

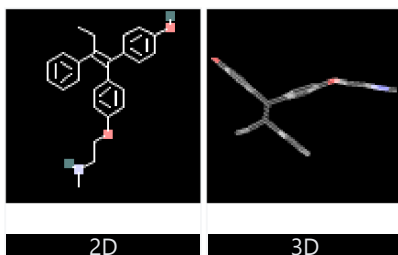
Endoxifen

Cite

Download

PubChem CID 10090750

Structure



Chemical Safety



[Laboratory Chemical Safety Summary \(LCSS\) Datasheet](#)

Molecular Formula $C_{25}H_{27}NO_2$

Synonyms

Endoxifen
112093-28-4
Z-Endoxifen
4-Hydroxy-N-desmethyltamoxifen
Endoxifen Z-Isomer

[View More...](#)

Molecular Weight 373.5 g/mol

Computed by PubChem 2.2 (PubChem release 2021.10.14)

Dates

Create: 2006-10-25
Modify: 2024-11-02

Description

4-Hydroxy-N-desmethyltamoxifen is a stilbenoid.

Contents

| | |
|-------------------------------------|---|
| Title and Summary | |
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| 2 Names and Identifiers | ▼ |
| 3 Chemical and Physical Properties | ▼ |
| 4 Related Records | ▼ |
| 5 Chemical Vendors | |
| 6 Drug and Medication Information | ▼ |
| 7 Pharmacology and Biochemistry | ▼ |
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| 13 Biological Test Results | ▼ |
| 14 Classification | ▼ |
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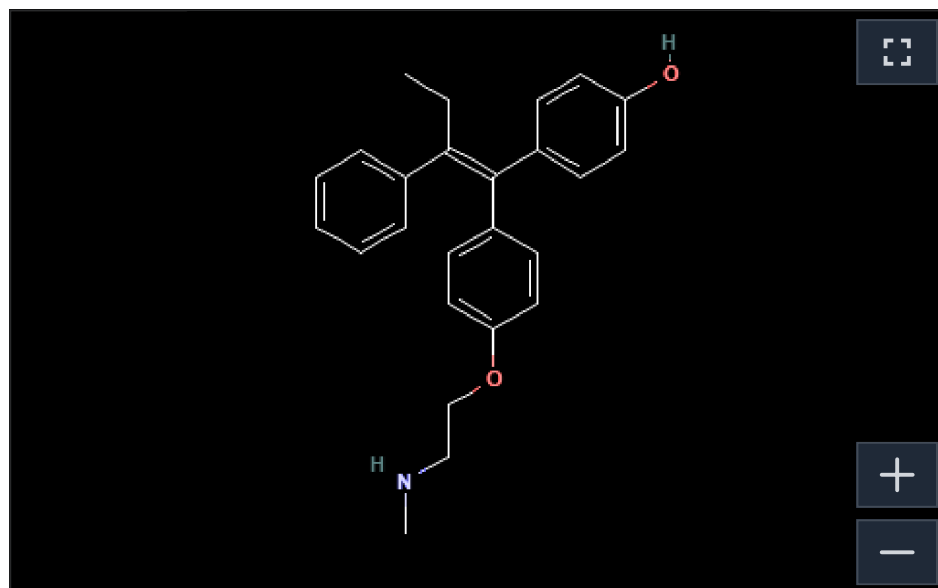
1 Structures



1.1 2D Structure



Chemical Structure
Depiction



► PubChem

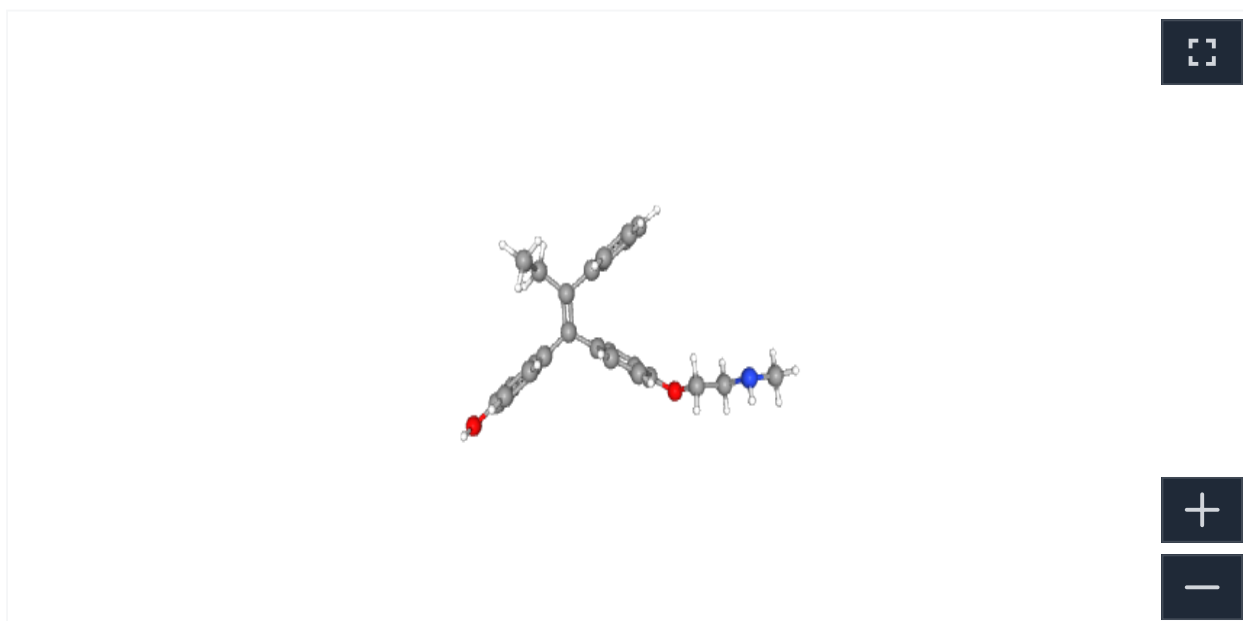
1.2 3D Conformer



Interactive Chemical Structure Model

Ball and Stick Sticks Wire-Frame Space-Filling

Show Hydrogens Animate



▶ PubChem

2 Names and Identifiers



2.1 Computed Descriptors



2.1.1 IUPAC Name



4-[(Z)-1-[4-[2-(methylamino)ethoxy]phenyl]-2-phenylbut-1-enyl]phenol

Computed by Lexichem TK 2.7.0 (PubChem release 2021.10.14)

▶ PubChem

2.1.2 InChI



InChI=1S/C25H27NO2/c1-3-24(19-7-5-4-6-8-19)25(20-9-13-22(27)14-10-20)21-11-15-23(16-12-21)28-18-17-26-2/h4-16,26-27H,3,17-18H2,1-2H3/b25-24-

Computed by InChI 1.0.6 (PubChem release 2021.10.14)

▶ PubChem

2.1.3 InChIKey



MHJBZVSGOZTKRH-IZHYLOQSSA-N

Computed by InChI 1.0.6 (PubChem release 2021.10.14)

▶ PubChem

2.1.4 SMILES



CC/C(=C(\C1=CC=C(C=C1)O)/C2=CC=C(C=C2)OCCNC)/C3=CC=CC=C3

Computed by OEChem 2.3.0 (PubChem release 2021.10.14)

▶ PubChem

2.2 Molecular Formula



C₂₅H₂₇NO₂

Computed by PubChem 2.2 (PubChem release 2021.10.14)

▶ PubChem

2.3 Other Identifiers



2.3.1 CAS



112093-28-4

▶ CAS Common Chemistry; ChemIDplus; DTP/NCI; EPA DSSTox; European Chemicals Agency (ECHA); F...

110025-28-0

▶ European Chemicals Agency (ECHA)

2.3.2 European Community (EC) Number



683-027-6

▶ European Chemicals Agency (ECHA)

808-709-4

▶ European Chemicals Agency (ECHA)

2.3.3 UNII



46AF8680RC

▶ FDA Global Substance Registration System (GSRS)

2.3.4 ChEBI ID



CHEBI:80555

▶ ChEBI

2.3.5 ChEMBL ID



CHEMBL1093458

▶ ChEMBL

2.3.6 DSSTox Substance ID



DTXSID80149880

▶ EPA DSSTox

2.3.7 HMDB ID



HMDB0060666

▶ Human Metabolome Database (HMDB)

2.3.8 KEGG ID



C16547

▶ KEGG

2.3.9 Nikkaji Number



J1.507.991F

▶ Japan Chemical Substance Dictionary (Nikkaji)

J393.650C

▶ Japan Chemical Substance Dictionary (Nikkaji)

2.3.10 NSC Number



749798

▶ DTP/NCI

746494

▶ DTP/NCI

2.3.11 PharmGKB ID



PA166124478

▶ PharmGKB

2.3.12 Pharos Ligand ID



57JTNU3YXJR1

▶ Pharos

2.3.13 Wikidata



Q27149598

▶ Wikidata

2.3.14 Wikipedia



Endoxifen

▶ Wikipedia

2.4 Synonyms



2.4.1 MeSH Entry Terms



4-hydroxy-N-demethyltamoxifen
4-hydroxy-N-desmethyltamoxifen
4-hydroxy-N-desmethyltamoxifen, (Z)-isomer
endoxifen

Z-endoxifen

► Medical Subject Headings (MeSH)

2.4.2 Depositor-Supplied Synonyms



| | |
|--------------------------------|---|
| Endoxifen 112093-28-4 | (Z)-4-Hydroxy-N-desmethyl Tamoxifen (contains up to 10% E isomer) Endoxifen (Z-isomer) |
| Z-Endoxifen | 4-[(Z)-1-[4-[2-(methylamino)ethoxy]phenyl]-2-phenylbut-1-enyl]phenol |
| 4-Hydroxy-N-desmethyltamoxifen | 4-Hydroxy-N-desmethyl-tamoxifen |
| Endoxifen Z-Isomer | CHEBI:80555 |
| N-Desmethyl-4-hydroxytamoxifen | 46AF8680RC |
| (Z)-Endoxifen | MFCD09840374 |
| 110025-28-0 | 4-[(1Z)-1-[4-[2-(methylamino)ethoxy]phenyl]-2-phenylbut-1-en-1-yl]phenol |
| 4OHNDtam | UNII-46AF8680RC |
| NSC-749798 | 4-hydroxy-N-desmethyl tamoxifen |

► PubChem

3 Chemical and Physical Properties



3.1 Computed Properties



| Property Name | Property Value | Reference |
|------------------------------|----------------|--|
| Molecular Weight | 373.5 g/mol | Computed by PubChem 2.2 (PubChem release 2021.10.14) |
| XLogP3-AA | 6.3 | Computed by XLogP3 3.0 (PubChem release 2021.10.14) |
| Hydrogen Bond Donor Count | 2 | Computed by Cactvs 3.4.8.18 (PubChem release 2021.10.14) |
| Hydrogen Bond Acceptor Count | 3 | Computed by Cactvs 3.4.8.18 (PubChem release 2021.10.14) |
| Rotatable Bond Count | 8 | Computed by Cactvs 3.4.8.18 (PubChem release 2021.10.14) |

| | | |
|-----------------------------------|------------------------|--|
| Exact Mass | 373.204179104 g/mol | Computed by PubChem 2.2 (PubChem release 2021.10.14) |
| Monoisotopic Mass | 373.204179104 g/mol | Computed by PubChem 2.2 (PubChem release 2021.10.14) |
| Topological Polar Surface Area | 41.5Å 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 | 467 | 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 | 1 | 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 Endocrine Disruptors



Potential endocrine disrupting compound

S109 | PARCEDC | List of 7074 potential endocrine disrupting compounds (EDCs) by PARC T4.2 | DOI:10.5281/zenodo.10944198

▶ [NORMAN Suspect List Exchange](#)

4 Related Records



4.1 Related Compounds with Annotation



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

▶ [PubChem](#)

4.2 Related Compounds



| | |
|---|--|
| Same Connectivity Count | 6 |
| Same Stereo Count | 2 |
| Same Isotope Count | 3 |
| Same Parent, Connectivity Count | 22 |
| Same Parent, Stereo Count | 11 |
| Same Parent, Isotope Count | 19 |
| Same Parent, Exact Count | 10 |
| Mixtures, Components, and Neutralized Forms Count | 22 |
| 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 | 215 |
| Same Count | 117 |
| Mixture Count | 98 |

▶ PubChem

4.3.2 Substances by Category



▶ PubChem

4.4 Entrez Crosslinks



| | |
|----------------|----|
| PubMed Count | 16 |
| Taxonomy Count | 2 |
| Gene Count | 17 |

▶ PubChem

5 Chemical Vendors



▶ PubChem

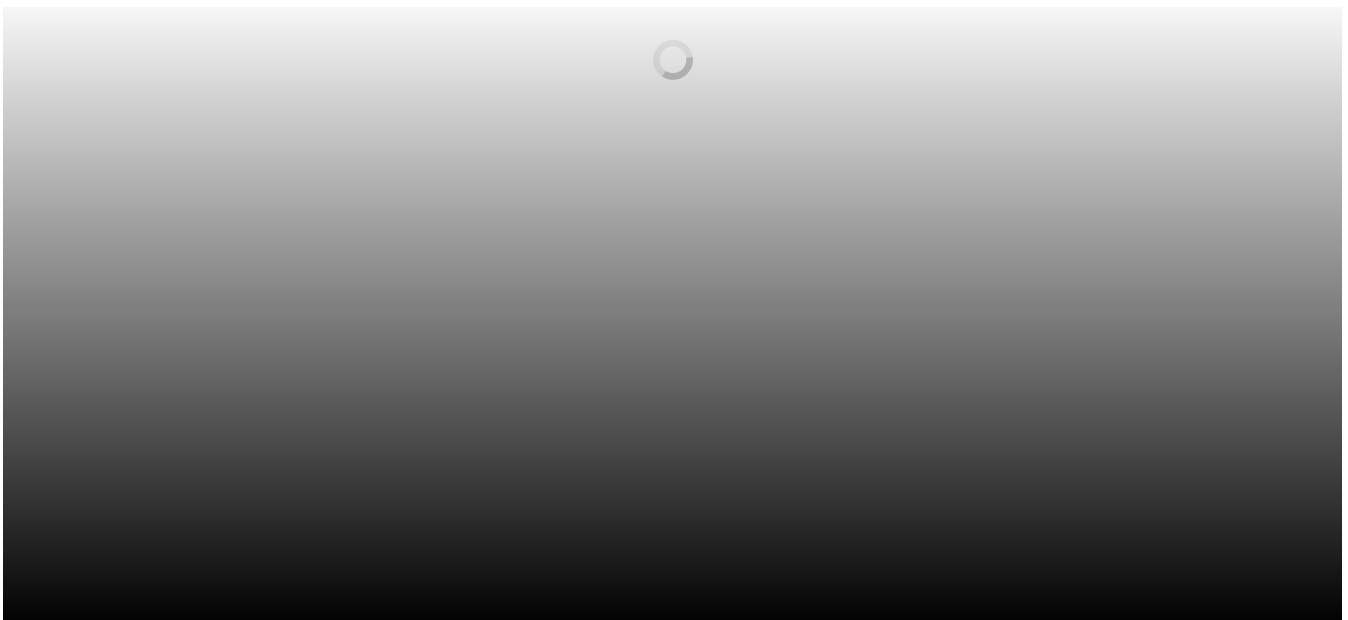
6 Drug and Medication Information



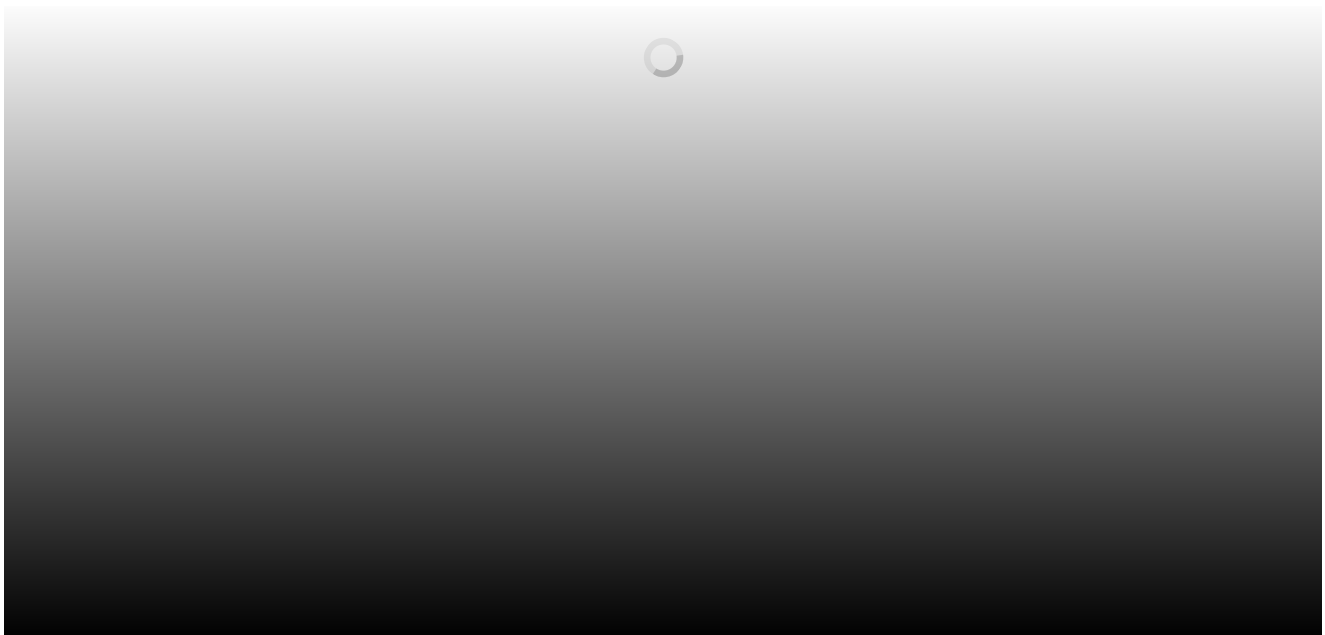
6.1 Clinical Trials



6.1.1 ClinicalTrials.gov



6.1.2 EU Clinical Trials Register



▶ [EU Clinical Trials Register](#)

7 Pharmacology and Biochemistry



7.1 Metabolism / Metabolites



Endoxifen has known human metabolites that include Endoxifen O-sulfate and Endoxifen O-glucuronide.

Endoxifen is a known human metabolite of [4-Hydroxytamoxifen](#) and [N-Desmethyltamoxifen](#).

S73 | METXBIODB | Metabolite Reaction Database from BioTransformer | DOI:10.5281/zenodo.4056560

▶ [NORMAN Suspect List Exchange](#)

7.2 Human Metabolite Information



7.2.1 Tissue Locations



Kidney
Liver

▶ [Human Metabolome Database \(HMDB\)](#)

7.2.2 Cellular Locations



Cytoplasm
Membrane

▶ [Human Metabolome Database \(HMDB\)](#)

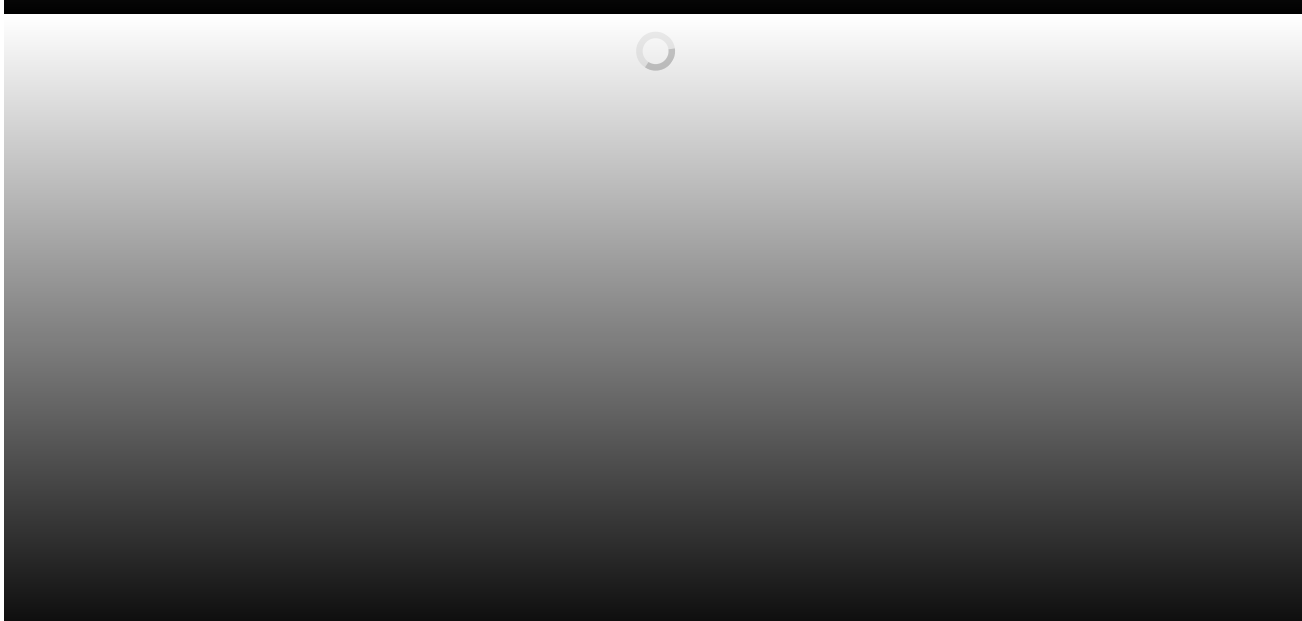
7.2.3 Metabolite Pathways



[Tamoxifen Action Pathway](#)
[Tamoxifen Metabolism Pathway](#)

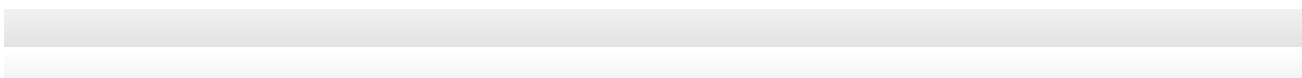
▶ [Human Metabolome Database \(HMDB\)](#)

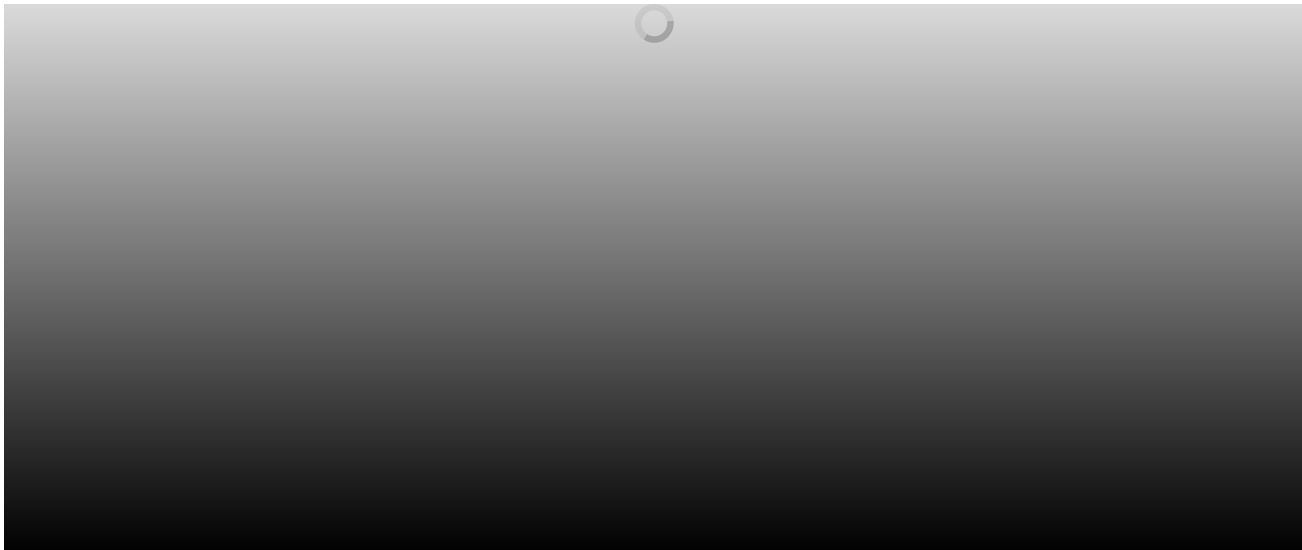
7.3 Biochemical Reactions



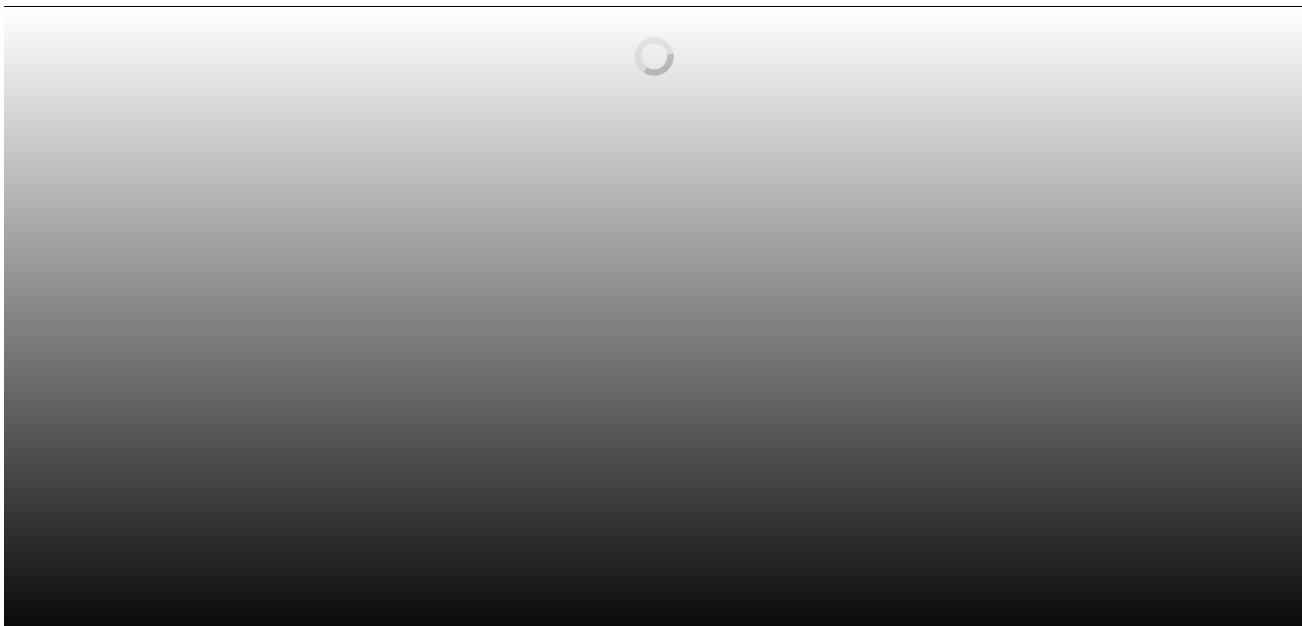
▶ [PubChem](#)

7.4 Transformations





▶ ChEMBL



▶ NORMAN Suspect List Exchange

8 Safety and Hazards



8.1 Hazards Identification





8.1.1 GHS Classification



1 of 2

View All

| | |
|--------------------------------|---|
| Pictogram(s) |   <div style="display: flex; justify-content: space-around; width: 100%;"> <div style="background-color: black; color: white; padding: 2px 5px; text-align: center;">Irritant</div> <div style="background-color: black; color: white; padding: 2px 5px; text-align: center;">Health Hazard</div> </div> |
| Signal | <u>Warning</u> |
| GHS Hazard Statements | <p>H302+H312+H332 (97.4%): Harmful if swallowed, in contact with skin or if inhaled [<u>Warning</u> Acute toxicity, oral; acute toxicity, dermal; acute toxicity, inhalation]</p> <p>H302 (100%): Harmful if swallowed [<u>Warning</u> Acute toxicity, oral]</p> <p>H312 (100%): Harmful in contact with skin [<u>Warning</u> Acute toxicity, dermal]</p> <p>H332 (100%): Harmful if inhaled [<u>Warning</u> Acute toxicity, inhalation]</p> <p>H361 (100%): Suspected of damaging fertility or the unborn child [<u>Warning</u> Reproductive toxicity]</p> <p>H413 (100%): May cause long lasting harmful effects to aquatic life [Hazardous to the aquatic environment, long-term hazard]</p> |
| Precautionary Statement Codes | <p>P203, P261, P264, P270, P271, P273, P280, P301+P317, P302+P352, P304+P340, P317, P318, P321, P330, P362+P364, P405, and P501</p> <p>(The corresponding statement to each P-code can be found at the GHS Classification page.)</p> |
| ECHA C&L Notifications Summary | <p><i>Aggregated GHS information provided per 39 reports by companies from 2 notifications to the ECHA C&L Inventory. Each notification may be associated with multiple companies.</i></p> <p><i>Information may vary between notifications depending on impurities, additives, and other factors. The percentage value in parenthesis indicates the notified classification ratio from companies that provide hazard codes. Only hazard codes with percentage values above 10% are shown.</i></p> |

► [European Chemicals Agency \(ECHA\)](#)

8.1.2 Hazard Classes and Categories



Acute Tox. 4 (100%)

Acute Tox. 4 (100%)

Acute Tox. 4 (100%)

Repr. 2 (100%)

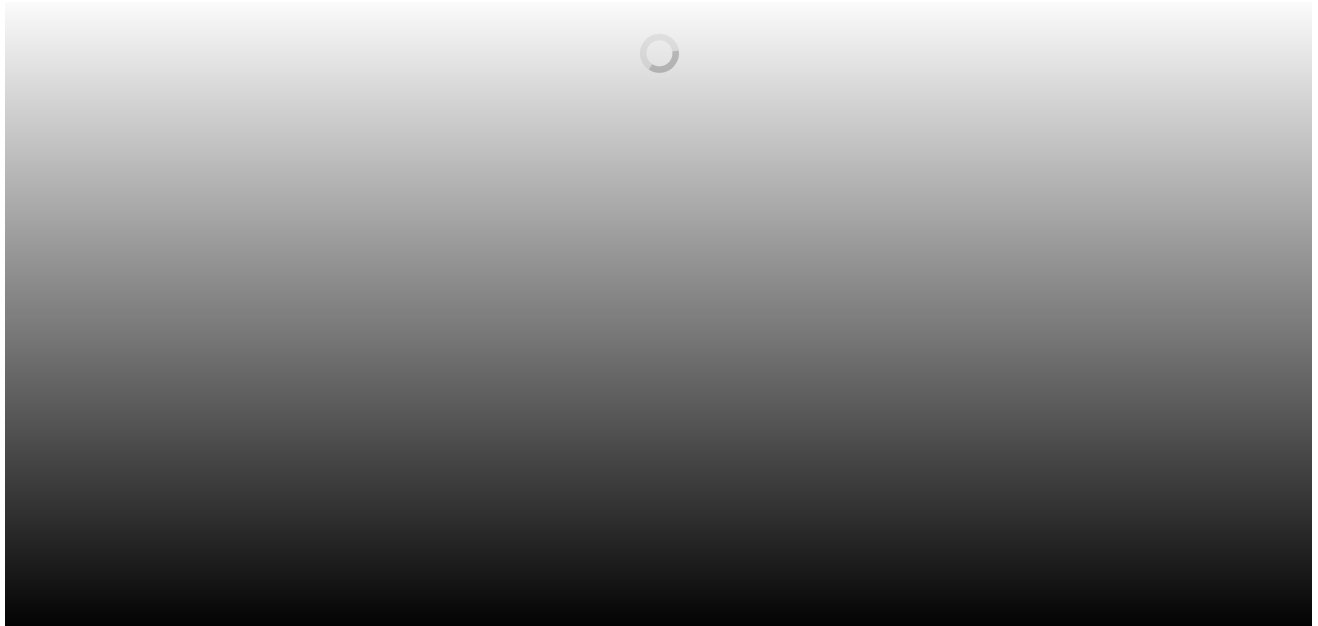
Aquatic Chronic 4 (100%)

► [European Chemicals Agency \(ECHA\)](#)

Aquatic Acute 1 (97.4%)

▶ European Chemicals Agency (ECHA)

9 Associated Disorders and Diseases

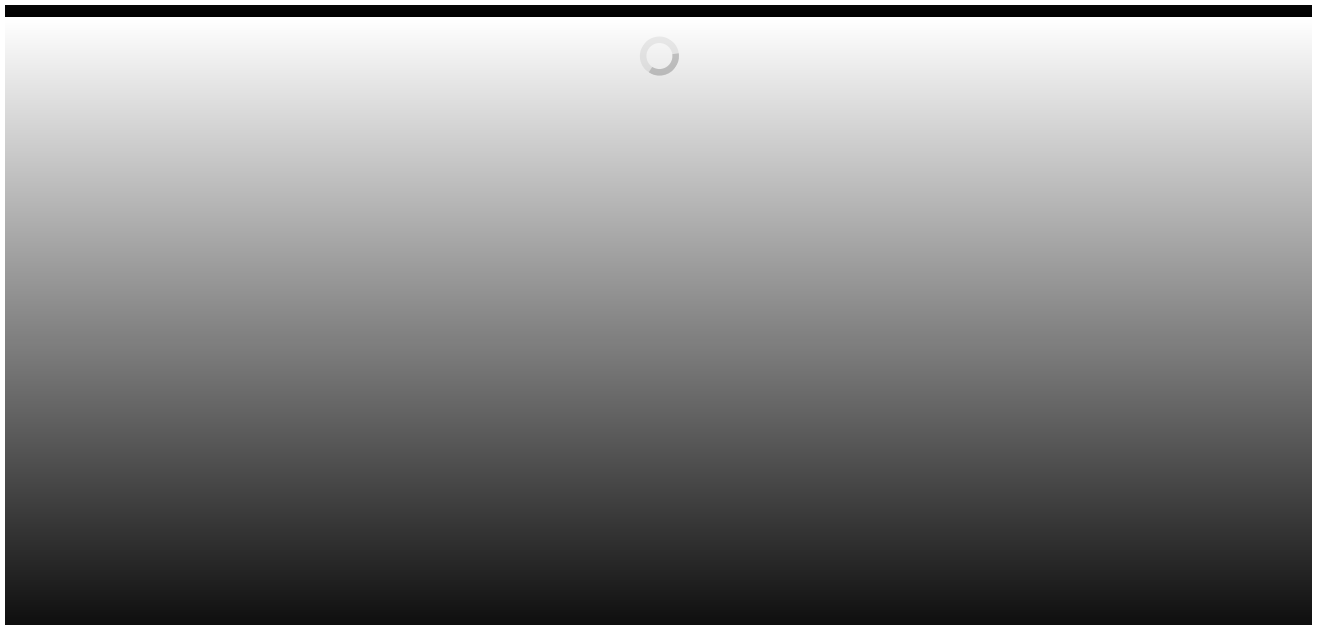


▶ Therapeutic Target Database (TTD)

10 Literature

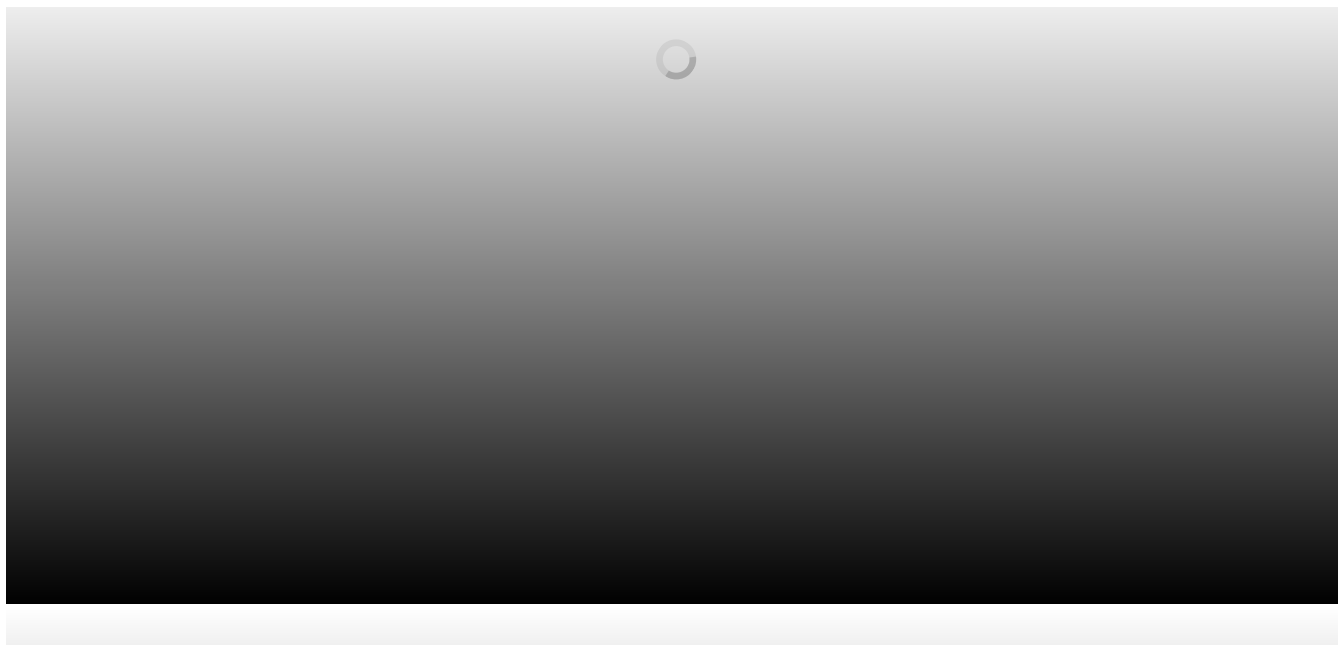


10.1 Consolidated References



▶ PubChem

10.2 NLM Curated PubMed Citations



▶ PubChem

10.3 Springer Nature References



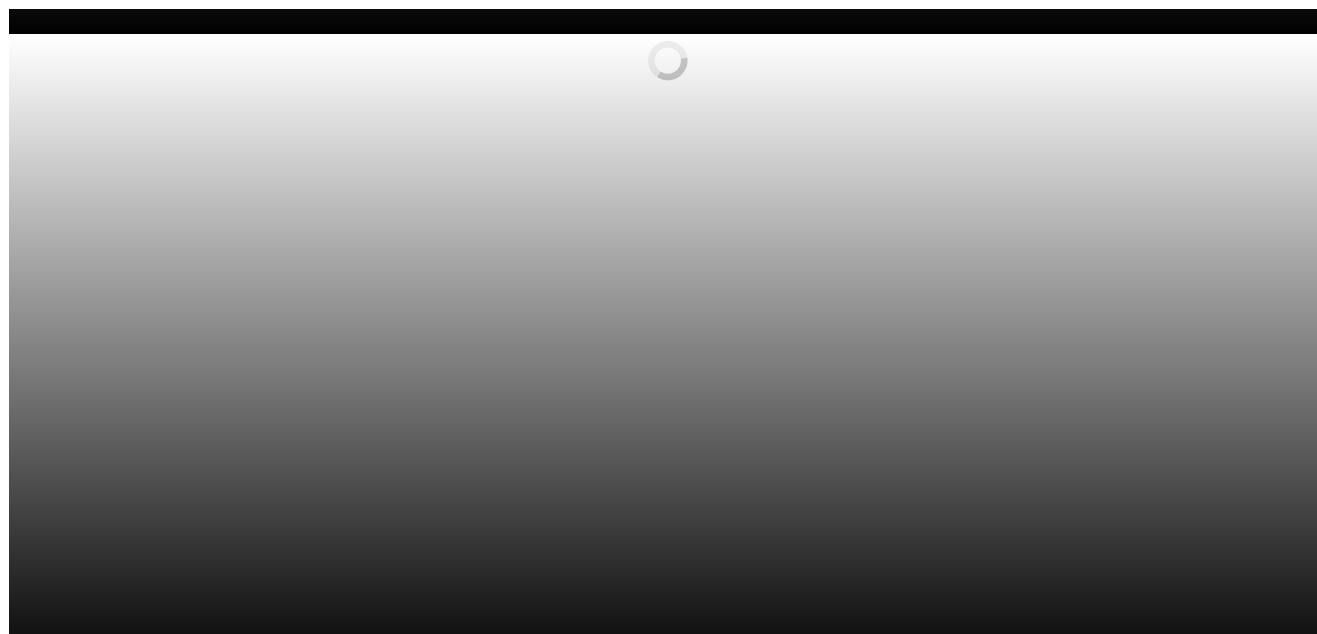
▶ Springer Nature

10.4 Chemical Co-Occurrences in Literature



▶ PubChem

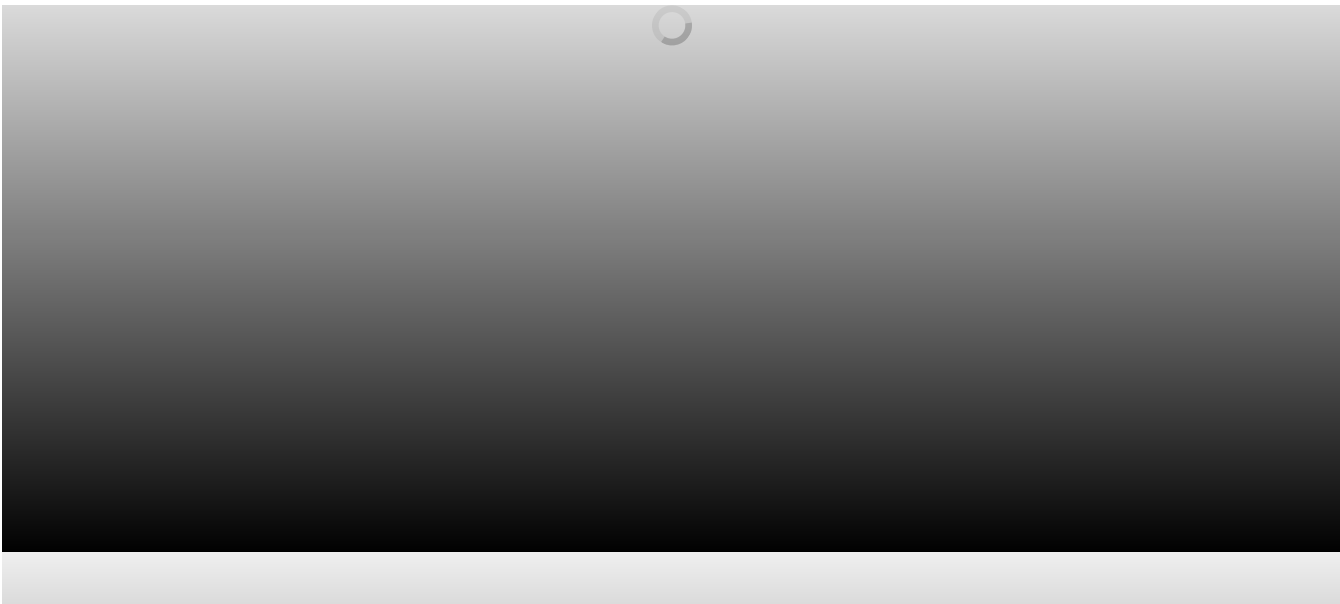
10.5 Chemical-Gene Co-Occurrences in Literature



▶ PubChem

10.6 Chemical-Disease Co-Occurrences in Literature



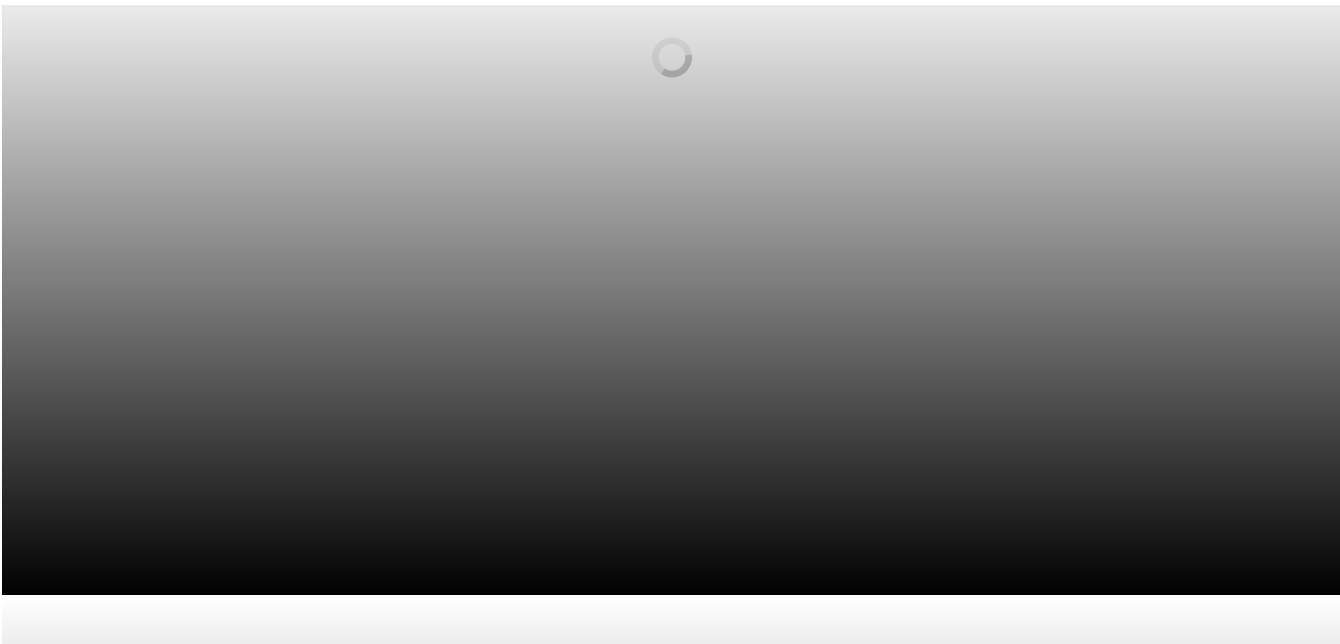


▶ PubChem

11 Patents



11.1 Depositor-Supplied Patent Identifiers



▶ PubChem

[Link to all deposited patent identifiers](#)

▶ PubChem

11.2 WIPO PATENTSCOPE

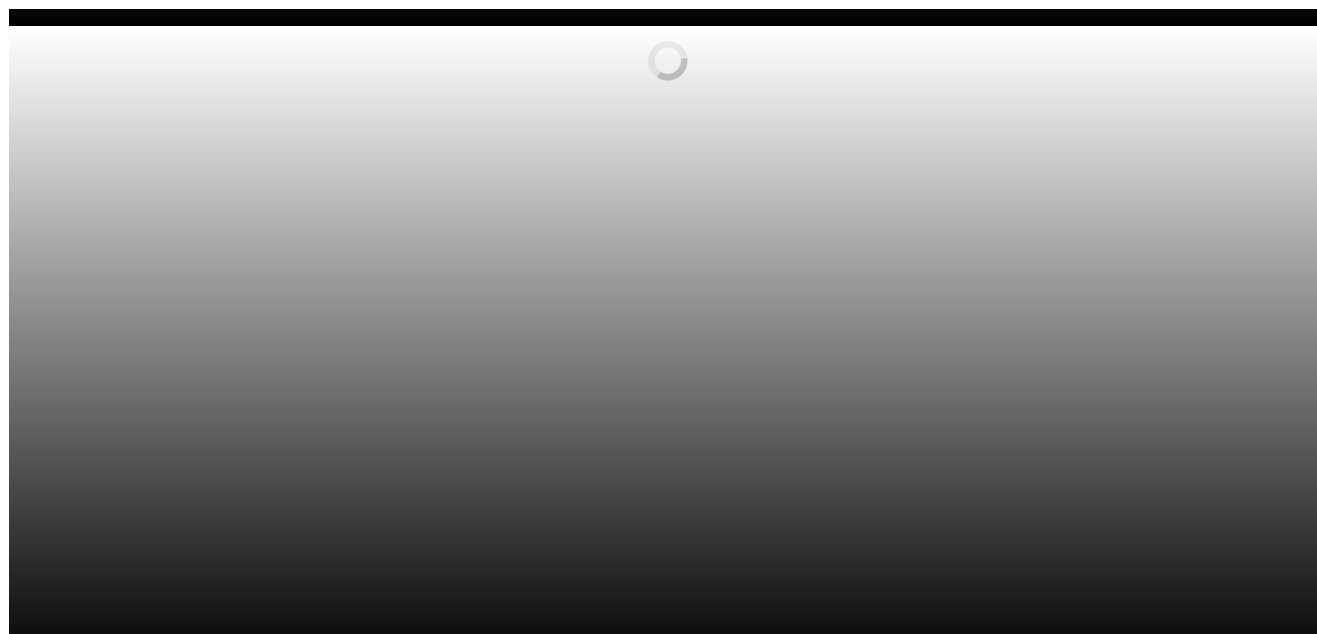


Patents are available for this chemical structure:

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

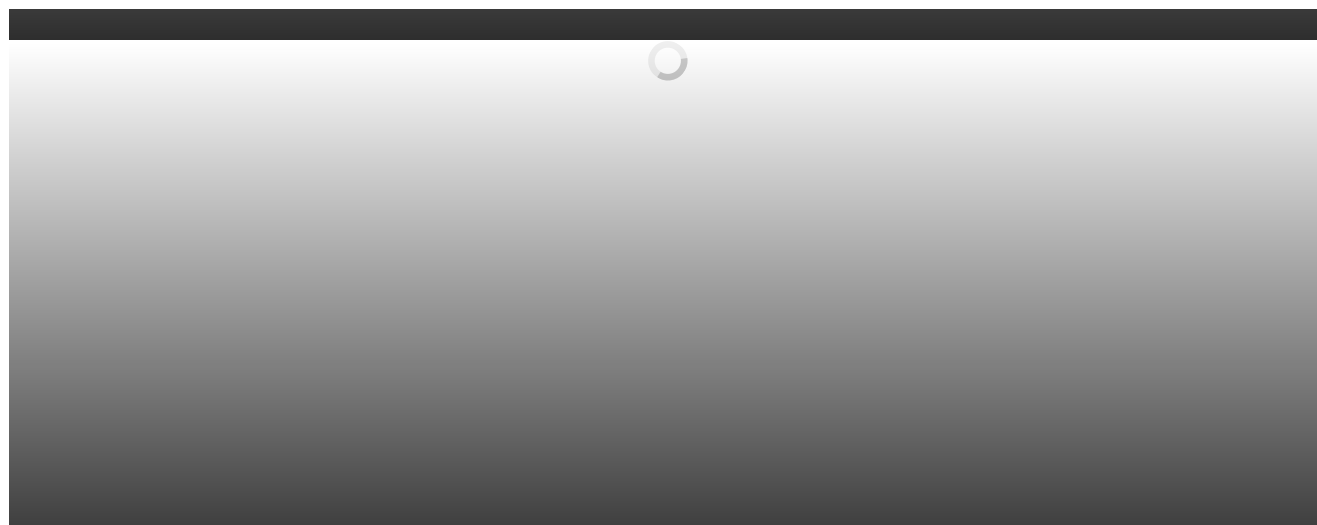
▶ PATENTSCOPE (WIPO)

11.3 Chemical Co-Occurrences in Patents



▶ PubChem

11.4 Chemical-Disease Co-Occurrences in Patents



▶ PubChem

11.5 Chemical-Gene Co-Occurrences in Patents

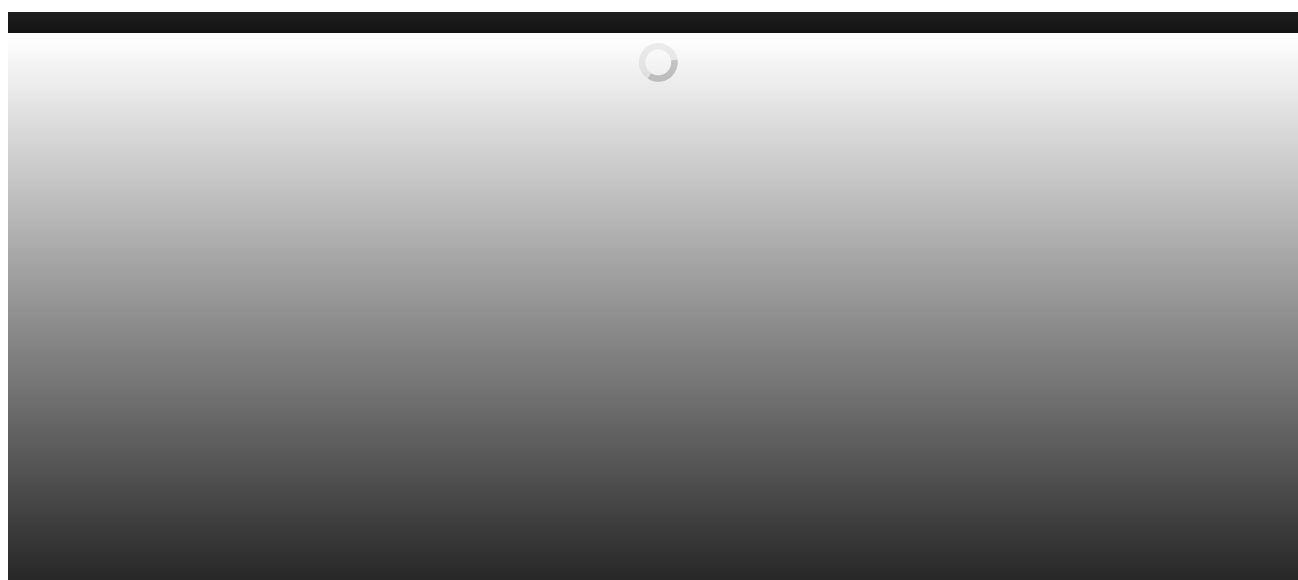


▶ PubChem

12 Interactions and Pathways



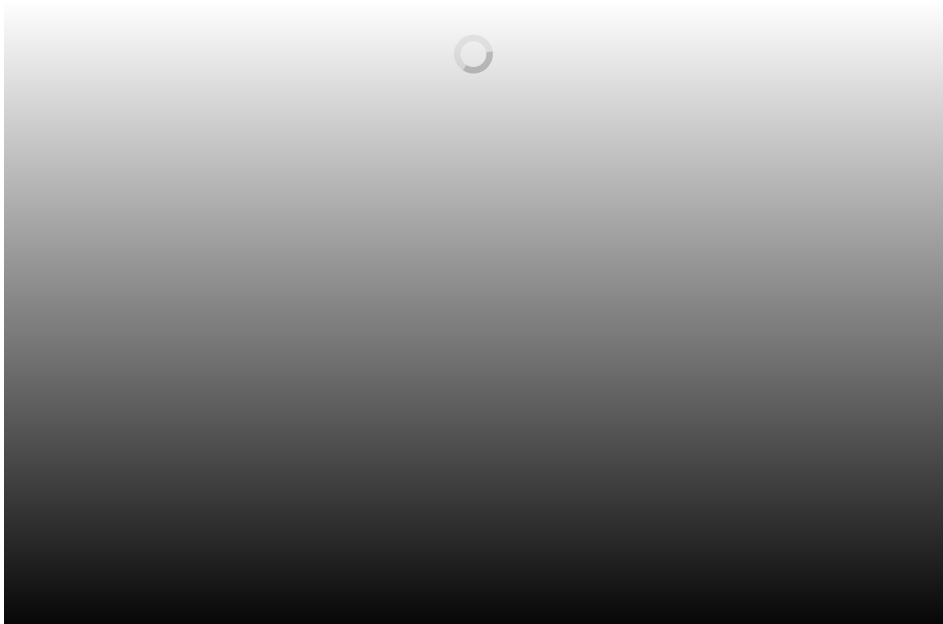
12.1 Protein Bound 3D Structures



▶ [RCSB Protein Data Bank \(RCSB PDB\)](#)

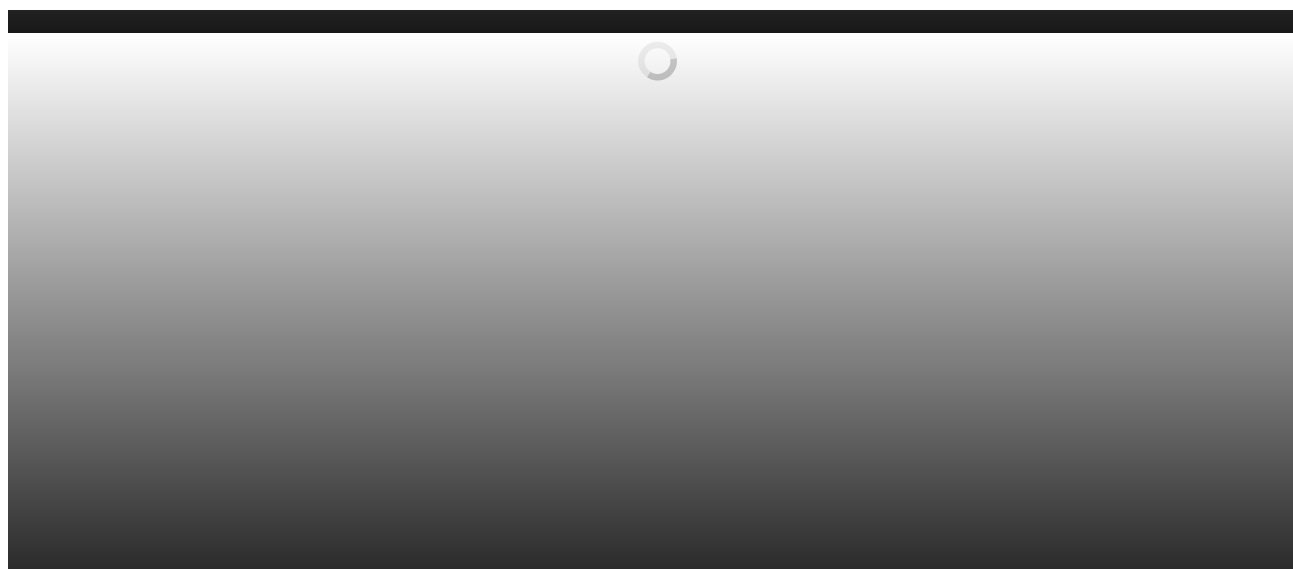
12.1.1 Ligands from Protein Bound 3D Structures



| | |
|---------------------|---|
| PDBe Ligand Code | 9XY |
| PDBe Structure Code | 5W9D |
| PDBe Conformer |  |

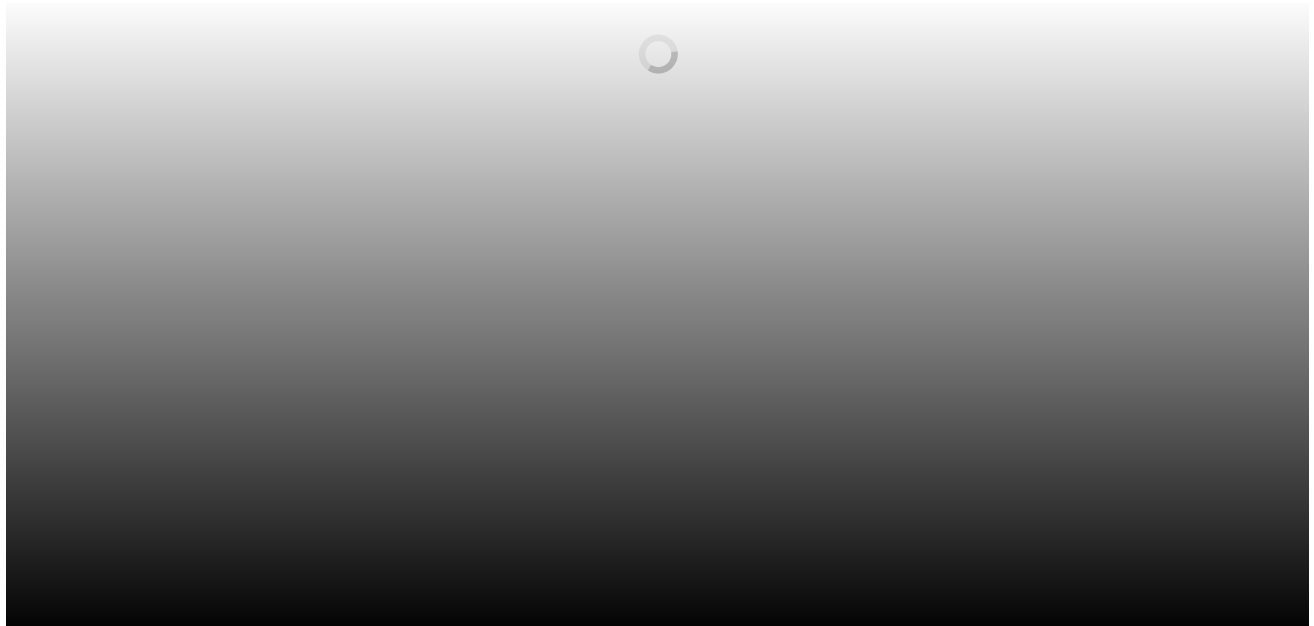
▶ [Protein Data Bank in Europe \(PDBe\)](#)

12.2 Chemical-Target Interactions



▶ Comparative Toxicogenomics Database (CTD); IUPHAR/BPS Guide to PHARMACOLOGY; Therapeutic ...

12.3 Pathways

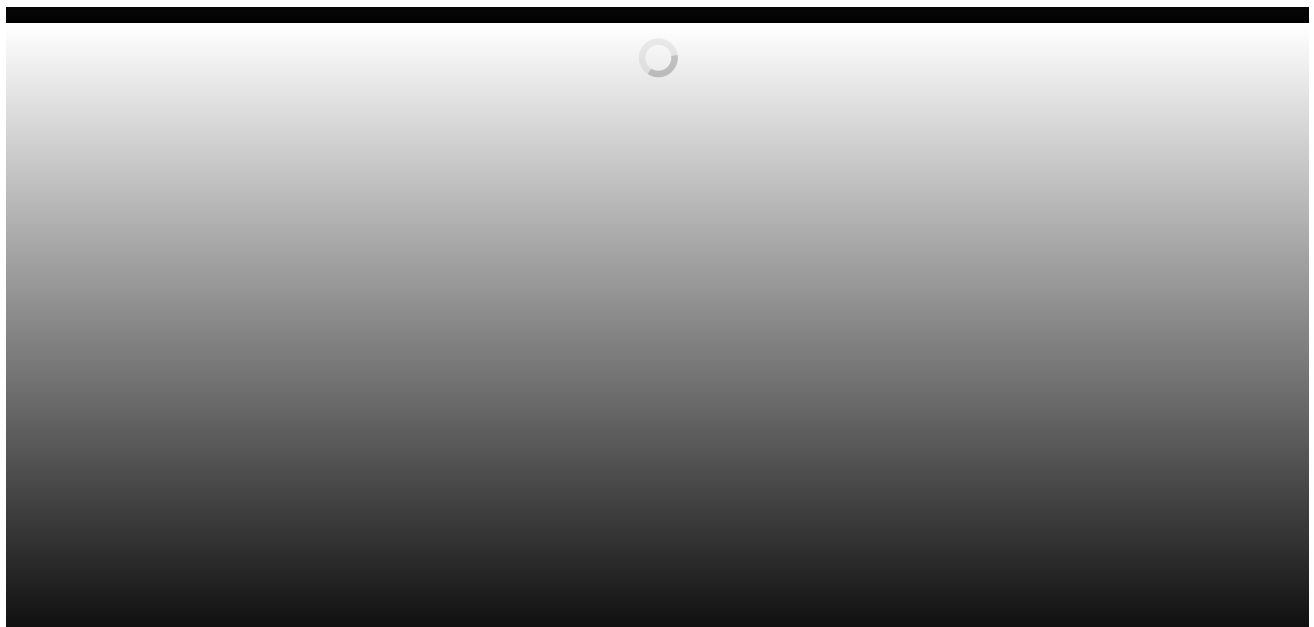


▶ PubChem

13 Biological Test Results



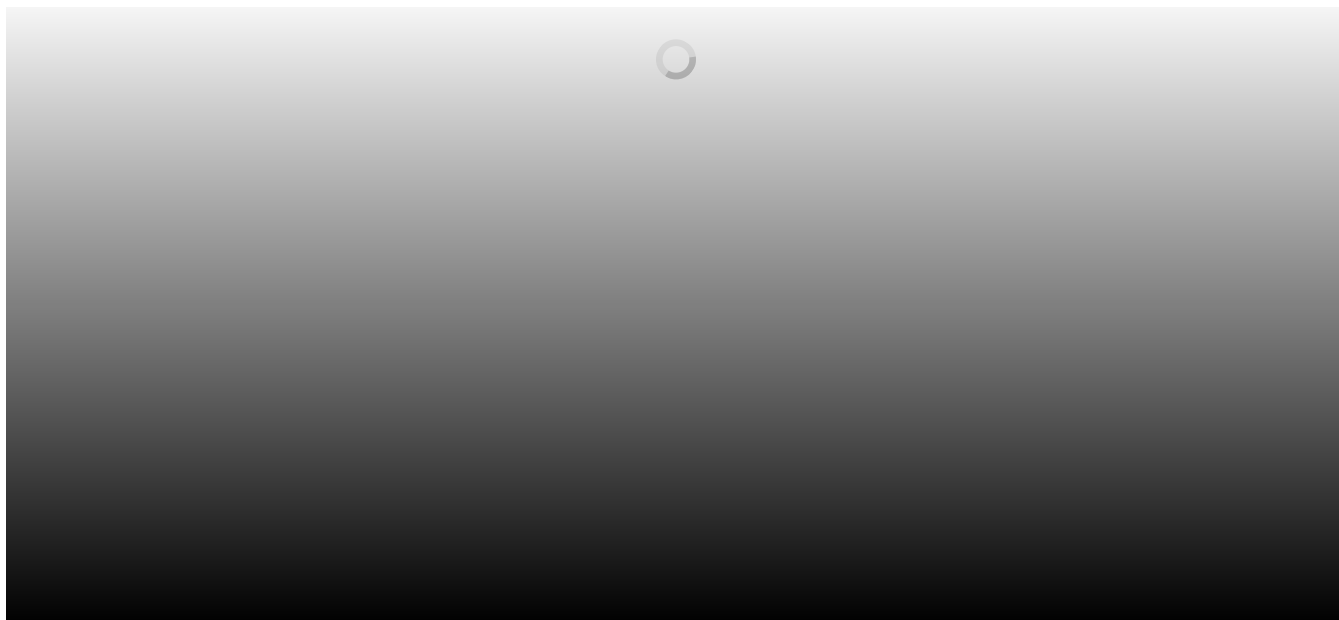
13.1 BioAssay Results



14 Classification

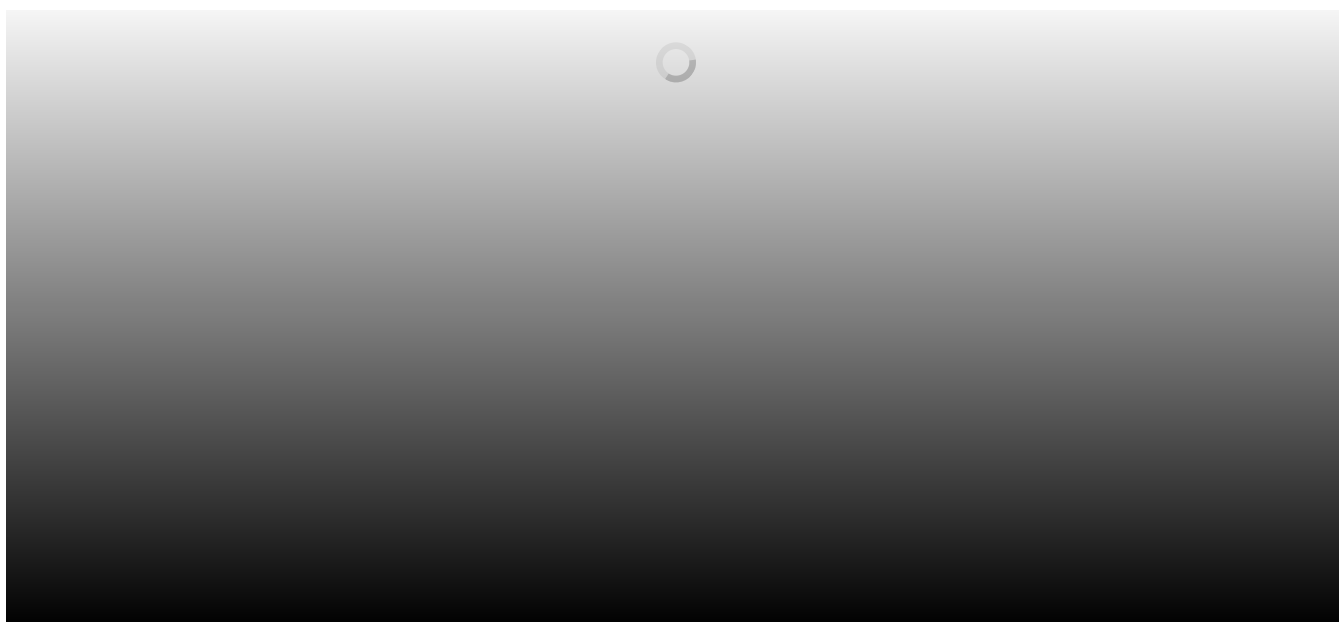


14.1 MeSH Tree



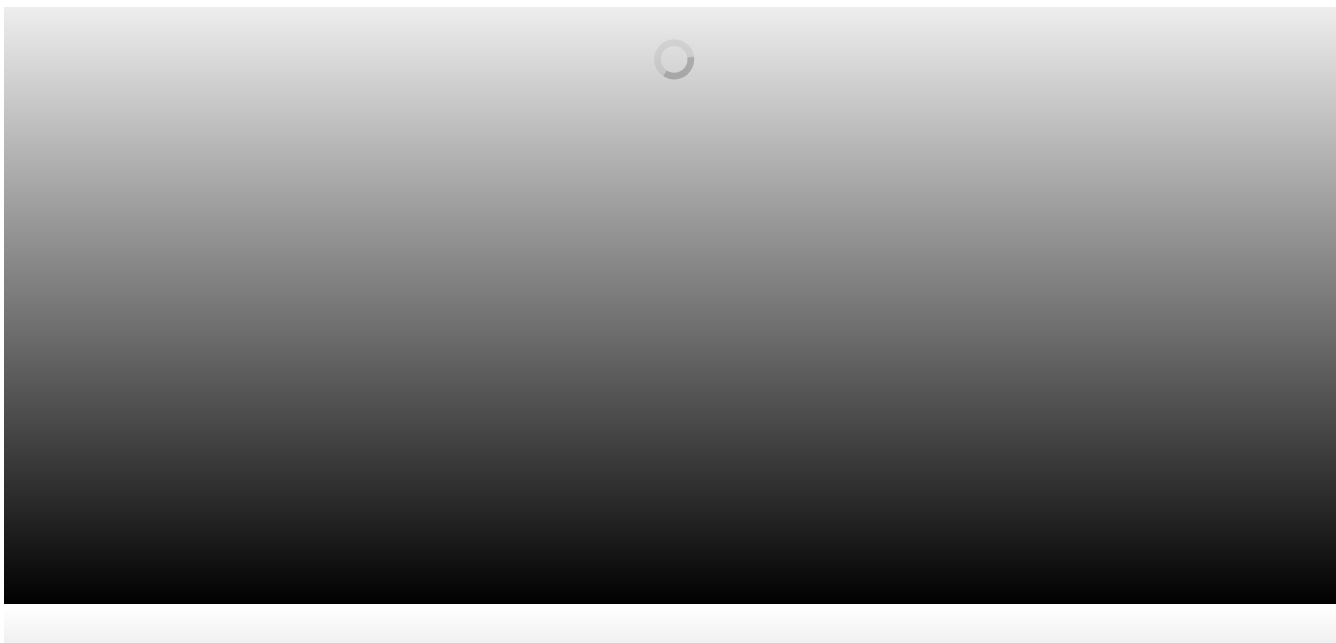
▶ Medical Subject Headings (MeSH)

14.2 ChEBI Ontology



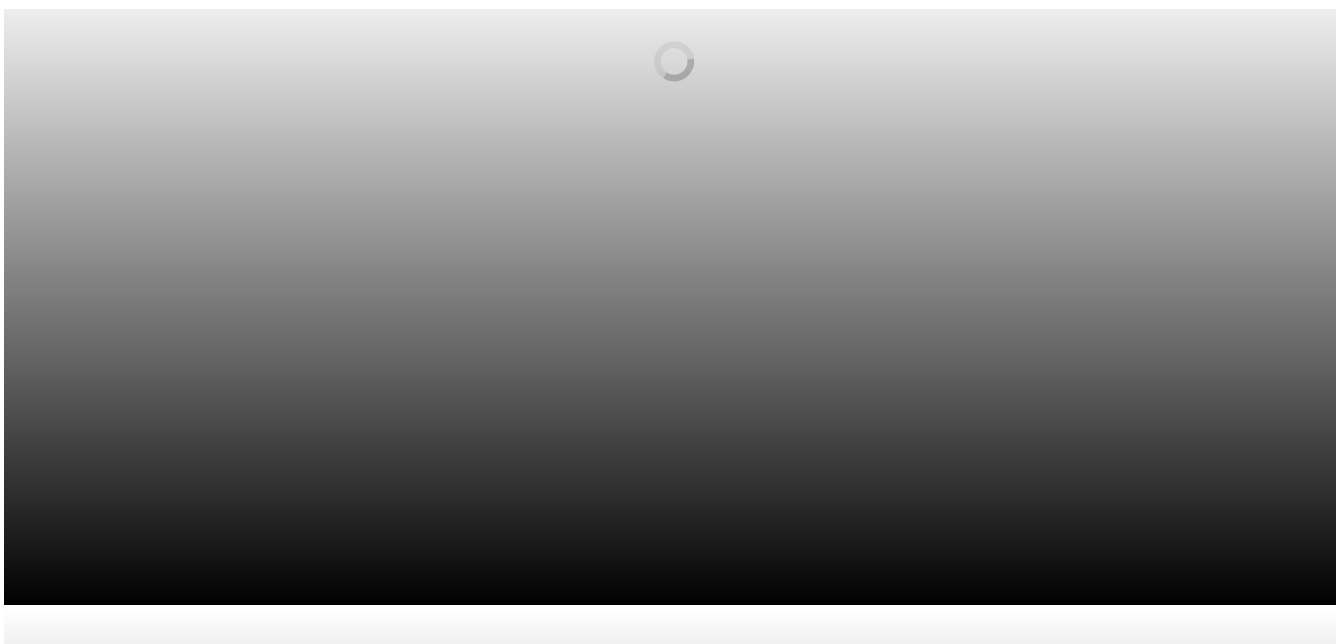
▶ ChEBI

14.3 ChemIDplus



▶ ChemIDplus

14.4 IUPHAR / BPS Guide to PHARMACOLOGY Target Classification



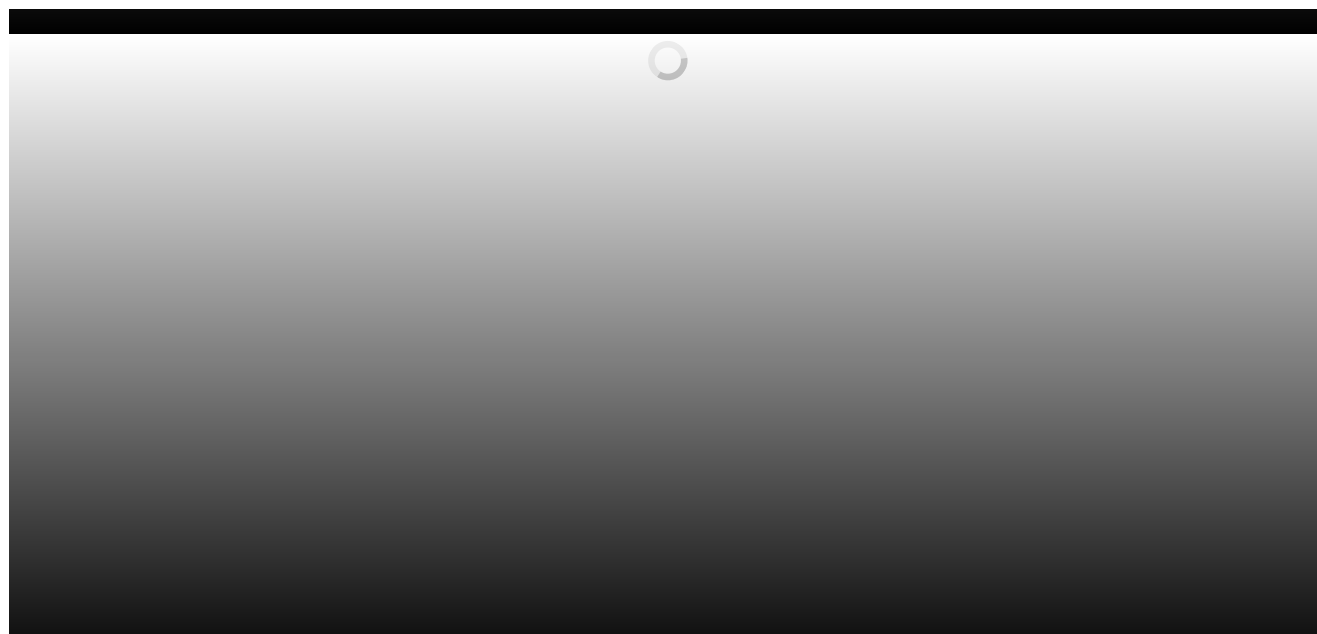
▶ IUPHAR/BPS Guide to PHARMACOLOGY

14.5 ChEMBL Target Tree



▶ ChEMBL

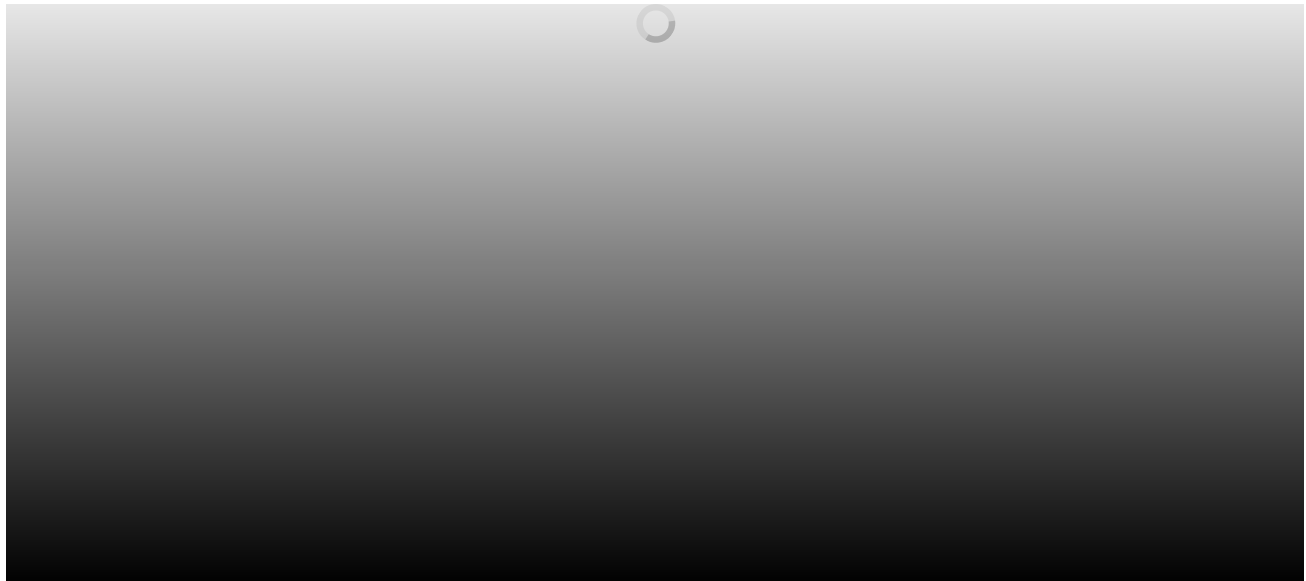
14.6 UN GHS Classification



▶ GHS Classification (UNECE)

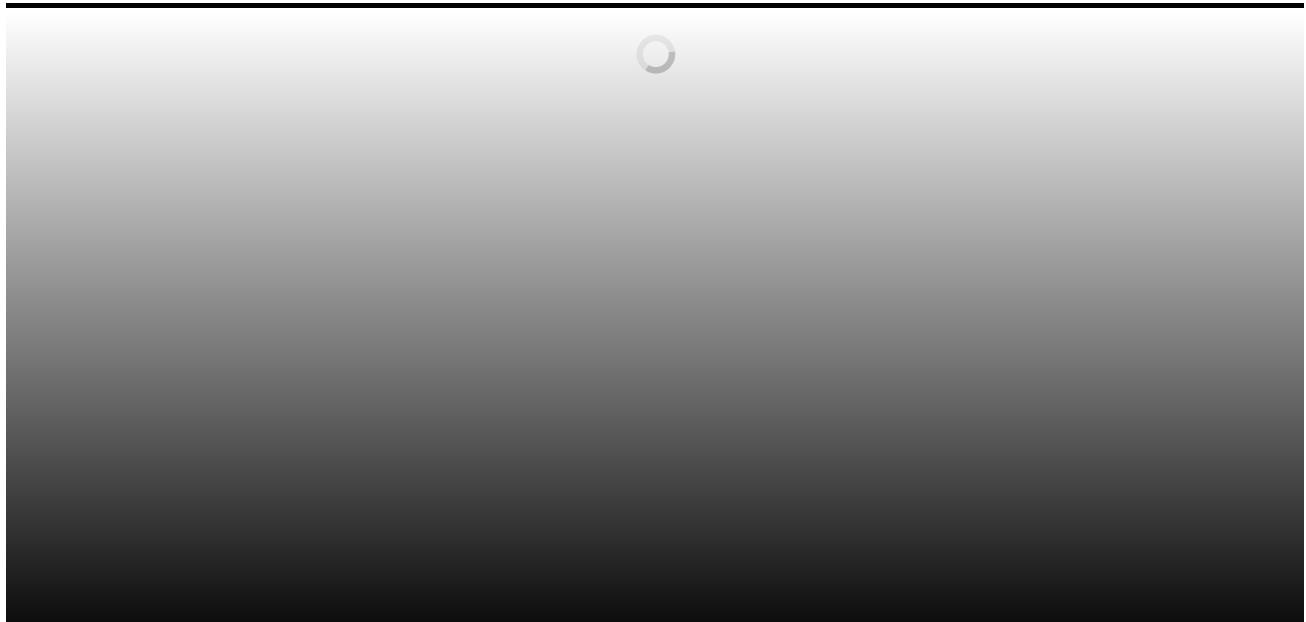
14.7 NORMAN Suspect List Exchange Classification





▶ NORMAN Suspect List Exchange

14.8 EPA DSSTox Classification



▶ EPA DSSTox

15 Information Sources



FILTER BY SOURCE

ALL SOURCES



1. CAS Common Chemistry

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Endoxifen

https://commonchemistry.cas.org/detail?cas_rn=112093-28-4

2. ChemIDplus

LICENSE

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

Endoxifen

<https://pubchem.ncbi.nlm.nih.gov/substance/?source=chemidplus&sourceid=0112093284>

ChemIDplus Chemical Information Classification

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

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Z-Endoxifen

<https://dtp.cancer.gov/dtpstandard/servlet/dwindex?searchtype=NSC&outputformat=html&searchlist=749798>

Endoxifen

<https://dtp.cancer.gov/dtpstandard/servlet/dwindex?searchtype=NSC&outputformat=html&searchlist=746494>

4. EPA DSSTox

LICENSE

<https://www.epa.gov/privacy/privacy-act-laws-policies-and-resources>

(Z)-Endoxifen

<https://comptox.epa.gov/dashboard/DTXSID80149880>

CompTox Chemicals Dashboard Chemical Lists

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

5. European Chemicals Agency (ECHA)

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<https://echa.europa.eu/web/guest/legal-notice>

4-[(1Z)-1-[4-[2-(methylamino)ethoxy]phenyl]-2-phenyl-1-buten-1-yl]phenol

<https://echa.europa.eu/substance-information/-/substanceinfo/100.208.548>

4-(1-{4-[2-(methylamino)ethoxy]phenyl}-2-phenylbut-1-en-1-yl)phenol

<https://echa.europa.eu/substance-information/-/substanceinfo/100.236.644>

808-709-4

<https://echa.europa.eu/information-on-chemicals/cl-inventory-database/-/discli/details/245913>

4-[(1Z)-1-[4-[2-(methylamino)ethoxy]phenyl]-2-phenyl-1-buten-1-yl]phenol (EC: 683-027-6)

<https://echa.europa.eu/information-on-chemicals/cl-inventory-database/-/discli/details/213563>

6. FDA Global Substance Registration System (GSRS)

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

ENDOXIFEN

<https://gsrs.ncats.nih.gov/ginas/app/beta/substances/46AF8680RC>

7. ChEBI

4-Hydroxy-N-desmethyltamoxifen

<https://www.ebi.ac.uk/chebi/searchId.do?chebiId=CHEBI:80555>

ChEBI Ontology

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

8. ChEMBL

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13. Therapeutic Target Database (TTD)

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25. PubChem

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26. **Medical Subject Headings (MeSH)**

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<https://www.ncbi.nlm.nih.gov/mesh/67055492>

MeSH Tree

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

27. **GHS Classification (UNECE)**

GHS Classification Tree

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28. **PATENTSCOPE (WIPO)**

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