

2009 NMR User Training Course I : New Software in HFNMR

Feb. 25, 2009

Part I : Lectures

Place : B1B Meeting Room, IBMS, Academia Sinica, Taipei

10:00-10:50

Introduction to Topspin2.1 by Dr. Casper Wu, Rezwave Co.

11:00-11:50

Application using Topspin2.1: APSY and standard experiments in HFNMR
by Dr. Chi-Fon Chang, HFNMR, Academia Sinica

Part II : Hands-On (Getting start on Topspin2.1)

Place : B1A Conference Room, IBMS, Academia Sinica, Taipei

13:30-14:00

Overview for Practical Session by Dr. Chi-Fon Chang

Tips on using Topspin2.1

Set up HFNMR standard experiments

Set up one APSY experiment

14:00-17:00

Group1 : AV600_CHEM, CHEMISTRY, B1, Academia Sinica (**14:00-15:30**)

Group2: AV600_CHEM, CHEMISTRY, B1, Academia Sinica (**15:30-17:00**)

Group3: AV600L, 1F , GRC, Academia Sinica

Group4: AVIII600, B1A, IBMS

Group5: AV600_IBMS, B1, IBMS

Application using Topspin2.1

APSY & Standard experiments in HFNMRC

Chi-Fon Chang, Ph.D.

02.25.2009

Nice/New functions in Topspin2.1 (few examples)

Example 1: multi windows

Window numbering

L = Lock display
B = BSMS display
<number> appears now in toolbar and inframe icon

The screenshot shows the Bruker TOPSPIN 2.1.1 software interface. The window title bar displays 'Bruker TOPSPIN 2.1.1 on Leda2 as nmrsu'. The toolbar contains various icons, including a green play button, a red 'L' icon, a yellow 'B' icon, and a yellow '2' icon. A red box highlights the 'Acquisition finished:' icon in the toolbar and the '1' icon in the window title bar. A yellow box explains the icons: L = Lock display, B = BSMS display, and <number> appears now in toolbar and inframe icon. The main window displays a spectrum plot and various parameters, including 'Installed probe: 5 mm DUL 13C-1HVD Z-GP D Z3494/345' and 'Program: SFO1 [MHz] 300.1316534'. The status bar at the bottom shows 'Acquisition information: no acquisition running', 'Lock' status, 'Sample' status, 'POWCHK' status, 'Spooler' status, 'BSMS status message: Δ Z3 -5', and 'Time: 12:23 Jan 03'.

Example 2: Acquisition and processing up to 8D

The image shows the Bruker TopSpin software interface. A warning dialog box titled "parmode" is open, displaying the following text:

Warning!

You are about to change the dimension of the current dataset. As a consequence an existing FID will be deleted!

Change acquisition dimension of dataset from 1D to **2D**

Buttons: OK, Cancel

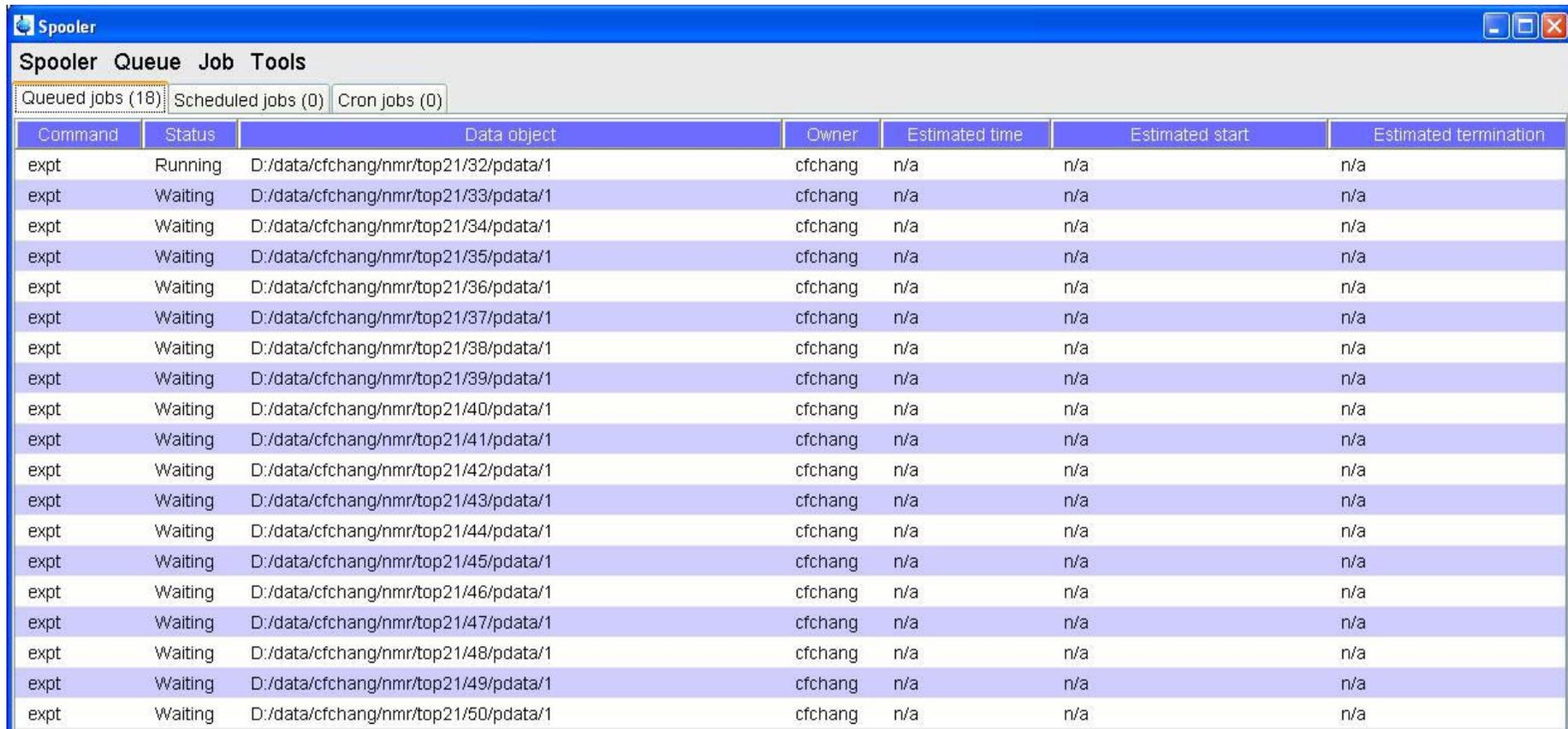
The background window shows the "AcquPARs" window for the dataset "exam1d_13C 1 8 F:\Bruker\topspin2.0". The "Experiment" section is expanded, showing the following parameters:

Parameter	F5	F4	F3	F2	F1	Frequency axis
PULPROG	zgpg30					Current pulse
AQ_mod	DQD					Acquisition mc
FhMODE	undefined	undefined	undefined	undefined	undefined	Acquisition mc
TD	65536	256	256	256	256	Size of fid
NS	256					Number of sca
DS	4					Number of dui
TD0	1					Loop count fo
Width						
SW [ppm]	236.5959	10.3278	10.3278	10.3278	10.3278	Spectral width
SWH [Hz]	17867.143	3099.709	3099.709	3099.709	3099.709	Spectral width
IN_F [μs]		322.61096191	322.61096191	322.61096191	322.61096191	Increment for
AQ [s]	1.8350580	0.0412942	0.0412942	0.0412942	0.0412942	Acquisition tir
FIDRES [Hz]	0.272478	12.106237	12.106237	12.106237	12.106237	Fid resolution
FW [Hz]	90000.00					Filter width
Receiver						
RG	32768					Receiver gain
DW [μs]	29.000					Dwell time

Example 3: Topshim is faster than gradientshim

Example 4: Spooler

(notice that not all commend will show on spooler, ex: multizg won't be there!!!!)



The screenshot shows the Spooler application window with a menu bar (Spooler, Queue, Job, Tools) and a toolbar with buttons for Queued jobs (18), Scheduled jobs (0), and Cron jobs (0). Below the toolbar is a table with the following columns: Command, Status, Data object, Owner, Estimated time, Estimated start, and Estimated termination. The table contains 18 rows of job information, all with a status of 'Waiting'.

Command	Status	Data object	Owner	Estimated time	Estimated start	Estimated termination
expt	Running	D:/data/cfchang/nmr/top21/32/pdata/1	cfchang	n/a	n/a	n/a
expt	Waiting	D:/data/cfchang/nmr/top21/33/pdata/1	cfchang	n/a	n/a	n/a
expt	Waiting	D:/data/cfchang/nmr/top21/34/pdata/1	cfchang	n/a	n/a	n/a
expt	Waiting	D:/data/cfchang/nmr/top21/35/pdata/1	cfchang	n/a	n/a	n/a
expt	Waiting	D:/data/cfchang/nmr/top21/36/pdata/1	cfchang	n/a	n/a	n/a
expt	Waiting	D:/data/cfchang/nmr/top21/37/pdata/1	cfchang	n/a	n/a	n/a
expt	Waiting	D:/data/cfchang/nmr/top21/38/pdata/1	cfchang	n/a	n/a	n/a
expt	Waiting	D:/data/cfchang/nmr/top21/39/pdata/1	cfchang	n/a	n/a	n/a
expt	Waiting	D:/data/cfchang/nmr/top21/40/pdata/1	cfchang	n/a	n/a	n/a
expt	Waiting	D:/data/cfchang/nmr/top21/41/pdata/1	cfchang	n/a	n/a	n/a
expt	Waiting	D:/data/cfchang/nmr/top21/42/pdata/1	cfchang	n/a	n/a	n/a
expt	Waiting	D:/data/cfchang/nmr/top21/43/pdata/1	cfchang	n/a	n/a	n/a
expt	Waiting	D:/data/cfchang/nmr/top21/44/pdata/1	cfchang	n/a	n/a	n/a
expt	Waiting	D:/data/cfchang/nmr/top21/45/pdata/1	cfchang	n/a	n/a	n/a
expt	Waiting	D:/data/cfchang/nmr/top21/46/pdata/1	cfchang	n/a	n/a	n/a
expt	Waiting	D:/data/cfchang/nmr/top21/47/pdata/1	cfchang	n/a	n/a	n/a
expt	Waiting	D:/data/cfchang/nmr/top21/48/pdata/1	cfchang	n/a	n/a	n/a
expt	Waiting	D:/data/cfchang/nmr/top21/49/pdata/1	cfchang	n/a	n/a	n/a
expt	Waiting	D:/data/cfchang/nmr/top21/50/pdata/1	cfchang	n/a	n/a	n/a

(click on Spooler → you can check or modify the running status)

qumulti

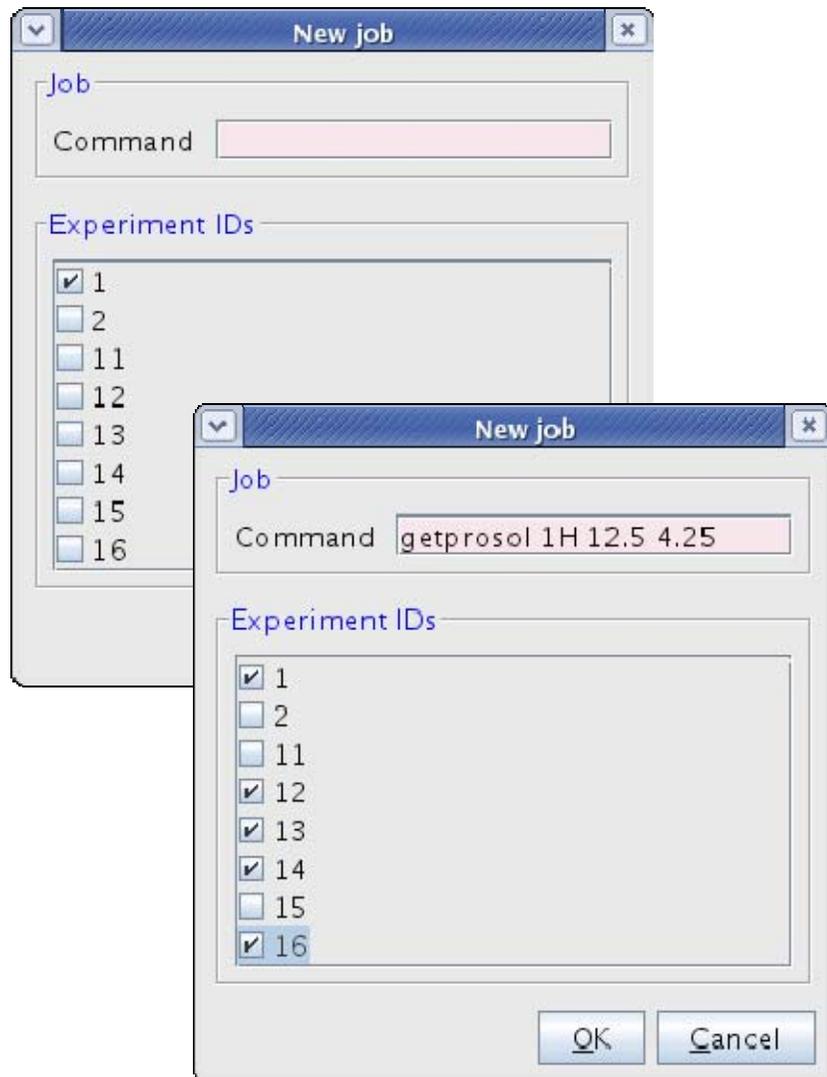
可以下同一個指令給多個實驗



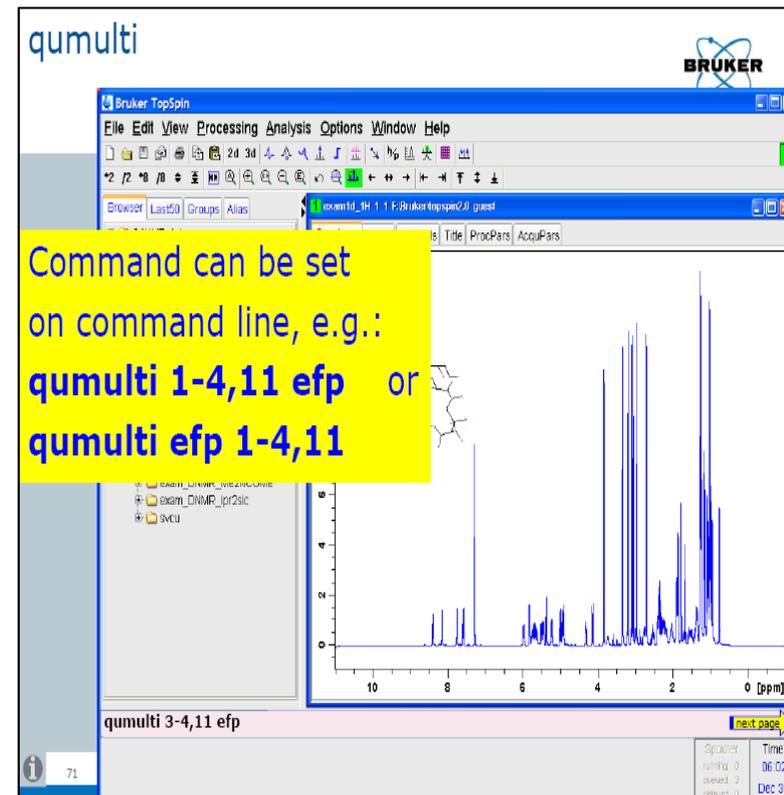
Each expno can be added manually to the dataset list.

The screenshot shows the Bruker TopSpin software interface. A 'New job' dialog box is open, showing the 'Command' field set to 'efp' and the 'Experiment IDs' list with checkboxes for 1, 3, 4, and 11. The '11' checkbox is selected. The background shows a chemical structure and an NMR spectrum. The dataset list on the left includes 'exam2d_HH', 'exam3d', 'exam_DNMR_Me2NCDMe', 'exam_DNMR_jpr2sic', and 'svcu'. The status bar at the bottom shows 'qumulti' and a 'next page' button.

> qumulti



> qumulti 1-4,11 efp



> qu efp

atmulti

可以下同一個指令給多個實驗;並指定開始的時間



Same functionalities
are available for the
list of delayed jobs
with command:
atmulti

New schedule

Schedule

Command

Time

Date

Experiment IDs

- 1
- 3
- 4
- 11

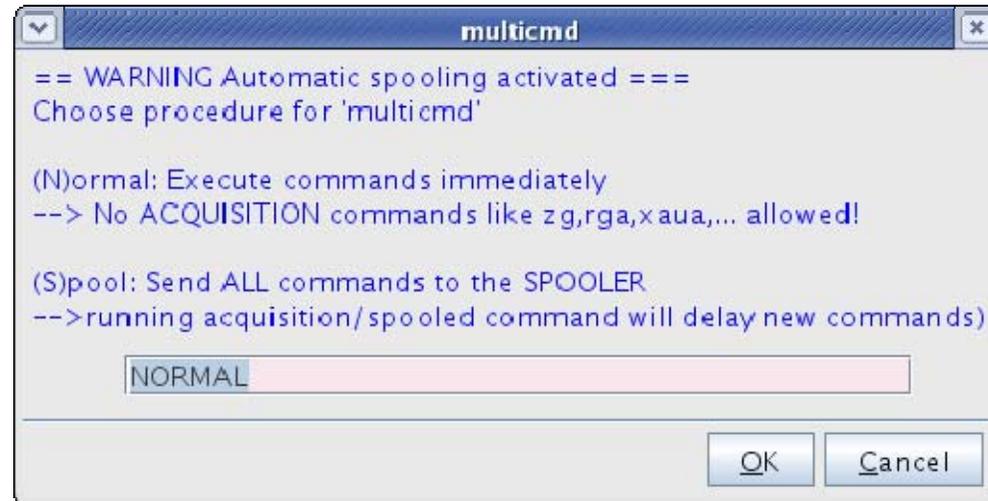
next page

OK Cancel Spin



multicmd

可以下多個指令給多個實驗



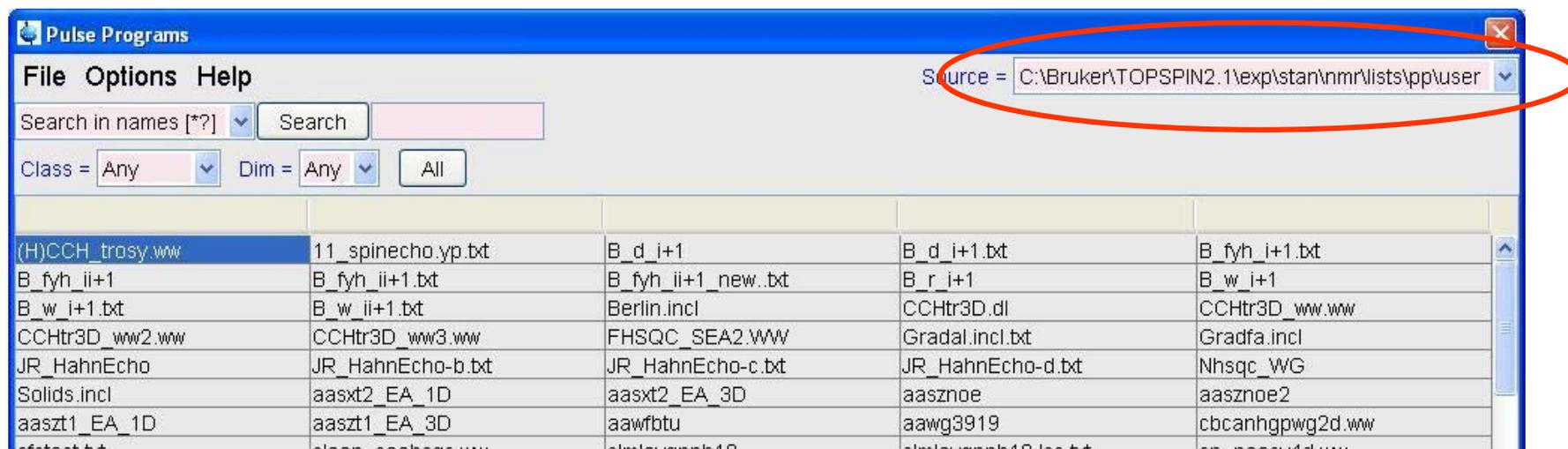
Example 5: “Users” directory for pulseprogram and parameter set

Bruker default pulse program directory (xxx\Topspin2.1\exp\stan\nmr\list\pp)

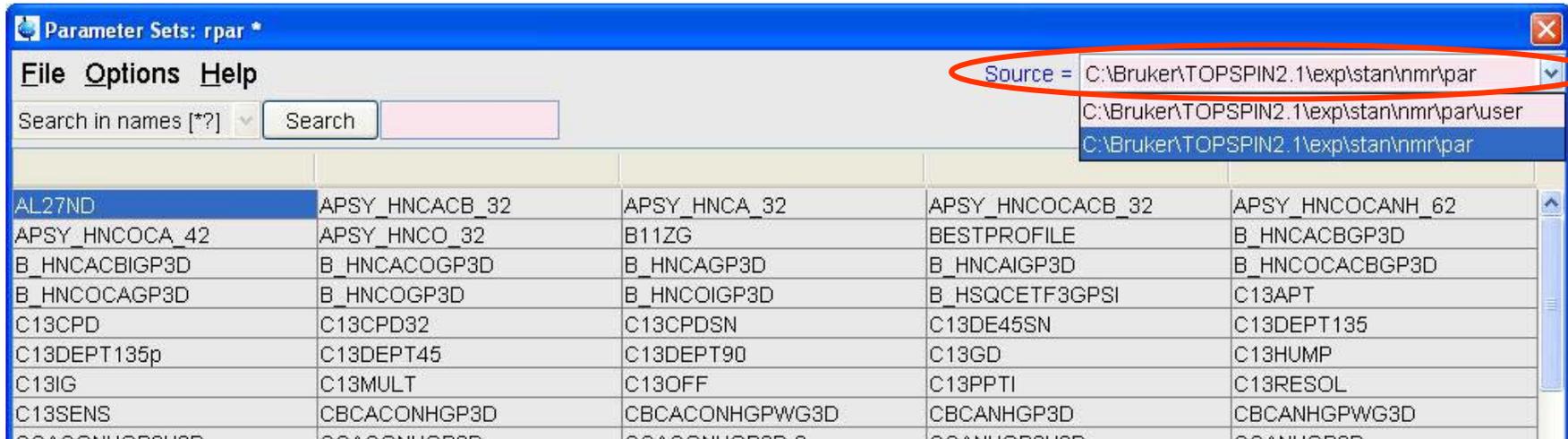


User's Pulse program directory

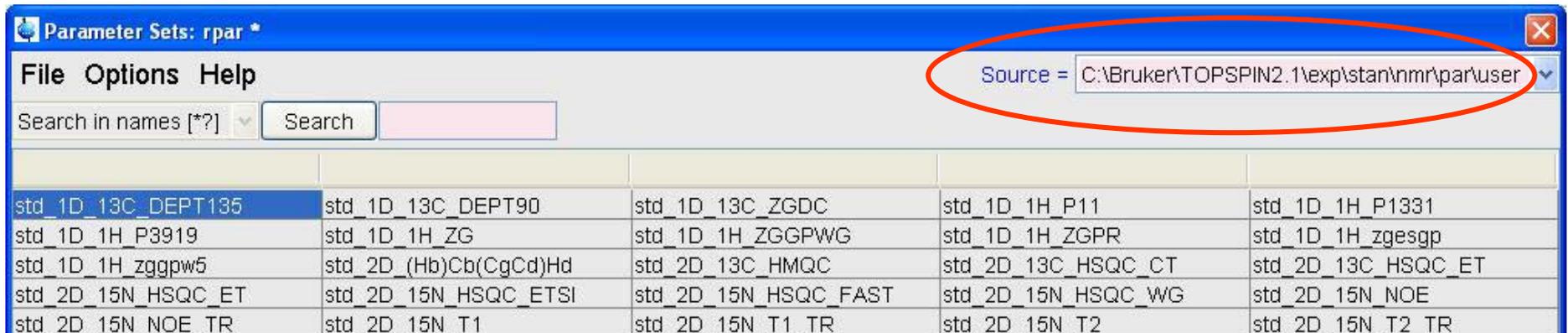
(HFNMRC staff or users : xxx\Topspin2.1\exp\stan\nmr\list\pp\user)



Bruker default Parameter Set directory (xxx\TOPSPIN2.1\exp\stan\nmr\par)



HFNMRC standard Parameter Set directory (xxx\TOPSPIN2.1\ejxjp\stan\nmr\par\user)



Example 6: new pulseprogram (Music type)

Pulse Programs

File Options Help

Source = /opt/topspin/exp/stan/nmr/lists/pp

Search in names [??] Search

Class = Any Dim = Any

All

music_cm_3d	music: Met(M) 3D sequence with inverse correlation for triple resonance using inept transfer steps CH2 selection F1(H(CH ₂)) ->
music_cm_3d_2	music: Met(M) 3D sequence with inverse correlation for triple resonance using inept transfer steps CH2 selection F1(H(CH ₂)) ->
music_de_3d	music: Asp(D) or Glu(E) 3D sequence with inverse correlation for triple resonance using inept transfer steps CH2 selection F1(H(CH ₂)) ->
music_de_3d_2	music: Asp(D) or Glu(E) 3D sequence with inverse correlation for triple resonance using inept transfer steps CH2 and CON selection
music_fhyw_3d	music: Phe(F)/His(H)/Tyr(Y) or Trp(W) 3D sequence with inverse correlation for triple resonance using inept transfer steps CH2 selection
music_fhyw_3d_2	music: Phe(F)/His(H)/Tyr(Y) or Trp(W) 3D sequence with inverse correlation for triple resonance using inept transfer steps CH2 selection
music_gly_3d	music: Gly(G) and/or Asn(N)/Gln(Q) sidechain 3D sequence with inverse correlation for triple resonance using inept transfer steps CH2
music_gly_3d_2	music: Gly(G) and/or Asn(N)/Gln(Q) sidechain 3D sequence with inverse correlation for triple resonance using inept transfer steps CH2
music_ile_3d	music: Ile(I) 3D sequence with inverse correlation for triple resonance using inept transfer steps CH3 selection F1(H(CH ₃)) -> F2(C->->Ca,t1)
music_ile_3d_2	music: Ile(I) 3D sequence with inverse correlation for triple resonance using inept transfer steps CH3 selection F1(H(CH ₃)) -> F2(C->->Ca,t1)
music_kr_3d	music: Lys(K) and/or Arg(R) 3D sequence with inverse correlation for triple resonance using inept transfer steps F1(H) -> F2(C->->Ca,t1) ->
music_kr_3d_2	music: Lys(K) and/or Arg(R) 3D sequence with inverse correlation for triple resonance using inept transfer steps F1(H) -> F2(C->->Ca,t1) ->
music_lavia_3d	music: Leu(L)/Ala(A) or Val(V)/Ile(I)/Ala(A) 3D sequence with inverse correlation for triple resonance using inept transfer steps CH3 selection
music_lavia_3d_2	music: Leu(L)/Ala(A) or Val(V)/Ile(I)/Ala(A) 3D sequence with inverse correlation for triple resonance using inept transfer steps CH3 selection
music_pro_1_3d	music: Pro 3D sequence with inverse correlation for triple resonance using inept transfer steps F1(Ha) -> F2(Ca) -> F2(C=O) -> F3(N(Pro),t1)
music_pro_1_3d.2	music: Pro 3D sequence with inverse correlation for triple resonance using inept transfer steps F1(Ha) -> F2(Ca) -> F2(C=O) -> F3(N(Pro))
music_pro_2_3d	music: Pro 3D sequence with inverse correlation for triple resonance using inept transfer steps F1(Ha) -> F2(Ca) -> F3(N(Pro),t1) > F2(Ca) ->
music_pro_2_3d.2	music: Pro 3D sequence with inverse correlation for triple resonance using inept transfer steps F1(Ha) -> F2(Ca) -> F3(N(Pro)) > F2(Ca,t1) ->
music_qn_3d	music: Gln(Q) and/or Asn(N) 3D sequence with inverse correlation for triple resonance using inept transfer steps NH2 selection F1(H(NH ₂))
music_qn_3d_2	music: Gln(Q) and/or Asn(N) 3D sequence with inverse correlation for triple resonance using inept transfer steps NH2 selection F1(H(NH ₂))
music_ser_3d	music: Ser 3D sequence with inverse correlation for triple resonance using inept transfer steps CH2 selection F1(H(CH ₂)) -> F2(C->->Ca,t1)
music_ser_3d_2	music: Ser 3D sequence with inverse correlation for triple resonance using inept transfer steps CH2 selection F1(H(CH ₂)) -> F2(C->->Ca,t1)
music_tavi_3d	music: Val(V)/Ile(I) and/or Thr(T)/Ala(A) music: 3D sequence with inverse correlation for triple resonance using inept transfer steps CH3
music_tavi_3d_2	music: Val(V)/Ile(I) and/or Thr(T)/Ala(A) 3D sequence with inverse correlation for triple resonance using inept transfer steps CH3 selection
music_trpe_2d	music: Trp(W)e 2D sequence with inverse correlation for triple resonance using inept transfer steps F1(H(Ne)) -> F3(Ne) -> F2(Ce) ->

OK Cancel Edit

Example 6: new pulseprogram (for APSY & 4D experiments)

File Options Help Source = /opt/topspin/exp/stan/nmr/lists/pp

Search in names [??] Search

Class = Any Dim = Any

All

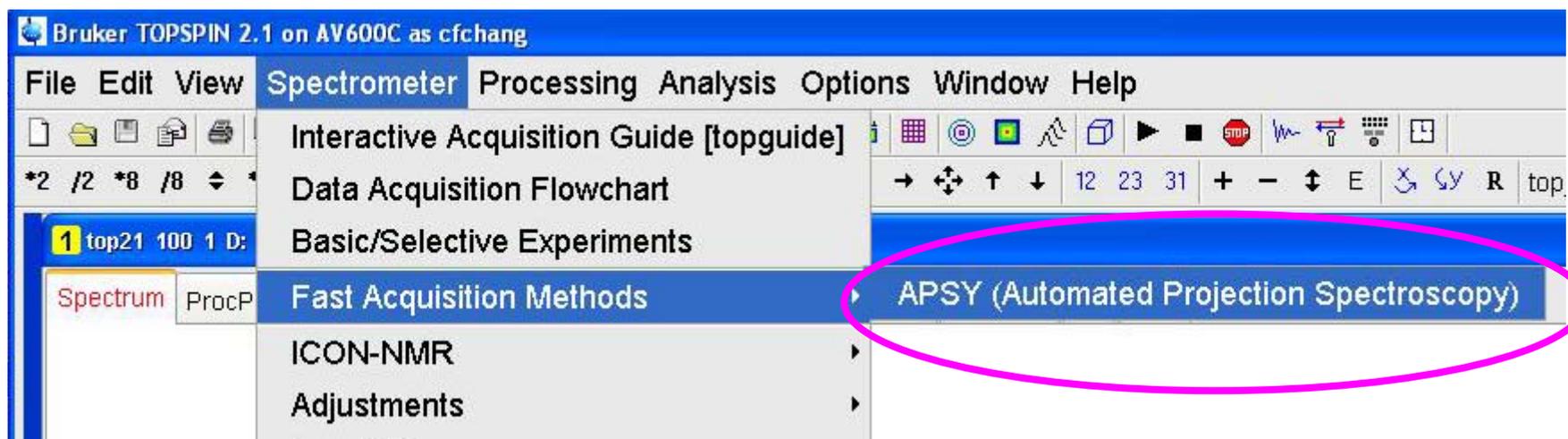
rd_hnca_32	3,2 RD-HNCA (APSY) 3D sequence with inverse correlation for triple resonance using multiple inept transfer steps F1(H) -> F3(N) -> F2(Ca,t1)
rd_hncacb_32	3,2 RD-HNCACB (APSY) 3D sequence with inverse correlation for triple resonance using multiple inept transfer steps F1(H) -> F3(N) -> F2(Ca
rd_hnco_32	3,2 RD-HNCO (APSY) 3D sequence with inverse correlation for triple resonance using multiple inept transfer steps F1(H) -> F3(N) ->
rd_hncoca_42	4,2 RD-HNCOCA (APSY) 4D sequence with inverse correlation for triple resonance using multiple inept transfer steps F1(H) -> F3(N) ->
rd_hncocacb_32	3,2 RD-HNCOACB (APSY) 3D sequence with inverse correlation for triple resonance using multiple inept transfer steps F1(H) -> F3(N) ->
rd_hncocanh_62	6,2 RD-seq.-HNCOCANH (APSY) 6D sequence with inverse correlation for triple resonance using multiple inept transfer steps F1(H, t1) ->

differences to 07/07/16

added hsqcnoesyhsqcncgp4d 4D HSQC-NOESY-HSQC
 hsqcnoesyhsqcccgp4d
 hsqcnoesyhsqccngp4d
 hsqcnoesyhsqcngp4d

OK Cancel Edit

Example 7: APSY



S. Hiller, F. Fiorito, K. Wüthrich and G. Wider, Proc. Nat. Acad. Sci. USA 102, 10876-10881 (2005).

Automated Projection Spectroscopy (APSY).

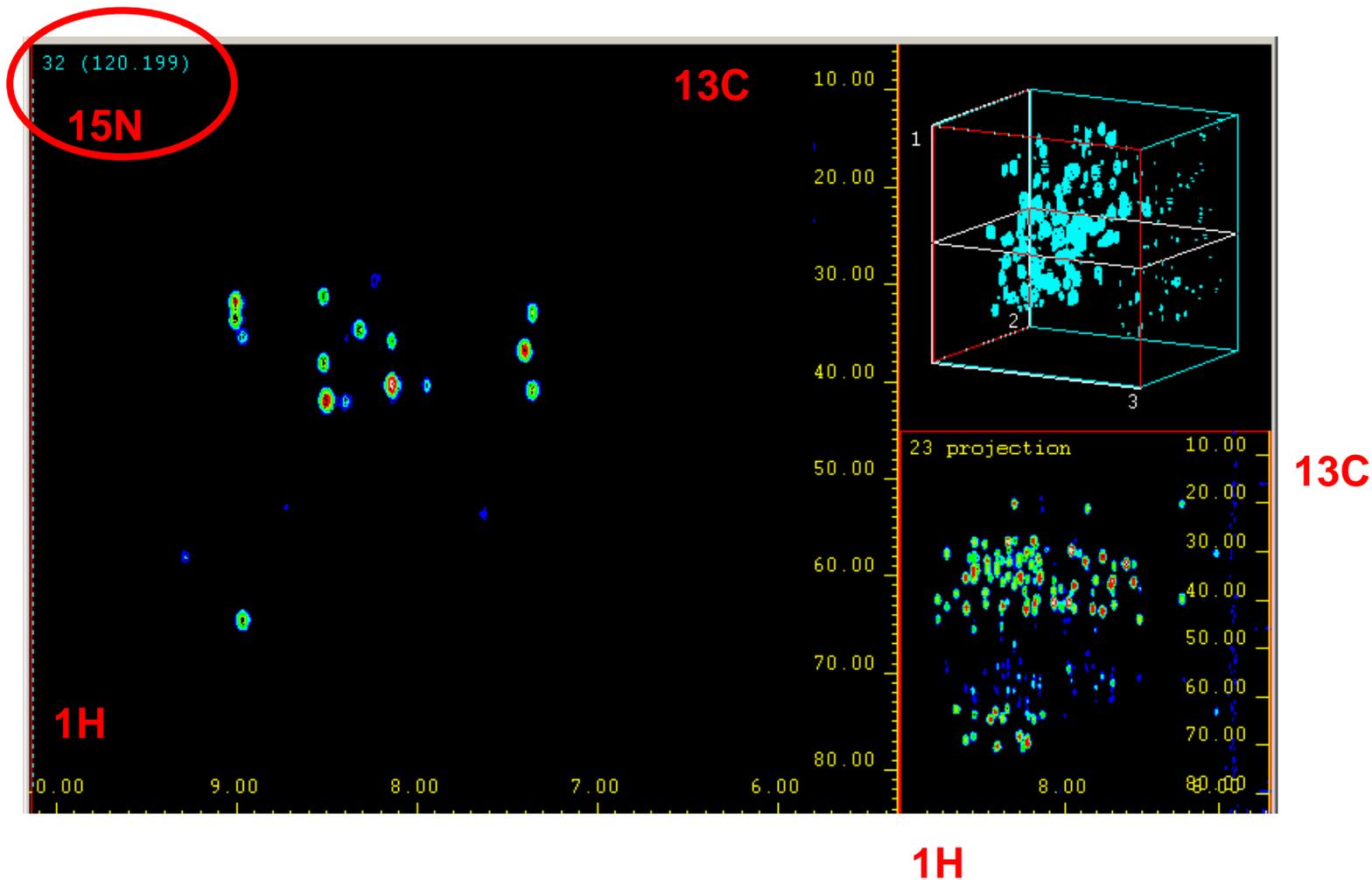
Brief Introduction to APSY

Automated Projection Spectroscopy (APSY)

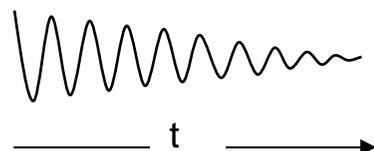
Part I: Acquisition using Projection Spectroscopy

Background:

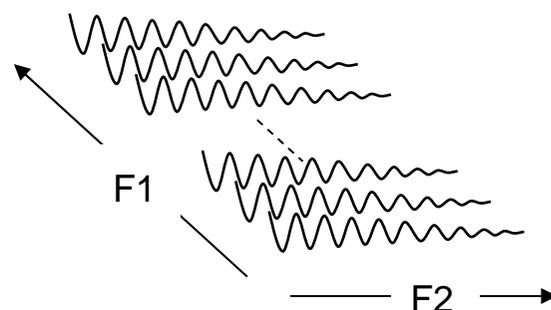
- Multidimensional NMR could help to solve the problem of overlapping



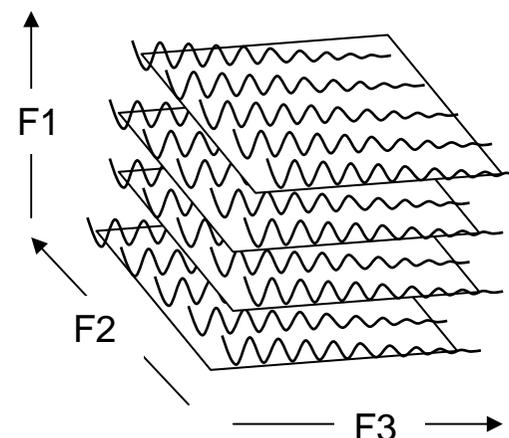
• However, multidimensional NMR is time consuming



一維實驗
1個FID, $t=30$ 秒



二維實驗
如 $F1=128$, i.e. 128個FID
則需 64分鐘



三維實驗
如 $F1=128$, $F2=64$
 $128*64$ 個FID, 則需 68.2小時

• How could we keep the resolution and also save the machine time?

→ Rapid Acquisition Methods !!

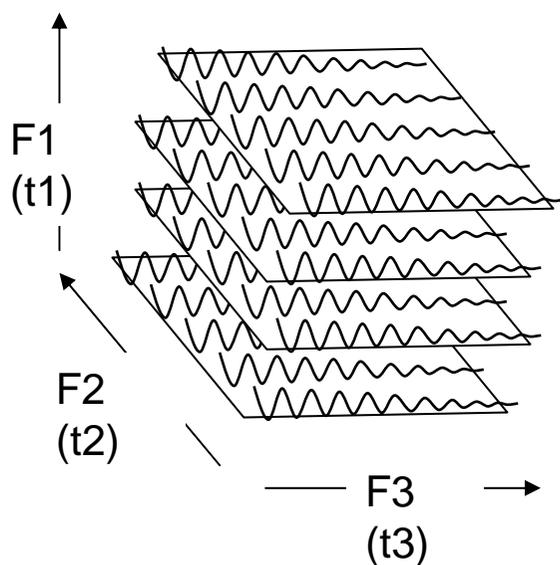
最新公告	活動公告
注意事項	<ul style="list-style-type: none"> • 2009 NMR User Training Course I : New Software in HFNMR... 報名時效已過 (2009.2.25) • 2008 NMR User Training Course II : Introduction to Fast NMR methods ... 報名時效已過 (2008.7.25) • 2007 NMR Users Training Course : Advanced NMR Topics - Introduction to Projection Reconstruction NMR ... 報名過
活動公告	

Method: Projection Spectroscopy

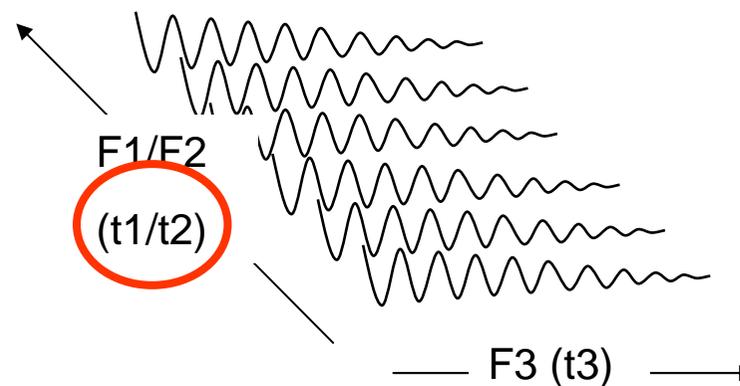
傳統三維實驗



三維縮減成二維實驗



傳統三維實驗
t1及t2 各自獨立增加



維度縮減實驗
t1及 t2 若同時增加
則可共用同一維度

Method: Projection Spectroscopy

$$t_1 = t \cdot \sin(\alpha) \quad \& \quad t_2 = t \cdot \cos(\alpha)$$

Example: 3D HNCO experiment

single evolution during t_1 only:

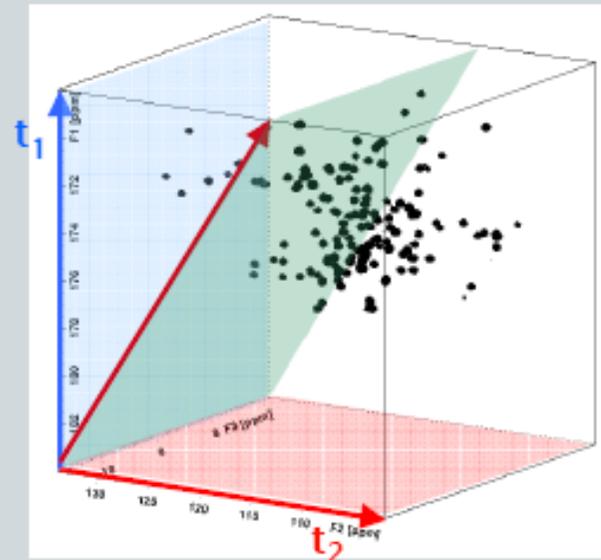
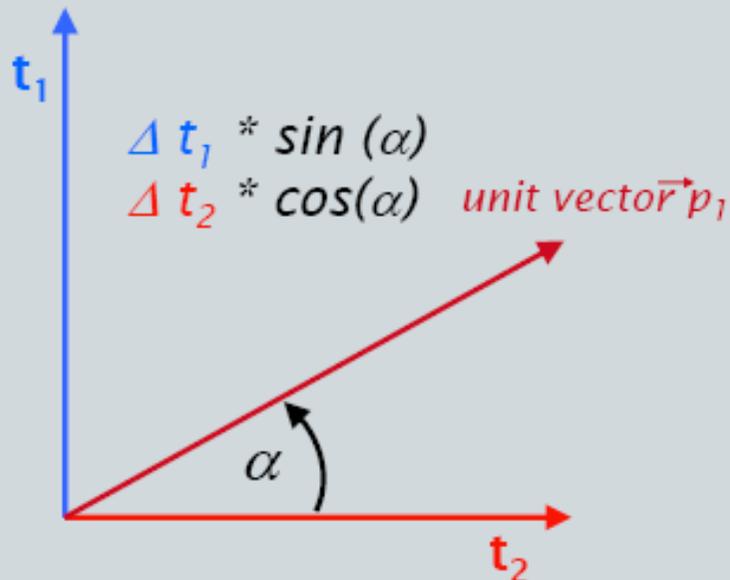
2D H,C plane ($\alpha = 90^\circ$)

single evolution during t_2 only:

2D H,N plane ($\alpha = 0^\circ$)

simultaneous evolution during t_1 and t_2 :

2D H,NC plane ($\alpha = n^\circ$)



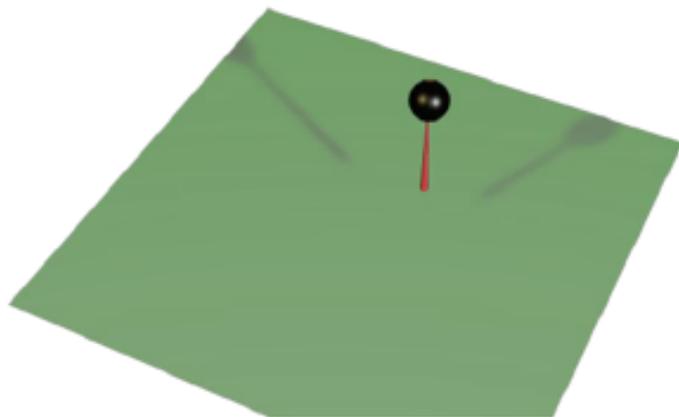
Method: Projection Spectroscopy

Consequence of **Reduction of dimensionality**:

Shift information of reduced dimensions is lost, but:

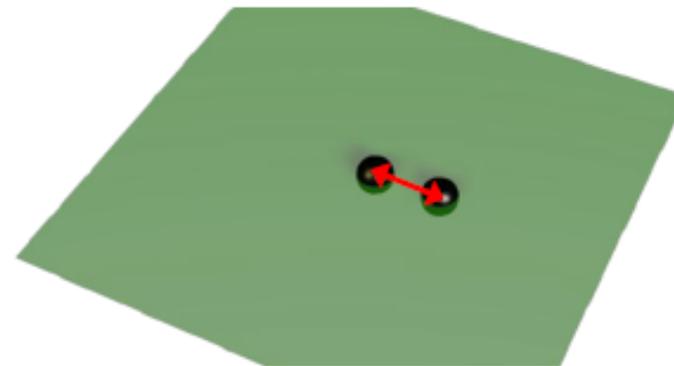
- Shift information is coded as a distance
- By additional splitting of single peaks

2-dimensional, one selected peak
With information about shift in Z



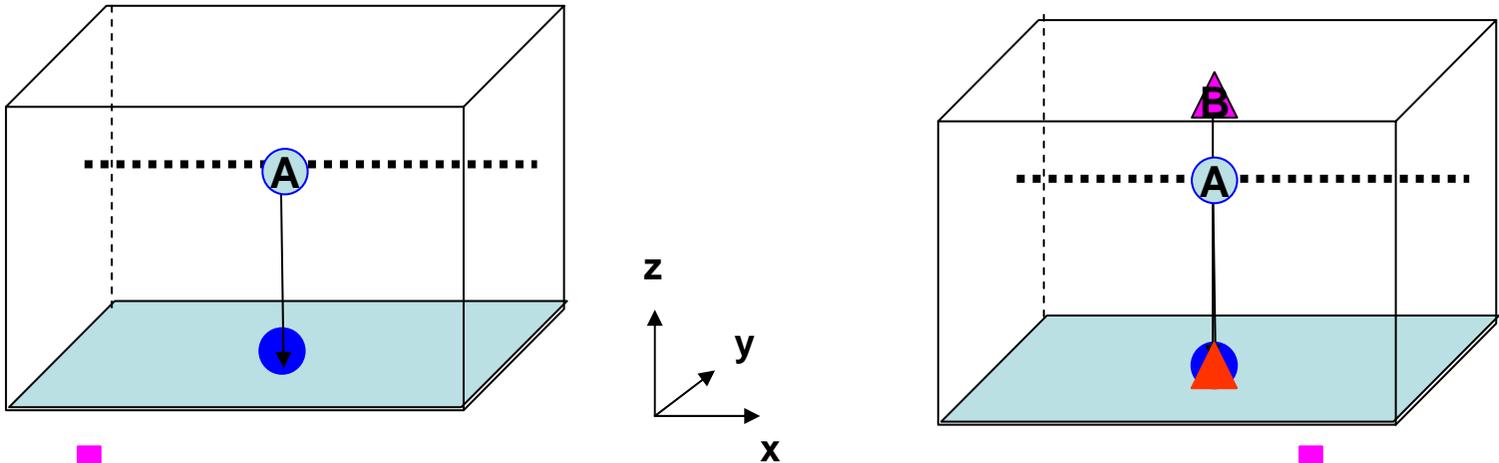
dimensionality:
full

2-dimensional, one selected peak
Information about shift in Z coded
in a **distance**

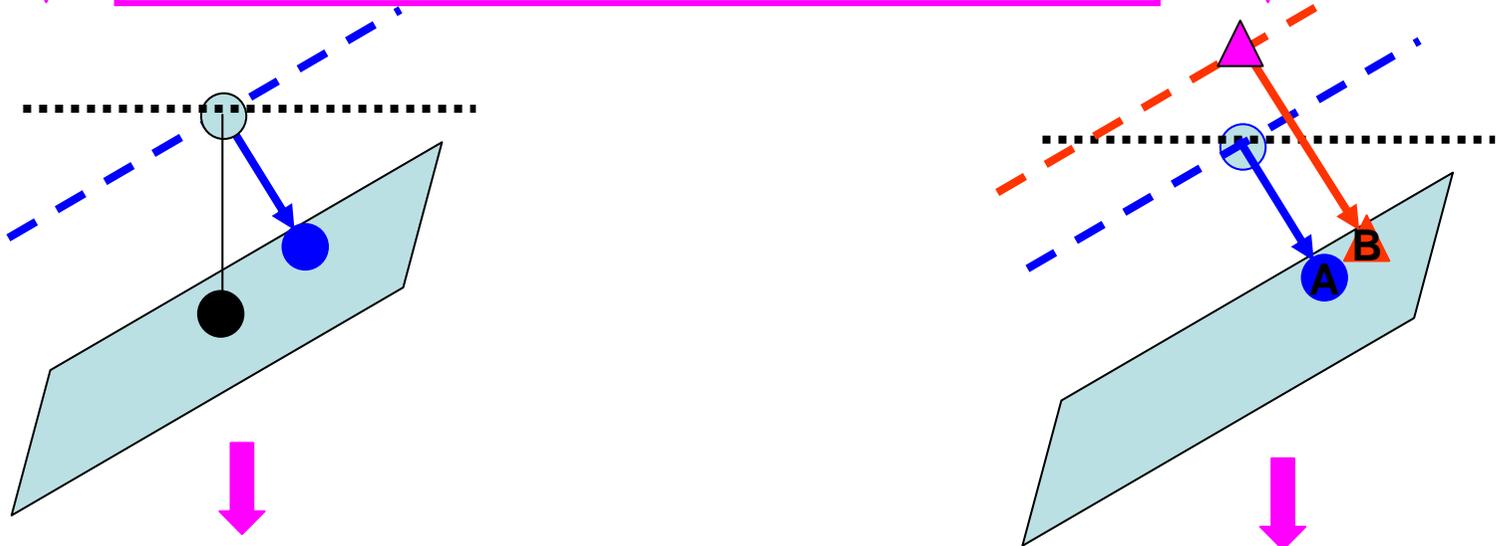


dimensionality:
reduced

Projection of peaks in 3D box to XY Plane



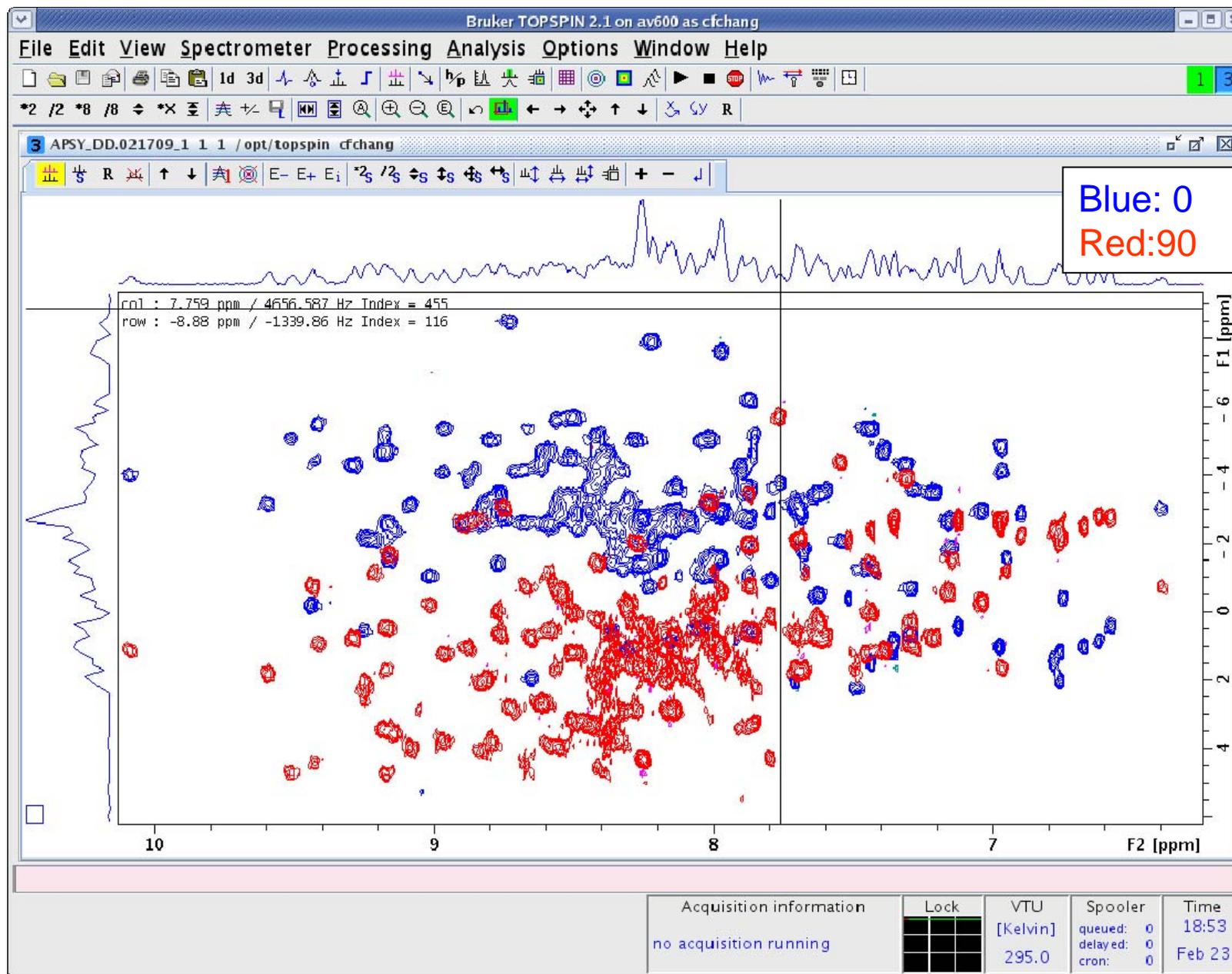
Projection of peaks in 3D box to 30deg Plane

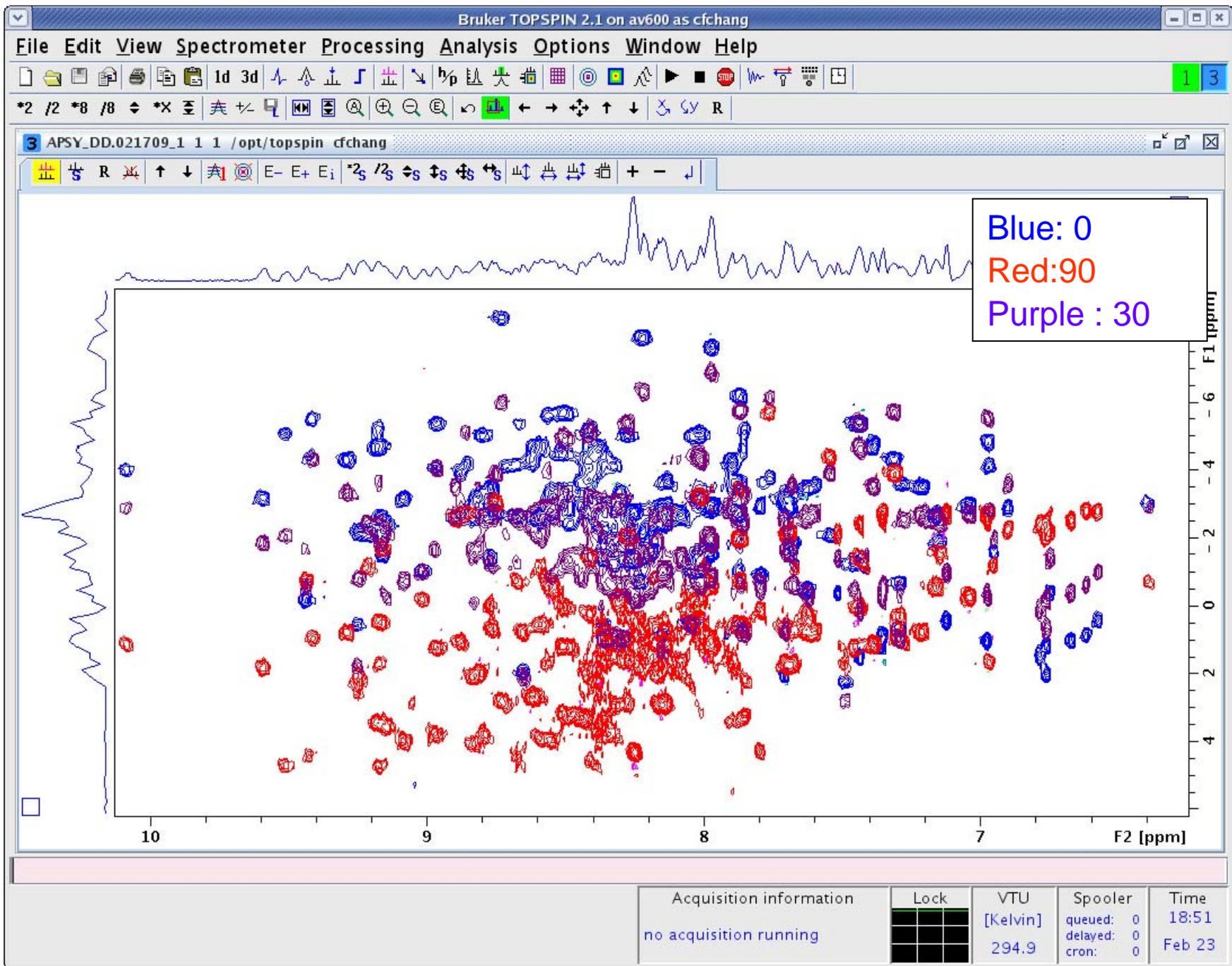


Peak's information on Z-axis is coded in distance of peaks at different projection angles

Overlap in XY could be resolved by different projection angles

Method: Projection Spectroscopy

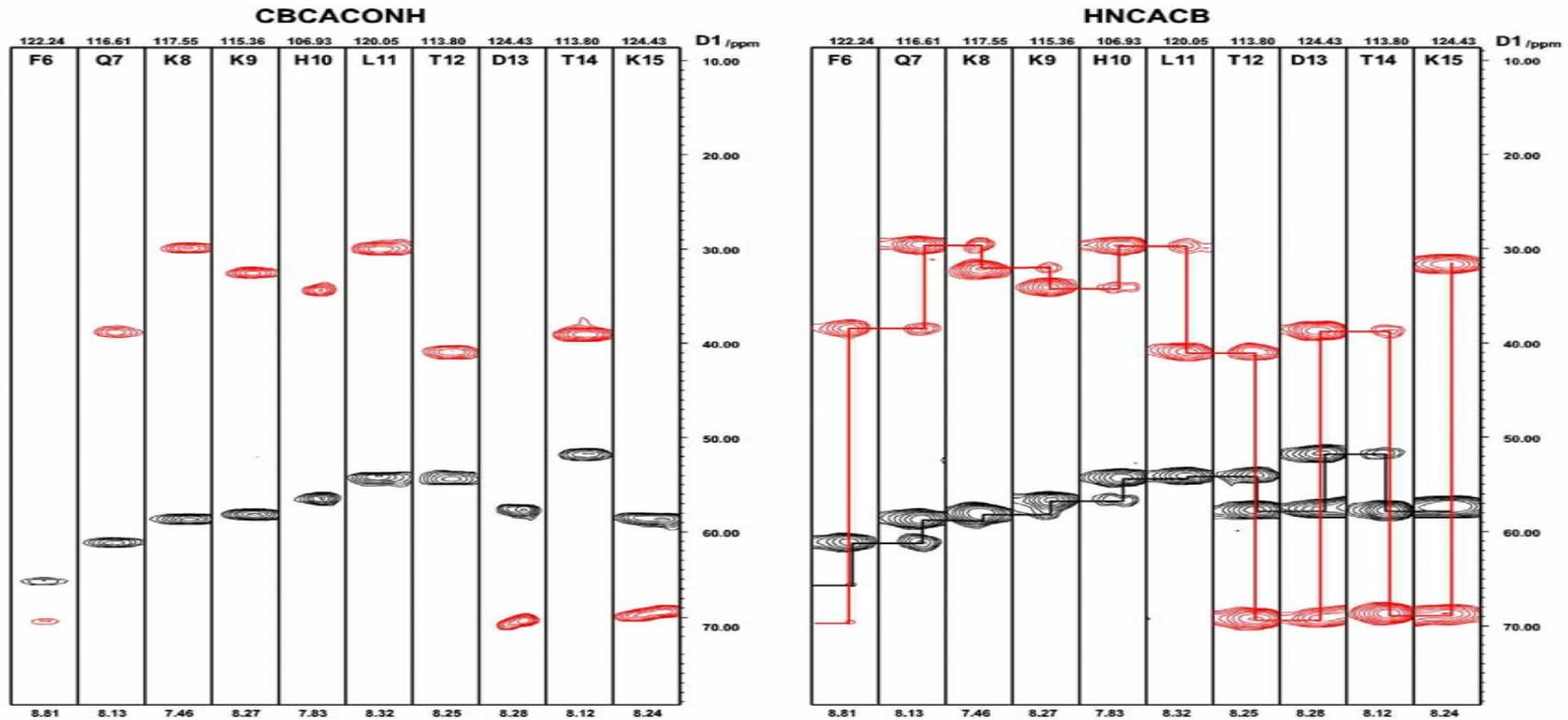




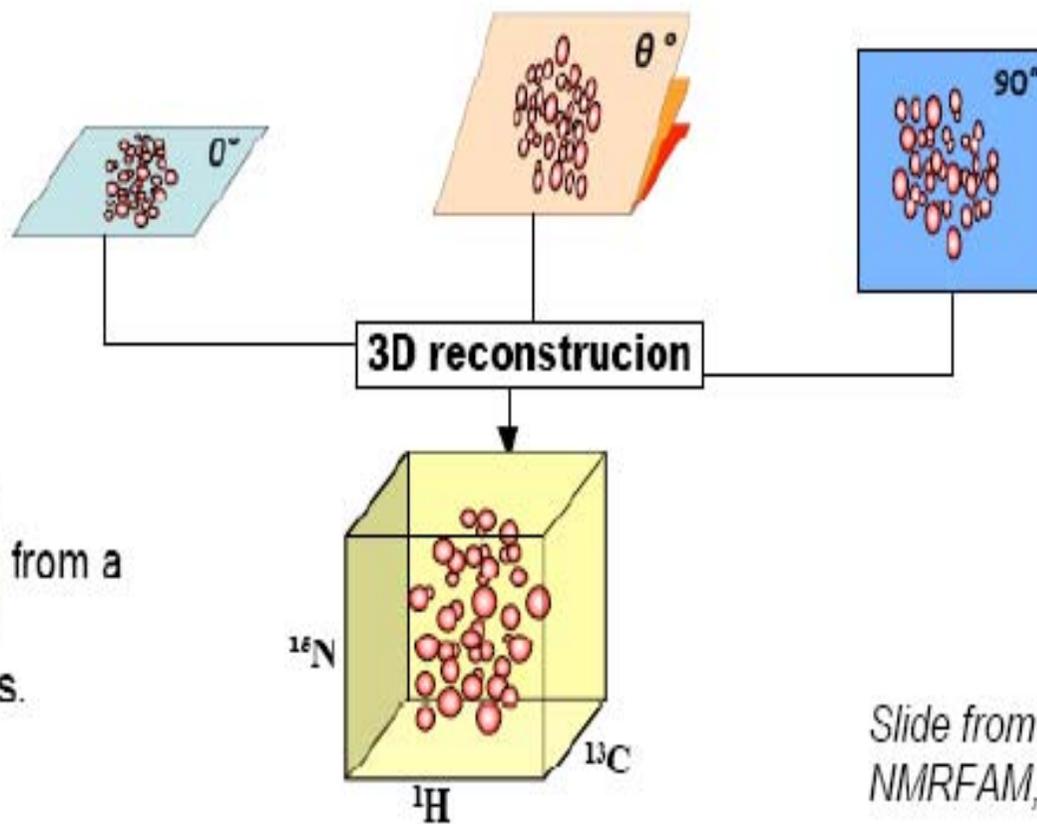
Part II: Automatic data analysis

Background:

- What we need is a peak lists with all chemical shift information
- Then, based on the peaks correlation between different spectra, chemical shift could be assigned



- Projection –Reconstruction Method



In principle, it is feasible to reconstruct a 3D spectrum from a number of 2D tilted planes collected at different angles.

*Slide from M. Tornelli
NMRFAM, UW-Madison*

- After reconstruction, go through traditional 3D data analysis process

Method: Automatic peak analysis

ATNOS : Peak picking program

- Pick peaks for each projection spectrum

GARPO: Geometric Analysis of Projections

Proc. Nat. Acad. Sci. USA 102, 10876-10881 (2005).

- Analyze all peaks from different angles, and select real peaks

Output: Final Peak List

```
28 *****
29 *** NOH. peaks ***
30 *****
31 # Number of dimensions 3
32 #INAME 1 N
33 #INAME 2 O
34 #INAME 3 H
35      1      114.5913      168.7465      7.4410 1 U  0.000E+00  0.000E+00 e 0  0  0  0  0
36      2      118.4312      173.2002      7.7997 1 U  0.000E+00  0.000E+00 e 0  0  0  0  0
37      3      126.6306      169.4641      9.1843 1 U  0.000E+00  0.000E+00 e 0  0  0  0  0
38      4      116.7820      171.1912      8.5505 1 U  0.000E+00  0.000E+00 e 0  0  0  0  0
39      5      122.6248      171.1549      7.7035 1 U  0.000E+00  0.000E+00 e 0  0  0  0  0
40      6      118.0694      175.2307      8.3105 1 U  0.000E+00  0.000E+00 e 0  0  0  0  0
41      7      120.6934      170.2307      8.8864 1 U  0.000E+00  0.000E+00 e 0  0  0  0  0
42      8      110.6688      171.3524      8.7585 1 U  0.000E+00  0.000E+00 e 0  0  0  0  0
43      9      116.7303      166.4779      7.9777 1 U  0.000E+00  0.000E+00 e 0  0  0  0  0
44     10      111.4506      174.4963      6.5844 1 U  0.000E+00  0.000E+00 e 0  0  0  0  0
45     11      111.2100      174.2705      6.5253 1 U  0.000E+00  0.000E+00 e 0  0  0  0  0
```

Summary for APSY

Set up a “parent”
experiment
(with optimize AQ and
Process parameters)

Collect different
projection angles
(based on “parent”
eda setting)

FT each projection
plan (based on “parent”
edp setting)

PK each projection
plan and Analyze all
peak list
Final Peak List

- The same as setting up regular experiment

- Define the projection angles (use default values)

- Could run all angles or let the program decide how many angles to collect

- Automatic FT (xfb)

- Change edp setting and re-process if necessary

- Automatic analyzing and show Result

- Change GARPO setting and re-analyze if necessary

Running APSY in HFNMRC

NMRs in HFNMRC

System	AV500_ IBMS	AV600_ IBMS	AV600_ CHEM	AVIII600_ IBMS	AV800_ IBMS
Hardware	AVANCE Cryoprobe	AVANCE Cryoprobe	AVANCE	AVANCEIII Cryoprobe ATM	AVANCE Cryoprobe
Operation	Linux*	Linux	Windows	Linux	Linux*
Software	Topshin2.1*	Topshin2.1	Topshin2.1	Topshin2.1	Topshin2.1*
APSY	YES *	YES	NO (demo)	YES	YES *
Process using Xwinmr?	YES	YES	YES	NO	YES
BSMS Keyboard	YES	YES	YES	NO	YES

* Will be available in March, 2009

How to run APSY in HFNMR

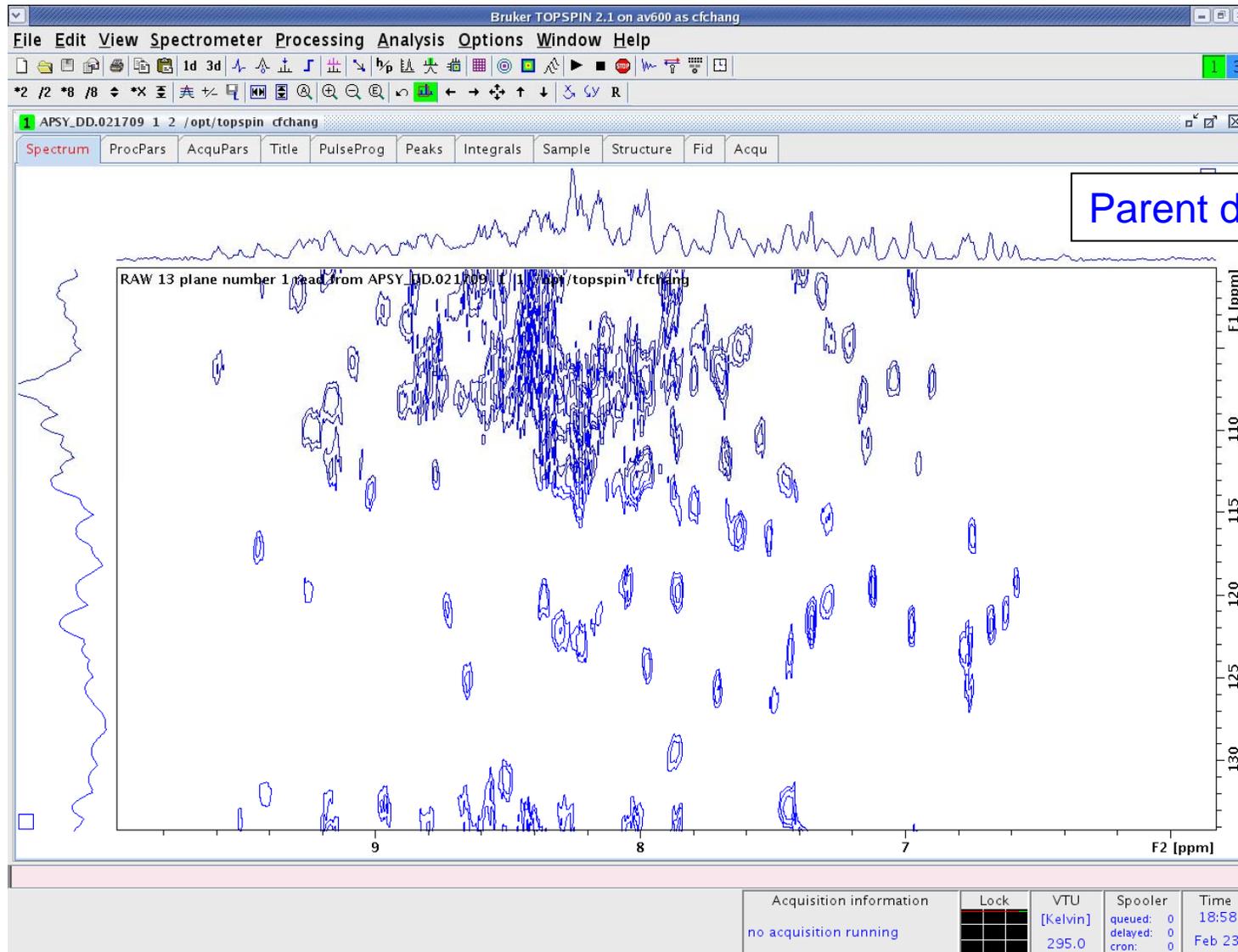
Set up a “parent”
experiment
(with optimize AQ and
Process parameters)

STEP1 : rpar std1_APSY*

The screenshot shows the Bruker TOPSPIN 2.1 software interface. The main window displays the title bar "Bruker TOPSPIN 2.1 on av600 as cfchang" and a menu bar with "File", "Edit", "View", "Spectrometer", "Processing", "Analysis", "Options", "Window", and "Help". Below the menu bar is a toolbar with various icons. The main workspace shows the file name "5 APSY_DD.021709 1 1 /opt/topspin cfchang" and a tabbed interface with "Spectrum", "ProcPars", "AcquPars", "Title", "PulseProg", "Peaks", "Integrals", "Sample", "Structure", "Fid", and "Acqu". The "Spectrum" tab is active, showing the text "APSY_HNCO_32 (3D to 2D) rd_hnco_32". A search dialog box is open in the foreground, titled "File Options Help", with a search field containing "std1_APSY*" and a "Search" button. The search results list several files, with "std1_APSY-HNCO_rd_hnco_32" highlighted in red.

File Name
std1_APSY-HN(CO)CACB_rd_hnco_cacb_32
std1_APSY-HN(CO)CA_rd_hnco_caca_42
std1_APSY-HNCACB_rd_hncacb_32
std1_APSY-HNCA_rd_hnca_32
std1_APSY-HNCOCANH rd_hnco_canh_62
std1_APSY-HNCO_rd_hnco_32

STEP2 : set up eda and edp , then collect the “parent” spectrum

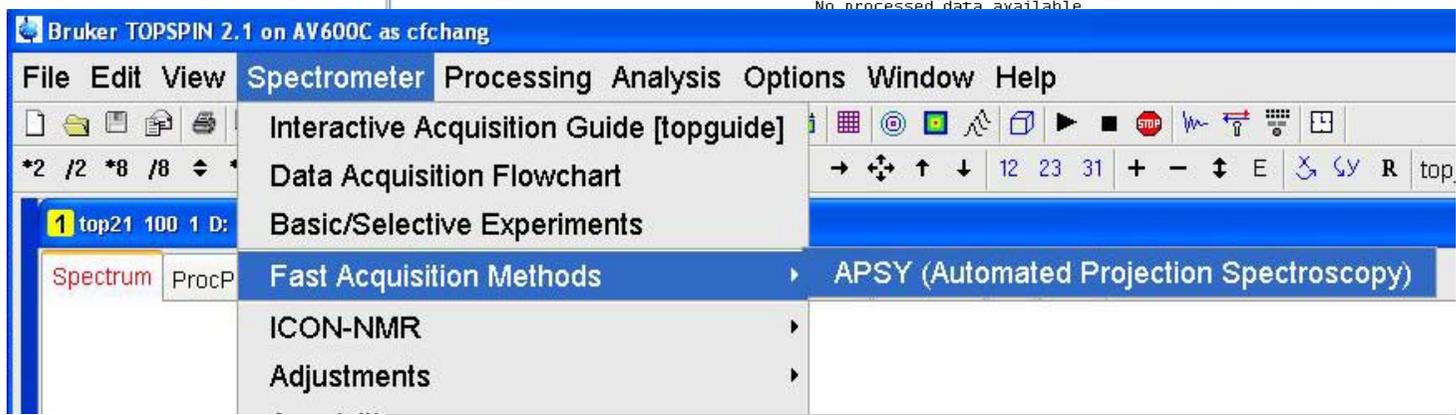
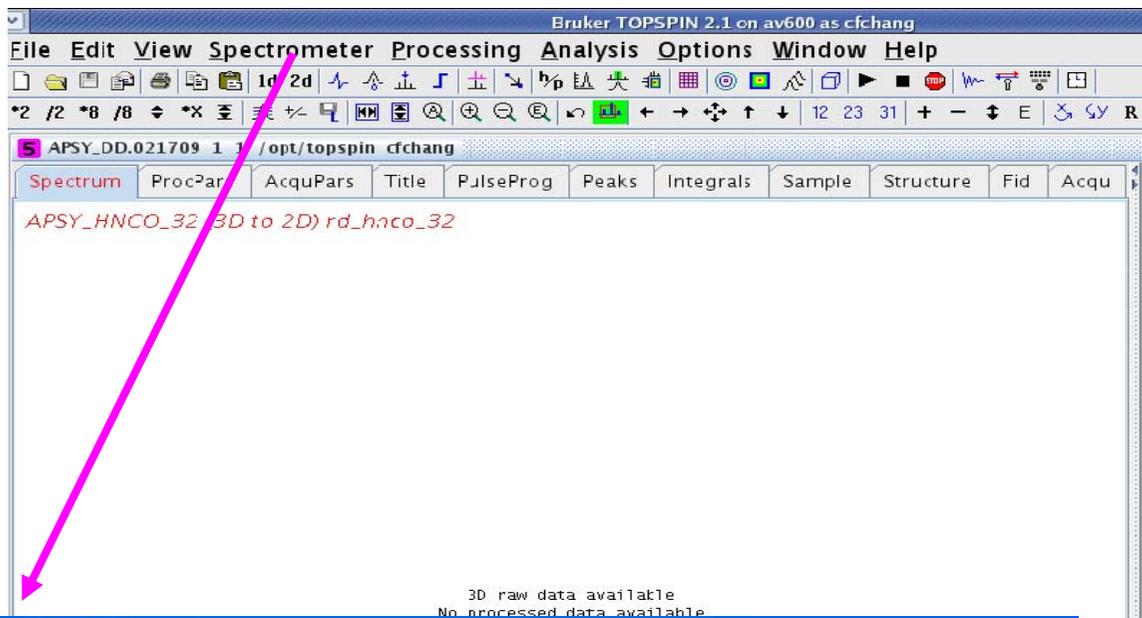


How to run APSY in HFNMR

Set up a "parent" experiment
(with optimize AQ and Process parameters)

Collect different projection angles
(based on "parent" eda setting)

STEP3 : open APSY manual



STEP4 : Set up different projection angles

The screenshot shows the Bruker TOPSPIN 2.1 interface. The main window displays the file `APSY_DD.021709 1 1 /opt/topspin cfchang`. The `APSY Management` panel on the right contains several buttons, with `Setup Proj. Angles [From Parent]` circled in pink. A pink arrow points from this button to the `angles.dat` file editor window. The editor shows the following content:

```
File Edit Search
/opt/topspin/data/cfchang/nmr/APSY_DD.021709/1/angles.dat
1 #Filename: AnglesFile_Dimensionality3.txt
2 #Location: <TOPSHIMHOME>/ApsyDir/Templates
3 #Creation: 25jan07,pgs,vs 0.20
4 #Modification: 02mar07,pgs,vs 0.25 (removed #No index)
5 #RunLocation: Starting DATASET of APSY-RUN
6 #RunName: angles.dat
7 #-----
8 #Structure: Angle=Alpha
9 #Range: 0 <= Alpha <= 90
10 # ==> lines starting with # are considered as comments
11 # ==> blank lines are skipped
12 # ==> lines containing less than one element are skipped
13 #-----
14 #File for Dimensionality 3
15 #
16 #Alpha
17 #---
18 0
19 90
20 30
21 60
22 20
23 70
24 40
25 50
26 10
27 80
28 55
29 35
30
```

A pink box highlights the list of angles in the editor. A text box at the bottom right explains the list:

0,90, +/- 30, +/- 60, +/- 20, +/- 70, +/- 40, +/- 50, +/- 10, +/- 80, +/- 55, +/- 35 → 22 angles

STEP5 : Set up GARPRO parameters



```
File Edit Search /opt/topspin/data/cfchang/nm
1 #Filename: TemplateParameterGapro.txt
2 #Location: <TOPSHIMHOME>/ApsyDir/Templates
3 #Creation: 26Jan07.pgs.vs 0.20
4 #Modification: 02Mar07.pgs.vs 0.25 (Smin1,Smin2,rmin)
5 #RunLocation: Starting DATASET of APSY-RUN
6 #RunName: parameter.gap
7 -----
8 #Structure: ParameterName ParameterValue
9 # ==> Lines starting with # are considered as comments
10 -----
11 #Parameter information
12 -----
13 #####Smin1:
14 #Determines the minimal support needed for a candidate.
15 #A good value for Smin1 is the dimensionality of the experiment.
16 #If Smin1 is set < 1.0, Smin1 will proportionally scale to the
17 #number of projections used.
18 #####Smin2:
19 #Determines the minimal support needed for a candidate.
20 #A good value for Smin1 is the dimensionality of the experiment.
21 #If Smin1 is set < 1.0, Smin1 will proportionally scale to the
22 #number of projections used.
23 #####DeltaNu:
24 #Peak matching tolerance in the direct dimension. A reasonable
25 #value is the digital resolution in the direct dimension.
26 #####rmin:
27 #Peak matching tolerance in Hz or in points (pt) in the indirect
28 #dimensions. If given in points, it will scale with the actual
29 #angle. A reasonable value is the largest digital resolution in
30 #the indirect dimension from all projections.
31 #Typical values are 30.0 Hz or 0.7 pt.
32 #####S/Nratio:
33 #Defines the signal-to-noise-ratio for peak picking. Typical
34 #values are 4-10.
35 #####waterline:
36 #Defines the half width of a strip along the waterline in Hz,
37 #from which no peaks were picked.
38 -----
39 Smin1: 3
40 Smin2: 3
41 DeltaNu: 7.0
42 rmin: 30.0 Hz
43 S/Nratio: 15
44 waterline: 500.0
45
```

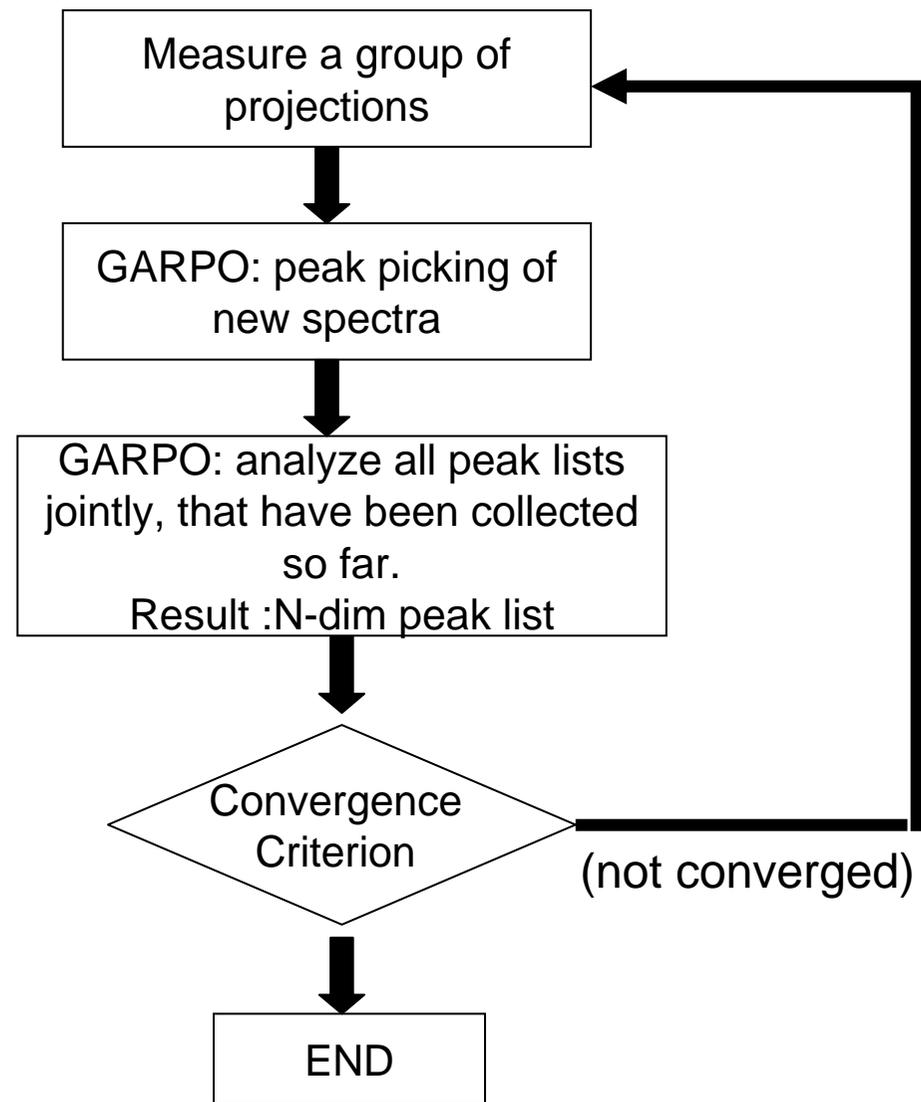
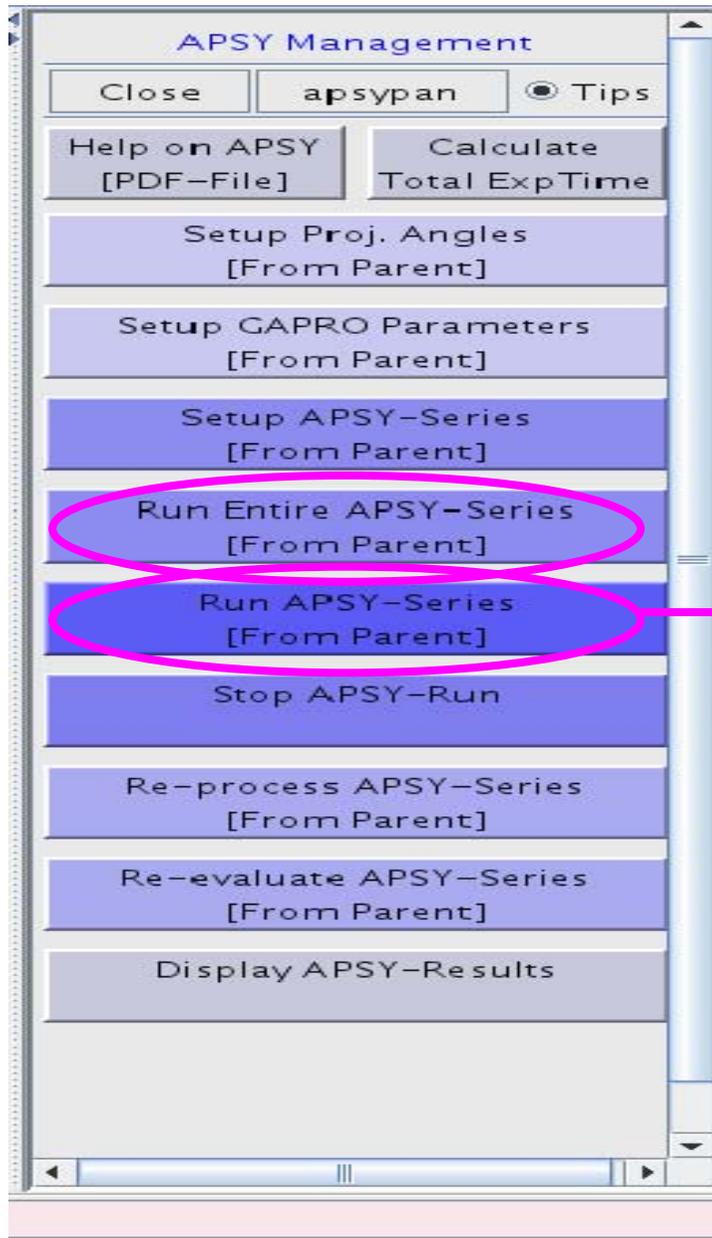
Smin1; Smin2 \geq dimension (ex: 3)
DeltaNu ~ digital resolution in Hz in the direct dimension
rmin~digital resolution in Hz in the indirect dimension
S/Nration: typical values are 3-10
Waterline: half-width water line in the direct dimension

STEP6 : Set up different projection angles

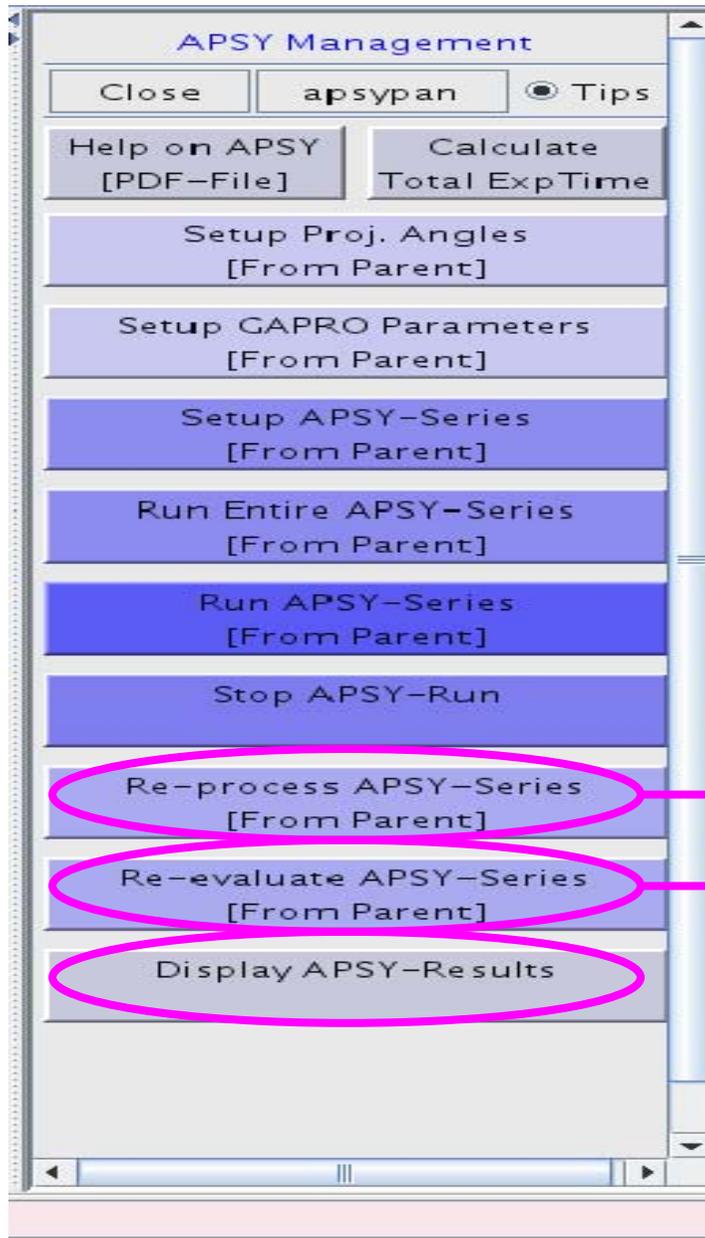
0,90, +/- 30, +/- 60, +/- 20, +/- 70, +/- 40, +/- 50, +/- 10, +/- 80, +/- 55, +/- 35 → 22 angles

(暫存檔)

STEP7 : Collect data for different projection angles



STEP8 : Final Peak List Result



```
27
28 *****
29 *** NOH.peaks ***
30 *****
31 # Number of dimensions 3
32 #INAME 1 N
33 #INAME 2 O
34 #INAME 3 H
35 1 114.5913 168.7465 7.4410 1 U 0.000E+00 0.000E+00 e 0 0 0 0
36 2 118.4312 173.2002 7.7997 1 U 0.000E+00 0.000E+00 e 0 0 0 0
37 3 126.6306 169.4641 9.1843 1 U 0.000E+00 0.000E+00 e 0 0 0 0
38 4 116.7820 171.1912 8.5505 1 U 0.000E+00 0.000E+00 e 0 0 0 0
39 5 122.6248 171.1549 7.7035 1 U 0.000E+00 0.000E+00 e 0 0 0 0
40 6 118.0694 175.2307 8.3105 1 U 0.000E+00 0.000E+00 e 0 0 0 0
41 7 120.6934 170.2307 8.8864 1 U 0.000E+00 0.000E+00 e 0 0 0 0
42 8 110.6688 171.3524 8.7585 1 U 0.000E+00 0.000E+00 e 0 0 0 0
43 9 116.7303 166.4779 7.9777 1 U 0.000E+00 0.000E+00 e 0 0 0 0
44 10 111.4506 174.4963 6.5844 1 U 0.000E+00 0.000E+00 e 0 0 0 0
45
46
```

If change edp parameters

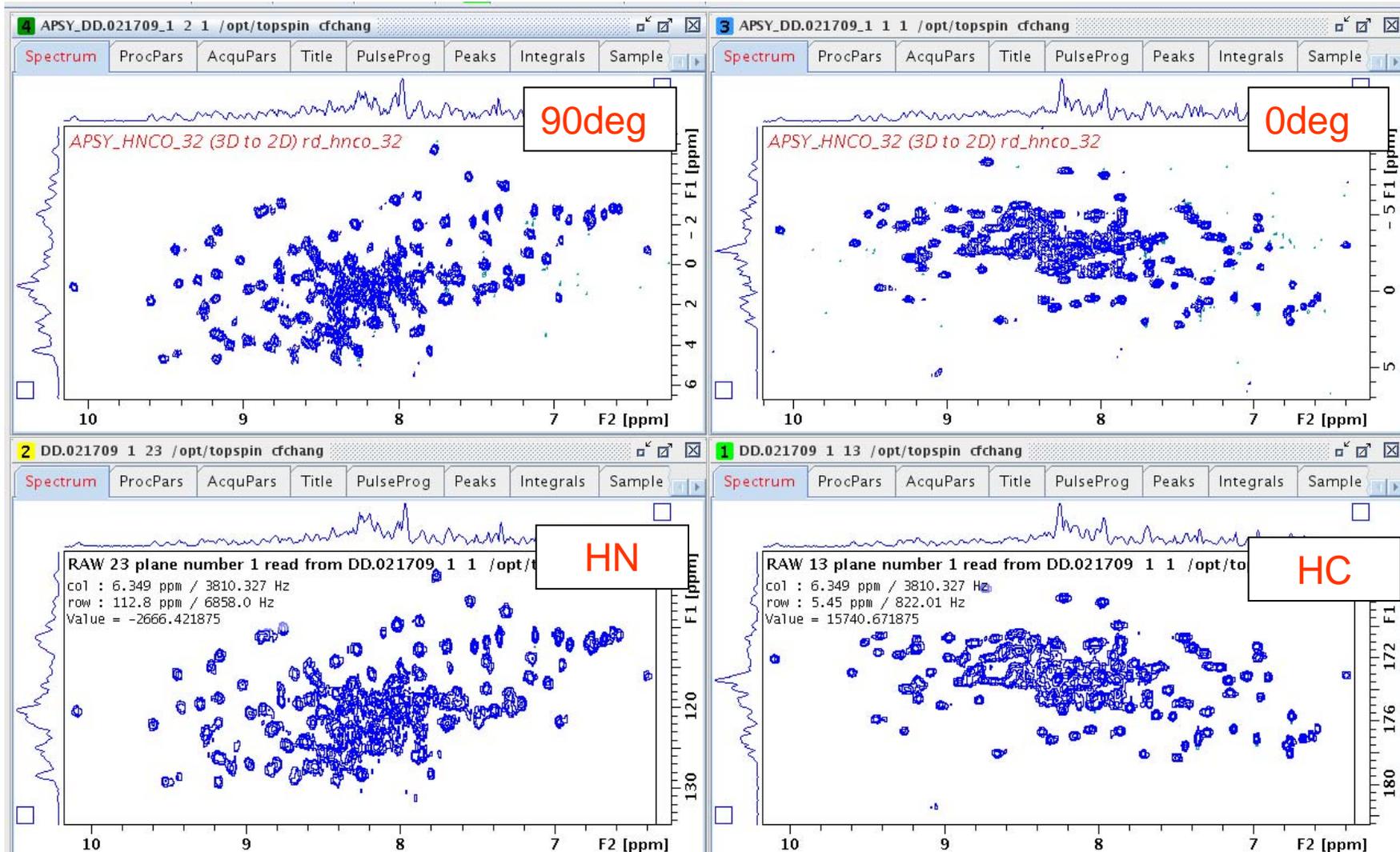
If change GAPRO parameters

Example

Sample : 145 assigned AA $^{13}\text{C}/^{15}\text{N}$ protein

System: AV600_IBMS (regular TXI probe)

Experiment : rd_hnco_32 vs. 3D HNCO, NS=8

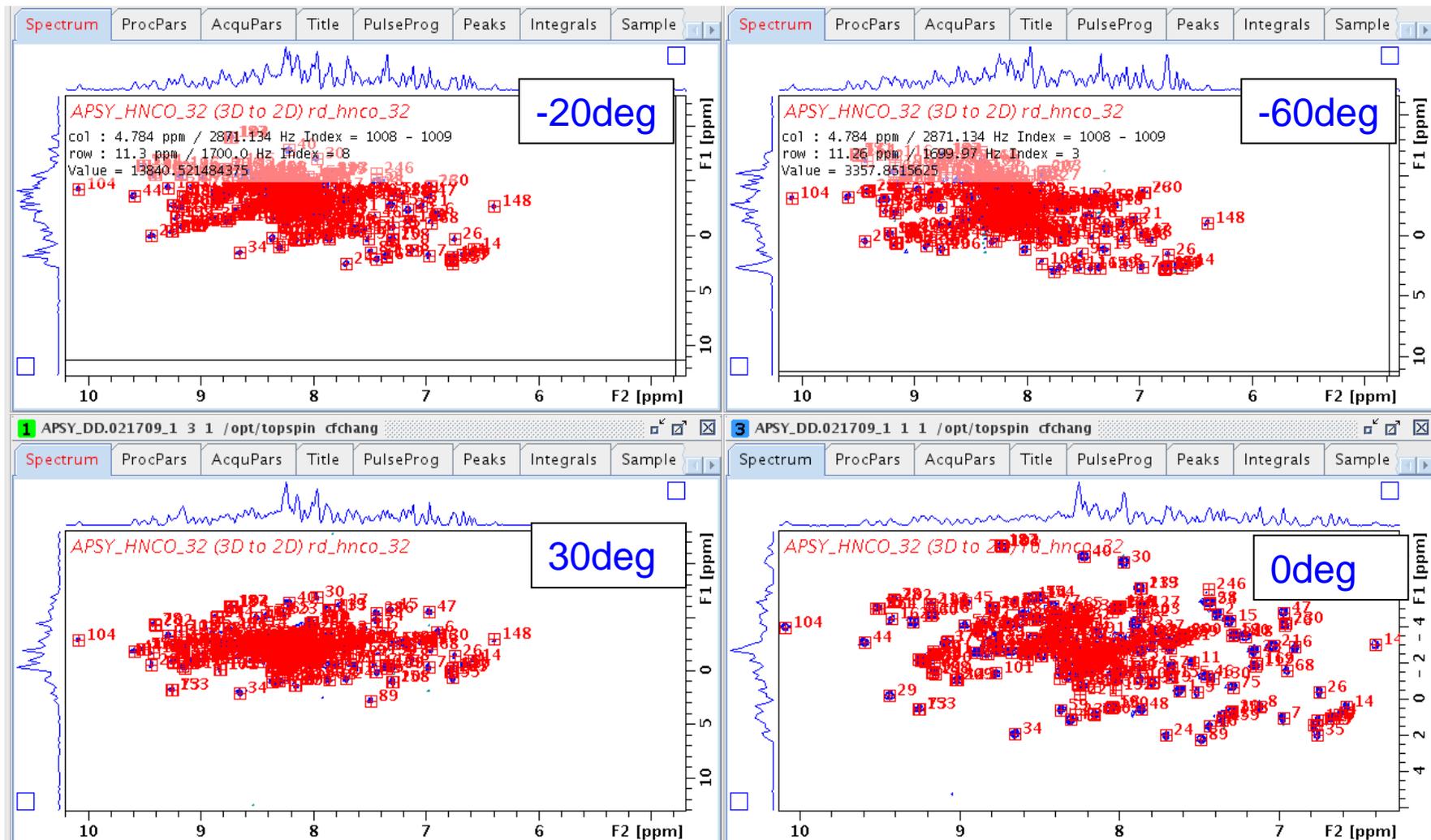


Example

Sample : 145 assigned AA 13C/15N protein

System: AV600_IBMS (regular TXI probe)

Experiment : rd_hnco_32, NS=8



Example

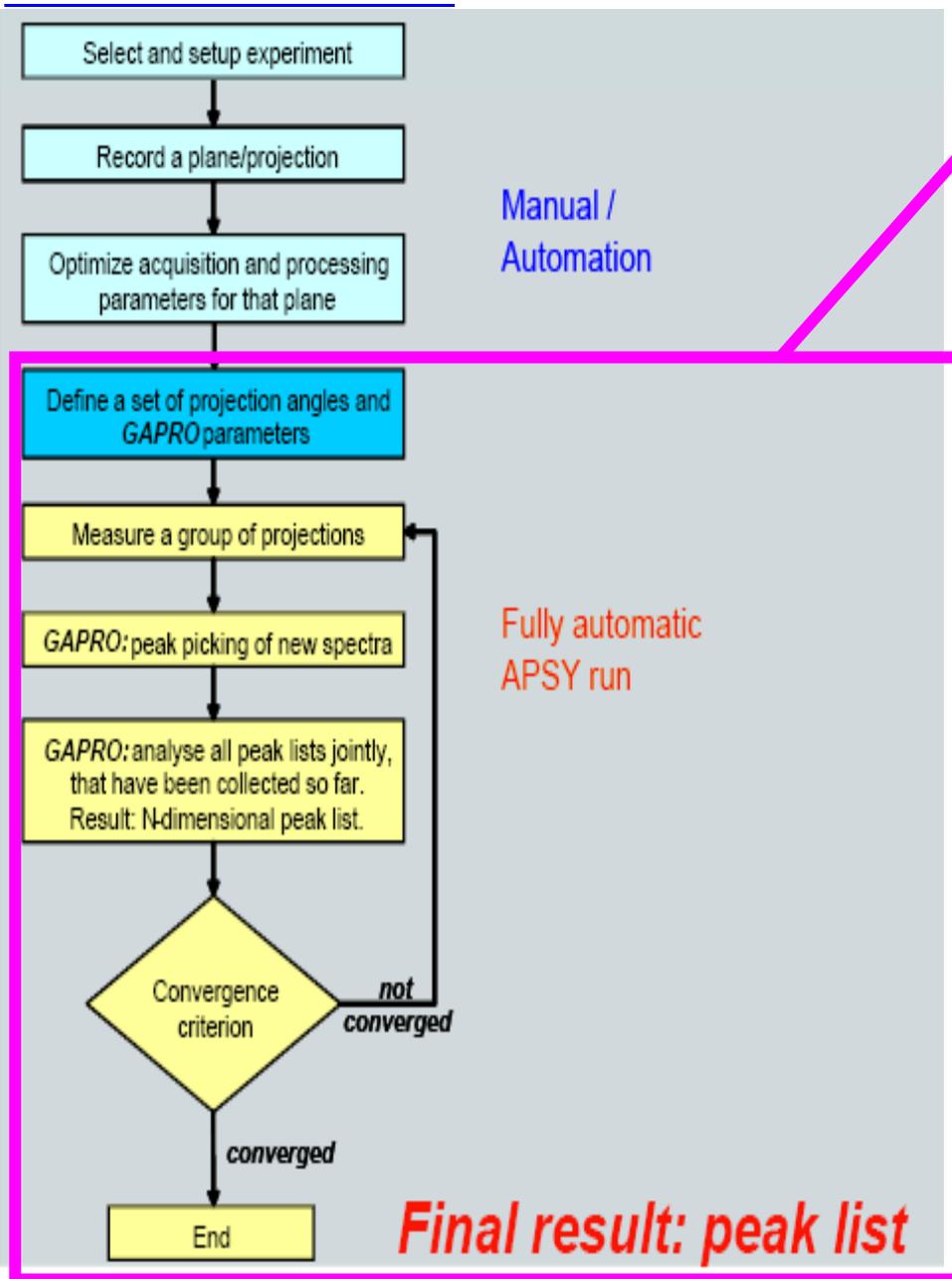
Sample : 145 assigned AA $^{13}\text{C}/^{15}\text{N}$ protein

System: AV600_IBMS (regular TXI probe)

Experiment : HNCO, NS=8, 2K*64(CO)*32(NH)

	3D HNCO	APSY-HNCO
Expt. Time	~ 6hours	~9min/angles ~3.5 hours for 22 angles
Peaks	~130/170	
(1) S/N=10		~130/242
(2) S/N=15		~125/170
(3) S/N=20		~120/170

APSY: Flow Chart



(From Bruker APSY document)



What's New in HFNMRC
(Standard Parameter Set)

Standard Parameter Sets in HFNMRC (std*)

std*_nD_exptname_pp

(1) Bruker pulseprogram

(pulseprogram from Bruker data base or with minor correction)

std0_nD_expt_pp : for small molecules (~100% D-solvent)

std1_nD_expt_pp : for biomolecules (~10% D-solvent)

(2) Implemented/modify version

(pulseprogram not in Bruker data base or with major modification)

std2_nD_expt_pp

(3) Others

(home-made experiments, or custom-requested experiments)

std3_**

Standard Parameter Sets in HFNMR (std1* or std2* or std3*)

Parameter Sets: rpar std1*

Source = /opt/topspin/exp/stan/nmr/par/user

File Options Help

Search in names [*?]

std1_1D_1H-ZG
std1_1D_1H-ZGGPPR
std1_1D_1H-ZGGPWS
std1_1D_1H-ZGGPWG
std1_1D_1H-ZGPR
std1_2D_13C-HSQC_hsqcctetgppsp
std1_2D_13C-HSQC_hsqcctetgpsi
std1_2D_13C-aroTROSY_trosyargpphwg
std1_2D_15N-CLEANEX_fhsqcxf3gpgh
std1_2D_15N-HSQC_hsqcctf3gpsi
std1_2D_15N-HSQC_hsqcctf3gpsi
std1_2D_15N-HSQC_hsqcctf3gpsi
std1_2D_15N-HSQC_hsqcctf3gpsi
std1_2D_15N-NOE_hsqcnoef3gpsi
std1_2D_15N-T1_hsqct1etf3gpsi
std1_2D_15N-T2_hsqct2etf3gpsi
std1_2D_15N-TR-CLEANEX_trosycxf3gpghsi19
std1_2D_15N-TROSY_trosyef3gpsi
std1_2D_15N-TROSY_trosyf3gpgh19
std1_3D_13C-HCCHCOSY_hcchcogp3d
std1_3D_13C-HCCHTOCSY_hcchdigp3d
std1_3D_13C-NOESYHSQC_noesyhsqctg3d
std1_3D_15N-NOESYHSQC_noesyhsqcf3gpsi3d
std1_3D_15N-NOESYHSQC_noesyhsqcf3gpsi3d
std1_3D_15N-TOCSYHSQC_dipsihsqcf3gpsi3d
std1_3D_15N-TR-NOESY_noesyretf3gp3d
std1_3D_15N-TR-TOCSY_dipsitretf3gp3d
std1_3D_CBCA(CO)NH_cbcacohgp3d
std1_3D_CBCA(CO)NH_cbcacohgpwg3d
std1_3D_HBHA(CO)NH_hbhaconhgp3d
std1_3D_HBHANH_hbhanhgp3d
std1_3D_HCCCONH-C_hccconhgp3d3
std1_3D_HCCCONH-H_hccconhgp3d2
std1_3D_HN(CA)CO_hncacogp3d
std1_3D_HN(CA)CO_hncacogpwg3d
std1_3D_HN(CO)CAB_hncocacogp3d

File Options Help

Search in names [*?]

std2_1D_P1331_15Ndec.ww
std2_2D_HMQC-JR-GE.WW
std2_2D_NCESY-JR-IP.WW
std2_3D-TR-HN(CA)CB.WW
std2_3D_CBCA(CO)NH_SC.WW
std2_3D_HN(CA)CB.WW
std2_3D_HN(CA)CB_SC.WW
std2_3D_HN(CA)CO.WW
std2_3D_HN(CA)CO_SC.WW
std2_3D_HN(CO)CA.WW
std2_3D_HN(CO)CA_SC.WW
std2_3D_HNCA.WW
std2_3D_HNCACB.WW
std2_3D_HNCACB_SC.WW
std2_3D_HNCA_SC.WW
std2_3D_HNCO.WW
std2_3D_HNCO_SC.WW
std2_3D_TR-HNCO.WW
std2_3D_TR_HN(CO)CA.WW
std2_3D_TR_HN(CO)CACB.WW
std2_3D_TR_HN(COCA)CB.WW
std2_3D_TR_HNCA.WW
std2_3D_TR_HNCACB.WW

File Options Help

Search in names [*?]

std3_NTU_CPMG_cpmgpr1d
std3_NTU_Diffusion_ledopgs1spr.cf
std3_NTU_NOESY_noesypr1d

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Notice

- 重要訊息：收費調整和預約制度修正等 (20060731)**
Dear HFNMRC users, 為反應核心低溫探頭維護成本及核心服務滿載之情形, 核心使用者委員會於本月12日委員會議中討論後針對核心使用辦法修正如下, 請大家配合: ...
-- [more detail] --
- 收費標準異動 (20060119)**
為反應低溫探頭定期維護所需之維護耗材費, 使用者委員會決議以循序漸進的方式調整, 民國95年前半年先微幅調漲, 後半年視國科會補助情形再作調整, 故自2月1日起500MHz 及600MHz 低溫探頭分 ...