An official website of the United States government Here is how you know

National Library of Medicine
National Center for Biotechnology Information

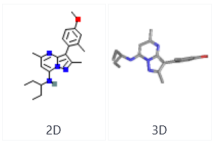
PubChem About Docs Submit Contact

Quick Search PubChem

Advanced Search Search History Help

COMPOUND

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

PubChem CID	9884878
Structure	 2D 3D
Molecular Formula	$C_{21}H_{28}N_4O$
Synonyms	DMP 904 DMP-904 202579-74-6 DMP904 4-(3-pentylamino)-DMMPP View More...
Molecular Weight	352.5 g/mol *Computed by PubChem 2.2 (PubChem release 2024.11.20)*
Dates	Create: 2006-10-25 Modify: 2026-05-23

Cite Download

CONTENTS

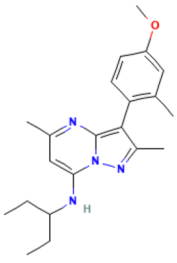
Title and Summary
1 Structures
2 Names and Identifiers
3 Chemical and Physical Properties
4 Related Records
5 Chemical Vendors
6 Literature
7 Patents
8 Interactions and Pathways
9 Biological Test Results
10 Classification
11 Information Sources

1 Structures

1.1 2D Structure

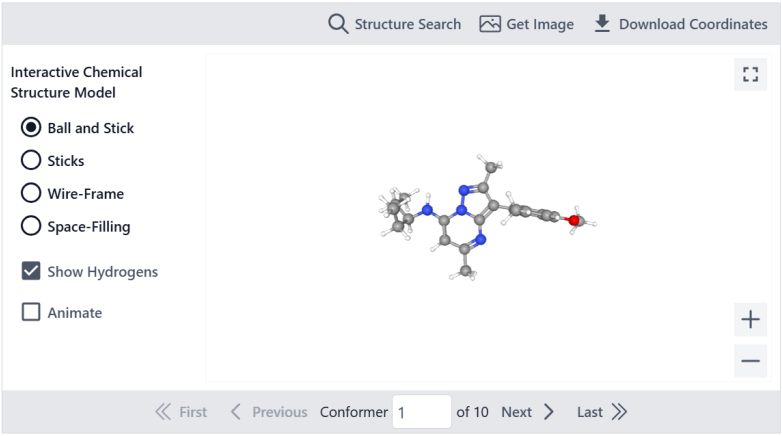
Structure Search Get Image Download Coordinates

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*-pentan-3-ylpyrazolo[1,5-a]pyrimidin-7-amine

Computed by Lexichem TK 2.7.0 (PubChem release 2024.11.20)

PubChem

2.1.2 InChI

InChI=1S/C21H28N4O/c1-7-16(8-2)23-19-12-14(4)22-21-20(15(5)24-25(19)21)18-10-9-17(26-6)11-13(18)3/h9-12,16,23H,7-8H2,1-6H3

Computed by InChI 1.07.0 (PubChem release 2024.11.20)

PubChem

2.1.3 InChIKey

QBBJSFUFEUXTNU-UHFFFAOYSA-N

Computed by InChI 1.07.0 (PubChem release 2024.11.20)

PubChem

2.1.4 SMILES

CCC(CC)NC1=CC(=NC2=C(C(=NN12)C)C3=C(C=C(C=C3)OC)C)C

Computed by OEChem 2.3.0 (PubChem release 2024.12.12)

PubChem

2.2 Molecular Formula

$C_{21}H_{28}N_4O$

Computed by PubChem 2.2 (PubChem release 2024.11.20)

PubChem

2.3 Other Identifiers

2.3.1 CAS

202579-74-6

ChemIDplus

2.3.2 ChEMBL ID

CHEMBL45187

▸ ChEMBL

2.3.3 HMDB ID

HMDB0251545

▸ Human Metabolome Database (HMDB)

2.3.4 Pharos Ligand ID

KQJWNJRJRVDY

▸ Pharos

2.4 Synonyms

2.4.1 Depositor-Supplied Synonyms

DMP 904
DMP-904
202579-74-6
DMP904
4-(3-pentylamino)-DMMPP
CHEMBL45187
3-(4-methoxy-2-methylphenyl)-2,5-dimethyl-N-pentan-3-ylpyrazolo[1,5-a]pyrimidin-7-amine
4-(3-pentylamino)-2,7-dimethyl-8-(2-methyl-4-methoxyphenyl)pyrazolo(1,5-a)pyrimidine
sp90--4
SCHEMBL13134050
SCHEMBL30787417
BDBM50087713
PDSP1_001297
PDSP2_001281
(1-Ethyl-propyl)-[3-(4-

▸ PubChem

3 Chemical and Physical Properties

3.1 Computed Properties

Property Name	Property Value	Reference
Molecular Weight	352.5 g/mol	Computed by PubChem 2.2 (PubChem release 2024.11.20)
XLogP3-AA	5.3	Computed by XLogP3 3.0 (PubChem release 2024.11.20)
Hydrogen Bond Donor Count	1	Computed by Cactvs 3.4.8.18 (PubChem release 2024.11.20)
Hydrogen Bond Acceptor Count	4	Computed by Cactvs 3.4.8.18 (PubChem release 2024.11.20)
Rotatable Bond Count	6	Computed by Cactvs 3.4.8.18 (PubChem release 2024.11.20)
Exact Mass	352.22631153 Da	Computed by PubChem 2.2 (PubChem release 2024.11.20)
Monoisotopic Mass	352.22631153 Da	Computed by PubChem 2.2 (PubChem release 2024.11.20)
Topological Polar Surface Area	51.5 Å^2	Computed by Cactvs 3.4.8.18 (PubChem release 2024.11.20)
Heavy Atom Count	26	Computed by PubChem
Formal Charge	0	Computed by PubChem
Complexity	444	Computed by Cactvs 3.4.8.18 (PubChem release 2024.11.20)
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 2010.07.16)

PubChem

4 Related Records

4.1 Related Compounds with Annotation

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

PubChem

4.2 Related Compounds

Same Parent, Exact Count	2
Mixtures, Components, and Neutralized Forms Count	4
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	41
Same Count	37
Mixture Count	4

PubChem

4.3.2 Substances by Category

6 categories Download

Chemical Vendors (11)

001Chemical
PubChem SID: 440015783 External ID: DY537965

Yuhao Chemical
PubChem SID: 347730414 External ID: YH44565

MolCore
PubChem SID: 446241751 External ID: DY537965
PubChem SID: 405469122 External ID: MC537965

Ambinter
PubChem SID: 370022981 External ID: Amb24093283

BenchChem
PubChem SID: 462758051 External ID: B3420801

Smolecule
PubChem SID: 471091114 External ID: S3708543
PubChem SID: 439405773 External ID: S636290

RR Scientific
PubChem SID: 481304777 External ID: R645122

Starshine Chemical
PubChem SID: 481708531 External ID: 2023-05-16B01444

BOC Sciences
PubChem SID: 488203408 External ID: 202579-74-6

Curation Efforts (7)

BindingDB (Curation Efforts, Research and Development)
PubChem SID: 103986741 External ID: 50087713

ChEMBL (Curation Efforts, Research and Development)
PubChem SID: 103225286 External ID: CHEMBL45187

ChemIDplus (Curation Efforts, Governmental Organizations, Research and Development)
PubChem SID: 381124436 External ID: 0202579746

Comparative Toxicogenomics Database (CTD) (Curation Efforts, Research and Development)
PubChem SID: 53789482 External ID: C417190

Human Metabolome Database (HMDB) (Curation Efforts, Research and Development)
PubChem SID: 447225294 External ID: HMDB0251545

SureChEMBL (Curation Efforts, Research and Development)
PubChem SID: 238135366 External ID: SCHEMBL13134050
PubChem SID: 515572261 External ID: SCHEMBL30787417

Governmental Organizations (2)

ChemIDplus (Curation Efforts, Governmental Organizations, Research and Development)
PubChem SID: 381124436 External ID: 0202579746

PATENTSCOPE (WIPO)
PubChem SID: 392269608 External ID: QBBJSFUFEUXTNU-UHFFFAOYSA-N

Journal Publishers (1)

Springer Nature
PubChem SID: 341307491 External ID: 26051416-190686973

Research and Development (10)

BindingDB (Curation Efforts, Research and Development)
PubChem SID: 103986741 External ID: 50087713

ChEMBL (Curation Efforts, Research and Development)
PubChem SID: 103225286 External ID: CHEMBL45187

ChemIDplus (Curation Efforts, Governmental Organizations, Research and Development)
PubChem SID: 381124436 External ID: 0202579746

Comparative Toxicogenomics Database (CTD) (Curation Efforts, Research and Development)
PubChem SID: 53789482 External ID: C417190

Google Patents
PubChem SID: 426151495 External ID: 17630807

Human Metabolome Database (HMDB) (Curation Efforts, Research and Development)
PubChem SID: 447225294 External ID: HMDB0251545

IBM
PubChem SID: 128997208 External ID: DDFC6E89F125914761CCE53E7B91FB79

MolGenie
PubChem SID: 502375933 External ID: 190013355553

SureChEMBL (Curation Efforts, Research and Development)
PubChem SID: 238135366 External ID: SCHEMBL13134050
PubChem SID: 515572261 External ID: SCHEMBL30787417

Legacy Depositors (14)

Active Biopharma (Chemical Vendors)
PubChem SID: 252109956 External ID: ABP000363

Apexmol (Chemical Vendors)
PubChem SID: 441107908 External ID: AMY15349

Bic Biotech (Chemical Vendors)
PubChem SID: 383418159 External ID: NSZB-A223252

BioChemPartner (Chemical Vendors)
PubChem SID: 375582928 External ID: BCP26370

ChemBank (Research and Development)
PubChem SID: 47880138 External ID: PDSP1_001297
PubChem SID: 48329089 External ID: PDSP2_001281

Chemieliva Pharmaceutical Co., Ltd (Chemical Vendors)
PubChem SID: 349712017 External ID: PBCM1230161

ChemSpider (Research and Development)
PubChem SID: 45631819 External ID: 8060552

DiscoveryGate (Subscription Services)
PubChem SID: 24171715 External ID: 9884878

Lan Pharmatech (Chemical Vendors)
PubChem SID: 433835309 External ID: LAN-B40658

NextBio (Subscription Services)
PubChem SID: 74754278 External ID: 9884878

SCRIPDB (Research and Development)
PubChem SID: 141141923 External ID: US20100249138A1-20100930-C00015_1

Thomson Pharma (Journal Publishers, Subscription Services)
PubChem SID: 14852066 External ID: 00005716

ZINC (Chemical Vendors)
PubChem SID: 256187102 External ID: ZINC1488097

▸ PubChem

4.4 Entrez Crosslinks

PubMed Count	4
Taxonomy Count	1
Gene Count	15

▸ PubChem

5 Chemical Vendors

9 vendors — Download

001Chemical	
PubChem SID: 440015783	Purchasable Chemical: DY537965
Yuhao Chemical	
PubChem SID: 347730414	Purchasable Chemical: YH44565
MolCore	
PubChem SID: 446241751	Purchasable Chemical: DY537965
PubChem SID: 405469122	Purchasable Chemical: MC537965
Ambinter	
PubChem SID: 370022981	Purchasable Chemical: Amb24093283
BenchChem	
PubChem SID: 462758051	Purchasable Chemical: B3420801
Smolecule	
PubChem SID: 471091114	Purchasable Chemical: S3708543
PubChem SID: 439405773	Purchasable Chemical: S636290
RR Scientific	
PubChem SID: 481304777	Purchasable Chemical: R645122
Starshine Chemical	
PubChem SID: 481708531	Purchasable Chemical: 2023-05-16B01444
BOC Sciences	
PubChem SID: 488203408	Purchasable Chemical: 202579-74-6

PubChem

6 Literature

6.1 Consolidated References

11 items — Download

Search — SORT BY Publication Date - Most Recent

Generating the Blood Exposome Database Using a Comprehensive Text Mining and Database Fusion Approach
Publication Name: Environmental Health Perspectives
Publication Date: 2019-09
PMCID: PMC6794490 **PMID:** 31557052 **DOI:** 10.1289/ehp4713

An insight on synthetic and medicinal aspects of pyrazolo[1,5-a]pyrimidine scaffold
Publication Name: European Journal of Medicinal Chemistry
Publication Date: 2017-01-27
PMID: 27894044 **DOI:** 10.1016/j.ejmech.2016.11.019

Discovery of potent, metabolically stable purine CRF-1 antagonists with differentiated binding kinetic profiles
Publication Name: Bioorganic & Medicinal Chemistry Letters
Publication Date: 2011-10-15
PMID: 21889333 **DOI:** 10.1016/j.bmcl.2011.08.040

6,7-Dihydro-5H-cyclopenta[d]pyrazolo[1,5-a]pyrimidines and their derivatives as novel corticotropin-releasing factor 1 receptor antagonists
Publication Name: Bioorganic & Medicinal Chemistry
Publication Date: 2011-09-15
PMID: 21865047 **DOI:** 10.1016/j.bmc.2011.07.055

Modulation of ascorbic acid metabolism by cytochrome P450 induction revealed by metabonomics and transcriptional profiling
Publication Name: Magnetic resonance in chemistry : MRC
Publication Date: 2009-11-06
PMID: 19768707 **DOI:** 10.1002/mrc.2503

First Previous Page 1 of 3 Next Last

PubChem

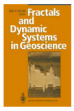
6.2 Springer Nature References

2 items Download

Statistical methods suitable for the analysis of plant tissue culture data

Publication Date: 1994

Publication Name: Plant Cell, Tissue and Organ Culture



Fractal Geometry and the Mining Industry, a Review

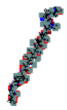
Publication Date: 1994

Publication Name: Fractals and Dynamic Systems in Geoscience

▸ Springer Nature

6.3 Chemical Co-Occurrences in Literature

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

Chemical	Selected evidence
8-(4-methoxy-2-methylphenyl)-2,7-dimethyl-N-pentan-3-yl-7H-pyrazolo[1,5-a]pyrimidin-8-ium-4-amine CID 53991888	2 articles View All Increased Hepatobiliary Clearance of Unconjugated Thyroxine Determines DMP 904-Induced Alterations in Thyroid Hormone Homeostasis in Rats PMID 15673846; DOI 10.1093/toxsci/kfi094; Toxicological sciences : an official journal of the Society of Toxicology 2005-01-19 Peripheral urocortin inhibits gastric emptying and food intake in mice: differential role of CRF receptor 2 PMID 11641109; DOI 10.1152/ajpregu.2001.281.5.r1401; American journal of physiology. Regulatory, integrative and comparative physiology 2001-11-01
Phenobarbital CID 4763	3 articles View All Hepatobiliary Disposition of Thyroid Hormone in Mrp2-Deficient TR− Rats: Reduced Biliary Excretion of Thyroxine Glucuronide Does Not Prevent Xenobiotic-Induced Hypothyroidism PMID 19211616; DOI 10.1093/toxsci/kfp026; Toxicological sciences : an official journal of the Society of Toxicology 2009-02-11 Increased Hepatobiliary Clearance of Unconjugated Thyroxine Determines DMP 904-Induced Alterations in Thyroid Hormone Homeostasis in Rats PMID 15673846; DOI 10.1093/toxsci/kfi094; Toxicological sciences : an official journal of the Society of Toxicology 2005-01-19 Modulation of ascorbic acid metabolism by cytochrome P450 induction revealed by metabonomics and transcriptional profiling PMID 19768707; DOI 10.1002/mrc.2503; Magnetic resonance in chemistry : MRC 2009-11-06
 Astressin B CID 73350132	1 article View All Peripheral urocortin inhibits gastric emptying and food intake in mice: differential role of CRF receptor 2 PMID 11641109; DOI 10.1152/ajpregu.2001.281.5.r1401; American journal of physiology. Regulatory, integrative and comparative physiology 2001-11-01

▸ PubChem

6.4 Chemical-Gene Co-Occurrences in Literature

Showing 3 of 41 View More Co-Occurrence and Evidence Data | Download

Gene/Protein/Enzyme	Selected evidence
corticotropin releasing hormone receptor 1	6 articles — View All Peripheral urocortin inhibits gastric emptying and food intake in mice: differential role of CRF receptor 2 PMID 11641109; DOI 10.1152/ajpregu.2001.281.5.r1401; American journal of physiology. Regulatory, integrative and comparative physiology 2001-11-01 Increased Hepatobiliary Clearance of Unconjugated Thyroxine Determines DMP 904-Induced Alterations in Thyroid Hormone Homeostasis in Rats PMID 15673846; DOI 10.1093/toxsci/kfi094; Toxicological sciences : an official journal of the Society of Toxicology 2005-01-19 6,7-Dihydro-5H-cyclopenta[d]pyrazolo[1,5-a]pyrimidines and their derivatives as novel corticotropin-releasing factor 1 receptor antagonists PMID 21865047; DOI 10.1016/j.bmc.2011.07.055; Bioorganic & Medicinal Chemistry 2011-09-15
corticotropin releasing hormone	4 articles — View All Peripheral urocortin inhibits gastric emptying and food intake in mice: differential role of CRF receptor 2 PMID 11641109; DOI 10.1152/ajpregu.2001.281.5.r1401; American journal of physiology. Regulatory, integrative and comparative physiology 2001-11-01 Increased Hepatobiliary Clearance of Unconjugated Thyroxine Determines DMP 904-Induced Alterations in Thyroid Hormone Homeostasis in Rats PMID 15673846; DOI 10.1093/toxsci/kfi094; Toxicological sciences : an official journal of the Society of Toxicology 2005-01-19 Discovery of potent, metabolically stable purine CRF-1 antagonists with differentiated binding kinetic profiles PMID 21889333; DOI 10.1016/j.bmcl.2011.08.040; Bioorganic & Medicinal Chemistry Letters 2011-10-15
thyroid stimulating hormone subunit beta	2 articles — View All Hepatobiliary Disposition of Thyroid Hormone in Mrp2-Deficient TR− Rats: Reduced Biliary Excretion of Thyroxine Glucuronide Does Not Prevent Xenobiotic-Induced Hypothyroidism PMID 19211616; DOI 10.1093/toxsci/kfp026; Toxicological sciences : an official journal of the Society of Toxicology 2009-02-11 Increased Hepatobiliary Clearance of Unconjugated Thyroxine Determines DMP 904-Induced Alterations in Thyroid Hormone Homeostasis in Rats PMID 15673846; DOI 10.1093/toxsci/kfi094; Toxicological sciences : an official journal of the Society of Toxicology 2005-01-19

▸ PubChem

6.5 Chemical-Disease Co-Occurrences in Literature

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

Disease	Selected evidence
Adenoma	1 article — View All Increased Hepatobiliary Clearance of Unconjugated Thyroxine Determines DMP 904-Induced Alterations in Thyroid Hormone Homeostasis in Rats PMID 15673846; DOI 10.1093/toxsci/kfi094; Toxicological sciences : an official journal of the Society of Toxicology 2005-01-19
Hypothyroidism	1 article — View All Hepatobiliary Disposition of Thyroid Hormone in Mrp2-Deficient TR− Rats: Reduced Biliary Excretion of Thyroxine Glucuronide Does Not Prevent Xenobiotic-Induced Hypothyroidism PMID 19211616; DOI 10.1093/toxsci/kfp026; Toxicological sciences : an official journal of the Society of Toxicology 2009-02-11
Hyperplasia	1 article — View All Increased Hepatobiliary Clearance of Unconjugated Thyroxine Determines DMP 904-Induced Alterations in Thyroid Hormone Homeostasis in Rats PMID 15673846; DOI 10.1093/toxsci/kfi094; Toxicological sciences : an official journal of the Society of Toxicology 2005-01-19

▸ PubChem

6.6 Chemical-Organism Co-Occurrences in Literature

Showing 3 of 8 View More Co-Occurrence and Evidence Data | Download

Organism	Selected evidence
rattus norvegicus (norway rat)	6 articles View All Increased Hepatobiliary Clearance of Unconjugated Thyroxine Determines DMP 904-Induced Alterations in Thyroid Hormone Homeostasis in Rats PMID 15673846; DOI 10.1093/toxsci/kfi094; Toxicological sciences : an official journal of the Society of Toxicology 2005-01-19 Hepatobiliary Disposition of Thyroid Hormone in Mrp2-Deficient TR− Rats: Reduced Biliary Excretion of Thyroxine Glucuronide Does Not Prevent Xenobiotic-Induced Hypothyroidism PMID 19211616; DOI 10.1093/toxsci/kfp026; Toxicological sciences : an official journal of the Society of Toxicology 2009-02-11 Modulation of ascorbic acid metabolism by cytochrome P450 induction revealed by metabonomics and transcriptional profiling PMID 19768707; DOI 10.1002/mrc.2503; Magnetic resonance in chemistry : MRC 2009-11-06
rattus sp. (rats)	3 articles View All Increased Hepatobiliary Clearance of Unconjugated Thyroxine Determines DMP 904-Induced Alterations in Thyroid Hormone Homeostasis in Rats PMID 15673846; DOI 10.1093/toxsci/kfi094; Toxicological sciences : an official journal of the Society of Toxicology 2005-01-19 Hepatobiliary Disposition of Thyroid Hormone in Mrp2-Deficient TR− Rats: Reduced Biliary Excretion of Thyroxine Glucuronide Does Not Prevent Xenobiotic-Induced Hypothyroidism PMID 19211616; DOI 10.1093/toxsci/kfp026; Toxicological sciences : an official journal of the Society of Toxicology 2009-02-11 Modulation of ascorbic acid metabolism by cytochrome P450 induction revealed by metabonomics and transcriptional profiling PMID 19768707; DOI 10.1002/mrc.2503; Magnetic resonance in chemistry : MRC 2009-11-06
homo sapiens (human)	6 articles View All Increased Hepatobiliary Clearance of Unconjugated Thyroxine Determines DMP 904-Induced Alterations in Thyroid Hormone Homeostasis in Rats PMID 15673846; DOI 10.1093/toxsci/kfi094; Toxicological sciences : an official journal of the Society of Toxicology 2005-01-19 Peripheral urocortin inhibits gastric emptying and food intake in mice: differential role of CRF receptor 2 PMID 11641109; DOI 10.1152/ajpregu.2001.281.5.r1401; American journal of physiology. Regulatory, integrative and comparative physiology 2001-11-01 Discovery of potent, metabolically stable purine CRF-1 antagonists with differentiated binding kinetic profiles PMID 21889333; DOI 10.1016/j.bmcl.2011.08.040; Bioorganic & Medicinal Chemistry Letters 2011-10-15

▸ PubChem

7 Patents

7.1 Depositor-Supplied Patent Identifiers

37 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: US-2021038604-A1
Priority Date: 2018-04-27

First Previous Page 1 of 8 Next Last

PubChem

Link to all deposited patent identifiers

PubChem

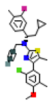
7.2 WIPO PATENTSCOPE

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

PATENTSCOPE (WIPO)

7.3 Chemical Co-Occurrences in Patents

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

Chemical	Selected evidence
R121919 CID 9821250	7 patents from 4 patent families View All Treatment and prevention of tauopathies and amyloid beta amyloidosis by modulating CRF receptor signaling EP-2522351-B1; Grant Date: 2017-09-06 Method for predicting a treatment response to a CRHR1 antagonist and/or a V1B antagonist in a patient with depressive and/or anxiety symptoms US-10837062-B2; Grant Date: 2020-11-17 Treatment of congenital adrenal hyperplasia US-11730739-B2; Grant Date: 2023-08-22
 4-(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	7 patents from 4 patent families View All Treatment and prevention of tauopathies and amyloid beta amyloidosis by modulating CRF receptor signaling EP-2522351-B1; Grant Date: 2017-09-06 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-10837062-B2; Grant Date: 2020-11-17

Antalarmin
CID 177990

7 patents from 4 patent families View All

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

Method for predicting a treatment response to a CRHR1 antagonist and/or a V1B antagonist in a patient with depressive and/or anxiety symptoms
US-10837062-B2; Grant Date: 2020-11-17

Treatment of congenital adrenal hyperplasia
US-11311544-B2; Grant Date: 2022-04-26

PubChem

7.4 Chemical-Disease Co-Occurrences in Patents

Showing 3 of 52 View More Co-Occurrence and Evidence Data Download

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

PubChem

7.5 Chemical-Gene Co-Occurrences in Patents

Showing 3 of 26 View More Co-Occurrence and Evidence Data Download

Gene	Selected evidence
crhr2	1 patent from 1 patent family View All Treatment and prevention of tauopathies and amyloid beta amyloidosis by modulating CRF receptor signaling EP-2522351-B1; Grant Date: 2017-09-06
crh	3 patents from 2 patent families View All Treatment and prevention of tauopathies and amyloid beta amyloidosis by modulating CRF receptor signaling EP-2522351-B1; Grant Date: 2017-09-06 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
insr	1 patent from 1 patent family View All Treatment and prevention of tauopathies and amyloid beta amyloidosis by modulating CRF receptor signaling EP-2522351-B1; Grant Date: 2017-09-06

PubChem

7.6 Chemical-Organism Co-Occurrences in Patents

Showing 3 of 24 View More Co-Occurrence and Evidence Data | Download

Organism	Selected evidence
chichester	1 patent from 1 patent family — View All Treatment and prevention of tauopathies and amyloid beta amyloidosis by modulating CRF receptor signaling EP-2522351-B1; Grant Date: 2017-09-06
armoracia rusticana (horseradish)	1 patent from 1 patent family — View All Treatment and prevention of tauopathies and amyloid beta amyloidosis by modulating CRF receptor signaling EP-2522351-B1; Grant Date: 2017-09-06
anura (frogs & toads)	1 patent from 1 patent family — View All Treatment and prevention of tauopathies and amyloid beta amyloidosis by modulating CRF receptor signaling EP-2522351-B1; Grant Date: 2017-09-06

▸ PubChem

8 Interactions and Pathways

8.1 Chemical-Target Interactions

17 items | Download

Search | SORT BY Data Source - A to Z

Gene	Taxonomy	Action	Evidence	Data Source
CRHR1	Homo sapiens (human)	4-(3-pentylamino)-2,7-dimethyl-8-(2-methyl-4-methoxyphenyl)pyrazolo(1,5-a)pyrimidine binds to and results in decreased activity of CRHR1 protein	PMID:11641109 PMID:15673846	Comparative Toxicogenomics Database (CTD)
Gulo	Rattus norvegicus (Norway rat)	4-(3-pentylamino)-2,7-dimethyl-8-(2-methyl-4-methoxyphenyl)pyrazolo(1,5-a)pyrimidine results in decreased expression of GULO mRNA	PMID:19768707	Comparative Toxicogenomics Database (CTD)
Slco1a1	Rattus norvegicus (Norway rat)	4-(3-pentylamino)-2,7-dimethyl-8-(2-methyl-4-methoxyphenyl)pyrazolo(1,5-a)pyrimidine results in increased expression of SLCO1A1 mRNA	PMID:15673846	Comparative Toxicogenomics Database (CTD)
UGT1A1	Rattus norvegicus (Norway rat)	4-(3-pentylamino)-2,7-dimethyl-8-(2-methyl-4-methoxyphenyl)pyrazolo(1,5-a)pyrimidine results in increased expression of UGT1A1 mRNA	PMID:15673846	Comparative Toxicogenomics Database (CTD)
AKR1A1	Rattus norvegicus (Norway rat)	4-(3-pentylamino)-2,7-dimethyl-8-(2-methyl-4-methoxyphenyl)pyrazolo(1,5-a)pyrimidine affects the expression of AKR1A1 mRNA	PMID:19768707	Comparative Toxicogenomics Database (CTD)

First | Previous | Page 1 of 4 | Next | Last

▸ Comparative Toxicogenomics Database (CTD)

9 Biological Test Results

9.1 BioAssay Results

PubChem

10 Classification

10.1 ChemIDplus

6 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)

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

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

ChemIDplus Chemical Information Classification > NLM Resources (File Locators)

PubMed Central

PubMed Central - Free digital archive of biomedical and life sciences journal literature from the National Institutes of Health

First Previous Page 1 of 2 Next Last

ChemIDplus

10.2 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

10.3 MolGenie Organic Chemistry Ontology

8 items — View in Classification Browser

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

MolGenie Organic Chemistry Ontology > ChEMBL chemical entities > substructural concepts > functional groups > nitrogen containing functional groups > amines > secondary amines

alkyl aryl secondary amines

MolGenie Organic Chemistry Ontology > ChEMBL chemical entities > substructural concepts > scaffolds > ring systems > plain ring systems > 3-membered ring systems > ring size 5,6,9

pyrazolo[1,5-a]pyrimidines

First Previous Page 1 of 2 Next Last

MolGenie

11 Information Sources

FILTER BY SOURCE

ALL SOURCES

1. **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

CHEMBL45187
https://www.ebi.ac.uk/chembl/explore/compound/CHEMBL45187

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

2. **ChemIDplus**

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

DMP904
https://pubchem.ncbi.nlm.nih.gov/substance/?source=chemidplus&sourceid=0202579746

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

3. **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

4-(3-pentylamino)-2,7-dimethyl-8-(2-methyl-4-methoxyphenyl)pyrazolo(1,5-a)pyrimidine
https://ctdbase.org/detail.go?type=chem&acc=C417190

4. **Human Metabolome Database (HMDB)**

LICENSE
HMDB is offered to the public as a freely available resource. Use and re-distribution of the data, in whole or in part, for commercial purposes requires explicit permission of the authors and explicit acknowledgment of the source material (HMDB) and the original publication (see the HMDB citing page). We ask that users who download significant portions of the database cite the HMDB paper in any resulting publications.
https://www.hmdb.ca/citing

3-(4-Methoxy-2-methylphenyl)-2,5-dimethyl-N-pentan-3-yl]pyrazolo[1,5-a]pyrimidin-7-amine
http://www.hmdb.ca/metabolites/HMDB0251545

5. Pharos

LICENSE
Data accessed from Pharos and TCRD is publicly available from the primary sources listed above. Please respect their individual licenses regarding proper use and redistribution.
https://pharos.nih.gov/about

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

6. Springer Nature

https://pubchem.ncbi.nlm.nih.gov/substance/341307491

7. PubChem

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

8. MolGenie

LICENSE
CC-BY 4.0
https://creativecommons.org/licenses/by/4.0/

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

9. PATENTSCOPE (WIPO)

SID 392269608
https://pubchem.ncbi.nlm.nih.gov/substance/392269608

Connect with NLM

National Library of Medicine
8600 Rockville Pike, Bethesda, MD
20894

Web Policies
FOIA
HHS Vulnerability Disclosure

Help
Accessibility
Careers

NLM | NIH | HHS | USA.gov