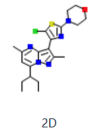
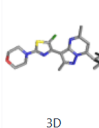


COMPOUND

Tildacerfont

PubChem CID	134694266
Structure	2D 3D
Molecular Formula	C ₂₀ H ₂₆ ClN ₅ OS
Synonyms	Tildacerfont [INN] 09QCEV5481 UNII-09QCEV5481 SPR-001 LY-2371712 View More...
Molecular Weight	420.0 g/mol <i>Computed by PubChem 2.2 (PubChem release 2025.09.15)</i>
Dates	Create: 2018-08-16 Modify: 2026-05-23
Description	Tildacerfont is a corticotropin-releasing factor receptor-1 antagonist containing an unfused thiazole ring ▶ DrugBank Tildacerfont is an orally bioavailable, selective nonsteroidal antagonist of the corticotropin-releasing factor type-1 (CRF1; CRF-1) receptor, that can potentially be used to prevent excess androgen production in congenital adrenal hyperplasia (CAH). Upon oral administration, tildacerfont targets, binds to and inhibits the CRF1 receptor located in the pituitary gland. This reduces adrenocorticotrophic hormone (ACTH) secretion and reduces the overproduction of adrenal androgens. CRF is a key regulator of the hypothalamic-pituitary-adrenal (HPA) axis and stimulates ACTH release from the anterior pituitary. CAH comprises a set of enzymatic defects in the cortisol synthetic pathway. A decrease in adrenal cortisol production impairs negative feedback on the HPA axis, which increases production of CRF and ACTH, the primary stimulus for cortisol and 19-carbon steroid production in the adrenal cortex. ▶ NCI Thesaurus (NCIt)

Cite

Download

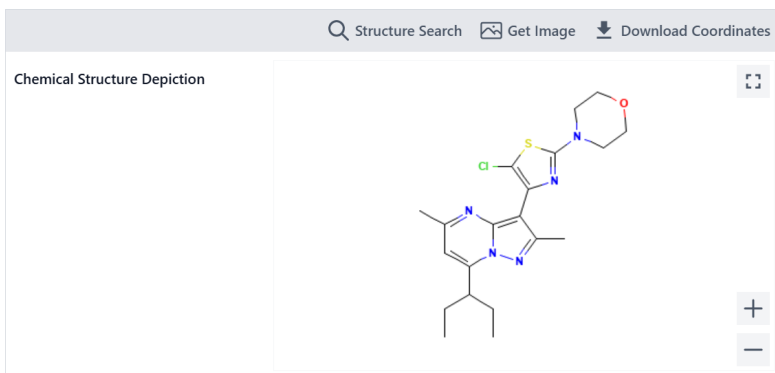
CONTENTS

Title and Summary	
1 Structures	
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5 Chemical Vendors	
6 Drug and Medication Information	
7 Associated Disorders and Diseases	
8 Literature	
9 Patents	
10 Interactions and Pathways	
11 Classification	
12 Information Sources	

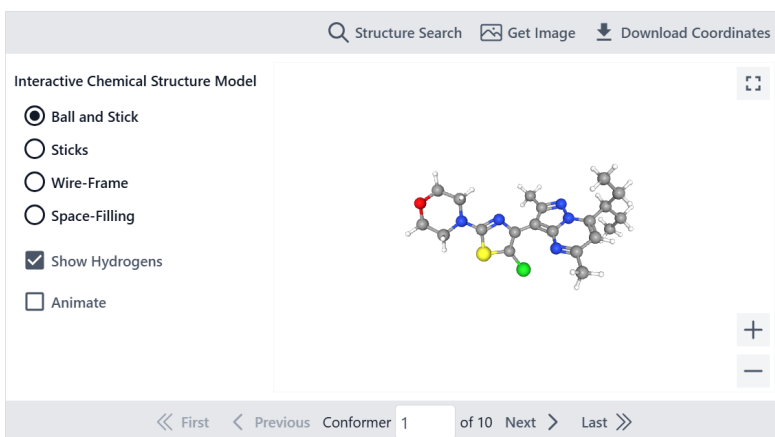
1 Structures



1.1 2D Structure



1.2 3D Conformer



2 Names and Identifiers



2.1 Computed Descriptors



2.1.1 IUPAC Name



4-[5-chloro-4-(2,5-dimethyl-7-pentan-3-ylpyrazolo[1,5-a]pyrimidin-3-yl)-1,3-thiazol-2-yl]morpholine

Computed by Lexichem TK 2.9.3 (PubChem release 2025.09.15)

PubChem

2.1.2 InChI



InChI=1S/C₂₀H₂₆ClN₅O₅/c1-5-14(6-2)15-11-12(3)22-19-16(13(4)24-26(15)19)17-18(21)28-20(23-17)25-7-9-27-10-8-25/h11,14H,5-10H2,1-4H3

Computed by InChI 1.07.4 (PubChem release 2025.09.15)

PubChem

2.1.3 InChIKey



CLKXPWDYIYIPFS-UHFFFAOYSA-N

Computed by InChI 1.07.4 (PubChem release 2025.09.15)

PubChem

2.1.4 SMILES



CCC(CC)C1=CC(=NC2=C(C(=NN12)C)C3=C(SC(=N3)N4CCOCC4)Cl)C

Computed by OEChem 4.2.0 (PubChem release 2025.09.15)

► [PubChem](#)

2.2 Molecular Formula



C₂₀H₂₆ClN₅OS

Computed by PubChem 2.2 (PubChem release 2025.09.15)

► [PubChem](#)

2.3 Other Identifiers



2.3.1 CAS



1014983-00-6

► [ChEMDplus](#); [DrugBank](#); [FDA Global Substance Registration System \(GSR\)](#)

2.3.2 UNII



09QCEV5481

► [FDA Global Substance Registration System \(GSR\)](#)

2.3.3 ChEMBL ID



[ChEMBL5095198](#)

► [ChEMBL](#); [Open Targets](#)

2.3.4 DrugBank ID



[DB18545](#)

► [DrugBank](#)

2.3.5 International Nonproprietary Names (INN)



TILDACERFONT

► [FDA Global Substance Registration System \(GSR\)](#)

2.3.6 NCI Thesaurus Code



[C171816](#)

► [NCI Thesaurus \(NCIt\)](#)

2.3.7 United States Adopted Name (USAN)



TILDACERFONT

► [FDA Global Substance Registration System \(GSR\)](#)

2.4 Synonyms



2.4.1 Depositor-Supplied Synonyms

Tildacerfont [INN]	PYRAZOLO(1,5-DIMETHYL-PY
09QCEV5481	Pyrazolo[1,5-a
UNII-09QCEV5481	Pyrazolo[1,5-a
SPR-001	pyrazolo[1,3-a
LY-2371712	RefChem:1900
LY2371712	SPR 001
3-(5-Chloro-2-morpholin-4-yl-thiazol-4-yl)-7-(1-ethyl-propyl)-2,5-dimethylpyrazolo(1,5-a)pyrimidine	LY 2371712
Pyrazolo(1,5-a)pyrimidine, 3-(4-chloro-2-(4-morpholinyl)-5-thiazolyl)-7-(1-ethylpropyl)-2,5-dimethyl-	3-(5-CHLORO
tildacerfontum	A)PYRIMIDINI
	1014983-00-6

PubChem

3 Chemical and Physical Properties

3.1 Computed Properties

Property Name	Property Value	Reference
Molecular Weight	420.0 g/mol	Computed by PubChem 2.2 (PubChem release 2025.09.15)
XLogP3-AA	4.7	Computed by XLogP3 3.0 (PubChem release 2025.09.15)
Hydrogen Bond Donor Count	0	Computed by Cactvs 3.4.8.24 (PubChem release 2025.09.15)
Hydrogen Bond Acceptor Count	6	Computed by Cactvs 3.4.8.24 (PubChem release 2025.09.15)
Rotatable Bond Count	5	Computed by Cactvs 3.4.8.24 (PubChem release 2025.09.15)
Exact Mass	419.1546593 Da	Computed by PubChem 2.2 (PubChem release 2025.09.15)
Monoisotopic Mass	419.1546593 Da	Computed by PubChem 2.2 (PubChem release 2025.09.15)
Topological Polar Surface Area	83.8 Å²	Computed by Cactvs 3.4.8.24 (PubChem release 2025.09.15)
Heavy Atom Count	28	Computed by PubChem
Formal Charge	0	Computed by PubChem
Complexity	521	Computed by Cactvs 3.4.8.24 (PubChem release 2025.09.15)
Isotope Atom Count	0	Computed by PubChem
Defined Atom Stereocenter Count	0	Computed by PubChem
Undefined Atom Stereocenter Count	0	Computed by PubChem
Defined Bond Stereocenter Count	0	Computed by PubChem
Undefined Bond Stereocenter Count	0	Computed by PubChem
Covalently-Bonded Unit Count	1	Computed by PubChem
Compound Is Canonicalized	Yes	Computed by PubChem (release 2025.09.15)

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



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



500833421

► [PubChem](#)

4.3.2 Related Substances



Same Count	15
------------	----

► [PubChem](#)

4.3.3 Substances by Category



6 categories 	
Chemical Vendors (5)	
Starshine Chemical	
PubChem SID: 480485375	External ID: 2023-05-7C01604
BOC Sciences	
PubChem SID: 482589706	External ID: 1014983-00-6
eNovation Chemicals	
PubChem SID: 523169329	External ID: Y4294652
Pharmacore Co., Limited	
PubChem SID: 504737740	External ID: 190931409
CymitQuimica	
PubChem SID: 470163615	External ID: CQ_1014983-00-6
Curation Efforts (4)	
ChEMBL (Curation Efforts, Research and Development)	
PubChem SID: 475978099	External ID: ChEMBL5095198
ChemIDplus (Curation Efforts, Governmental Organizations, Research and Development)	
PubChem SID: 375892238	External ID: 1014983006
FDA Global Substance Registration System (GSRS) (Curation Efforts, Governmental Organizations)	
PubChem SID: 375579093	External ID: 09QCEV5481
SureChEMBL (Curation Efforts, Research and Development)	
PubChem SID: 514272603	External ID: SCHEMBL29462437

Governmental Organizations (4)	
ChemIDplus (Curation Efforts, Governmental Organizations, Research and Development)	
PubChem SID: 375892238	External ID: 1014983006
FDA Global Substance Registration System (GSRS) (Curation Efforts, Governmental Organizations)	
PubChem SID: 375579093	External ID: 09QCEV5481
PATENTSCOPE (WIPO)	
PubChem SID: 440666221	External ID: CLKXPWDYEYIPFS-UHFFFAOYSA-N
PubChem Reference Collection	
PubChem SID: 500833421	External ID: 190003
Journal Publishers (1)	
Springer Nature	
PubChem SID: 461456260	External ID: 28052277-230853427
Research and Development (5)	
ChEMBL (Curation Efforts, Research and Development)	
PubChem SID: 475978099	External ID: ChEMBL5095198
ChemIDplus (Curation Efforts, Governmental Organizations, Research and Development)	
PubChem SID: 375892238	External ID: 1014983006
MolGenie	
PubChem SID: 503044770	External ID: 190118133205
Probes & Drugs portal	
PubChem SID: 507524322	External ID: PD205328
SureChEMBL (Curation Efforts, Research and Development)	
PubChem SID: 514272603	External ID: SCHEMBL29462437
Legacy Depositors (1)	
Amadis Chemical (Chemical Vendors)	
PubChem SID: 497987339	External ID: A1247571

► PubChem

5 Chemical Vendors



5 vendors		Download
Starshine Chemical		
PubChem SID: 480485375	Purchasable Chemical: 2023-05-7C01604	
BOC Sciences		
PubChem SID: 482589706	Purchasable Chemical: 1014983-00-6	
eNovation Chemicals		
PubChem SID: 523169329	Purchasable Chemical: Y4294652	
Pharmacore Co., Limited		
PubChem SID: 504737740	Purchasable Chemical: 190931409	
CymitQuimica		
PubChem SID: 470163615	Purchasable Chemical: CQ_1014983-00-6	

► PubChem

6 Drug and Medication Information



6.1 Drug Indication



3 items		Download
MeSH Heading	EFO Term	Max Phase
Adrenal Hyperplasia, Congenital	congenital adrenal hyperplasia	Phase 2
Adrenal Hyperplasia, Congenital	classic congenital adrenal hyperplasia due to 21-hydroxylase deficiency	Phase 2
Polycystic Ovary Syndrome	polycystic ovary syndrome	Phase 2

► ChEMBL

6.2 Clinical Trials



6.2.1 ClinicalTrials.gov



4 items		Download
A Phase 2 Study to Evaluate the Safety, Efficacy and PK of Tildacerfont in Children Aged 2-17 Years With CAH CTID: NCT05128942 Phase: Phase 2 Status: Terminated Date: 2025-12-24		
Study of SPR001 in Adults With Classic Congenital Adrenal Hyperplasia CTID: NCT03257462 Phase: Phase 2 Status: Completed Date: 2025-10-22		
A Study of Safety and Efficacy of Tildacerfont in Females With Polycystic Ovary Syndrome and Elevated Adrenal Androgens CTID: NCT05370521 Phase: Phase 2 Status: Terminated Date: 2025-10-09		
Study to Evaluate the Safety and Efficacy of SPR001 in Subjects With Classic Congenital Adrenal Hyperplasia CTID: NCT03687242 Phase: Phase 2 Status: Completed Date: 2025-04-01		

► ClinicalTrials.gov

6.2.2 EU Clinical Trials Register



2 items		Download
A Randomized, Double-Blind, Placebo-Controlled Study to Evaluate the Efficacy and Safety of SPR001 (Tildacerfont) in Reducing Supraphysiologic Glucocorticoid Use in Adult Subjects with Classic Congenital Adrenal Hyperplasia EudraCT: 2019-004765-40 Phase: Phase 2 Status: Trial now transitioned Date: 2020-11-17		
A Randomized, Double-Blind, Placebo-Controlled, Dose-Ranging Study to Evaluate the Efficacy and Safety of SPR001 (Tildacerfont) in Adult Subjects with Classic Congenital Adrenal Hyperplasia EudraCT: 2019-004764-22 Phase: Phase 2 Status: Trial now transitioned, GB - no longer in EU/EEA, Ongoing Date: 2020-10-15		

▶ [EU Clinical Trials Register](#)

6.3 EMA Drug Information



3 items	Download
Category/Dataset: Orphan designations	
Active Substance: pyrazolo[1,5-a]pyrimidine, 3-[4-chloro-2-(4-morpholinyl)-5-thiazolyl]-7-(1-ethylpropyl)-2,5-dimethyl-pyrazolo[1,3-a]pyrimidine	
Status: Positive	
Therapeutic Use: Treatment of congenital adrenal hyperplasia	
Publish Date: 2018-03-12 Update Date: 2018-03-12	
Category/Dataset: Paediatric investigation plans (PIP)	
Product/no.: PIP number: EMEA-002970-PIP01-21 Active Substance: tildacerfont	
Status: PIP decision type: P: decision agreeing on a investigation plan, with or without partial waiver(s) and or deferral(s)	
Pharmaceutical Form: Granules;Tablet Administration Route: Oral use	
Therapeutic Use: Endocrinology-Gynaecology-Fertility-Metabolism	
Condition/Indication: Treatment of congenital adrenal hyperplasia	
Publish Date: 2022-01-31	
Category/Dataset: Paediatric investigation plans (PIP)	
Product/no.: PIP number: EMEA-002970-PIP01-21 Active Substance: tildacerfont	
Status: PIP decision type: P: decision agreeing on a investigation plan, with or without partial waiver(s) and or deferral(s)	
Pharmaceutical Form: Tablet;Granules Administration Route: Oral use	
Therapeutic Use: Endocrinology-Gynaecology-Fertility-Metabolism	
Condition/Indication: Treatment of congenital adrenal hyperplasia	
Publish Date: 2022-01-31	

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

6.4 Drug Development Summary



Max Phase	Phase 2
-----------	---------

▶ [ChEMBL](#)

7 Associated Disorders and Diseases



3 items	Download
Source Disease	Data Source
Adrenal Hyperplasia, Congenital	ChEMBL
Adrenal Hyperplasia, Congenital	ChEMBL
Polycystic Ovary Syndrome	ChEMBL

▶ [Therapeutic Target Database \(TTD\)](#)

8 Literature



8.1 Consolidated References



9 items	Download
Search	SORT BY Publication Date - Most Recent
Interleukin 15 and autoimmune disorders: pathophysiology, therapeutic potential, and clinical implications	
Publication Name: Inflammation research : official journal of the European Histamine Research Society ... [et al.]	
Publication Date: 2025-10-17	
PMID: 41107624 DOI: 10.1007/s00011-025-02084-7	
Non-classical congenital adrenal hyperplasia: current insights into clinical implications, diagnosis and treatment	
Publication Name: Endocrine	
Publication Date: 2025-07-23	
PMID: 40699527 DOI: 10.1007/s12020-025-04341-5	
Recent advances in treatments for congenital adrenal hyperplasia	
Publication Name: Nature reviews. Endocrinology	
Publication Date: 2025-02-11	
PMID: 39934411 DOI: 10.1038/s41574-025-01089-w	
Congenital Adrenal Hyperplasia	
Publication Name: Children with Differences in Sex Development	
Publication Date: 2024	
DOI: 10.1007/978-981-97-1639-5_30	
Congenital Adrenal Hyperplasia	
Publication Name: Pediatric Endocrinology	
Publication Date: 2024	
DOI: 10.1007/978-3-031-66296-6_11	
« First < Previous Page 1 of 2 Next > Last »	

► PubChem

8.2 Springer Nature References



9 items	Download
Search	SORT BY Publication Date - Oldest
Recent advances in treatments for congenital adrenal hyperplasia	
PMID: 39934411	
Publication Date: 2025	
Publication Name: Nature Reviews Endocrinology	
Management challenges and therapeutic advances in congenital adrenal hyperplasia	
PMID: 35411073	
Publication Date: 2022	
Publication Name: Nature Reviews Endocrinology	
Congenital Adrenal Hyperplasia	
Publication Date: 2024	
Publication Name: Children with Differences in Sex Development	
Congenital Adrenal Hyperplasia	
Publication Date: 2024	
Publication Name: Pediatric Endocrinology	
Neue Behandlungsstrategien bei adrenogenitalem Syndrom/21-Hydroxylase-Mangel	
Publication Date: 2022	
Publication Name: Journal für Klinische Endokrinologie und Stoffwechsel	

► Springer Nature

8.3 Chemical Co-Occurrences in Literature



Showing 3 of 66 View More Co-Occurrence and Evidence Data ↗		Download
Chemical	Selected evidence	
 Androstenedione CID 6128	8 articles	View All ↗
	Recent advances in treatments for congenital adrenal hyperplasia PMID 39934411; DOI 10.1038/s41574-025-01089-w; Nature reviews. Endocrinology 2025-02-11	
	Neue Behandlungsstrategien bei adrenogenitalem Syndrom/21-Hydroxylase-Mangel DOI 10.1007/s41969-022-00159-y; Journal für Klinische Endokrinologie und Stoffwechsel 2022-01-01	
	Congenital Adrenal Hyperplasia DOI 10.1007/978-981-97-1639-5_30; Children with Differences in Sex Development 2024-01-01	
 Cortisol CID 5754	8 articles	View All ↗
	Recent advances in treatments for congenital adrenal hyperplasia PMID 39934411; DOI 10.1038/s41574-025-01089-w; Nature reviews. Endocrinology 2025-02-11	
	Management challenges and therapeutic advances in congenital adrenal hyperplasia PMID 35411073; DOI 10.1038/s41574-022-00655-w; Nature reviews. Endocrinology 2022-04-11 (Review Article)	
	Non-classical congenital adrenal hyperplasia: current insights into clinical implications, diagnosis and treatment PMID 40699527; DOI 10.1007/s12020-025-04341-5; Endocrine 2025-07-23 (Review Article)	
 [(E,3R)-2-amino-3-hydroxyoctadec-4-enyl] dihydrogen phosphate CID 44341320	1 article	View All ↗
	Interleukin 15 and autoimmune disorders: pathophysiology, therapeutic potential, and clinical implications PMID 41107624; DOI 10.1007/s00011-025-02084-7; Inflammation research : official journal of the European Histamine Research Society ... [et al.] 2025-10-17 (Review Article)	

► PubChem

8.4 Chemical-Gene Co-Occurrences in Literature



Showing 3 of 3 View More Co-Occurrence and Evidence Data		Download
Gene/Protein/Enzyme	Selected evidence	
interleukin 15	1 article	View All
Interleukin 15 and autoimmune disorders: pathophysiology, therapeutic potential, and clinical implications PMID 41107624; DOI 10.1007/s00011-025-02084-7; Inflammation research : official journal of the European Histamine Research Society ... [et al.] 2025-10-17 (Review Article)		
cd8 subunit alpha	1 article	View All
Interleukin 15 and autoimmune disorders: pathophysiology, therapeutic potential, and clinical implications PMID 41107624; DOI 10.1007/s00011-025-02084-7; Inflammation research : official journal of the European Histamine Research Society ... [et al.] 2025-10-17 (Review Article)		
insulin	1 article	View All
Non-classical congenital adrenal hyperplasia: current insights into clinical implications, diagnosis and treatment PMID 40699527; DOI 10.1007/s12020-025-04341-5; Endocrine 2025-07-23 (Review Article)		

PubChem

8.5 Chemical-Disease Co-Occurrences in Literature

Showing 3 of 27 View More Co-Occurrence and Evidence Data		Download
Disease	Selected evidence	
Adrenal Hyperplasia, Congenital	4 articles	View All
Recent advances in treatments for congenital adrenal hyperplasia PMID 39934411; DOI 10.1038/s41574-025-01089-w; Nature reviews. Endocrinology 2025-02-11		
Management challenges and therapeutic advances in congenital adrenal hyperplasia PMID 35411073; DOI 10.1038/s41574-022-00655-w; Nature reviews. Endocrinology 2022-04-11 (Review Article)		
Non-classical congenital adrenal hyperplasia: current insights into clinical implications, diagnosis and treatment PMID 40699527; DOI 10.1007/s12020-025-04341-5; Endocrine 2025-07-23 (Review Article)		
Congenital adrenal hyperplasia due to 21 hydroxylase deficiency	3 articles	View All
Management challenges and therapeutic advances in congenital adrenal hyperplasia PMID 35411073; DOI 10.1038/s41574-022-00655-w; Nature reviews. Endocrinology 2022-04-11 (Review Article)		
Novel treatments for congenital adrenal hyperplasia PMID 35199280; DOI 10.1007/s11154-022-09717-w; Reviews in Endocrine and Metabolic Disorders 2022-02-23 (Review Article)		
Non-classical congenital adrenal hyperplasia: current insights into clinical implications, diagnosis and treatment PMID 40699527; DOI 10.1007/s12020-025-04341-5; Endocrine 2025-07-23 (Review Article)		
Autoimmune Diseases	1 article	View All
Interleukin 15 and autoimmune disorders: pathophysiology, therapeutic potential, and clinical implications PMID 41107624; DOI 10.1007/s00011-025-02084-7; Inflammation research : official journal of the European Histamine Research Society ... [et al.] 2025-10-17 (Review Article)		

PubChem

9 Patents

9.1 Depositor-Supplied Patent Identifiers



34 items		Download
Search	SORT BY	Priority Date - Most Recent
Amorphous solid dispersion of tildacerfont formulations		
Publication Number: WO-2025188842-A8		
Priority Date: 2024-03-08		
Amorphous solid dispersion of tildacerfont formulations		
Publication Number: WO-2025188842-A1		
Priority Date: 2024-03-08		
Methods and compositions for treating polycystic ovary syndrome		
Publication Number: WO-2025038392-A1		
Priority Date: 2023-08-11		
Tildacerfont cocrystal formulations		
Publication Number: WO-2024243431-A1		
Priority Date: 2023-05-24		
Melanocortin 2-type receptor antagonist		
Publication Number: WO-2024237266-A1		
Priority Date: 2023-05-16		
<< First < Previous Page 1 of 7 Next > Last >>		

► PubChem

Link to all deposited patent identifiers

► PubChem

9.2 WIPO PATENTSCOPE



Patents are available for this chemical structure:

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

► PATENTSCOPE (WIPO)

10 Interactions and Pathways



10.1 Chemical-Target Interactions



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

► IUPHAR/BPS Guide to PHARMACOLOGY; Therapeutic Target Database (TTD)

11 Classification



11.1 NCI Thesaurus Tree



1 item	View in Classification Browser
NCI Thesaurus > Drug, Food, Chemical or Biomedical Material > Pharmacologic Substance > Hormone Therapy Agent > Hormone Antagonist	
Tildacerfont	
An orally bioavailable, selective nonsteroidal antagonist of the corticotropin-releasing factor type-1 (CRF1; CRF-1) receptor, that can potentially be used to prevent excess androgen production in congenital adrenal hyperplasia (CAH). Upon oral administration, tildacerfont targets, binds to and inhibits the CRF1 receptor located in the pituitary gland. This reduces adrenocorticotrophic hormone (ACTH) secretion and reduces the overproduction of adrenal androgens. CRF is a key regulator of the hypothalamic-pituitary-adrenal (HPA) axis and stimulates ACTH release from the anterior pituitary. CAH comprises a set of enzymatic defects in the cortisol synthetic pathway. A decrease in adrenal cortisol production impairs negative feedback on the HPA axis, which increases production of CRF and ACTH, the primary stimulus for cortisol and 19-carbon steroid production in the adrenal cortex.	

► [NCI Thesaurus \(NCIt\)](#)

11.2 ChemIDplus



5 items

[View in Classification Browser](#)

ChemIDplus Chemical Information Classification > NLM Resources (File Locators)

ClinicalTrials.gov

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

ChemIDplus Chemical Information Classification > NLM Resources (File Locators)

DrugPortal

Drug Information Portal - Portal to selected drug information from the U.S. National Library of Medicine and other key U.S. Government agencies

ChemIDplus Chemical Information Classification > 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

Registry Number

► [ChemIDplus](#)

11.3 MolGenie Organic Chemistry Ontology



18 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 > PubChemLite chemical entities > substructural concepts > scaffolds > ring systems > plain ring systems > 3-membered ring systems > ring size 5,6,9

pyrazolo[1,5-a]pyrimidines

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

⌵ [Show alternative paths](#)

aromatic chlorides

⏪ First < Previous Page 1 of 4 Next > Last ⏩

► [MolGenie](#)

11.4 Chemicals in PubChem from Regulatory Sources



2 items

View in Classification Browser

Chemicals in PubChem from Regulatory Sources > EU EMA

Orphan drugs and substances

Drug and substance information from orphan designations

Chemicals in PubChem from Regulatory Sources > EU EMA

Paediatric drugs and substances

Drug and substance information from paediatric investigation plans

► PubChem

12 Information Sources



FILTER BY SOURCE

ALL SOURCES

1. ChEMBL

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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>

TILDACERFONT

<https://www.ebi.ac.uk/chembl/explore/compound/CHEMBL5095198>

2. Open Targets

LICENSE

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

TILDACERFONT

<https://platform.opentargets.org/drug/CHEMBL5095198>

3. ChemIDplus

LICENSE

<https://www.nlm.nih.gov/copyright.html>

Tildacerfont [INN]

<https://pubchem.ncbi.nlm.nih.gov/substance/?source=chemidplus&sourceid=1014983006>

ChemIDplus Chemical Information Classification

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

4. DrugBank

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