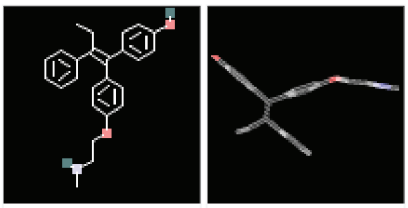
PubChem

COMPOUND SUMMARY

Endoxifen

Cite | Download

PubChem CID	10090750
Structure	 2D 3D
Chemical Safety	Irritant Health Hazard 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.

ChEBI

Contents

Title and Summary

1 Structures

2 Names and Identifiers

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8 Safety and Hazards

9 Associated Disorders and Diseases

10 Literature

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12 Interactions and Pathways

13 Biological Test Results

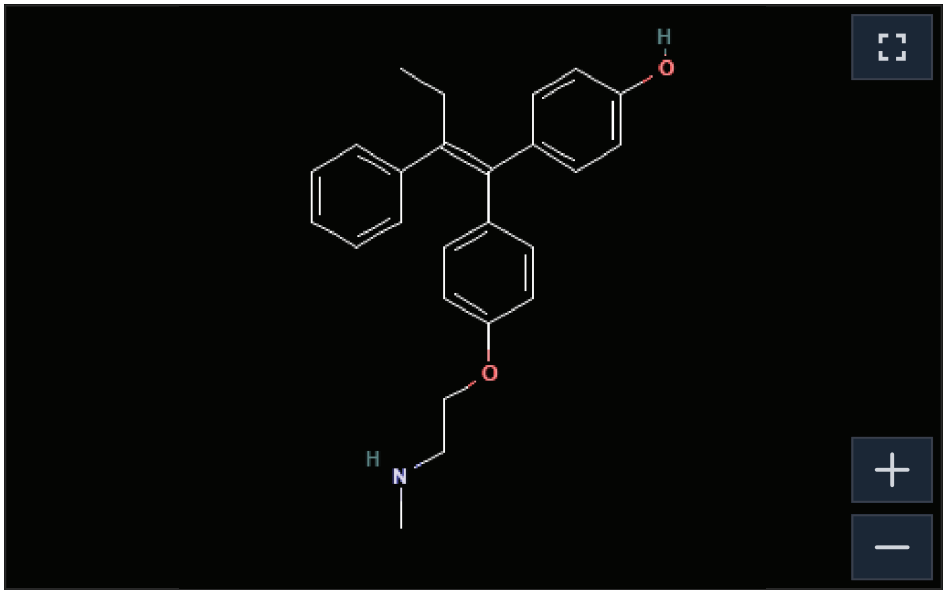
14 Classification

15 Information Sources

1 Structures

1.1 2D Structure

Chemical Structure Depiction



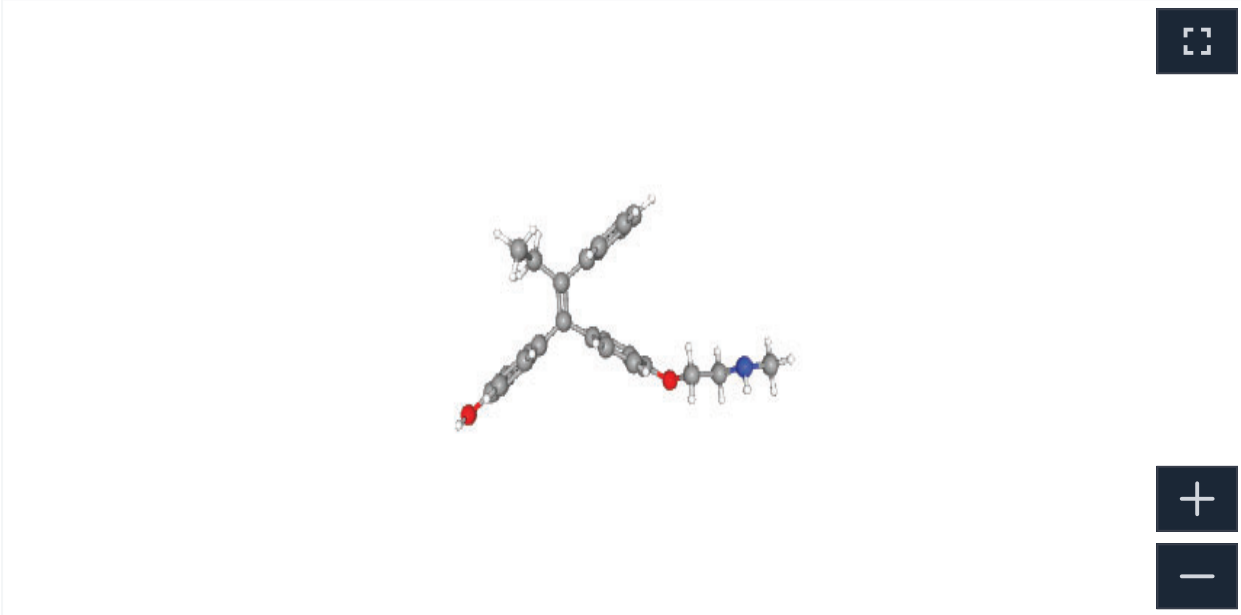
PubChem

1.2 3D Conformer

Interactive Chemical Structure Model

Ball and Stick Sticks Wire-Frame Space-Filling

Show Hydrogens Animate



First Previous Conformer 1 of 6 Next Last

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

$C_{25}H_{27}NO_2$

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

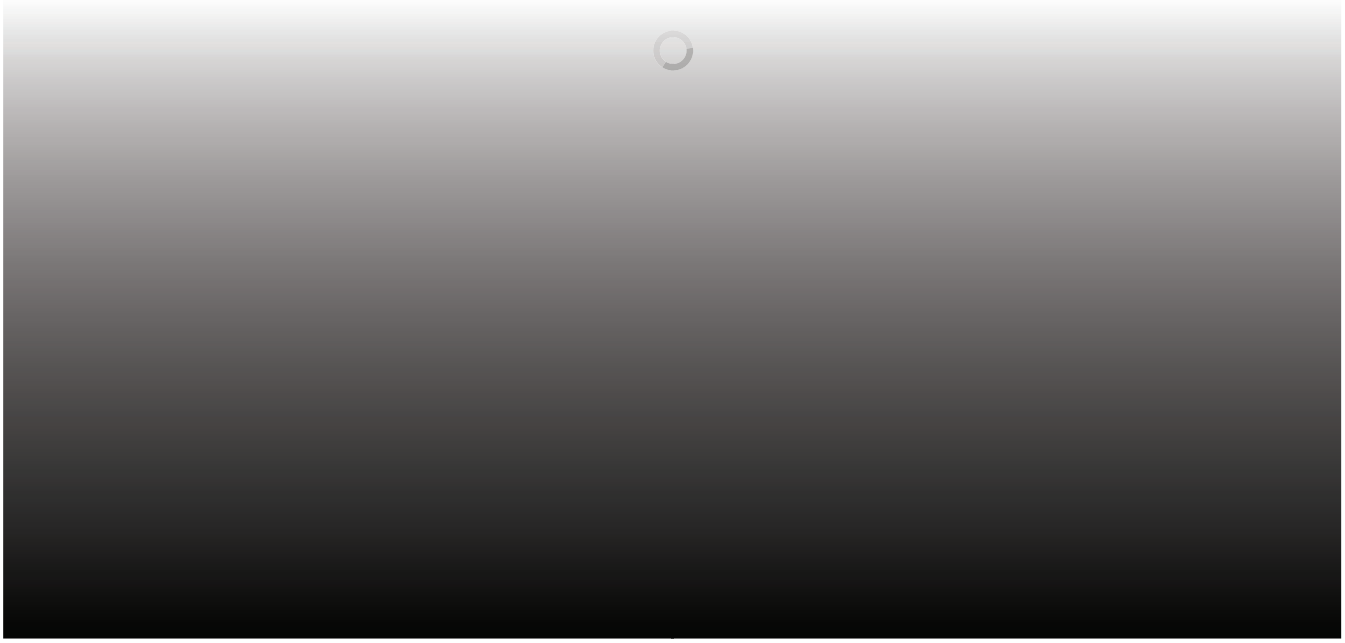
4.3 Substances

4.3.1 Related Substances

All Count	215
Same Count	117
Mixture Count	98

PubChem

4.3.2 Substances by Category



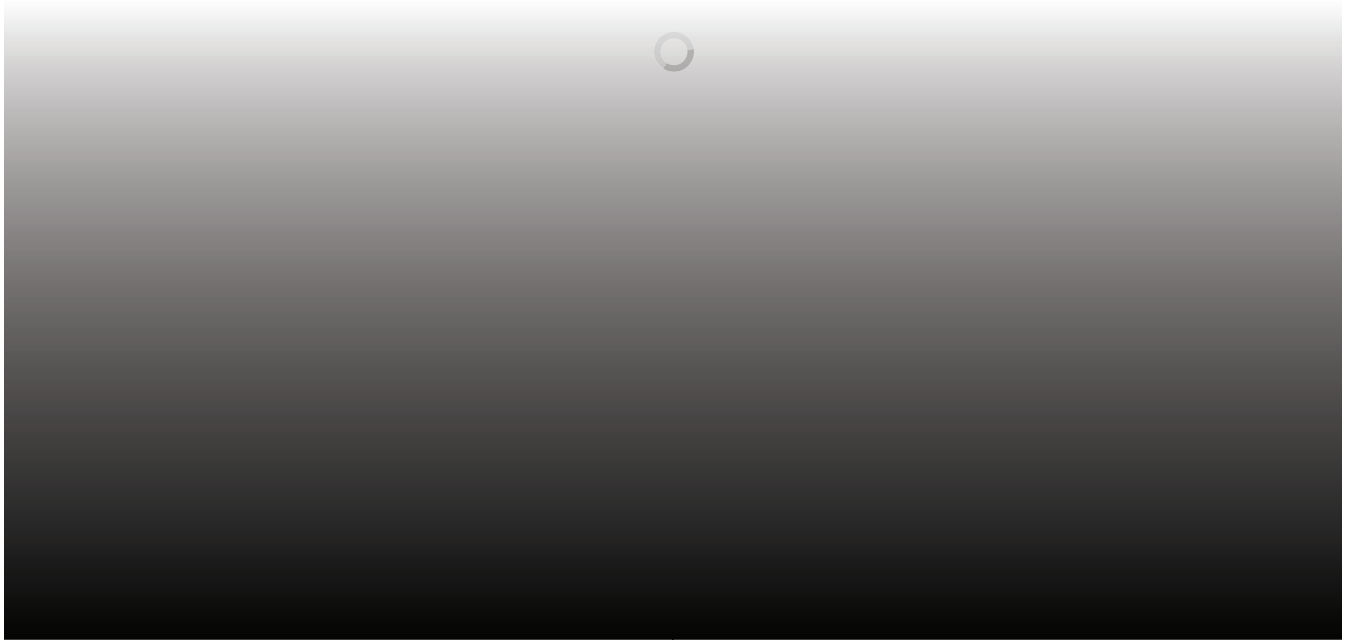
PubChem

4.4 Entrez Crosslinks

PubMed Count	16
Taxonomy Count	2
Gene Count	17

PubChem

5 Chemical Vendors

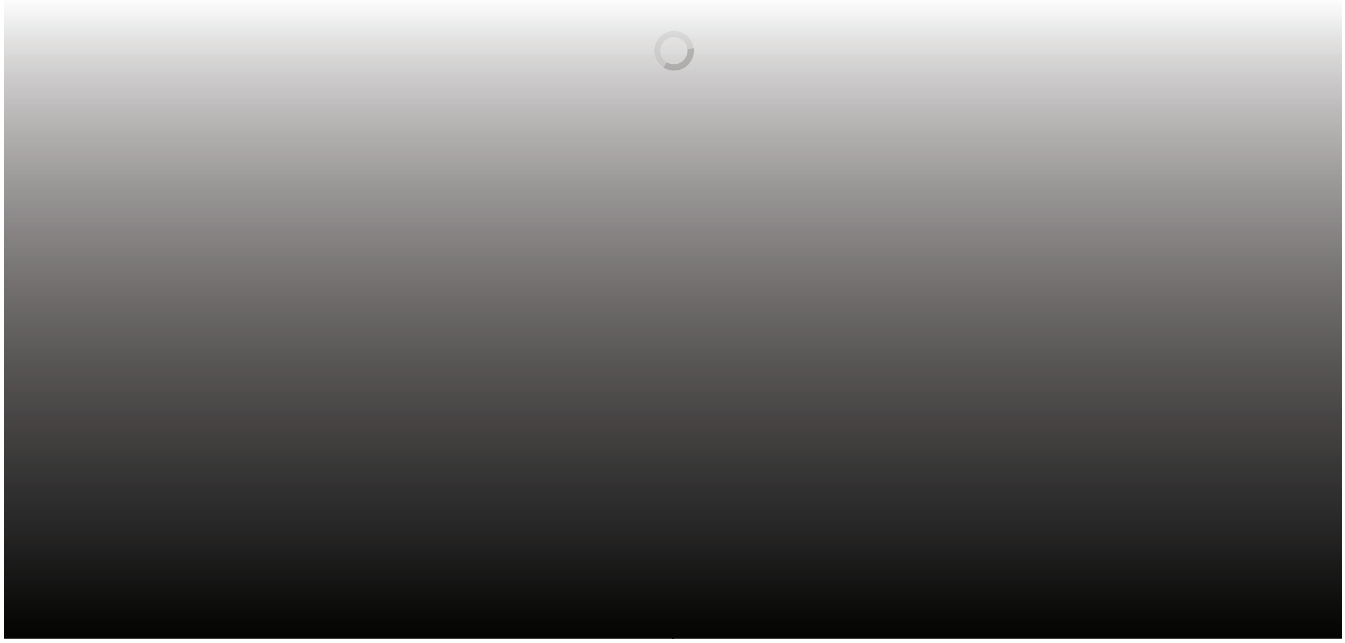


- PubChem

6 Drug and Medication Information

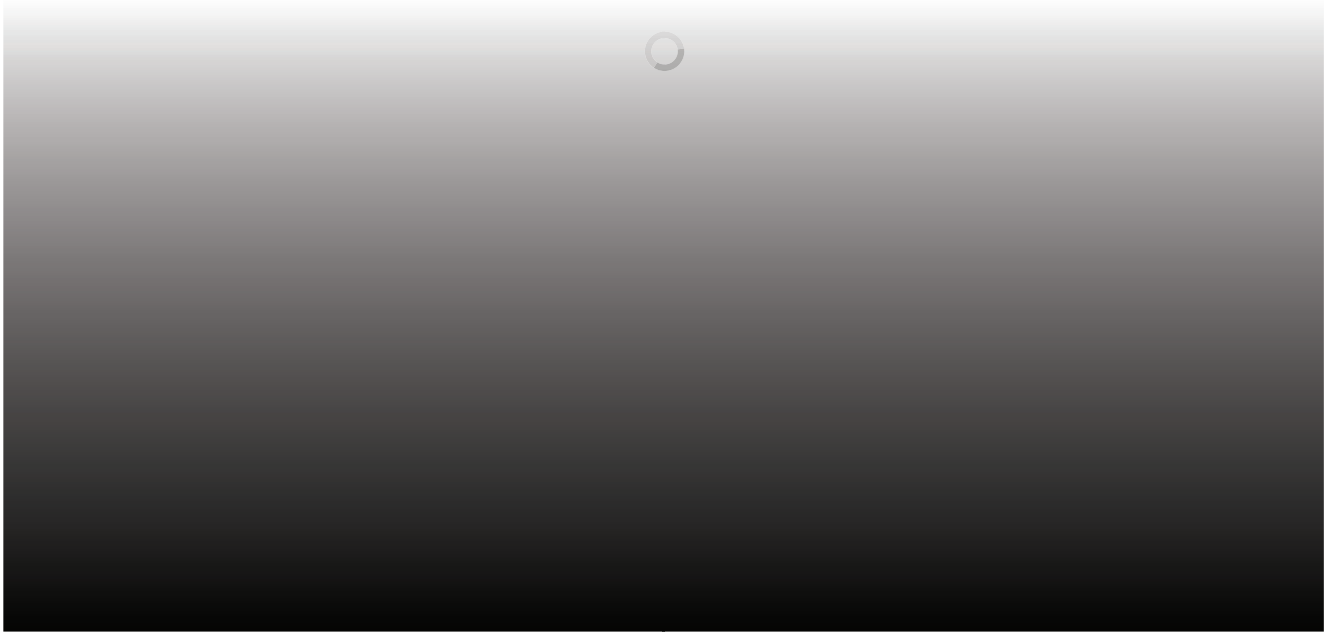
6.1 Clinical Trials

6.1.1 ClinicalTrials.gov



- 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

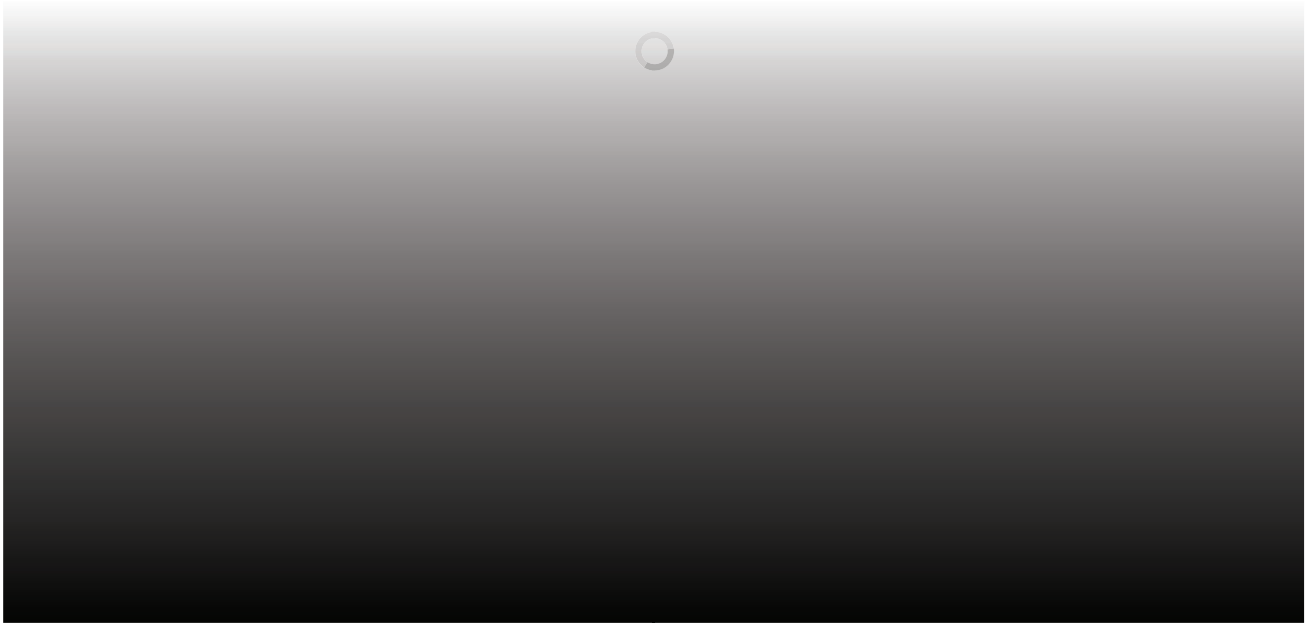
- Human Metabolome Database (HMDB)

7.2.3 Metabolite Pathways

Tamoxifen Action Pathway
Tamoxifen Metabolism Pathway

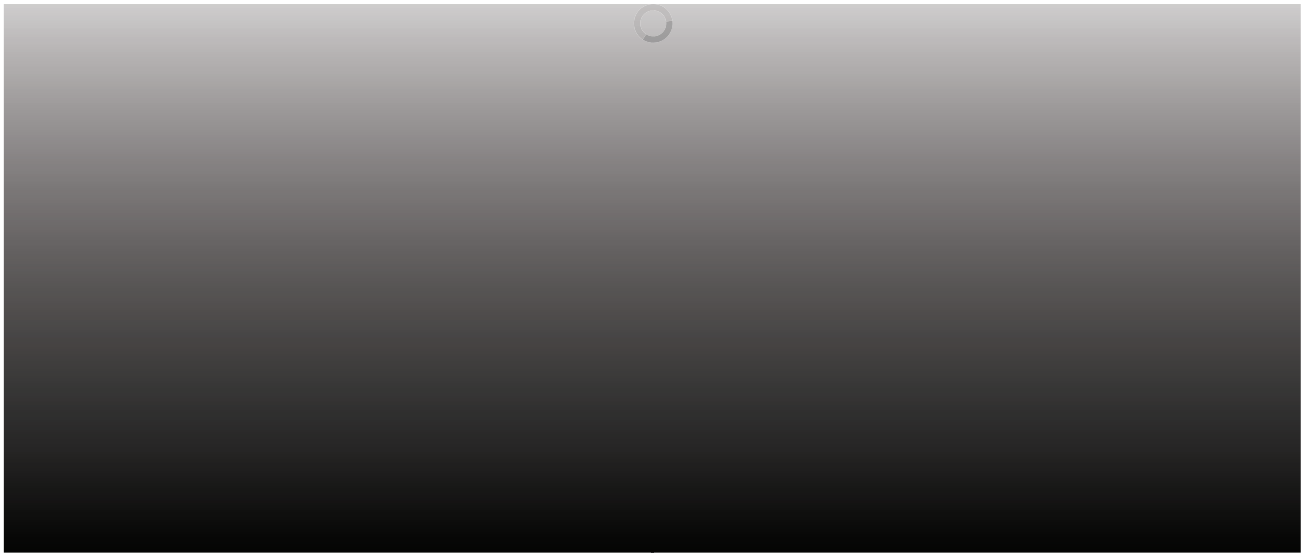
- Human Metabolome Database (HMDB)

7.3 Biochemical Reactions

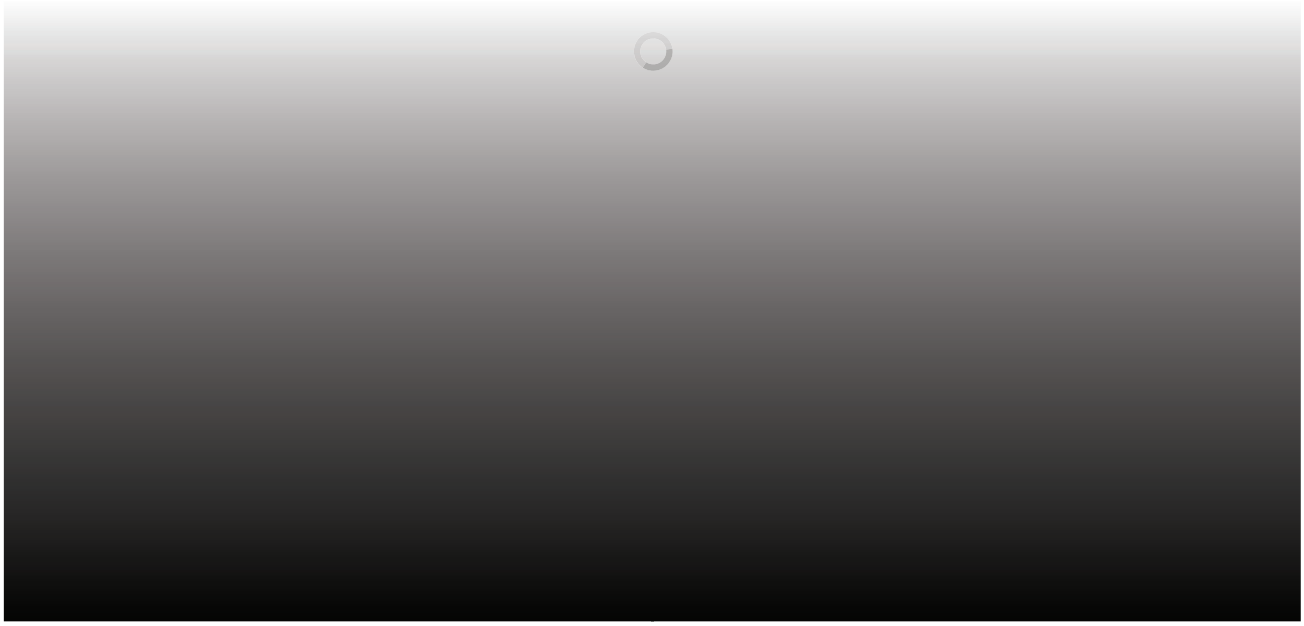


- PubChem

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)	
Signal	Warning
GHS Hazard Statements	H302+H312+H332 (97.4%): Harmful if swallowed, in contact with skin or if inhaled [Warning Acute toxicity, oral; acute toxicity, dermal; acute toxicity, inhalation] H302 (100%): Harmful if swallowed [Warning Acute toxicity, oral] H312 (100%): Harmful in contact with skin [Warning Acute toxicity, dermal] H332 (100%): Harmful if inhaled [Warning Acute toxicity, inhalation] H361 (100%): Suspected of damaging fertility or the unborn child [Warning Reproductive toxicity] H413 (100%): May cause long lasting harmful effects to aquatic life [Hazardous to the aquatic environment, long-term hazard]
Precautionary Statement Codes	P203, P261, P264, P270, P271, P273, P280, P301+P317, P302+P352, P304+P340, P317, P318, P321, P330, P362+P364, P405, and P501 (The corresponding statement to each P-code can be found at the GHS Classification page.)
ECHA C&L Notifications Summary	*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.* *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.*

- 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

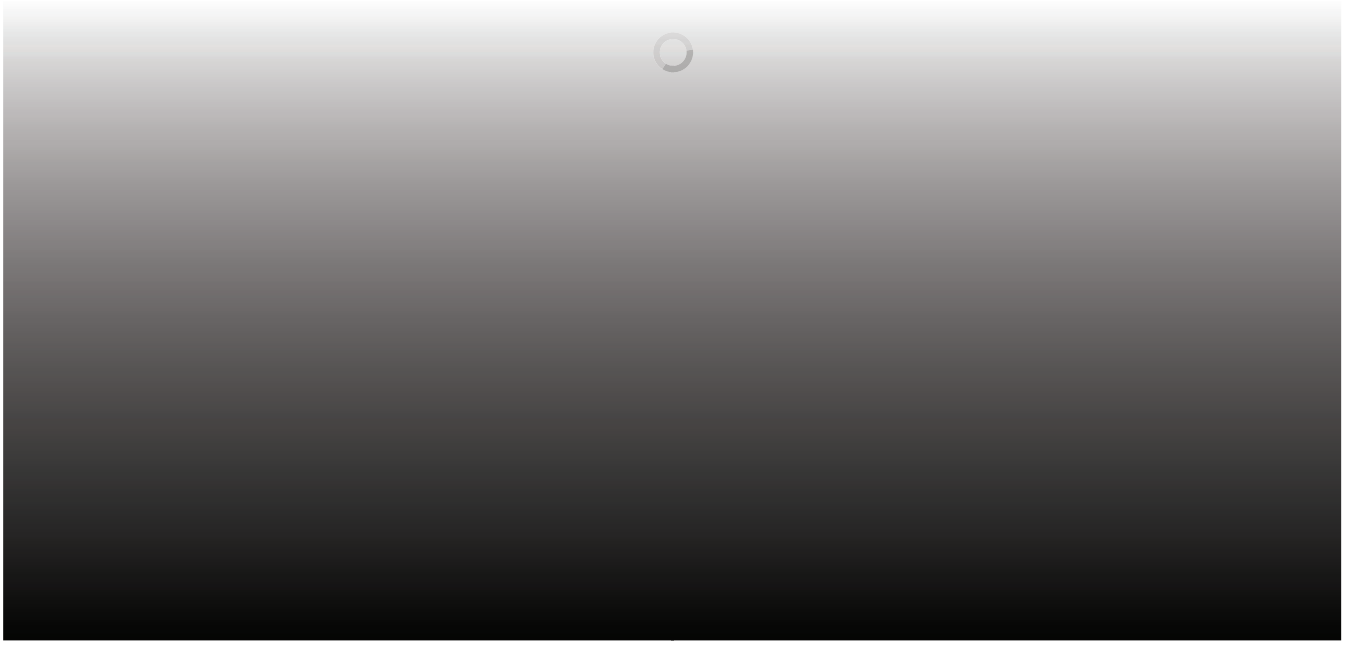
- Therapeutic Target Database (TTD)

10 Literature

10.1 Consolidated References

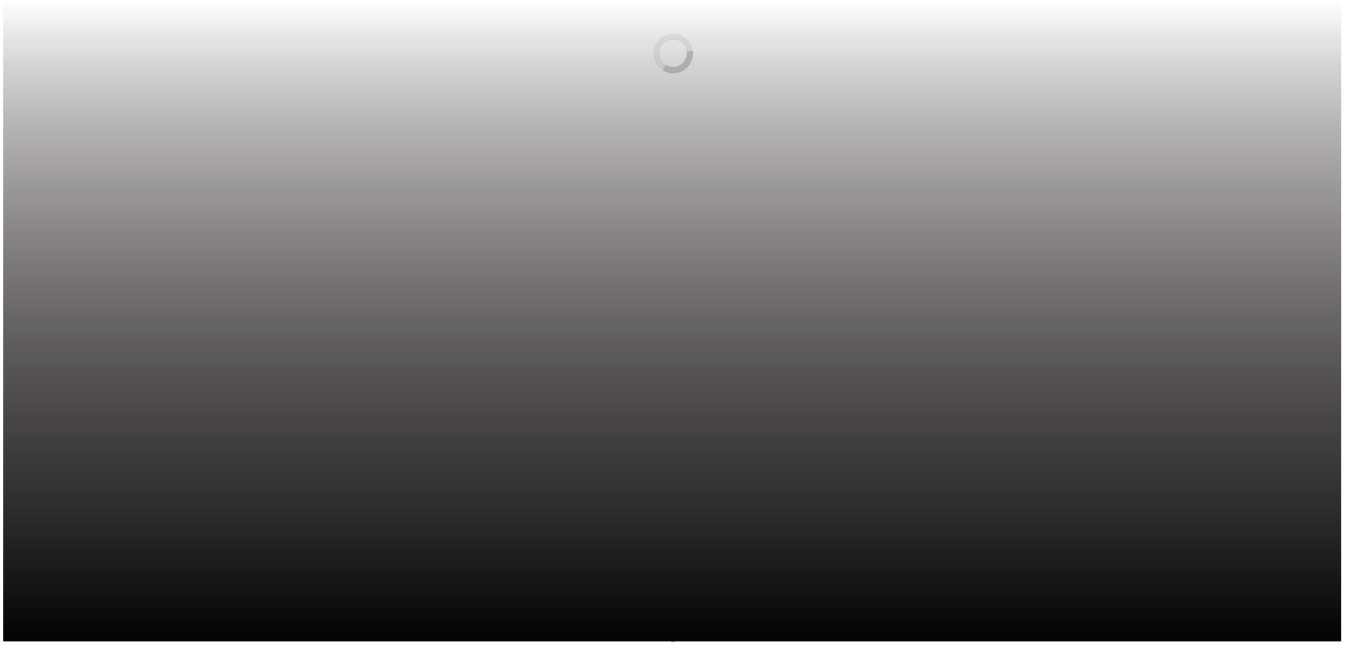
PubChem

10.2 NLM Curated PubMed Citations



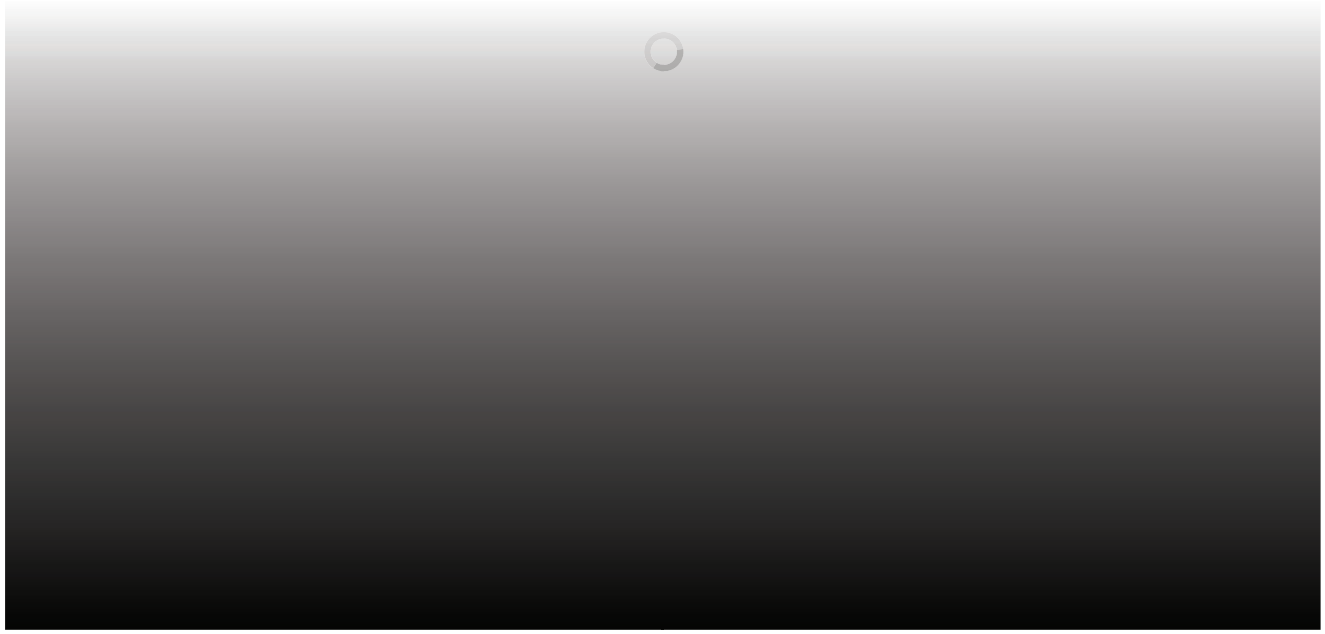
PubChem

10.3 Springer Nature References



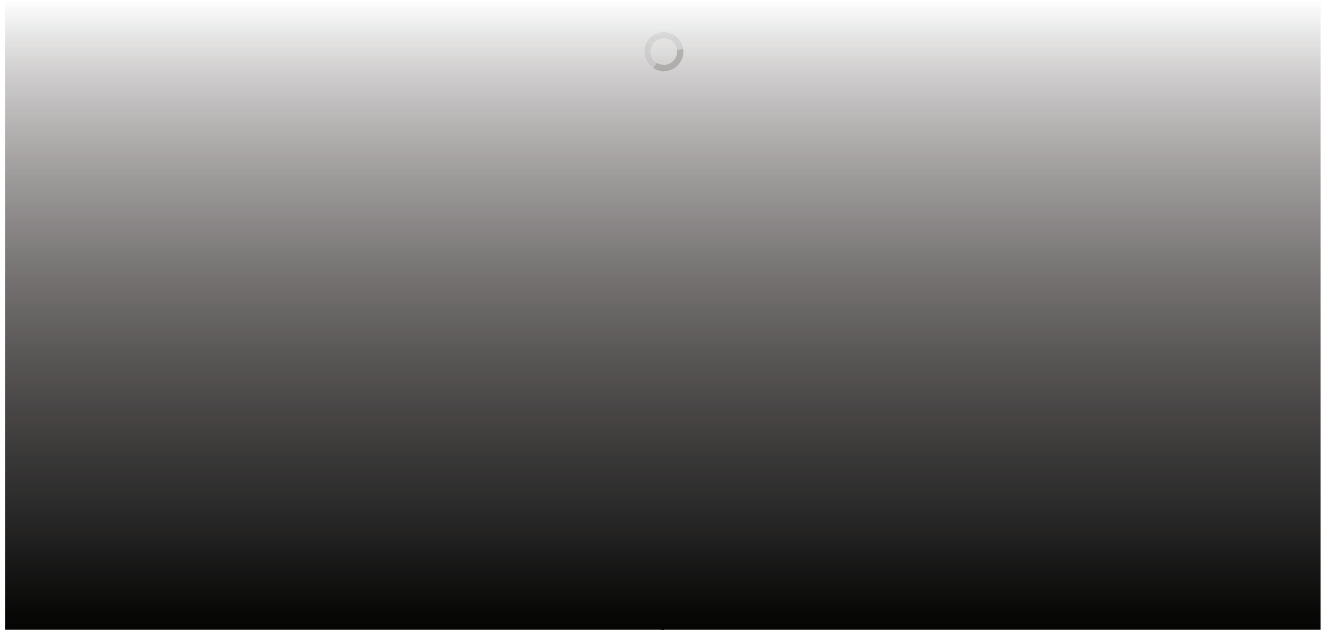
Springer Nature

10.4 Chemical Co-Occurrences in Literature



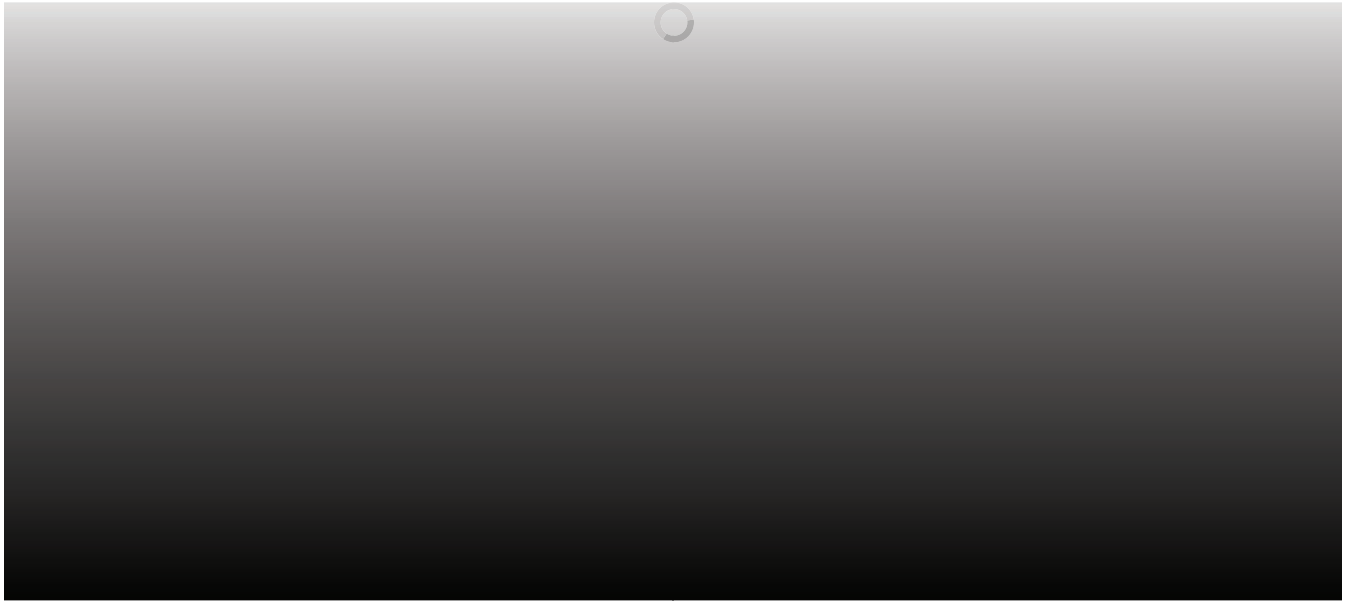
PubChem

10.5 Chemical-Gene Co-Occurrences in Literature



PubChem

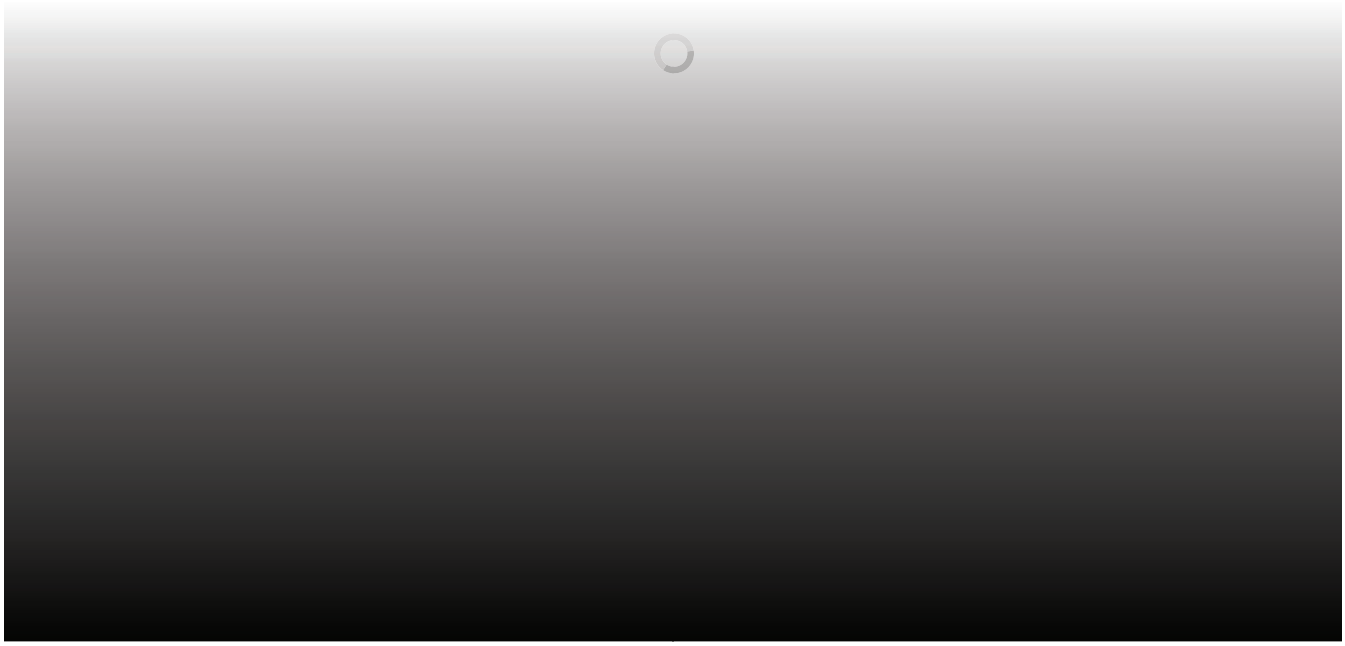
10.6 Chemical-Disease Co-Occurrences in Literature



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

[redacted]

- 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

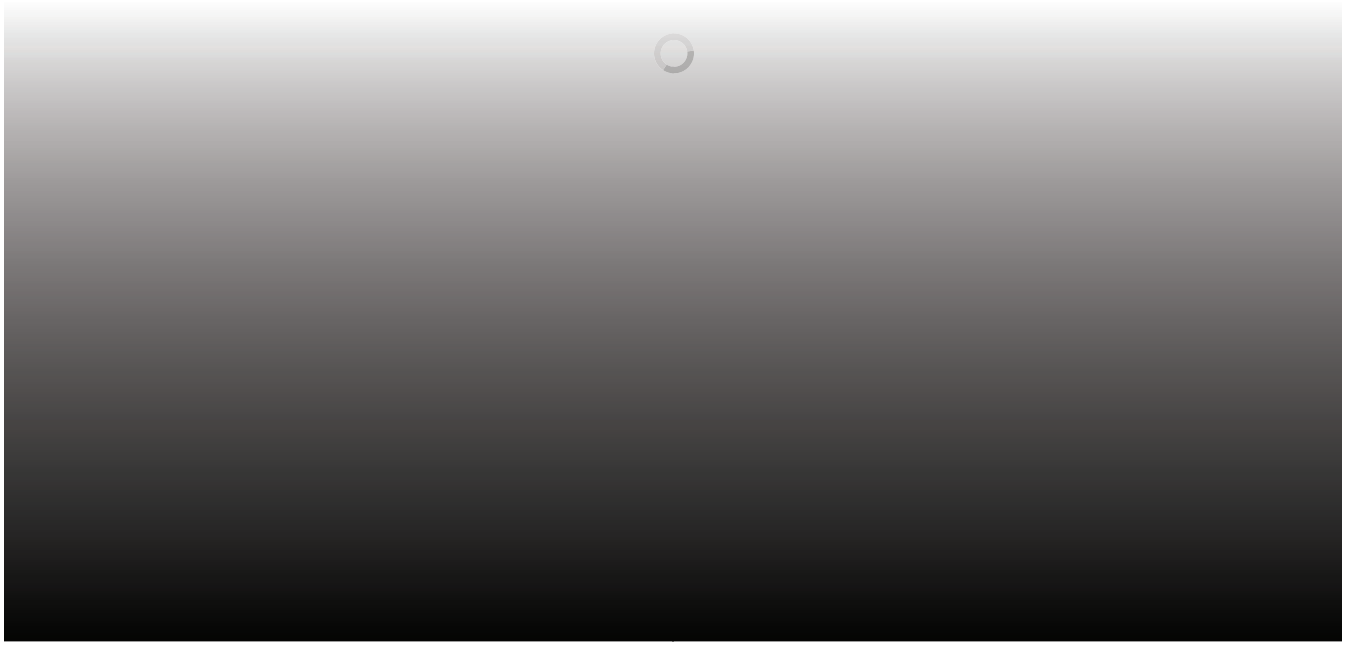
13 Biological Test Results

13.1 BioAssay Results

- PubChem

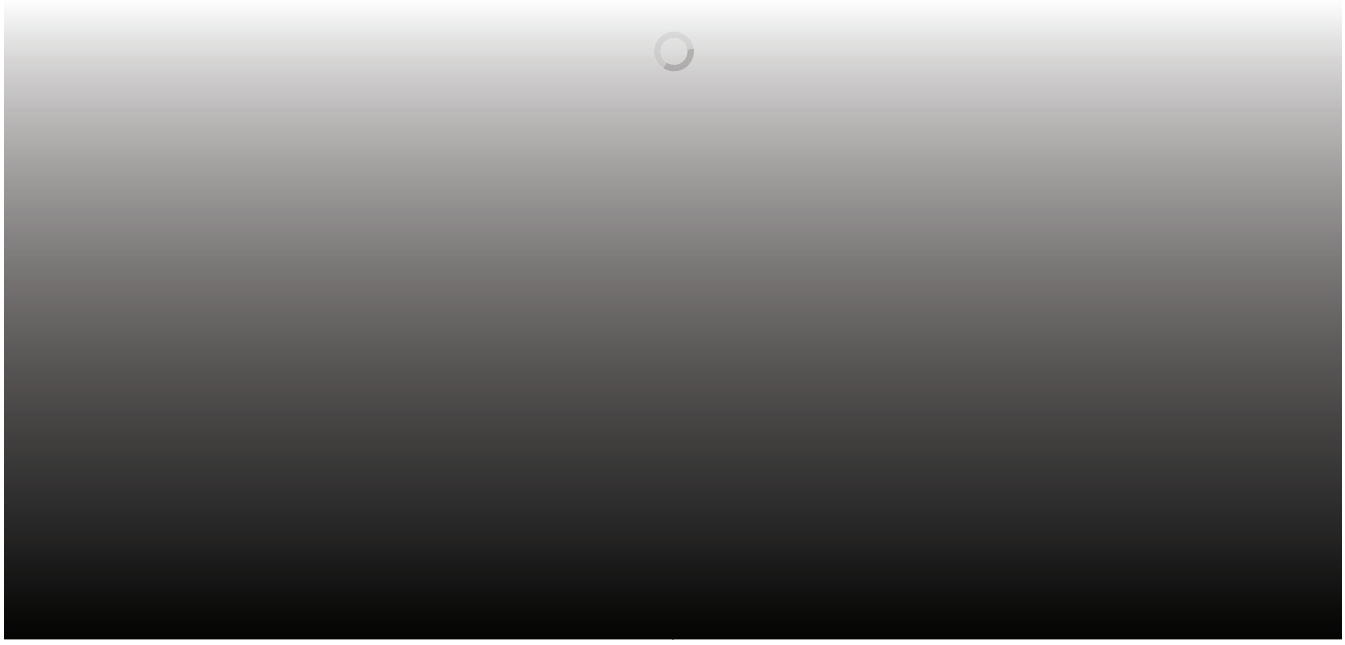
14 Classification

14.1 MeSH Tree



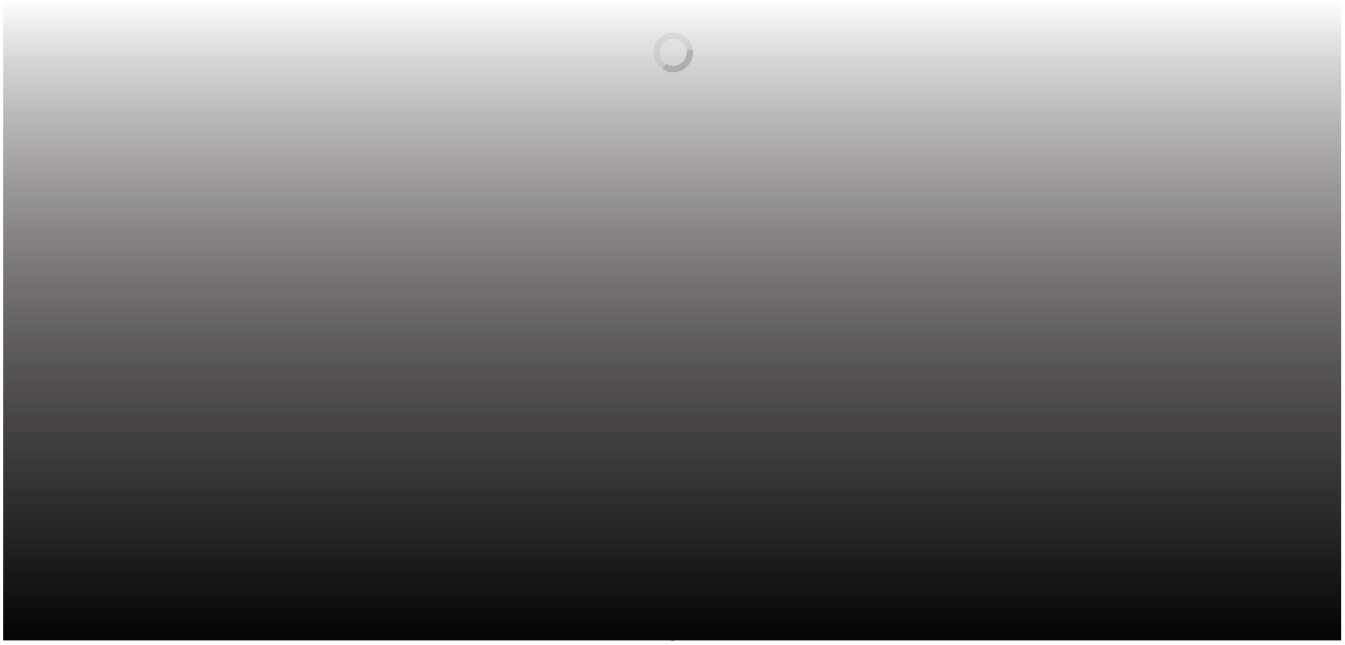
- Medical Subject Headings (MeSH)

14.2 ChEBI Ontology



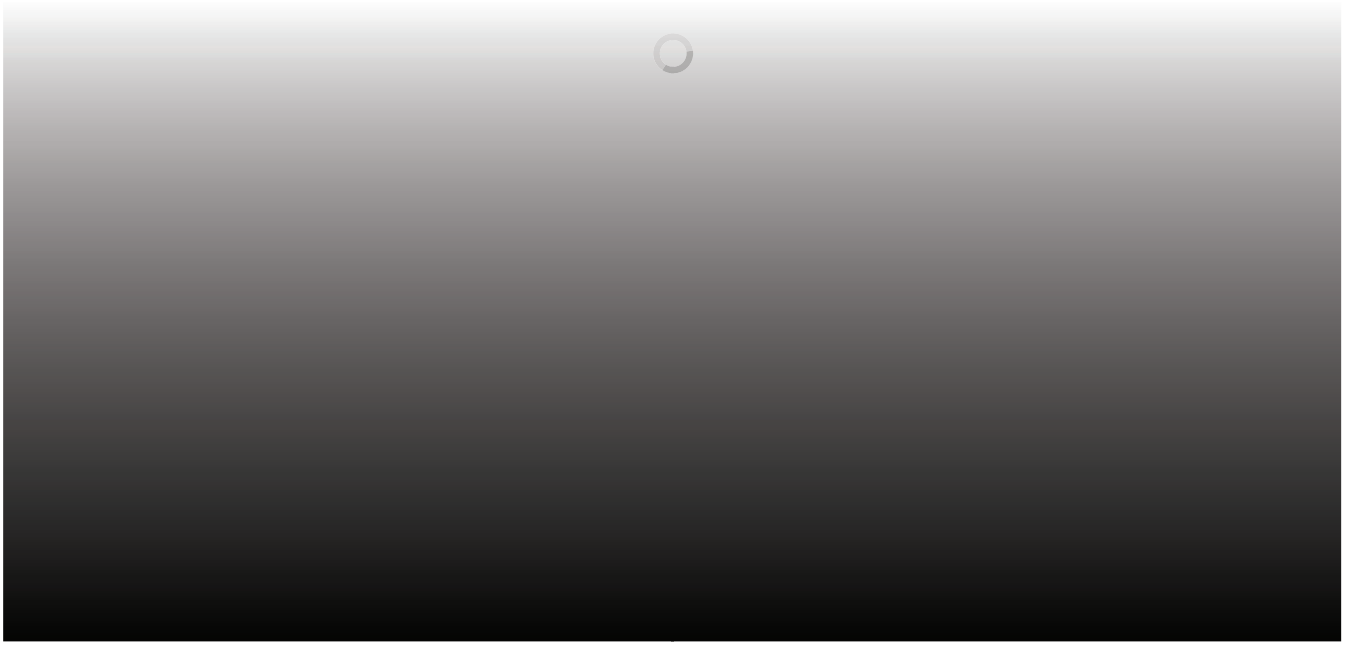
- ChEBI

14.3 ChemIDplus



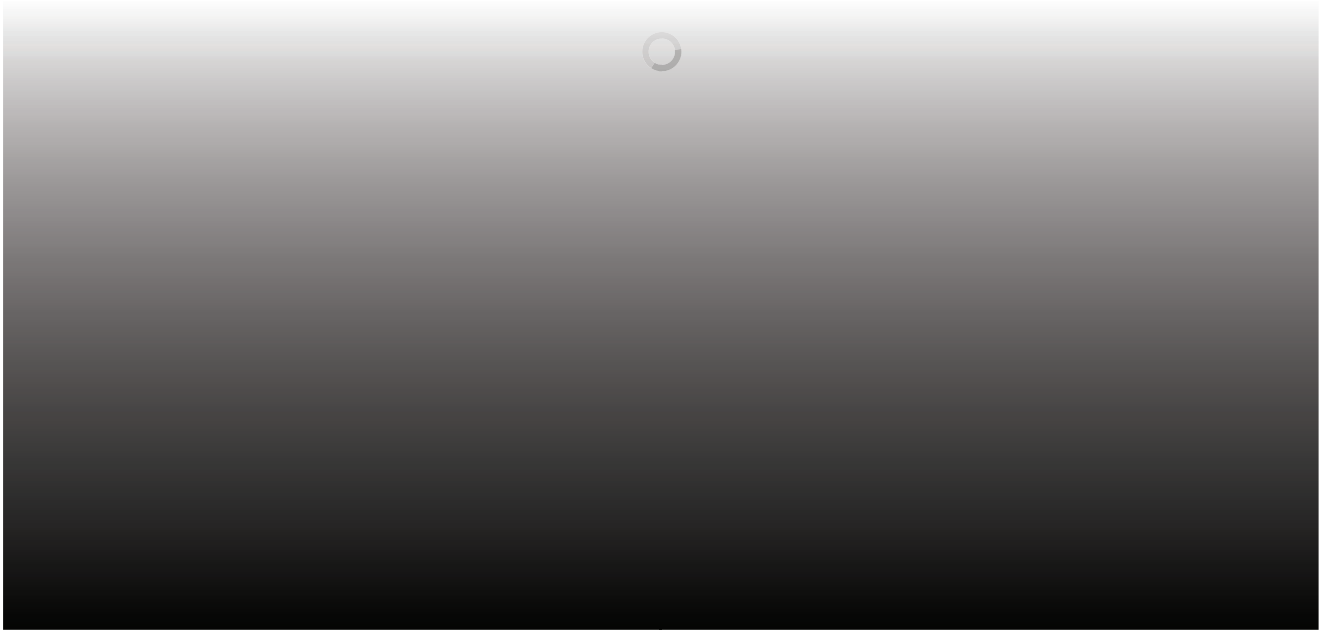
- ChemIDplus

14.4 IUPHAR / BPS Guide to PHARMACOLOGY Target Classification



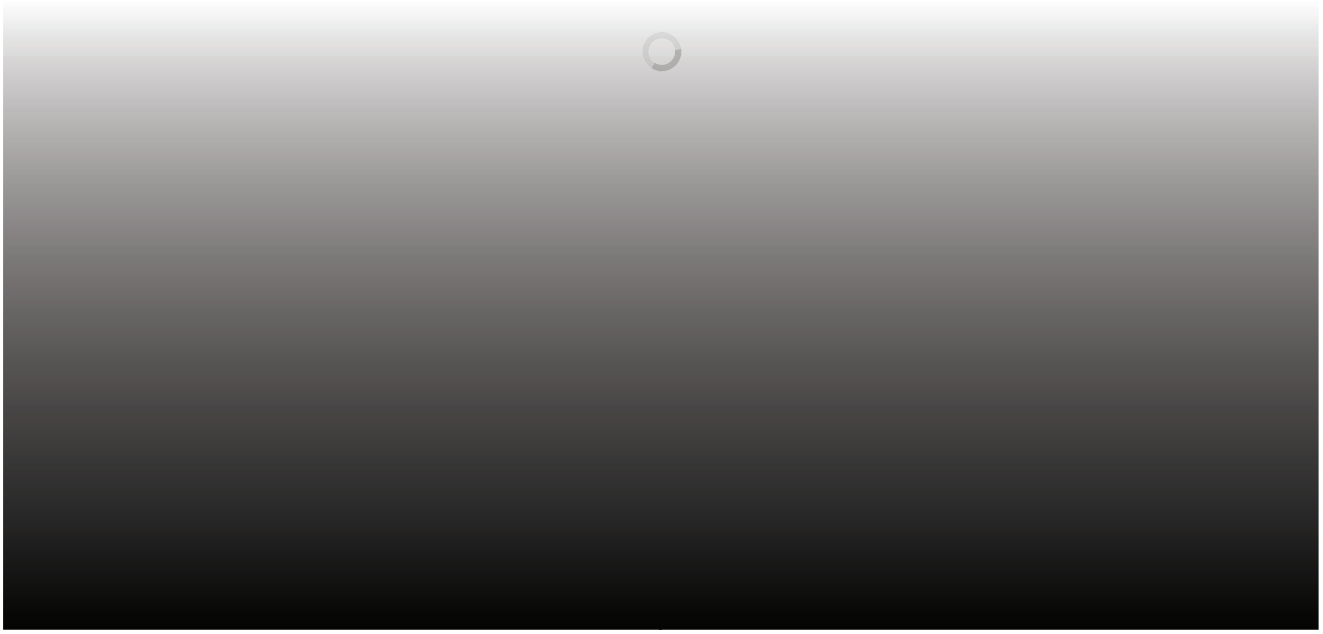
- IUPHAR/BPS Guide to PHARMACOLOGY

14.5 ChEMBL Target Tree



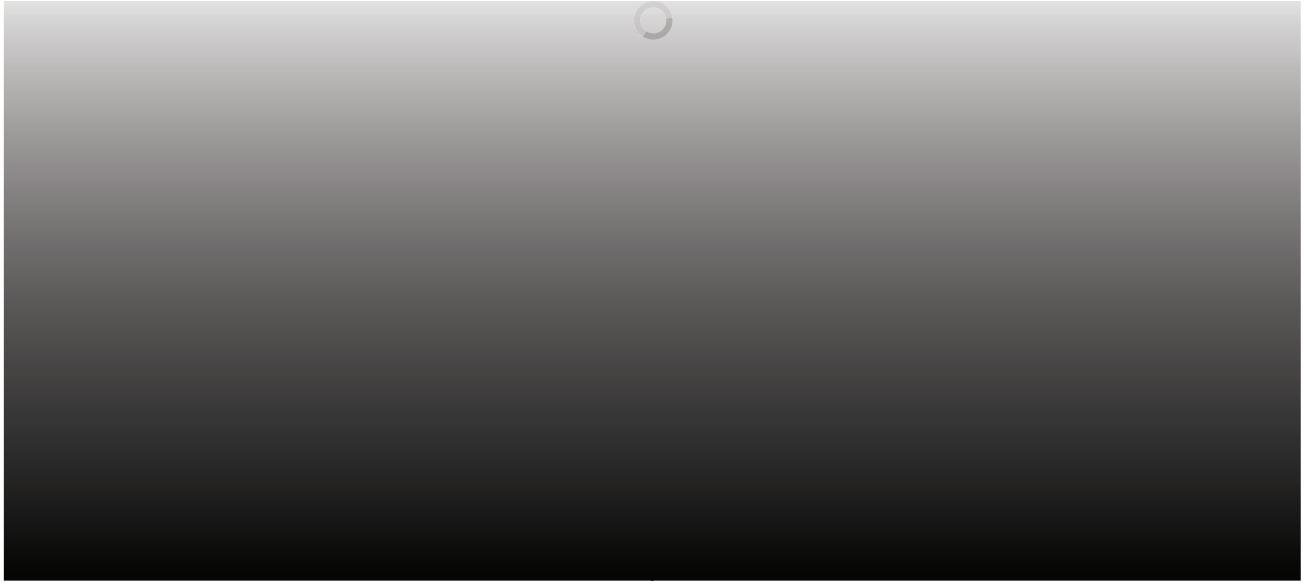
- ChEMBL

14.6 UN GHS Classification



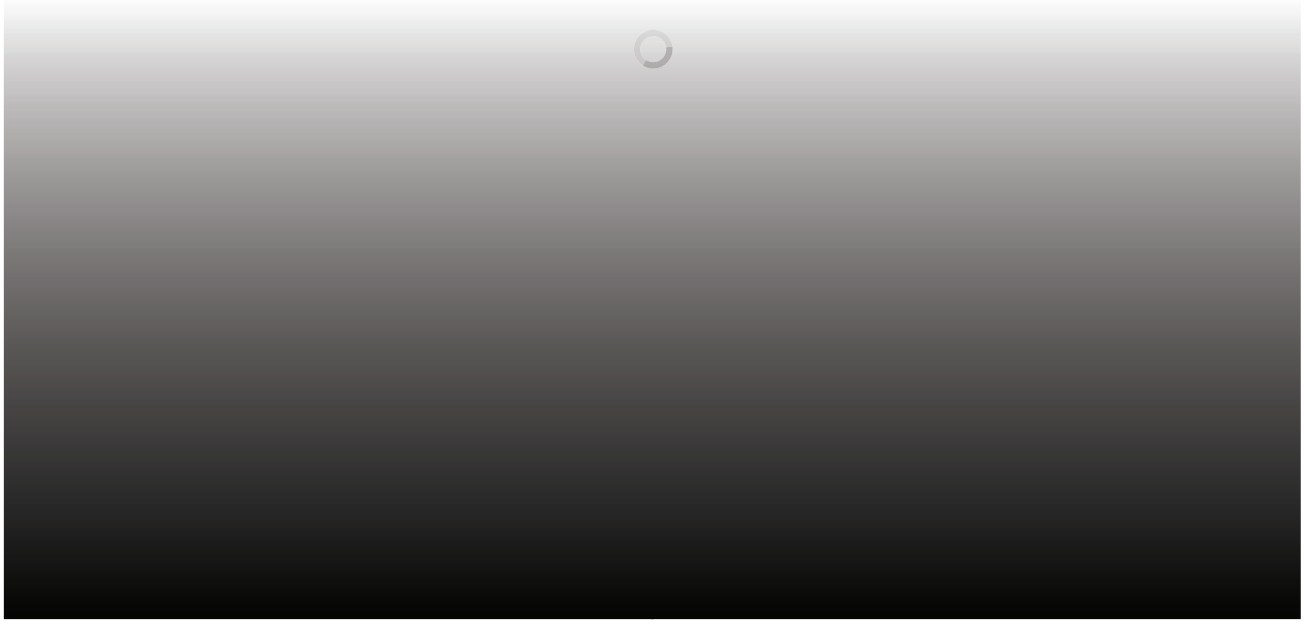
- GHS Classification (UNECE)

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

LICENSE
The data from CAS Common Chemistry is provided under a CC-BY-NC 4.0 license, unless otherwise stated.
https://creativecommons.org/licenses/by-nc/4.0/

Endoxifen

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

2. ChemIDplus

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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

3. DTP/NCI

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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://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

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http://www.ebi.ac.uk/Information/termsofuse.html

https://www.ebi.ac.uk/chembl/compound_report_card/CHEMBL1093458/

ChEMBL Protein Target Tree

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

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NORMAN Suspect List Exchange Classification

https://www.norman-network.com/nds/SLE/

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https://www.guidetopharmacology.org/GRAC/LigandDisplayForward?ligandId=10203

Guide to Pharmacology Target Classification

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

13. Therapeutic Target Database (TTD)

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https://idrblab.net/ttd/data/drug/details/D0W4EB

14. EU Clinical Trials Register

https://www.clinicaltrialsregister.eu/

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http://www.hmdb.ca/citing

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http://www.hmdb.ca/metabolites/HMDB0060666

16. Japan Chemical Substance Dictionary (Nikkaji)

http://jglobal.jst.go.jp/en/redirect?Nikkaji_No=J1.507.991F

http://jglobal.jst.go.jp/en/redirect?Nikkaji_No=J393.650C

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http://www.ebi.ac.uk/pdbe-srv/pdbechem/chemicalCompound/show/9XY

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

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4-hydroxy-N-desmethyltamoxifen

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

http://www.unece.org/trans/danger/publi/ghs/ghs_welcome_e.html

28. PATENTSCOPE (WIPO)

SID 391753311

https://pubchem.ncbi.nlm.nih.gov/substance/391753311