

How to access the data on this CD

Accessing the ITC data:

The ITC data is present both in its raw form and as processed origin graph. The raw data can be accessed using any version of origin however the processed data can also be accessed using the origin viewer available for free download here:

<http://www.originlab.com/viewer/dl.aspx>

Accessing the NMR side chain assignment data:

You will need the CCPN analysis software (v. 2.1.3) to access the assignment files.

CCPN analysis is available for free download here if required:

<http://www.ccpn.ac.uk/ccpn/software/downloads-v2>

Included on the CD are the processed spectra in .aza and .aza.par form for the three constant time CHSQC experiments in the apo, ADP and AMPPNP bound state.

Also included is a CCPN analysis file entitled chsqcoverlay. In this file are the aligned overlays of the apo, ADP and AMPPNP spectra. The apo and ADP spectra have associated assignments. The AMPPNP is not assigned in this file due to technical difficulties with the CCPN format convertor software in exporting the assignments from the original project. To this extent the AMPPNP assignments can be found in the CCPN analysis file amppnp3.

When opening these files the relevant path positions of the spectra will have to be updated both linking the .aza.par file to the .aza file and linking the ccpn project to the .aza.par files. The exact path details of the update will, of course, depend where you have saved the data in order to access it.

The CCPN analysis file amppnp3 contains peak assignments for spectra other than the constant time CHSQC given and as such many of the windows present will show up blank, or with peaks that appear to match to nothing visible, as other spectra are not provided.

If you have any problems accessing the data please contact either Dr. Mark Williams (m.williams@mail.cryst.bbk.ac.uk) or myself (eleanorpolly.smith@gmail.com).