

NLM Division of Specialized Information Services

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ChemIDplus

- Over 400,000 chemicals covered
 - Lite and Advanced interfaces
- Covers chemicals with biomedical activity
- Points to over 100 sources of more information
- Name, formula, structure display and searching
 - Spell checking of input names
 - InChI, InChIKey and SMILES creation
 - Substructure , similarity, and identity searching



Recent ChemIDplus changes

- Search Engine sitemap created
 - All ChemIDplus records indexed in Google
 - Updates to sitemap weekly
- Switch to JavaScript chemical draw and display
 - Speed of loading pages greatly improved
 - Marvin for JavaScript for 2D input and output
 - JSMol for 3D display (coming).
- Improved mobile use
- New browse feature .. “starts with”
- Automatic updates to PubChem



Current SIS Drug Information

- NLM Drug Information Portal
 - <http://druginfo.nlm.nih.gov>
- Over 50,000 drug records
- Data stored in ChemIDplus
- Covers NLM and other US Government resources
- Coverage starts with Clinical Trials
- Monitor drug data including Twitter, ListServes, Web
- Searchable by name and category
 - Spell checking, autosuggest, embedded drug names

List of Resources Searched

Summary

- ▶ [i](#) Summary of drug information (MedlinePlusDrug)
- ▶ [i](#) Summary of dietary supplement and herbal information (MedlinePlusSupp)
- ▶ [i](#) Summary of consumer health information (MedlinePlusTopics)
- ▶ [i](#) Summary of HIV/AIDS treatment (AIDSinfo)
- ▶ [i](#) Summary of the effect on breastfeeding (LactMed)
- ▶ [i](#) Summary of Drug-Induced Liver Injury (LiverTox)
- ▶ [i](#) Manufacturers drug label (DailyMed)
- ▶ [i](#) Summary of ingredients and label information (Dietary Supplements Labels Database)
- ▶ [i](#) Clinical trials (ClinicalTrials.gov)
- ▶ [i](#) Drug Identification and Image Display (Pillbox *beta*)

Detailed Summary

- ▶ [i](#) Summary of reviewed biological and physical data (HSDB)
- ▶ [i](#) References from scientific journals (Medline/PubMed)
- ▶ [i](#) References from toxicological journals (TOXLINE)
- ▶ [i](#) Biological activities and chemical structures (PubChem)
- ▶ [i](#) Biological activities against HIV/AIDS and other viruses (NIAID ChemDB)
- ▶ [i](#) Toxicological and chemical resources (ChemIDplus)

Additional Resources

- ▶ [i](#) Information from the US Food & Drug Administration (Drugs@FDA)
- ▶ [i](#) Information from the US Drug Enforcement Administration (DEA)
- ▶ [i](#) Search engine for other government resources (USA.gov)



Recent NLM Drug Portal Changes

- FDA Substance Registration System (SRS) search
 - FDA SRS replaced regularly
 - UNII and names going to the Drug Portal
 - Names lower cased by algorithm
 - Structure exchange between NLM and FDA
- Addition of new sources to the Drug Portal
 - LiverTox
 - Dietary Supplements Label Database
 - Medline Health (coming)
- Weekly transfer of drug names into SIS web site search
- Mobile version improved



FDA Substance Registry Search

- Hosted by NLM (<http://fdasis.nlm.nih.gov>)
- Covers over 62,000 substances
 - Drugs, additives
 - Biologics, devices
- Searchable by Name and UNII
- Spell checker, autosuggest
- Links out to ChemIDplus, Drug Portal, ITIS, NCBI Taxonomy, NCI Thesaurus, USDA Plants
- InChIKey used to search the web



Collaborative Efforts

- FDA SRS
- PubChem
- ClinicalTrials.gov
- EPA SRS
- Comparative Toxicogenomics Database
- Chemical Entities of Biological Interest
- AIDInfo
- LiverTox
- PillBox
- NCI CADD group (Marc Nicklaus)