

List of referenced Web sites

Without trying to be exhaustive, the most important Web sites referenced in this book are listed below. Additional sites may be found using any of the many available search engines, using keywords from the list of references presented at the end of each chapter. For example, the string “LHASA Organic Synthesis” will produce several relevant hits pointing to LHASA research and entry points for further searches. Although all the sites listed below were checked at the time of editing of this book (March 2004), the reader should be aware that the Web is a volatile medium and that sites continuously appear and disappear.

Academic Chemical Information Services and Research

Computer-Chemie-Centrum, Erlangen, Germany.

www.ccc.uni-erlangen.de

CDS (Chemical Data Service), U.K.

<http://cds.dl.ac.uk>

CMBI, Nijmegen University, the Netherlands – successor to CAOS/CAMM Center.

www.cmbi.kun.nl

Molecular Modeling

Accelrys – molecular modeling and cheminformatics software.

www.accelrys.com

Tripos – molecular modeling and cheminformatics software.

www.tripos.com

Quantum Chemical Literature Database (QCLDB).

www.jaici.or.jp

MOLDEN – molecular modeling program.

www.cmbi.kun.nl/~schaft/molden

UPACK – crystal modeling program.

www.crystal.chem.uu.nl/~vaneyck

Modeling interface software.

<http://gdis.seul.org>

RASMOL – molecular visualization.

<http://www.bernstein-plus-sons.com/software/rasmol>

File format conversion for molecular modeling.

<http://openbabel.sourceforge.net>

Open source Java molecular viewer.

<http://jmol.sourceforge.net>

Chime – molecular visualization.

www.mdl.com/products/framework/chime/index.jsp

Crystallography and Crystallographic Databases

Brookhaven National Laboratory. Former location of the PDB (see next link).

www.bnl.gov/world

Protein Databank (PDB).

www.rcsb.org/pdb

(Chemical) database services including, among others, ICSD.

www.stn-international.de

CRYSTMET (crystallographic metals and alloys database).

www.tothcanada.com

CSD, Cambridge Crystallographic Data Centre, U.K.

www.ccdc.cam.ac.uk

ICSD (Inorganic Crystal Structure Database).

www.fiz-informationsdienste.de

U.K. Collaborative Computing Project Number 4 in Protein Crystallography (CCP4).

<http://www.ccp4.ac.uk>

U.K. Collaborative Computing Project 11 (CCP11), in bioinformatics.

www.ccp11.ac.uk

ICSD for WWW-interface with free demo access.

<http://icsd.ill.fr>

Crystal Data Identification File.

www.nist.gov/srd/jcps.htm

Bioinformatics

European Bioinformatics Institute - nucleic acid sequence databases.

www.ebi.ac.uk

EMBL Nucleotide Sequence Database (EMBL-Bank).

www.ebi.ac.uk/embl

EBI Macromolecular Structure Database (MSD).

www.ebi.ac.uk/msd

European Molecular Biology Network.

www.embnet.org

Nucleic Acid Database (NDB).

<http://ndbserver.rutgers.edu>

Dutch Bioinformatics Applications Services.

www.bioasp.nl

Human Genome Project at Sanger Institute, U.K.

www.sanger.ac.uk/HGP

International Human Genome Sequencing Consortium.

www.ensembl.org

U.K. SEQUENCE NETWORK.

www.hgmp.mrc.ac.uk/About/SEQNET

Protein Sequence Database.

<http://pir.georgetown.edu>

Genbank DNA Sequence Database and other bioinformatics software.

www.ncbi.nlm.nih.gov/Genbank

Reaction Databases and Synthesis Planning

Computer-assisted synthesis planning - overview of the LHASA system.

www.cmbi.kun.nl/cheminf/olp

Reaction-retrieval software and databases.

www.mdl.com

LHASA U.K. – synthesis planning.

www.chem.leeds.ac.uk/luk/

Reaction databases – ChemInform.

www.fiz-chemie.de

Reaction databases – Accelrys.

www.accelrys.com

Beilstein Database.

www.beilstein-institut.de

(for Crossfire see: www.mdl.com)

Beilstein Crossfire access in the U.K., Ireland, and Scandinavia.

www.mimas.ac.uk

Journal of Synthetic Methods. Organic Reactions Database (via MDL).

www.thomsonderwent.com

Org Syn. Organic Reactions Database.

www.orgsyn.org

Drug Discovery

DEREK – toxicity prediction.

www.chem.leeds.ac.uk/luk/derek

Data mining tools; classifier construction.

www.rulequest.com

MDL's discovery tools

www.beilstein.com/products

ClogP & QSAR software.

www.biobyte.com

ADME-prediction software.

www.schrodinger.com

pKa-prediction software.

www.acdlabs.com

NCI/NIH Databases.

<http://dtp.nci.nih.gov>

Educational

Mol4D educational software.

www.cmbi.kun.nl/wetche/organic

Collection of (bio)chemical applications using Chime.

www.umass.edu/microbio/chime

World Index of Molecular Visualization Resources.

www.molvisindex.org

Communication between Chime and an HTML page.

<http://www3.sympatico.ca/diane.demers/moi>

Organic Reaction Animations.

<http://chemwww.byu.edu/ora>

Chemistry software tools for education; Spartan.

www.wavefunction.com

Chemistry (teaching) software; CAChe.

www.cachesoftware.com

Molecule of the Month page.

www.bris.ac.uk/Depts/Chemistry/MOTM/motm.htm

C4 consortium – collection of organic and bio-organic compounds.

<http://c4.cabrillo.cc.ca.us>

Freeware Web-based interface to computational chemistry.

www.webmo.net

Spectroscopy, Chromatography, and Physical Chemistry

Spectroscopic software and spectral databases; SpecInfo.

www.chemicalconcepts.com

Database for chiral chromatography.

<http://chirbase.u-3mrs.fr>

Thermophysical properties database – Detherm.

<http://www.dechema.de>

See also <http://cds.dl.ac.uk/cds/datasets/physchem/detherm/detherm.html>

Miscellaneous

Bibliographic software.

www.endnote.com

MDL software linking data sources.

www.litlink.com/products/knowledge/litlink_server

Popular system for delivering multimedia content.

www.macromedia.com

Dutch academic computer network.

www.surfnet.nl

U.K. academic computer network – Joint Information Systems Committee (JISC).

www.jisc.ac.uk

Royal Dutch Chemical Society.

www.kncv.nl

Gesellschaft Deutscher Chemiker.

www.gdch.de

Molecular Diversity Preservation International (MDPI).

www.mdpi.org

Chemical information services.

www.fiz-karlsruhe.de

Internet Journal of Chemistry.

http://www.ijc.com

World Wide Molecular Matrix Project.

http://wwmm.ch.cam.ac.uk