

Structural Biology cost model

Cost for spectrometer time and personell can be found on our home page xxx, different prices apply for different categories of users

For samples up to 150 residues

Assessment of sample

Initial startup, discussion of sample prep and scientific questions

Nhsqc - measure s/N and number of peaks

hetNOE - judge overall appearance

Spectra to run:

Nhsqc/Trosy/sofast

Chsqc_ali, Chsqc_aro

hetNOE

Man hours:	8
Spectrometer hours:	16

Backbone assignment

setting up, running and processing TA

Setting up ccpn project

Manual check of TA results

Spectra to run:

Nhsqc

HNCO, HNCA, HNcoCA, HNCACB, HNcoCACB, HNcaCO

Nnoesy

Man hours:	12-20
Spectrometer hours:	100

Side chain assignment

Setting up and processing Ntocsy, CCH tocsy, Cnoe_ali, Cnoe_aro, tdCCHnoesy.

Analysing spectra in ccpn and transfer peak picking and assignment to Cnoesy_ali

Man hours:	80-100
Spectrometer hours:	192

Structure calculations:

Transferring data from ccpn to cyana, setup of calc

Checking structure

Loop back to spectra
Water refinement
Deposition of data

Man hours: 40

Total time

Spectrometer hours: 300-320
Man hours: 140-150

For sample over 150 residues

Assessment of sample

Initial startup, discussion of sample prep and scientific questions
Nhsqc - measure s/N and number of peaks
hetNOE - judge overall appearance

Spectra to run:

Nhsqc/Trosy/sofast
Chsqc_ali, Chsqc_aro
hetNOE

Man hours: 8
Spectrometer hours: 16

Backbone assignment

setting up, running and processing TA on deuterated sample
Setting up ccpn project
Manual check of TA results

Spectra to run:

Nhsqc
HNCO, HNCA, HNcoCA, HNCACB, HNcoCACB, HNcaCO
Nnoesy

Man hours: 20-30
Spectrometer hours: 100

Side chain assignment

Setting up and processing CCH tocsy, Cnoe_ali H2O, Cnoe_ali D2O, Cnoe_aro, tdCCHnoesy/4D.
Analysing spectra in ccpn and transfer peak picking and assignment to Cnoesy_ali

Man hours: 100

Spectrometer hours: 288

Structure calculations:

Transferring data from ccpn to cyana, setup of calc

Checking structure

Loop back to spectra

Water refinement

Deposition of data

Man hours: 40+

Total time

Spectrometer hours: min 308

Man hours: min 180