

## Software

We encourage open access to NMR databases and software. Tools for data processing, analysis and data submission are installed, and conform with international standards.

An extensive range of NMR software is available, with some of the more popular packages listed below.

### NMR processing

- **Azara 2.7** (<http://www.bio.cam.ac.uk/azara/>)
- Munin
- **NMRLab/MetaboLab** (<http://nmrlab.org.uk/>)
- **NMRPipe/TALOS** (<http://spin.niddk.nih.gov/bax/software/NMRPipe/NMRPipe.html>)
- **TopSpin 2.1** (<http://www.bruker-biospin.com/topspin.html>) (acquisition) and 2.0 (off-line processing)
- **VnmrJ** (<http://www.varianinc.com/cgi-bin/nav?products/nmr/software/vnmrj&cid=KQPIHILPFP>) (acquisition only)

### Assignment

- **Autoassign** ([http://www-nmr.cabm.rutgers.edu/NMRsoftware/nmr\\_software.html](http://www-nmr.cabm.rutgers.edu/NMRsoftware/nmr_software.html))
- **CcpNmr 1.0** (<http://www.ccpn.ac.uk/ccpn/software/ccpnmr-suite>)
- **NMRView 5.2.2** (<http://onemoonscientific.com/nmrview/>)
- **NMRViewJ 6.1** (<http://onemoonscientific.com/nmrview/>)
- **Sparky 3** (<http://www.cgl.ucsf.edu/home/sparky/>)

### Validation

- **Procheck 3.5.4** (<http://www.biochem.ucl.ac.uk/~roman/procheck/procheck.html>)
- **Queen 1.1** (<http://www.cmbi.kun.nl/software/queen/>)
- **Whatif 5.0** (<http://swift.cmbi.kun.nl/whatif/>)

### Structure calculation

- **Aria 2.2** (<http://www.pasteur.fr/recherche/unites/Binfs/aria/>)
- Dyana/Candid

### Molecular Graphics

- **Dino 0.9.0-rc5** (<http://www.dino3d.org/intro.php>)
- **MolMol 2K.1** (<http://hugin.ethz.ch/wuthrich/software/molmol/>)
- **PyMol 0.97** (<http://pymol.sourceforge.net/>)
- **Raster3D 2.7c** (<http://skuld.bmsc.washington.edu/raster3d/raster3d.html>)
- **VMD 1.8.2** (<http://www.ks.uiuc.edu/Research/vmd/>)

We offer access to **computer hardware** including:

- workstations (Pentium IV 3GHz, 1GB RAM to Intel Core2Duo 2.66GHz with 4GB RAM)
- Kubuntu-Desktop 9.04 Linux operating system
- terabyte RAID server on which dedicated disk drives (300 GB) can be purchased
- access to a **1000 node cluster** (<http://www.bear.bham.ac.uk/>)
- printers, both high speed B&W and colour laser
- data backup by tape and CD/DVD
- dedicated sftp site and ssh remote access
- hardware firewall
- gigabit ethernet