Exploring 3D Molecular Structures Using NCBI Resources

A Field Guide

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Online Resources

Course Resources

Course home page	http://www.ncbi.nlm.nih.gov/Class/Structure/course.html
PowerPoint slides	ftp://ftp.ncbi.nih.gov/pub/sayers/Structure/
Workshop I exercises	http://www.ncbi.nlm.nih.gov/Class/Structure/handson_I.html
Workshop II exercises	http://www.ncbi.nlm.nih.gov/Class/Structure/handson_II.html
Alignment Guide	http://www.ncbi.nlm.nih.gov/Class/Structure/align_guide.html
Amino Acid Explorer	http://www.ncbi.nlm.nih.gov/Class/Structure/aa/aa_explorer.cgi
PSSM Viewer	http://www.ncbi.nlm.nih.gov/Class/Structure/pssm/pssm_viewer.cgi

General NCBI

NCBI home page	http://www.ncbi.nlm.nih.gov
About NCBI	http://www.ncbi.nlm.nih.gov/About
NCBI news	http://www.ncbi.nlm.nih.gov/About/newsletter.html

NCBI Structure Sites

Structure main page	http://www.ncbi.nlm.nih.gov/Structure
MMDB main page	http://www.ncbi.nlm.nih.gov/Structure/MMDB/mmdb.shtml
CDD main page	http://www.ncbi.nlm.nih.gov/Structure/cdd/cdd.shtml
VAST page	http://www.ncbi.nlm.nih.gov/Structure/VAST/vast.shtml
PubChem page	http://pubchem.ncbi.nlm.nih.gov
NCBI Handbook	http://www.ncbi.nlm.nih.gov/books/bv.fcgi?rid=handbook.chapter.ch3

NCBI Structure Tools

Cn3D	http://www.ncbi.nlm.nih.gov/Structure/CN3D/cn3d.shtml
CD-Search	http://www.ncbi.nlm.nih.gov/Structure/cdd/wrpsb.cgi
VAST Search	http://www.ncbi.nlm.nih.gov/Structure/VAST/vastsearch.html
CDART	http://www.ncbi.nlm.nih.gov/Structure/lexington/lexington.cgi?cmd=rps
NCBI Threader	http://www.ncbi.nlm.nih.gov/Structure/RESEARCH/threading.shtml
Entrez Structure	http://www.ncbi.nlm.nih.gov/entrez/query.fcgi?db=Structure
Entrez 3D Domains	http://www.ncbi.nlm.nih.gov/entrez/query.fcgi?db=Domains
Entrez Domains	http://www.ncbi.nlm.nih.gov/entrez/query.fcgi?db=cdd
COG	http://www.ncbi.nlm.nih.gov/COG/
MMDB URLs	http://www.ncbi.nlm.nih.gov/Structure/MISC/linking.html#mmdbsrv

Other Databases

PDB	http://www.rcsb.org/pdb/
Pfam	http://pfam.wustl.edu/
SMART	http://smart.embl-heidelberg.de/

NCBI Structure FTP Resources

CDD	ftp://ftp.ncbi.nih.gov/pub/mmdb/cdd/
Cn3D	ftp://ftp.ncbi.nih.gov/cn3d/
CDART	ftp://ftp.ncbi.nih.gov/pub/mmdb/cdart/
RPS-BLAST	ftp://ftp.ncbi.nih.gov/blast/

Literature

Structural Biology

1. Bourne, P.E. and Weissig, H., eds. *Structural Bioinformatics*. John Wiley & Sons. Hoboken, NJ. 2003.
2. McPherson, A. *Introduction to Macromolecular Crystallography*. John Wiley & Sons. Hoboken, NJ. 2002.
3. Cavanagh, J., Fairbrother, W.J., Palmer, A.G., and Skelton, N.J. *Protein NMR Spectroscopy.* Academic Press, San Diego. 1996.

NCBI Databases

1. Chen, J. et al, (2003) MMDB: Entrez's 3D-structure database. *Nucleic Acids Res* **31**, 474-477.
2. Marchler-Bauer, A. et al, (2003) CDD: a curated Entrez database of conserved domain alignments. *Nucleic Acids Res* **31**, 383-387.

VAST

1. Gibrat, J.-F. et al, (1996) Surprising similarities in structure comparison. *Curr Opin Struct Biol* **6**, 377-385.
2. Madej, T. et al, (1995) Threading a database of protein cores. *Proteins* **23**, 356-369.

CDART

1. Geer, L.Y. et al, (2002) CDART: protein homology by domain architecture. *Genome Res* **12**, 1619-23.

Other relevant NCBI publications are linked from http://www.ncbi.nih.gov/Structure/.