

Chemistry Resources of Interest

This list is maintained by [Jeff Christoff](#) and was last updated on 8-12-2004. Suggestions for changes are encouraged!

Books

"Foye's Principles of Medicinal Chemistry, Fifth Edition", David A. Williams, and Thomas L. Lemke, Editors, Lippincott, Williams, and Wilkins, Baltimore, (2002), 1114 pages.

For a review, please see Lien, E.J. Am. J. Pharm, Ed., 2002, 66(3), 344-345.

"Medicinal Chemistry Case Study Workbook", Bruce L. Currie, Victoria F. Roche, and S. William Zito, Editors, Lippincott, Williams, and Wilkins, Baltimore, (1996), 300 pages.

For a review, please see Matuszak, A.J. Am. J. Pharm, Ed., 1996, 60(4), 432-433.

Professional Organizations

- [American Association of Colleges of Pharmacy \(AACP\)](#)
- [American Association of Pharmaceutical Scientists \(AAPS\)](#)
- [American Pharmaceutical Association \(APhA\)](#)
- [American Association for the Advancement of Science \(AAAS\)](#)

Software

2D and 3D Drawing Programs

[ISIS/Draw](#)

What is ISIS/Draw? ISIS/Draw is a chemical drawing program used to create publication quality chemical structures and graphics using flexible drawing tools and pre-drawn structure templates and fragments. Preparing reports and presentations. Creating structure queries. Drawing structures for registration. Viewing chemical structures. You can use ISIS/Draw for these purposes and more. MDL offers this free license of ISIS/Draw for academic and personal use at home. This is not a "crippled" version, nor does it only create static GIF images. This is the complete ISIS/Draw package! Download it directly from [Free ISIS/Draw License](#).

[ChemSketch](#)

ChemSketch is another free modeling and drawing package that includes a few more features than ISIS/Draw. It includes a number of short-cut drawing features that can speed up the drawing of complex structures including nucleotide and polypeptide sequences. It can import and export to most of the common file formats (including MOL, CHM, SKC, and GIF, TIFF, and PCX) and includes a basic programming language module (ChemBasic) that allows the user to develop custom functions, templates, and preview windows. It also includes a 3D viewer that can be configured to work with both ChemSketch and ISIS/Draw as an add-in application. Some features are disabled in the freeware version and ACD does not provide user support unless you purchase the commercial version. Other add-on components include modules for calculating

logP, logD, and pKa, an NMR/IR/MS spectrum predictor, and an HPLC/GC simulator. Users must register to [download ChemSketch](#), but registration is free.

Viewers and Plug-ins

[Chemscape Chime Plug-in](#)

What is Chime? Chime is a browser plug-in that allows for the visualization of molecular structures from within your Web browser. It is a product of MDL Incorporated and is based on the RasMol program written by Roger Sayle. Molecules, usually as 3-dimensional coordinate files such as pdb, xyz, or mol, can be viewed, dynamically rotated, sized, colored, and selected to highlight areas of interest. It is free, easily installed, and is available for both the PC and Macintosh/PPC operating systems. There are several good places to learn about using Chime, including [Creating Enhanced Web Pages for Chemistry](#), [Chime Applications](#), and [New to Molecular Visualization?](#) I have created other simple examples to demonstrate how you can use Chime to augment a report or "electronic lecture": one on [Viagra®](#) and one on the [mechanism of aspirin](#).

[RasMol Viewer](#)

What is RasMol? RasMol is a molecular graphics program intended for the visualisation of proteins, nucleic acids and small molecules. The program is aimed at display, teaching and generation of publication quality images. The program was developed at the University of Edinburgh's Biocomputing Research Unit and the Biomolecular Structure Department at Glaxo Research and Development, Greenford, UK by Roger Sayle.

RasMol reads in molecular co-ordinate files in a number of formats and interactively displays the molecule on the screen in a variety of colour schemes and representations. RasMol can read a prepared list of commands from a `script' file (or via interprocess communication) to allow a given image or viewpoint to be restored quickly. RasMol can also create a script file containing the commands required to regenerate the current image, or create a dynamic session. Finally the rendered image may be written out in a variety of formats including both raster and vector PostScript, GIF, PPM, BMP, PICT, Sun rasterfile or as a MolScript input script or Kinemage. The best site displaying the functionality of RasMol is still the "original" [RasMol Home Page](#) by Eric Martz.

Commercial Products (\$)

ChemWindow by [Bio-Rad Laboratories](#)

ChemDraw and Chem3D by [CambridgeSoft](#)

Alchemy 2000 and ChemPrint by [Tripos](#)

HSC Chemistry by [Outokumpu Research Oy](#)

Hyperchem by [Hypercube](#)

Chemistry 4-D Draw/NamExpert/Nomenclator by [ChemInnovation](#)

3D Structure Libraries

[3D Pharmaceutical Structures](#)

Developed by Akira Dobashi's group at Tokyo University of Pharmacy and Life Sciences, this database is an excellent source of 3D structures of biologically active small molecules. You will

need a copy of the [Chime plug-in](#) installed on your workstation to view 3D structures and dynamic simulations.

[Molecules of the Month](#)

Developed by the Chemistry IT Centre of the University of Oxford, this site includes a variety of demonstrations, historical accounts of drug discovery, and several "hot" compounds such as Viagra® and Prozac®. You will need Chime to view the 3D structures and dynamic demonstrations.

[ChemFinder WebServer](#)

On the face of it, a way to search for chemical compounds over the World Wide Web is not a novel concept. WWW-based chemical search engines have existed since at least 1995, including [SciFinder Scholar](#) and [STN Easy](#) from the [Chemical Abstracts Service Academic Program](#). General-purpose databases of WWW contents (such as Yahoo and Alta Vista) have existed far longer. So what's the deal with this ChemFinder WebServer?

The key, you might say, is in the chemistry. It's one thing to pop over to Lycos and do a search for all references to Aluminum Hydroxide. It's another thing to actually find them, especially if the information you want is at a site in Australia under the listing Aluminium Hydroxide. Or if there is simply a passing mention of the compound with CAS RN 21645-51-2. Or a compound with the molecular formula $\text{Al}(\text{OH})_3$. By working from a single master list of chemical compounds, the ChemFinder WebServer avoids these problems, and lets you find the information you want, faster. In generating this database, we have also taken pains to identify and correct the obvious errors (like 'mehtyl', as well as invalid CAS RNs) that account for 3-5% of of all chemical information on the WWW. Very likely we have introduced some new and exciting mistakes of our own, but we are confident that the overall quality of the ChemFinder WebServer data far surpasses the bulk of the information that it indexes.

Because the ChemFinder WebServer is a chemical database, it can also provide information that a general-purpose WWW index cannot, including physical property data and 2D chemical structures. This information is somewhat sparse at the moment, but is very good for the several thousand most-common compounds. We are constantly working on getting more data, and we expect the ChemFinder WebServer only to keep improving. Access to ChemFinder WebServer is free, but you will need the [ChemDraw WebServer plugin](#) (also free) to create structure queries and view the results from this database.

[Cranium](#)

A software package capable of predicting values for more than 20 physical properties for pure components and mixtures. Cranium runs under the Windows operating system, and a lite version is available free of charge.

[Genamics SoftwareSeek](#)

This is a new repository and database of freely-distributable and commercial tools for use in molecular biology, molecular modeling, biochemistry, and chemistry. The database presently has more than 1200 entries.

[SciFinder Scholar](#) and [SciFinder](#)

Chemical Abstracts Service recently announced [SciFinder Scholar](#), an academic version of CAS' award winning [SciFinder](#), an electronic interface to the chemical literature in CAS databases. Released in December 1997, SciFinder Scholar has the following features:

- Explore the literature by topic with natural language questions
- Identify the work of specific authors
- Explore chemical substances by name, structure, formulas, or registry numbers
- Get reactions, starting from structures of interest
- Find specific CA journal or patent abstracts by entering the abstract/patent numbers

Tutorials

[Medicinal Chemistry and Biochemistry Tutorials](#)

Marc Harrold (Duquesne) has made available to Section members several excellent ToolBook-based tutorials, including a review of new drug approvals for 1996 and medicinal chemistry and biochemistry tutorials. The programs can be downloaded for local use (Marc includes a runtime version of ToolBook so purchasing the program is NOT necessary to view the tutorials) or viewed interactively online using the Neuron browser from [Asymetrix](#). Please let Marc know if you find the tutorials useful in your courses or if you plan on incorporating them into your curriculum.

[Biochemistry Tutorials](#)

Pat Woster (Wayne State) has made available to Section members access to tutorials and other information from Wayne State's Pharmaceutical Biochemistry course. Tutorials available include (1) [Protein Structure and Function](#), (2) [Enzymes - Kinetics and Catalysis](#), and (3) [Carbohydrate Metabolism](#).

[Metabolism Tutorials](#)

Pat Davis (Texas) has made available to Section members access to some Metabolism Tutorials created with Flash software. These tutorials are designed to help students integrate:

1. functional group recognition
2. enzymes involved in phase-1 and phase-2 biotransformations
3. the reaction definitions
4. the metabolic products generated by these transformations

[Medicinal Chemistry Lectures](#)

Pat Woster (Wayne State) has made available to Section members access to medicinal chemistry lecture content from his Medicinal Chemistry Module on topics including:

PSC 3320 - Principles of Drug Action

[PHA 4110 - Autonomic Pharmacology/Fluid and Electrolytes/Immunology and Inflammatory Diseases](#)

[PHA 4140 - Gastroenterology, Fluids and Electrolytes, Immunology](#)

[PHA 4150 - Cardiovascular Pharmacotherapeutics](#)

[PHA 4210 - Infectious Disease and Dermatology Module](#)

[PHA 4220 - Neurology and Psychiatry](#)

[Biochemical Tutorials in Chime](#)

A **[Visitor-Maintained Indices \(VMI\)](#)**TM Site by **[Eric Martz](#)** and **[Trevor D. Kramer](#)**. Server courtesy **[Philip Bourne](#)** and the **[San Diego Supercomputer Center](#)**. You will need Chime or other viewers.

<p>Category: Biochemistry Tutorials in Chime, Ready-to-Use</p>	<p><i>Category Description:</i> Biochemistry tutorials employing MDL's Chime on specific proteins, metabolic pathways, or other biochemical topics, ready to use in classes or for individual study. Some can be downloaded for local or off-line use. Most of these resources work best in Netscape 4.08-4.7x-4.8 (not 6 or 7!), but some also work in Internet Explorer. All require MDL's Chime plugin. Please submit resources targeted to K-12 audiences to the K-12 category.</p> <p>http://www.umass.edu/microbio/chime/pipehttp://www.umass.edu/microbio/chime/pipehttp://www.umass.edu/microbio/chime/pipehttp://www.umass.edu/microbio/chime/pipehttp://www.umass.edu/microbio/chime/pipe</p> <p>Titles,alphabetized, with full descriptions. Subjects,cross-indexed.</p> <p>Author Indices:</p> <p>Detailed.Resource descriptions shown under each entry. Compact.Click on an author to see the resource description.</p> <p>Find newest additions. Submit a new Ready-to-Use Chime Tutorial Revise (or delete) a previously-submitted resource.</p> <p>Back to List of Categories</p>
---	--

<p>Category: Biochemistry Structure Visualization Tutorials (not employing Chime)</p>	<p><i>Category Description:</i> Biochemistry tutorials (not employing MDL's Chime as the primary imaging method). Tutorials on specific proteins, metabolic pathways, or other biochemical topics, ready to use in classes or for individual study, employing non-Chime methods such as still images, VRML, or Shockwave. Submit tutorials employing MDL's Chime to the Biochemistry: Chime category. Submit resources targeted to K-12 audiences to the K-12 category. Submit tutorials relying primarily upon Deep</p>
--	--

	<p>View/Swiss-PDBViewer to that category.</p> <p>Titles,alphabetized, with full descriptions.</p> <p>Subjects,cross-indexed.</p> <p>Author Indices:</p> <p style="padding-left: 40px;">Detailed.Resource descriptions shown under each entry.</p> <p style="padding-left: 40px;">Compact.Click on an author to see the resource description.</p> <p>Find newest additions.</p> <p>Submit a new <i>Biochemistry Tutorial (not primarily in Chime)</i></p> <p>Revise (or delete) a previously-submitted resource.</p>
--	--

Websites

[ChemCenter: The American Chemical Society \(ACS\) Online](#)

o [Publications Division](#)

o [Medicinal Chemistry Division](#)

[Chemical Abstracts Service \(CAS\)](#)

o [CAS SciFinder Scholar](#)

[ChemPointers at UCLA](#)

[ChemWeb](#)

[Chemisty Links from the FDA](#)

[Information Retrieval in Chemistry](#)

[Links for Chemists](#)

Links for Chemists is an index of over 8,400 chemistry resources on the web. This site is the copyright of The University of Liverpool, [Department](#) of Chemistry

[Medline via PubMed](#)

[PubMed, a service of the National Library of Medicine, provides access to over 12 million MEDLINE citations back to the mid-1960's and additional life science journals. PubMed includes links to many sites providing full text articles and other related resources.](#)

[Scirus](#)

Scirus is the most comprehensive science-specific search engine available on the Internet. Driven by the latest search engine technology, it enables scientists, students and anyone searching for scientific information to chart and pinpoint data, locate university sites and find reports and articles quickly and easily. It was launched by Elsevier Science, the leading international publisher of scientific information.

[Virtual Pharmacy Library at UOKHSC](#)

Structure Databases

[NIH Molecular Modeling Home Page](#)

[NIH Molecular Biology Database](#)

[NLM Center for Biotechnology Information](#)

[Entrez Macromolecule Search Engine](#)

[Cn3D Structure Viewer](#)

Physicochemical Properties

[ChemIDplus](#)

ChemID*plus* is a searchable chemical substance database developed by the [Division of Specialized Information Services](#) of the National Library of Medicine and TOXNET. It is capable of both name/synonym searches on over 350,000 substances (including 65,000 structures) as well as structure/substructure searching (you will need the [ISIS/Draw](#) program to create and transfer structures to ChemID*plus*). Structures are displayed using the Chemscape Chime plug-in, available from [MDL](#) or from the ChemID*plus* home page.