

COMPOUND SUMMARY

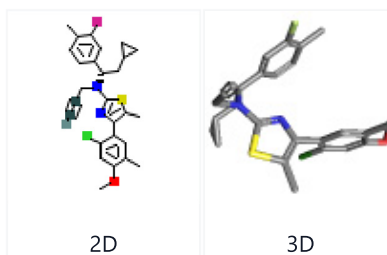
Crinecerfont

 Cite Download

PubChem CID

5282340

Structure



Molecular Formula

C₂₇H₂₈ClFN₂OS

Synonyms

Crinecerfont
752253-39-7
SSR125543
SSR 125543
SSR-125543

[View More...](#)

Molecular Weight

483.0 g/mol

Computed by PubChem 2.2 (PubChem release 2021.10.14)

Dates

Create: Modify:
2005-10-11 2025-02-01

Description

SSR 125543 is an amine.

[► ChEBI](#)

CRINECERFONT is a small molecule drug with a maximum clinical trial phase of III (across all indications) and has 2 investigational indications.

[► Open Targets](#)

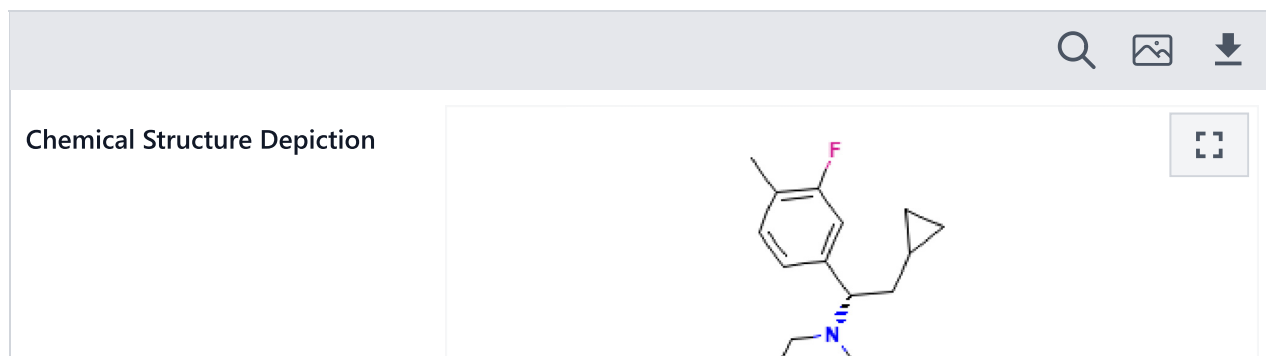
Contents

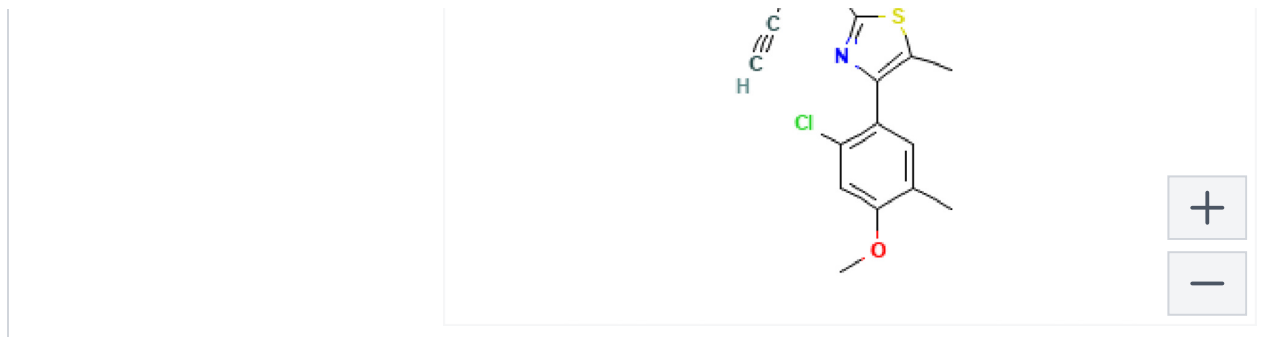
Title and Summary	
1 Structures	▼
2 Names and Identifiers	▼
3 Chemical and Physical Properties	▼
4 Related Records	▼
5 Chemical Vendors	
6 Drug and Medication Information	▼
7 Use and Manufacturing	▼
8 Associated Disorders and Diseases	
9 Literature	▼
10 Patents	▼
11 Interactions and Pathways	▼
12 Biological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

1 Structures



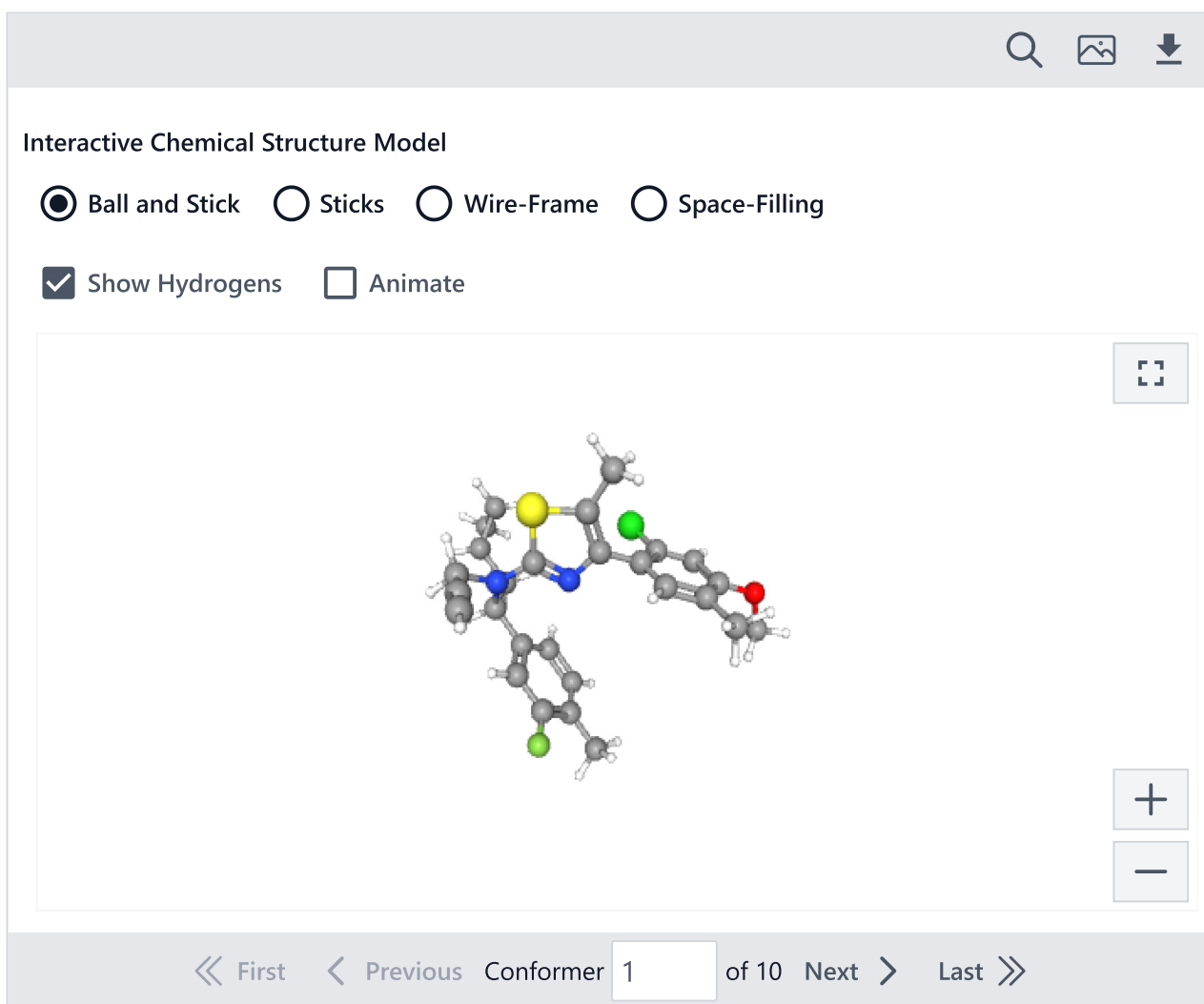
1.1 2D Structure





► PubChem

1.2 3D Conformer



► PubChem

2 Names and Identifiers



2.1 Computed Descriptors



2.1.1 IUPAC Name



4-(2-chloro-4-methoxy-5-methylphenyl)-N-[(1S)-2-cyclopropyl-1-(3-fluoro-4-methylphenyl)ethyl]-5-methyl-N-prop-2-ynyl-1,3-thiazol-2-amine

Computed by Lexichem TK 2.7.0 (PubChem release 2021.10.14)

► [PubChem](#)

2.1.2 InChI



InChI=1S/C27H28ClFN2OS/c1-6-11-31(24(13-19-8-9-19)20-10-7-16(2)23(29)14-20)27-30-26(18(4)33-27)21-12-17(3)25(32-5)15-22(21)28/h1,7,10,12,14-15,19,24H,8-9,11,13H2,2-5H3/t24-/m0/s1

Computed by InChI 1.0.6 (PubChem release 2021.10.14)

► [PubChem](#)

2.1.3 InChIKey



IEAKXXNRGSLYTQ-DEOSSOPVSA-N

Computed by InChI 1.0.6 (PubChem release 2021.10.14)

► [PubChem](#)

2.1.4 SMILES



CC1=C(C=C(C=C1)[C@H](CC2CC2)N(CC#C)C3=NC(=C(S3)C)C4=C(C=C(C(=C4)C)OC)Cl)F

Computed by OEChem 2.3.0 (PubChem release 2024.12.12)

► [PubChem](#)

2.2 Molecular Formula



C₂₇H₂₈ClFN₂OS

Computed by PubChem 2.2 (PubChem release 2021.10.14)

► PubChem

2.3 Other Identifiers



2.3.1 CAS



752253-39-7

► CAS Common Chemistry; ChemIDplus; DrugBank; EPA DSSTox; FDA Global Substance Registratio...

2.3.2 UNII



MFT24BX55I

► FDA Global Substance Registration System (GSRS)

2.3.3 ChEBI ID



CHEBI:34969

► ChEBI

2.3.4 ChEMBL ID



CHEMBL291657

► ChEMBL

2.3.5 DrugBank ID



DB18518

► DrugBank

2.3.6 DSSTox Substance ID



DTXSID10996687

▶ EPA DSSTox

2.3.7 KEGG ID



D12366

▶ KEGG

2.3.8 NCI Thesaurus Code



C174708

▶ NCI Thesaurus (NCIt)

2.3.9 Nikkaji Number



J2.788.046K

▶ Japan Chemical Substance Dictionary (Nikkaji)

2.3.10 Pharos Ligand ID



W3JYT8TJURTS

▶ Pharos

2.3.11 Wikidata



Q27088874

▶ Wikidata

2.3.12 Wikipedia



Crinecerfont

▶ Wikipedia

2.4 Synonyms



2.4.1 MeSH Entry Terms



4-(2-chloro-4-methoxy-5-methylphenyl)-N-((1S)-2-cyclopropyl-1-(3-fluoro-4-methylphenyl)ethyl)-5-methyl-N-prop-2-ynyl-1,3-thiazol-2-amine

crinecerfont

NBI 74788

NBI-74788

► Medical Subject Headings (MeSH)

2.4.2 Depositor-Supplied Synonyms



Crinecerfont

752253-39-7

SSR125543

SSR 125543

SSR-125543

06-RORI

Crinecerfont [USAN]

Nbi-74788

4-(2-chloro-4-methoxy-5-methylphenyl)-N-[(1S)-2-cyclopropyl-1-(3-fluoro-4-methylphenyl)ethyl]-5-methyl-N-prop-2-ynyl-1,3-thiazol-2-amine

► PubChem

3 Chemical and Physical Properties



3.1 Computed Properties



Property Name	Property Value	Reference
Molecular Weight	483.0 g/mol	Computed by PubChem 2.2 (PubChem release 2021.10.14)

XLogP3-AA	8	Computed by XLogP3 3.0 (PubChem release 2021.10.14)
Hydrogen Bond Donor Count	0	Computed by Cactvs 3.4.8.18 (PubChem release 2021.10.14)
Hydrogen Bond Acceptor Count	5	Computed by Cactvs 3.4.8.18 (PubChem release 2021.10.14)
Rotatable Bond Count	8	Computed by Cactvs 3.4.8.18 (PubChem release 2021.10.14)
Exact Mass	482.1594906 Da	Computed by PubChem 2.2 (PubChem release 2021.10.14)
Monoisotopic Mass	482.1594906 Da	Computed by PubChem 2.2 (PubChem release 2021.10.14)
Topological Polar Surface Area	53.6 Å ²	Computed by Cactvs 3.4.8.18 (PubChem release 2021.10.14)
Heavy Atom Count	33	Computed by PubChem
Formal Charge	0	Computed by PubChem
Complexity	699	Computed by Cactvs 3.4.8.18 (PubChem release 2021.10.14)
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 2021.10.14)

► PubChem

3.2 Chemical Classes



3.2.1 Drugs



3.2.1.1 Human Drugs



Paediatric drug

- ▶ [European Medicines Agency \(EMA\)](#)

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 [here](#) 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	7
Same Stereo Count	4
Same Isotope Count	3
Same Parent, Connectivity Count	10
Same Parent, Stereo Count	6
Same Parent, Isotope Count	6
Same Parent, Exact Count	3
Mixtures, Components, and Neutralized Forms Count	6
Similar Compounds (2D)	View in PubChem Search

[Similar Conformers \(3D\)](#)[View in PubChem Search](#)[▶ PubChem](#)

4.3 Substances



4.3.1 Related Substances



All Count	102
Same Count	58
Mixture Count	44

[▶ PubChem](#)

4.3.2 Substances by Category



7 categories	↓
Chemical Vendors (26)	+
Curation Efforts (13)	+
Governmental Organizations (6)	+
Journal Publishers (1)	+
NIH Initiatives (1)	+
Research and Development (15)	+
Legacy Depositors (10)	+

[▶ PubChem](#)

4.4 Entrez Crosslinks



PubMed Count	3
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Gene Count	1
------------	---

[▶ PubChem](#)

4.5 NCBI LinkOut



Provider	Information
Ingenuity Pathways Analysis	Chemical Information: molecular interactions

[▶ NCBI](#)

5 Chemical Vendors



25 vendors	
eMolecules PubChem SID: 490801745 Purchasable Chemical: 301245448	
BenchChem PubChem SID: 446438046 Purchasable Chemical: B1669616	
001Chemical PubChem SID: 440048050 Purchasable Chemical: DY570262	
Win-Win Chemical PubChem SID: 496163285 Purchasable Chemical: 38507	
Mcule PubChem SID: 493553177 Purchasable Chemical: MCULE-5744636773 PubChem SID: 494193126 Purchasable Chemical: MCULE-6859372505	
Smolecule PubChem SID: 438454854 Purchasable Chemical: S524452	
CHIRALEN PubChem SID: 491446067 Purchasable Chemical: 275564	
InvivoChem PubChem SID: 500196892 Purchasable Chemical: V18805	
AbaChemScene PubChem SID: 463561210 Purchasable Chemical: CS-0025238	



AKos Consulting & SolutionsPubChem SID: [481563851](#)Purchasable Chemical: [AKOS040751318](#)**Amadis Chemical**PubChem SID: [498216771](#)Purchasable Chemical: [A1241944](#)**MedChemexpress MCE**PubChem SID: [461503573](#)Purchasable Chemical: [HY-106203](#)**Key Organics/BIONET**PubChem SID: [486525901](#)Purchasable Chemical: [TS-08701](#)**EvitaChem**PubChem SID: [485958977](#)Purchasable Chemical: [evt-265434](#)**Debye Scientific Co., Ltd**PubChem SID: [496741488](#)Purchasable Chemical: [DA-78023](#)**THE BioTek**PubChem SID: [434249251](#)Purchasable Chemical: [bt-265434](#)**TargetMol**PubChem SID: [494448094](#)Purchasable Chemical: [T31095](#)**AA BLOCKS**PubChem SID: [479914414](#)Purchasable Chemical: [AA005MPZ](#)**BOC Sciences**PubChem SID: [441158728](#)Purchasable Chemical: [752253-39-7](#)**RR Scientific**PubChem SID: [481391142](#)Purchasable Chemical: [R746744](#)**Starshine Chemical**PubChem SID: [480486690](#)

Purchasable Chemical: 2023-05-7C02919

AstaTech, Inc.PubChem SID: [505061391](#)Purchasable Chemical: [AT46091](#)**A2B Chem**PubChem SID: [480588866](#)Purchasable Chemical: [AC62627](#)**J&H Chemical Co.,Ltd**PubChem SID: [469608935](#)Purchasable Chemical: [JH469047](#)**10X CHEM**PubChem SID: [491552545](#)Purchasable Chemical: [TX005NYF](#)

▶ PubChem

6 Drug and Medication Information

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6.1 Drug Indication

?

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Treatment of atypical haemolytic uremic syndrome, Treatment of paroxysmal nocturnal haemoglobinuria

▶ European Medicines Agency (EMA)

Treatment of congenital adrenal hyperplasia

▶ European Medicines Agency (EMA)

2 items ↓	
Indication	Max Phase
congenital adrenal hyperplasia	Phase III
depressive disorder	Phase II

▶ Open Targets

6.2 FDA Orange Book

?

↗

4 items ↓				
Trade Name	Application Number	Product Number	Applicant	Approval Date
CRENESSITY	218808	001	NEUROCRINE BIOSCIENCES INC	Dec 13, 2024
CRENESSITY	218808	002	NEUROCRINE BIOSCIENCES INC	Dec 13, 2024
CRENESSITY	218808	003	NEUROCRINE BIOSCIENCES	Dec 13, 2024

▶ FDA Orange Book

6.3 FDA National Drug Code Directory



4 items					
Product NDC	Start Marketing Date	Dosage Form	Strength	Labeler	
70370-5025	2024-12-13	CAPSULE	25 mg/1	Neurocrine Biosciences, Inc.	
70370-5050	2024-12-13	CAPSULE	50 mg/1	Neurocrine Biosciences, Inc.	
70370-5100	2024-12-13	CAPSULE	100 mg/1	Neurocrine Biosciences, Inc.	
70370-5250	2024-12-13	SOLUTION	50 mg/mL	Neurocrine Biosciences, Inc.	

▶ National Drug Code (NDC) Directory

6.4 Drug Labels



Drug and label

1 item		
CRENESSITY (CRINECERFONT) CAPSULE CRENESSITY (CRINECERFONT) SOLUTION		
Drug: crinecerfont Download: PDF Data File: XML		
Ingredient (UNII): CRINECERFONT (UNII:MFT24BX55I)		
Category: Human prescription Company: Neurocrine Biosciences, Inc. Date: 2024-12-01		

▶ DailyMed

Active ingredient and drug

1 item						
Ingredient	Drug	Active Moiety	Label	Data File	Data SetID	
CRINECERFONT (UNII:MFT24BX55I)	crinecerfont	CRINECERFONT (UNII:MFT24BX55I)	PDF	XML	fd3a6fbd-9137-428a-ba46-df6606f07d28	

▶ DailyMed

6.5 Clinical Trials



6.5.1 ClinicalTrials.gov



5 items	
Safety, Tolerability, Pharmacokinetics, and Pharmacodynamics of NBI-74788 (Crinecerfont) in Pediatric Participants With Congenital Adrenal Hyperplasia CTID: NCT04045145 Phase: Phase 2 Status: Completed Date: 2024-07-18	
Global Safety and Efficacy Registration Study of Crinecerfont for Congenital Adrenal Hyperplasia CTID: NCT04490915 Phase: Phase 3 Status: Active, not recruiting Date: 2024-07-15	
Global Safety and Efficacy Registration Study of Crinecerfont in Pediatric Patients With Classic Congenital Adrenal Hyperplasia (CAHtalyst Pediatric Study) CTID: NCT04806451 Phase: Phase 3 Status: Active, not recruiting Date: 2024-05-07	
Safety, Tolerability, Pharmacokinetics, and Pharmacodynamics of NBI-74788 in Adults With Congenital Adrenal Hyperplasia CTID: NCT03525886 Phase: Phase 2 Status: Completed Date: 2022-05-03	
A Trial Evaluating the Efficacy and Tolerability of SSR125543 in Outpatients With Major Depressive Disorder CTID: NCT01034995	

► [ClinicalTrials.gov](#)

6.5.2 EU Clinical Trials Register



3 items	

A Randomized, Double-Blind, Placebo-Controlled Study to Evaluate the Safety and Efficacy of Crinecerfont (NBI-74788) in Pediatric Subjects with Classic Congenital Adrenal Hyperplasia, Followed by Open-Label Treatment

EudraCT: [2020-004381-19](#)

Phase: Phase 3 Status: Ongoing, Trial now transitioned

Date: 2021-06-07

A Randomized, Double-Blind, Placebo-Controlled Study to Evaluate the Safety and Efficacy of Crinecerfont (NBI-74788) in Adult Subjects with Classic Congenital Adrenal Hyperplasia, Followed by Open-Label Treatment

EudraCT: [2019-004873-17](#)

Phase: Phase 3 Status: GB - no longer in EU/EEA, Ongoing, Trial now transitioned

Date: 2020-10-15

An eight-week, multinational, multicenter, double-blind, active- and placebo-controlled clinical trial evaluating the efficacy and tolerability of three fixed doses of SSR125543 (20 mg daily, 50 mg daily and 100 mg daily) in outpatients with major depressive disorder.

EudraCT: [2009-010339-42](#)

Phase: Phase 2 Status: Completed

► [EU Clinical Trials Register](#)

6.6 EMA Drug Information



1 of 2

Type	Paediatric investigation
Active Substance	Crinecerfont
Therapeutic Area	Endocrinology-Gynaecology-Fertility-Metabolism
Drug Form	Capsule, hard, Oral solution
Administration Route	Subcutaneous use, Intravenous use
Decision Type	P: decision agreeing on a investigation plan, with or without partial waiver(s) and or deferral(s)
Decision Date	2021-03-17

► [European Medicines Agency \(EMA\)](#)

2 of 2

Type	Paediatric investigation
Active Substance	Crinecerfont
Therapeutic Area	Endocrinology-Gynaecology-Fertility-Metabolism
Drug Form	Capsule, hard, Oral solution
Administration Route	Oral use, Gastric use
Decision Type	P: decision agreeing on a investigation plan, with or without partial waiver(s) and or deferral(s)
Decision Date	2021-03-17

► [European Medicines Agency \(EMA\)](#)

7 Use and Manufacturing



7.1 Uses



7.1.1 Use Classification



Human Drugs -> EU pediatric investigation plans

► [European Medicines Agency \(EMA\)](#)

Human Drugs -> FDA Approved Drug Products with Therapeutic Equivalence Evaluations (Orange Book) -> Active Ingredients

► [FDA Orange Book](#)

8 Associated Disorders and Diseases



4 items 	
Source Disease	Data Source
Anxiety disorder [ICD-11: 6B00-6B0Z]	Therapeutic Target Database (TTD)
Congenital adrenal hyperplasia [ICD-11: 5A71.01]	Therapeutic Target Database (TTD)
congenital adrenal hyperplasia	Open Targets

[depressive disorder](#)[Open Targets](#)[► Open Targets; Therapeutic Target Database \(TTD\)](#)

9 Literature



9.1 Consolidated References



36 items



SORT BY

Publication Date - Most Recent



Phase 3 Trial of Crinicerfont in Pediatric Congenital Adrenal Hyperplasia

Publication Name: The New England journal of medicine

Publication Date: 2024-08-08

PMID: [38828945](#) DOI: [10.1056/nejmoa2404655](#)

Phase 3 Trial of Crinicerfont in Adult Congenital Adrenal Hyperplasia

Publication Name: The New England journal of medicine

Publication Date: 2024-08-08

PMCID: [PMC11309900](#) PMID: [38828955](#) DOI: [10.1056/nejmoa2404656](#)

Current and future perspectives on clinical management of classic 21-hydroxylase deficiency

Publication Name: Endocrine Journal

Publication Date: 2023-10-30

PMID: [37380491](#) DOI: [10.1507/endocrj.ej23-0075](#)

Crinicerfont in a First Clinical Application of a CRH Antagonist: Further Potential Uses Are Still an Open Chapter!

Publication Name: The Journal of clinical endocrinology and metabolism

Publication Date: 2023-08-31

PMID: [37650613](#) DOI: [10.1210/clinem/dgad513](#)

Dissecting the Relationship Between Neuropsychiatric and Neurodegenerative Disorders

Publication Name: Molecular Neurobiology

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9.2 NLM Curated PubMed Citations



All NLM Curated PubMed Citations



► PubChem

9.3 Springer Nature References



23 items

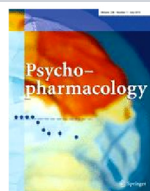


Search



SORT BY

Publication Date - Oldest

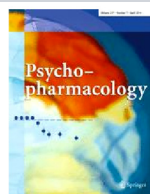


The CRF1 receptor antagonist SSR125543 prevents stress-induced cognitive deficit associated with hippocampal dysfunction: Comparison with paroxetine and d-cycloserine

PMID: [23407783](#)

Publication Date: 2013

Publication Name: Psychopharmacology



CRF1 receptor antagonists do not reverse pharmacological disruption of prepulse inhibition in rodents

PMID: [24186076](#)

Publication Date: 2013

Publication Name: Psychopharmacology



Development of CRF1 Receptor Antagonists as Antidepressants and Anxiolytics

Publication Date: 2006

Publication Name: CNS Drugs



Effects of a stressor and corticotrophin releasing factor on ethanol deprivation-induced ethanol intake and anxiety-like behavior in alcohol-preferring P rats

PMID: [21643675](#)

Publication Date: 2011

Publication Name: Psychopharmacology



Reduced vasopressin receptors activation mediates the anti-depressant effects of fluoxetine and venlafaxine in bulbectomy model of depression

PMID: [26700241](#)

► [Springer Nature](#)

9.4 Chemical Co-Occurrences in Literature

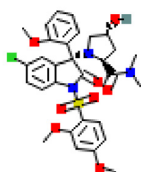


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Chemical

Selected evidence



Nelivaptan

CID 9895468

12 articles

[View All](#)

Antidepressant-Like Effects of the Corticotropin-Releasing Factor 1 Receptor Antagonist, SSR125543, and the Vasopressin 1b Receptor Antagonist, SSR149415, in a DRL-72 s Schedule in the Rat

PMID 16452986; DOI 10.1038/sj.npp.1301036; Neuropsychopharmacology : official publication of the American College of Neuropsychopharmacology 2006-02-01

Name matches: *ssr149415 ssr125543*

The corticotropin-releasing factor 1 receptor antagonist, SSR125543, and the vasopressin 1b receptor antagonist, SSR149415, prevent stress-induced cognitive impairment in mice

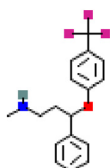
PMID 21356230; DOI 10.1016/j.pbb.2011.02.019; Pharmacology, biochemistry, and behavior 2011-05-01

Name matches: *ssr149415 ssr125543*

Effects of the vasopressin (V1B) receptor antagonist, SSR149415, and the corticotropin-releasing factor 1 receptor antagonist, SSR125543, on FG 7142-induced increase in acetylcholine and norepinephrine release in the rat

PMID 16781820; DOI 10.1016/j.neuroscience.2006.05.006; Neuroscience 2006-09-01

Name matches: *ssr149415 ssr125543*



Fluoxetine

CID 3386

14 articles

[View All](#)

Blockade of CRF(1) or V(1b) receptors reverses stress-induced suppression of neurogenesis in a mouse model of depression

PMID 14699428; DOI 10.1038/sj.mp.4001464; Molecular Psychiatry 2003-12-23

Name matches: *fluoxetine ssr125543a*

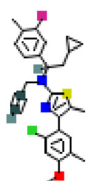
Corticolimbic Transcriptome Changes are State-Dependent and Region-Specific in a Rodent Model of Depression and of Antidepressant Reversal

PMID 18536703; DOI 10.1038/npp.2008.76; Neuropsychopharmacology : official publication of the American College of Neuropsychopharmacology 2008-06-04

Name matches: fluoxetine *ssr125543*

The corticotropin-releasing factor 1 receptor antagonist, SSR125543, and the vasopressin 1b receptor antagonist, SSR149415, prevent stress-induced cognitive impairment in mice

PMID 21356230; DOI 10.1016/j.pbb.2011.02.019; Pharmacology, biochemistry, and behavior 2011-05-01

Name matches: fluoxetine *ssr125543*

4-(2-chloro-4-methoxy-5-methylphenyl)-N-[2-cyclopropyl-1-(3-fluoro-4-methylphenyl)ethyl]-5-methyl-N-prop-2-ynyl-1,3-thiazol-2-amine

CID 9956923

5 articles

View All [↗](#)

4-(2-Chloro-4-methoxy-5-methylphenyl)-N-[(1S)-2-cyclopropyl-1-(3-fluoro-4-methylphenyl)ethyl]5-methyl-N-(2-propynyl)-1,3-thiazol-2-amine Hydrochloride (SSR125543A): A Potent and Selective Corticotrophin-Releasing Factor1Receptor Antagonist. I. Biochemical and Pharmacological Characterization

PMID 11907190; DOI 10.1124/jpet.301.1.322; The Journal of pharmacology and experimental therapeutics 2002-04-01

4-(2-Chloro-4-methoxy-5-methylphenyl)-N-[(1S)-2-cyclopropyl-1-(3-fluoro-4-methylphenyl)ethyl]5-methyl-N-(2-propynyl)-1, 3-thiazol-2-amine Hydrochloride (SSR125543A), a Potent and Selective Corticotrophin-Releasing Factor1 Receptor Antagonist. II. Characterization in Rodent Models of Stress-Related Disorders

PMID 11907191; DOI 10.1124/jpet.301.1.333; The Journal of pharmacology and experimental therapeutics 2002-04-01

Effects of the CRF1 antagonist SSR125543A on aggressive behaviors in hamsters

PMID 15006456; DOI 10.1016/j.pbb.2003.12.023; Pharmacology, biochemistry, and behavior 2004-03-01

[▶ PubChem](#)

9.5 Chemical-Gene Co-Occurrences in Literature

Showing 3 of 45 [View More](#) [↗](#)**Gene/Protein/Enzyme****Selected evidence**

corticotropin releasing hormone receptor 1

20 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

The CRF1 receptor antagonist SSR125543 attenuates long-term cognitive deficit induced by acute inescapable stress in mice, independently from the hypothalamic pituitary adrenal axis
PMID 22659580; DOI 10.1016/j.pbb.2012.05.013; Pharmacology, biochemistry, and behavior 2012-09-01

Control of Stress-Induced ACTH Secretion by Vasopressin and CRH: Additional Evidence
PMID 27221315; DOI 10.1159/000445480; Neuropsychobiology 2016-01-01

ethylene-responsive
transcription factor crf1

16 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
Name matches: crf1; crhr1 ssr125543

The CRF1 receptor antagonist SSR125543 attenuates long-term cognitive deficit induced by acute inescapable stress in mice, independently from the hypothalamic pituitary adrenal axis
PMID 22659580; DOI 10.1016/j.pbb.2012.05.013; Pharmacology, biochemistry, and behavior 2012-09-01
Name matches: crf1; crhr1 ssr125543

Control of Stress-Induced ACTH Secretion by Vasopressin and CRH: Additional Evidence
PMID 27221315; DOI 10.1159/000445480; Neuropsychobiology 2016-01-01
Name matches: crf1; crhr1 ssr125543

corticotropin releasing hormone

23 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

Control of Stress-Induced ACTH Secretion by Vasopressin and CRH: Additional Evidence
PMID 27221315; DOI 10.1159/000445480; Neuropsychobiology 2016-01-01
Name matches: crh ssr125543

Drug-Dependent Requirement of Hippocampal Neurogenesis in a Model of Depression and of Antidepressant Reversal
PMID 18406399; DOI 10.1016/j.biopsych.2008.02.022; Biological Psychiatry 2008-08-15

9.6 Chemical-Disease Co-Occurrences in Literature

Showing 3 of 70 [View More](#)

Disease

Selected evidence

Congenital adrenal hyperplasia due to 21 hydroxylase deficiency

6 articles

[View All](#)
Crinercerfont Lowers Elevated Hormone Markers in Adults With 21-Hydroxylase Deficiency Congenital Adrenal Hyperplasia

PMID 34653252; DOI 10.1210/clinem/dgab749; The Journal of clinical endocrinology and metabolism 2021-10-15

 Name matches: 21-hydroxylase deficiency; 21ohd *crinercerfont*; *nbi-74788*
Crinercerfont, a CRF1 Receptor Antagonist, Lowers Adrenal Androgens in Adolescents With Congenital Adrenal Hyperplasia

PMID 37216921; DOI 10.1210/clinem/dgad270; The Journal of clinical endocrinology and metabolism 2023-05-22

 Name matches: 21-hydroxylase deficiency; 21ohd *crinercerfont*
Current and future perspectives on clinical management of classic 21-hydroxylase deficiency

PMID 37380491; DOI 10.1507/endocrj.ej23-0075; Endocrine Journal 2023-10-30 (Review Article)

 Name matches: 21-hydroxylase deficiency; 21ohd *crinercerfont*
Anxiety Disorders

13 articles

[View All](#)
Drug-Dependent Requirement of Hippocampal Neurogenesis in a Model of Depression and of Antidepressant Reversal

PMID 18406399; DOI 10.1016/j.biopsych.2008.02.022; Biological Psychiatry 2008-08-15

 Name matches: anxiety disorders *ssr125543*
Effects of a stressor and corticotrophin releasing factor on ethanol deprivation-induced ethanol intake and anxiety-like behavior in alcohol-preferring P rats

PMID 21643675; DOI 10.1007/s00213-011-2366-5; Psychopharmacology 2011-06-04

 Name matches: anxiety *ssr125543*
4-(2-Chloro-4-methoxy-5-methylphenyl)-N-[(1S)-2-cyclopropyl-1-(3-fluoro-4-methylphenyl)ethyl]5-methyl-N-(2-propynyl)-1, 3-thiazol-2-amine Hydrochloride (SSR125543A), a Potent and Selective Corticotrophin-Releasing Factor1 Receptor Antagonist. II. Characterization in Rodent Models of Stress-Related Disorders

PMID 11907191; DOI 10.1124/jpet.301.1.333; The Journal of pharmacology and experimental therapeutics 2002-04-01

Name matches: **anxiety**; **anxiety disorders** *ssr125543a*

Depressive Disorder

18 articles

[View All](#)

Drug-Dependent Requirement of Hippocampal Neurogenesis in a Model of Depression and of Antidepressant Reversal

PMID 18406399; DOI 10.1016/j.biopsych.2008.02.022; Biological Psychiatry 2008-08-15

Name matches: **depression** *ssr125543*

4-(2-Chloro-4-methoxy-5-methylphenyl)-N-[(1S)-2-cyclopropyl-1-(3-fluoro-4-methylphenyl)ethyl]5-methyl-N-(2-propynyl)-1, 3-thiazol-2-amine Hydrochloride (SSR125543A), a Potent and Selective Corticotrophin-Releasing Factor1 Receptor Antagonist. II. Characterization in Rodent Models of Stress-Related Disorders

PMID 11907191; DOI 10.1124/jpet.301.1.333; The Journal of pharmacology and experimental therapeutics 2002-04-01

Name matches: **depression** *ssr125543a*

Blockade of CRF(1) or V(1b) receptors reverses stress-induced suppression of neurogenesis in a mouse model of depression

PMID 14699428; DOI 10.1038/sj.mp.4001464; Molecular Psychiatry 2003-12-23

Name matches: **depression** *ssr125543a*

[PubChem](#)

10 Patents



10.1 Depositor-Supplied Patent Identifiers



103 items





SORT BY

Priority Date - Most Recent



Method of treating late-onset congenital adrenal hyperplasia due to 21-hydroxylase deficiency by individually tailored glucocorticoid regimen

Publication Number: **US-2022323461-A1**

Priority Date: 2021-04-12

Crf1 receptor antagonist for the treatment of congenital adrenal hyperplasia

Publication Number: **WO-2021252669-A1**

Priority Date: 2020-06-10

Crf receptor antagonists and methods of usePublication Number: [WO-2021062246-A1](#)

Priority Date: 2019-09-27

Crf receptor antagonists and methods of usePublication Number: [EP-4034111-A1](#)

Priority Date: 2019-09-27

Processes for the synthesis of valbenazinePublication Number: [WO-2021050977-A1](#)

Priority Date: 2019-09-13

[<< First](#) [< Previous](#) Page **1** of 21 [Next >](#) [Last >>](#)[▶ PubChem](#)**Link to all deposited patent identifiers**[▶ PubChem](#)

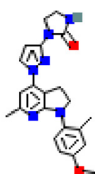
10.2 WIPO PATENTSCOPE



Patents are available for this chemical structure:

<https://patentscope.wipo.int/search/en/result.jsf?inchikey=IEAKXXNRGSLYTQ-DEOSSOPVSA-N>[▶ PATENTSCOPE \(WIPO\)](#)

10.3 Chemical Co-Occurrences in Patents

Showing 3 of 100 [View More](#)**Chemical****Selected evidence****Emicerfont**

5 patents from 3 patent families

[View All](#)[Gene predictors of response to treatment with CRHR1 antagonists](#)

JP-6857130-B2; Grant Date: 2021-04-14

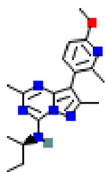
[Treatment of congenital adrenal hyperplasia](#)

US-11311544-B2; Grant Date: 2022-04-26

CID 11223423

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



Pexacerfont

CID 9884366

5 patents from 3 patent families

View All

Gene predictors of response to treatment with CRHR1 antagonists

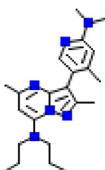
JP-6857130-B2; Grant Date: 2021-04-14

Treatment of congenital adrenal hyperplasia

US-11311544-B2; Grant Date: 2022-04-26

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



3-(6-(Dimethylamino)-4-methylpyridin-3-yl)-2,5-dimethyl-N,N-dipropylpyrazolo[1,5-a]pyrimidin-7-amine

CID 9821250

5 patents from 2 patent families

View All

Crf1 receptor antagonists for the treatment of congenital adrenal hyperplasia

KR-102258522-B1; Grant Date: 2021-05-31

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

10.4 Chemical-Disease Co-Occurrences in Patents



Showing 3 of 100 View More



Disease

Selected evidence

Adrenal Hyperplasia, Congenital

5 patents from 3 patent families

View All

Crf1 receptor antagonists for the treatment of congenital adrenal hyperplasia

KR-102258522-B1; Grant Date: 2021-05-31

	Gene predictors of response to treatment with CRHR1 antagonists JP-6857130-B2; Grant Date: 2021-04-14 Methods of treatment with gene predictors of response to treatment with CRHR1 antagonists JP-6905468-B2; Grant Date: 2021-07-21	
Congenital adrenal hyperplasia due to 11-Beta-hydroxylase deficiency	3 patents from 1 patent family Treatment of congenital adrenal hyperplasia US-11311544-B2; Grant Date: 2022-04-26	View All 
Adrenogenital Syndrome	5 patents from 3 patent families Crf1 receptor antagonists for the treatment of congenital adrenal hyperplasia KR-102258522-B1; Grant Date: 2021-05-31 Gene predictors of response to treatment with CRHR1 antagonists JP-6857130-B2; Grant Date: 2021-04-14 Methods of treatment with gene predictors of response to treatment with CRHR1 antagonists JP-6905468-B2; Grant Date: 2021-07-21	View All 

► PubChem

10.5 Chemical-Gene Co-Occurrences in Patents



Showing 3 of 34 View More 



Gene	Selected evidence	
crhr1	5 patents from 4 patent families Gene predictors of response to treatment with CRHR1 antagonists JP-6857130-B2; Grant Date: 2021-04-14 Crf1 receptor antagonists for the treatment of congenital adrenal hyperplasia KR-102258522-B1; Grant Date: 2021-05-31 Method for predicting a treatment response to a CRHR1 antagonist and/or a V1B antagonist in a patient with depressive and/or anxiety symptoms	View All 

cyp21a2	3 patents from 1 patent family	View All
Treatment of congenital adrenal hyperplasia US-11311544-B2; Grant Date: 2022-04-26		
steroid 11-beta-hydroxylase	3 patents from 1 patent family	View All
Treatment of congenital adrenal hyperplasia US-11311544-B2; Grant Date: 2022-04-26		

► [PubChem](#)

11 Interactions and Pathways

11.1 Chemical-Target Interactions

4 items						
Protein	Gene	Taxonomy	Action	Evidence IDs	Data Source	
Corticotropin-releasing factor receptor 1	LINC02210-CRHR1	Homo sapiens (human)	Antagonist		Therapeutic Target Database (TTD)	
	CRHR1	Homo sapiens (human)	Inhibitor		Drug Gene Interaction database (DGIdb)	
Corticotropin-releasing factor receptor 1		Homo sapiens (human)	Antagonist	PMID:11907190	IUPHAR/BPS Guide to PHARMACOLOGY	

► [Drug Gene Interaction database \(DGIdb\)](#); [IUPHAR/BPS Guide to PHARMACOLOGY](#); [Therapeutic T...](#)

12 Biological Test Results

12.1 BioAssay Results

76 items 	
Search 	SORT BY Activity Value - Increasing 
Binding affinity towards human Corticotropin releasing factor receptor 1 by the displacement of [125I]CRF from CHO cells Activity Outcome: Active Activity Type: Ki Activity Value: 0.24 μM BioAssay AID: 53966 Target Name: CRHR1 - corticotropin releasing hormone receptor 1 (human) Substance SID: 103258755 Compound CID: 5282340	
Binding affinity towards human Corticotropin releasing factor receptor 1 by the displacement of [125I]CRF from CHO cells Activity Outcome: Active Activity Type: Ki Activity Value: 0.24 μM BioAssay AID: 53966 Target Name: LINC02210-CRHR1 - LINC02210-CRHR1 readthrough (human) Substance SID: 103258755 Compound CID: 5282340	
Primary qHTS to identify gynecologic anti-cancer compounds using libraries of approved drugs and bioactive compounds Activity Outcome: Inactive Activity Value: 1 μM BioAssay AID: 1345084 Substance SID: 363680369 Compound CID: 5282340	
Cytochrome P450 family 2 subfamily D member 6 (CYP2D6) small molecule antagonists: luciferase cell-based qHTS assay Activity Outcome: Active Activity Type: Potency Activity Value: 2.6837 μM BioAssay AID: 1645840 Target Name: CYP2D6 - cytochrome P450 family 2 subfamily D member 6 (gene/pseudogene) (human) Substance SID: 363680369 Compound CID: 5282340	
Primary qHTS for inhibitors of nuclear receptor binding SET domain protein 2 (NSD2)	
 First  Previous Page 1 of 16 Next  Last 	

 PubChem

13 Classification



13.1 MeSH Tree



1 item

View in Classification Browser

MeSH Tree > Chemicals and Drugs Category > Organic Chemicals > Amines > Supplementary Records
[crinecerfont](#)

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

13.2 NCI Thesaurus Tree



1 item

View in Classification Browser

NCI Thesaurus > Drug, Food, Chemical or Biomedical Material > Pharmacologic Substance >
Hormone Therapy Agent > Hormone Antagonist
[Crinecerfont](#)

► [NCI Thesaurus \(NCIt\)](#)

13.3 ChEBI Ontology



1 item

View in Classification Browser

ChEBI Ontology > chemical entity > molecular entity > main group molecular entity > p-block molecular entity >
carbon group molecular entity > organic molecular entity > organic amino compound > amine
[SSR 125543](#)

► [ChEBI](#)

13.4 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]
[Crinecerfont \(USAN\)](#)

► [KEGG](#)

13.5 ChemIDplus



12 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 > Other Resources (Internet Locators)

ChEBI

Chemical Entities of Biological Interest - Dictionary of molecular entities focused on "small" chemical compounds. ChEBI is part of the EMBL-European Bioinformatics Institute.

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

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of 3
Next >
Last »

► [ChemIDplus](#)

13.6 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 NRI27914, R121919, antalarmin, CP 154 526, CP

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

13.7 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 consequences

[▶ ChEMBL](#)

13.8 EPA DSSTox Classification



3 items

View in Classification Browser

CompTox Chemicals Dashboard Chemical Lists > LIST

[\[CPDAT\] 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

[\[FDAUNII0421\] 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

[\[CPDATv2\] Chemical and Products Database v2](#)

Short_Description: Chemicals contained in the EPA's Chemical and Products Database: Version 2 (last updated March 13th 2024)

[▶ EPA DSSTox](#)

13.9 PFAS and Fluorinated Organic Compounds in PubChem



1 item

View in Classification Browser

PFAS and Fluorinated Compounds in PubChem > Organofluorine compounds > Fluorinated aromatic substances > Fluorinated aromatic ring(s) with non-fluorinated aliphatic side chain(s) > Contains 01 Fluorine atom

Exact mass range 250-500

Cases where the chemical structure exact mass is in the range of 250-500 Daltons

[▶ PubChem](#)

13.10 MolGenie Organic Chemistry Ontology



39 items
View in Classification Browser

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

MolGenie Organic Chemistry Ontology > ChEBI chemical entities > substructural concepts > functional groups > oxygen containing functional groups > ethers
aryl alkyl ethers

MolGenie Organic Chemistry Ontology > ChEMBL chemical entities > compounds > organic compounds > aromatic compounds
aromatic chlorides

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

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► MolGenie

14 Information Sources



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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

https://commonchemistry.cas.org/detail?cas_rn=752253-39-7

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SSR 125543

<https://pubchem.ncbi.nlm.nih.gov/substance/?source=chemidplus&sourceid=0752253397>

ChemIDplus Chemical Information Classification

<https://pubchem.ncbi.nlm.nih.gov/source/ChemIDplus>

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4-(2-Chloro-4-methoxy-5-methylphenyl)-N-[2-cyclopropyl-1-(3-fluoro-4-methylphenyl)ethyl]-5-methyl-N-(prop-2-yn-1-yl)-1,3-thiazol-2-amine

<https://comptox.epa.gov/dashboard/DTXSID10996687>

CompTox Chemicals Dashboard Chemical Lists

<https://comptox.epa.gov/dashboard/chemical-lists/>

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<https://gsrs.ncats.nih.gov/ginas/app/beta/substances/MFT24BX55I>

6. ChEBI

SSR 125543

<https://www.ebi.ac.uk/chebi/searchId.do?chebiId=CHEBI:34969>

ChEBI Ontology

<http://www.ebi.ac.uk/chebi/userManualForward.do#ChEBI%20Ontology>

7. Open Targets

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<https://platform.opentargets.org/drug/CHEMBL291657>

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

<https://www.ebi.ac.uk/chembl/explore/compound/CHEMBL291657>

ChEMBL Protein Target Tree

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

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<https://dailymed.nlm.nih.gov/dailymed/search.cfm?labeltype=all&query=CRINECERFONT>

11. Drug Gene Interaction database (DGIdb)

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The data used in DGIdb is all open access and where possible made available as raw data dumps in the downloads section.

<http://www.dgldb.org/downloads>

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<https://www.dgldb.org/drugs/ncit:C174708>

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<https://www.guidetopharmacology.org/GRAC/LigandDisplayForward?ligandId=3533>

Guide to Pharmacology Target Classification

<https://www.guidetopharmacology.org/targets.jsp>

13. Therapeutic Target Database (TTD)

SSR125543

<https://idrblab.net/ttd/data/drug/details/D05IIN>

14. EU Clinical Trials Register

<https://www.clinicaltrialsregister.eu/>

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17. Japan Chemical Substance Dictionary (Nikkaji)

http://jglobal.jst.go.jp/en/redirect?Nikkaji_No=J2.788.046K

18. KEGG

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<https://www.kegg.jp/entry/D12366>

Target-based classification of drugs

http://www.genome.jp/kegg-bin/get_htext?br08310.keg

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NCI Thesaurus

<https://ncit.nci.nih.gov>

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<https://pharos.nih.gov/about>

SSR125543A

<https://pharos.nih.gov/ligands/W3JYT8TJURTS>

22. Springer Nature

<https://pubchem.ncbi.nlm.nih.gov/substance/?source=15745&sourceid=33059069-373786447>

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25. PubChem

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

PFAS and Fluorinated Compounds in PubChem

https://gitlab.com/uniluxembourg/lcsb/eci/pubchem-docs/-/raw/main/pfas-tree/PFAS_Tree.pdf?inline=false

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<https://www.ncbi.nlm.nih.gov/mesh/2102536>

MeSH Tree

<http://www.nlm.nih.gov/mesh/meshhome.html>

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MolGenie Organic Chemistry Ontology

<https://github.com/MolGenie/ontology/>

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