4D-NMR Experiments with Avance Spectrometer

Topspin 1.3

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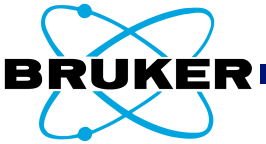
General procedure to setup a 4D-experiment



GETTING STARTED:

simply read standard parameter set with 'rpar HNCOCAGP3D' and select the corresponding 4D pulse program, then load pulses with 'getprosol'

DEFINING THE SPECTRAL WINDOWS FOR THE INDIRECT DIMENSIONS:

1. use CNST20 to define spectral width for CO-dimension
2. set SW{F1} and SW{F2} in the eda-window to define spectral window, e.g. for N and CA

DEFINING THE NUMBER OF INCREMENTS FOR THE INDIVIDUAL DIMENSIONS:

3. Use TD{F1} and TD{F2} to define number of incrments for the F1- and F2-dimensions.
Use 'parmode' = 3D.
4. Use L3 to define number of increments for F3-dimension.
Use 'parmode' = 2D.

SELECTING DIMENSIONS:

5. use the acquisition parameter ZGOPTN to define which dimensions should be measured:

examples a) 'ZGOPTN = -DNH_EVOL' would give the NH plane

b) 'ZGOPTN = -DCA_EVOL -DNH_EVOL' will give a regular 3D HNCOCA spectrum

c) 'ZGOPTN = -DCA_EVOL -DNH_EVOL -DCO_EVOL' will give a 4D HNCOCA spectrum

Example of a 4D Pulse Program

1. Defining the 4th dimension:

Parameters like spectral window and number of time increments for the first three frequency dimensions can be directly set within the ‚eda' window of XWIN-NMR.

Parameters for the 4th dimension cannot be set with the ‚eda' window, and therfore will be coded in the pulse program

2. Writing a 4D pulse program:

Starting from a corresponding 3D-pulse program, just a few modifications have to be done:

b) Automated calculation of the time increment for the evolution delay of the 4th dimension

c) Adding the evolution for the 4th dimension

d) Adding actors for the evolution in the 4th dimension, e.g. TPPI phase incrementation, incrementation of evolution delay

Example of a 4D Pulse Program

Automated calculation of the time increment for the evolution delay of the 4th dimension:

"in20=1/(4*bf2*(cnst20/1000000))"

Adding evolution period for the 4th dimension (here, the CO evolution):

```
d20                                          ;start t3 evolution
(center (p14:sp5 ph1):f2 (p22 ph1):f3 )      ;refocuss J(CO,N) and
J(CaCO)
d20                                          ;end t3 evolution
```

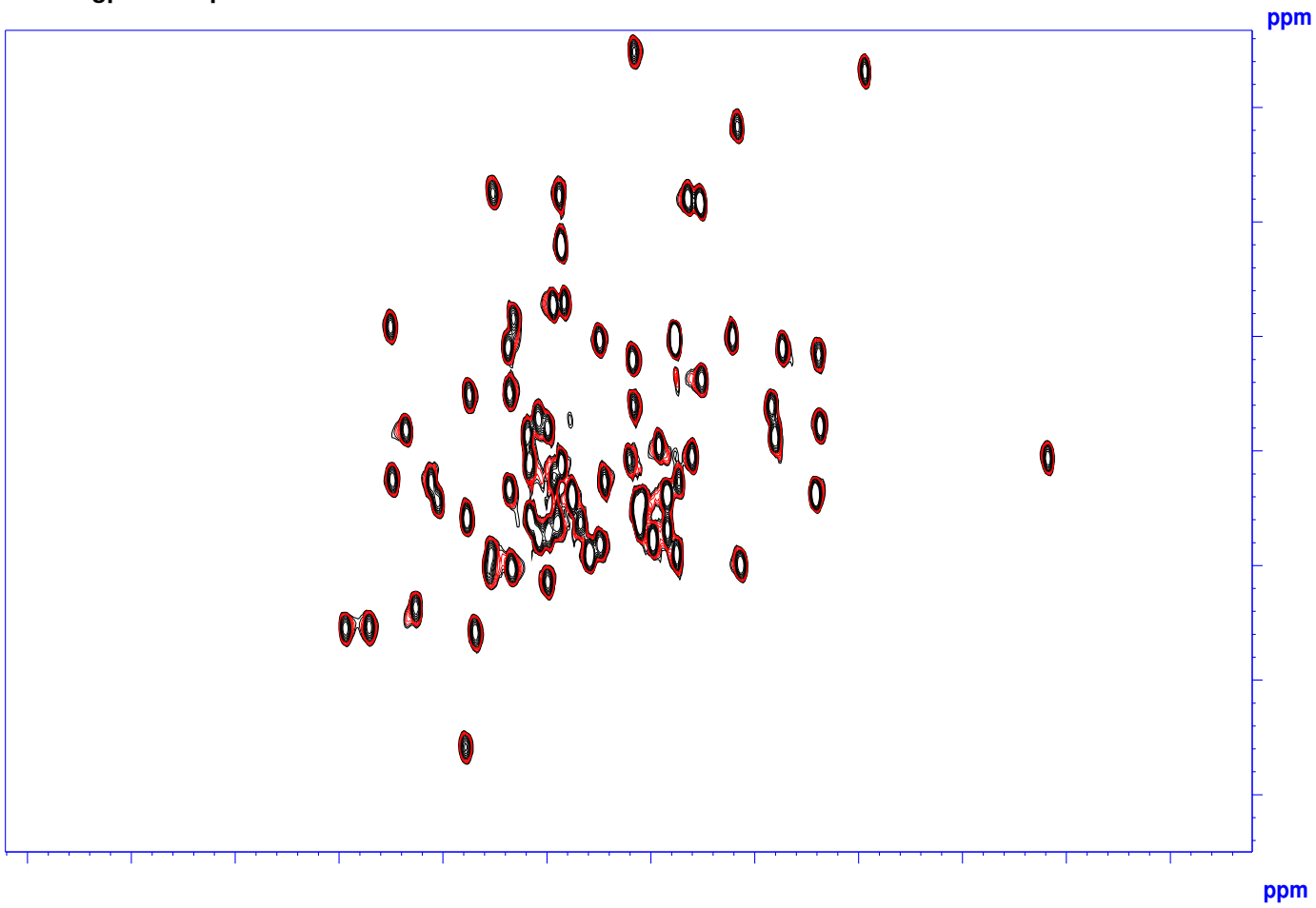
Example of a 4D Pulse Program

Factors for quadrature and evolution;

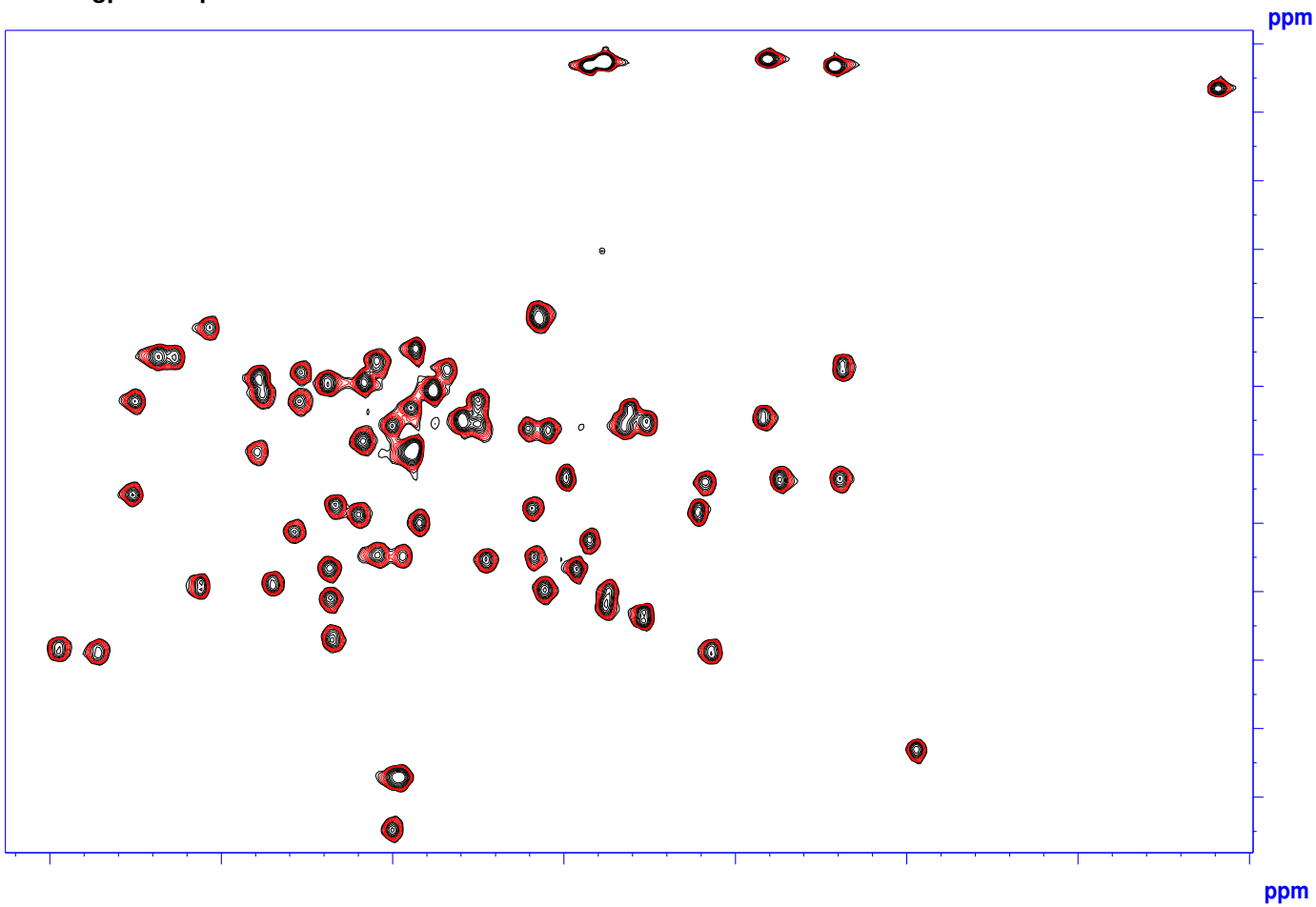
```
/*Definitions for individual planes*/
# ifdef CA_EVOL
  d11 do:f3 wr #0 if #0 ip4 zd
  lo to 3 times 2
  d11 id0
  lo to 4 times l1
# endif

# ifdef NH_EVOL
  d11 do:f3 wr #0 if #0 igrad EA ip6*2 zd
  lo to 5 times 2
  d11 id10
  d11 id29
  d11 dd30
  lo to 6 times l2
# endif
# ifdef CO_EVOL
  d11 do:f3 wr #0 if #0 id20 ip3 zd
  lo to 7 times l3
# endif
```

individual or combinations of dimensions can be selected by setting the acquisition parameter ZGOPTNS.

NH plane of 4D-HNCOCA experiment



CA plane of 4D-HNCOCA experiment



CO plane of 4D-HNCOCA experiment

hncocagp4d CO plane