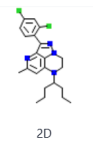
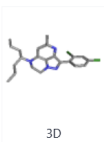


COMPOUND

Nbi-34041

PubChem CID	9888194
Structure	<div> 2D</div> <div> 3D</div>
Molecular Formula	C ₂₂ H ₂₆ Cl ₂ N ₄
Synonyms	NBI-34041 268545-87-5 874OEY3JEJ SB723620 SB-723620 View More...
Molecular Weight	417.4 g/mol <small>Computed by PubChem 2.2 (PubChem release 2025.04.14)</small>
Dates	Create: 2006-10-25 Modify: 2026-05-23
Description	high-affinity CRF1 (corticotropin-releasing factor receptor 1) receptor antagonist for attenuating elevated stress response ► Medical Subject Headings (MeSH)

Cite

Download

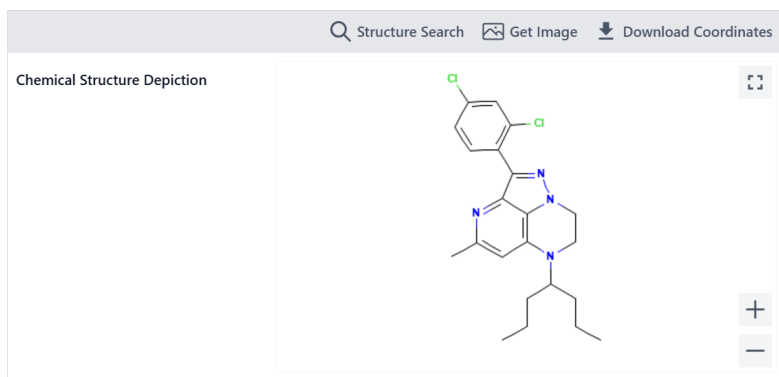
CONTENTS

Title and Summary

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

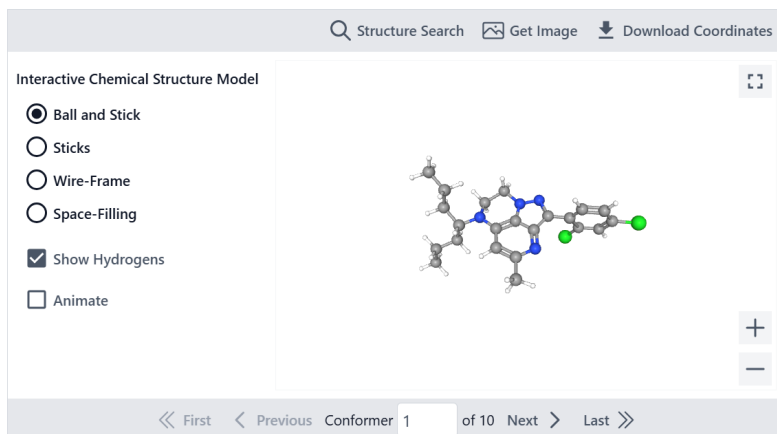
1 Structures

1.1 2D Structure



[► PubChem](#)

1.2 3D Conformer



[PubChem](#)

2 Names and Identifiers



2.1 Computed Descriptors



2.1.1 IUPAC Name



3-(2,4-dichlorophenyl)-9-heptan-4-yl-6-methyl-1,2,5,9-tetrazatricyclo[6.3.1.0^{4,12}]dodeca-2,4,6,8(12)-tetraene

Computed by Lexichem TK 2.7.0 (PubChem release 2025.04.14)

[PubChem](#)

2.1.2 InChI



InChI=1S/C22H26Cl2N4/c1-4-6-16(7-5-2)27-10-11-28-22-19(27)12-14(3)25-21(22)20(26-28)17-9-8-15(23)13-18(17)24/h8-9,12-13,16H,4-7,10-11H2,1-3H3

Computed by InChI 1.07.2 (PubChem release 2025.04.14)

[PubChem](#)

2.1.3 InChIKey



AKLMUGFDGONMAA-UHFFFAOYSA-N

Computed by InChI 1.07.2 (PubChem release 2025.04.14)

[PubChem](#)

2.1.4 SMILES



CCCC(CCC)N1CCN2C3=C1C=C(N=C3C(=N2)C4=C(C(C=C(C4)Cl)Cl)C

Computed by OEChem 2.3.0 (PubChem release 2025.04.14)

[PubChem](#)

2.2 Molecular Formula



C₂₂H₂₆Cl₂N₄

Computed by PubChem 2.2 (PubChem release 2025.04.14)

[PubChem](#)

2.3 Other Identifiers

2.3.1 CAS

268545-87-5
[▶ ChemDplus; FDA Global Substance Registration System \(GSRS\)](#)

2.3.2 UNII

874OEY3JEJ
[▶ FDA Global Substance Registration System \(GSRS\)](#)

2.3.3 ChEMBL ID

CHEMBL188907
[▶ ChEMBL](#)

2.3.4 Nikkaji Number

J2.861.989H
[▶ Japan Chemical Substance Dictionary \(Nikkaji\)](#)

2.3.5 Pharos Ligand ID

6X1UZBXJTLJH
[▶ Pharos](#)

2.3.6 Wikidata

Q27269794
[▶ Wikidata](#)

2.4 Synonyms

2.4.1 MeSH Entry Terms

NBI-34041
[▶ Medical Subject Headings \(MeSH\)](#)

2.4.2 Depositor-Supplied Synonyms

NBI-34041	CHEMBL18890
268545-87-5	3-(2,4-Dichloro
874OEY3JEJ	orb1695949
SB723620	SCHEMBL1660
SB-723620	SCHEMBL2946
1-(2,4-Dichlorophenyl)-5-(heptan-4-yl)-7-methyl-4,5-dihydro-3H-2,2a,5,8-tetraazaacenaphthylene	SCHEMBL2946
6H-1,3,6,8a-Tetraazaacenaphthylene, 2-(2,4-dichlorophenyl)-7,8-dihydro-4-methyl-6-(1-propylbutyl)-	GTPL10375
RefChem:164906	NBI34041
NBI 34041	BDBM5017132
UNII-874OEY3JEJ	AKOS0407532

[▶ PubChem](#)

3 Chemical and Physical Properties

3.1 Computed Properties

Property Name	Property Value	Reference
Molecular Weight	417.4 g/mol	Computed by PubChem 2.2 (PubChem release 2025.04.14)
XLogP3-AA	6.3	Computed by XLogP3 3.0 (PubChem release 2025.04.14)
Hydrogen Bond Donor Count	0	Computed by Cactvs 3.4.8.18 (PubChem release 2025.04.14)
Hydrogen Bond Acceptor Count	3	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	416.1534522 Da	Computed by PubChem 2.2 (PubChem release 2025.04.14)
Monoisotopic Mass	416.1534522 Da	Computed by PubChem 2.2 (PubChem release 2025.04.14)
Topological Polar Surface Area	34 Å²	Computed by Cactvs 3.4.8.18 (PubChem release 2025.04.14)
Heavy Atom Count	28	Computed by PubChem
Formal Charge	0	Computed by PubChem
Complexity	515	Computed by Cactvs 3.4.8.18 (PubChem release 2025.04.14)
Isotope Atom Count	0	Computed by PubChem
Defined Atom Stereocenter Count	0	Computed by PubChem
Undefined Atom Stereocenter Count	0	Computed by PubChem
Defined Bond Stereocenter Count	0	Computed by PubChem
Undefined Bond Stereocenter Count	0	Computed by PubChem
Covalently-Bonded Unit Count	1	Computed by PubChem
Compound Is Canonicalized	Yes	Computed by PubChem (release 2025.04.14)

[PubChem](#)

4 Related Records

4.1 Related Compounds with Annotation

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

[PubChem](#)

4.2 Related Compounds

Mixtures, Components, and Neutralized Forms 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

500808324

▶ PubChem

4.3.2 Related Substances 🔍 🔗

All Count	51
Same Count	48
Mixture Count	3

▶ PubChem

4.3.3 Substances by Category 🔍 🔗

5 categories Download	
Chemical Vendors (20) —	
MedChemexpress MCE	External ID: HY-14128
TargetMol	External ID: T33607
001Chemical	External ID: DY545531
BenchChem	External ID: B1676988
Ambinter	External ID: Amb24088299
A2B Chem	External ID: BJ61438
AbaChemScene	External ID: CS-0003216
EvitaChem	External ID: evt-276591
Starshine Chemical	External ID: 2023-05-7C03426
BOC Sciences	External ID: 268545-87-5
RR Scientific	External ID: R659338
AKos Consulting & Solutions	External ID: AKOS040753222
Biorbyt	External ID: orb1695949
Mcule	External ID: MCULE-2888217136
MolCore	External ID: DY545531
	External ID: MC545531
BLD Pharm	External ID: BD01850809
InvivoChem	External ID: V26279
Smolecule	External ID: S536786
MuseChem	External ID: I008251

Curation Efforts (10)	
BindingDB (Curation Efforts, Research and Development)	
PubChem SID: 104057570	External ID: 50171325
ChEMBL (Curation Efforts, Research and Development)	
PubChem SID: 103459940	External ID: ChEMBL188907
ChemDplus (Curation Efforts, Governmental Organizations, Research and Development)	
PubChem SID: 313370849	External ID: 0268545875
Egon Willighagen, Department of Bioinformatics - BiGCaT, Maastricht University	
PubChem SID: 385744693	External ID: Q27269794
FDA Global Substance Registration System (GSRS) (Curation Efforts, Governmental Organizations)	
PubChem SID: 313183377	External ID: 8740EY3JEJ
IUPHAR/BPS Guide to PHARMACOLOGY (Curation Efforts, Research and Development)	
PubChem SID: 384403655	External ID: 10375
SureChEMBL (Curation Efforts, Research and Development)	
PubChem SID: 311391177	External ID: SCHEMBL16606732
PubChem SID: 514292023	External ID: SCHEMBL29482254
PubChem SID: 514292027	External ID: SCHEMBL29482258
Wikidata	
PubChem SID: 386581331	External ID: Q27269794
Governmental Organizations (5)	
ChemDplus (Curation Efforts, Governmental Organizations, Research and Development)	
PubChem SID: 313370849	External ID: 0268545875
FDA Global Substance Registration System (GSRS) (Curation Efforts, Governmental Organizations)	
PubChem SID: 313183377	External ID: 8740EY3JEJ
Japan Chemical Substance Dictionary (Nikkaji)	
PubChem SID: 273928003	External ID: J2.861.989H
PATENTSCOPE (WIPO)	
PubChem SID: 389793900	External ID: AKLMUGFDGONMAA-UHFFFAOYSA-N
PubChem Reference Collection	
PubChem SID: 500808324	External ID: 164906
Research and Development (12)	
Ace Therapeutics	
PubChem SID: 491486620	External ID: SMD294
BindingDB (Curation Efforts, Research and Development)	
PubChem SID: 104057570	External ID: 50171325
ChEMBL (Curation Efforts, Research and Development)	
PubChem SID: 103459940	External ID: ChEMBL188907
ChemDplus (Curation Efforts, Governmental Organizations, Research and Development)	
PubChem SID: 313370849	External ID: 0268545875
Google Patents	
PubChem SID: 407428903	External ID: 125133
IBM	
PubChem SID: 245277788	External ID: 63ACC015D1A38C318FC67A861CC85174
IUPHAR/BPS Guide to PHARMACOLOGY (Curation Efforts, Research and Development)	
PubChem SID: 384403655	External ID: 10375
MolGenie	
PubChem SID: 503181970	External ID: 190000883310
Probes & Drugs portal	
PubChem SID: 482136032	External ID: PD121603
SureChEMBL (Curation Efforts, Research and Development)	
PubChem SID: 311391177	External ID: SCHEMBL16606732
PubChem SID: 514292023	External ID: SCHEMBL29482254
PubChem SID: 514292027	External ID: SCHEMBL29482258

Legacy Depositors (10)

3WAY PHARM INC (Chemical Vendors)

PubChem SID: 438580247	External ID: SWK-03701
PubChem SID: 438580817	External ID: SWOT-111720

Bic Biotech (Chemical Vendors)

PubChem SID: 383452841	External ID: NSZB-A261839
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ChemSpider (Research and Development)

PubChem SID: 45635133	External ID: 8063866
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DiscoveryGate (Subscription Services)

PubChem SID: 24174361	External ID: 9888194
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NextBio (Subscription Services)

PubChem SID: 76816332	External ID: 9888194
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SCRIPDB (Research and Development)

PubChem SID: 140044994	External ID: US06514982-20030204-C00028_7
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THE BioTek (Chemical Vendors)

PubChem SID: 434301417	External ID: bt-276591
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Thomson Pharma (Journal Publishers, Subscription Services)

PubChem SID: 14855764	External ID: 00036898
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ZINC (Chemical Vendors)

PubChem SID: 260041786	External ID: ZINC28465228
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► PubChem

4.4 Entrez Crosslinks



PubMed Count 2

► PubChem

5 Chemical Vendors



19 vendors

Download

MedChemexpress MCE

PubChem SID: 497390160	Purchasable Chemical: HY-14128
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TargetMol

PubChem SID: 494450347	Purchasable Chemical: T33607
------------------------	------------------------------

001Chemical

PubChem SID: 440023341	Purchasable Chemical: DY545531
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BenchChem

PubChem SID: 446025129	Purchasable Chemical: B1676988
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Ambinter

PubChem SID: 370016647	Purchasable Chemical: Amb24088299
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A2B Chem

PubChem SID: 495764150	Purchasable Chemical: B161438
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AbaChemScene

PubChem SID: 497386296	Purchasable Chemical: CS-0003216
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EvitaChem

PubChem SID: 486050013	Purchasable Chemical: evt-276591
------------------------	----------------------------------

Starshine Chemical

PubChem SID: 480487197	Purchasable Chemical: 2023-05-7C03426
------------------------	---------------------------------------

BOC Sciences

PubChem SID: 441153794	Purchasable Chemical: 268545-87-5
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RR Scientific

PubChem SID: 481317420	Purchasable Chemical: R659338
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AKos Consulting & Solutions

PubChem SID: 481565754	Purchasable Chemical: AKOS040753222
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Biorbyt	PubChem SID: 516448060	Purchasable Chemical: orb1695949
Mcule	PubChem SID: 494207225	Purchasable Chemical: MCULE-2888217136
MolCore	PubChem SID: 446249309	Purchasable Chemical: DY545531
	PubChem SID: 405476682	Purchasable Chemical: MC545531
BLD Pharm	PubChem SID: 523014307	Purchasable Chemical: BD01850809
InvivoChem	PubChem SID: 500585988	Purchasable Chemical: V26279
Smolecule	PubChem SID: 438486481	Purchasable Chemical: S536786
MuseChem	PubChem SID: 355190251	Purchasable Chemical: 1008251

► PubChem

6 Associated Disorders and Diseases



This data is in our database, but it has not yet made it through processing. Please check back soon...

► Therapeutic Target Database (TTD)

7 Literature



7.1 Consolidated References



5 items

Download

Discovery of N-(1-Ethylpropyl)-[3-methoxy-5-(2-methoxy-4-trifluoromethoxyphenyl)-6-methyl-pyrazin-2-yl]amine 59 (NGD 98-2): An Orally Active Corticotropin Releasing Factor-1 (CRF-1) Receptor Antagonist

Publication Name: Journal of Medicinal Chemistry

Publication Date: 2011-05-27

PMID: 21618986 DOI: 10.1021/jm200365y

Developing small molecule nonpeptidergic drugs for the treatment of anxiety disorders: is the challenge still ahead?

Publication Name: Current topics in behavioral neurosciences

Publication Date: 2010

PMID: 21309119 DOI: 10.1007/7854_2009_14

High-Affinity CRF1 Receptor Antagonist NBI-34041: Preclinical and Clinical Data Suggest Safety and Efficacy in Attenuating Elevated Stress Response

Publication Name: Neuropsychopharmacology : official publication of the American College of Neuropsychopharmacology

Publication Date: 2007-02-07

PMID: 17287823 DOI: 10.1038/sj.npp.1301328

Design and Synthesis of Tricyclic Corticotropin-Releasing Factor-1 Antagonists

Publication Name: Journal of Medicinal Chemistry

Publication Date: 2005-08-10

PMID: 16134945 DOI: 10.1021/jm049085v

Design and Synthesis of Tricyclic Imidazo[4,5-b]pyridin-2-ones as Corticotropin-Releasing Factor-1 Antagonists

Publication Name: Journal of Medicinal Chemistry

Publication Date: 2005-07-09

PMID: 16078829 DOI: 10.1021/jm050384+

► PubChem

7.2 NLM Curated PubMed Citations



All NLM Curated PubMed Citations

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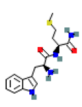
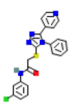
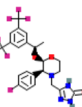
► Medical Subject Headings (MeSH)

7.3 Chemical Co-Occurrences in Literature



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

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Chemical	Selected evidence
 H-Trp-Met-NH2 CID 13306579	<p>1 article View All</p> <p>Developing small molecule nonpeptidergic drugs for the treatment of anxiety disorders: is the challenge still ahead? PMID 21309119; DOI 10.1007/7854_2009_14; Current topics in behavioral neurosciences 2010-01-01 (Review Article)</p>
 N-(3-chlorophenyl)-2-[(4-phenyl-5-pyridin-4-yl-1,2,4-triazol-3-yl)sulfanyl]acetamide CID 1122655	<p>1 article View All</p> <p>Developing small molecule nonpeptidergic drugs for the treatment of anxiety disorders: is the challenge still ahead? PMID 21309119; DOI 10.1007/7854_2009_14; Current topics in behavioral neurosciences 2010-01-01 (Review Article)</p>
 Aprepitant CID 13541356	<p>1 article View All</p> <p>Developing small molecule nonpeptidergic drugs for the treatment of anxiety disorders: is the challenge still ahead? PMID 21309119; DOI 10.1007/7854_2009_14; Current topics in behavioral neurosciences 2010-01-01 (Review Article)</p>

► PubChem

7.4 Chemical-Gene Co-Occurrences in Literature



Showing 3 of 56 View More Co-Occurrence and Evidence Data

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Gene/Protein/Enzyme	Selected evidence
corticotropin releasing hormone receptor 1	<p>5 articles View All</p> <p>High-Affinity CRF1 Receptor Antagonist NBI-34041: Preclinical and Clinical Data Suggest Safety and Efficacy in Attenuating Elevated Stress Response PMID 17287823; DOI 10.1038/sj.npp.1301328; Neuropsychopharmacology : official publication of the American College of Neuropsychopharmacology 2007-02-07</p> <p>Developing small molecule nonpeptidergic drugs for the treatment of anxiety disorders: is the challenge still ahead? PMID 21309119; DOI 10.1007/7854_2009_14; Current topics in behavioral neurosciences 2010-01-01 (Review Article)</p> <p>Design and Synthesis of Tricyclic Imidazo[4,5-b]pyridin-2-ones as Corticotropin-Releasing Factor-1 Antagonists PMID 16078829; DOI 10.1021/jm050384+; Journal of Medicinal Chemistry 2005-07-09</p>
corticotropin releasing hormone	<p>4 articles View All</p> <p>High-Affinity CRF1 Receptor Antagonist NBI-34041: Preclinical and Clinical Data Suggest Safety and Efficacy in Attenuating Elevated Stress Response PMID 17287823; DOI 10.1038/sj.npp.1301328; Neuropsychopharmacology : official publication of the American College of Neuropsychopharmacology 2007-02-07</p>

	Design and Synthesis of Tricyclic Imidazo[4,5- b]pyridin-2-ones as Corticotropin-Releasing Factor-1 Antagonists PMID 16078829; DOI 10.1021/jm050384+; Journal of Medicinal Chemistry 2005-07-09
	Design and Synthesis of Tricyclic Corticotropin-Releasing Factor-1 Antagonists PMID 16134945; DOI 10.1021/jm049085v; Journal of Medicinal Chemistry 2005-08-10
tachykinin precursor 3	1 article View All
	Developing small molecule nonpeptidergic drugs for the treatment of anxiety disorders: is the challenge still ahead? PMID 21309119; DOI 10.1007/7854_2009_14; Current topics in behavioral neurosciences 2010-01-01 (Review Article)

► PubChem

7.5 Chemical-Disease Co-Occurrences in Literature



Showing 2 of 2 View More Co-Occurrence and Evidence Data Download	
Disease	Selected evidence
Anxiety Disorders	3 articles View All Developing small molecule nonpeptidergic drugs for the treatment of anxiety disorders: is the challenge still ahead? PMID 21309119; DOI 10.1007/7854_2009_14; Current topics in behavioral neurosciences 2010-01-01 (Review Article) High-Affinity CRF1 Receptor Antagonist NBI-34041: Preclinical and Clinical Data Suggest Safety and Efficacy in Attenuating Elevated Stress Response PMID 17287823; DOI 10.1038/sj.npp.1301328; Neuropsychopharmacology : official publication of the American College of Neuropsychopharmacology 2007-02-07 Design and Synthesis of Tricyclic Corticotropin-Releasing Factor-1 Antagonists PMID 16134945; DOI 10.1021/jm049085v; Journal of Medicinal Chemistry 2005-08-10
Depressive Disorder	1 article View All High-Affinity CRF1 Receptor Antagonist NBI-34041: Preclinical and Clinical Data Suggest Safety and Efficacy in Attenuating Elevated Stress Response PMID 17287823; DOI 10.1038/sj.npp.1301328; Neuropsychopharmacology : official publication of the American College of Neuropsychopharmacology 2007-02-07

► PubChem

7.6 Chemical-Organism Co-Occurrences in Literature



Showing 3 of 5 View More Co-Occurrence and Evidence Data Download	
Organism	Selected evidence
rattus norvegicus (norway rat)	2 articles View All High-Affinity CRF1 Receptor Antagonist NBI-34041: Preclinical and Clinical Data Suggest Safety and Efficacy in Attenuating Elevated Stress Response PMID 17287823; DOI 10.1038/sj.npp.1301328; Neuropsychopharmacology : official publication of the American College of Neuropsychopharmacology 2007-02-07 Discovery of N-(1-Ethylpropyl)-[3-methoxy-5-(2-methoxy-4-trifluoromethoxyphenyl)-6-methyl-pyrazin-2-yl]amine 59 (NGD 98-2): An Orally Active Corticotropin Releasing Factor-1 (CRF-1) Receptor Antagonist PMID 21618986; DOI 10.1021/jm200365y; Journal of Medicinal Chemistry 2011-05-27
homo sapiens (human)	4 articles View All High-Affinity CRF1 Receptor Antagonist NBI-34041: Preclinical and Clinical Data Suggest Safety and Efficacy in Attenuating Elevated Stress Response PMID 17287823; DOI 10.1038/sj.npp.1301328; Neuropsychopharmacology : official publication of the American College of Neuropsychopharmacology 2007-02-07 Design and Synthesis of Tricyclic Imidazo[4,5- b]pyridin-2-ones as Corticotropin-Releasing Factor-1 Antagonists PMID 16078829; DOI 10.1021/jm050384+; Journal of Medicinal Chemistry 2005-07-09 Design and Synthesis of Tricyclic Corticotropin-Releasing Factor-1 Antagonists PMID 16134945; DOI 10.1021/jm049085v; Journal of Medicinal Chemistry 2005-08-10

cricetulus griseus (chinese hamster)

1 article

[View All](#)

Design and Synthesis of Tricyclic Imidazo[4,5- b]pyridin-2-ones as Corticotropin-Releasing Factor-1 Antagonists
PMID 16078829; DOI 10.1021/jm050384+; Journal of Medicinal Chemistry 2005-07-09

[PubChem](#)

8 Patents



8.1 Depositor-Supplied Patent Identifiers



159 items		Download
Search	SORT BY	Priority Date - Most Recent
Mc2r modulator compounds		
Publication Number: WO-2024175925-A1		
Priority Date: 2023-02-23		
Mc2r modulator compounds		
Publication Number: WO-2024175928-A1		
Priority Date: 2023-02-23		
Mc2r modulator compounds		
Publication Number: WO-2024175927-A1		
Priority Date: 2023-02-23		
Treatment of congenital adrenal hyperplasia and polycystic ovary syndrome		
Publication Number: WO-2023163945-A1		
Priority Date: 2022-02-23		
Methods for treating testicular and ovarian adrenal rest tumors		
Publication Number: WO-2019210266-A1		
Priority Date: 2018-04-27		
<< First < Previous Page 1 of 32 Next > Last >>		

[PubChem](#)

[Link to all deposited patent identifiers](#)

[PubChem](#)

8.2 WIPO PATENTSCOPE



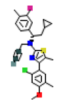
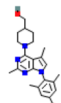
Patents are available for this chemical structure:

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

[PATENTSCOPE \(WIPO\)](#)

8.3 Chemical Co-Occurrences in Patents



Showing 3 of 100 View More Co-Occurrence and Evidence Data ↗		Download
Chemical	Selected evidence	
 4-(2-Chloro-4-methoxy-5-methylphenyl)-N-((1S)-2-cyclopropyl-1-(3-fluoro-4-methylphenyl)ethyl)-5-methyl-N-2-propyn-1-yl-2-thiazolamine CID 5282340	6 patents from 2 patent families	View All ↗
	Treatment of congenital adrenal hyperplasia US-10905690-B2; Grant Date: 2021-02-02 Method for predicting a treatment response to a CRHR1 antagonist and/or a V1B antagonist in a patient with depressive and/or anxiety symptoms US-10837062-B2; Grant Date: 2020-11-17	
 4-Piperidinemethanol, 1-(7-(4-bromo-2,6-dimethylphenyl)-2,5-dimethyl-7H-pyrrolo(2,3-d)pyrimidin-4-yl)- CID 10478567	7 patents from 3 patent families	View All ↗
	Treatment of congenital adrenal hyperplasia US-10905690-B2; Grant Date: 2021-02-02 Method for predicting a treatment response to a CRHR1 antagonist and/or a V1B antagonist in a patient with depressive and/or anxiety symptoms US-10837062-B2; Grant Date: 2020-11-17 Genetic predictors of a response to treatment with crhr1 antagonists EP-3277835-B1; Grant Date: 2019-01-09	
 R121919 CID 9821250	6 patents from 2 patent families	View All ↗
	Treatment of congenital adrenal hyperplasia US-10905690-B2; Grant Date: 2021-02-02 Method for predicting a treatment response to a CRHR1 antagonist and/or a V1B antagonist in a patient with depressive and/or anxiety symptoms US-10837062-B2; Grant Date: 2020-11-17	

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8.4 Chemical-Disease Co-Occurrences in Patents



Showing 3 of 21 View More Co-Occurrence and Evidence Data ↗		Download
Disease	Selected evidence	
Bipolar Disorder	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	
Depressive Disorder	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	
Psychomotor Disorders	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	

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8.5 Chemical-Gene Co-Occurrences in Patents



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Gene	Selected evidence	
avpr1b	2 patents from 1 patent family 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	View All
avp	2 patents from 1 patent family 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	View All
crhr1	2 patents from 1 patent family 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	View All

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8.6 Chemical-Organism Co-Occurrences in Patents



Showing 3 of 8 View More Co-Occurrence and Evidence Data		Download
Organism	Selected evidence	
salvia officinalis (garden sage)	2 patents from 1 patent family 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	View All
entandrophragma utile	1 patent from 1 patent family 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	View All
anthonomus pomorum (apple weevil)	2 patents from 1 patent family 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	View All

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9 Interactions and Pathways



9.1 Chemical-Target Interactions



3 items Download					
Protein	Gene	Taxonomy	Action	Evidence	Data Source
	CRHR2	Homo sapiens (human)			Drug Gene Interaction database (DGIdb)
Corticotropin-releasing factor receptor 1	CRHR1	Homo sapiens (human)	Antagonist	PMID:16078829	IUPHAR/BPS Guide to PHARMACOLOGY
	ALAS2	Homo sapiens (human)	Inhibitor		Drug Gene Interaction database (DGIdb)

► Drug Gene Interaction database (DGIdb); IUPHAR/BPS Guide to PHARMACOLOGY; Therapeutic Target Databas...

10 Biological Test Results



10.1 BioAssay Results



6 items	Download
<input type="text" value="Search"/>	SORT BY Activity Value - Increasing
Antagonist activity at human CRF-1 receptor	
Activity Outcome: Active Activity Type: Ki Activity Value: 0.004000 µM	
BioAssay AID: 609182	
Target Name: CRHR1 - corticotropin releasing hormone receptor 1 (human)	
Substance SID: 103459940 Compound CID: 9888194	
Antagonist activity at human CRF-1 receptor	
Activity Outcome: Active Activity Type: Ki Activity Value: 0.004000 µM	
BioAssay AID: 609182	
Target Name: LINC02210-CRHR1 - LINC02210-CRHR1 readthrough (human)	
Substance SID: 103459940 Compound CID: 9888194	
Binding affinity for corticotropin-releasing factor-1 expressed in leukocyte tyrosine kinase cells	
Activity Outcome: Active Activity Type: Ki Activity Value: 0.004500 µM	
BioAssay AID: 239687	
Target Name: LINC02210-CRHR1 - LINC02210-CRHR1 readthrough (human)	
Substance SID: 103459940 Compound CID: 9888194	
Binding affinity for corticotropin-releasing factor-1 expressed in leukocyte tyrosine kinase cells	
Activity Outcome: Active Activity Type: Ki Activity Value: 0.004500 µM	
BioAssay AID: 239687	
Target Name: CRHR1 - corticotropin releasing hormone receptor 1 (human)	
Substance SID: 103459940 Compound CID: 9888194	
Binding affinity for human corticotropin releasing factor receptor 1 expressed in Ltk- cells using [125I]sauvagine	
Activity Outcome: Active Activity Type: Ki Activity Value: 0.005012 µM	
BioAssay AID: 254614	
Target Name: CRHR1 - corticotropin releasing hormone receptor 1 (human)	
Substance SID: 103459940 Compound CID: 9888194	
<< First < Previous Page 1 of 2 Next > Last >>	

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11 Classification



11.1 MeSH Tree



1 item	View in Classification Browser
MeSH Tree > Chemicals and Drugs Category > Polycyclic Compounds > Polycyclic Aromatic Hydrocarbons > Naphthalenes > Acenaphthenes	
⌕ Show alternative paths	
NBI-34041	
high-affinity CRF1 (corticotropin-releasing factor receptor 1) receptor antagonist for attenuating elevated stress response	
MeSH Concept: M0515983	
MeSH Descriptor: C524544	

► Medical Subject Headings (MeSH)

11.2 ChemIDplus



8 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 (NCSTU).	
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 > NLM Resources (File Locators)	
MeSH Medical Subject Heading and Supplementary Concept Records - ChemIDplus includes only the chemical names and chemical MeSH headings from this file. This search retrieves information from both MeSH headings and Supplementary Concept Records	
ChemIDplus Chemical Information Classification > NLM Resources (File Locators)	
PubChem PubChem Substance Database - The PubChem Substance Database contains the chemical structures of small organic molecules and information on their biological activities	
ChemIDplus Chemical Information Classification > NLM Resources (File Locators)	
PubMed PubMed - PubMed comprises over 20 million citations for biomedical literature from MEDLINE, life science journals, and online books	
« First < Previous Page 1 of 2 Next > Last »	

► ChemIDplus

11.3 IUPHAR / BPS Guide to PHARMACOLOGY Target Classification



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

► IUPHAR/BPS Guide to PHARMACOLOGY

11.4 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

11.5 MolGenie Organic Chemistry Ontology



14 items	View in Classification Browser
MolGenie Organic Chemistry Ontology > PubChemLite chemical entities > substructural concepts > functional groups > nitrogen containing functional groups > amines > tertiary amines	
alkyl aryl tertiary amines	
MolGenie Organic Chemistry Ontology > PubChemLite chemical entities > compounds > organic compounds > aromatic compounds	
⌵ Show alternative paths	
aromatic chlorides	
MolGenie Organic Chemistry Ontology > PubChemLite chemical entities > calculated properties	
drug like compounds	
Using a Fragment Based Druglikeness from OpenChemLib > -1	
MolGenie Organic Chemistry Ontology > ChEMBL chemical entities > compounds > organic compounds > aromatic compounds	
⌵ Show alternative paths	
aromatic chlorides	
MolGenie Organic Chemistry Ontology > ChEMBL chemical entities > substructural concepts > scaffolds > simple organic compound scaffolds	
biaryls	
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► MolGenie

12 Information Sources



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1. ChEMBL

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CHEMBL188907

<https://www.ebi.ac.uk/chembl/explore/compound/CHEMBL188907>

ChEMBL Protein Target Tree

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

2. ChemIDplus

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NBI-34041

<https://pubchem.ncbi.nlm.nih.gov/substance/?source=chemidplus&sourceid=0268545875>

ChemIDplus Chemical Information Classification

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3. FDA Global Substance Registration System (GSRS)

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<https://gsrs.ncats.nih.gov/ginas/app/beta/substances/874OEY3JE/>

4. 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.dgidb.org/downloads>

NBI-34041

<https://www.dgidb.org/drugs/iuphar.ligand:10375>

5. IUPHAR/BPS Guide to PHARMACOLOGY

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<https://www.guidetopharmacology.org/GRAC/LigandDisplayForward?ligandId=10375>

Guide to Pharmacology Target Classification

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

6. Therapeutic Target Database (TTD)

NBI-34041

<https://ttd.idrblab.cn/data/drug/details/D07QWW>

7. Japan Chemical Substance Dictionary (Nikkaji)

http://jglobal.jst.go.jp/en/redirect?Nikkaji_No=J2.861.989H

8. Pharos

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

2-(2,4-Dichloro-phenyl)-4-methyl-6-(1-propyl-butyl)-7,8-dihydro-6H-1,3,6,8a-tetraaza-acenaphthylene

<https://pharos.nih.gov/ligands/6X1UZXJLJH>

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NBI-34041

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MeSH Tree

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

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MolGenie Organic Chemistry Ontology

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

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