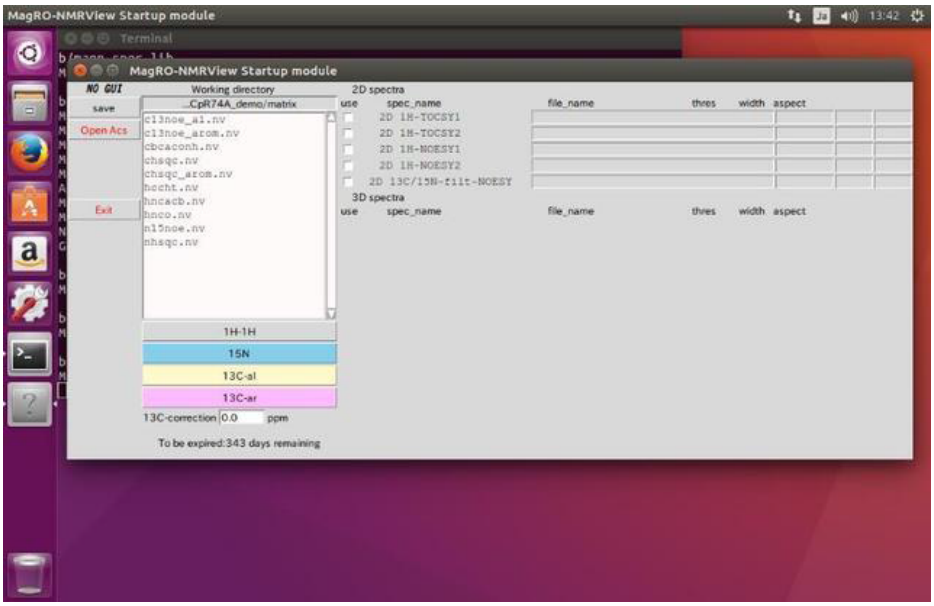
MagRO NMRView Noise filter Guide

MagRO NMRView and Filt Robot can be used for noise filtration of NMR spectra using Deep Learning Technology

Try demo of CNN filter (run the filter)

2017/11/21

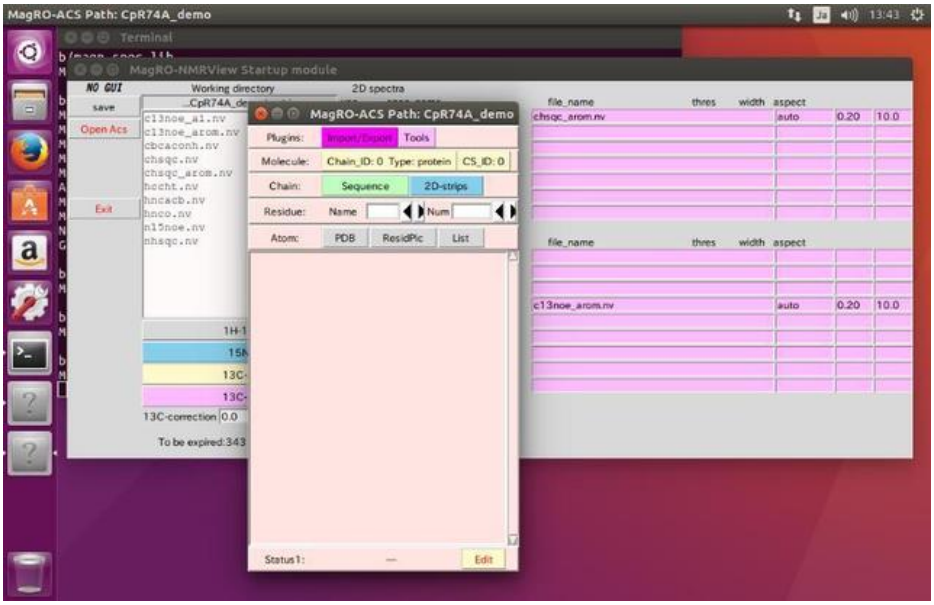
So just type,
./run_demo.csh
then you will see the GUI:



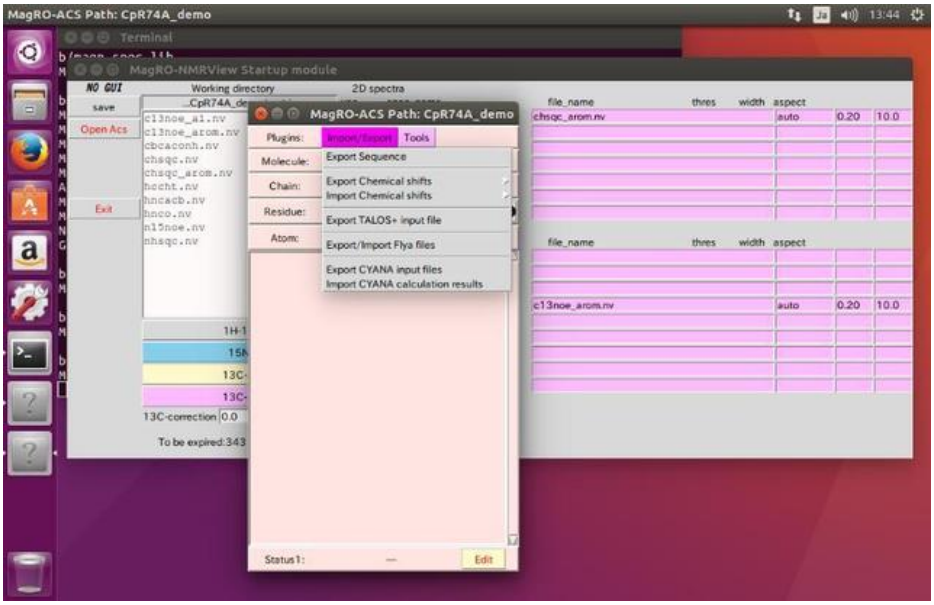
The interface for setting up spectrum data sets for the fully automated peak picking and noise filter ing. (detailed algorithm and benchmarks will be shown in our publication soon: now under review)

The default state, 10 spectra
2D 1H-15N HSQC, 1H-13C CT-HSQC for aliphatic and aromatic
3D HNCO, CBCA(CO)NH, HNCACB, HCCH-TOCSY for aliphatic
3D 15N-edited NOESY, 13C-edited NOESY for aliphatic and aromatic
(the program also supports 3D HBHA(CO)NH, H(CCCO)NH, CC(CO)NH and so on...)

Press "OpenAcs" to open small window (light pink):



Press "Import/Export" button to open FLYA module:



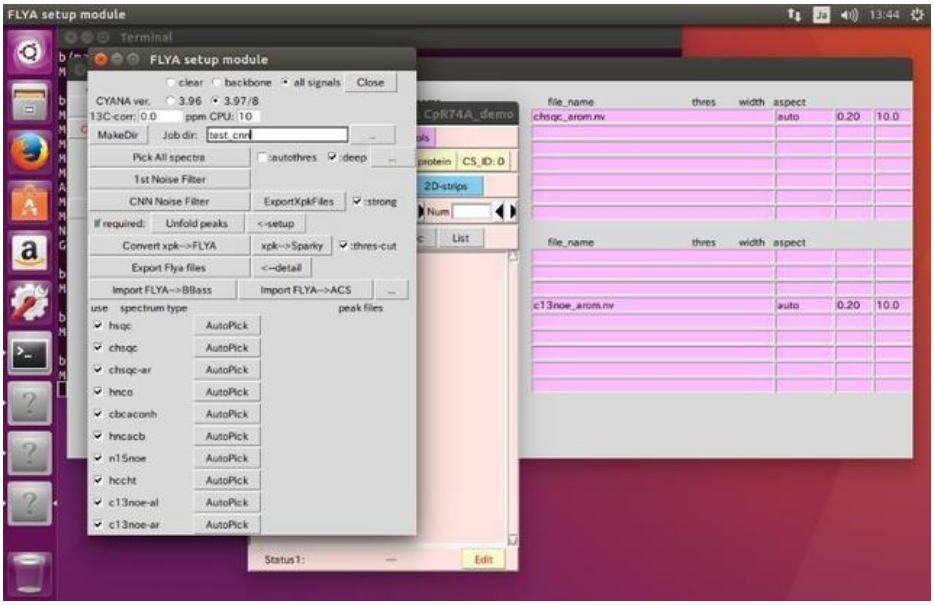
So now you are ready to start automated peak picking and noise filtration.

0.setting for the automated jobs

press check-button "all signals"

change CPU numbers (default:4)

and type the directory name (Job dir:) that you would like to place the peak lists.

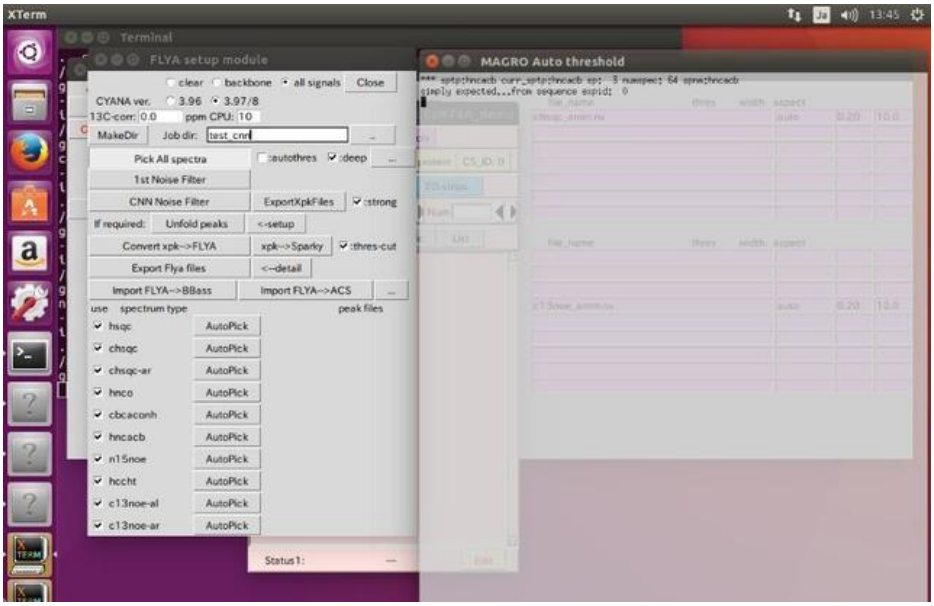


1. fully automated peak picking

This peak picker is quite fast, but it is not powerful enough to detect shoulder peaks. If you check "deep" check-button, the peak picker will determine optimal data threshold (baseline level) and a little larger number of peaks than expected from the protein sequence.

Press "Pick All spectra" to begin the picking jobs (will take a few minutes).

After the picking jobs you will find *_auto.xpk files as lists of picked peaks.



[caution]

The peak picker does not care the sign of signals and base-line nose signals from bulk water. So the peak lists may contain more than 20,000 peaks depending on the type of spectrum and data quality.

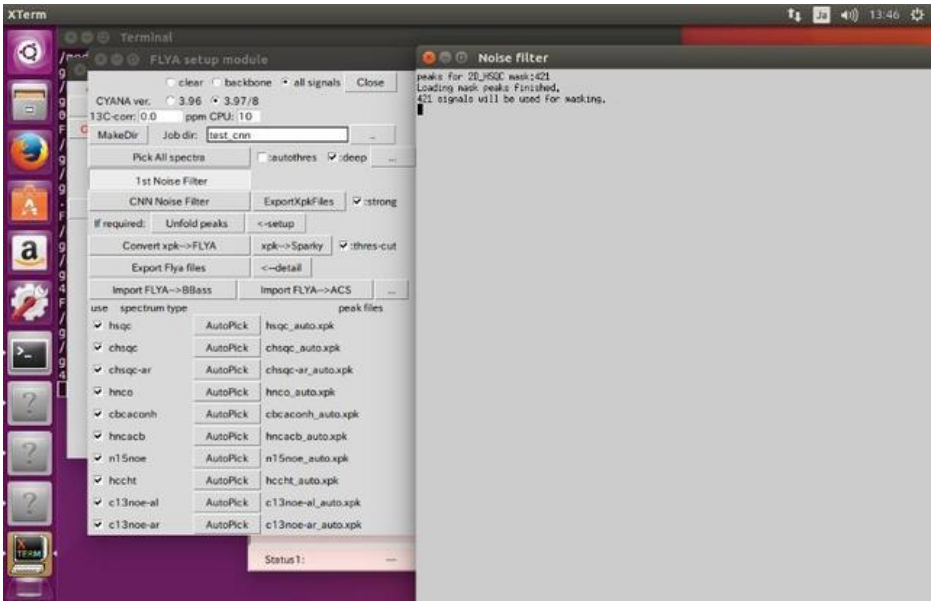
2. HSQC masked filter

The program can roughly filter 3D peak lists using peak lists derived from 2D 1H-15N or 1H-13C HSQC spectrum. The peak lists automatically selects peak lists for the masking corresponding to each 3D peak lists (same HSQC projection type).

This step can be skipped but this should increase the performance of the image generation stage.

Press "1st Noise filter " button to start the filtration (may take a few minutes).

When the all jobs are finished, you will find *_filt.xpk files in the job directory.



[caution]

If the peak pattern of the HSQC spectrum for masking job is largely different from the targeted 3D spectrum projection, the real signals can be filtered.

You have to be careful to check the peak pattern in HSQC spectrum is similar to the targeted 3D spectra before do this job.

3.CNN filtration

This task requires CNTK 2.0-CPU only version. Please check if you try this on your own system.

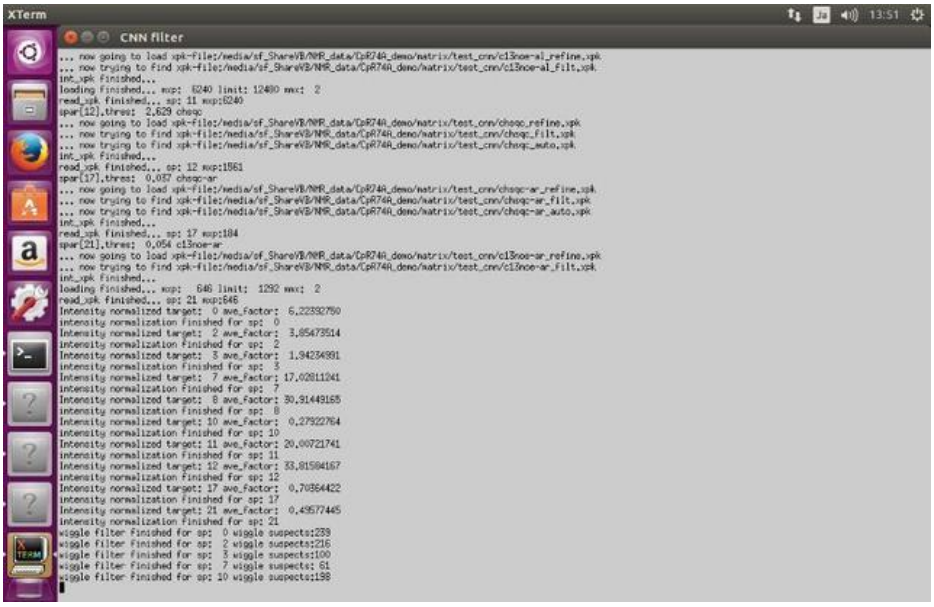
Just press "CNN Noise filter" button to start the filtering jobs.

Firstly generation of extracted gray scale images from 2D and 3D spectrum data (may take 20-30 min depending on the number of detected signals)

[caution]

If you apply a large number of data, or total size of spectrum data is more than 1GB, we would recommend you to increase the virtual memory size to 6-8GB.

When the all jobs are finished, you will find *_cnn.xpk files in the job directory.



Fully automated peak picker will take more than 40,000 peaks but after the CNN-filtration the total number of peaks will be ~10,000 peaks which may be suitable for automated signal assignment and structure determination performed by FLYA/CYANA.