

In CCPNMRV3 :

- Assign > Assignment Inspector > Right clic on the header > Column Settings...

Check only : Value(ppm), NmrAtom, SequenceCode, ResidueType, AtomName, Total Peak Count

- Save > Close > ctrl a > right clic> Export visible Table > save it in .csv
- In View>Peak Table> select the N or C NOESY spectra

Check only in columns Settings : POS F1, POS F2, POS F3 and Volume

- Save > Close > ctrl a > right clic> Export visible Table > save it in .csv

Do the same for the other NOESY.

```
uniqueId,"Value
(ppm)","Value Error
(ppm)","SequenceCode,ResidueType,AtomName,"Total
Peak Count"
143,173.073111116886,0,43-1,None,C,
145,44.7815707186237,0,43-1,None,CA,
144,175.404697612044,None,43,ALA,C,
146,50.1030611375232,0.184284867346688,43,ALA,CA,
147,17.8848422996301,0.0702525036454874,43,ALA,CB,
15,7.93837832968314,0.0114269196686178,43,ALA,H,
430,4.40339598437056,0.0112321177191982,43,ALA,HA,
431,1.14186252963931,0.0134205242938577,43,ALA,HB,
14,124.81377686881,3.01578298584783E-06,43,ALA,N,
193,176.771590959746,0,45-1,None,C,
195,62.6417444513904,0.128760707338567,45-1,None,CA,
197,31.615977214165,0.0820089774868514,45-1,None,CB,
492,49.9767797041912,0.0333255337186087,45-1,None,CD,
698,62.632984161377,None,45-1,None,CD2,
491,26.9761517047882,0.0859981015289865,45-1,None,CG,
490,4.20995203086308,0.00614990268790723,45-1,None,HA,
```

The CSV of the full attribution of the protein extract from CCPNMRV3

```
[object,Pos F1,Pos F2,Pos F3,Volume
"PK:noesy_HSQC_Si1841_lag.1.277: @(8.394, 8.389, 126.03)>" ,8.39395139857336,8.3893333951683,126.025033812623,169800153361.851
"PK:noesy_HSQC_Si1841_lag.1.278: @(8.393, 4.12, 126.03)>" ,8.39303901724364,4.11970053896418,126.03302547551,54079422843.4623
"PK:noesy_HSQC_Si1841_lag.1.279: @(8.394, 1.191, 126.04)>" ,8.39447875647235,1.19084001404252,126.040126888102,21722018850.0452
"PK:noesy_HSQC_Si1841_lag.1.280: @(8.393, 0.363, 126.02)>" ,8.39253575435935,0.362690888546545,126.020780222963,16653072417.9061
"PK:noesy_HSQC_Si1841_lag.1.281: @(8.688, 8.687, 127.05)>" ,8.68832665158592,8.68694572331333,127.04907953941,99923818212.4587
"PK:noesy_HSQC_Si1841_lag.1.282: @(8.689, 6.616, 127.1)>" ,8.68917270952467,6.61572981163462,127.098016152902,15181728146.9459
"PK:noesy_HSQC_Si1841_lag.1.283: @(8.689, 3.394, 127.05)>" ,8.68895883521895,3.3944063758191,127.051110077052,27509209196.4003
"PK:noesy_HSQC_Si1841_lag.1.284: @(8.688, 1.176, 127.05)>" ,8.68839222977025,1.17623560677256,127.05330687711,15856318317.0078
"PK:noesy_HSQC_Si1841_lag.1.285: @(8.689, 0.962, 127.03)>" ,8.68882146879496,0.961635826473163,127.031632023426,14145510609.2607
"PK:noesy_HSQC_Si1841_lag.1.286: @(8.689, 0.596, 127.03)>" ,8.68890145430766,0.595931395055361,127.032231443183,6945638268.63276
"PK:noesy_HSQC_Si1841_lag.1.287: @(8.69, 0.355, 127.04)>" ,8.68977135885889,0.355033329582,127.038404900458,6544752452.1314
"PK:noesy_HSQC_Si1841_lag.1.288: @(8.688, -1.077, 127.06)>" ,8.68783978324771,-1.0766027124647,127.060396707954,11384925362.7034
"PK:noesy_HSQC_Si1841_lag.1.289: @(6.613, 6.618, 112.07)>" ,6.61305507960641,6.61839348351673,112.067187031141,188910374295.197
"PK:noesy_HSQC_Si1841_lag.1.290: @(6.616, 4.466, 111.95)>" ,6.61602447966507,4.46597738594282,111.948136965599,4890750740.25771
"PK:noesy_HSQC_Si1841_lag.1.291: @(6.612, 3.4, 111.92)>" ,6.61194273449493,3.40002885363156,111.922992735222,5855678105.85992
"PK:noesy_HSQC_Si1841_lag.1.292: @(6.615, 0.965, 111.95)>" ,6.61516053676696,0.965151554831771,111.947884740884,7127824973.49348
"PK:noesy_HSQC_Si1841_lag.1.293: @(6.617, 0.589, 111.94)>" ,6.61728288527802,0.58932596657639,111.94250257431,3870861270.45688
```

The CSV of the peak of NOE extract from CCPNMRV3

For CCPNMRV3 to cyana

Creat a File with the three csv files and name it 13C.csv 15N.cvs and attrib.csv.

My file is demo for the exemple.

In the file of the software execute main.py via the terminal :

\$python3 main.py

This window should appear.

The image displays two side-by-side screenshots of a software window titled "CCPNMR to Cyana". The window has a dark theme with purple accents. The title bar shows standard window controls (minimize, maximize, close). The main content area is titled "CCPNMRV3 to Cyana" and has a status "Ready".

The left screenshot shows the initial state of the application:

- Amino Acid Start:** An empty text input field.
- Enter protein sequence:** A text input field containing the sequence "APEKKVLFWYDPMKPDTKFDKPGKSPFMDMDLVPKYADESG".
- Working Space:** A text input field with the placeholder "Select working directory".
- Browse Location:** A purple button.
- Cyana Version:** Two radio buttons, "Version 2" (selected) and "Version 3".
- Launch:** A purple button.

The right screenshot shows the same application with the following values entered:

- Amino Acid Start:** The value "43".
- Enter protein sequence:** The same sequence "APEKKVLFWYDPMKPDTKFDKPGKSPFMDMDLVPKYADESG".
- Working Space:** The value "D:/cc_python/demo".
- Browse Location:** A purple button.
- Cyana Version:** Two radio buttons, "Version 2" and "Version 3" (selected).
- Launch:** A purple button.

File the different information on the right the parameters for the demo.

Clic on Launch and 3 new files are creat in the working space: prot.seq, attrib_cyana.prot, 15N.peaks and 13C.peaks.