system disease > brain disease > mental or behavioural disorder > stress-related disorder

Show alternative paths

post-traumatic stress disorder

An anxiety disorder precipitated by an experience of intense fear or horror while exposed to a traumatic (especially life-threatening) event. The disorder is characterized by intrusive recurring thoughts or images of the traumatic event; avoidance of anything associated with the event; a state of hyperarousal and diminished emotional responsiveness. These symptoms are present for at least one month and the disorder is usually long-term.

Disease Classification > nervous system disease > central nervous system disease > brain disease > mental or behavioural disorder > drug dependence

Show alternative paths

alcohol dependence

Physical and psychological dependence on alcohol.

Disease Classification > nervous system disease > central nervous system disease > brain disease > mental or behavioural disorder > mood disorder > depressive disorder

Show alternative paths

major depressive disorder

An episode of depression lasting two or more weeks without an intervening episode of mania.

Disease Classification > endocrine system disease > adrenal gland disease > adrenogenital syndrome

Show alternative paths

congenital adrenal hyperplasia

Congenital adrenal hyperplasia (CAH) is an inherited endocrine disorder caused by a steroidogenic enzyme deficiency that is characterized by adrenal insufficiency and variable degrees of hyper or hypo androgyny manifestations, depending of the type and the severity of the disease.

Open Targets

14 Information Sources

FILTER BY SOURCE

ALL SOURCES

1. **CAS Common Chemistry**

LICENSE
The data from CAS Common Chemistry is provided under a CC-BY-NC 4.0 license, unless otherwise stated.
https://creativecommons.org/licenses/by-nc/4.0/

Verucerfont
https://commonchemistry.cas.org/detail?cas_rn=885220-61-1

2. **ChemIDplus**

LICENSE
https://www.nlm.nih.gov/copyright.html

Verucerfont [USAN:INN]
https://pubchem.ncbi.nlm.nih.gov/substance/?source=chemidplus&sourceid=0885220611

ChemIDplus Chemical Information Classification
https://pubchem.ncbi.nlm.nih.gov/source/chemidplus

3. **DrugBank**

LICENSE
Creative Common's Attribution-NonCommercial 4.0 International License (http://creativecommons.org/licenses/by-nc/4.0/legalcode)
https://www.drugbank.ca/legal/terms_of_use

Verucerfont
https://www.drugbank.ca/drugs/DB12512

4. ## EPA DSSTox

LICENSE
https://www.epa.gov/privacy/privacy-act-laws-policies-and-resources

Verucerfont
https://comptox.epa.gov/dashboard/DTXSID501032013

CompTox Chemicals Dashboard Chemical Lists
https://comptox.epa.gov/dashboard/chemical-lists/

5. ## European Chemicals Agency (ECHA)

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https://echa.europa.eu/web/guest/legal-notice

2,5-dimethyl-3-[2-methyl-4-(methyloxy)phenyl]-N-[(1S)-1-(3-methyl-1,2,4-oxadiazol-5-yl)propyl]pyrazolo[1,5-a]pyrimidin-7-amine
https://chem.echa.europa.eu/100.158.110

2,5-dimethyl-3-[2-methyl-4-(methyloxy)phenyl]-N-[(1S)-1-(3-methyl-1,2,4-oxadiazol-5-yl)propyl]pyrazolo[1,5-a]pyrimidin-7-amine (EC: 629-872-6)
https://chem.echa.europa.eu/substance-search?searchText=629-872-6

6. ## FDA Global Substance Registration System (GSRS)

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https://www.fda.gov/about-fda/about-website/website-policies#linking

VERUCERFONT
https://gsrs.ncats.nih.gov/ginas/app/beta/substances/X60608B091

7. ## ChEMBL

LICENSE
Access to the web interface of ChEMBL is made under the EBI's Terms of Use (http://www.ebi.ac.uk/Information/termsofuse.html). The ChEMBL data is made available on a Creative Commons Attribution-Share Alike 3.0 Unported License (http://creativecommons.org/licenses/by-sa/3.0/).
http://www.ebi.ac.uk/Information/termsofuse.html

VERUCERFONT
https://www.ebi.ac.uk/chembl/explore/compound/CHEMBL1287935

ChEMBL Protein Target Tree
https://www.ebi.ac.uk/chembl/g/#browse/targets

8. ## Comparative Toxicogenomics Database (CTD)

LICENSE
It is to be used only for research and educational purposes. Any reproduction or use for commercial purpose is prohibited without the prior express written permission of NC State University.
http://ctdbase.org/about/legal.jsp

NBI 77860
https://ctdbase.org/detail.go?type=chem&acc=C556497

9. ## Drug Gene Interaction database (DGIdb)

LICENSE
The data used in DGIdb is all open access and where possible made available as raw data dumps in the downloads section.
http://www.dgidb.org/downloads

VERUCERFONT
https://www.dgidb.org/drugs/ncit:C152869

10. ## IUPHAR/BPS Guide to PHARMACOLOGY

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https://www.guidetopharmacology.org/about.jsp#license

verucerfont
https://www.guidetopharmacology.org/GRAC/LigandDisplayForward?ligandId=10378

Guide to Pharmacology Target Classification
https://www.guidetopharmacology.org/targets.jsp

11. ## Therapeutic Target Database (TTD)

GSK561679
https://ttd.idrblab.cn/data/drug/details/D0ZC0M

12. ## Open Targets

LICENSE
Datasets generated by the Open Targets Platform are freely available for download.
https://platform-docs.opentargets.org/licence

VERUCERFONT
https://platform.opentargets.org/drug/CHEMBL1287935

Disease Classification
https://platform.opentargets.org/downloads/clinical_target/access

13. ## ClinicalTrials.gov

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https://clinicaltrials.gov/

14. ## EU Clinical Trials Register

https://www.clinicaltrialsregister.eu/

15. ## European Medicines Agency (EMA)

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https://www.kegg.jp/kegg/legal.html

https://www.kegg.jp/entry/D09695

Target-based classification of drugs
http://www.genome.jp/kegg-bin/get_htext?br08310.keg

17. ## Metabolomics Workbench

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https://www.metabolomicsworkbench.org/data/StructureData.php?RegNo=153488

18. ## NCI Thesaurus (NCIt)

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https://ncithesaurus.nci.nih.gov/ncitbrowser/ConceptReport.jsp?dictionary=NCI_Thesaurus&ns=ncit&code=C152869

NCI Thesaurus
https://ncit.nci.nih.gov

19. ## NORMAN Suspect List Exchange

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3-(4-methoxy-2-methylphenyl)-2,5-dimethyl-n-[1-(3-methyl-1,2,4-oxadiazol-5-yl)propyl]pyrazolo[1,5-a]pyrimidin-7-amine

NORMAN Suspect List Exchange Classification
https://www.norman-network.com/nds/SLE/

20. ## Pharos

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https://pharos.nih.gov/about

3-(4-methoxy-2-methylphenyl)-2,5-dimethyl-N-((S)-1-(3-methyl-1,2,4-oxadiazol-5-yl)propyl)pyrazolo[1,5-a]pyrimidin-7-amine
https://pharos.nih.gov/ligands/4W43ZXF751KD

21. ## Springer Nature

https://pubchem.ncbi.nlm.nih.gov/substance/341473837

22. ## Wikidata

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https://www.wikidata.org/wiki/Q21098847

23. Wikipedia

Verucerfont
https://en.wikipedia.org/wiki/Verucerfont

24. PubChem

https://pubchem.ncbi.nlm.nih.gov

25. GHS Classification (UNECE)

GHS Classification
https://unece.org/about-ghs

26. MolGenie

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MolGenie Organic Chemistry Ontology
https://github.com/MolGenie/ontology/

27. PATENTSCOPE (WIPO)

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