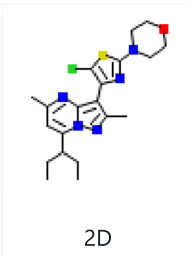
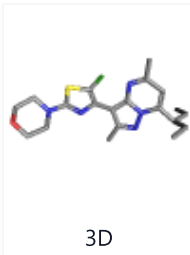


COMPOUND SUMMARY

Tildacerfont

Cite

Download

PubChem CID	134694266
Structure	<div style="display: flex; justify-content: space-around;"> <div style="text-align: center;">  <p>2D</p> </div> <div style="text-align: center;">  <p>3D</p> </div> </div>
Molecular Formula	C₂₀H₂₆ClN₅OS
Synonyms	<p>Tildacerfont [INN] 09QCEV5481 UNII-09QCEV5481 SPR001 SPR-001</p> <p>View More...</p>
Molecular Weight	<p>420.0 g/mol</p> <p><i>Computed by PubChem 2.2 (PubChem release 2021.10.14)</i></p>
Dates	<p>Create: 2018-08-16 Modify: 2025-02-01</p>
Description	<p>Tildacerfont is a corticotropin-releasing factor receptor-1 antagonist containing an unfused thiazole ring</p> <p>▶ DrugBank</p> <p>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</p>

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 \(NCIt\)](#)

TILDACERFONT is a small molecule drug with a maximum clinical trial phase of II (across all indications) and has 3 investigational indications.

▶ [Open Targets](#)

Contents

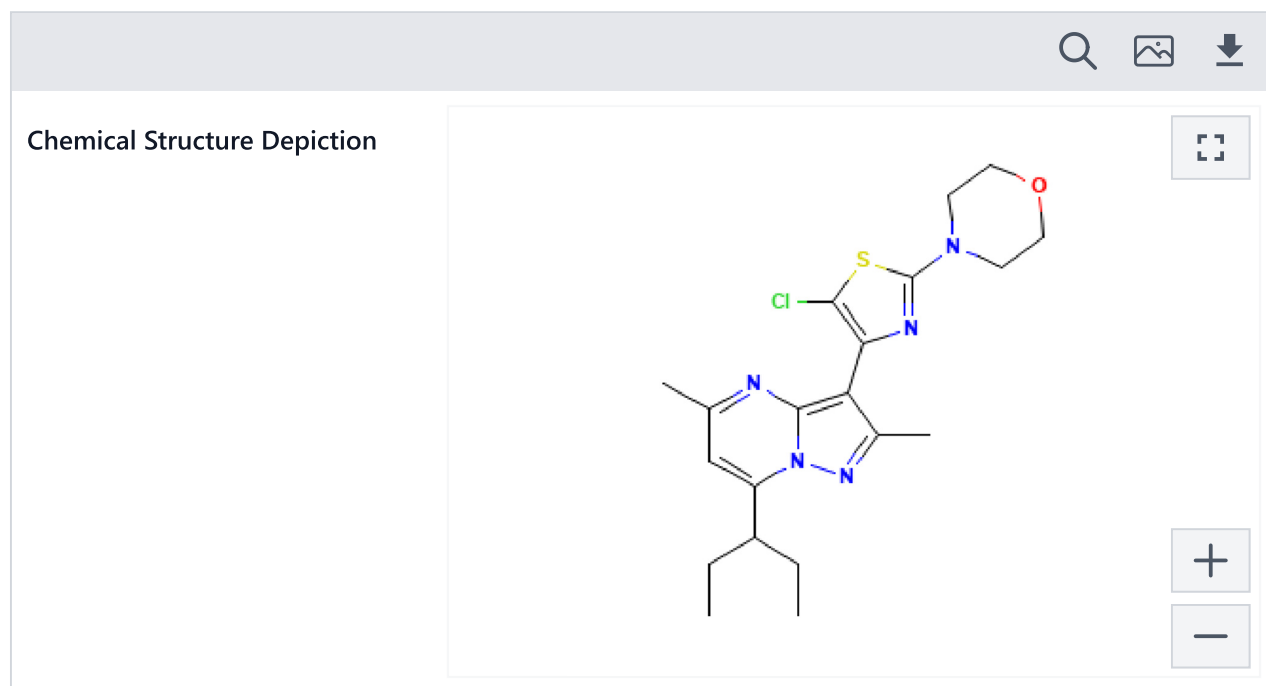
Title and Summary	
1 Structures	▼
2 Names and Identifiers	▼
3 Chemical and Physical Properties	▼
4 Related Records	▼
5 Chemical Vendors	
6 Drug and Medication Information	▼
7 Use and Manufacturing	▼
8 Associated Disorders and Diseases	
9 Literature	▼
10 Patents	▼
11 Classification	▼

12 Information Sources

1 Structures

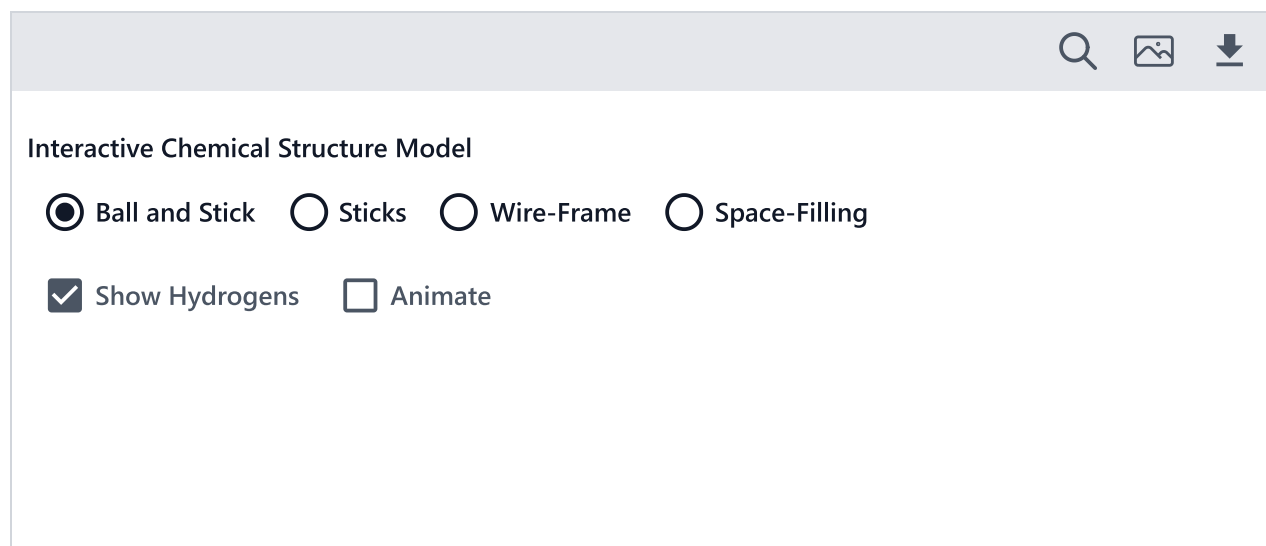


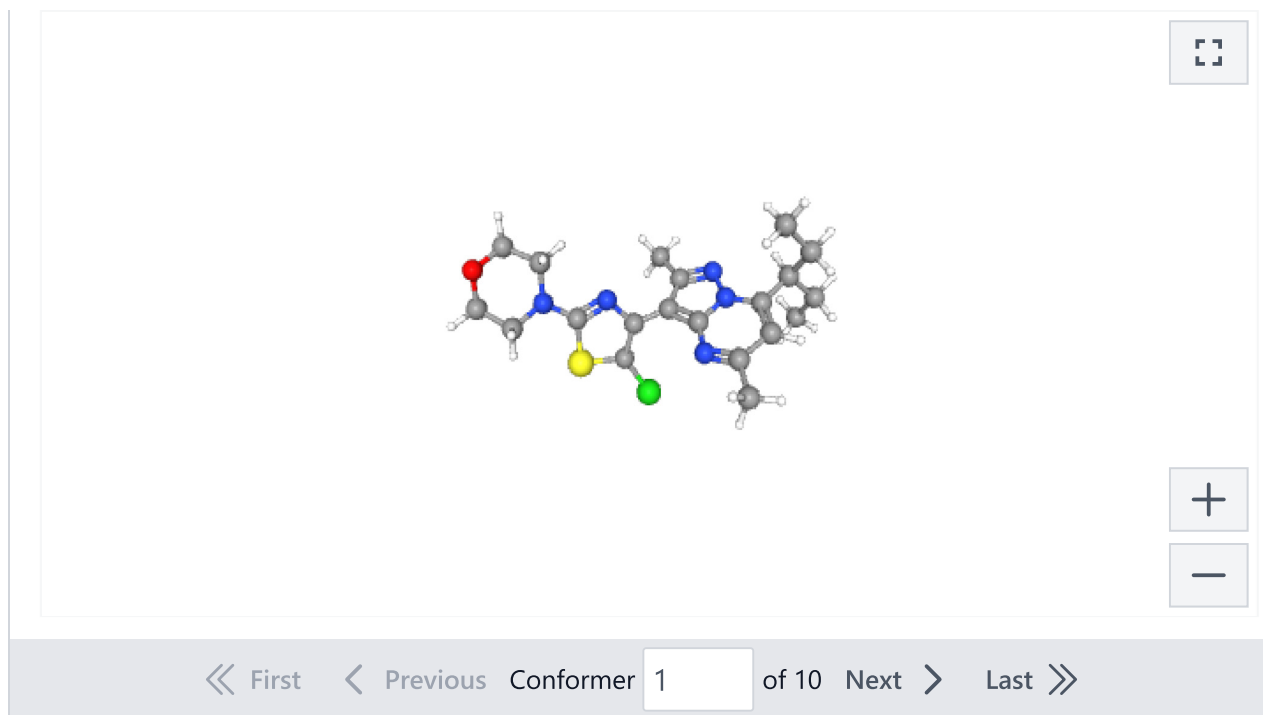
1.1 2D Structure



► [PubChem](#)

1.2 3D Conformer





► [PubChem](#)

2 Names and Identifiers ? ↗

2.1 Computed Descriptors ? ↗

2.1.1 IUPAC Name ? ↗

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 2.7.0 (PubChem release 2021.10.14)

► [PubChem](#)

2.1.2 InChI ? ↗

InChI=1S/C20H26ClN5OS/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 1.0.6 (PubChem release 2021.10.14)

► [PubChem](#)

2.1.3 InChIKey



CLKXPWDYEYIPFS-UHFFFAOYSA-N

Computed by InChI 1.0.6 (PubChem release 2021.10.14)

▶ [PubChem](#)

2.1.4 SMILES



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

Computed by OEChem 2.3.0 (PubChem release 2024.12.12)

▶ [PubChem](#)

2.2 Molecular Formula



C₂₀H₂₆ClN₅OS

Computed by PubChem 2.2 (PubChem release 2021.10.14)

▶ [PubChem](#)

2.3 Other Identifiers



2.3.1 CAS



1014983-00-6

▶ [ChemIDplus](#); [DrugBank](#); [FDA Global Substance Registration System \(GSRS\)](#)

2.3.2 UNII



09QCEV5481

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

2.3.3 ChEMBL ID



CHEMBL5095198

▶ ChEMBL

2.3.4 DrugBank ID



DB18545

▶ DrugBank

2.3.5 NCI Thesaurus Code



C171816

▶ NCI Thesaurus (NCIt)

2.4 Synonyms



2.4.1 Depositor-Supplied Synonyms



Tildacerfont [INN]

09QCEV5481

UNII-09QCEV5481

SPR001

SPR-001

LY-2371712

3-(5-Chloro-2-morpholin-4-yl-thiazol-4-yl)-7-(1-ethyl-propyl)-2,5-dimethylpyrazolo(1,5-a)pyrimidine

Pyrazolo(1,5-a)pyrimidine, 3-(4-chloro-2-(4-morpholinyl)-5-thiazolyl)-7-(1-ethylpropyl)-2,5-dimethyl-

tildacerfontum

P
E
P
d
P
d
T
C
S
L
L

▶ 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 2021.10.14)
XLogP3-AA	4.7	Computed by XLogP3 3.0 (PubChem release 2021.10.14)
Hydrogen Bond Donor Count	0	Computed by Cactvs 3.4.8.18 (PubChem release 2021.10.14)
Hydrogen Bond Acceptor Count	6	Computed by Cactvs 3.4.8.18 (PubChem release 2021.10.14)
Rotatable Bond Count	5	Computed by Cactvs 3.4.8.18 (PubChem release 2021.10.14)
Exact Mass	419.1546593 Da	Computed by PubChem 2.2 (PubChem release 2021.10.14)
Monoisotopic Mass	419.1546593 Da	Computed by PubChem 2.2 (PubChem release 2021.10.14)
Topological Polar Surface Area	83.8 Å ²	Computed by Cactvs 3.4.8.18 (PubChem release 2021.10.14)
Heavy Atom Count	28	Computed by PubChem
Formal Charge	0	Computed by PubChem
Complexity	521	Computed by Cactvs 3.4.8.18 (PubChem release 2021.10.14)
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 2021.10.14)

▶ [PubChem](#)

3.2 Chemical Classes



3.2.1 Drugs



3.2.1.1 Human Drugs



Paediatric drug

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

4 Related Records



4.1 Related Compounds with Annotation



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

▶ [PubChem](#)

4.2 Related Compounds



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 8

► PubChem

4.3.3 Substances by Category



5 categories



Chemical Vendors (1)



Starshine Chemical

PubChem SID: [480485375](#)

External ID: 2023-05-7C01604

Curation Efforts (3)



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](#)

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: [CLKXPWDYIYIPFS-UHFFFAOYSA-N](#)

PubChem Reference Collection

PubChem SID: [500833421](#)

External ID: 190003

Journal Publishers (1)



Springer NaturePubChem SID: [461456260](#)

External ID: 28052277-230853427

Research and Development (3)**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

[▶ PubChem](#)

5 Chemical Vendors



1 vendor

**Starshine Chemical**PubChem SID: [480485375](#)

Purchasable Chemical: 2023-05-7C01604

[▶ PubChem](#)

6 Drug and Medication Information



6.1 Drug Indication



Treatment of congenital adrenal hyperplasia

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

3 items



Indication	Max Phase
classic congenital adrenal hyperplasia due to 21-hydroxylase deficiency	Phase II
congenital adrenal hyperplasia	Phase II

polycystic ovary syndrome

Phase II

► [Open Targets](#)

6.2 Clinical Trials



6.2.1 ClinicalTrials.gov



2 items



Study to Evaluate the Safety and Efficacy of SPR001 in Subjects With Classic Congenital Adrenal Hyperplasia

CTID: [NCT03687242](#)

Phase: Phase 2 Status: Completed

Date: 2020-01-30

Study of SPR001 in Adults With Classic Congenital Adrenal Hyperplasia

CTID: [NCT03257462](#)

Phase: Phase 2 Status: Completed

Date: 2019-06-26

► [ClinicalTrials.gov](#)

6.2.2 EU Clinical Trials Register



2 items



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

[▶ EU Clinical Trials Register](#)

6.3 EMA Drug Information



1 of 2	
Type	Paediatric investigation
Active Substance	Tildacerfont
Therapeutic Area	Endocrinology-Gynaecology-Fertility-Metabolism
Drug Form	Tablet, Granules
Administration Route	Oral use
Decision Type	P: decision agreeing on a investigation plan, with or without partial waiver(s) and or deferral(s)
Decision Date	2022-01-31

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

2 of 2	
Type	Paediatric investigation
Active Substance	Tildacerfont
Therapeutic Area	Endocrinology-Gynaecology-Fertility-Metabolism
Drug Form	Granules, Tablet
Administration Route	Oral use
Decision Type	P: decision agreeing on a investigation plan, with or without partial waiver(s) and or deferral(s)
Decision Date	2022-01-31

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

7 Use and Manufacturing



7.1 Uses



7.1.1 Use Classification




Human Drugs -> EU pediatric investigation plans

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

8 Associated Disorders and Diseases



3 items 	
Source Disease	Data Source
classic congenital adrenal hyperplasia due to 21-hydroxylase deficiency	Open Targets
congenital adrenal hyperplasia	Open Targets
polycystic ovary syndrome	Open Targets


▶ [Open Targets](#)

9 Literature



9.1 Consolidated References



4 items 	
<p>Congenital Adrenal Hyperplasia Publication Name: Children with Differences in Sex Development Publication Date: 2024 DOI: 10.1007/978-981-97-1639-5_30</p>	
<p>Management challenges and therapeutic advances in congenital adrenal hyperplasia Publication Name: Nature reviews. Endocrinology Publication Date: 2022-04-11 PMID: PMC8999997 PMID: 35411073 DOI: 10.1038/s41574-022-00655-w</p>	
<p>Novel treatments for congenital adrenal hyperplasia Publication Name: Reviews in Endocrine and Metabolic Disorders Publication Date: 2022-02-23 PMID: PMC9156475 PMID: 35199280 DOI: 10.1007/s11154-022-09717-w</p>	

Neue Behandlungsstrategien bei adrenogenitalem Syndrom/21-Hydroxylase-Mangel

Publication Name: Journal für Klinische Endokrinologie und Stoffwechsel

Publication Date: 2022

DOI: [10.1007/s41969-022-00159-y](https://doi.org/10.1007/s41969-022-00159-y)

► [PubChem](#)

9.2 Springer Nature References



6 items ↓

Search 🔍 SORT BY Publication Date - Oldest ▼

<p>Novel treatments for congenital adrenal hyperplasia</p> <p>PMID: 35199280</p> <p>Publication Date: 2022</p> <p>Publication Name: Reviews in Endocrine and Metabolic Disorders</p>
<p>Management challenges and therapeutic advances in congenital adrenal hyperplasia</p> <p>PMID: 35411073</p> <p>Publication Date: 2022</p> <p>Publication Name: Nature Reviews Endocrinology</p>
<p>Neue Behandlungsstrategien bei adrenogenitalem Syndrom/21-Hydroxylase-Mangel</p> <p>Publication Date: 2022</p> <p>Publication Name: Journal für Klinische Endokrinologie und Stoffwechsel</p>
<p>Congenital Adrenal Hyperplasia</p> <p>Publication Date: 2024</p> <p>Publication Name: Children with Differences in Sex Development</p>
<p>Congenital Adrenal Hyperplasia</p> <p>Publication Date: 2024</p>

⏪ First ⏪ Previous Page 1 of 2 Next ⏩ Last ⏩

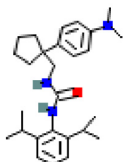
► [Springer Nature](#)

9.3 Chemical Co-Occurrences in Literature

Showing 3 of 37 [View More](#)

Chemical

Selected evidence



Nevanimibe
CID 131679

3 articles

[View All](#)

Neue Behandlungsstrategien bei adrenogenitem Syndrom/21-Hydroxylase-Mangel

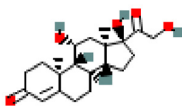
DOI 10.1007/s41969-022-00159-y; Journal für Klinische Endokrinologie und Stoffwechsel 2022-01-01

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)



(8R,9R,10S,11R,13R,14R,17S)-11,17-dihydroxy-17-(2-hydroxyacetyl)-10,13-dimethyl-2,6,7,8,9,11,12,14,15,16-decahydro-1H-cyclopenta[a]phenanthren-3-one

CID 40488894

3 articles

[View All](#)

Neue Behandlungsstrategien bei adrenogenitem Syndrom/21-Hydroxylase-Mangel

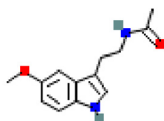
DOI 10.1007/s41969-022-00159-y; Journal für Klinische Endokrinologie und Stoffwechsel 2022-01-01

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)



Melatonin
CID 896

2 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

[▶ PubChem](#)

9.4 Chemical-Gene Co-Occurrences in Literature

Showing 1 of 1 [View More](#)**Gene/Protein/Enzyme****Selected evidence**[proopiomelanocortin](#)

1 article

[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)

[▶ PubChem](#)

9.5 Chemical-Disease Co-Occurrences in Literature

Showing 3 of 5 [View More](#)**Disease****Selected evidence**[Congenital adrenal hyperplasia due to 21 hydroxylase deficiency](#)

2 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)

[Adrenal Hyperplasia, Congenital](#)

2 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)

Puberty, Precocious

1 article

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)

 [PubChem](#)

10 Patents



10.1 WIPO PATENTSCOPE



Patents are available for this chemical structure:

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

 [PATENTSCOPE \(WIPO\)](#)

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 cortical synthetic pathway. A decrease in adrenal cortical production

 [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](#)

11.3 MolGenie Organic Chemistry Ontology



18 items

View in Classification Browser

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

aromatic chlorides

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

biaryls

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

MolGenie Organic Chemistry Ontology > PubChemLite chemical entities > substructural concepts > functional groups > nitrogen containing functional groups > amines > tertiary amines

alkyl aryl tertiary amines

[▶ MolGenie](#)

12 Information Sources



FILTER BY SOURCE

ALL SOURCES

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

2. ChemIDplus

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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>

3. DrugBank

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https://www.drugbank.ca/legal/terms_of_use

Tildacerfont

<https://www.drugbank.ca/drugs/DB18545>

4. FDA Global Substance Registration System (GSRS)

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

Tildacerfont

<https://gsrs.ncats.nih.gov/ginas/app/beta/substances/09QCEV5481>

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<https://clinicaltrials.gov/ct2/about-site/terms-conditions#Use>

<https://clinicaltrials.gov/>

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https://ncithesaurus.nci.nih.gov/ncitbrowser/ConceptReport.jsp?dictionary=NCI_Thesaurus&ns=ncit&code=C171816

NCI Thesaurus

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

7. 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>

8. EU Clinical Trials Register

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

9. European Medicines Agency (EMA)

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Tildacerfont (P/0036/2022)

<https://www.ema.europa.eu/en/medicines/human/paediatric-investigation-plans/mea-002970-pip01-21>

Tildacerfont (P/0036/2022)

<https://www.ema.europa.eu/en/medicines/human/paediatric-investigation-plans/emea-002970-pip01-21>

10. Springer Nature

<https://pubchem.ncbi.nlm.nih.gov/substance/?source=15745&sourceid=28052277-230853427>

11. PubChem

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

12. MolGenie

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MolGenie Organic Chemistry Ontology

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

13. PATENTSCOPE (WIPO)

SID 440666221

<https://pubchem.ncbi.nlm.nih.gov/substance/440666221>