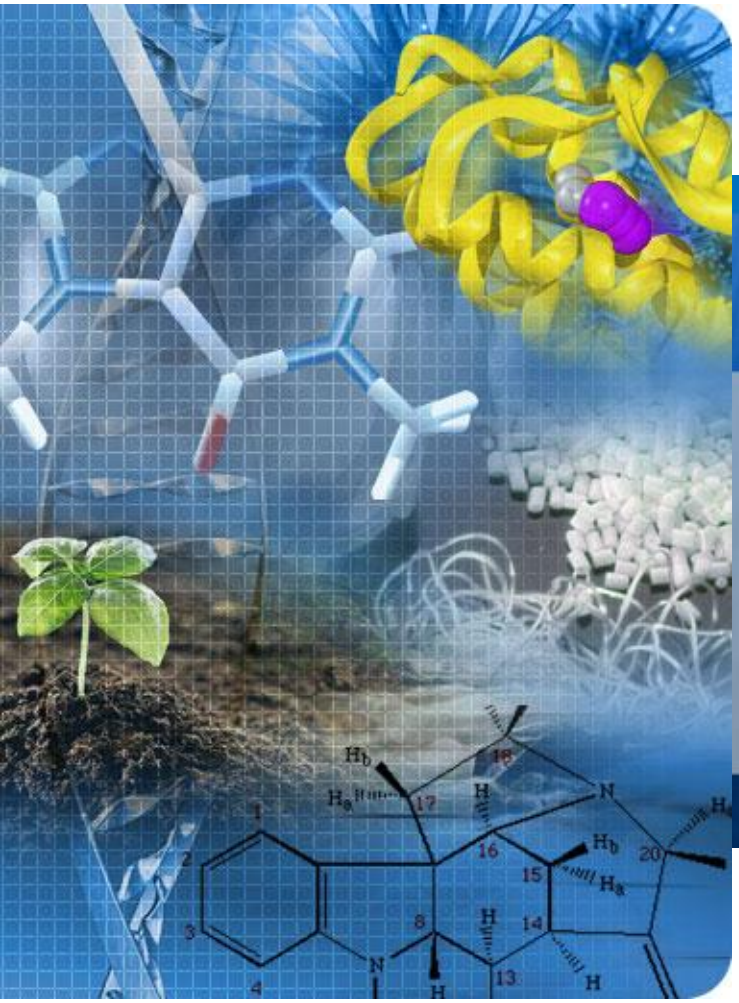


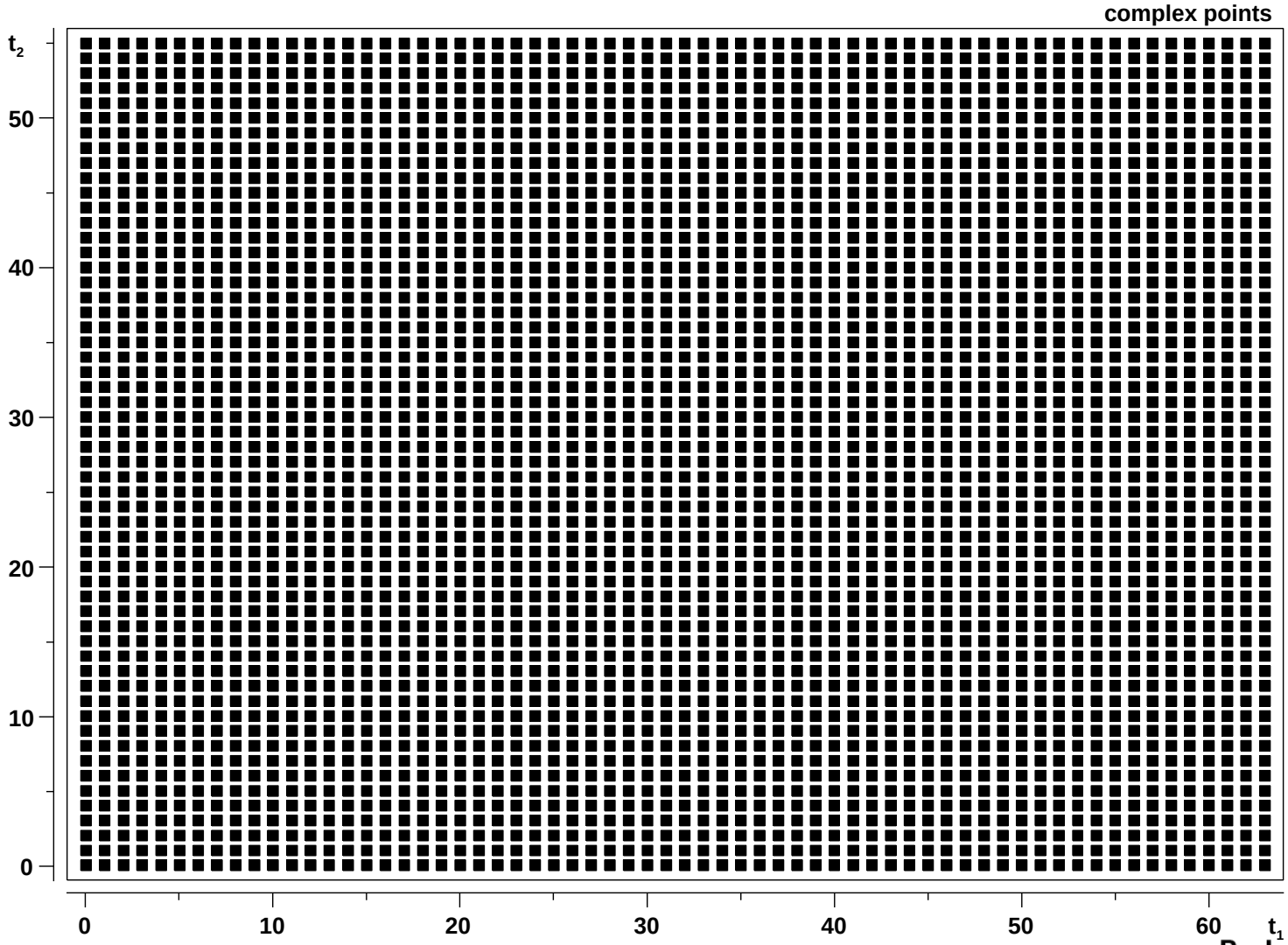
Non Uniform Sampling

Eric Johnson

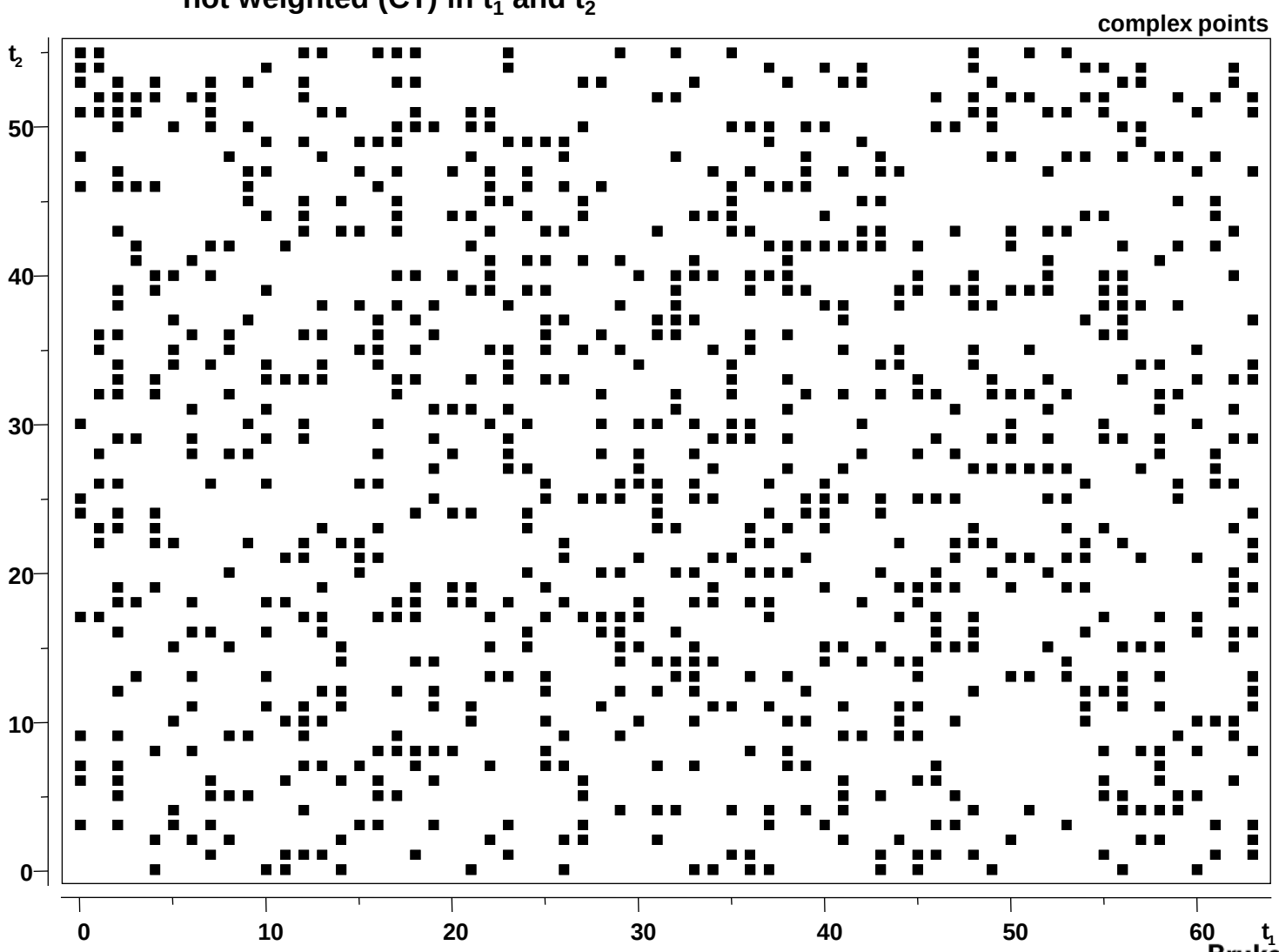
Symposium on Frontiers in Biomolecular NMR
Vanderbilt University
May 4, 2012

Introduction

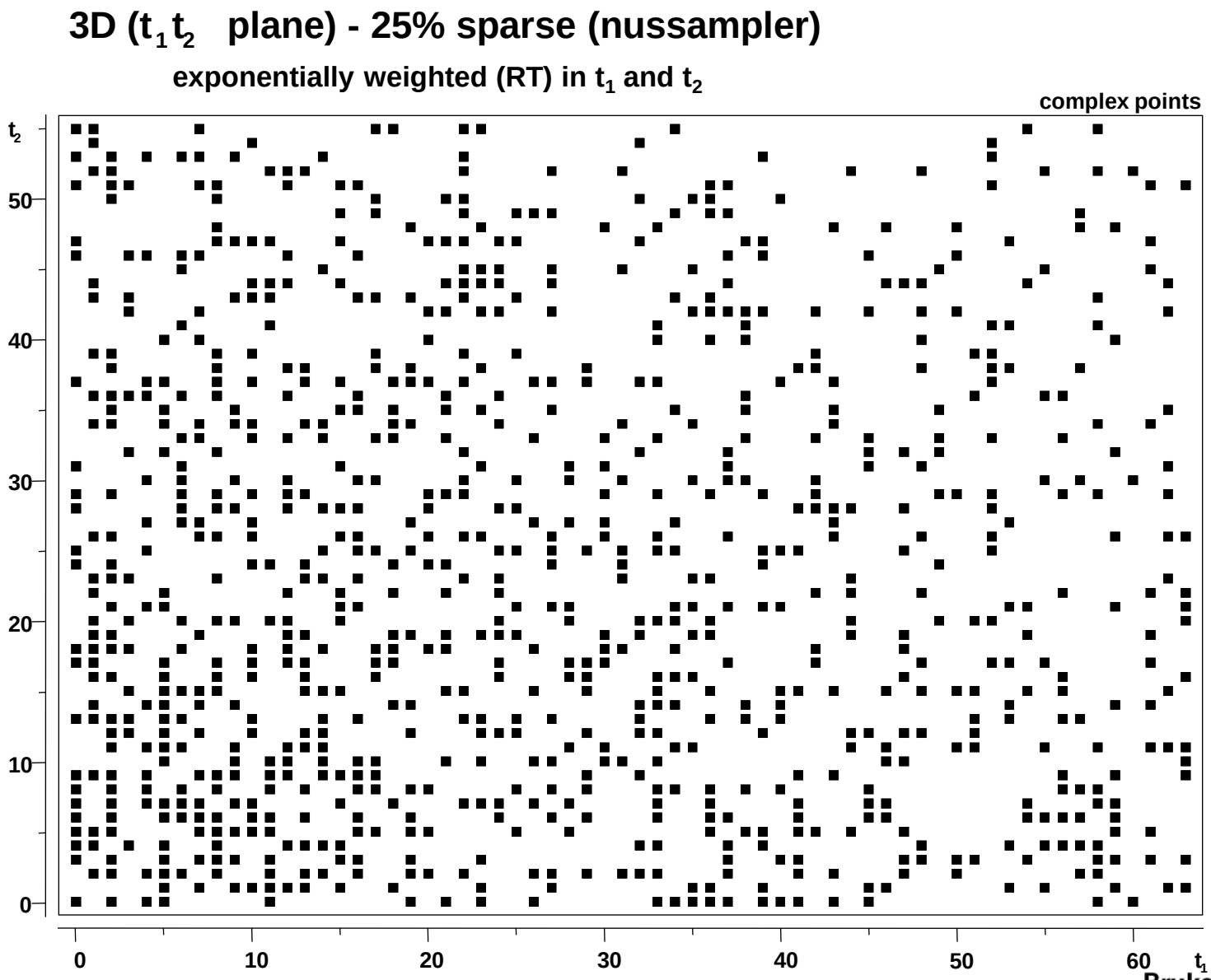
3D ($t_1 t_2$ plane)



Introduction

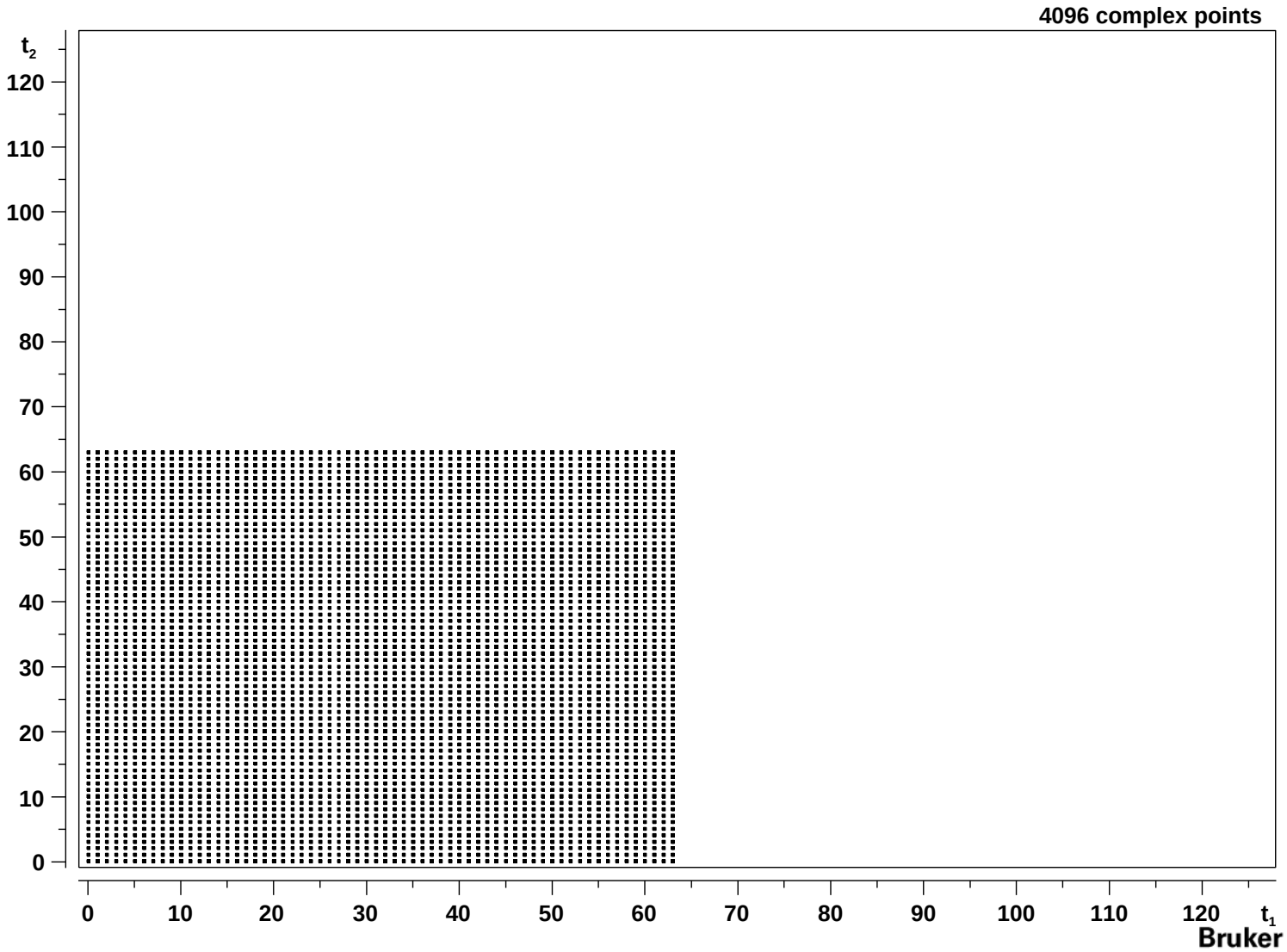


Introduction

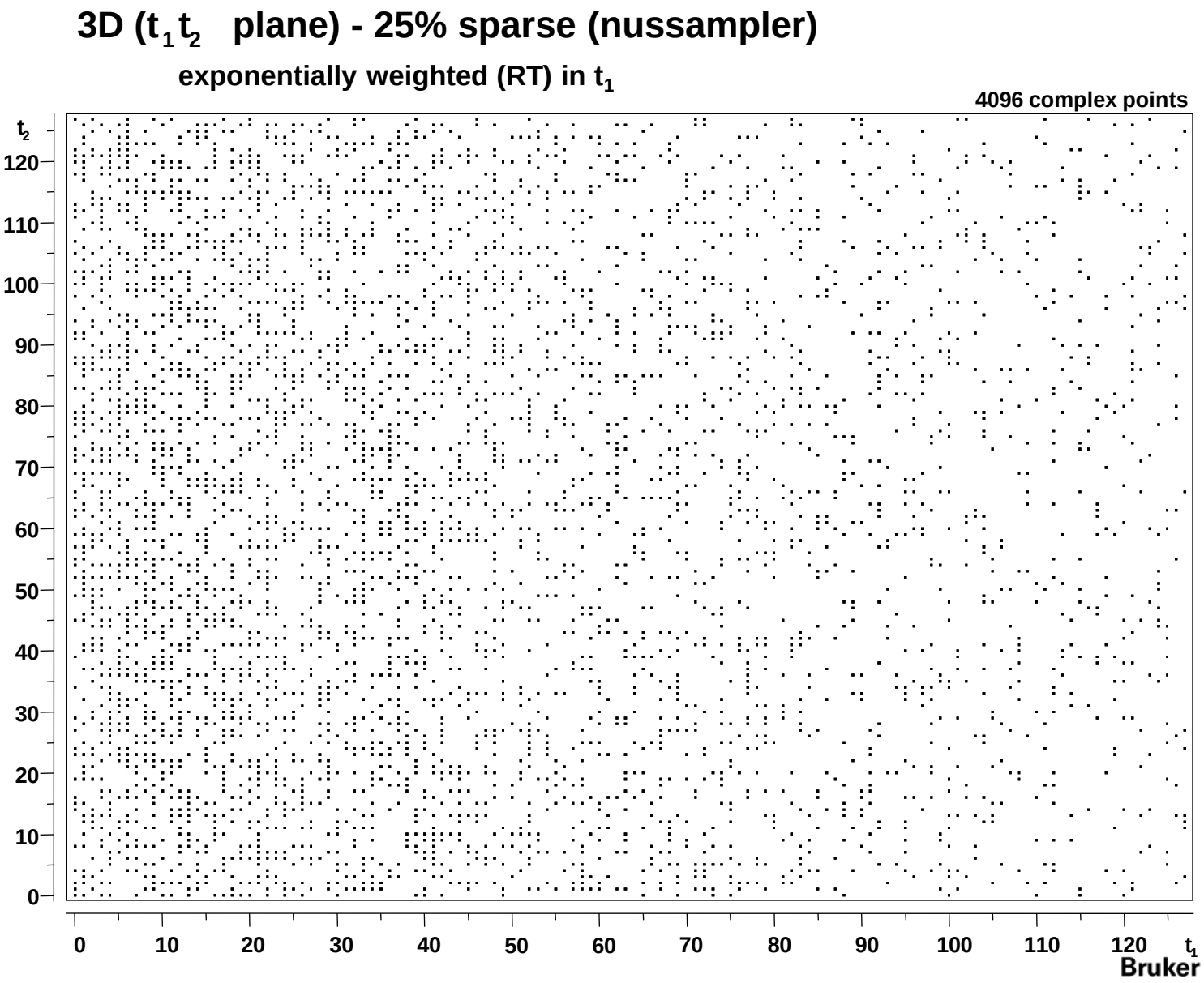


Introduction

3D ($t_1 t_2$ plane)



Introduction



Introduction

Multi Dimensional Decomposition (MDD)

MDD-NMR	Orekhov et al.

Maximum Entropy (MaxEnt)

Rowland Toolkit	Hoch et al.
Forward Maximum Entropy	Wagner et al.
Azara (CCPN)	Laue et al.

Multidimensional Fourier Transformation (MFT)

MFT	Kozminski et al.

Modifications to pulse sequences

mc (TopSpin 2.1)

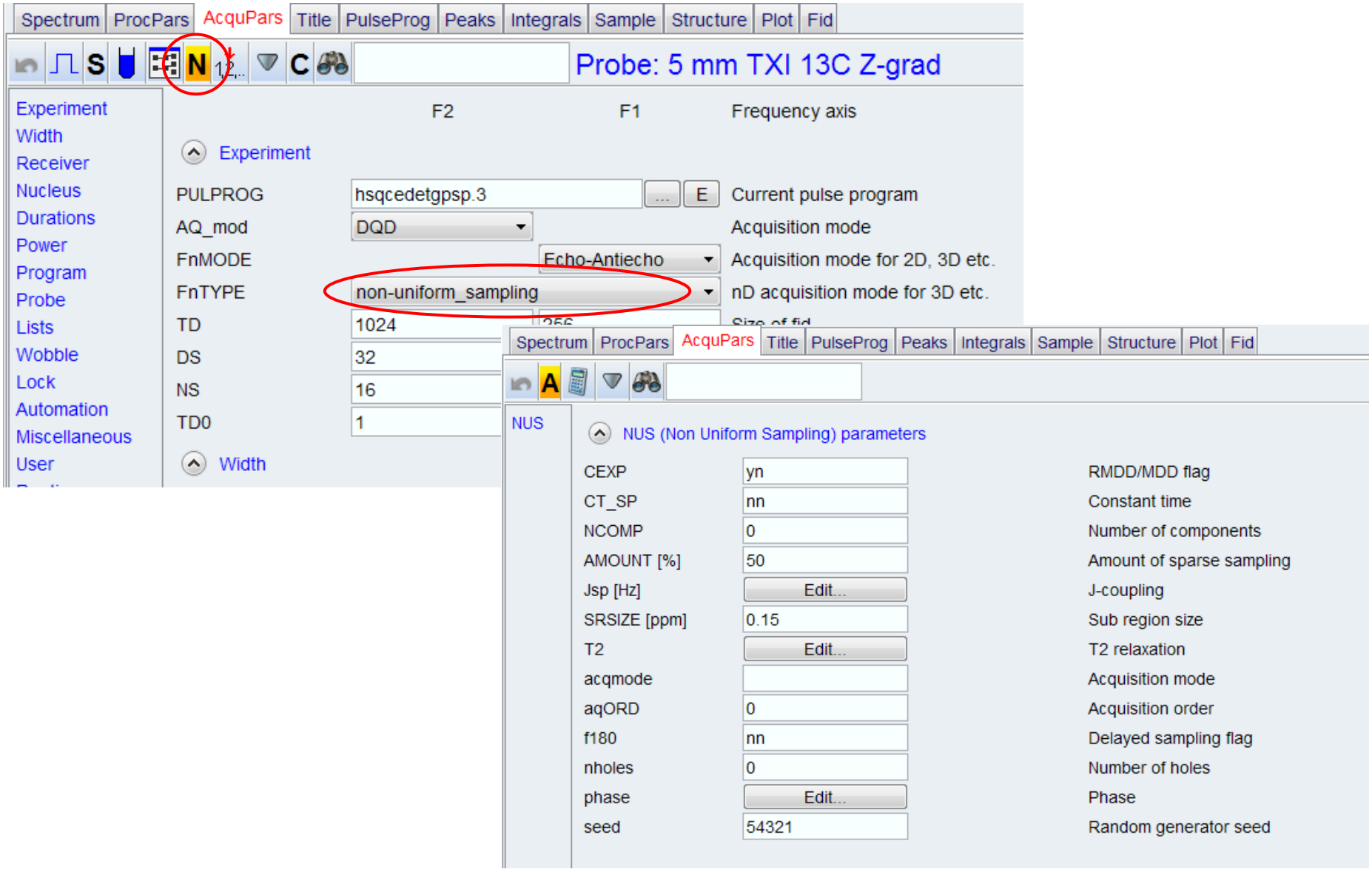
```
d11 do:f3 mc #0 to 2
  F1PH(rd10 & rd29 & rd30 & rp5 & ip4, id0)
  F2PH(ip5, id10 & id29 & dd30)
```

new mc (TopSpin 3.0 +)

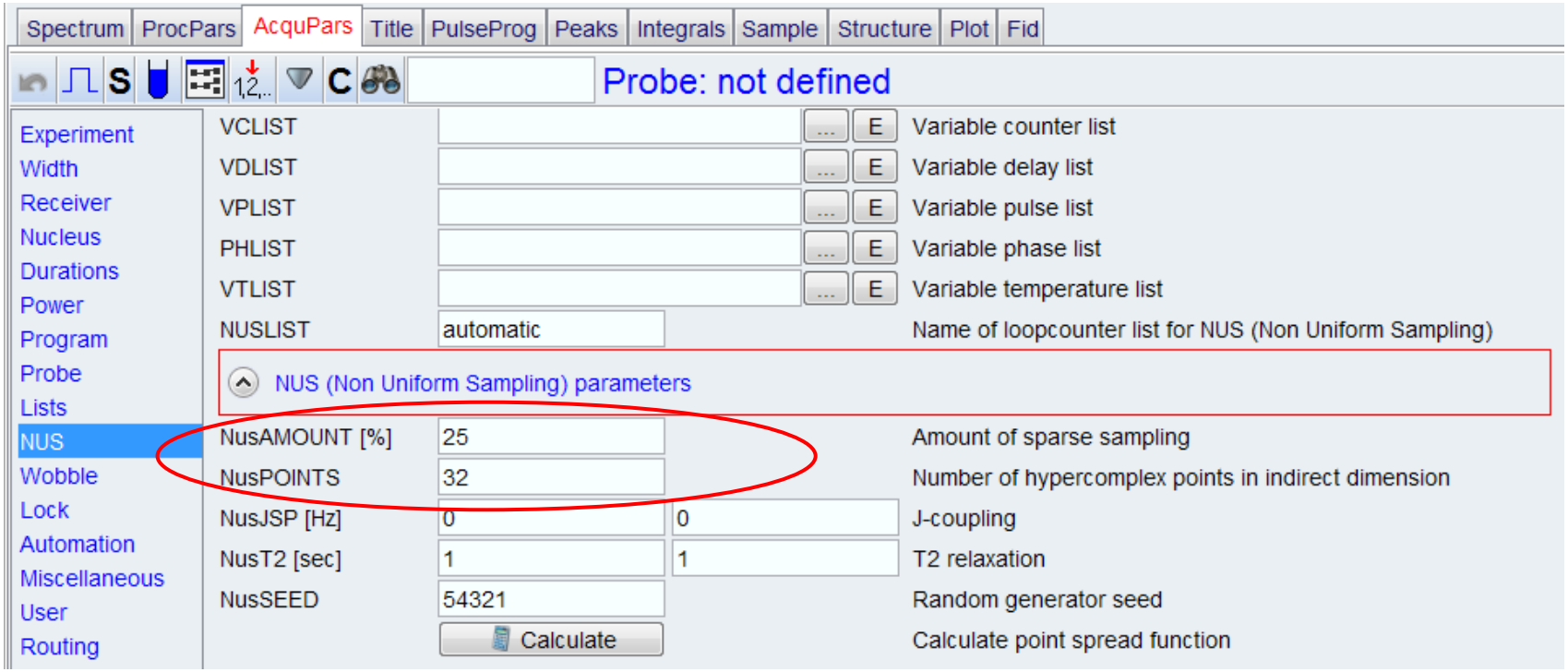
```
d11 do:f3 mc #0 to 2
  F1PH(calph(ph4, +90), caldel(d0, +in0))
  F2PH(calph(ph5, +90), caldel(d10, +in10) & caldel(d29, +in29) & caldel(d30, -in30))
```

+ both mc versions supported

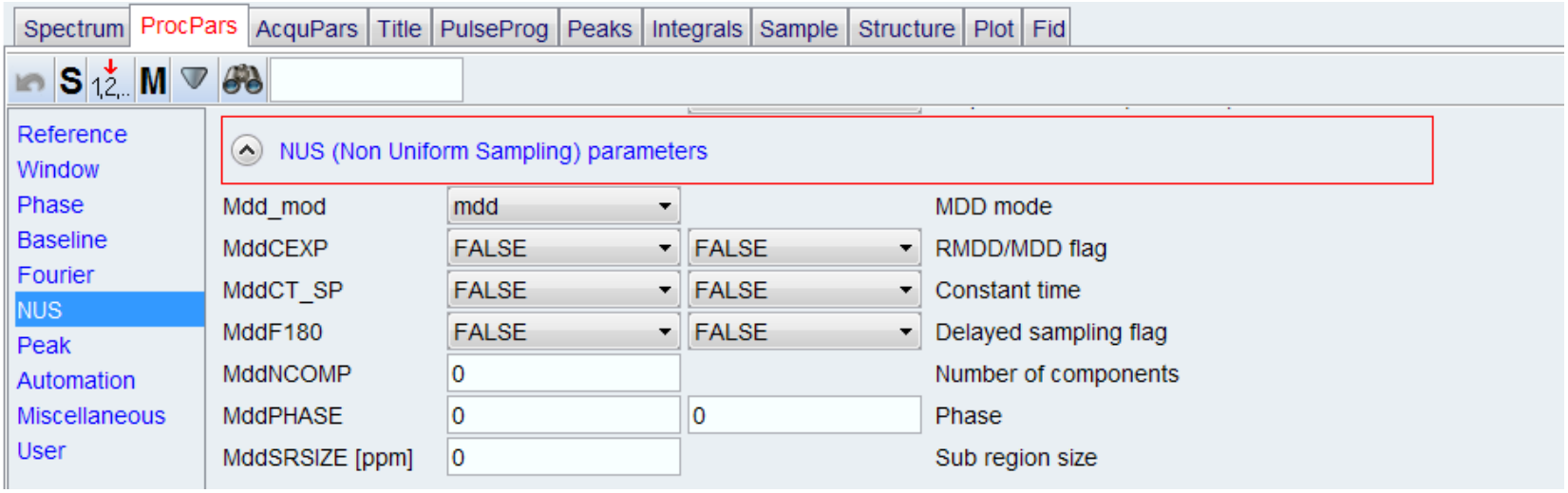
Acquisition parameters (TS3.0)



Acquisition parameters (TS3.1)



Processing parameters (TS3.1)



Improvements in TS3.1

TS3.0

- NUS processing was only supported under Linux

TS3.1

- NUS processing on Linux, Windows and Macintosh
- First data point is always same point as traditional sampling

  (you can use "rser 1" to check the 1st fid)
- Now includes two processing methods

  1. MDD (multi-dimensional decomposition)
  2. CS (compressed sensing)

Processing

- Only indirect dimension(s) is non-uniformly sampled
- Missing points are calculated with RMDD/MDD
- NUS dataset is then processed with FFT

- For 2D NUS datasets:

  “xfb”

- For nD NUS datasets:

  “ftnd”

Multi dimensional transforms

ftnd has the following options

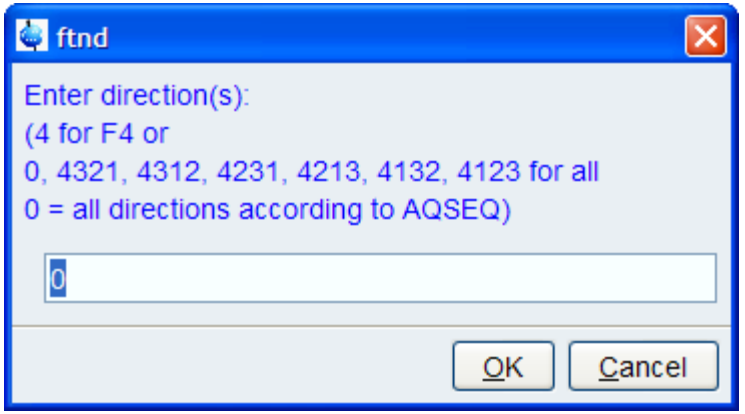
Dimension:

ftnd 0 = transform in order of acqu

ftnd 4321 or any sequence starting in 4…

fntd 4, 3, 2, 1 = transform only this dimension

Or just type “ftnd”:



Multi dimensional transforms

ftnd has the following options:

dlp: **d**elayed **l**inear **p**rediction

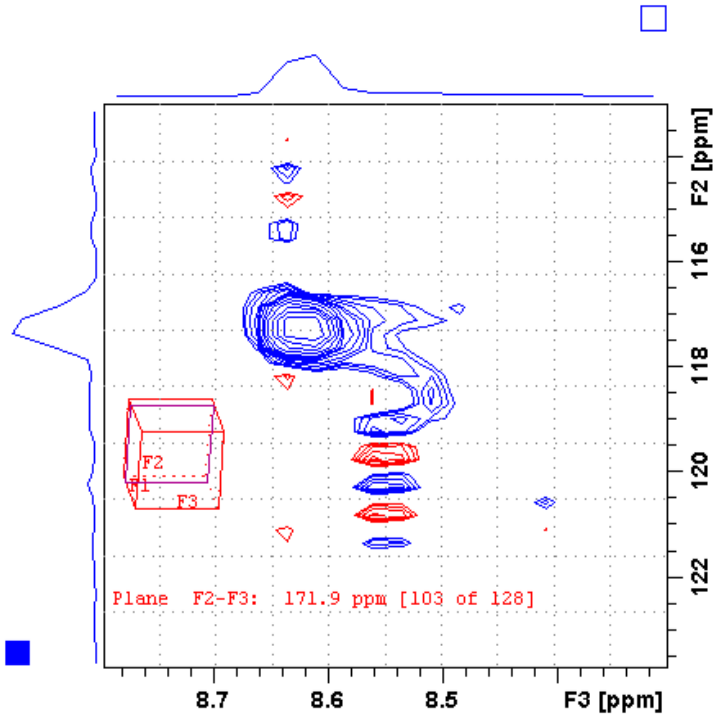
ftnd 0:	ftnd 0 dlp:
1. Processing in F3 (WM – FT)	1. Processing in F3 (WM – FT)
2. Processing in F2 (LP – WM - FT)	2. Processing in F2 (FT)
3. Processing in F1 (LP - WM – FT)	3. Processing in F1 (LP - WM – FT)
	4. Processing in F2 (IFT)
	5. Processing in F2 (LP - WM - FT)

dlp: linear prediction is performed only after FT is done in all other dimentions

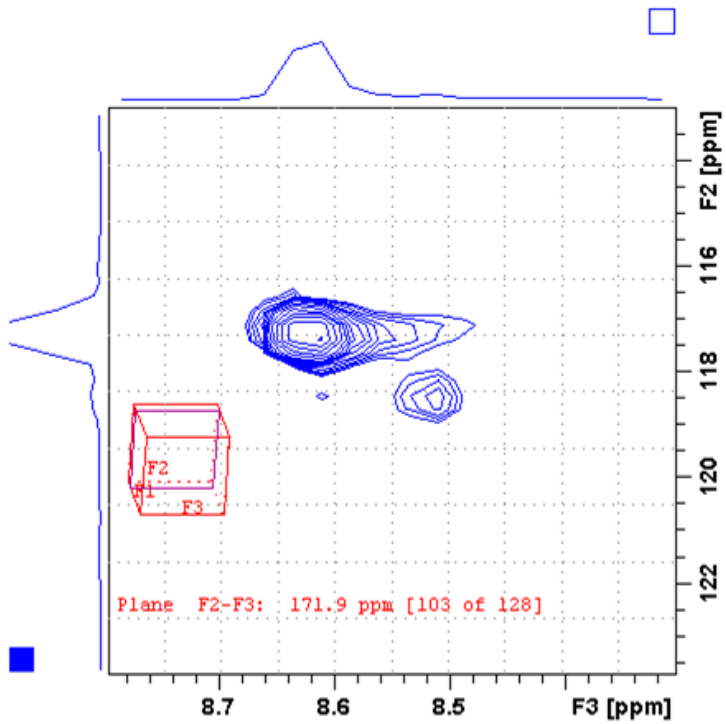
Multi dimensional transforms

dlp: **d**elayed **l**inear **p**rediction

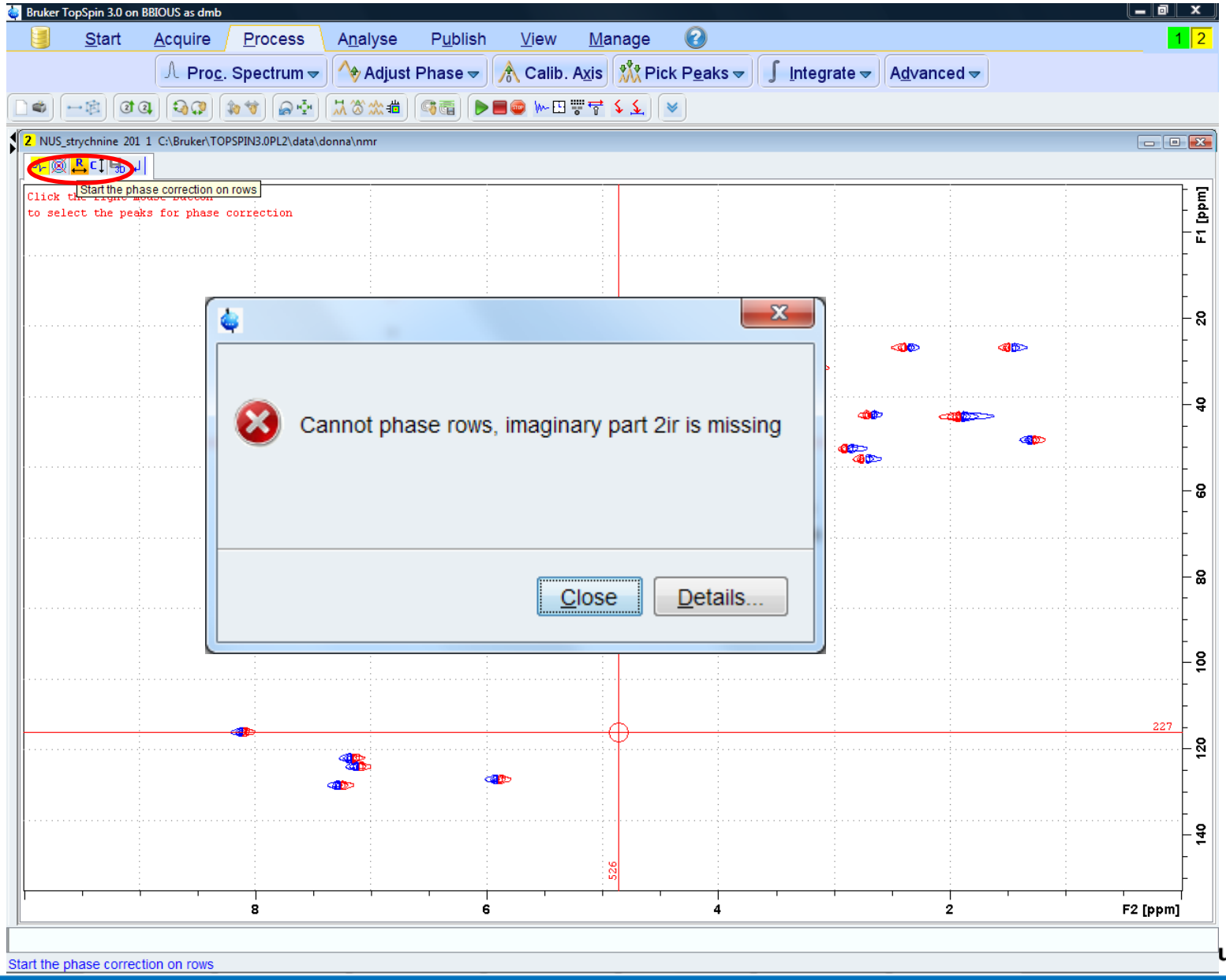
without



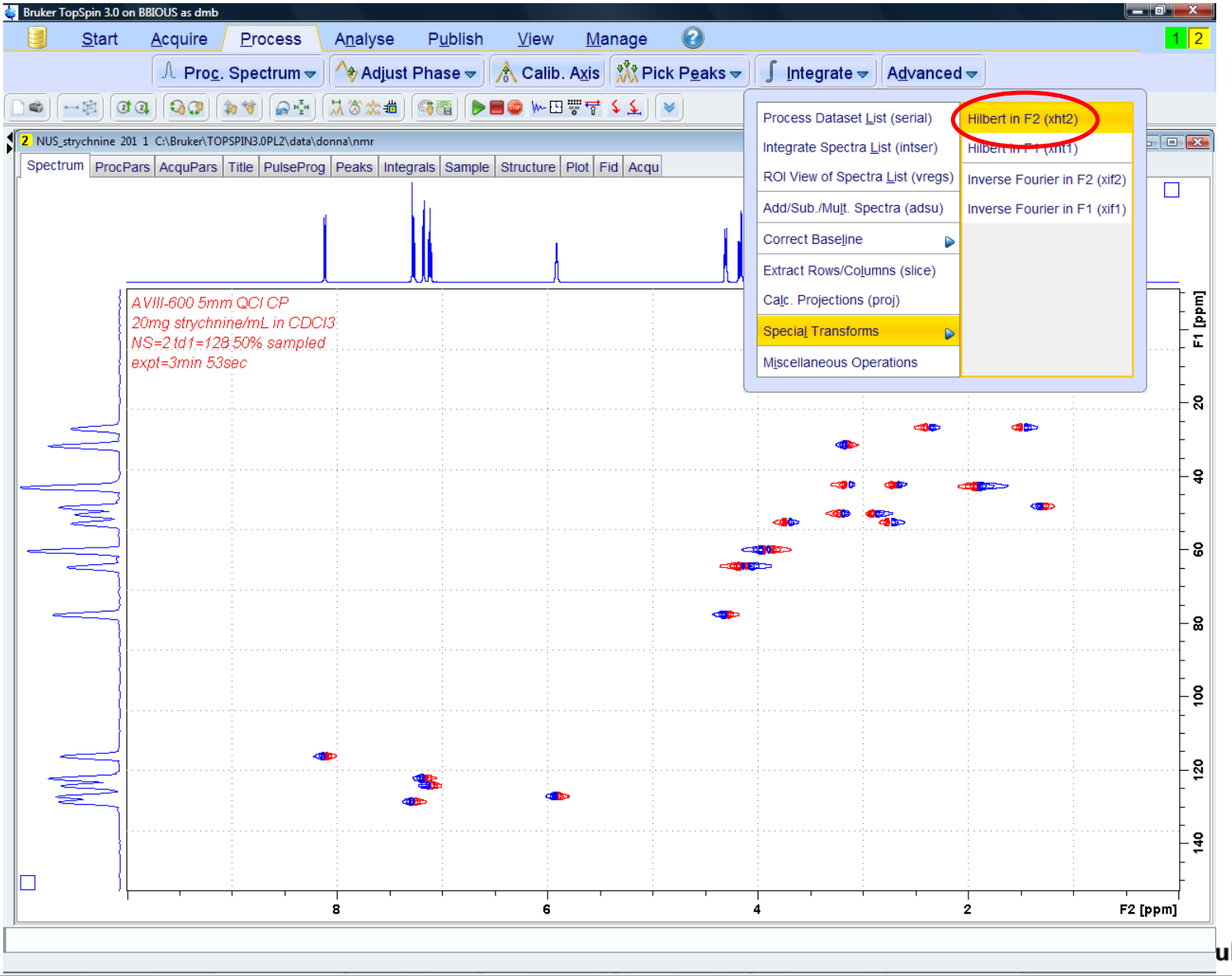
with



Phasing – Hilbert transform

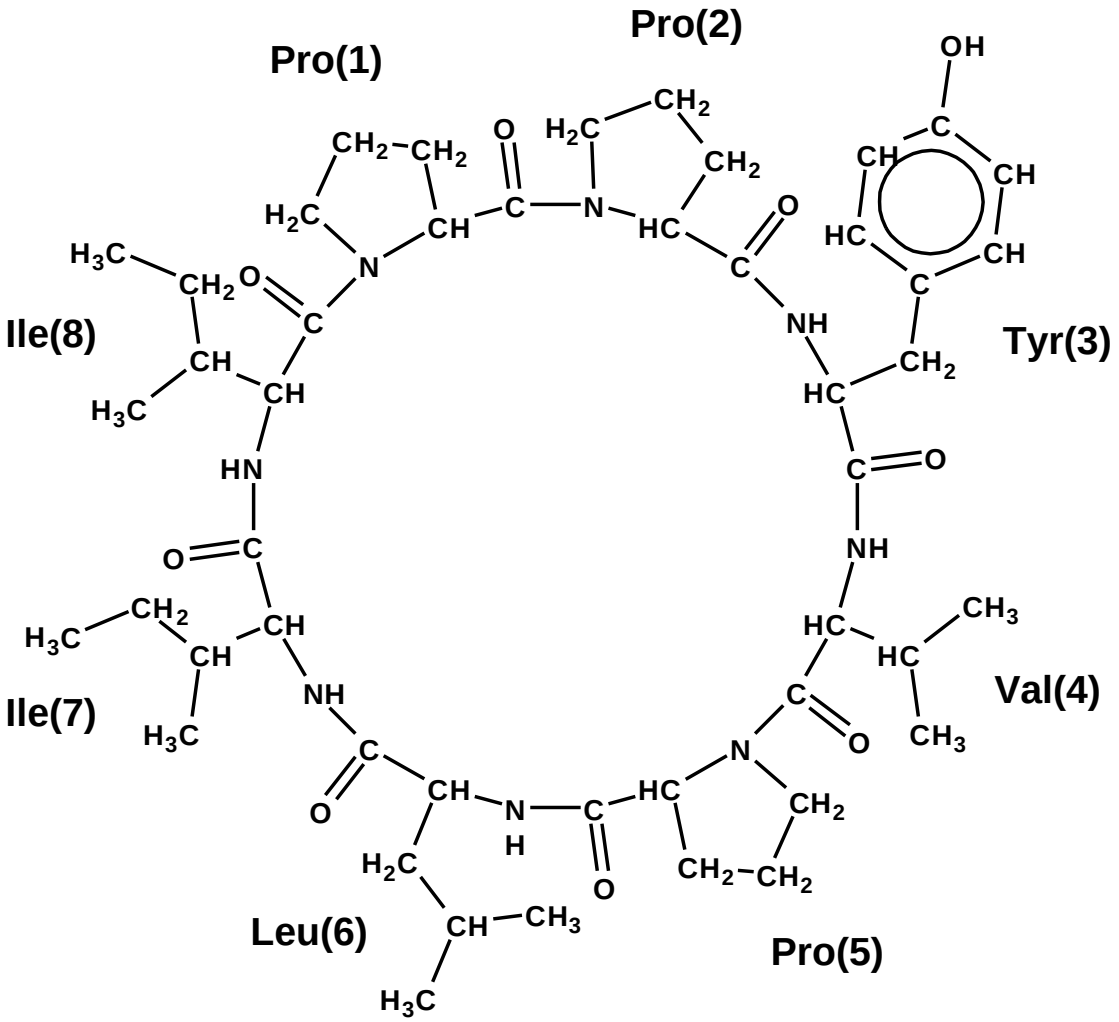


Phasing – Hilbert transform



Applications

Hymenistatin



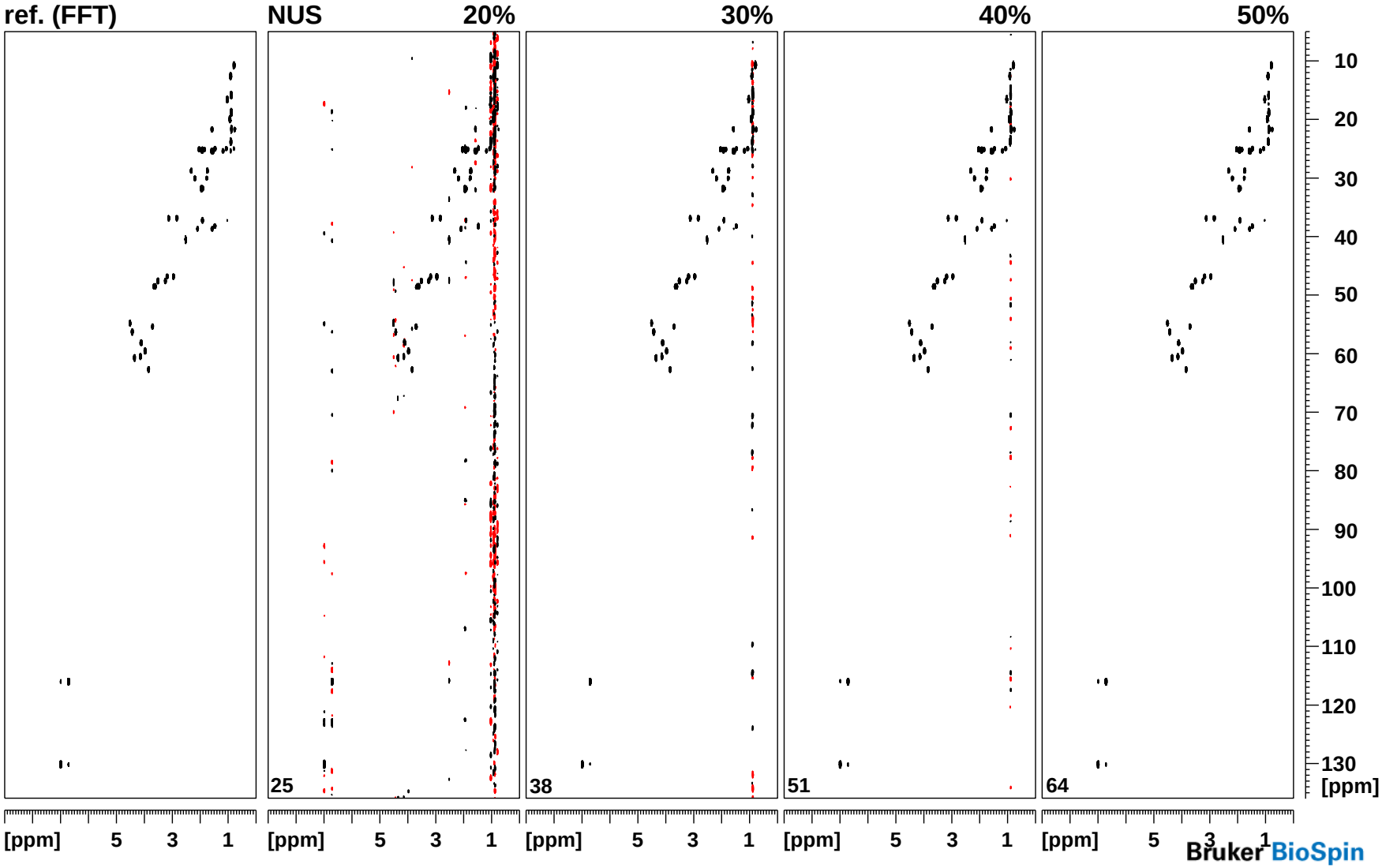
number of cross peaks (estimated maximum):

HSQC (^{13}C)	48
HMBC (^{13}C)	199
COSY	187
TOCSY	339

R.K. Konat, D.F. Mierke, H.Kessler, B. Kutscher, M. Bernd & R. Voegeli, Helv. Chim. Acta 76, 1649 (1993)

Applications

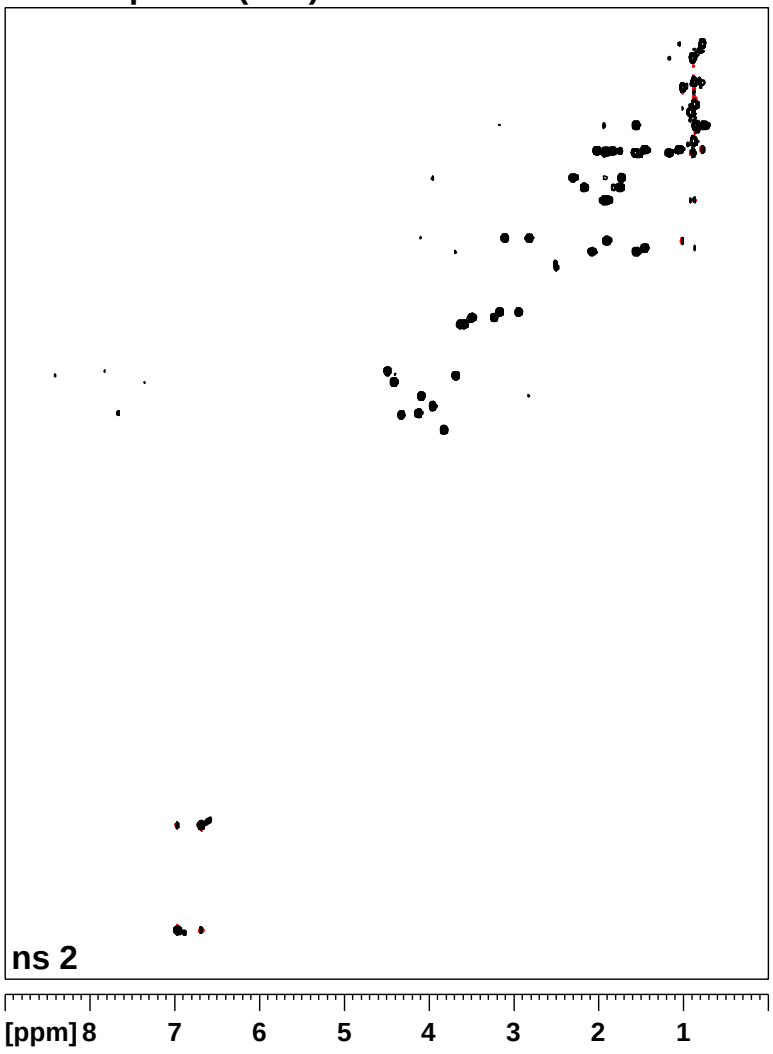
HSQC: td = 256



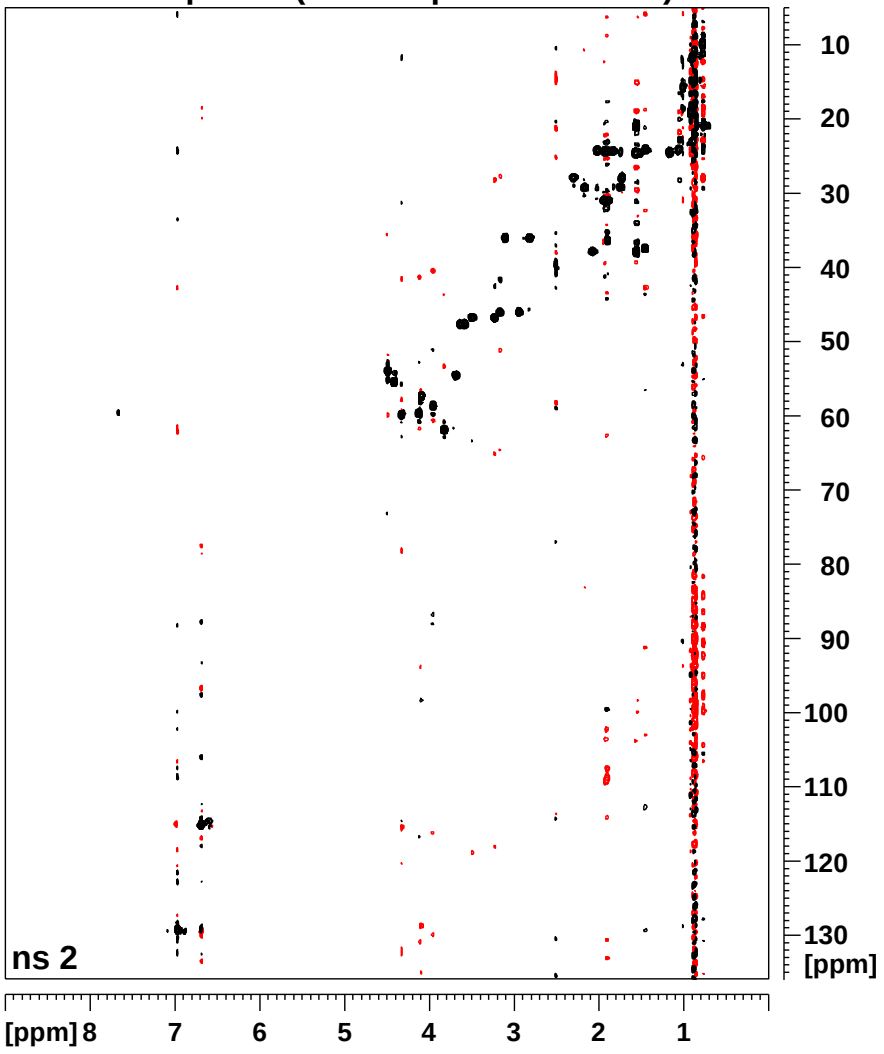
Applications

HSQC

ref. 256 points (FFT)



25% of 256 points (nussampler/MDD-NMR)

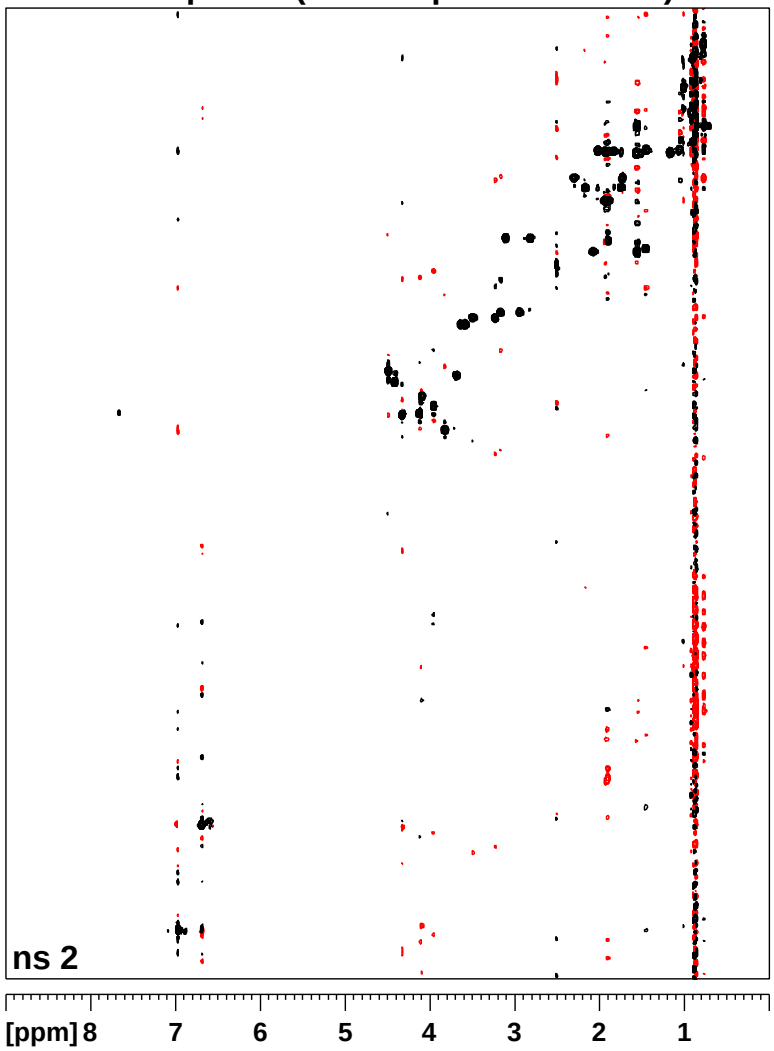


20mM Hymenistatin

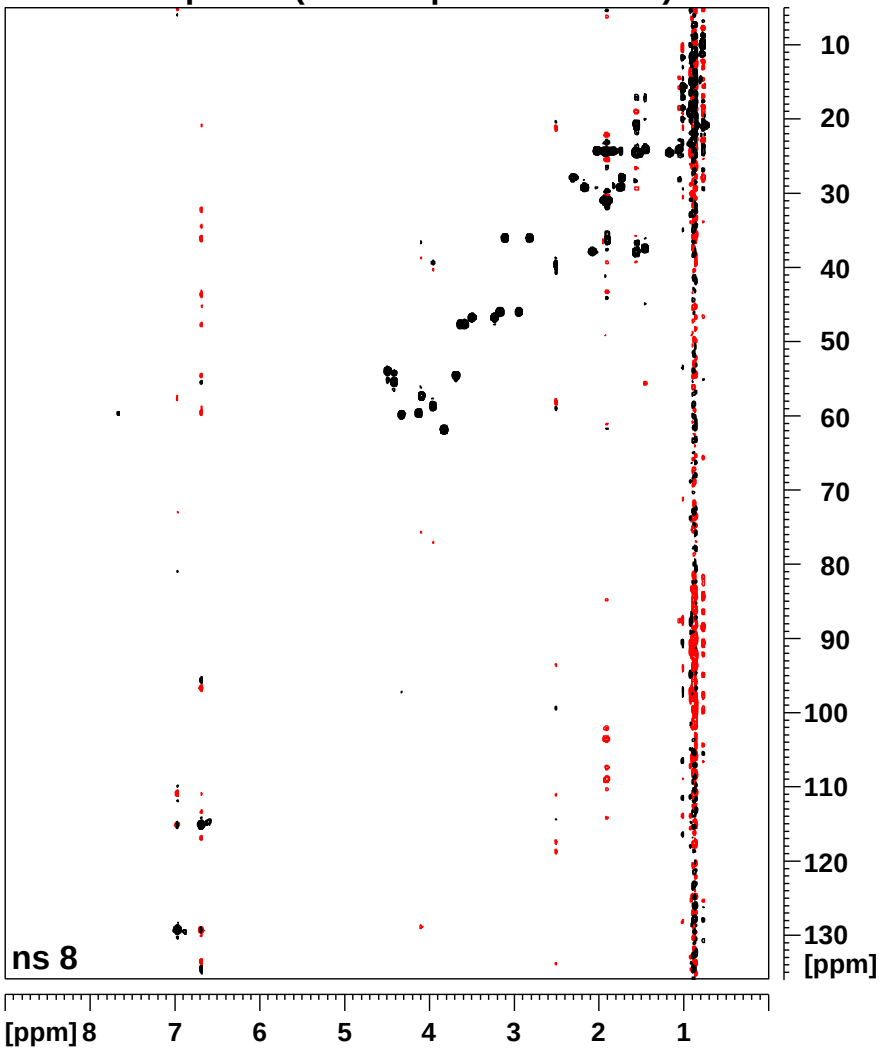
Applications

HSQC

25% of 256 points (nussampler/MDD-NMR)



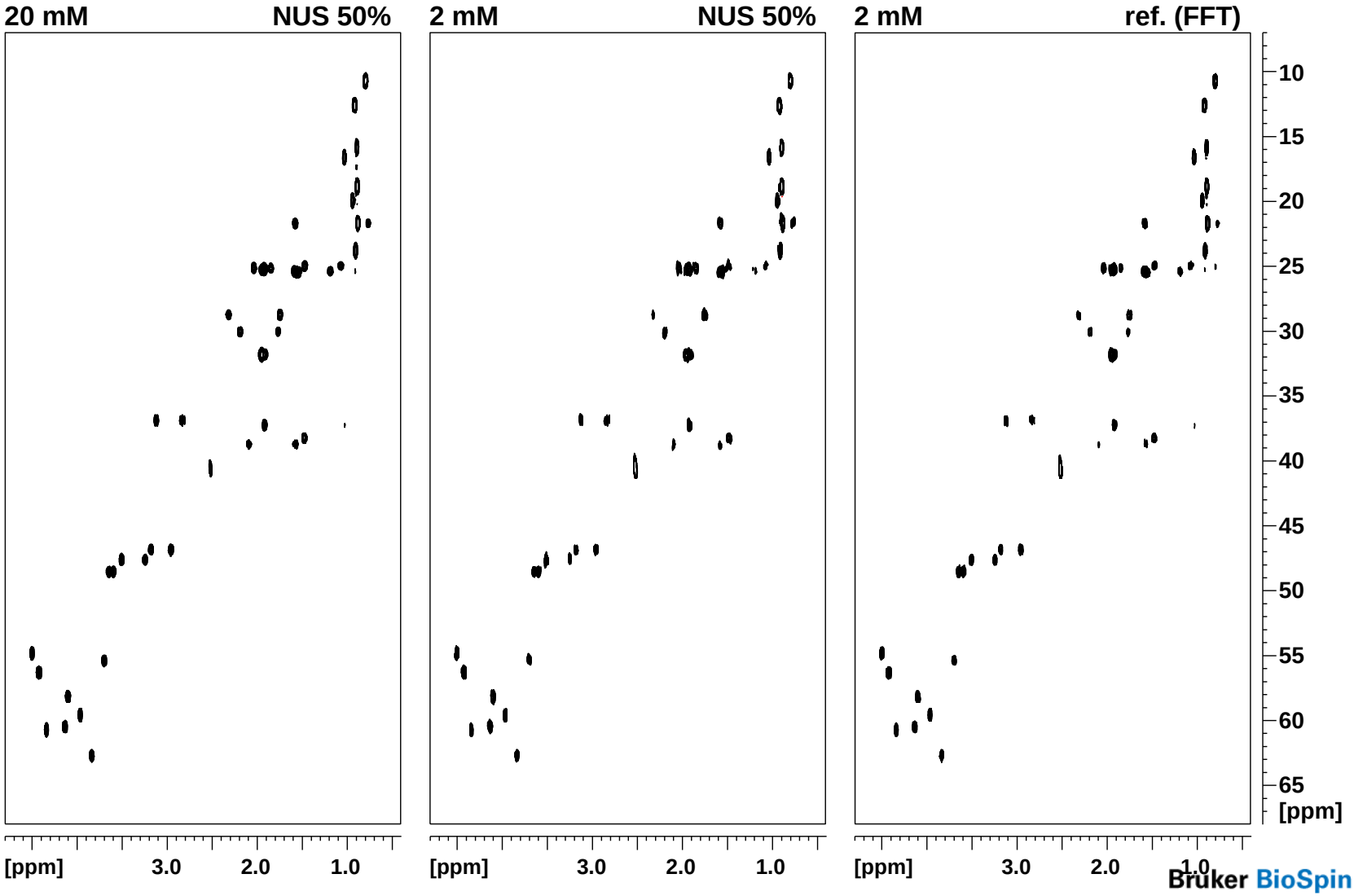
25% of 256 points (nussampler/MDD-NMR)



20mM Hymenistatin

Applications

HSQC: td = 256



Hymenistatin (2mM: 894ug in 0.5ml)

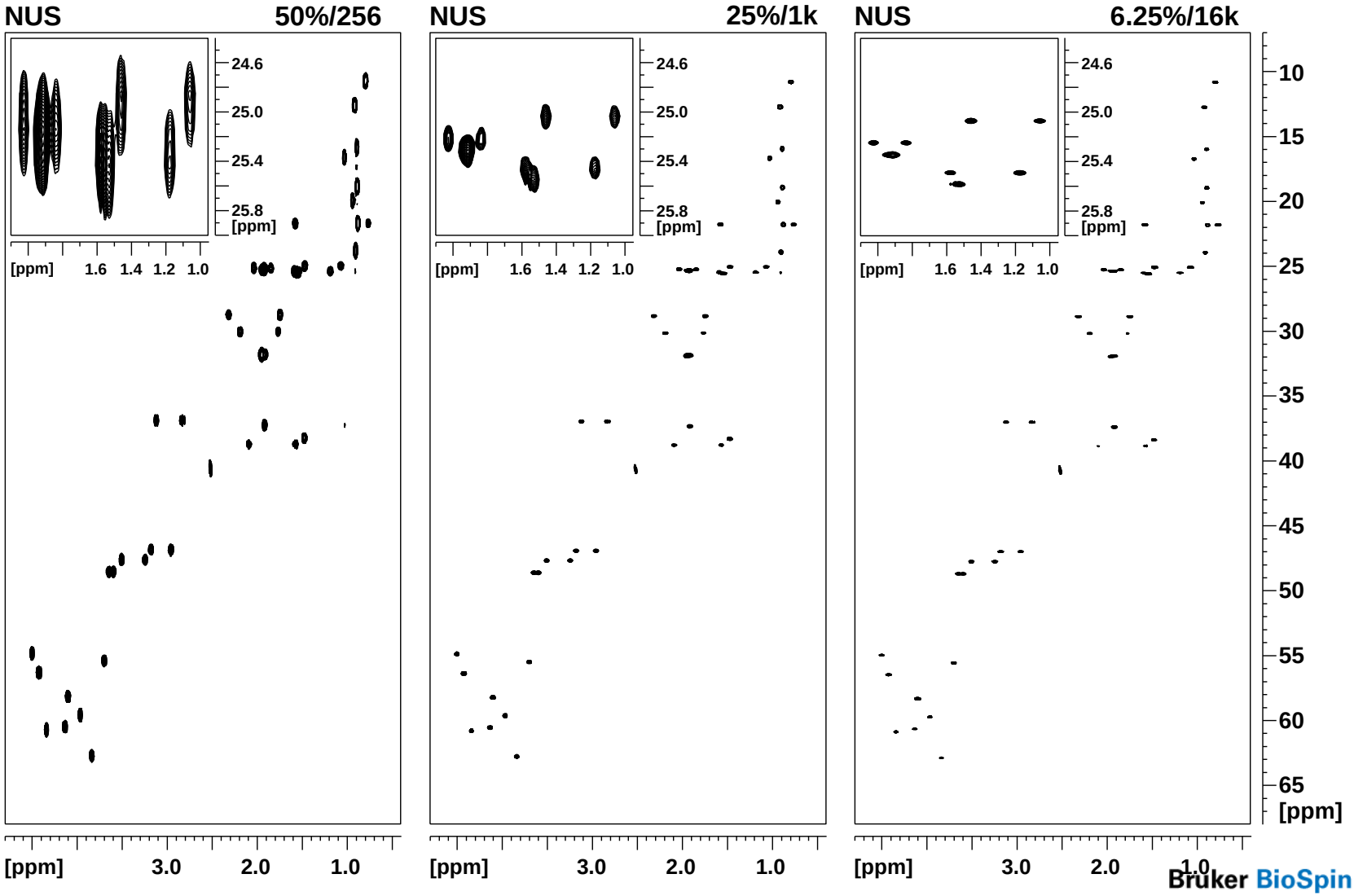
Applications

HSQC

td1	amount	NCP	expt (min)	proc. (FT + mddnmr) (m:s)	si1
256	50%	64	10.5	4:34	512
512	25%	64	10.5	5:06	1k
1k	25%	128	20	11:07	2k
2k	12.5%	128	20	12:18	4k
4k	12.5%	256	38.5	27:31	8k
8k	6.25%	256	38.5	31:24	16k
16k	6.25%	512	76	67:50	32k

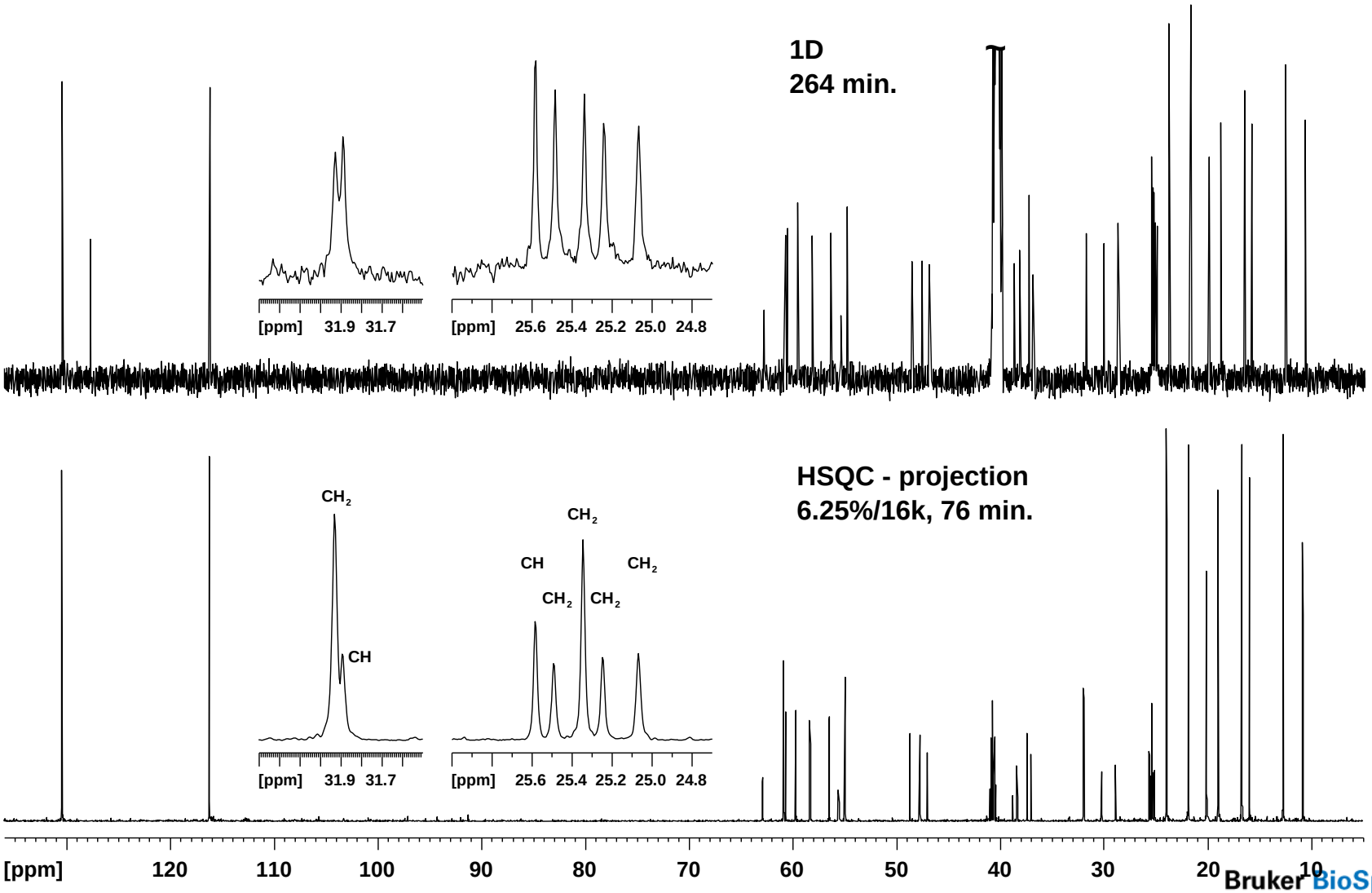
Applications

HSQC



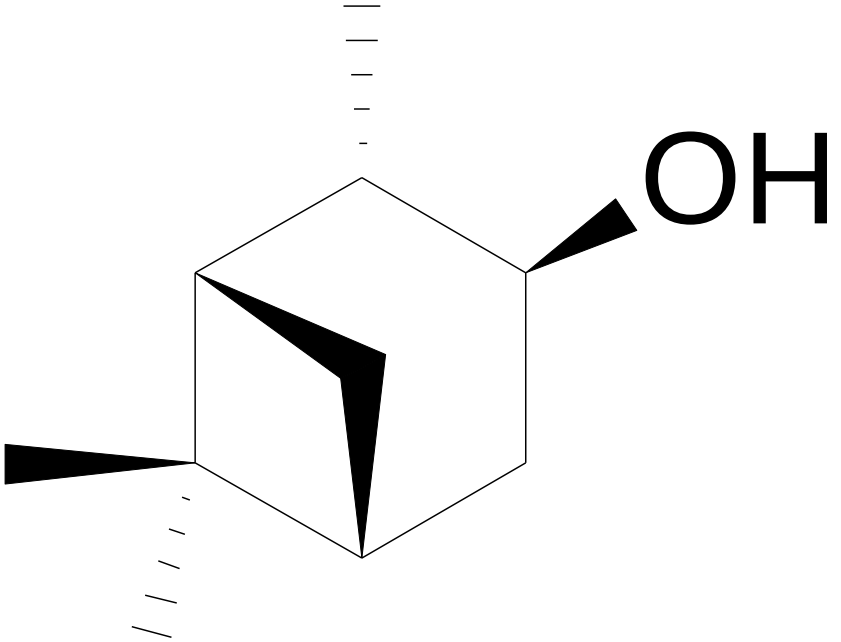
Applications

HSQC



Applications

(+)-Isopinocampheol ((+)-IPC)



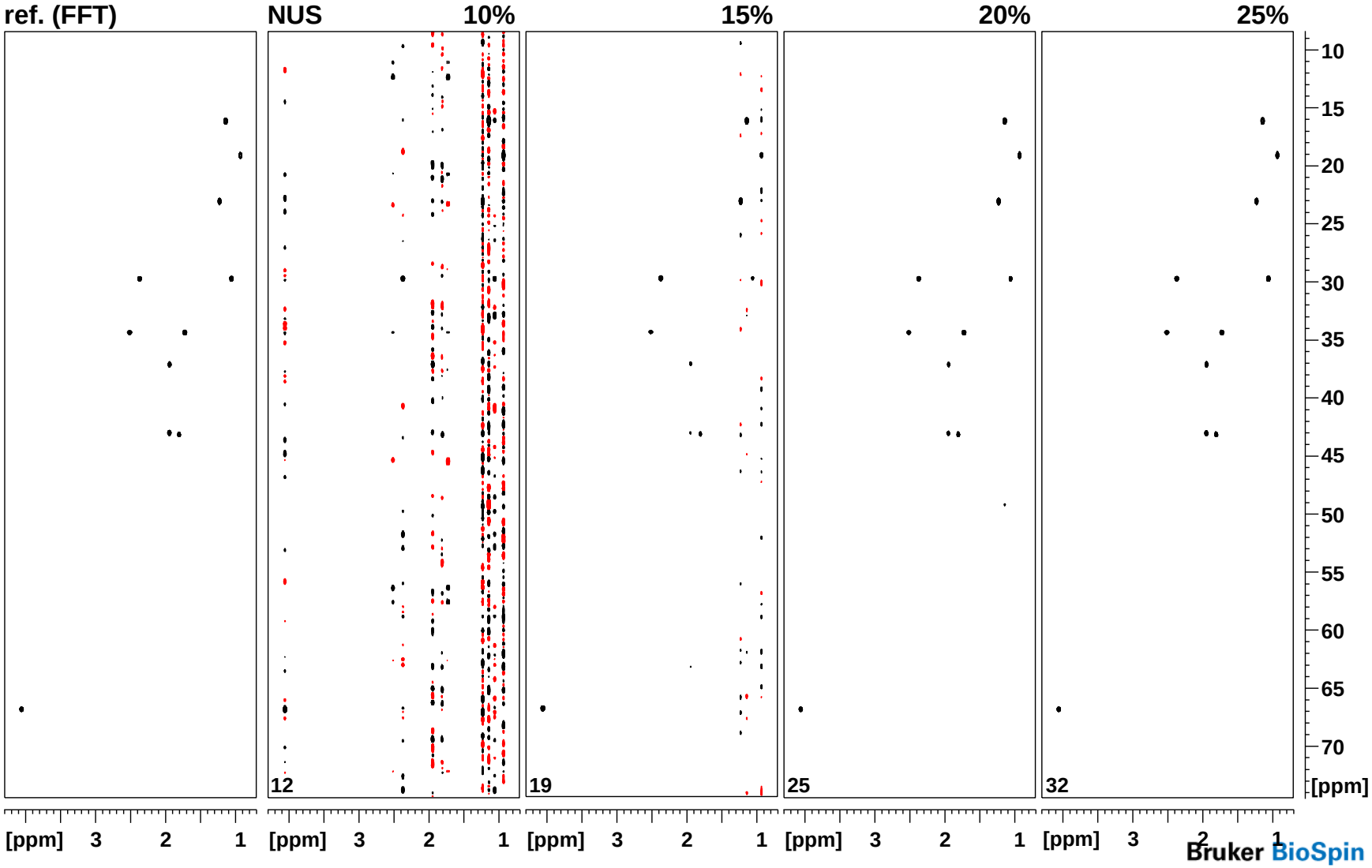
number of cross peaks (estimated maximum):

HSQC (^{13}C)	11
HMBC (^{13}C)	54
COSY	36
TOCSY	83

courtesy C. Thiele

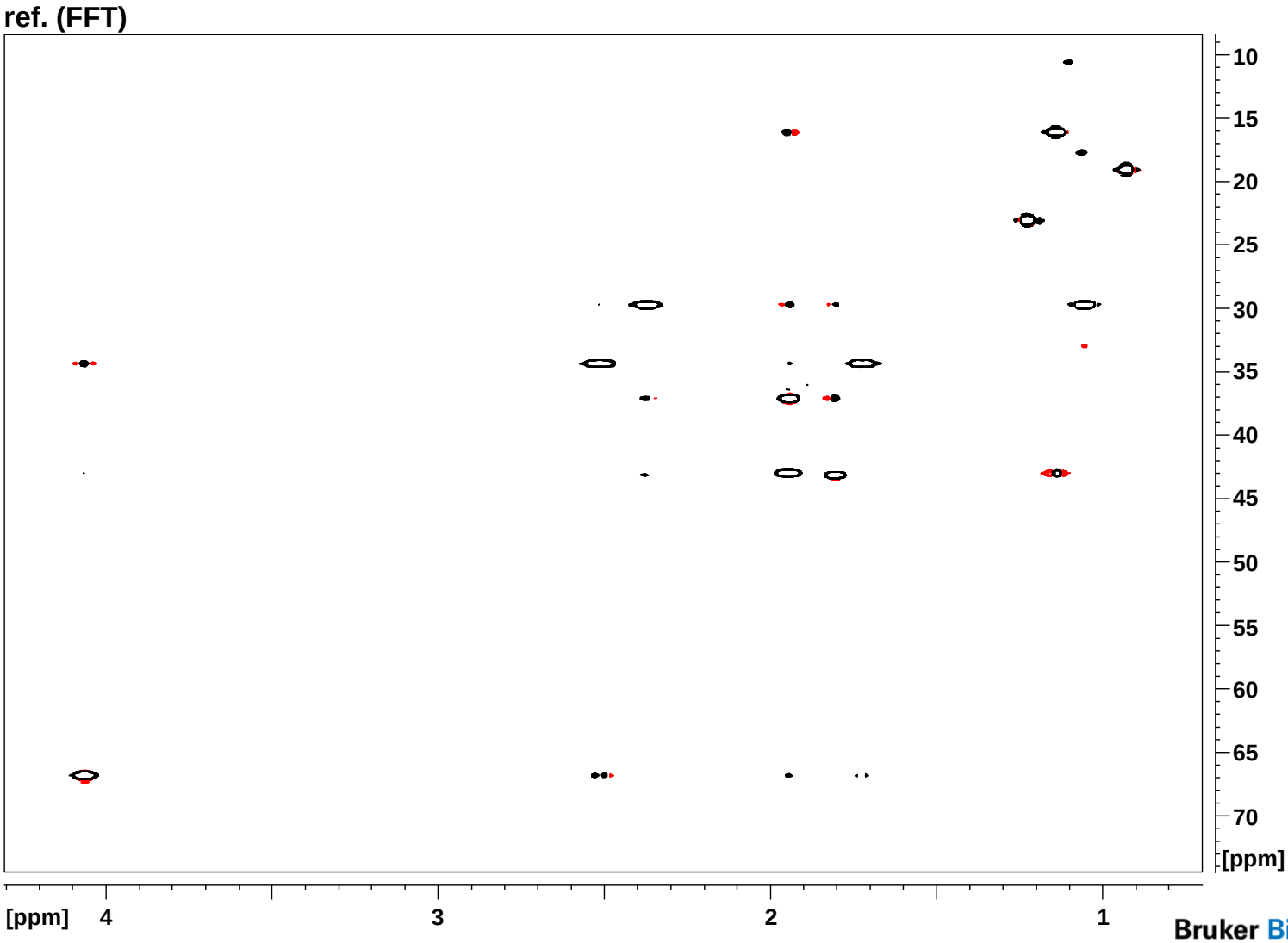
Applications

HSQC: td = 256



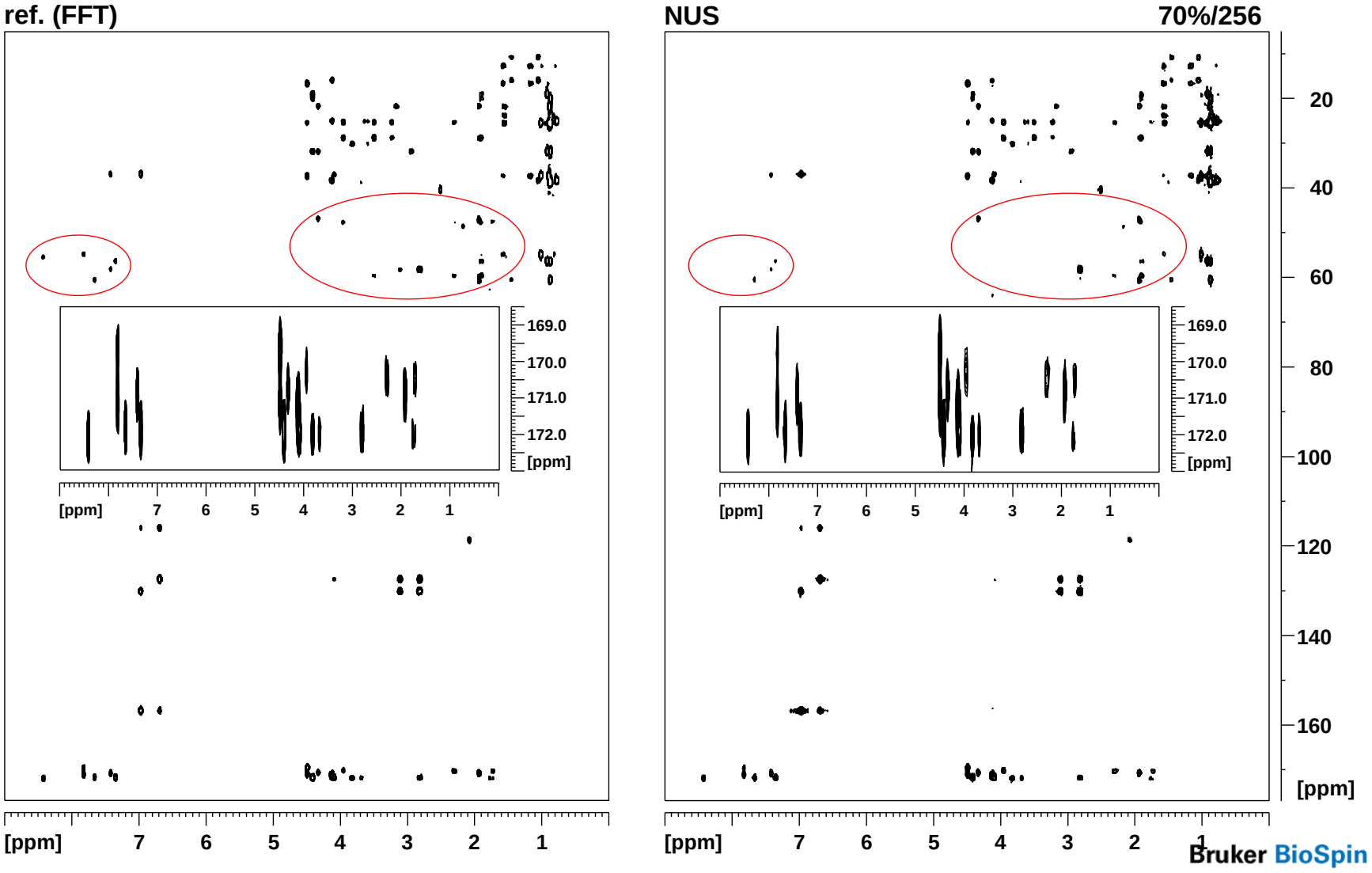
Applications

HSQC: COSY peaks in HSQC-si



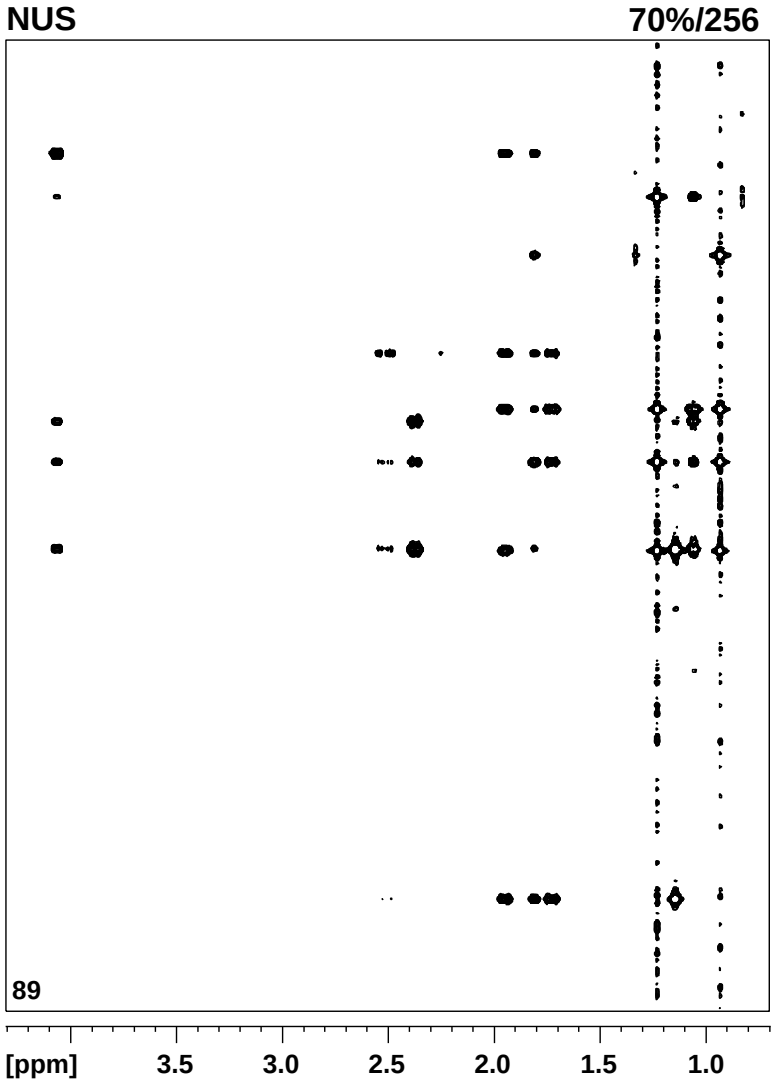
Applications

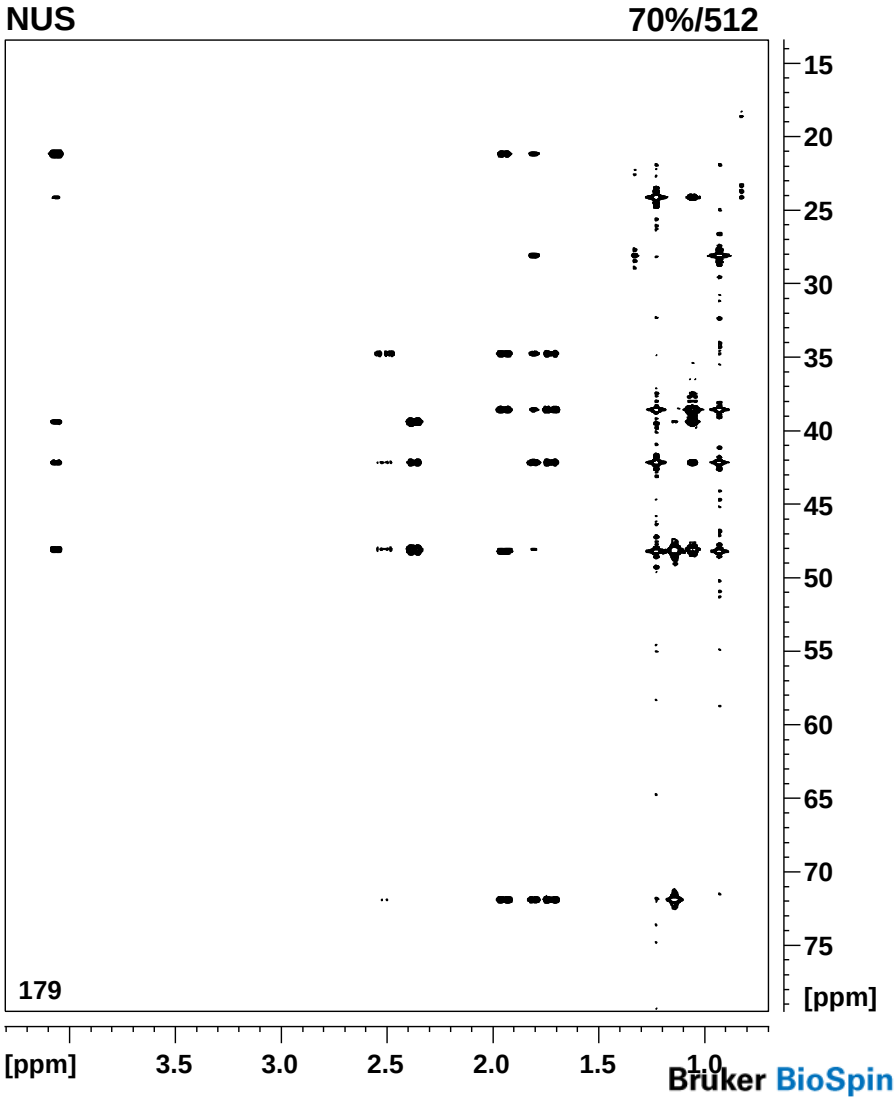
HMBC



Applications

HMBC

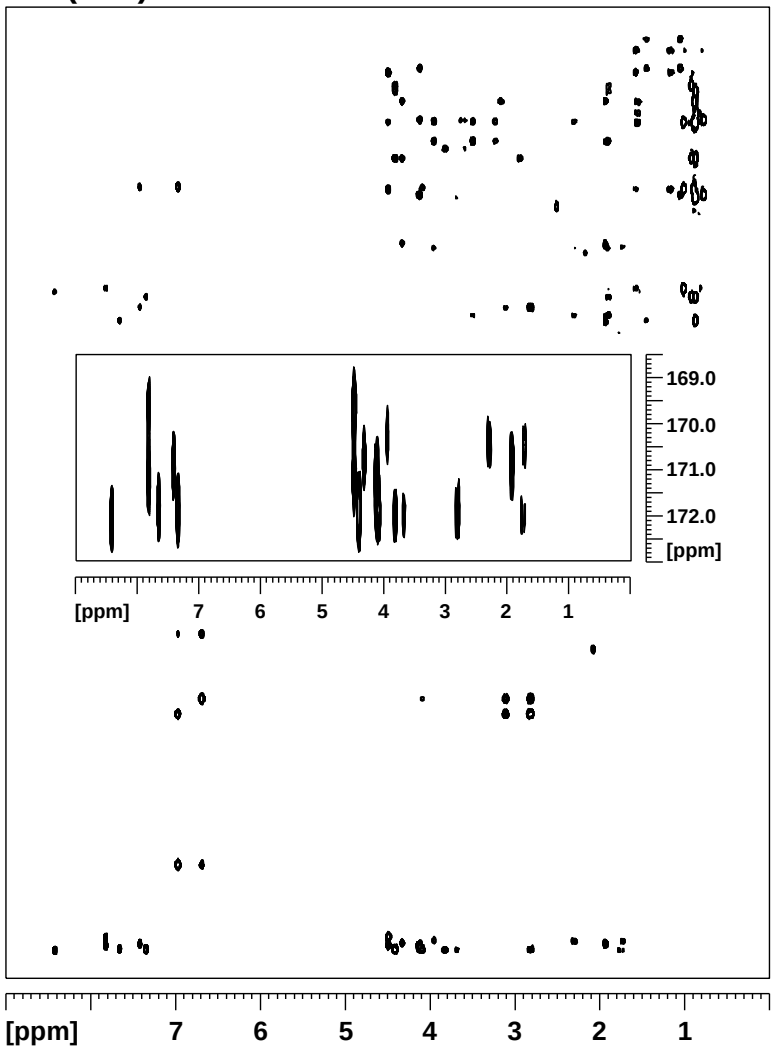




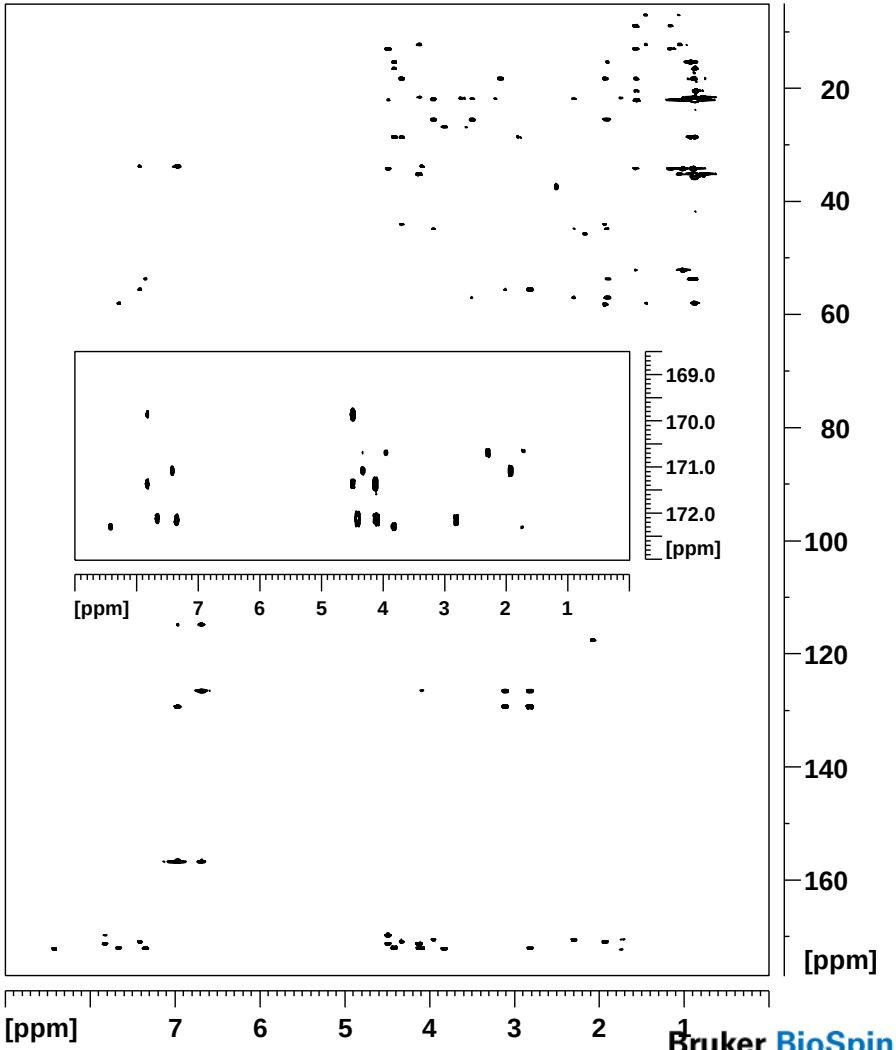
Applications

HMBC

ref. (FFT)



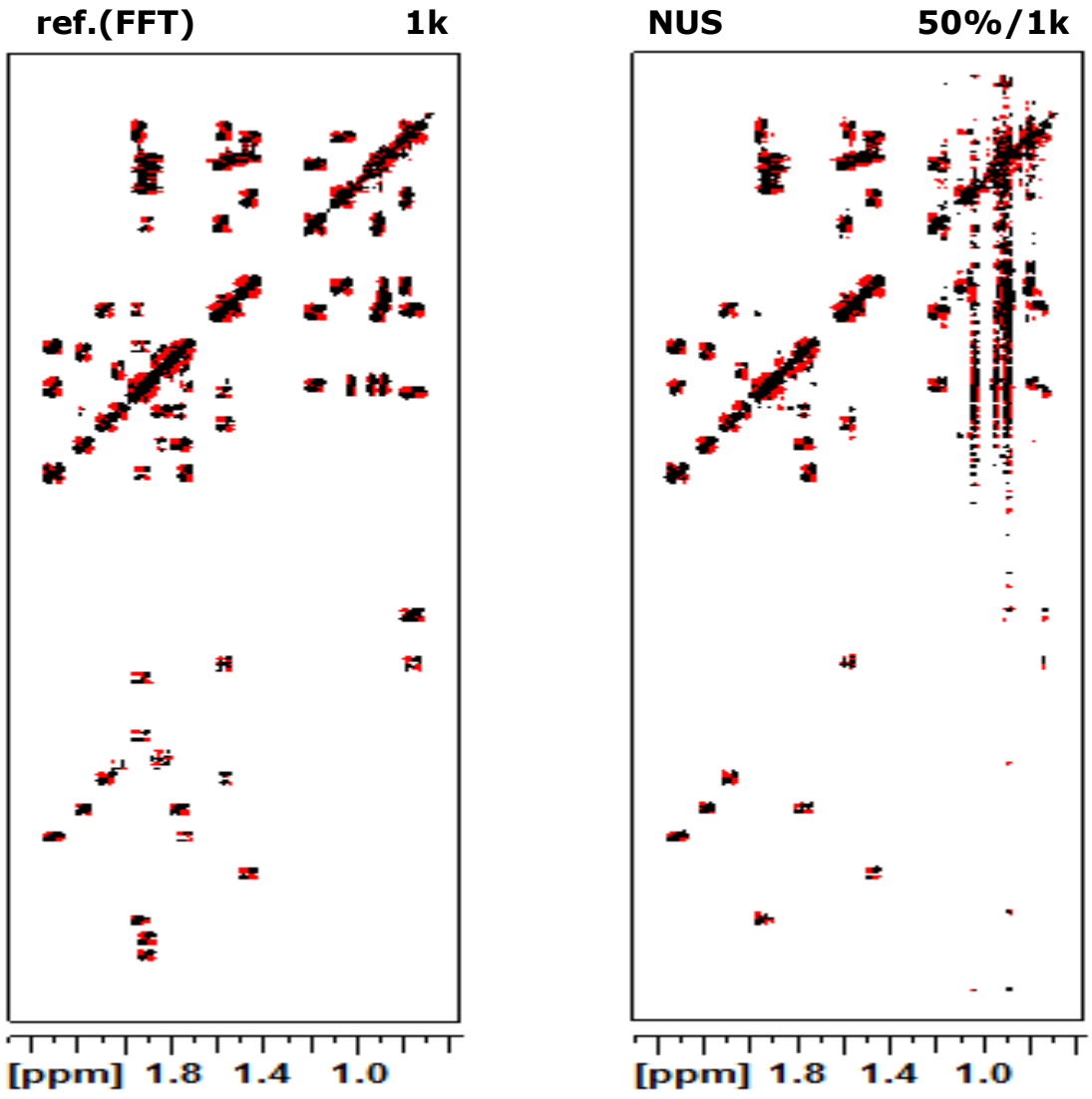
NUS 25%/4k



Bruker BioSpin

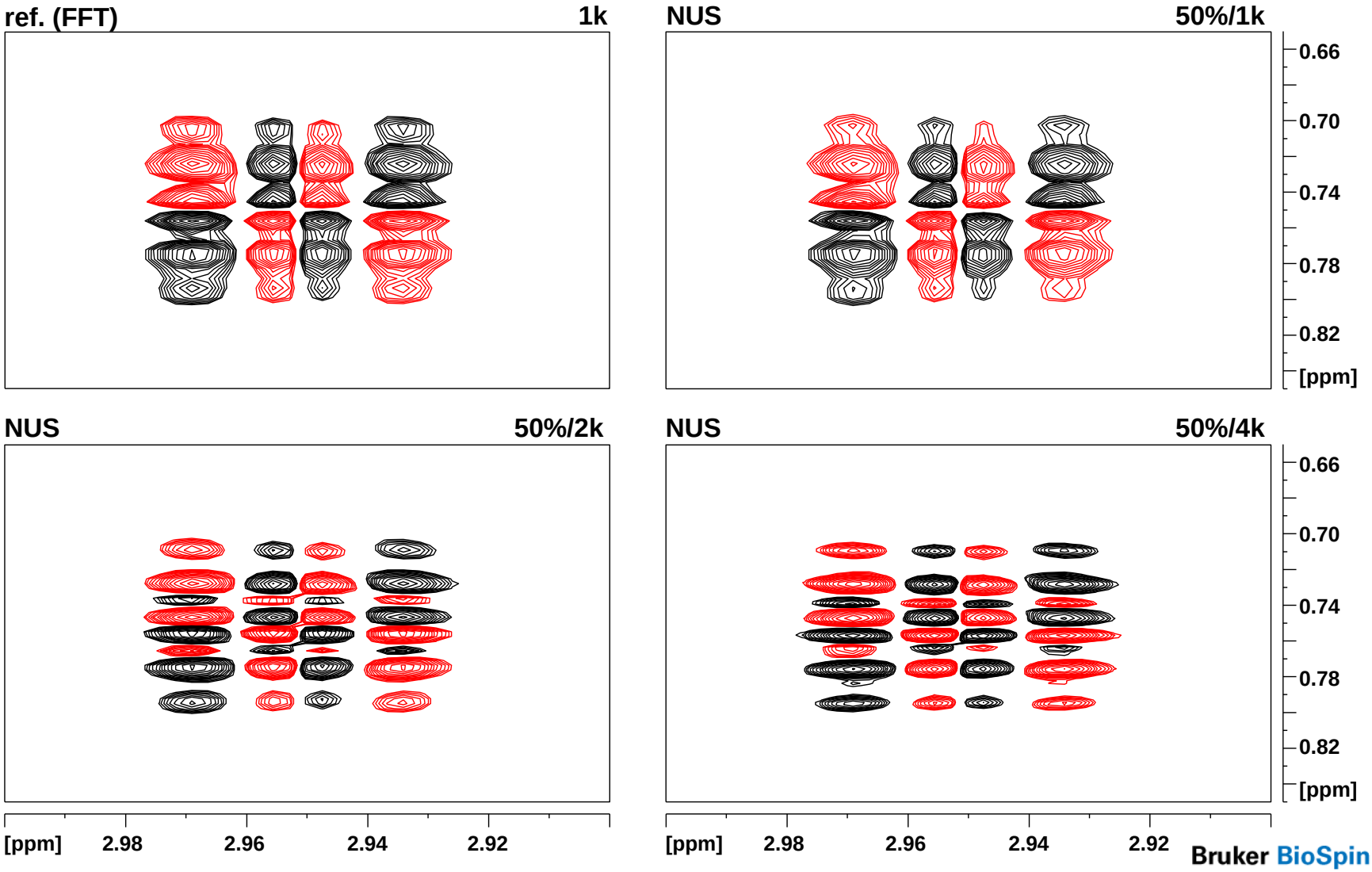
Applications

COSY - dfph



Applications

COSY - dfph

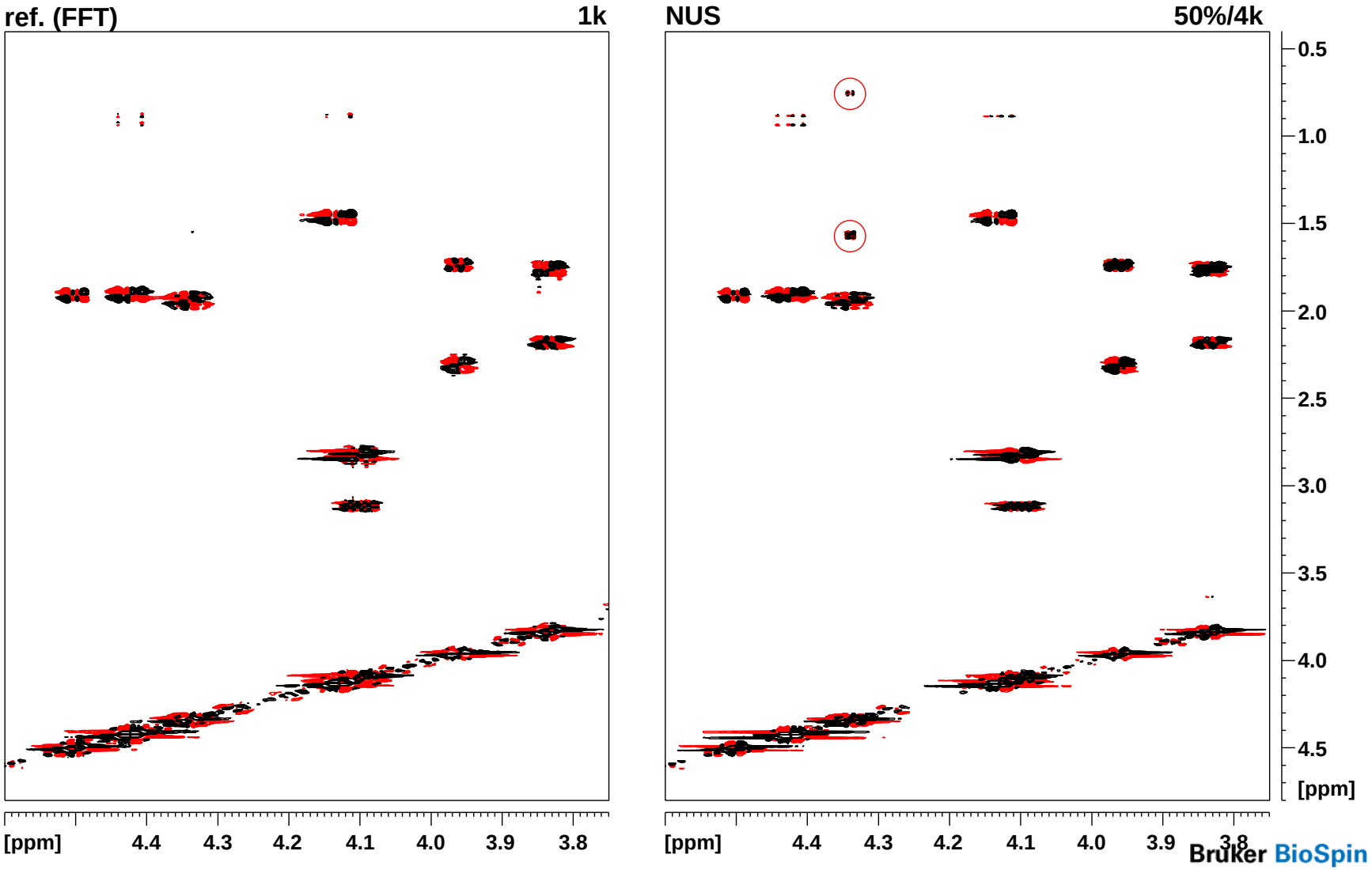


Bruker BioSpin

20mM Hymenistatin NCOMP = 120 25%/4k not possible

Applications

COSY - dfph



Bruker BioSpin

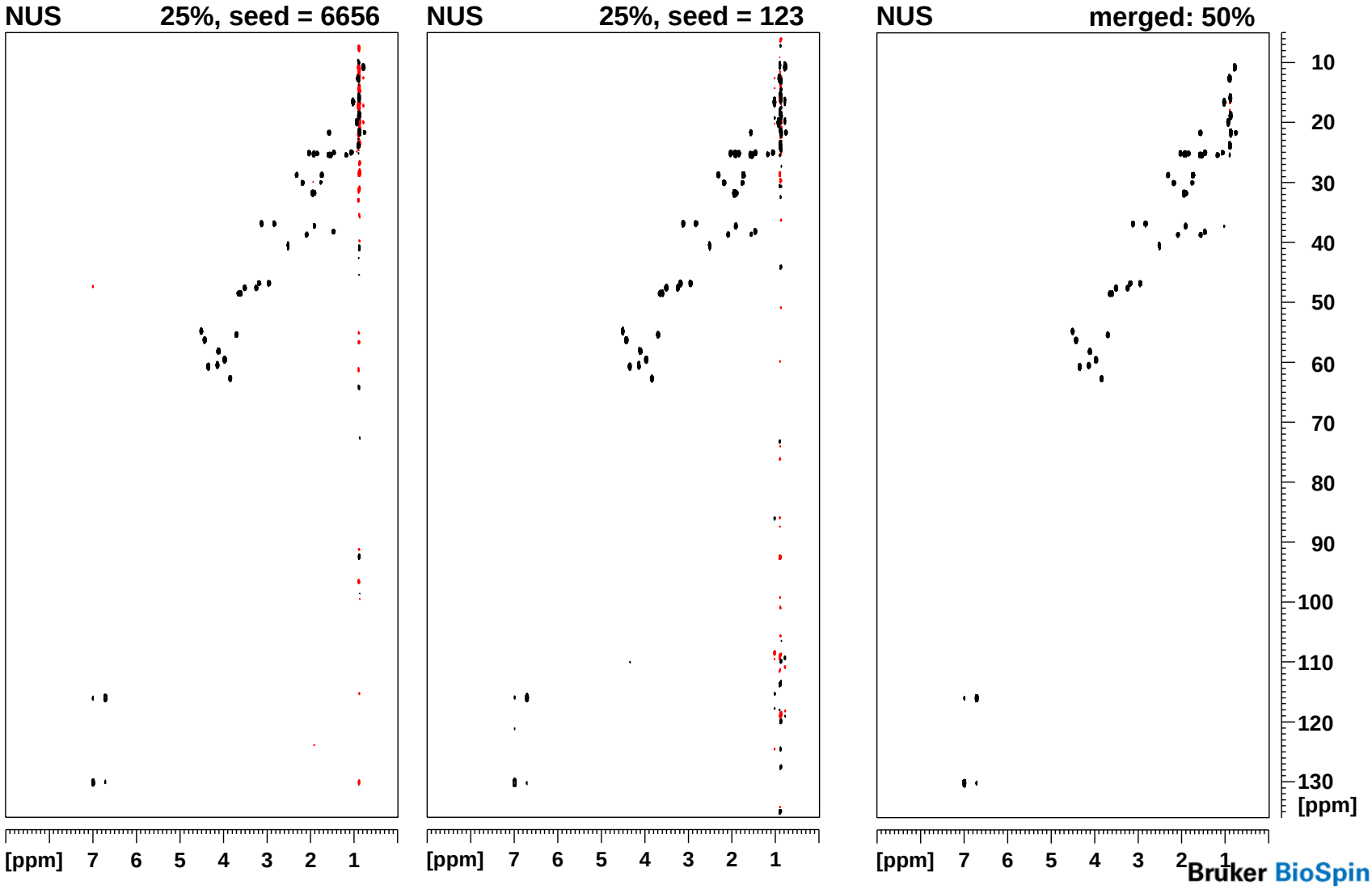
20mM Hymenistatin

NCOMP = 120

25%/4k not possible

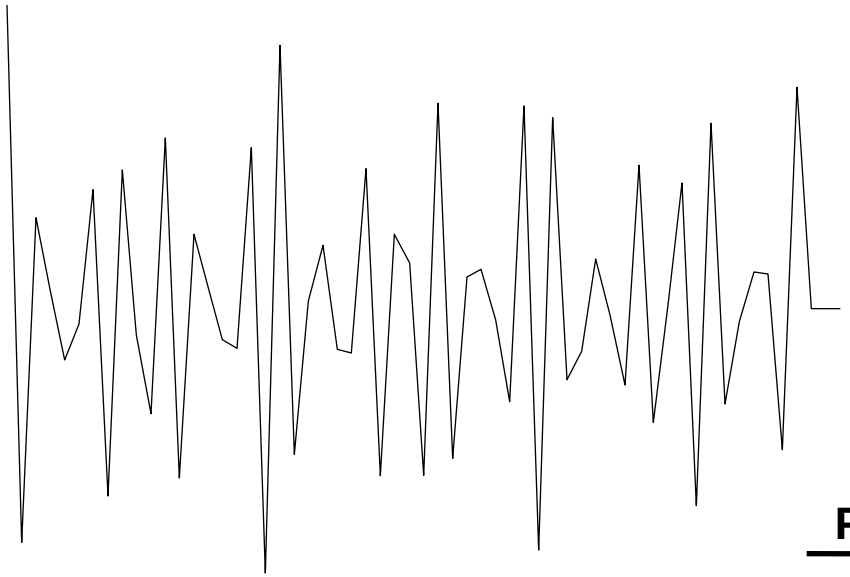
Applications

HSQC: td = 256

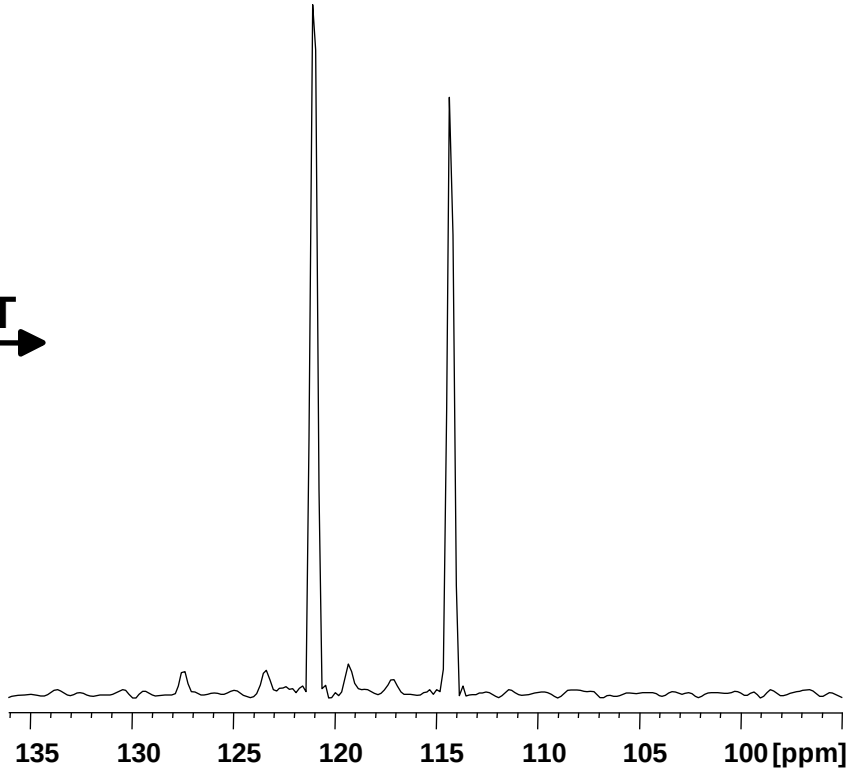


Applications

col from first t_2F_3 plane (HNCO)



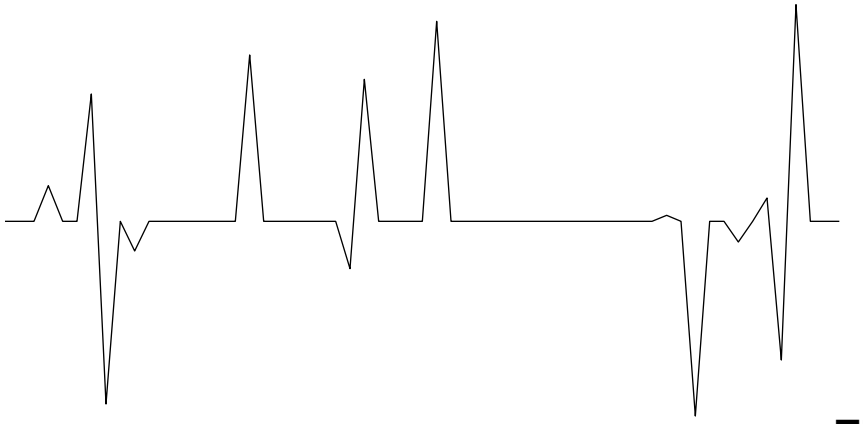
FFT



Ubiquitin

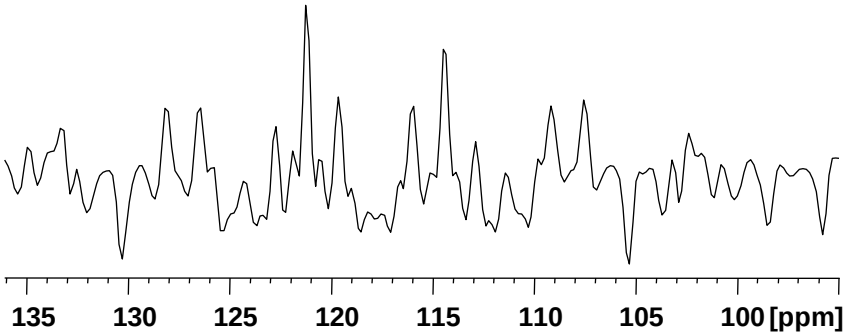
Applications

col from first t_2F_3 plane (HNCO)



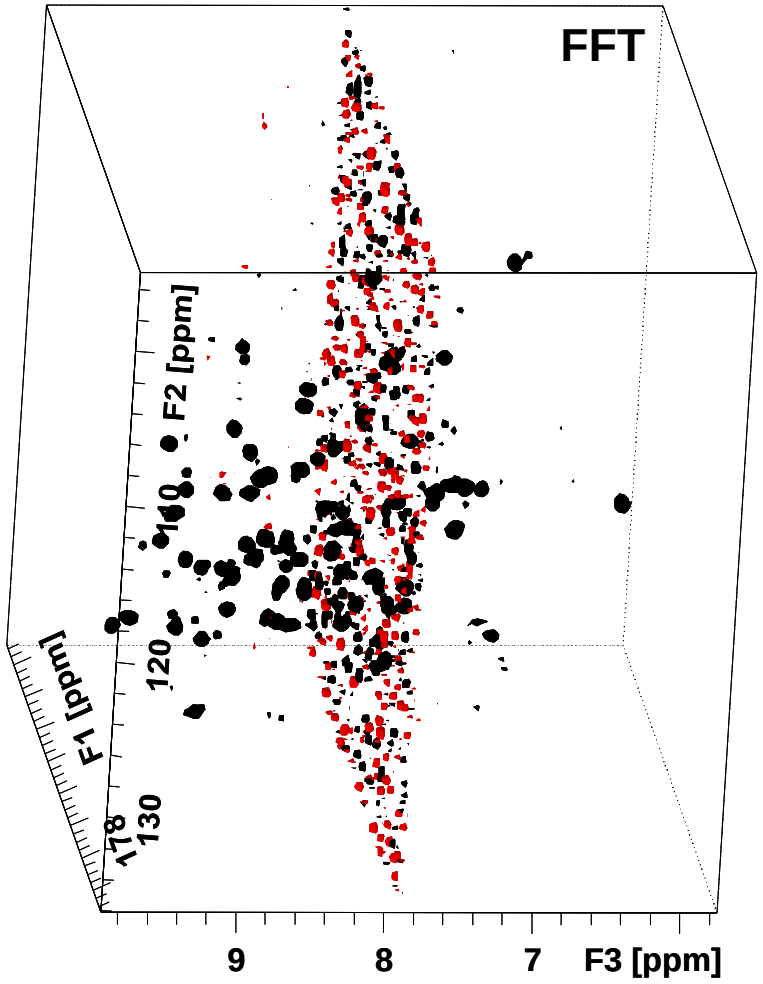
FFT

25% sparse (nussampler)



Applications

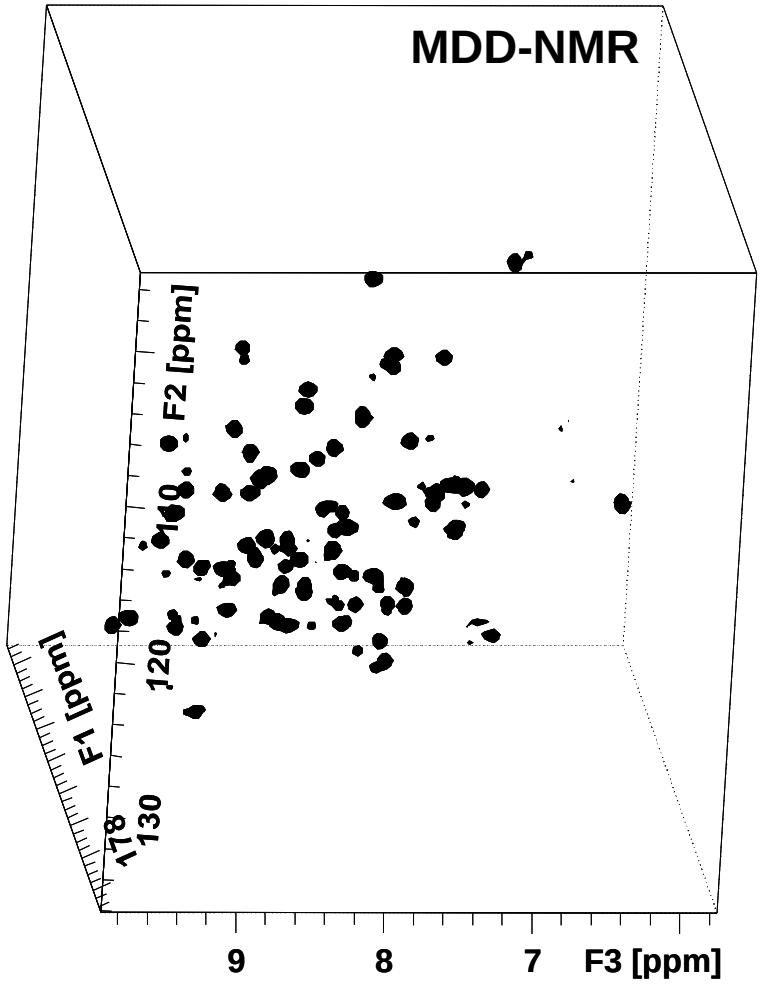
HNCO - 25% sparse (nussampler)



Ubiquitin

Applications

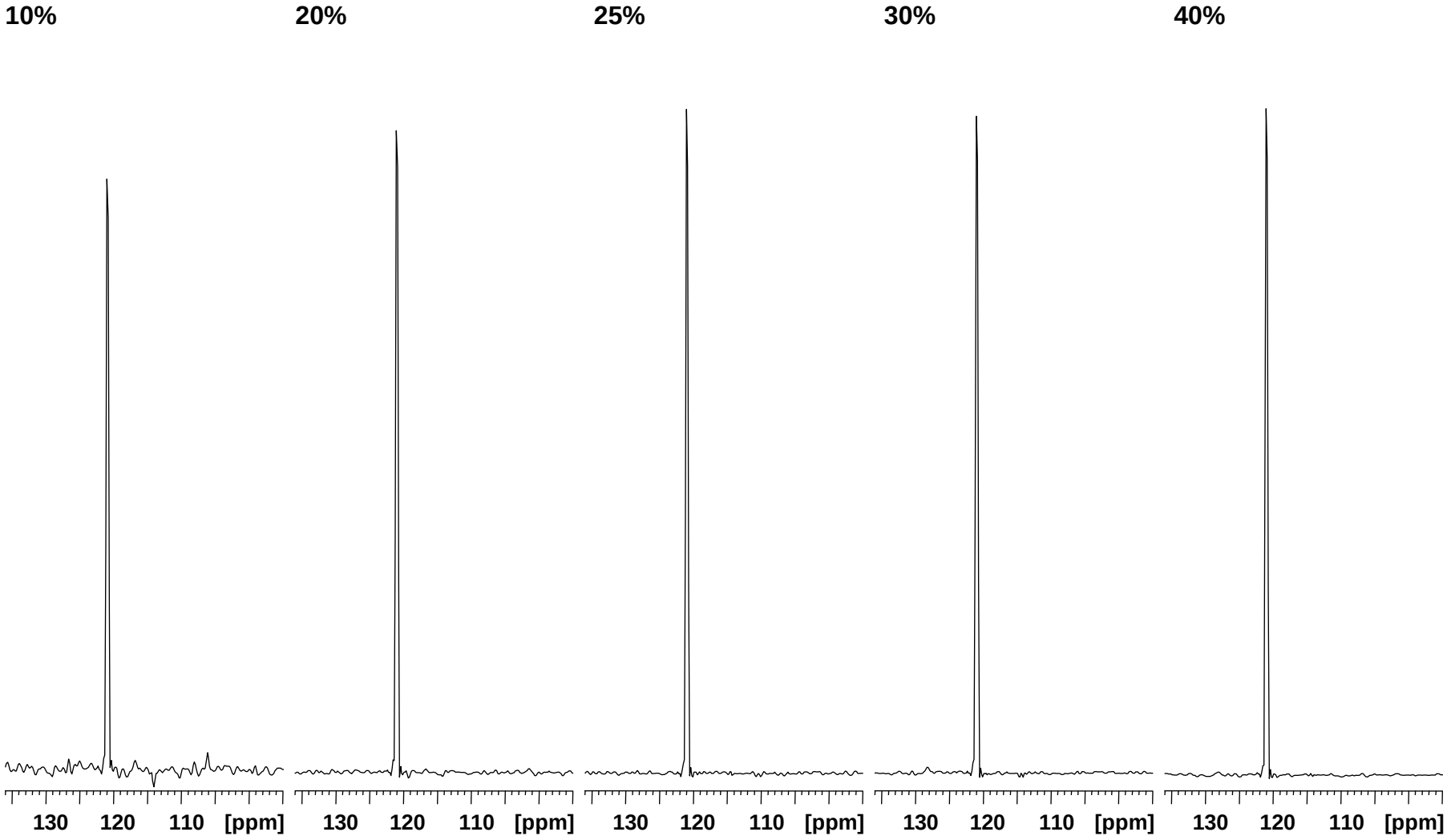
HNCO - 25% sparse (nussampler)



Ubiquitin

Applications

HNCO - col from F_2F_3 plane (172.8 ppm) - sparse (nussampler/MDD-NMR)

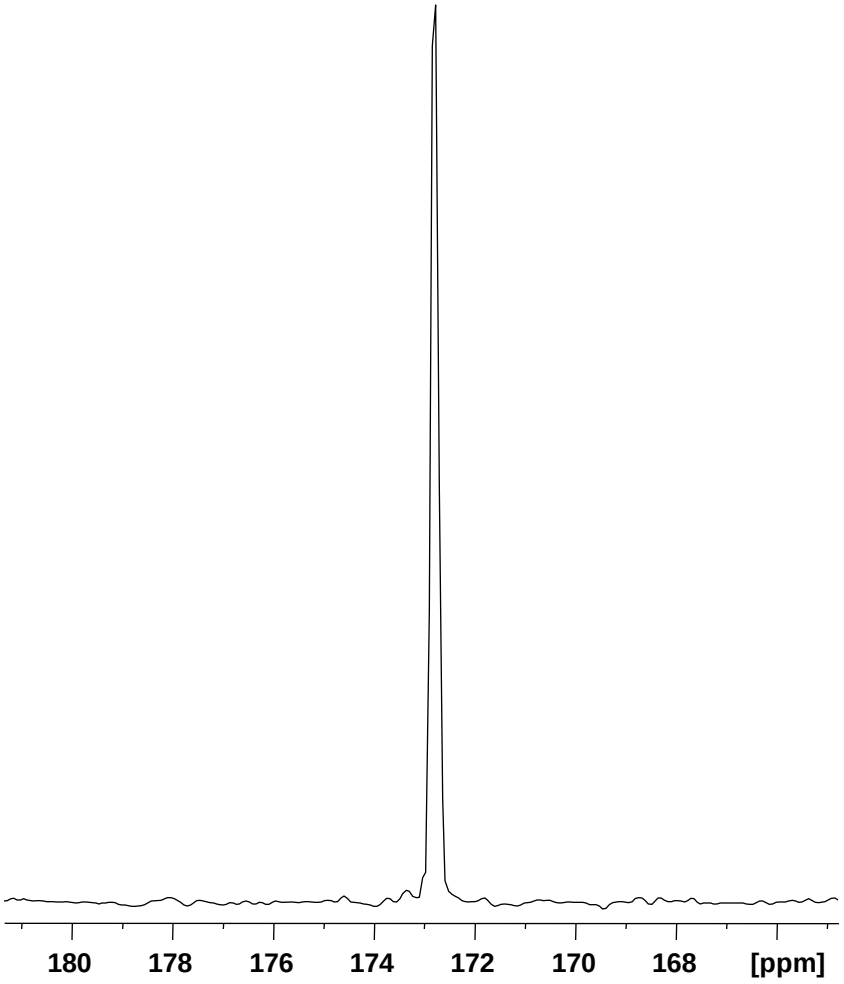


Ubiquitin

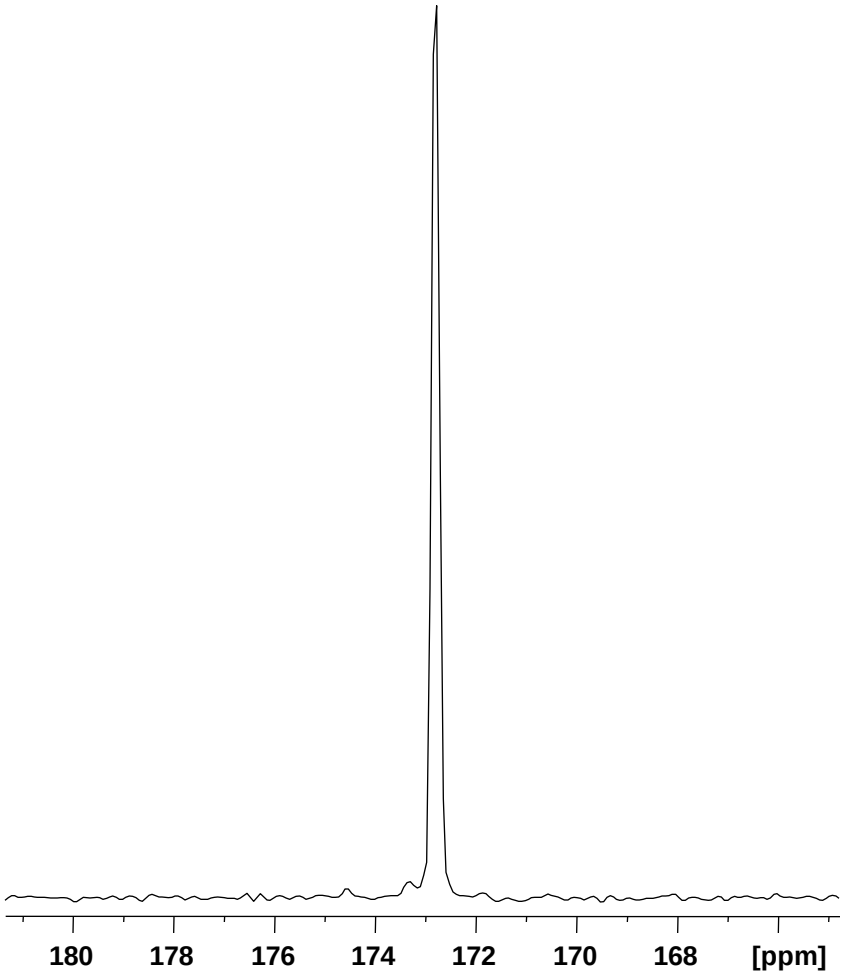
Applications

col from F_1F_3 plane (121.0 ppm) - 25% sparse (nussampler/MDD-NMR)

not weighted in t_1

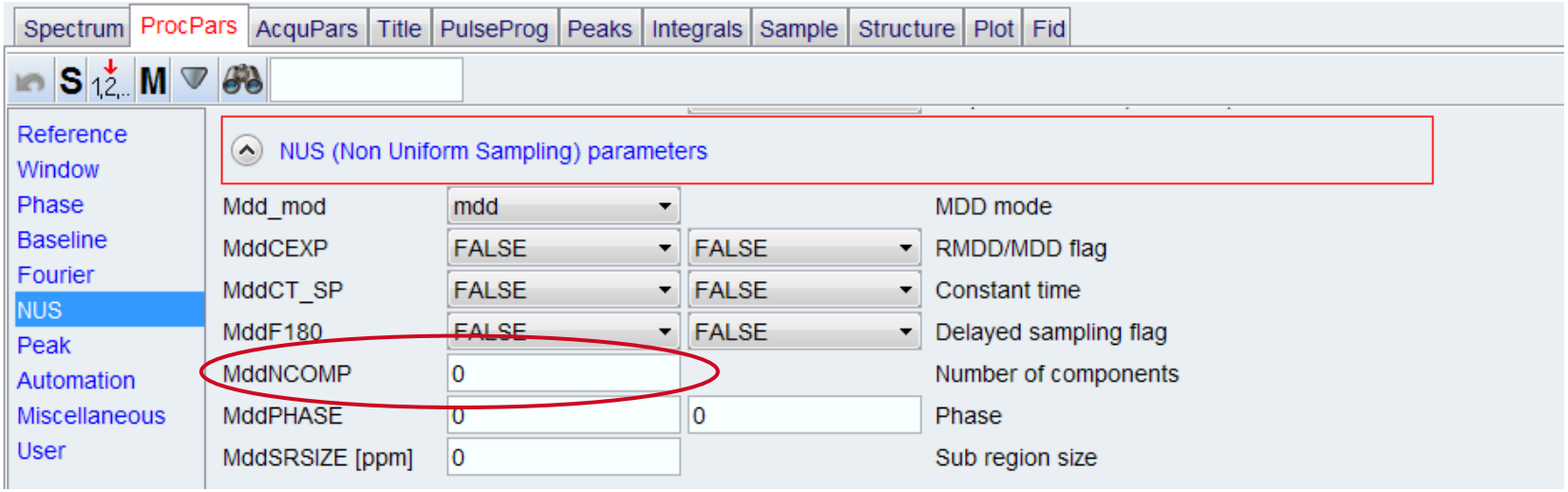


exponentially weighted in t_1



Ubiquitin

Additional processing parameters



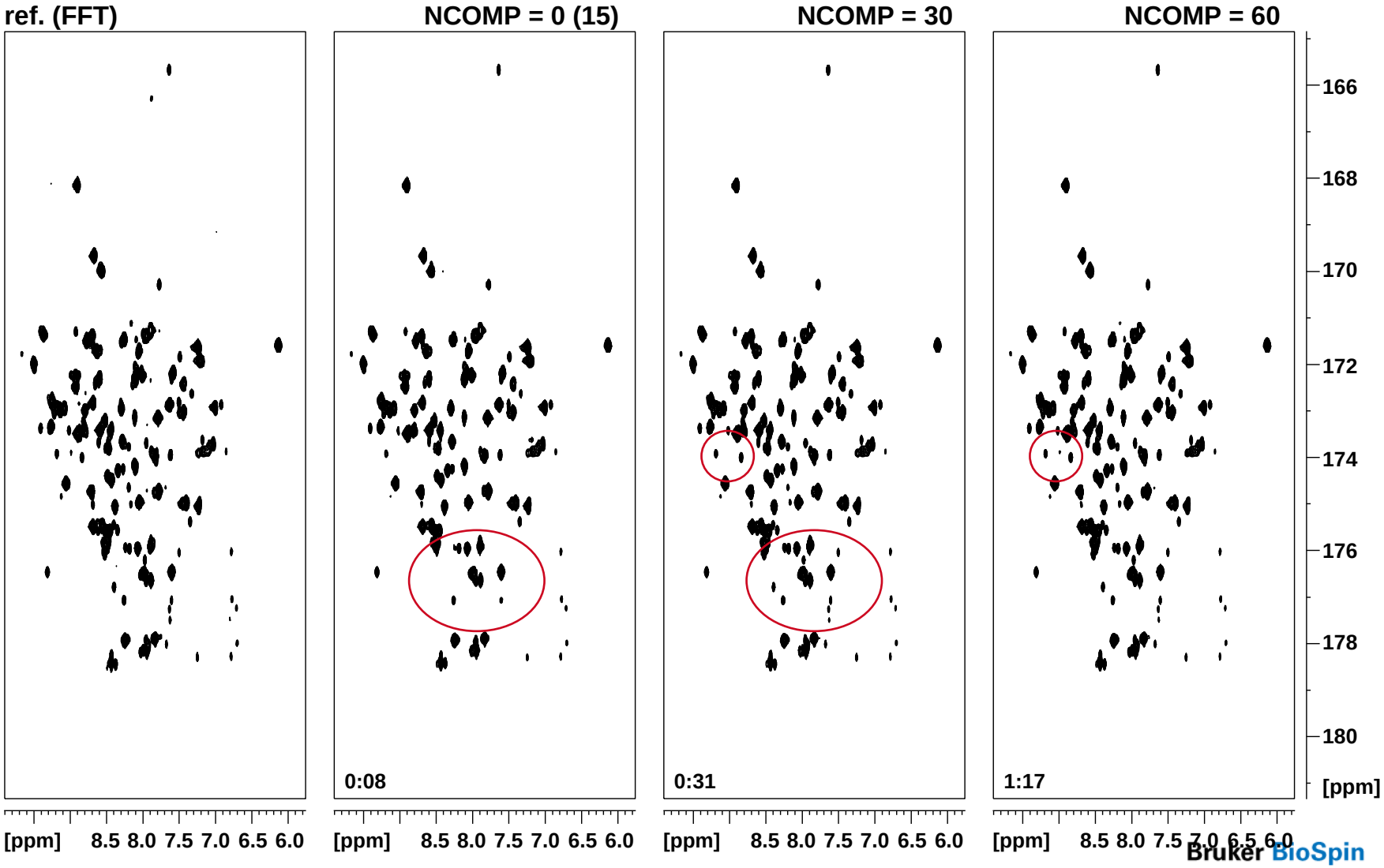
Number of components

- default is 15
- can be increased if peaks are missing
- processing times can get very long

Additional processing parameters

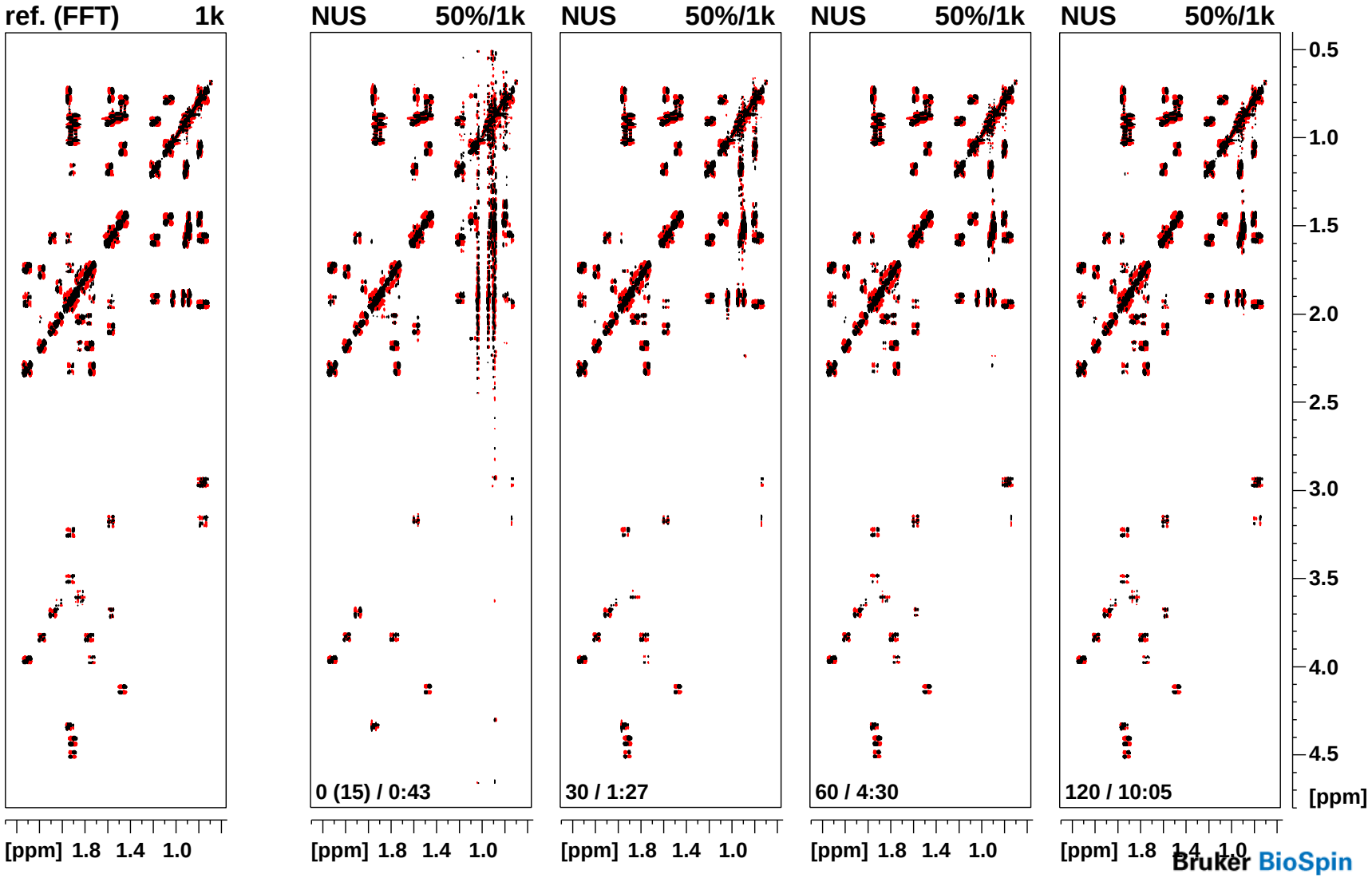
HNCO: F1F3 projection

NUS 25%, CEXP: nnn

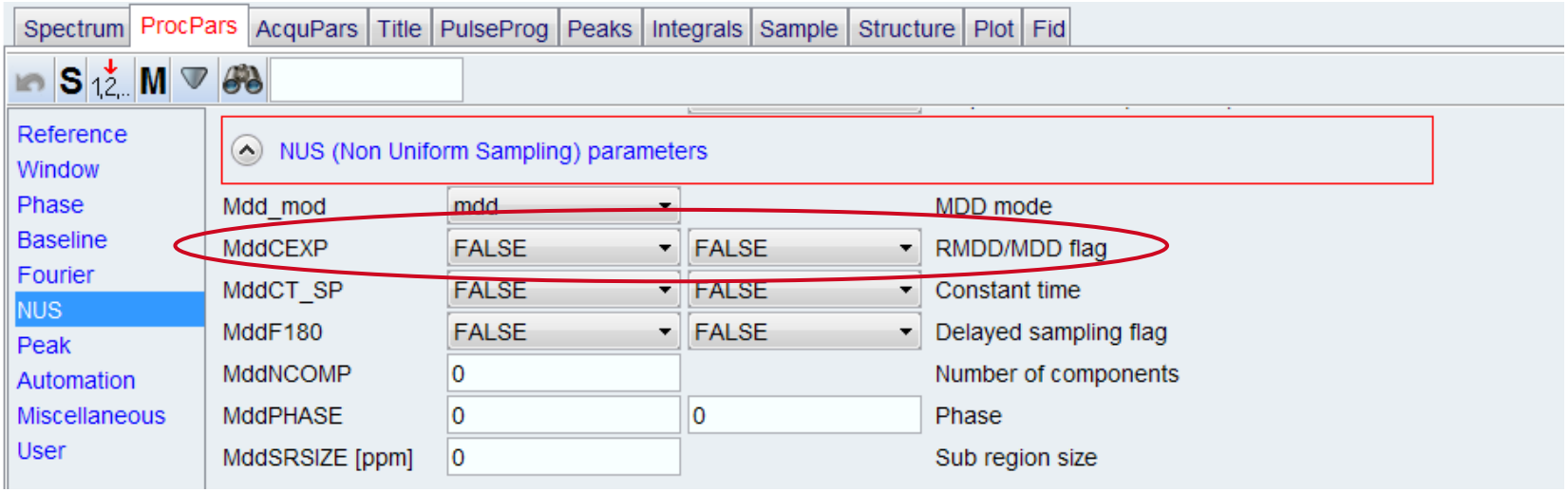


Additional processing parameters

COSY - dfph



Additional processing parameters

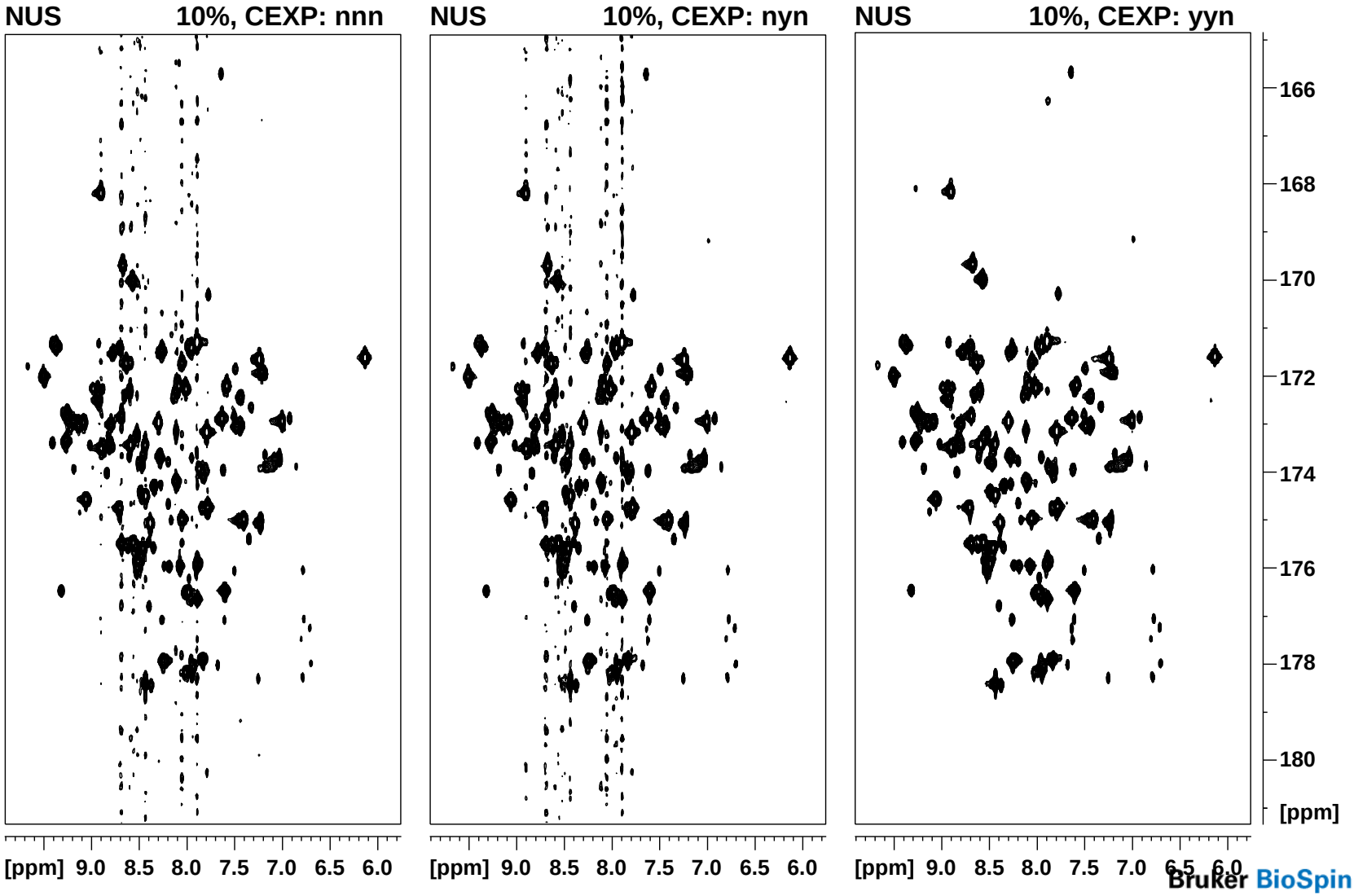


Recursive MDD

- required for 2D
- can also help with nD
- processing times are longer

Additional processing parameters

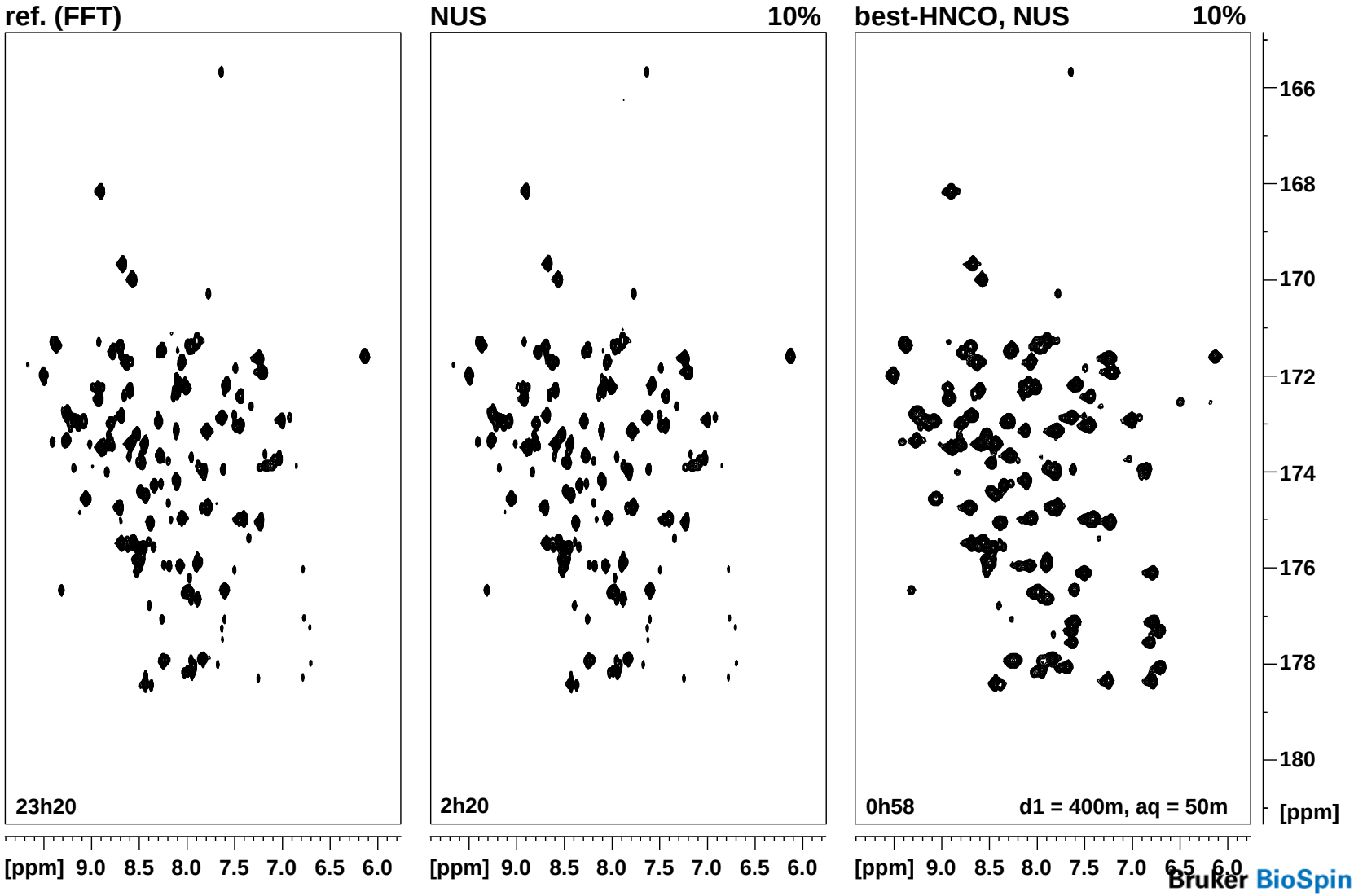
HNCO: F1F3 projection



Bruker BioSpin

Implementation

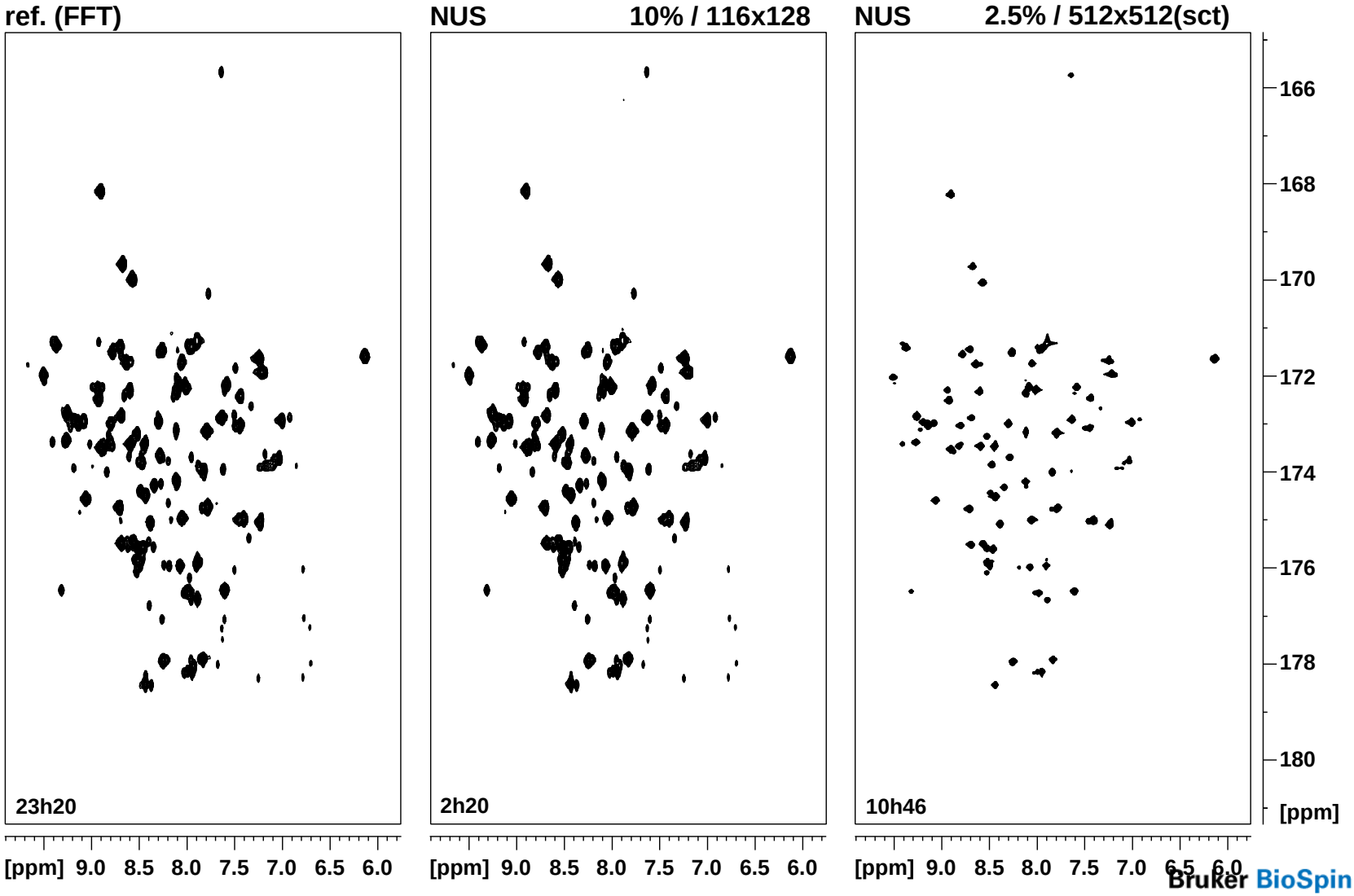
HNCO: F1F3 projection



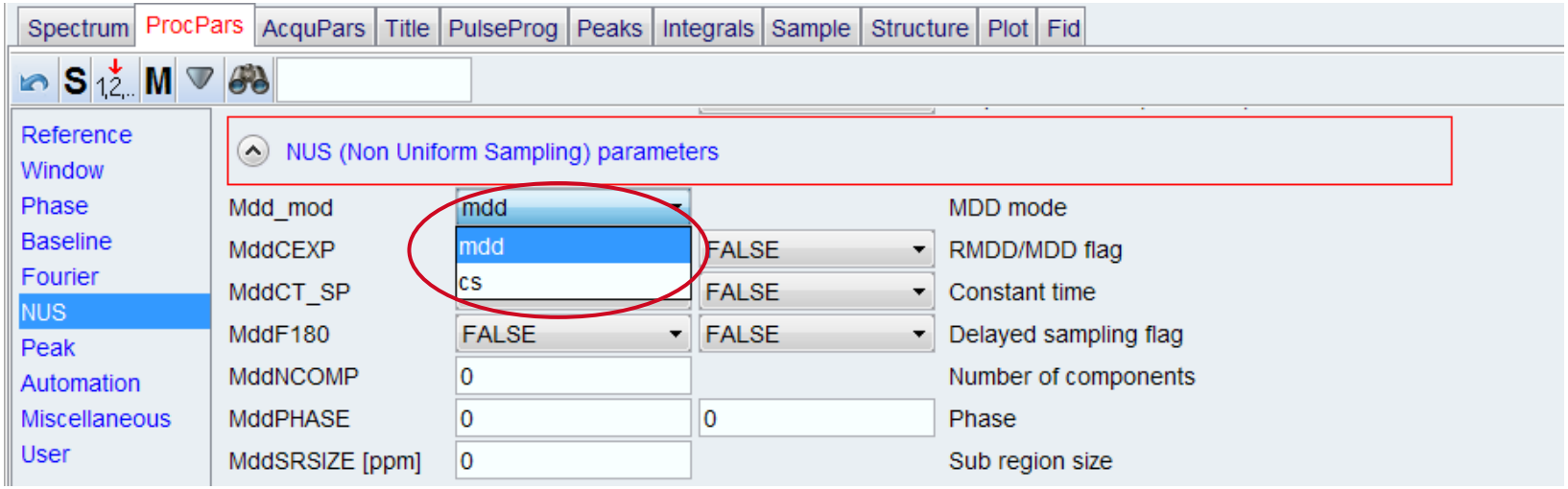
Bruker BioSpin

Implementation

HNCO: F1F3 projection



New processing algorithm

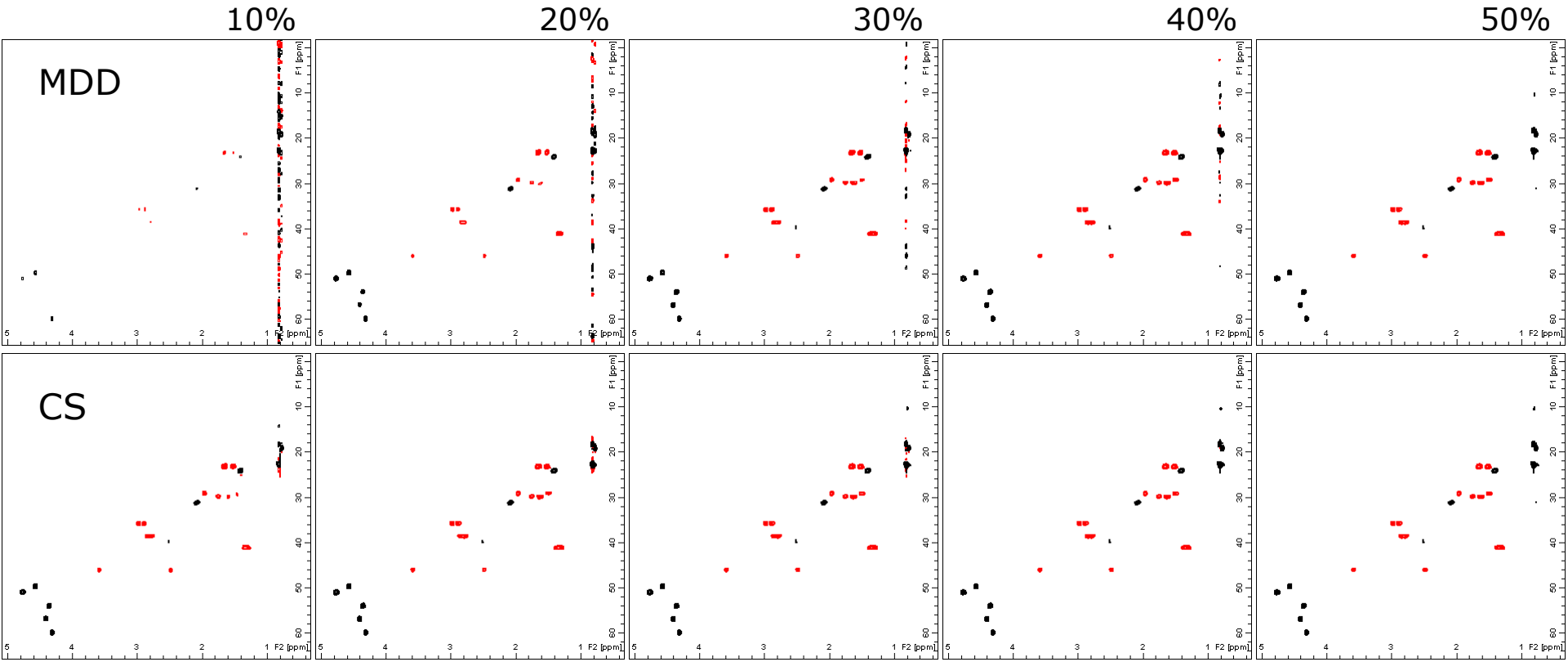


CS - Compressed Sensing

- significantly improves 2D processing
- can be helpful for nD as well
- additional license needed

MDD vs. CS processing

50mM Gramicidin
edited HSQC
td=256



MDD vs. CS processing

50mM Gramicidin
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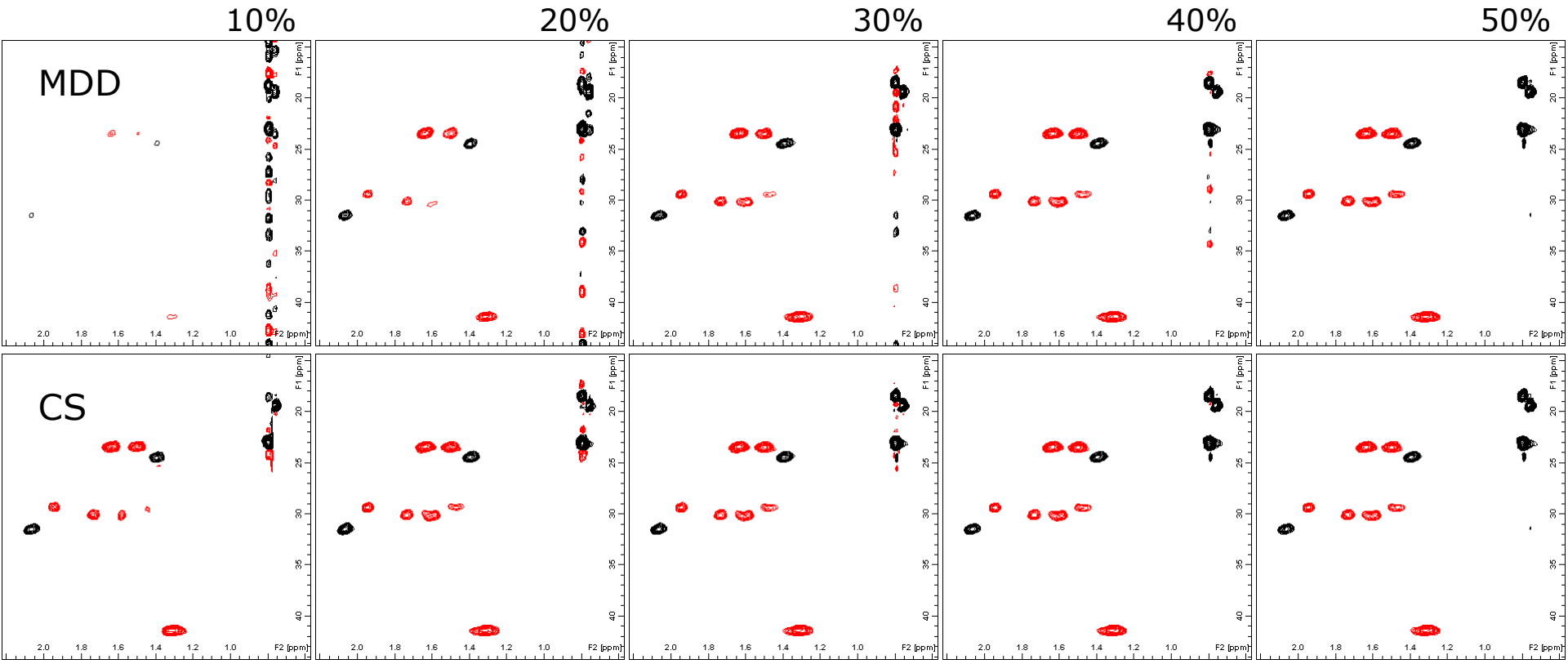
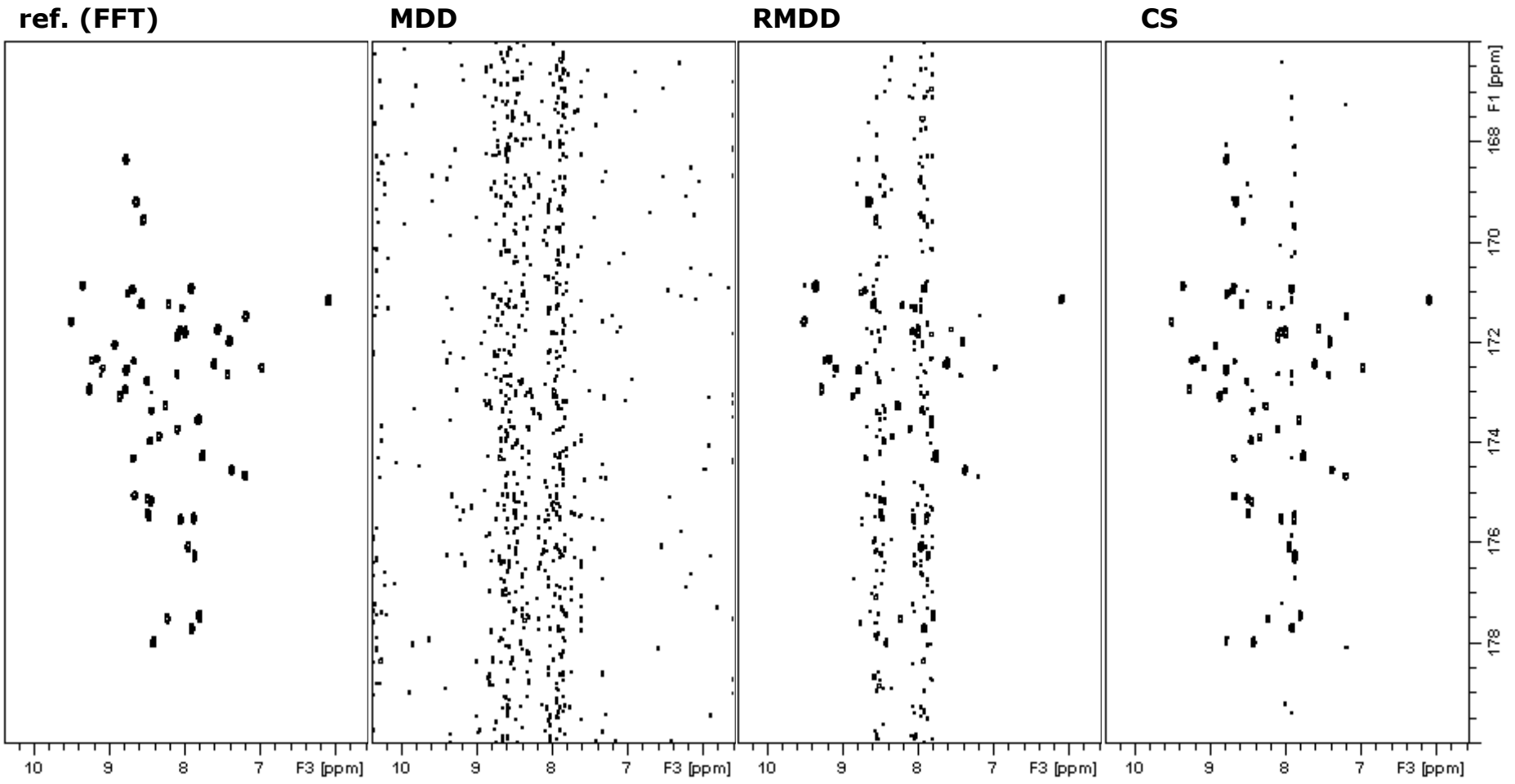


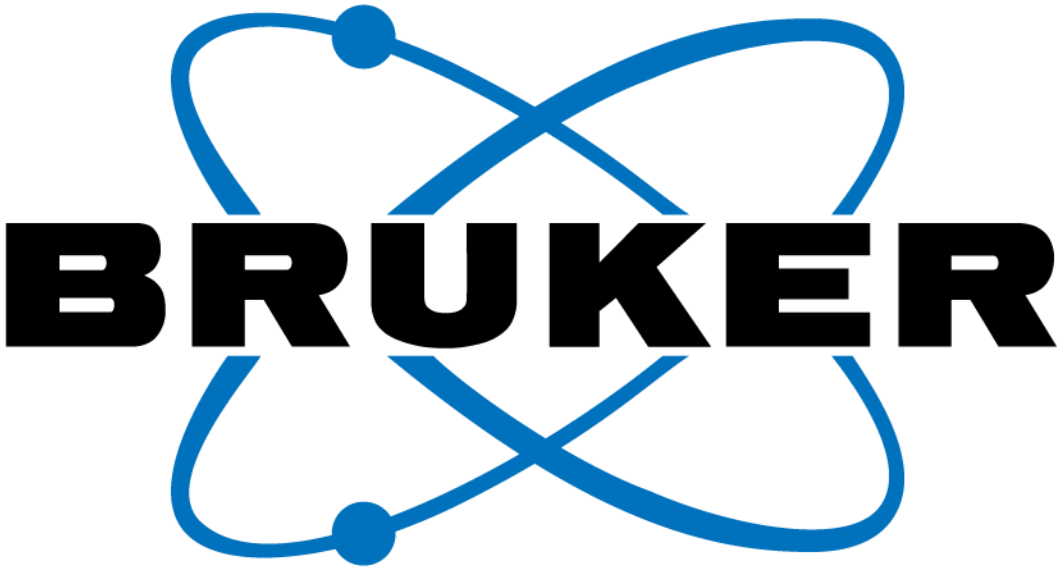
Pushing the limits

HNCO: F1F3 projection



Ubiquitin NUS 4% / 80x128 17min acquisition

Thank You



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