

## Supplementary Information

# **NXO beta structure mimicry: An ultra-short turn/hairpin mimic that folds in water**

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## Materials and Methods

All reactions were carried out in oven-dried glassware under argon unless otherwise noted. Melting points were measured on a Buchi B-545 melting point apparatus and are uncorrected. Infrared spectra were recorded on an FT-IR spectrometer and are reported in wave numbers ( $\text{cm}^{-1}$ ). Circular Dichroism was measured on a JASCO J-815 (cell length 10mm), from 190-260nm, at 295K and at a concentration of 0.1mmol. Routine  $^1\text{H}$ - and  $^{13}\text{C}$ -NMR spectra were recorded on a Bruker AC-200 (at 200 MHz and 50 MHz, respectively) pulse Fourier-transform NMR spectrometer. Chemical shifts  $\delta$  are reported in ppm relative to the resonance of tetramethylsilane (TMS). For compound **1**, NMR experiments were also performed on an Agilent/Varian VNMRs 600 MHz spectrometer equipped with inverse HCN probe, using standard vendor-supplied pulse sequences. For 1D-NOESY, ROESY and TOCSY experiments selective excitation of chosen protons was performed by a DPGSE excitation block using selective gaussian inversion pulses optimized for the selected spectral region. In both 1D-, 2D-NOESY and ROESY experiments zero-order coherences were suppressed by a scheme proposed by Keeler, see: Thrippleton, M. J.; Keeler, J. *Angew. Chem. Int. Ed.* **2003**, *42*, 3938. Combustion analyses were performed by the analytical laboratory, Vienna University. Mass spectra were obtained by MALDI-TOF-MS (on an Axima TOF<sup>2</sup>) using the matrix  $\alpha$ -cyano-4-hydroxycinnamic acid dissolved in methanol and *i*-propanol. Crude residues were purified by flash chromatography using silica gel 40-63 $\mu\text{m}$  and distilled reagent grade petroleum ether (bp 40-60°C) and ethyl acetate.

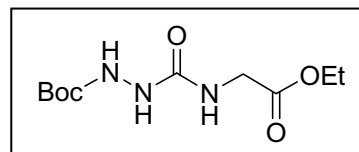
Conformation searching and Molecular Dynamics calculations were performed using Molecular Operating Environment, Version 2007.09 (MOE, © 1997-2007 [Chemical Computing Group Inc.](#)). To obtain input geometries, stochastic conformational searches employing the OPLS-AA forcefield potential parameters were performed with soft distance constraints derived from qualitatively assigned experimental NOE intensities. Criteria were thus registered from the assignment of crosspeaks in the ROESY experiment (for details *vide infra*) as very weak, weak, weak to medium, medium, medium to strong, strong with restraints below 5.5, 5, 4.5, 4, 3.5 and 3Å, respectively. Conformational space was explored with an energy cutoff of 20kcal using 0.0001Å Cartesian perturbation before 0.001Å RMS-gradient minimization with full dihedral minimization and bond rotation in 30° steps for a minimum of

$>10^6$  random geometries. The lowest energy conformers thus obtained were freed of restraints, partial charges on titratable groups adjusted according to standardized  $pK_A$  values and then subjected to Molecular Dynamics simulations in an NVT ensemble. Solvents as in the NMR experiment were treated implicitly by a generalized Born solvation model setting the exterior dielectric to the value of  $\epsilon = 78.5$  or 47 Debye for water and dimethylsulfoxide, respectively. Calculations were run for the indicated time of 100ns, excluding any atom constraints in the OPLS-AA forcefield. Dynamics were run at 290K and 297K with a timestep of 0.001ps, using the Nose-Poincaré-Anderson algorithm for solving the equations of motion. Pressure and temperature responses were set to 0.5 and 0.1ps relaxation time, respectively. Trajectory coordinates were stored at 0.5ps intervals for data analysis. Qualitatively assessed NOE intensities were compared to the calculated distances by an  $r^{-6}$  time-averaged treatment of calculated distances. The occurrence of a hydrogen bond was registered if the donor-acceptor distance was  $<3.5\text{\AA}$  with a donor-hydrogen-acceptor angle of  $90^\circ < \text{angle} < 180^\circ$ .

*Ab initio* (at HF/B3LYP/MP2 levels of theory using 6-31G and 6-311G++ (d,p) basis sets) calculations were performed using the GAUSSIAN G09 program package (see: Frisch M. J., *et al.* Gaussian 09, Revision A.1, **2009**. Gaussian, Inc., Wallingford CT). Continuum solvents (water, dimethylsulfoxide, methanol ( $\epsilon = 32.5$  Debye)) were model by an SCRF approach.

### Preparation of compound 3

A solution of glycine ethyl ester hydrochloride (4.0 g, 28.66 mmol) and DIPEA (14.87 mL, 85.97 mmol) in CH<sub>2</sub>Cl<sub>2</sub> (15 mL) was added slowly over a period of 30mins to a triphosgene

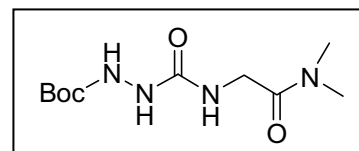


solution (3.4 g, 11.46 mmol) in CH<sub>2</sub>Cl<sub>2</sub> (10 mL). After stirring further for 15mins under argon, a solution of Boc-hydrazine (3.79 g, 28.66 mmol) in CH<sub>2</sub>Cl<sub>2</sub> (15 mL) was added in one portion. The reaction mixture was further refluxed for 2hrs, evaporated to dryness and the residue obtained was dissolved in ethyl acetate (50 mL). The ethyl acetate solution was washed with 10% aq. NaHCO<sub>3</sub> (15 mL), brine (15mL), dried over Na<sub>2</sub>SO<sub>4</sub> and concentrated to give 5.6 g of crude compound which was purified by column chromatography to give **3** as an off-white solid (3.63 g, 48%).

mp 137-138°C. Elemental analysis found: C, 45.71; H, 7.28; N, 16.48. Calc. for C<sub>10</sub>H<sub>19</sub>N<sub>3</sub>O<sub>5</sub>: C, 45.97; H, 7.33; N, 16.08. <sup>1</sup>H NMR (200 MHz, CDCl<sub>3</sub>): δ<sub>H</sub>=7.2 (bs, 1H), 7.05 (s, 1H), 6.2 (t, *J*=5.5 Hz, 1H), 4.11 (q, *J*=7 Hz, 2H), 3.92 (d, *J*=5.7 Hz, 2H), 1.39 (s, 9H), 1.2 (t, *J*=7 Hz, 3H); <sup>13</sup>C NMR (50 MHz, CDCl<sub>3</sub>): δ<sub>C</sub>=171.1, 158.9, 156.4, 81.5, 61.2, 41.8, 28.1, 14.0;

### Preparation of compound 4

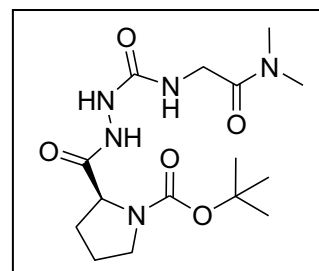
The solution of **3** (3.8 g, 14.54 mmol) in 33% w/v dimethylamine in ethanol (20 mL) was stirred overnight at room temperature. The solvent was removed by rotary evaporation and was well dried under high vacuum to give **4** as an off-white solid (3.78g, quant.).



mp 134-135°C. Elemental analysis found: C, 45.82; H, 7.39; N, 21.39. Calc. for C<sub>10</sub>H<sub>20</sub>N<sub>4</sub>O<sub>4</sub>: C, 46.14; H, 7.74; N, 21.52. <sup>1</sup>H NMR (200 MHz, CDCl<sub>3</sub>): δ<sub>H</sub>=7.35 (bs, 1H), 7.07 (s, 1H), 6.48 (t, *J*=4.3 Hz, 1H), 4.0 (d, *J*=4.3 Hz, 2H), 2.92 (s, 3H), 2.89 (s, 3H), 1.38 (s, 9H); <sup>13</sup>C NMR (50 MHz, CDCl<sub>3</sub>): δ<sub>C</sub>=169.2, 158.7, 156.3, 81.1, 41.8, 36.0, 35.6, 28.1;

### Preparation of compound 6

Ethyl acetate saturated with HCl (10 mL) was added slowly with stirring at 0°C to the solution of **4** (1.87 g, 7.2 mmol) in ethyl acetate (10 mL). The reaction mixture was stirred at room temperature for 30mins. Solvent was evaporated and the reaction mixture was well dried under high vacuum to afford hydrochloride salt **5** in quantitative yield. It was then dissolved in CH<sub>2</sub>Cl<sub>2</sub> (15 mL) and triethylamine (3.0 mL, 21.6 mmol) was added to free the amine group.

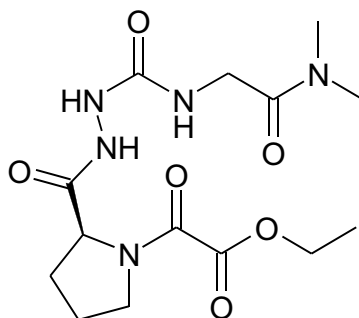


It was then dissolved in CH<sub>2</sub>Cl<sub>2</sub> (15 mL) and triethylamine (3.0 mL, 21.6 mmol) was added to free the amine group.

In another flask, Boc-L-proline (1.55 g, 7.2 mmol), HOBt (1.02 g, 7.56 mmol) and DCC (Dicyclohexylcarbodiimide, 1.56 g, 7.56 mmol) were dissolved in CH<sub>2</sub>Cl<sub>2</sub> (15 mL) and stirred for 15 mins at room temperature under argon. To this mixture, the above-mentioned solution of free amine was added at once and the resulting mixture stirred overnight under argon at room temperature. The precipitated DCHU (Dicyclohexylurea) was removed by filtration and the filtrate was evaporated. Additional DCHU was removed by subsequent trituration with cold ethyl acetate and filtration. The ethyl acetate solution was concentrated and the crude compound obtained was purified by column chromatography to give **6** as a white solid (2.1g, 81%).

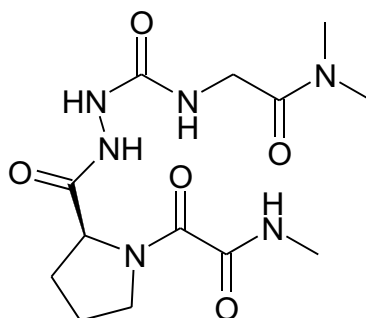
mp 74-75°C. Elemental analysis found: C, 50.21; H, 6.96; N, 19.43. Calc. for C<sub>15</sub>H<sub>27</sub>N<sub>5</sub>O<sub>5</sub>: C, 50.41; H, 7.61; N, 19.59. <sup>1</sup>H NMR (200 MHz, CDCl<sub>3</sub>): δ<sub>H</sub>=8.89 (bs, 1H), 7.75 (bs, 1H), 6.56 (bs, 1H), 3.87-4.22 (m, 3H), 3.41 (m, 2H), 2.91 (s, 3H), 2.88 (s, 3H), 1.68-2.1 (m, 4H), 1.36 (s, 9H); <sup>13</sup>C NMR (50 MHz, CDCl<sub>3</sub>): δ<sub>C</sub>=172.5, 169.1, 158.3, 155.3, 80.3, 58.7, 53.4, 47.1, 41.8, 36.1, 35.7, 28.3, 24.5.

## Preparation of compound 8



To the solution of **6** (3.79 g, 10.6 mmol) in ethyl acetate (10 mL), ethyl acetate saturated with HCl (10 mL) was added slowly with stirring at 0°C. The reaction mixture was stirred further at room temperature for 30mins. Solvent was evaporated and the reaction mixture was well dried under high vacuum to afford hydrochloride salt **7** in quantitative yield. It was then dissolved in DMF (30 mL), and with good stirring sodium bicarbonate (4.5 g, 53.02 mmol) was added. The reaction mixture was cooled to 0°C and ethyl oxalylchloride (1.4 mL, 12.73 mmol) was added slowly with stirring and the resulting mixture stirred for further 30mins under argon at room temperature. The mixture was diluted with ethyl acetate (100 mL) and filtered through celite to remove excess sodium bicarbonate and by-product salts. The filtrate was concentrated under reduced pressure to afford crude **8** as a thick sticky mass (1.1 g, 29%). Compound **8** was found to be unstable and was used for further reaction without purification.

## Preparation of compound 1



To the solution of crude **8** (1.1 g, 3.08 mmol) in ethanol (10 mL), 33% methylamine solution in ethanol (10 mL) was added. The reaction mixture was stirred at room temperature for 30mins. The white solid precipitated was filtered and washed with ethanol (10 mL) to afford **1** as a white solid (0.75g, 71%).

mp 201-202°C. Elemental analysis found: C, 43.54; H, 6.16; N, 22.88. Calc. for  $C_{13}H_{22}N_6O_5 \cdot H_2O$ : C, 43.33; H, 6.71; N, 23.32. IR (KBr)  $\nu_{max}/cm^{-1}$  4000-3336, 3214, 3016, 1640, 1554, 1436, 1412, 1340, 1257, 1126, 994, 816, 758, 731, 611.

$^1H$  NMR (400 MHz,  $d_6$ -DMSO):  $\delta_H$  =9.82 (bs, 1H), 9.74 (bs, 1H), 8.63 (d,  $J=1.5$ Hz, 1H), 8.57 (d,  $J=1.5$ Hz, 1H), 8.12 (s, 1H), 8.07 (s, 1H), 6.38 (s, 1H), 6.31 (s, 1H), 4.94 (bs, 1H), 4.34 (bs, 1H), 3.95-3.77 (m, 6H), 3.57-3.50 (m, 2H), 2.95 (s, 6H), 2.86 (s, 6H), 2.68 (d,  $J=1.5$ Hz, 3H), 2.60 (d,  $J=1.5$ Hz, 3H), 2.27-1.78 (m, 8H).

$^{13}C$  NMR (100 MHz,  $d_6$ -DMSO):  $\delta_C$  =172.9, 171.8, 169.5, 169.4, 162.7, 162.1, 161.6, 160.9, 158.7, 158.5, 60.7, 60.3, 49.5, 49.0, 42.1, 36.5, 35.9, 32.9, 29.6, 26.4, 26.3, 25.7, 25.3;

MS (MALDI-TOF):  $m/z$  found 365.15 (100) [ $M+Na^+$ ]; calc. for  $C_{13}H_{22}N_6O_5+Na^+$ : 365.15.

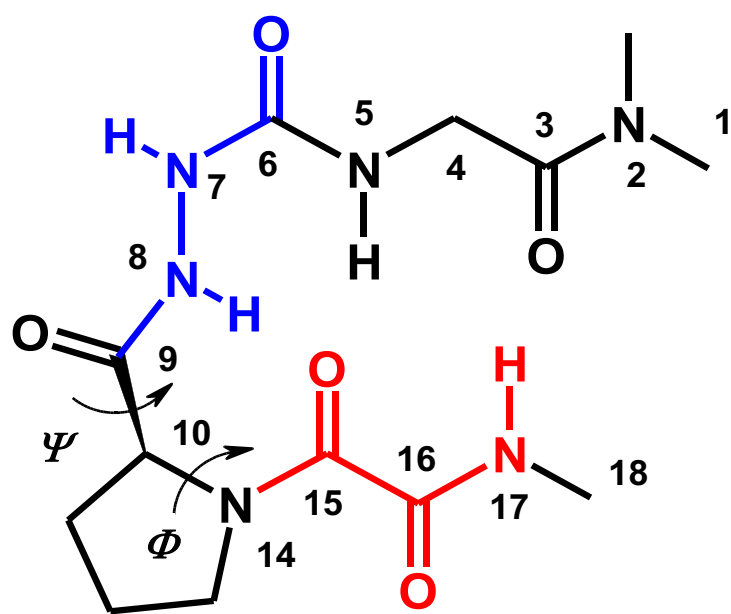
The D-Proline-derived analog of **1**, compound **9**, was prepared entirely analogously using Boc-D-proline. The final step yielded white solid material in 18% yield, mp 202-203°C.

MS (MALDI-TOF):  $m/z$  found 365.15 (100) [ $M+Na^+$ ]; calc. for  $C_{13}H_{22}N_6O_5+Na^+$ : 365.15.



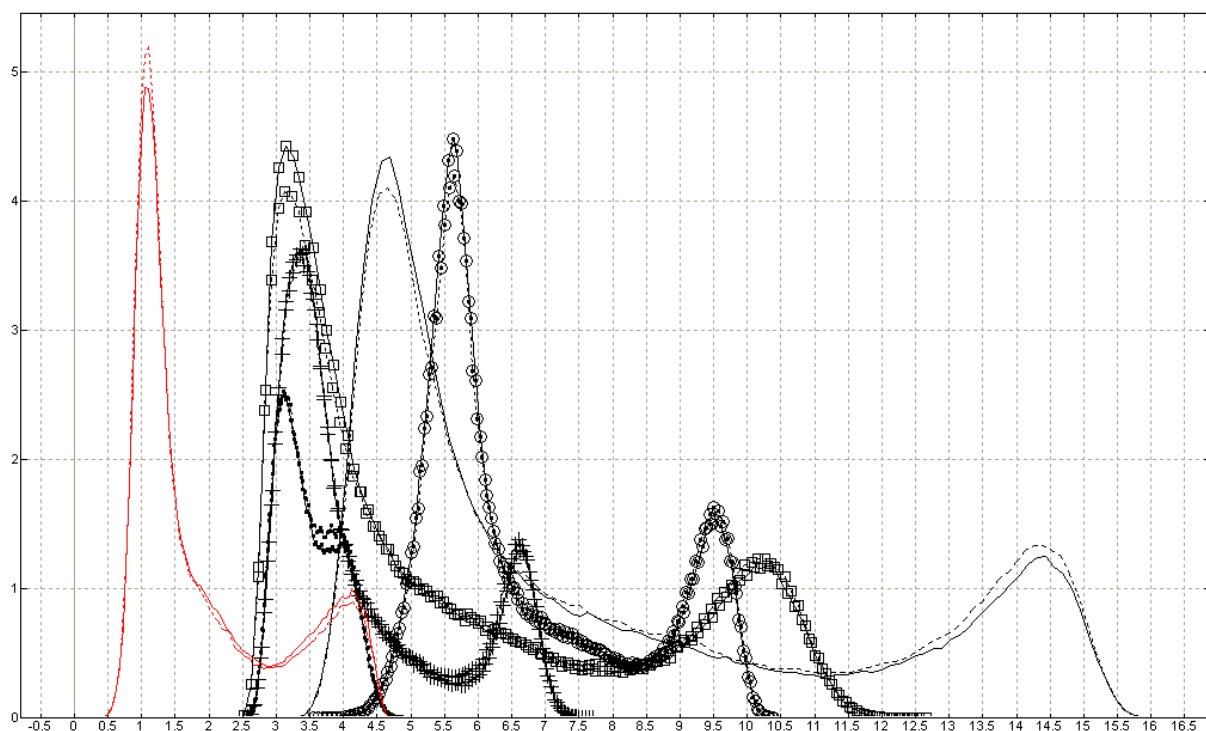
Atom	Chemical shift, ppm		Atom	Chemical shift, ppm	
	<b><sup>13</sup>C</b>	<b><sup>1</sup>H</b>		<b><sup>13</sup>C</b>	<b><sup>1</sup>H</b>
Conformer	<b>1a</b>		Conformer	<b>1b</b>	
1a	35,980	2,927	1a	35,980	2,918
1b	35,482	2,842	1b	35,482	2,821
3	169,075	-	3	168,960	-
4	41,640	3,920	4	41,640	3,920
		3,870			3,800
5	-	6,300	5	-	6,343
6	157,977	-	6	158,169	-
7	-	8,118	7	-	8,075
8	-	9,807	8	-	9,733
9	171,389	-	9	172,455	-
10	59,846	4,314	10	60,191	4,940
		2,078			2,190
11	29,105	1,825	11	32,416	1,983
		1,913			1,767
12	25,220	1,847	12	21,878	1,740
		3,802			3,515
13	49,001	3,802	13	48,534	3,453
		-			-
15	161,051	-	15	160,407	-
16	161,549	-	16	162,246	-
17	-	8,679	17	-	8,590
18	25,994	2,578	18	25,909	2,656

**Table 1.** 600 MHz (<sup>1</sup>H NMR) and 150 MHz (<sup>13</sup>C NMR), respectively, chemical shifts  $\delta$  of ensemble conformers **1a** and **1b** in d<sub>6</sub>-DMSO, measured at 5mM concentration.

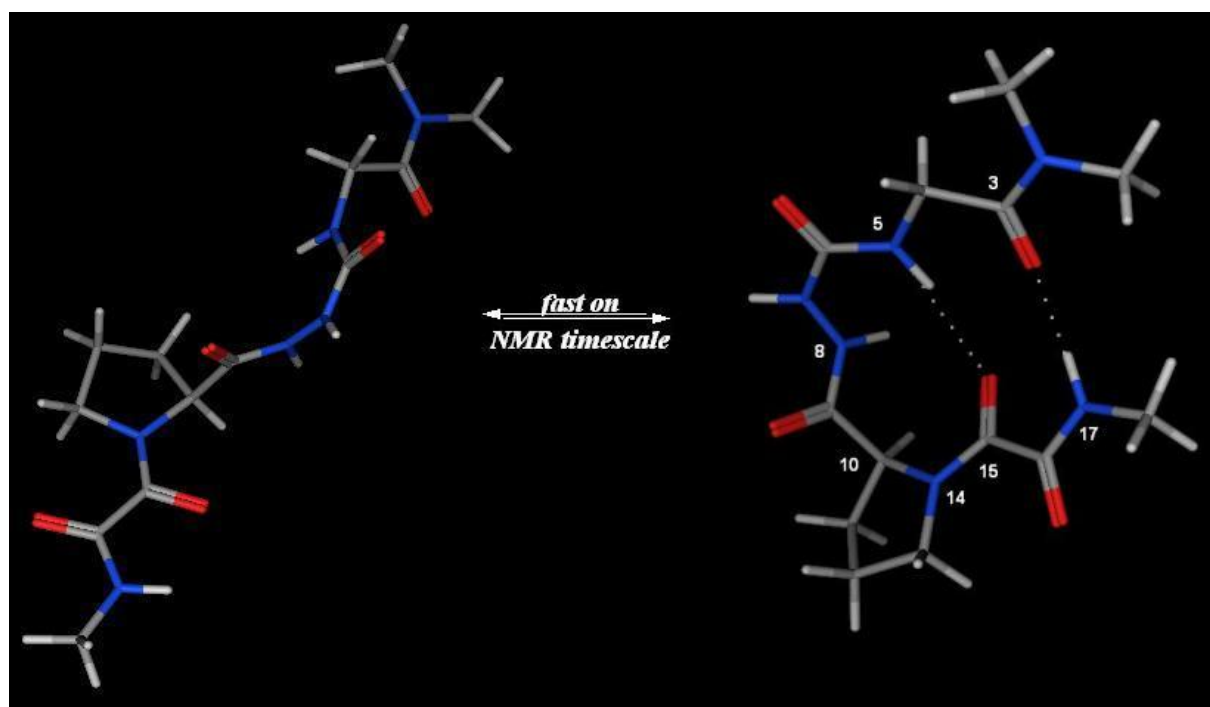


***N*<sup>L</sup>ProO-modified  $\beta$ -turn mimic 1**

**Figure 1.** Numbering of 1 as used throughout the text.



**Figure 2. 1**, percentage-weighted histogram of all-atom RMSD (red lines) and selected distances (black, abscissa values in Å) from a 100ns Molecular Dynamics run. Solid and dotted lines indicate H<sub>2</sub>O (290K) and DMSO (297K) trajectories, respectively. Distances (atoms, graph markers): 1-18, lines; 3-17, hollow squares; 5-15, hollow crosses; 4-16, hollow circles; 8-15, dots.



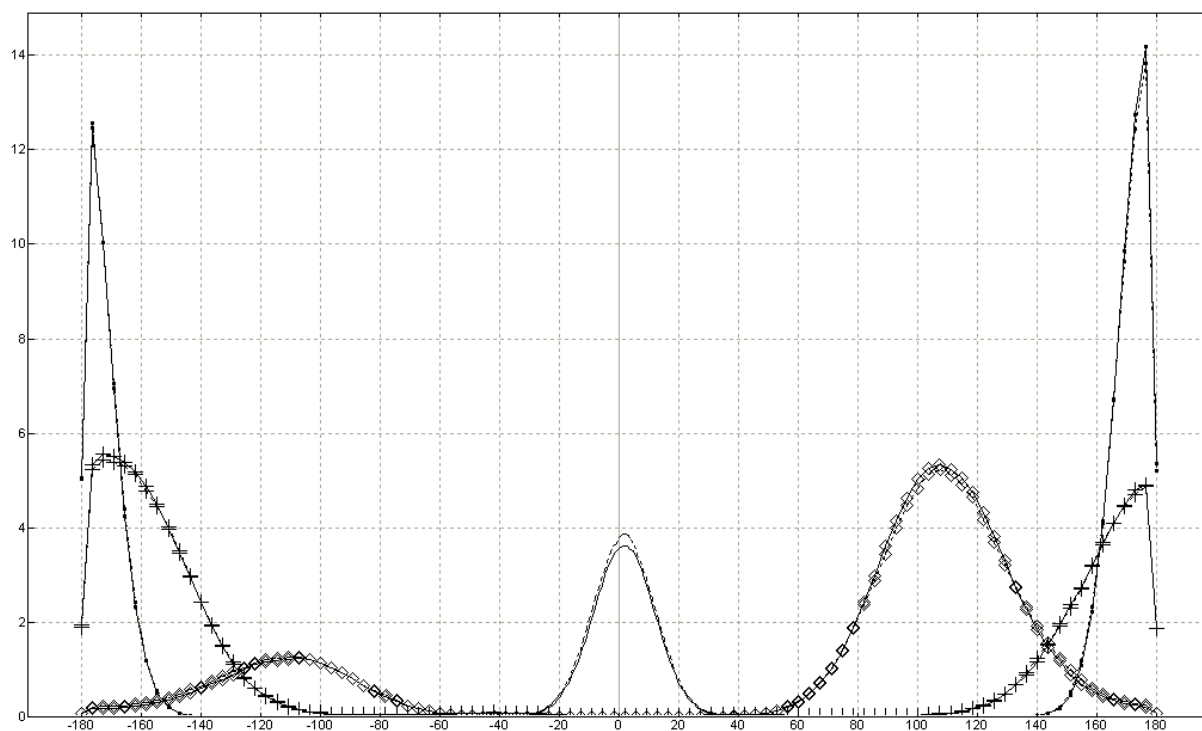
**Figure 3.** The open-fold equilibrium in **1**, from a 100ns MD trajectory in water at 290K with the OPLS-AA parameter set. At this temperature, the open-fold interconversion rate was simulated in the order of magnitude of  $10^{-11}$ s. Dotted lines indicate hydrogen bonding.

	<b>H<sub>2</sub>O, extended, 290K</b>	<b>H<sub>2</sub>O, folded, 290K</b>	<b>DMSO, extended, 297K</b>	<b>DMSO, folded, 297K</b>
<b>E, total potential energy</b>	-41.74	-44.15	-41.55	-44.0
<b>E, angle bend</b>	10.03	9.08	10.03	9.08
<b>E, torsion (proper and improper)</b>	2.25	5.44	2.26	5.43
<b>E, van der Waals</b>	10.29	7.78	10.30	7.81
<b>E, electrostatic</b>	-45.15	-51.16	-45.18	-51.25
<b>E, solvation</b>	-21.72	-17.68	-21.51	-17.47

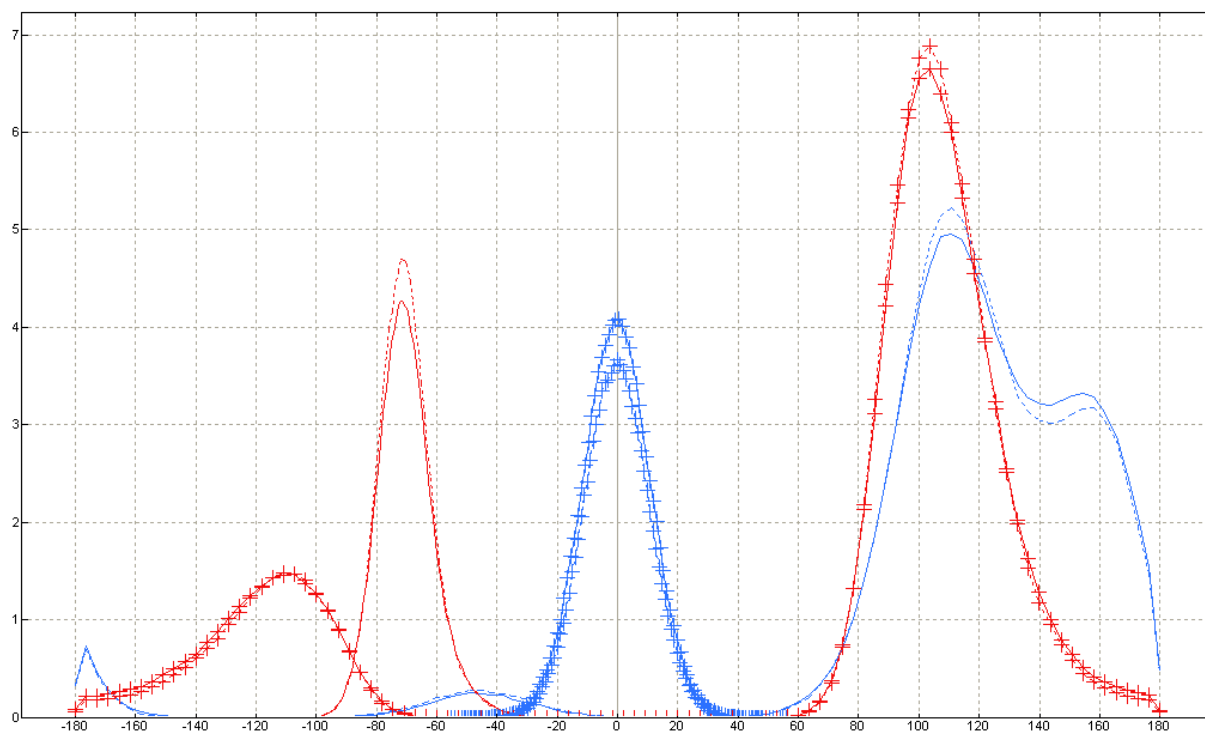
**Table 2.** Energies in the folded and unfolded conformers of **1** from MD. For structures see Picture above. Calculated by minimizing the most abundantly sampled conformation in RMSD around the respective extended and folded RMSD peak values with OPLS-AA parameters and implicitly treated solvation using the Born model. All values are in kcalmol<sup>-1</sup>.

	H <sub>2</sub> O, 290K	DMSO, 297K
<b>(C15)O←HN5, % sampled</b>	38.8	37.2
<b>(C15)O←HN5, visits</b>	29368	28637
<b>(C15)O←HN5, avg. lifetime [ps]</b>	2.80	2.74
<b>(C15)O←HN8, % sampled</b>	35.2	34.9
<b>(C15)O←HN8, visits</b>	34504	33576
<b>(C15)O←HN8, avg. lifetime</b>	2.09	2.12
<b>(C3)O←HN17, % sampled</b>	26.2	24.8
<b>(C3)O←HN17, visits</b>	26516	25258
<b>(C3)O←HN17, avg. lifetime</b>	2.06	2.09

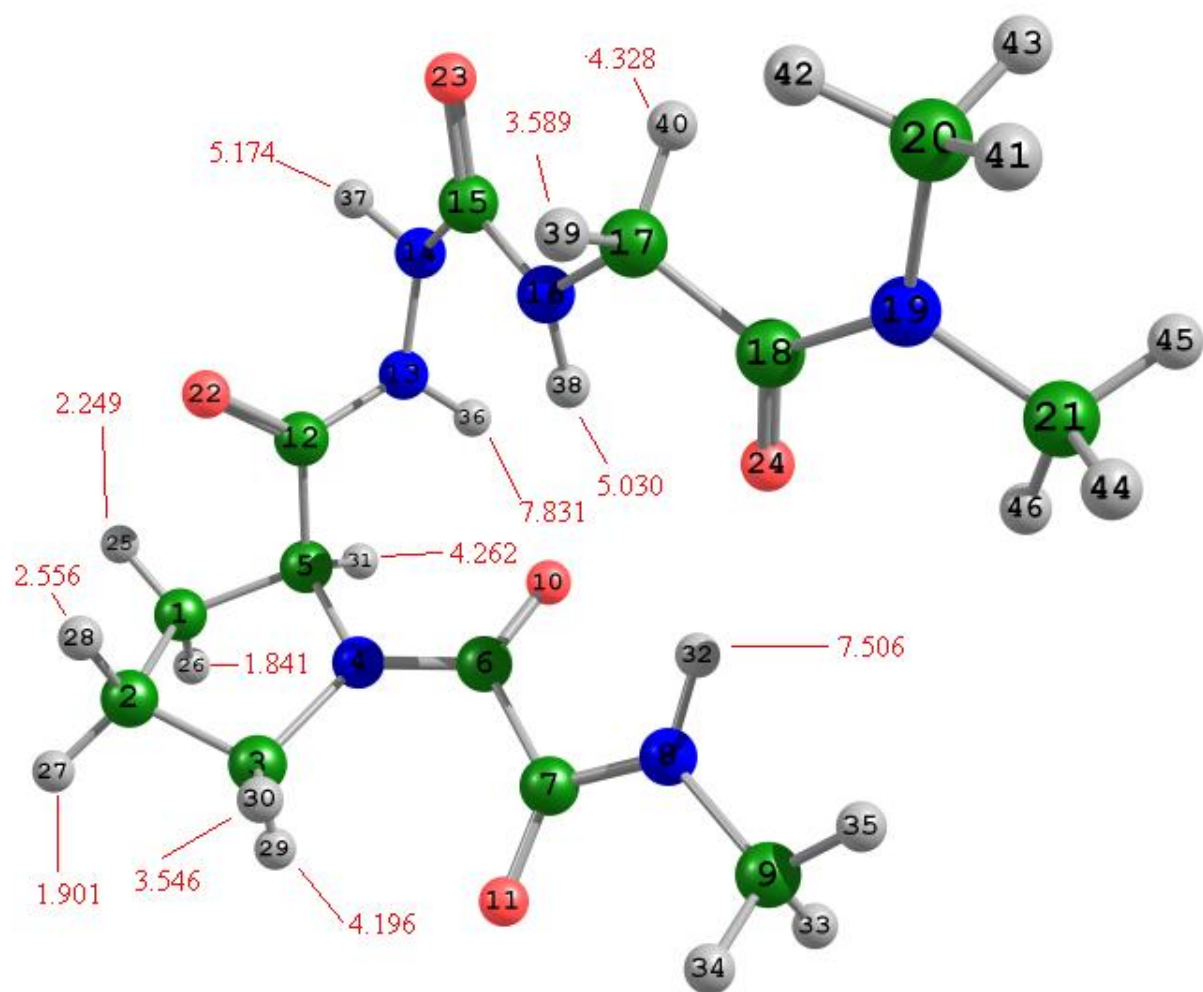
**Table 3.** Hydrogen bonding characteristics of the folded conformer of **1** during 100ns MD runs with OPLS-AA parameters using the Born model of solvation.



**Figure 4. 1**, percentage-weighted histogram of selected torsions during the MD runs. Solid and dotted lines indicate H<sub>2</sub>O (290K) and DMSO (297K) trajectories, respectively. H-N7-N8-H: diamonds; O15-C15-C16-O16: crosses; H-N7-C6-N5: dots; H8-N8-C9-C10: solid lines.



**Figure 5. 1**, percentage-weighted histogram of backbone  $\Phi$  (red) and  $\Psi$  (blue) during the MD runs. Dotted and solid lines indicate H<sub>2</sub>O (290K) and DMSO (297K) trajectories, respectively.  $\Phi$  or  $\Psi$  ( $i+1$ ): no markers;  $\Phi$  or  $\Psi$  ( $i+2$ ): crosses.

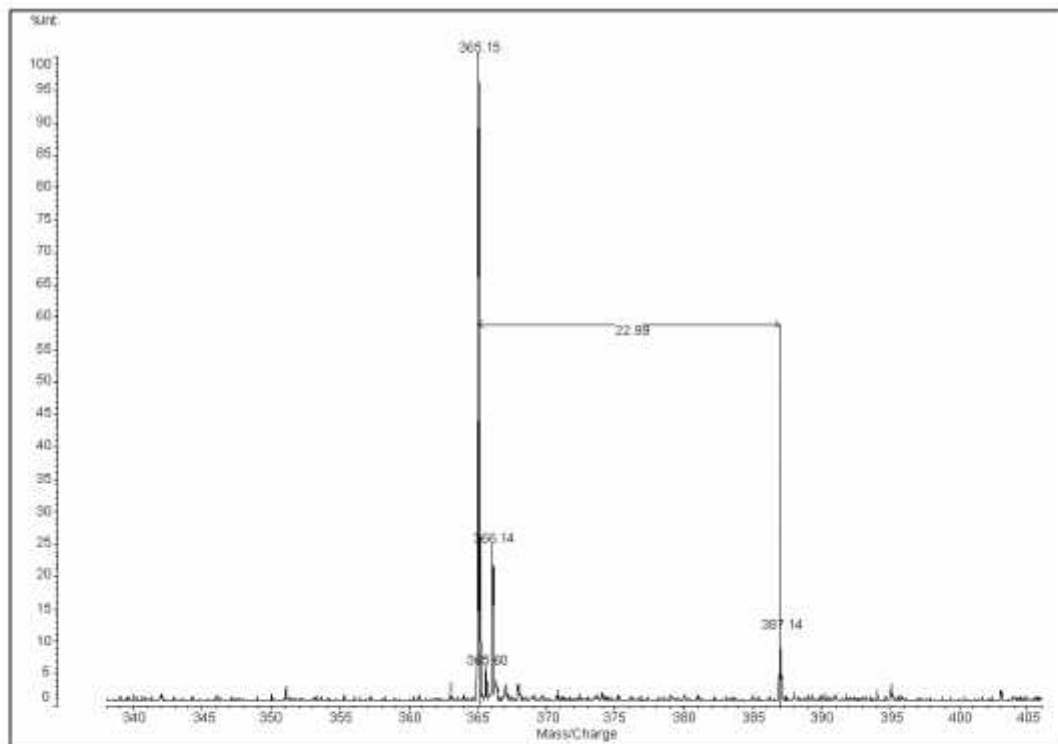
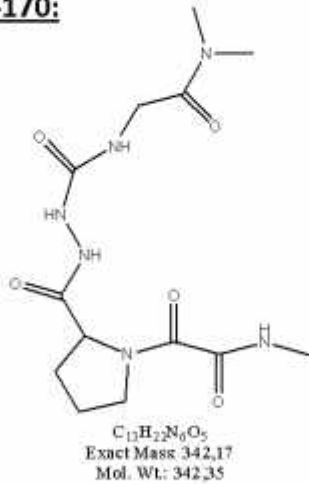


**Figure 6.** Relative minimum geometry from *ab initio* calculations at B3LYP/6-311G++(d,p) and substantiated as equilibrium conformer **1a** by comparison with MD and NMR. Given in the figure is the calculated value of the  $^1\text{H}$  NMR chemical shift in ppm relative to TMS.





### JP-170:



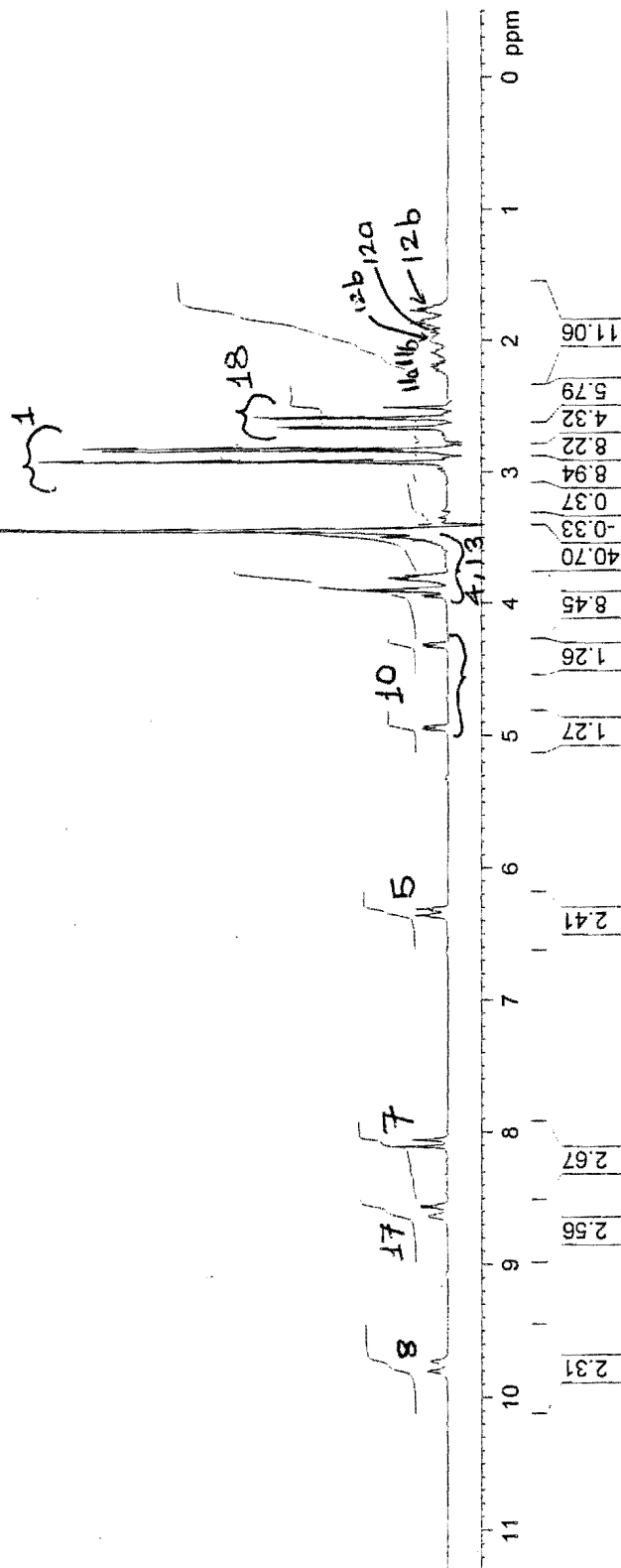
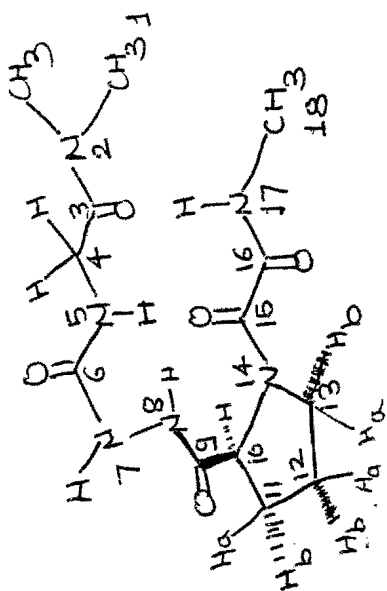
The theoretical molecular ion of JP-170 ( $[M+H]^+$  343.17) was not detected. The peak at  $m/z$  365.15 might represent an alkali adduct of the synthesized substance ( $[M+Na]^+$  theor. 365.15) and  $m/z$  387.14 might represent another Na adduct ( $[M+2Na-H]^+$ ). No further relevant  $m/z$  values were detected.

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 PROCNO 1

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 Time\_ 18.02  
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 SOLVENT DMSO  
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 AQ 2.5559540 se  
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 DW 78.000 us  
 DE 6.00 us  
 TE 297.2 K  
 D1 1.00000000 se  
 TDO 1

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 PL1 6.00 dB  
 SFO1 400.1330010 MHz

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 GB 0  
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FK70 DMSO - 13C 17C

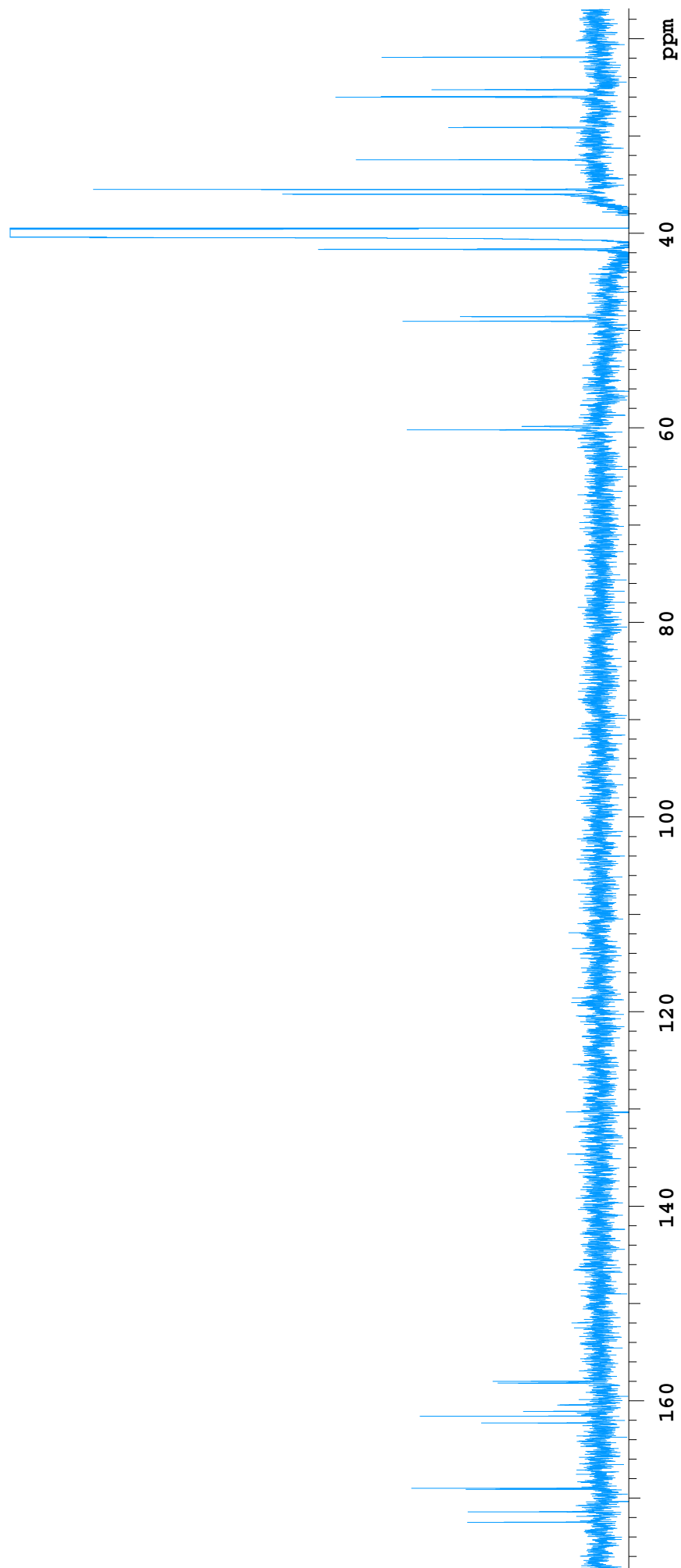
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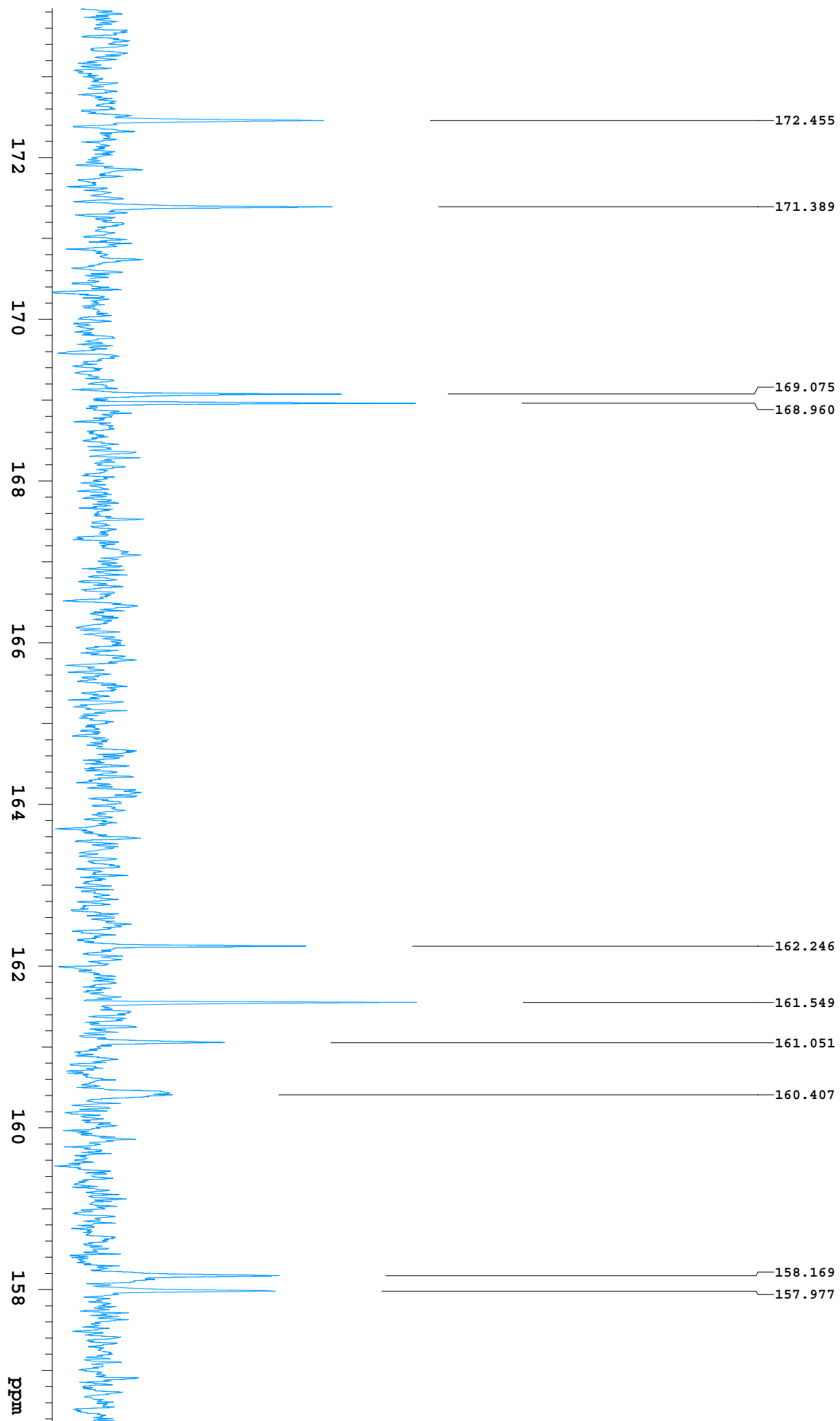
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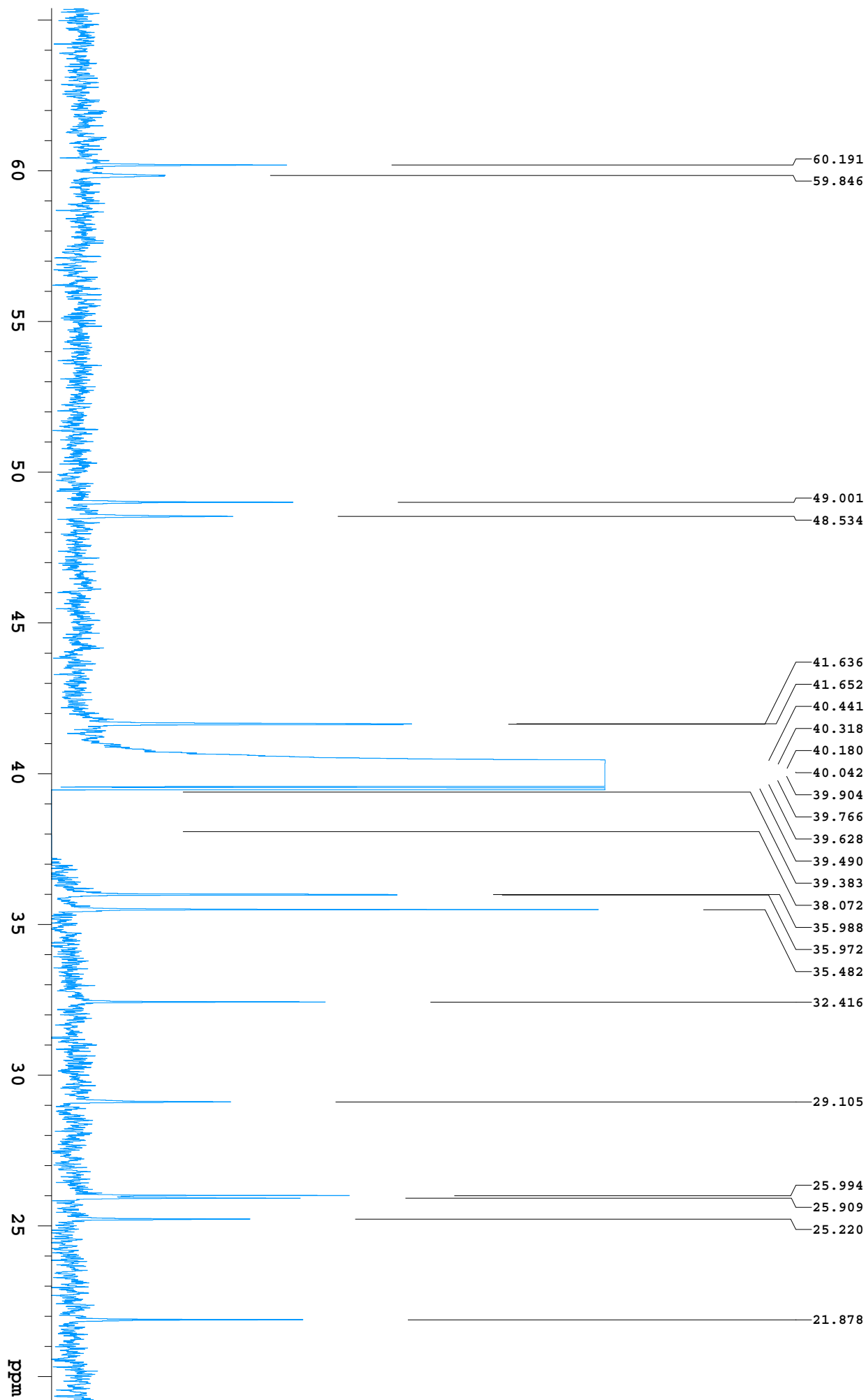
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Pulse Sequence: CARBON (s2pul)  
Solvent: dms0  
Data collected on: May 28 2010







FK70 dmso 1H 17C

Sample Name:

Data Collected on:  
Varian-NMR-vnmrs600  
Archive directory:

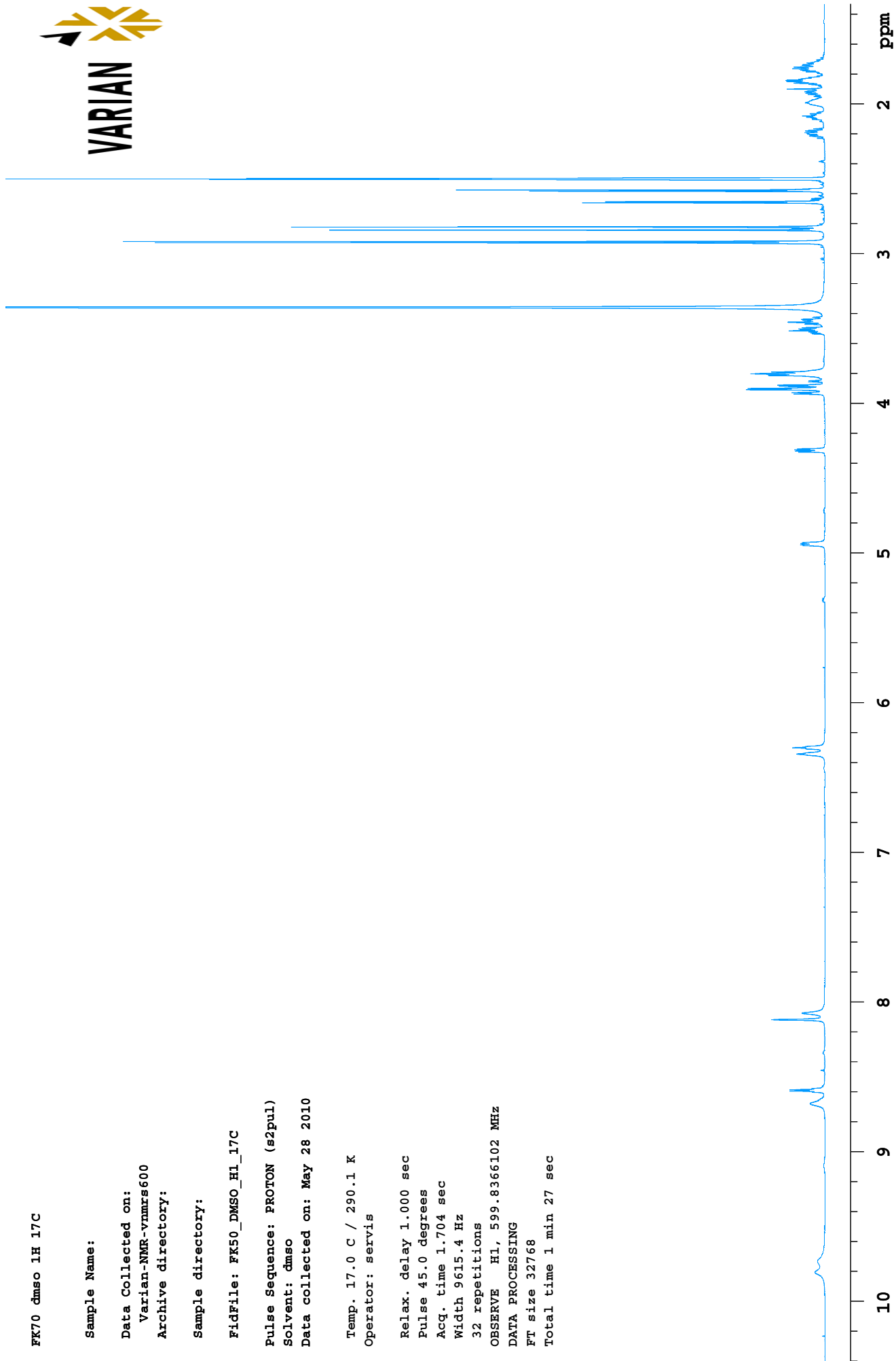
Sample directory:

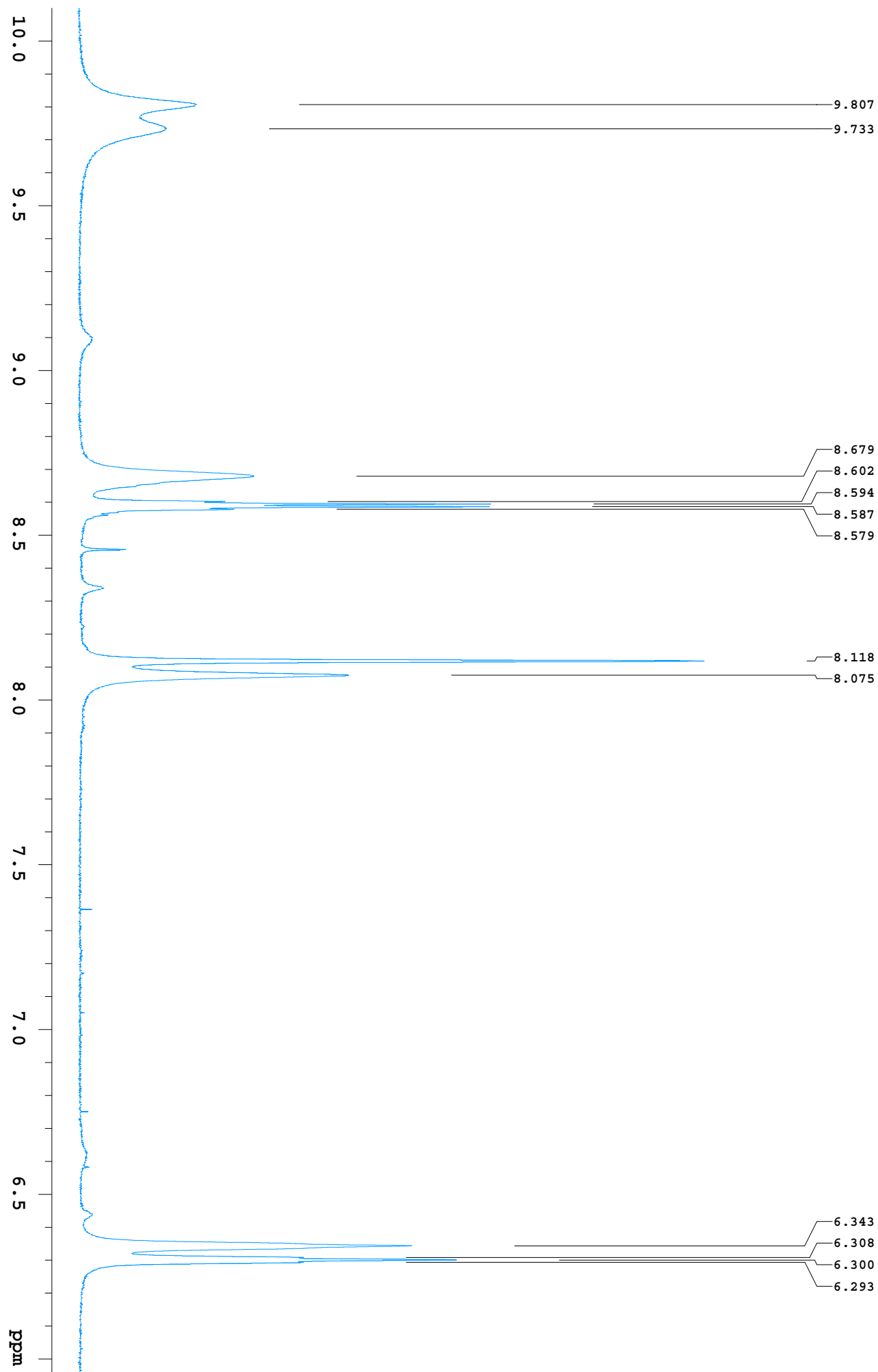
FidFile: FK50\_DMSO\_H1\_17C

Pulse Sequence: PROTON (s2pul)  
Solvent: dmso  
Data collected on: May 28 2010

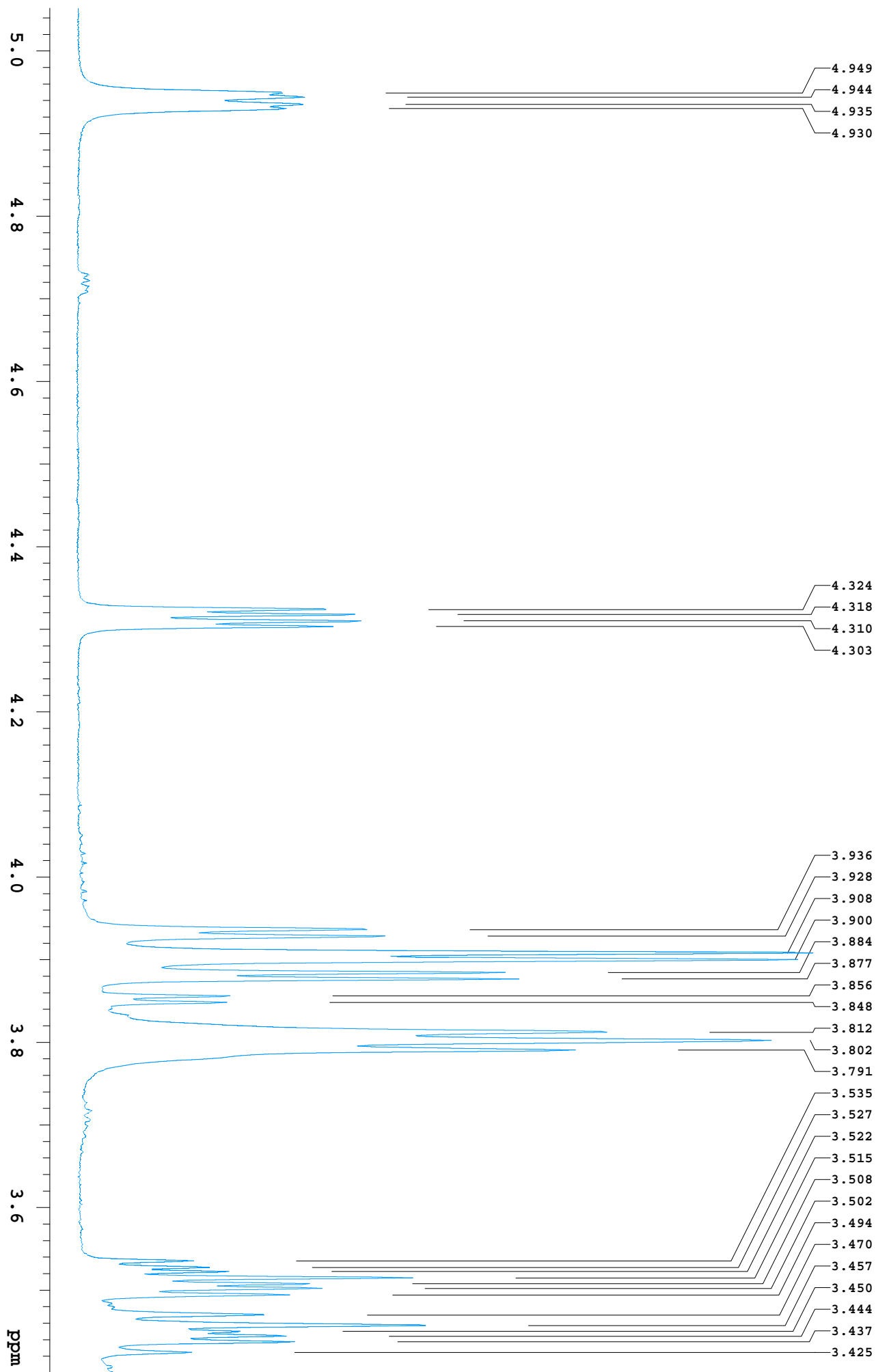
Temp. 17.0 C / 290.1 K  
Operator: servis

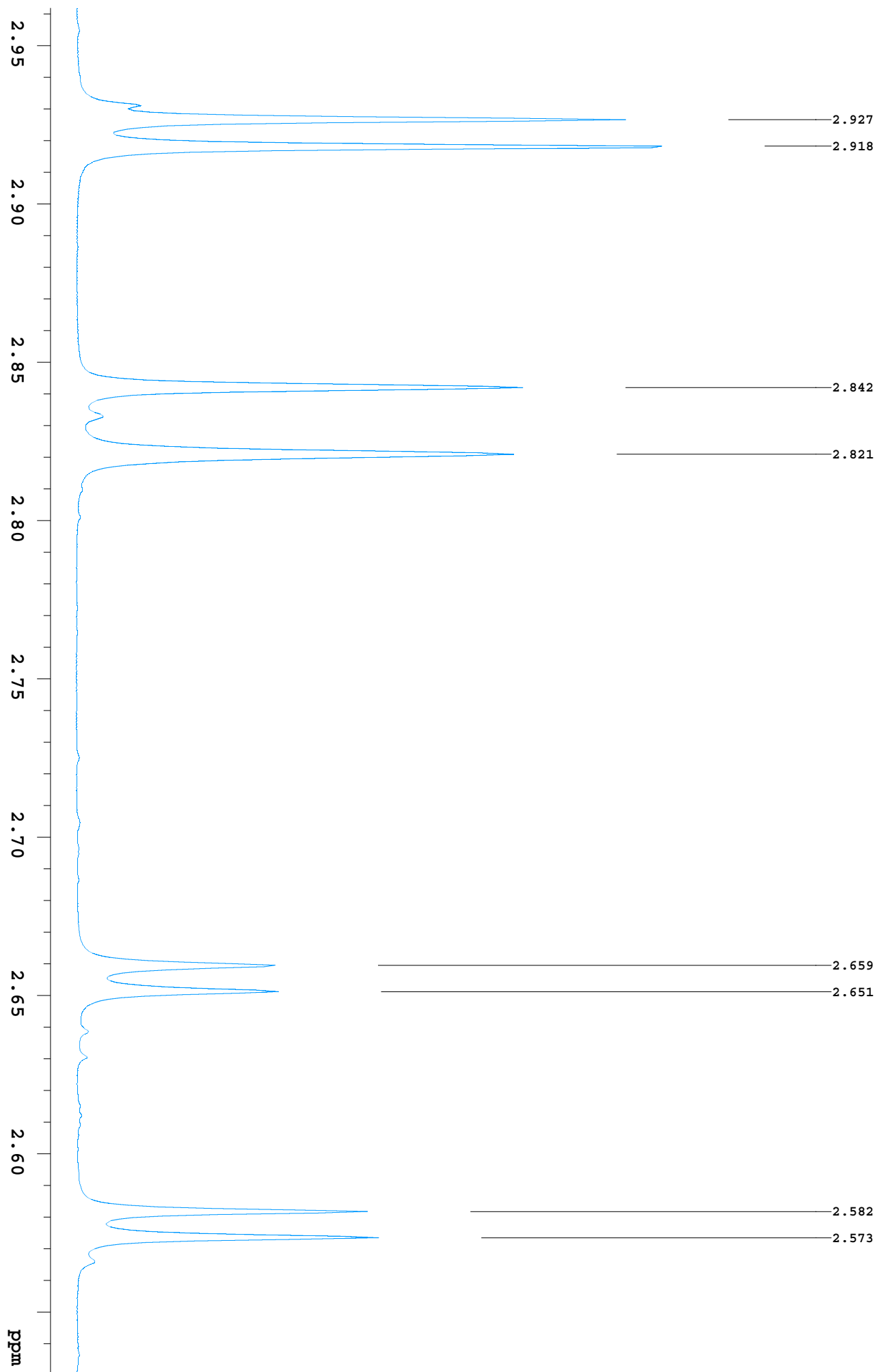
Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 1.704 sec  
Width 9615.4 Hz  
32 repetitions  
OBSERVE H1, 599.8366102 MHz  
DATA PROCESSING  
FT size 32768  
Total time 1 min 27 sec

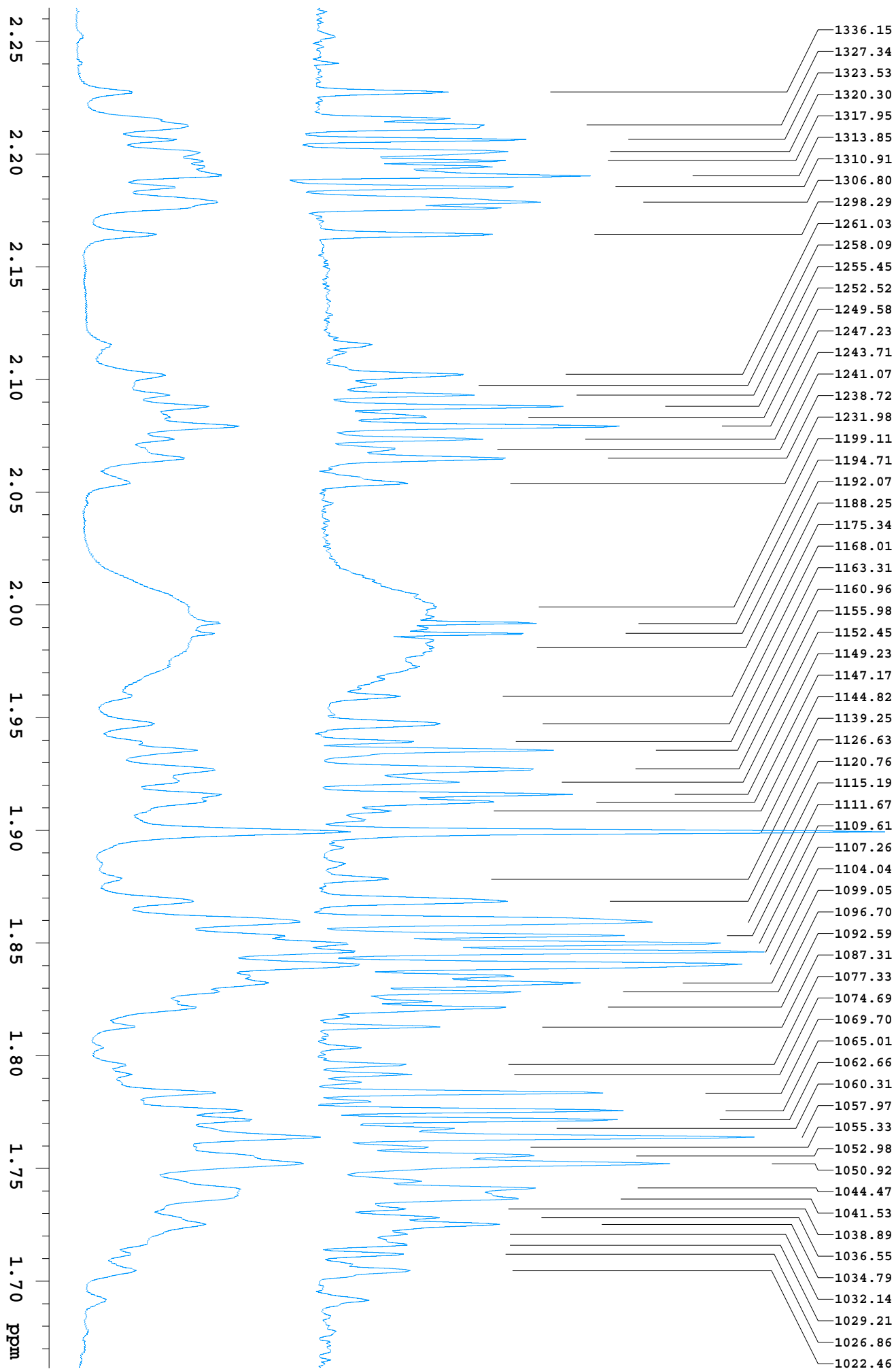












FK70 dmso 37C DQCOSY  
28.05.2010

Sample Name:

Data Collected on:  
Varian-NMR-vnmrs600  
Archive directory:

Sample directory:

FidFile: FK70\_dmso\_37C\_DQCOSY\_28May2010

Pulse Sequence: gDQCOSY

Solvent: dmso

Data collected on: May 28 2010

Temp. 37.0 C / 310.1 K  
Operator: servis

Relax. delay 1.000 sec  
Mixing 0.080 sec  
Acq. time 0.150 sec  
Width 9615.4 Hz  
2D Width 9615.4 Hz  
Single scan  
2 x 200 increments

OBSERVE H1, 599.8365881 MHz

DATA PROCESSING

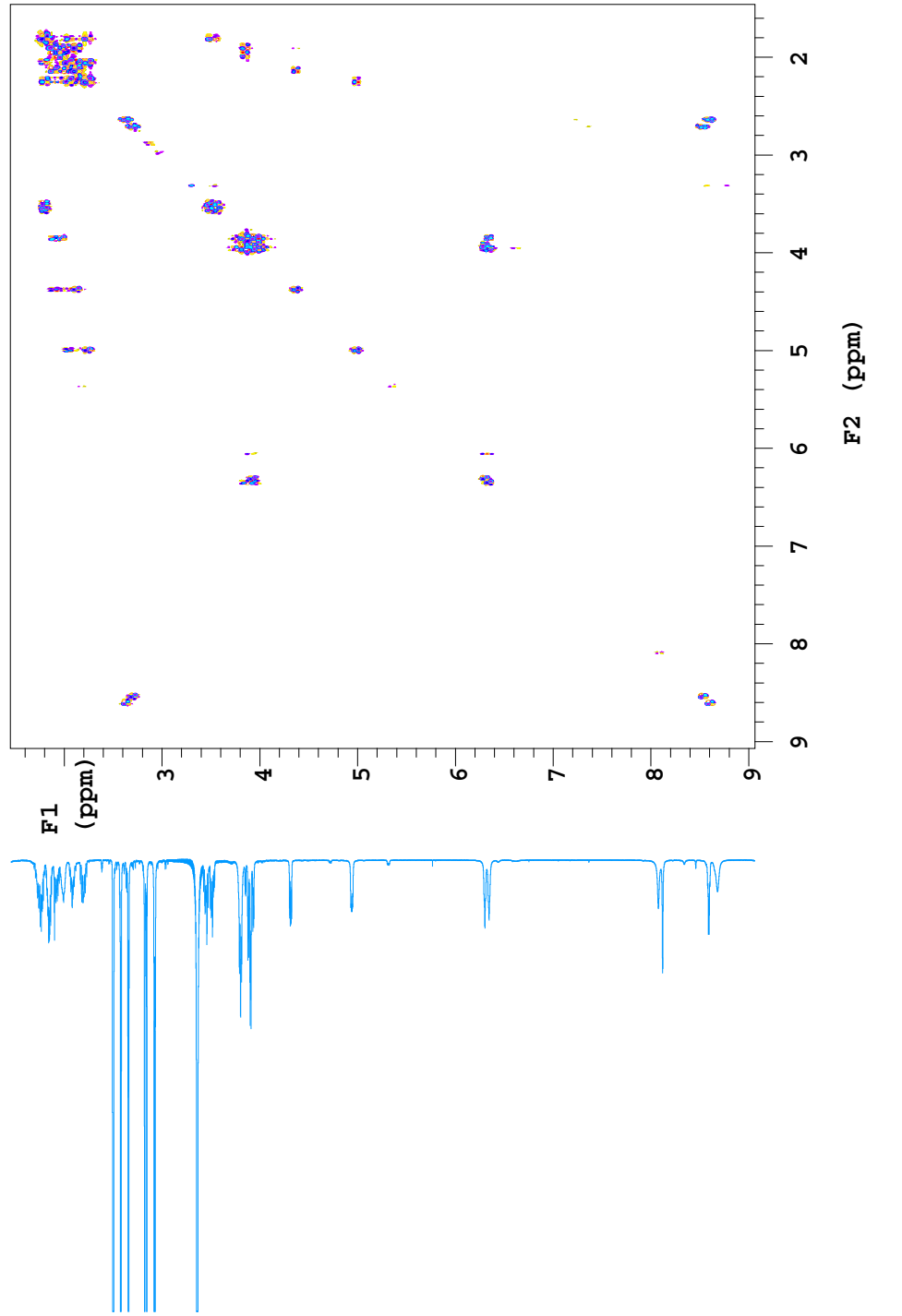
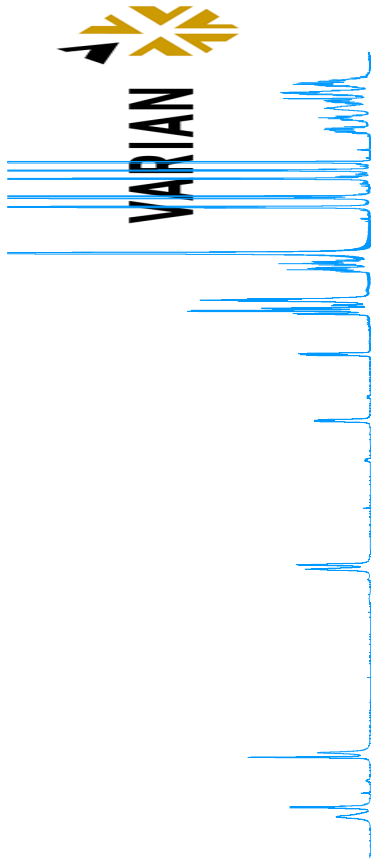
Sq. sine bell 0.125 sec  
Shifted by -0.100 sec

F1 DATA PROCESSING

Sq. sine bell 0.035 sec  
Shifted by -0.028 sec

FT size 4096 x 4096

Total time 8 min 27 sec



FK70 dmso 37C DQCOSY  
28.05.2010

Sample Name:

Data Collected on:  
Varian-NMR-vnmrs600  
Archive directory:

Sample directory:

FidFile: FK70\_dmso\_37C\_DQCOSY\_28May2010

Pulse Sequence: gDQCOSY

Solvent: dmso

Data collected on: May 28 2010

Temp. 37.0 C / 310.1 K  
Operator: servis

Relax. delay 1.000 sec

Mixing 0.080 sec

Acq. time 0.150 sec

Width 9615.4 Hz

2D Width 9615.4 Hz

Single scan

2 x 200 increments

OBSERVE H1, 599.8365881 MHz

DATA PROCESSING

Sq. sine bell 0.125 sec

Shifted by -0.100 sec

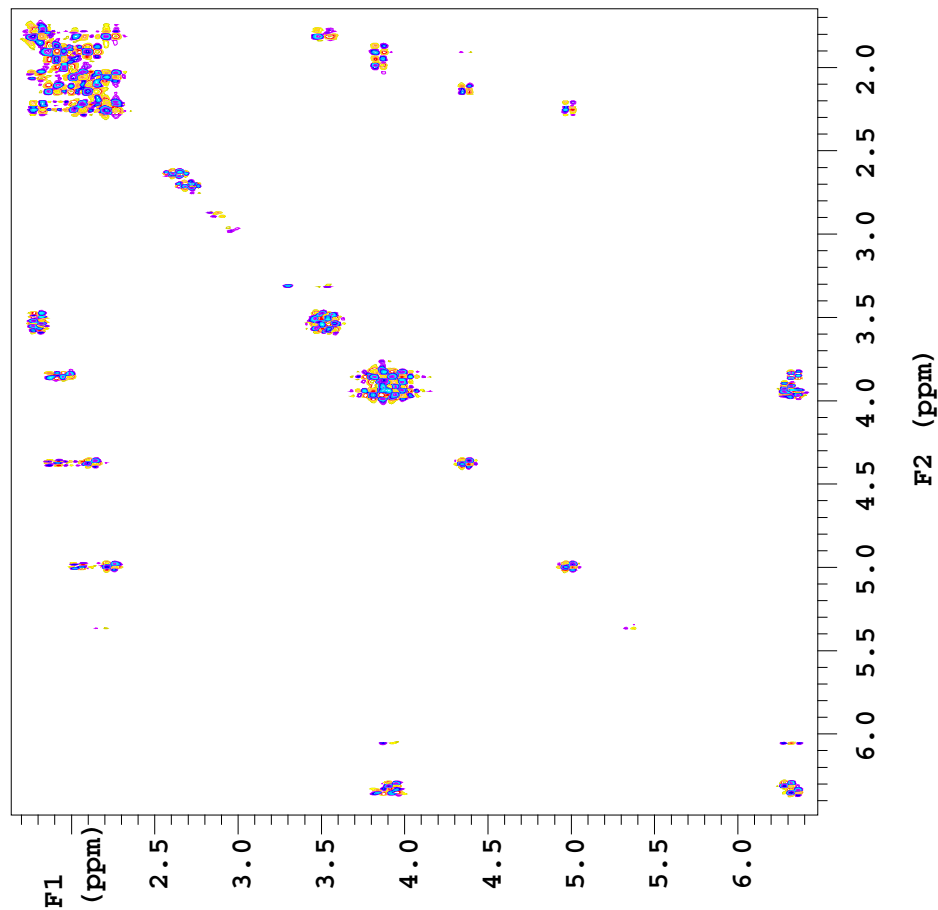
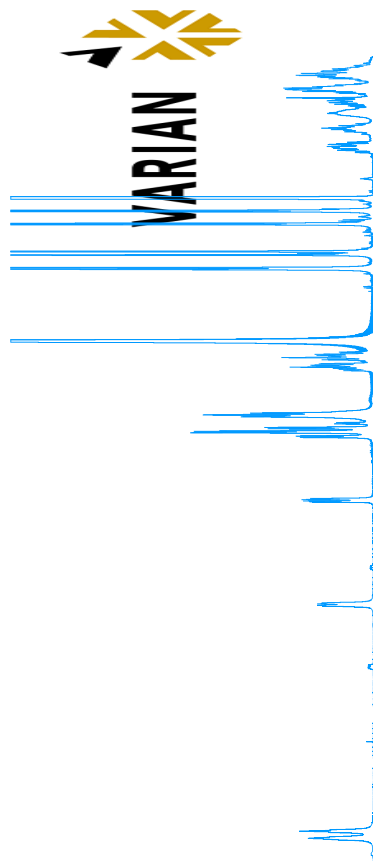
F1 DATA PROCESSING

Sq. sine bell 0.035 sec

Shifted by -0.028 sec

FT size 4096 x 4096

Total time 8 min 27 sec



FK70 dmso 37C DQCOSY  
28.05.2010

Sample Name:

Data Collected on:  
Varian-NMR-vnmrs600  
Archive directory:

Sample directory:

FidFile: FK70\_dmso\_37C\_DQCOSY\_28May2010

Pulse Sequence: gDQCOSY

Solvent: dmso

Data collected on: May 28 2010

Temp. 37.0 C / 310.1 K

Operator: servis

Relax. delay 1.000 sec

Mixing 0.080 sec

Acq. time 0.150 sec

Width 9615.4 Hz

2D Width 9615.4 Hz

Single scan

2 x 200 increments

OBSERVE H1, 599.8365881 MHz

DATA PROCESSING

Sq. sine bell 0.125 sec

Shifted by -0.100 sec

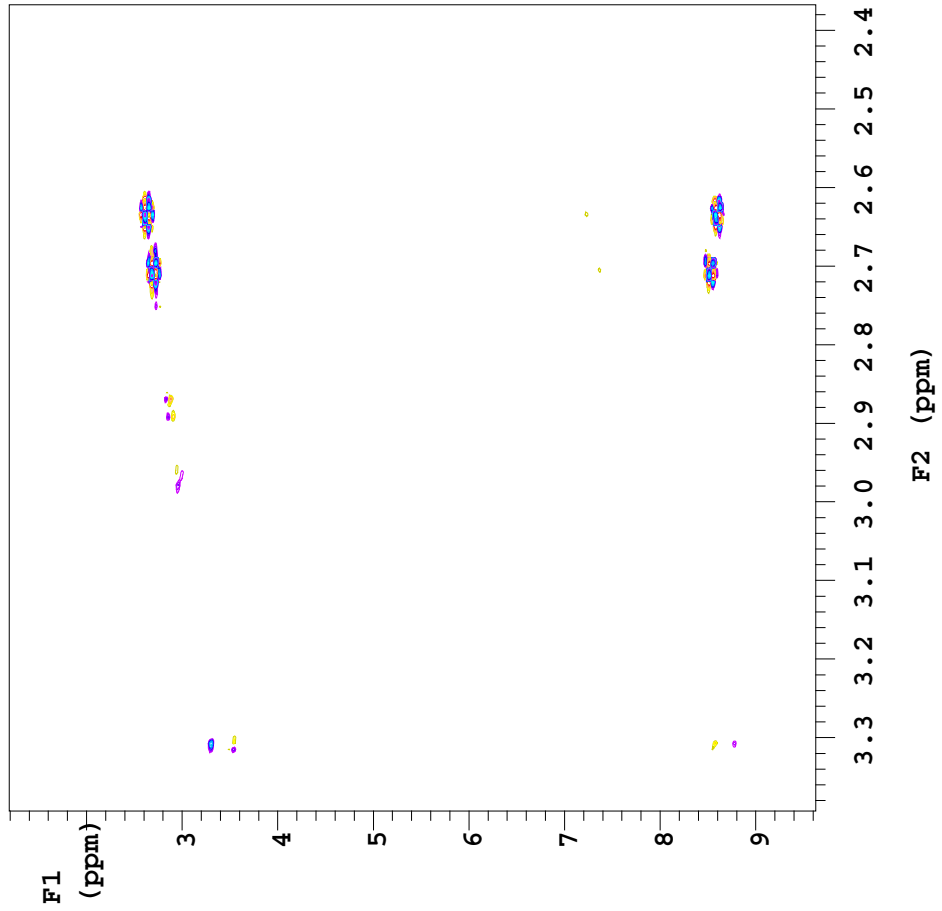
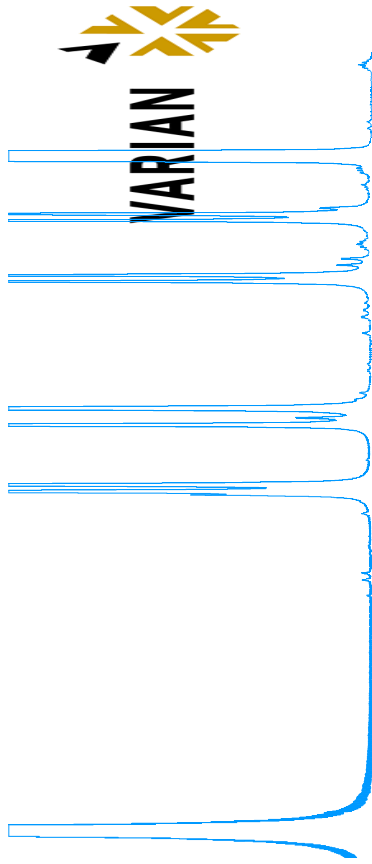
F1 DATA PROCESSING

Sq. sine bell 0.035 sec

Shifted by -0.028 sec

FT size 4096 x 4096

Total time 8 min 27 sec



FK70 dmso 37C DQCOSY  
28.05.2010

Sample Name:

Data Collected on:  
Varian-NMR-vnmrs600  
Archive directory:

Sample directory:

FidFile: FK70\_dmso\_37C\_DQCOSY\_28May2010

Pulse Sequence: gDQCOSY

Solvent: dmso

Data collected on: May 28 2010

Temp. 37.0 C / 310.1 K

Operator: servis

Relax. delay 1.000 sec

Mixing 0.080 sec

Acq. time 0.150 sec

Width 9615.4 Hz

2D Width 9615.4 Hz

Single scan

2 x 200 increments

OBSERVE H1, 599.8365530 MHz

DATA PROCESSING

Sq. sine bell 0.125 sec

Shifted by -0.100 sec

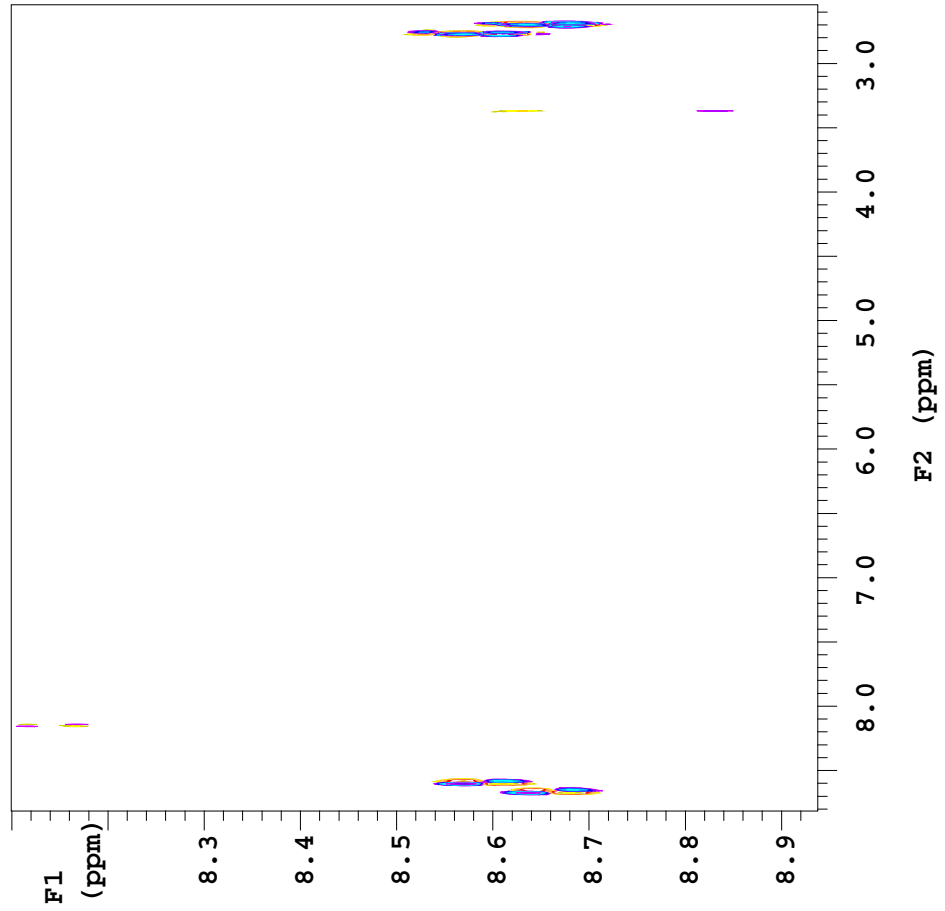
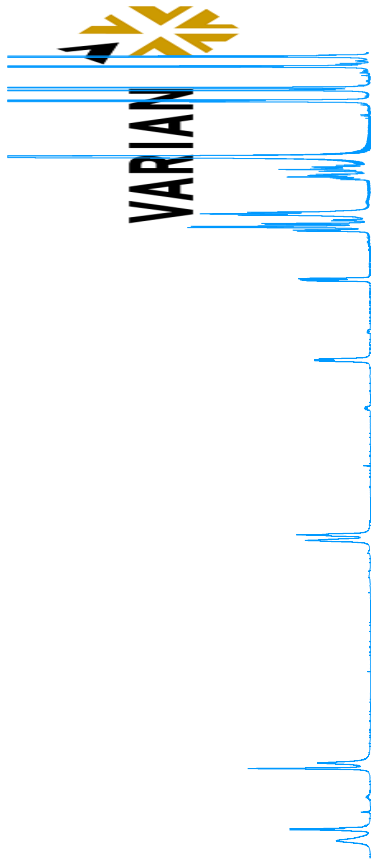
F1 DATA PROCESSING

Sq. sine bell 0.035 sec

Shifted by -0.028 sec

FT size 4096 x 4096

Total time 8 min 27 sec



FK70 dmso 37C DQCOSY  
28.05.2010

Sample Name:

Data Collected on:  
Varian-NMR-vnmrs600  
Archive directory:

Sample directory:

FidFile: FK70\_dmso\_37C\_DQCOSY\_28May2010

Pulse Sequence: gDQCOSY

Solvent: dmso

Data collected on: May 28 2010

Temp. 37.0 C / 310.1 K

Operator: servis

Relax. delay 1.000 sec

Mixing 0.080 sec

Acq. time 0.150 sec

Width 9615.4 Hz

2D Width 9615.4 Hz

Single scan

2 x 200 increments

OBSERVE H1, 599.8365530 MHz

DATA PROCESSING

Sq. sine bell 0.125 sec

Shifted by -0.100 sec

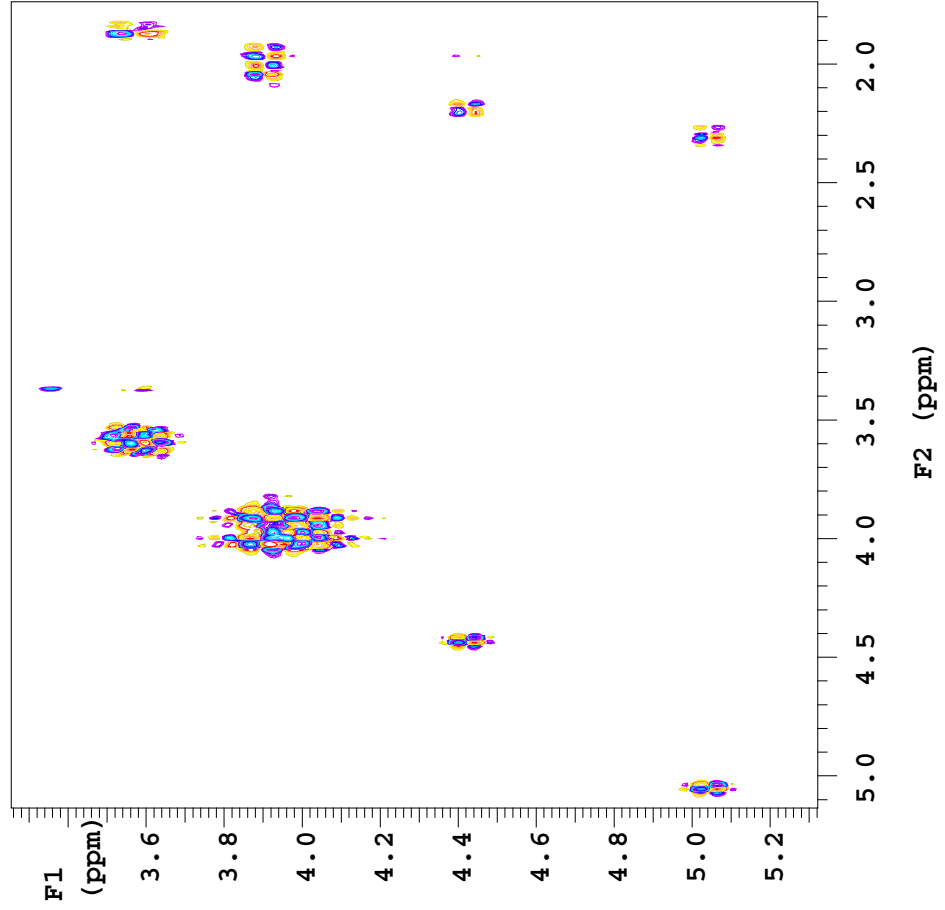
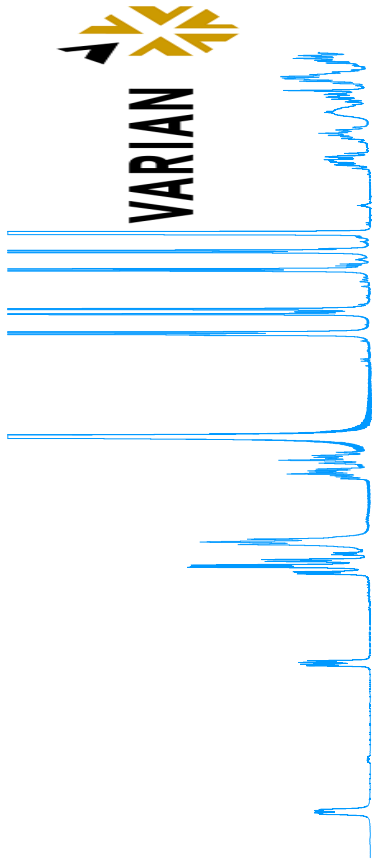
F1 DATA PROCESSING

Sq. sine bell 0.035 sec

Shifted by -0.028 sec

FT size 4096 x 4096

Total time 8 min 27 sec





FK70 dmso 17C HMBC  
28.05.2010

Sample Name:

FK70  
Data Collected on:  
Varian-NMR-vnmrs600  
Archive directory:

Sample directory:

FidFile: FK50\_DMSO\_HMBCAD\_17C

Pulse Sequence: gHMBCAD

Solvent: dmso

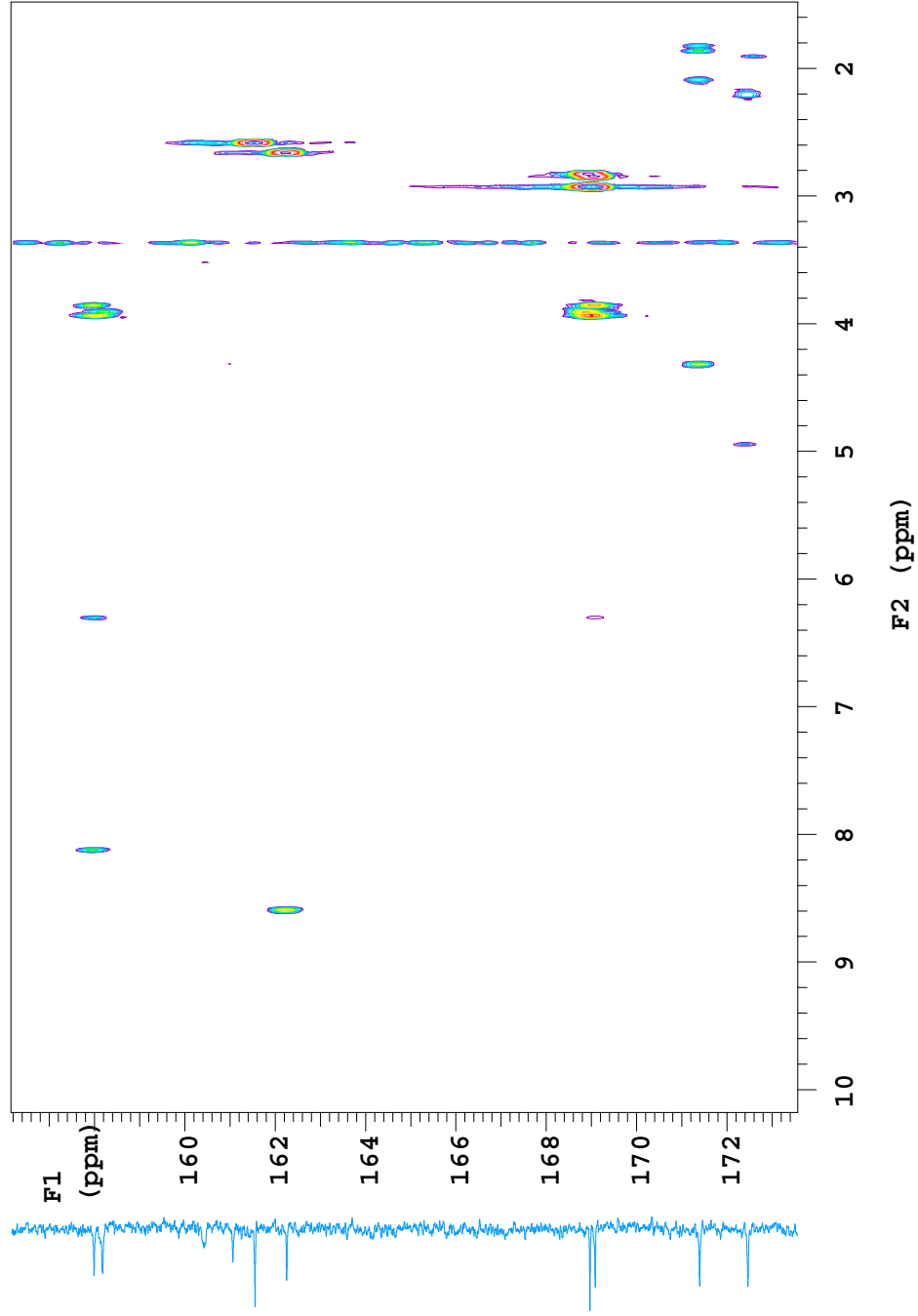
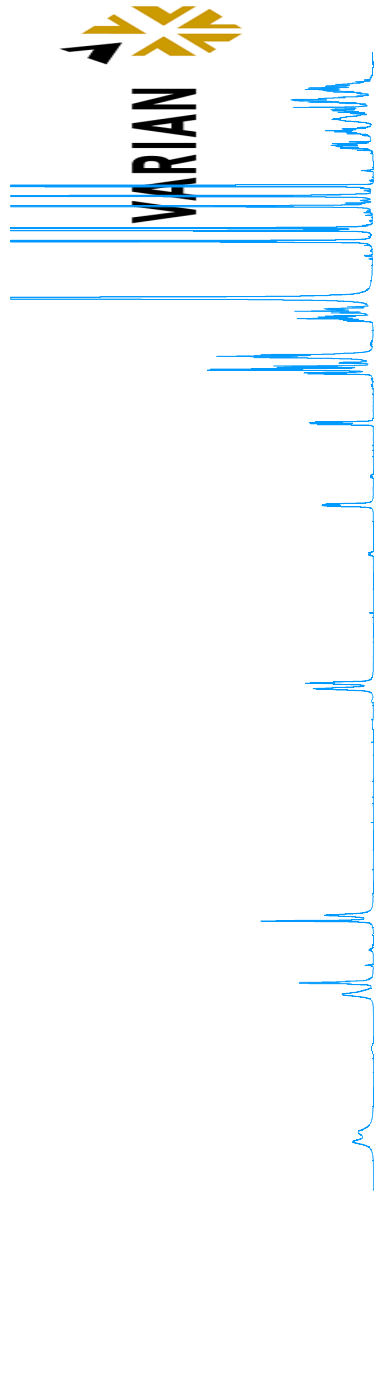
Data collected on: May 28 2010

Temp. 17.0 C / 290.1 K  
Operator: servis

Relax. delay 1.000 sec  
Acq. time 0.150 sec  
Width 9615.4 Hz  
2D Width 27146.3 Hz  
16 repetitions

2 x 256 increments  
OBSERVE H1, 599.8366087 MHZ  
DATA PROCESSING

Sq. sine bell 0.075 sec  
F1 DATA PROCESSING  
Gauss apodization 0.009 sec  
FT size 4096 x 4096  
Total time 2 hr, 54 min



FK70 dmso 17C HMBC  
28.05.2010

Sample Name:

FK70  
Data Collected on:  
Varian-NMR-vnmrs600  
Archive directory:

Sample directory:

FidFile: FK50\_DMSO\_HMBCAD\_17C

Pulse Sequence: gHMBCAD

Solvent: dmso

Data collected on: May 28 2010

Temp. 17.0 C / 290.1 K

Operator: servis

Relax. delay 1.000 sec

Acq. time 0.150 sec

Width 9615.4 Hz

2D Width 27146.3 Hz

16 repetitions

2 x 256 increments

OBSERVE H1, 599.8366087 MHZ

DATA PROCESSING

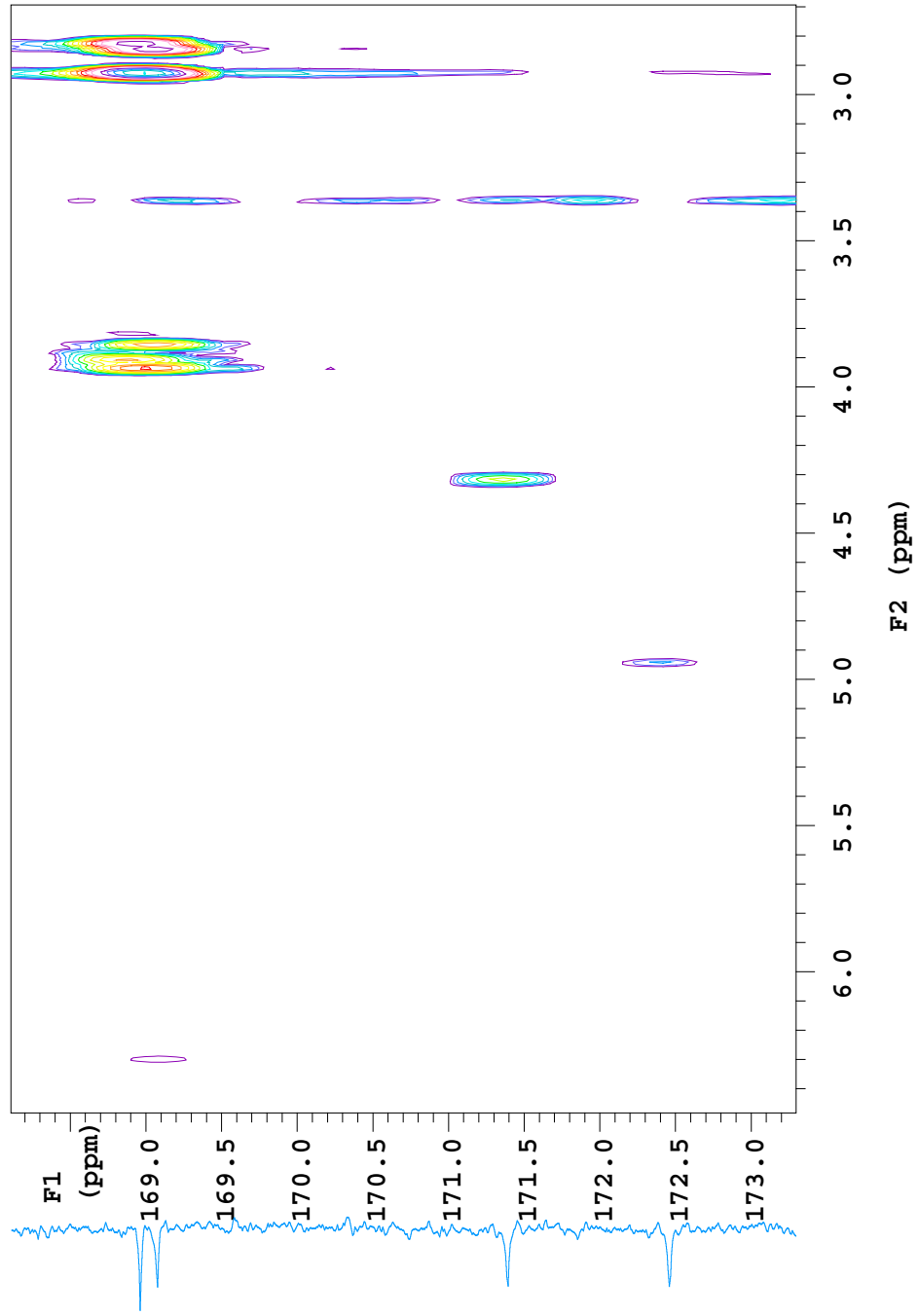
Sq. sine bell 0.075 sec

F1 DATA PROCESSING

Gauss apodization 0.009 sec

FT size 4096 x 4096

Total time 2 hr, 54 min



FK70 dmso 17C HMBC  
28.05.2010

Sample Name:

FK70  
Data Collected on:  
Varian-NMR-vnmrs600  
Archive directory:

Sample directory:

FidFile: FK50\_DMSO\_HMBCAD\_17C

Pulse Sequence: gHMBCAD

Solvent: dmso

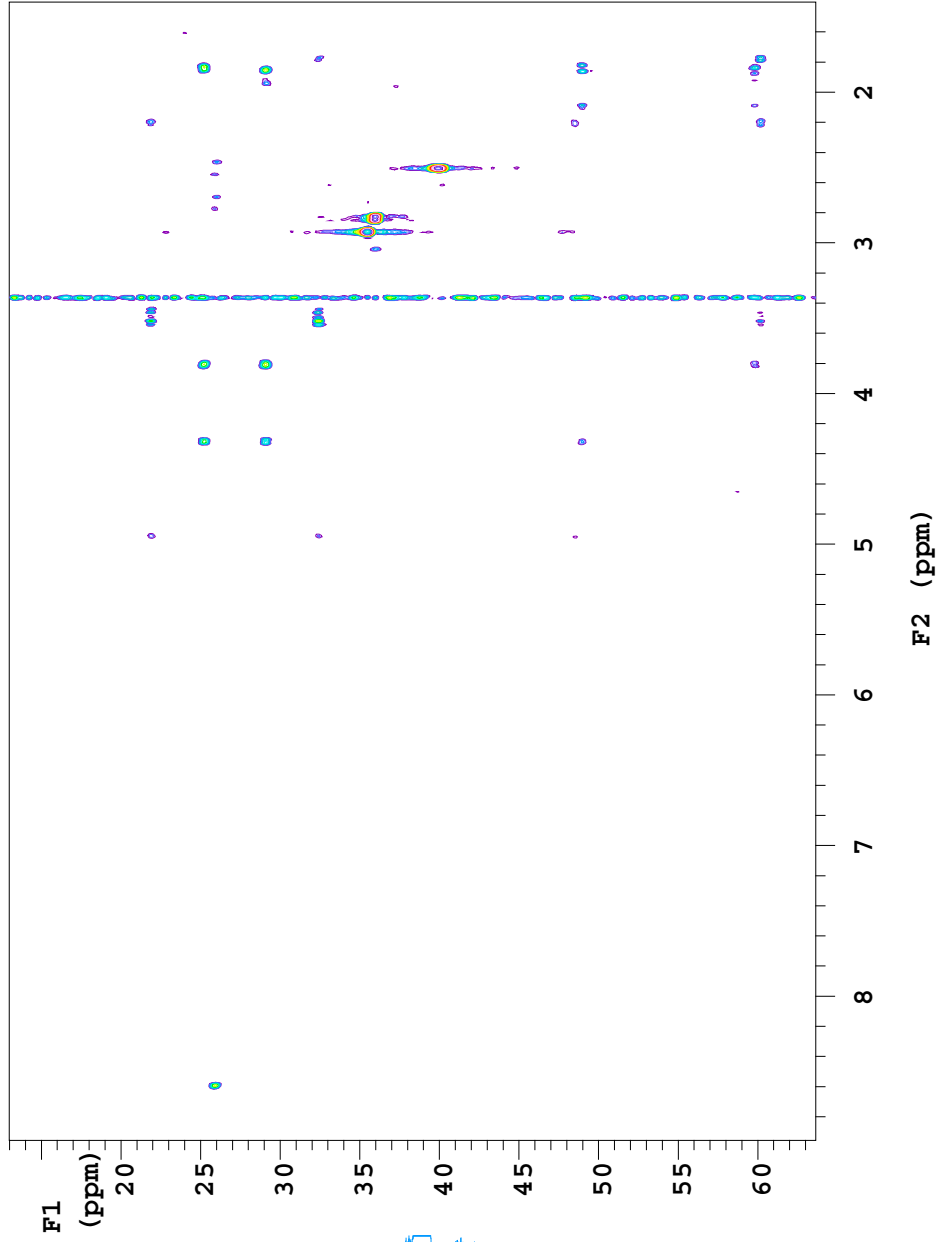
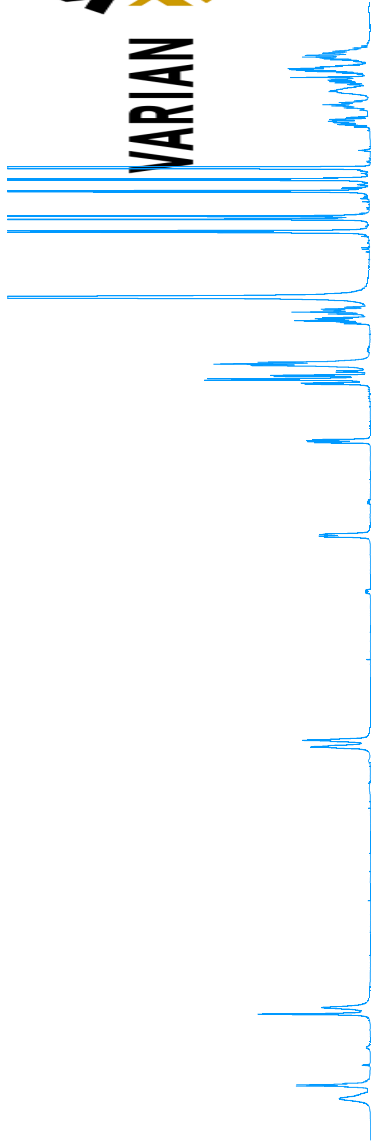
Data collected on: May 28 2010

Temp. 17.0 C / 290.1 K  
Operator: servis

Relax. delay 1.000 sec  
Acq. time 0.150 sec  
Width 9615.4 Hz  
2D Width 27146.3 Hz  
16 repetitions

2 x 256 increments  
OBSERVE H1, 599.8366087 MHz  
DATA PROCESSING

Sq. sine bell 0.075 sec  
F1 DATA PROCESSING  
Gauss apodization 0.009 sec  
FT size 4096 x 4096  
Total time 2 hr, 54 min



FK70 dmso 17C HMBC  
28.05.2010

Sample Name:

FK70  
Data Collected on:  
Varian-NMR-vnmrs600  
Archive directory:

Sample directory:

FidFile: FK50\_DMSO\_HMBCAD\_17C

Pulse Sequence: gHMBCAD

Solvent: dmso

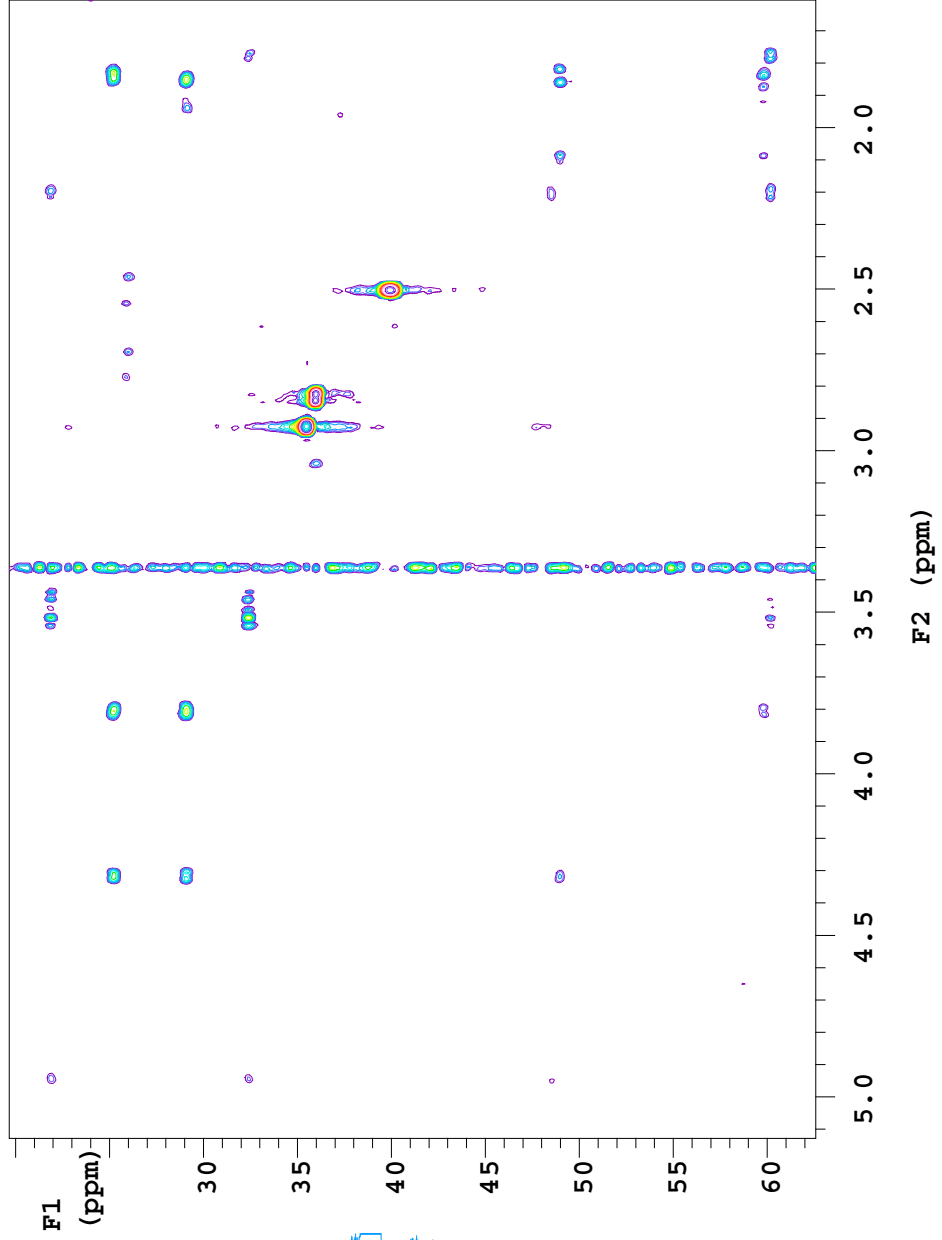
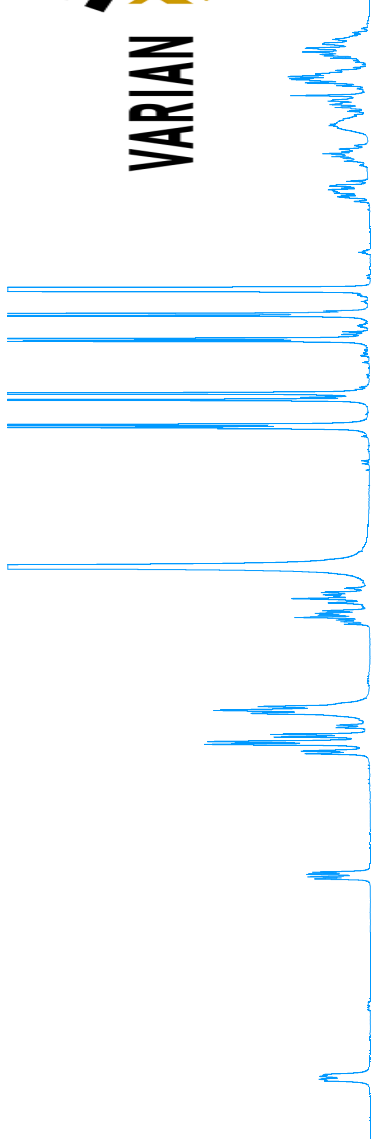
Data collected on: May 28 2010

Temp. 17.0 C / 290.1 K  
Operator: servis

Relax. delay 1.000 sec  
Acq. time 0.150 sec  
Width 9615.4 Hz  
2D Width 27146.3 Hz  
16 repetitions

2 x 256 increments  
OBSERVE H1, 599.8366087 MHz  
DATA PROCESSING

Sq. sine bell 0.075 sec  
F1 DATA PROCESSING  
Gauss apodization 0.009 sec  
FT size 4096 x 4096  
Total time 2 hr, 54 min



FK70 dmso gHSQCAD 17C

Sample Name:

FK70

Data Collected on:

Varian-NMR-vnmrs600

Archive directory:

Sample directory:

FidFile: FK50\_DMSO\_HSQCAD\_17C

Pulse Sequence: HSQCAD

Solvent: dmso

Data collected on: May 28 2010

Temp. 17.0 C / 290.1 K

Operator: servis

Relax. delay 1.000 sec

Acq. time 0.150 sec

Width 2185.3 Hz

2D Width 16590.6 Hz

16 repetitions

2 x 256 increments

OBSERVE H1, 599.8366123 MHz

DECOUPLE C13, 150.8358255 MHz

Power 43 dB

on during acquisition

off during delay

W40\_coldprobe modulated

DATA PROCESSING

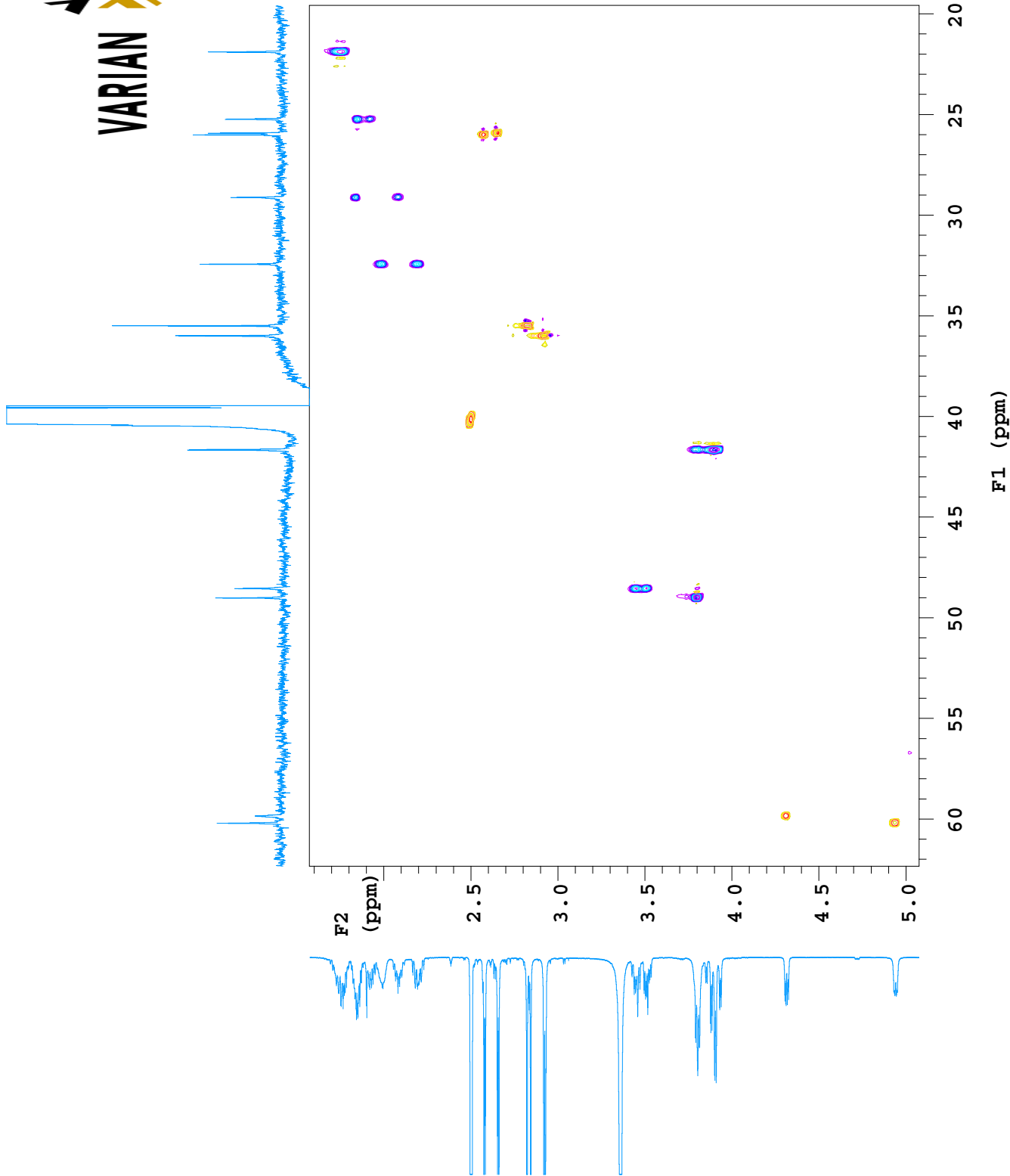
Gauss apodization 0.054 sec

F1 DATA PROCESSING

Gauss apodization 0.028 sec

FT size 512 x 4096

Total time 2 hr, 44 min



FK70 dmso gHSQCAD 17C

Sample Name:

FK70

Data Collected on:

Varian-NMR-vnmrs600

Archive directory:

Sample directory:

FidFile: FK50\_DMSO\_HSQCAD\_17C

Pulse Sequence: HSQCAD

Solvent: dmso

Data collected on: May 28 2010

Temp. 17.0 C / 290.1 K

Operator: servis

Relax. delay 1.000 sec

Acq. time 0.150 sec

Width 2185.3 Hz

2D Width 16590.6 Hz

16 repetitions

2 x 256 increments

OBSERVE H1, 599.8366123 MHz

DECOUPLE C13, 150.8358255 MHz

Power 43 dB

on during acquisition

off during delay

W40\_coldprobe modulated

DATA PROCESSING

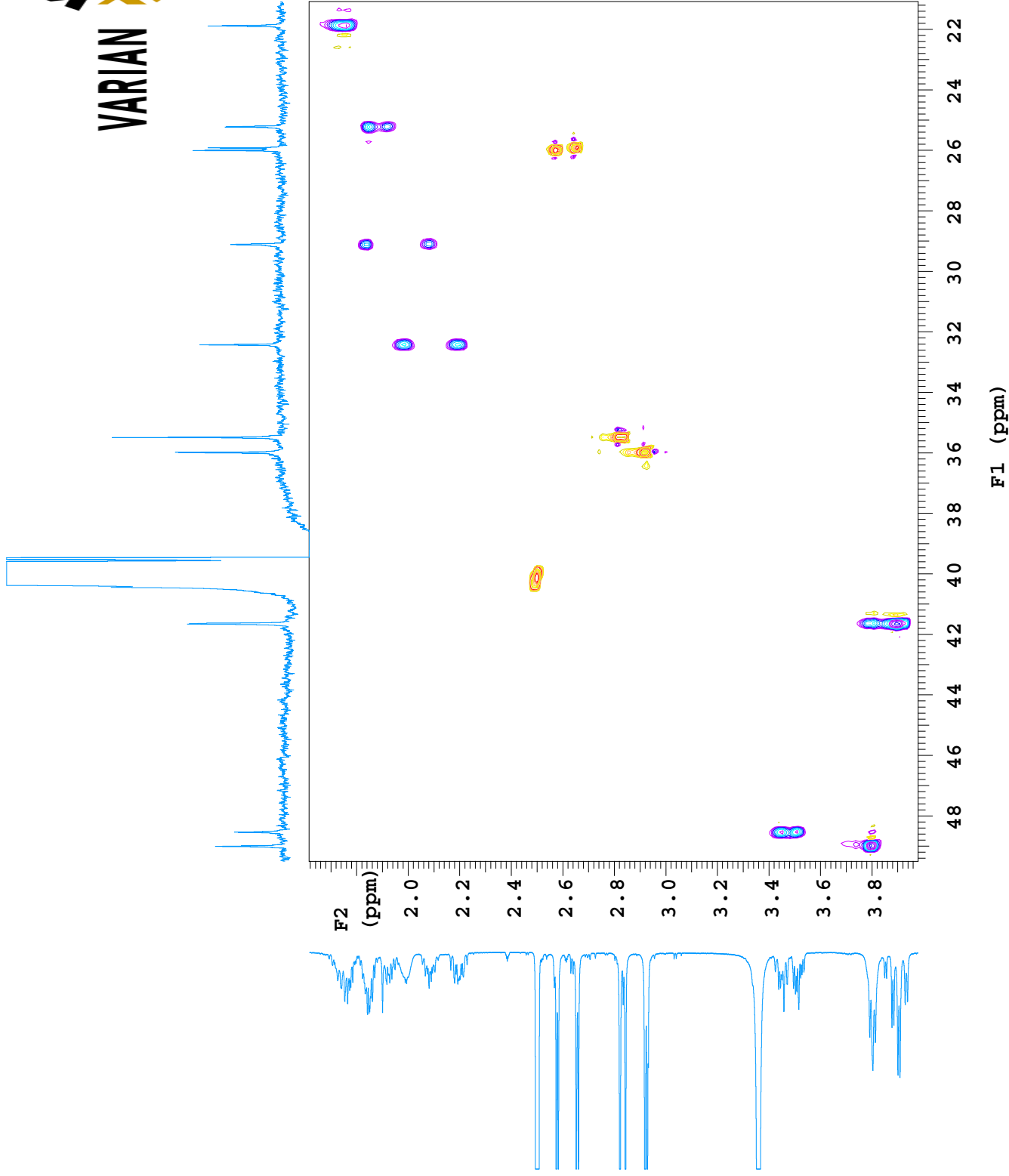
Gauss apodization 0.054 sec

F1 DATA PROCESSING

Gauss apodization 0.028 sec

FT size 512 x 4096

Total time 2 hr, 44 min



FK70 dmso gHSQCAD 17C

Sample Name:

FK70

Data Collected on:

Varian-NMR-vmrms600

Archive directory:

Sample directory:

FidFile: FK50\_DMSO\_HSQCAD\_17C

Pulse Sequence: HSQCAD

Solvent: dmso

Data collected on: May 28 2010

Temp. 17.0 C / 290.1 K

Operator: servis

Relax. delay 1.000 sec

Acq. time 0.150 sec

Width 2185.3 Hz

2D Width 16590.6 Hz

16 repetitions

2 x 256 increments

OBSERVE H1, 599.8366123 MHz

DECOUPLE C13, 150.8358255 MHz

Power 43 dB

on during acquisition

off during delay

W40\_coldprobe modulated

DATA PROCESSING

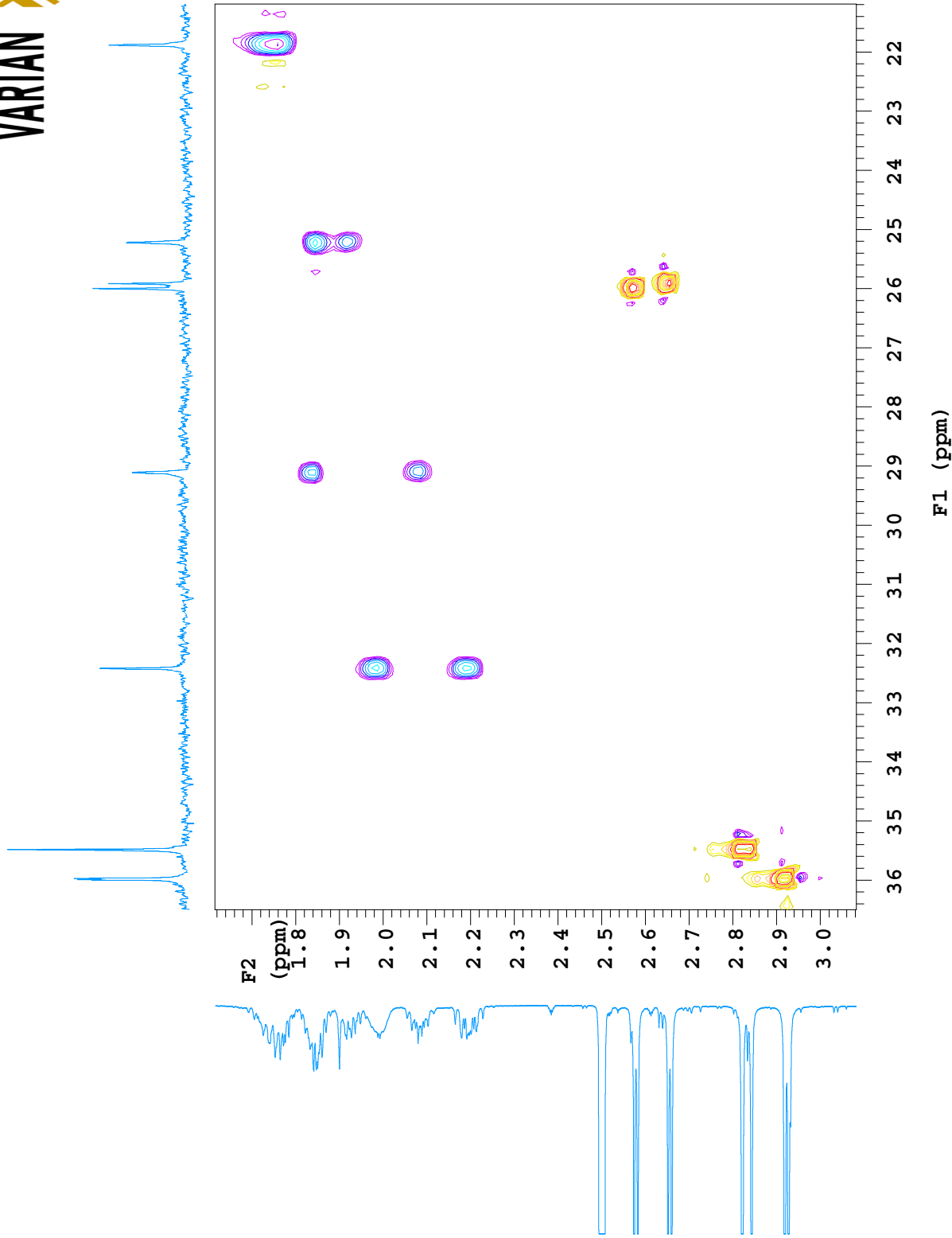
Gauss apodization 0.054 sec

F1 DATA PROCESSING

Gauss apodization 0.028 sec

FT size 512 x 4096

Total time 2 hr, 44 min



FK70 dmso 17C ROESYAD  
28.05.2010

Sample Name:  
FK70  
Data Collected on:  
Varian-NMR-vnmrs600  
Archive directory:  
/home/servis/vnmrsys/data  
Sample directory:  
FK70\_20100528\_01  
FidFile: FK50\_DMSO\_ROESY\_17C

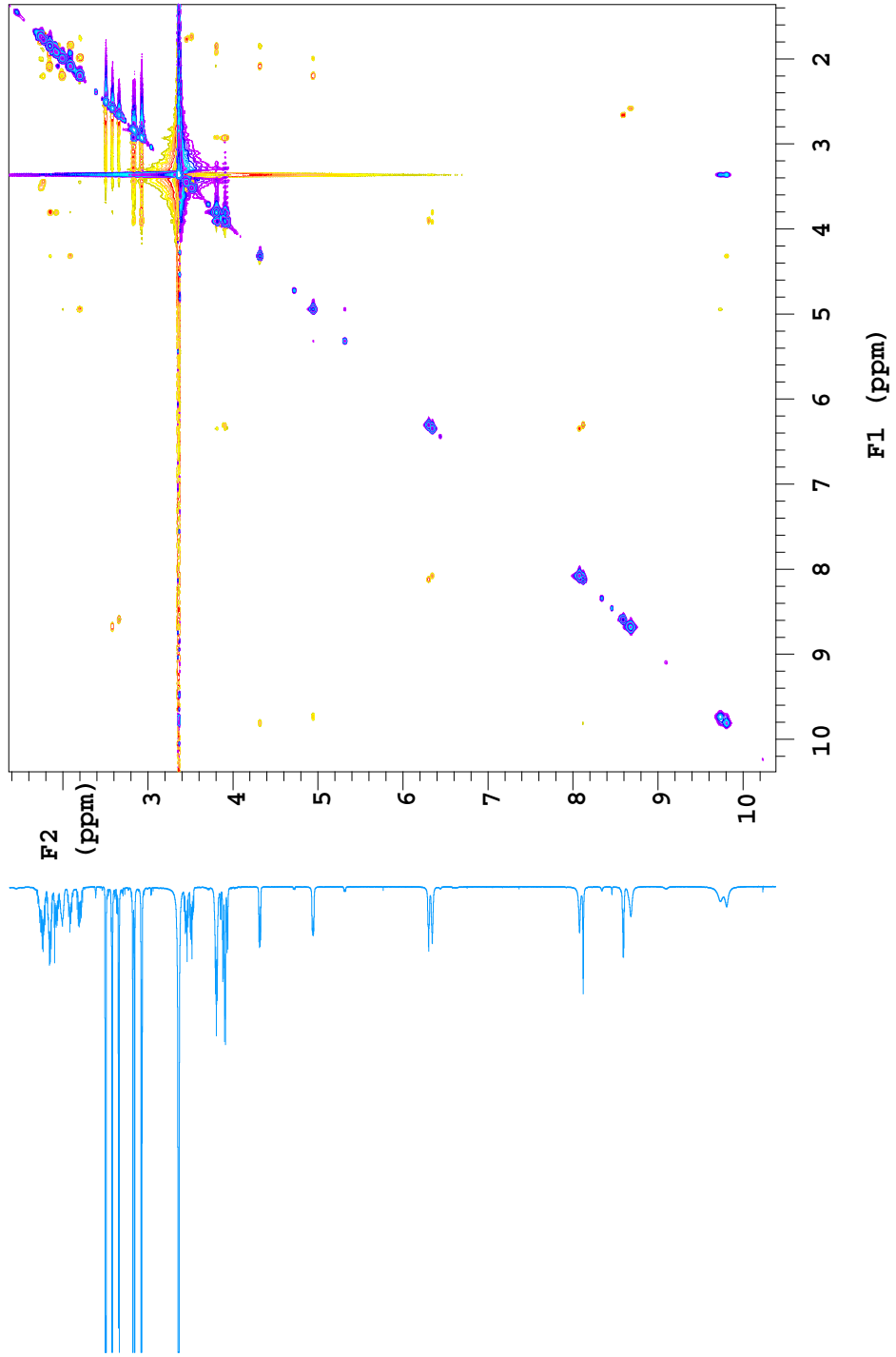
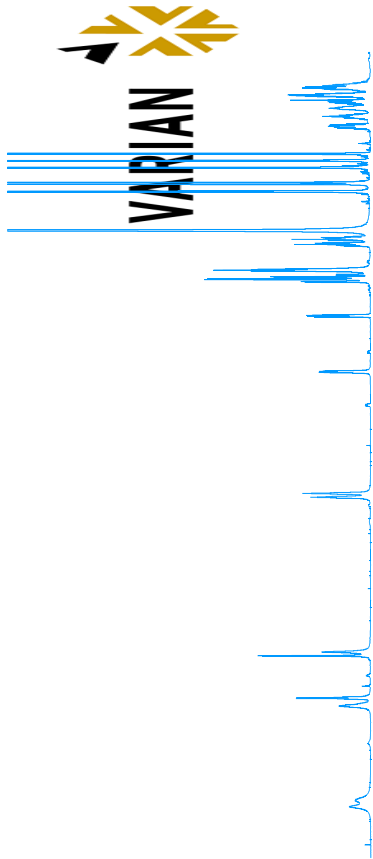
Pulse Sequence: ROESYAD  
Solvent: dmso  
Data collected on: May 31 2010

Temp. 17.0 C / 290.1 K  
Operator: servis

Relax. delay 1.000 sec  
Acq. time 0.150 sec  
Width 9615.4 Hz  
2D Width 9615.4 Hz  
12 repetitions  
2 x 256 increments

OBSERVE H1, 599.8366109 MHZ  
DATA PROCESSING

Gauss apodization 0.069 sec  
F1 DATA PROCESSING  
Gauss apodization 0.025 sec  
FT size 4096 x 4096  
Total time 2 hr, 41 min





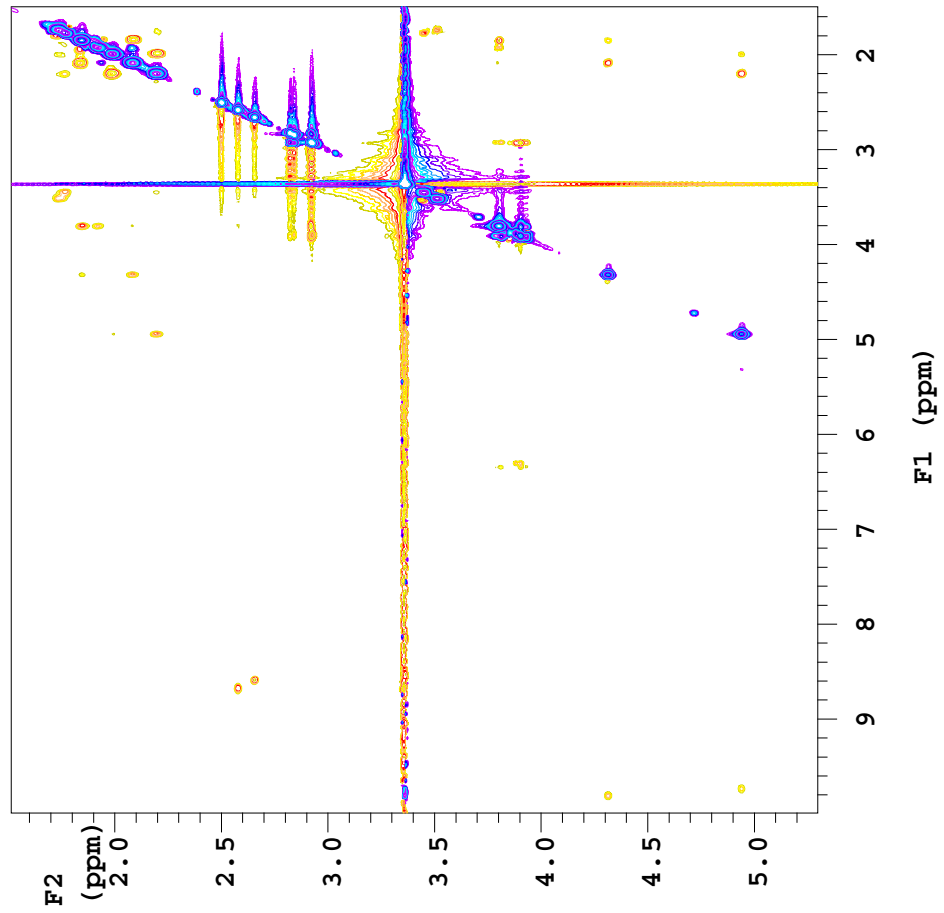
FK70 dmso 17C ROESYAD  
28.05.2010

Sample Name:  
FK70  
Data Collected on:  
Varian-NMR-vnmrs600  
Archive directory:  
/home/servis/vnmrsys/data  
Sample directory:  
FK70\_20100528\_01  
Fidfile: FK50\_DMSO\_ROESY\_17C

Pulse Sequence: ROESYAD  
Solvent: dmso  
Data collected on: May 31 2010

Temp. 17.0 C / 290.1 K  
Operator: servis

Relax. delay 1.000 sec  
Acq. time 0.150 sec  
Width 9615.4 Hz  
2D Width 9615.4 Hz  
12 repetitions  
2 x 256 increments  
OBSERVE H1, 599.8366109 MHZ  
DATA PROCESSING  
Gauss apodization 0.069 sec  
F1 DATA PROCESSING  
Gauss apodization 0.025 sec  
FT size 4096 x 4096  
Total time 2 hr, 41 min



FK70 dmso 17C ROESYAD  
28.05.2010

Sample Name:

FK70  
Data Collected on:  
Varian-NMR-vnmrs600  
Archive directory:  
/home/servis/vnmrsys/data  
Sample directory:  
FK70\_20100528\_01  
FidFile: FK50\_DMSO\_ROESY\_17C

Pulse Sequence: ROESYAD

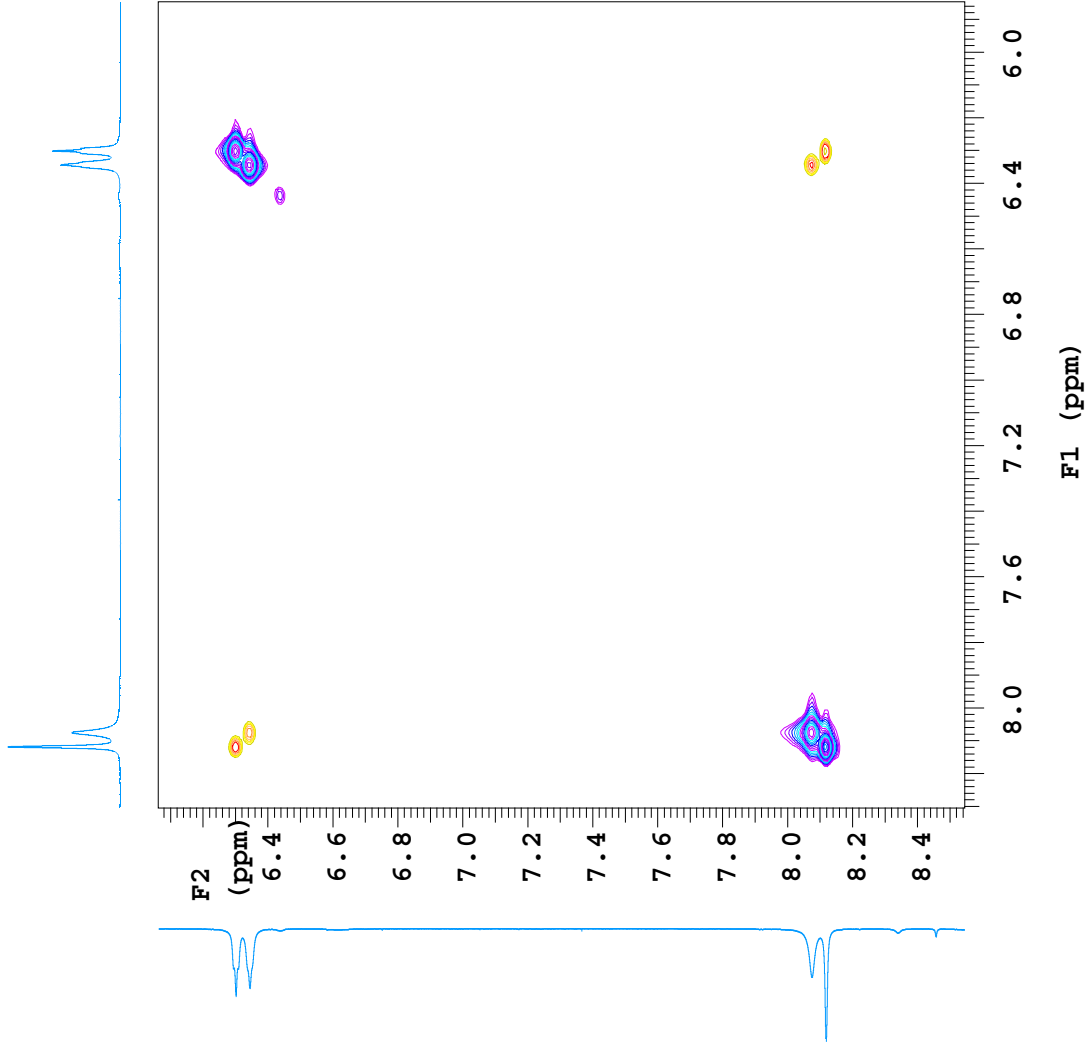
Solvent: dmso  
Data collected on: May 31 2010

Temp. 17.0 C / 290.1 K  
Operator: servis

Relax. delay 1.000 sec  
Acq. time 0.150 sec  
Width 9615.4 Hz  
2D Width 9615.4 Hz  
12 repetitions  
2 x 256 increments

OBSERVE H1, 599.8366109 MHZ  
DATA PROCESSING

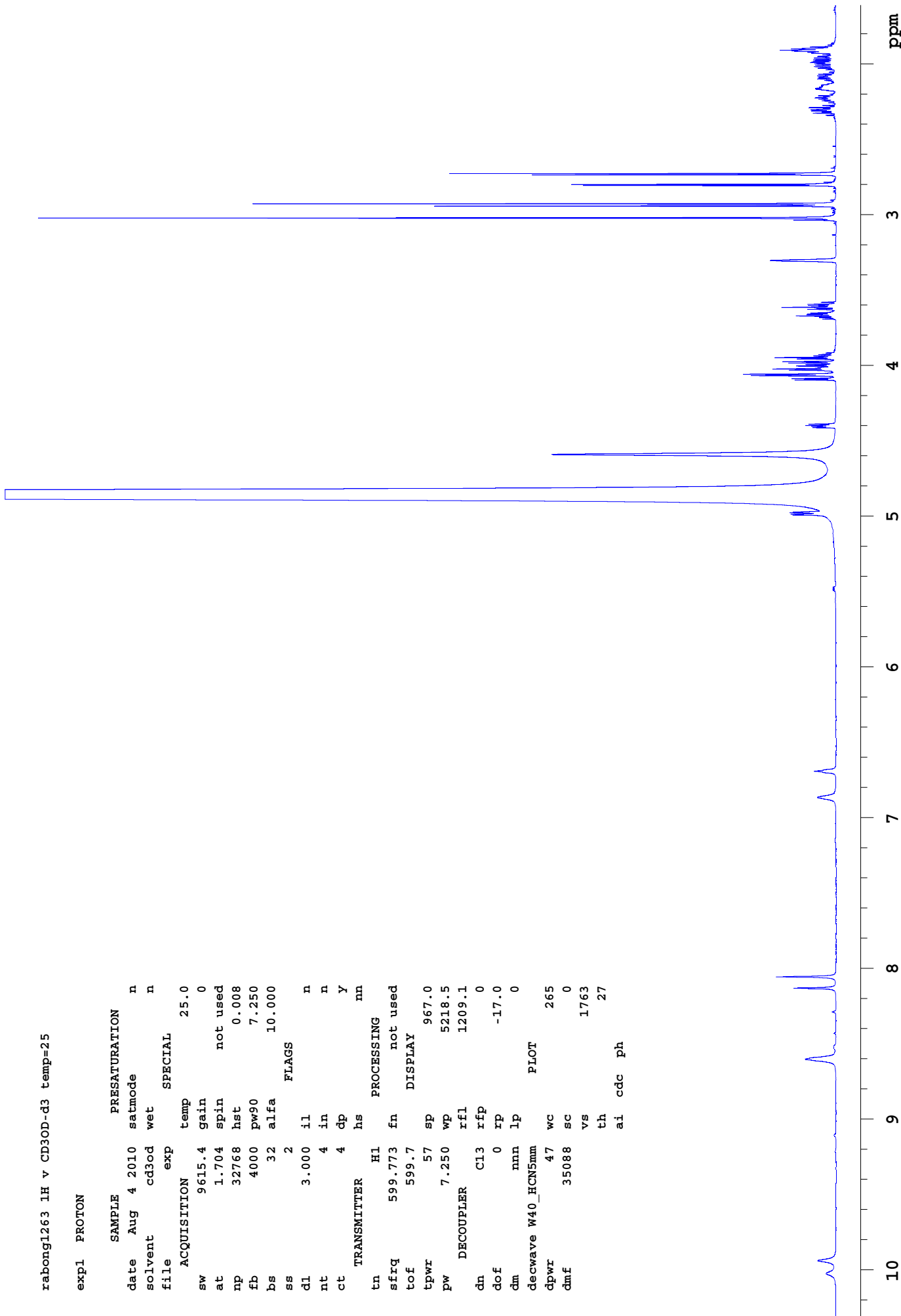
Gauss apodization 0.069 sec  
F1 DATA PROCESSING  
Gauss apodization 0.025 sec  
FT size 4096 x 4096  
Total time 2 hr, 41 min



rabong1263 1H v CD3OD-d3 temp=25

expl PROTON

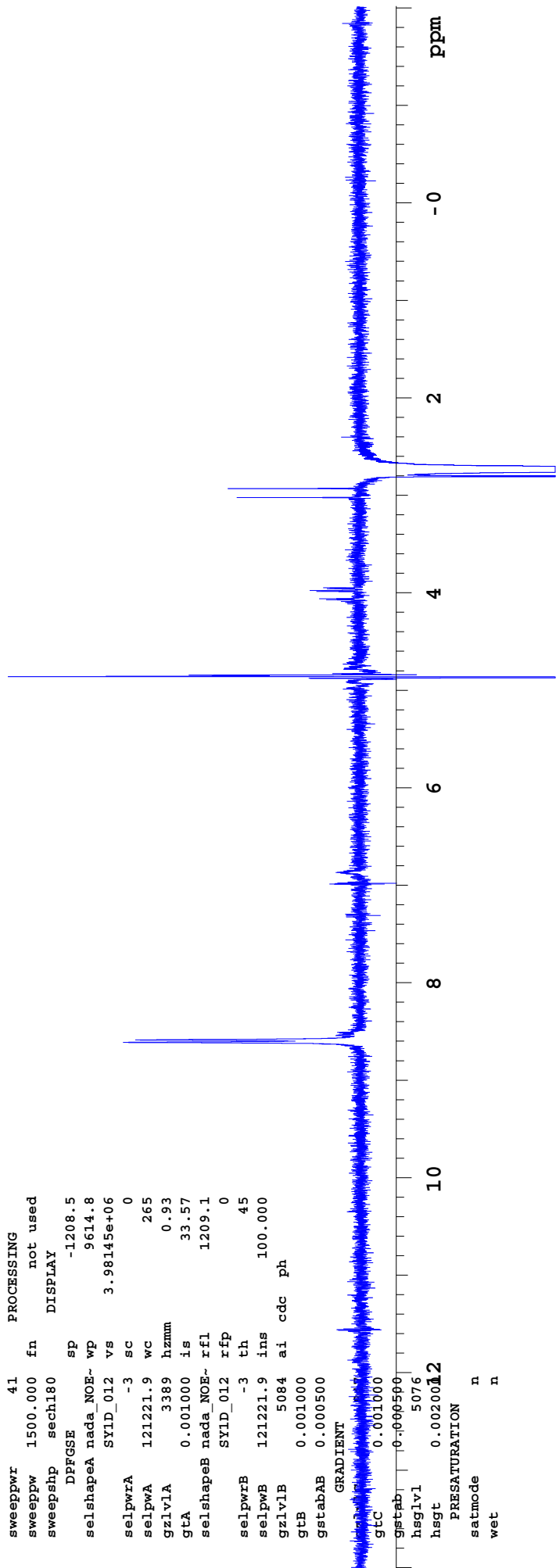
SAMPLE		PRESATURATION	
date	Aug 4 2010	satmode	n
solvent	cd3od	wet	n
file	exp	SPECIAL	
ACQUISITION		temp	25.0
sw	9615.4	gain	0
at	1.704	spin	not used
np	32768	hst	0.008
fb	4000	pw90	7.250
bs	32	alfa	10.000
ss	2	FLAGS	
d1	3.000	i1	n
nt	4	in	n
ct	4	dp	y
TRANSMITTER		hs	nn
tn	H1	PROCESSING	
sfrq	599.773	fn	not used
tof	599.7	DISPLAY	
tpwr	57	sp	967.0
pw	7.250	wp	5218.5
DECOUPLER		rfl	1209.1
dn	C13	rfp	0
dof	0	rp	-17.0
dm	nnn	lp	0
decwave W40_HCN5mm		PLOT	
dpwr	47	wc	265
dmf	35088	sc	0
		vs	1763
		th	27
		ai	cdc
			ph



1H CD3OD-d3 temp=25  
 Selective band center: 2.73 (ppm); width  
 : 29.7 (Hz)

exp2 NOESY1D

sw	9615.4	dn	C13
at	1.704	dm	mn
np	32768		SAMPLE
fb	4000	date	Aug 4 2010
bs	32	solvent	cd3od
ss	64	file	exp
d1	1.000		SPECIAL
nt	2024	temp	25.0
ct	2024	gain	0
		spn	not used
tn	H1	pw90	7.250
sfrq	599.773		FLAGS
tof	599.7	sspul	Y
tpwr	57	il	n
pw	7.250	in	n
		dp	Y
mixN	0.250	hs	nn
sweepwr	41		PROCESSING
sweepppw	1500.000	fn	not used
sweepshp	sech180		DISPLAY
		DPFGSE	-1208.5
selshapeA	nada_NOE-	wp	9614.8
	SYID_012	vs	3.98145e+06
selpwrA	-3	sc	0
selpwa	121221.9	wc	265
gzlv1A	3389	hzmm	0.93
gtA	0.001000	is	33.57
selshapeB	nada_NOE-	rfl	1209.1
	SYID_012	rfp	0
selpwrB	-3	th	45
selpwb	121221.9	ins	100.000
gzlv1B	5084	ai	cdc ph
gtB	0.001000		
gstabAB	0.000500		
		GRADIENT	
gtc	0.001000		
gstab	0.000500		
hsglv1	5076		
hsgt	0.0020012		
		PRESATURATION	
satmode	n		
wet	n		



1H CD30D-d3 temp=25  
Selective band center: 2.73 (ppm); width: 29.7 (Hz)

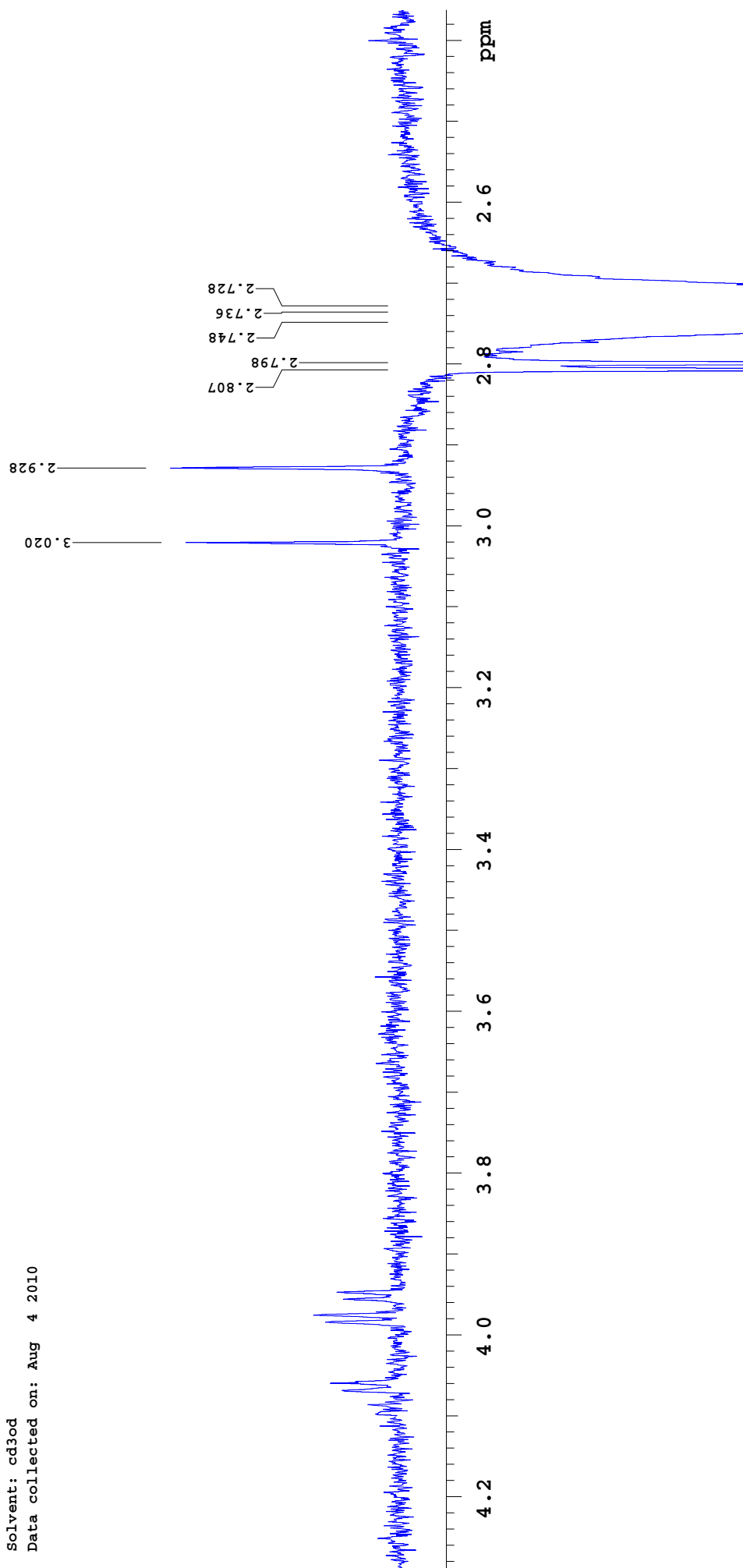
Sample Name:

Data Collected on:  
Varian-NMR-vnmrs600  
Archive directory:

Sample directory:

FidFile: NOESY1D

Pulse Sequence: NOESY1D  
Solvent: cd3od  
Data collected on: Aug 4 2010



1H CD3OD-d3 temp=25  
Selective band center: 2.73 (ppm); width: 29.7 (Hz)

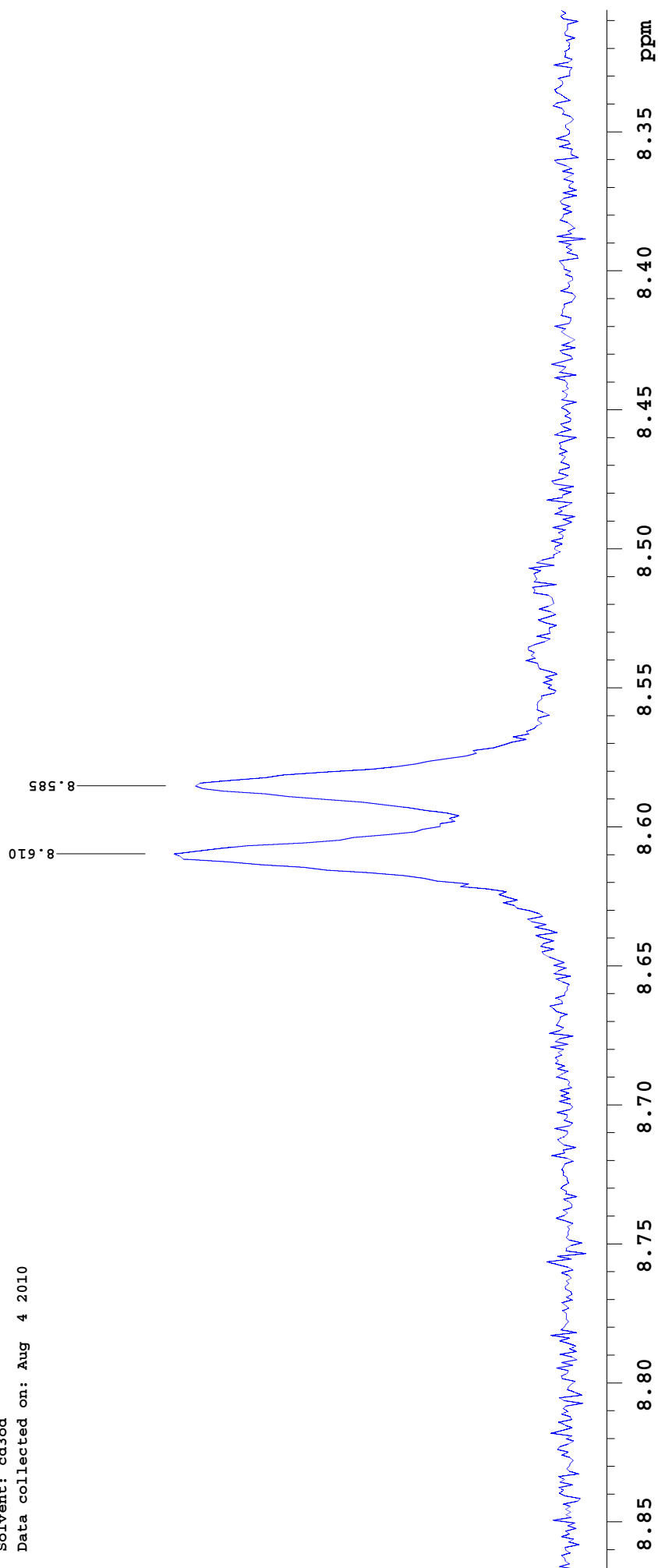
Sample Name:

Data Collected on:  
Varian-NMR-vnmrs600  
Archive directory:

Sample directory:

FidFile: NOESY1D

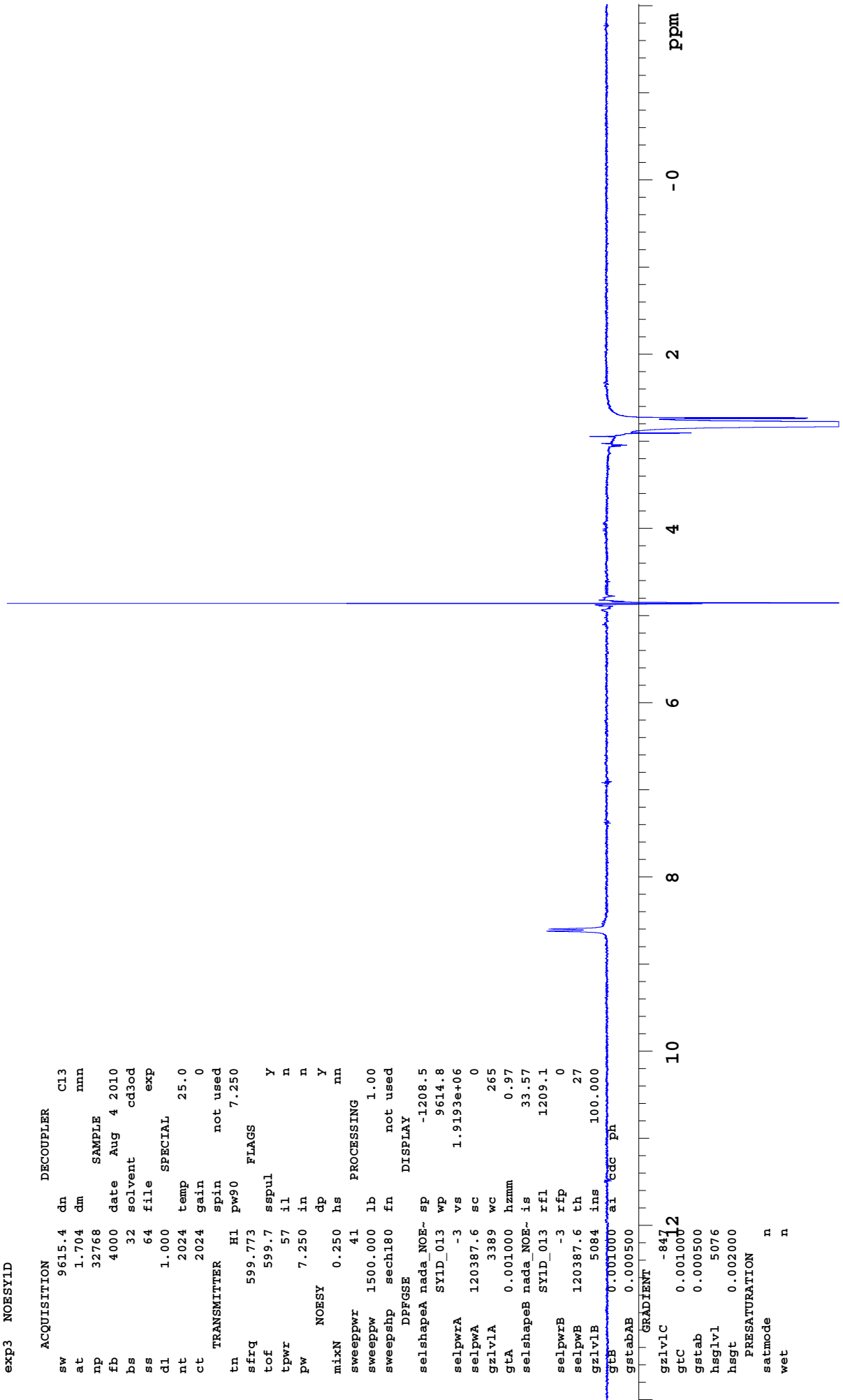
Pulse Sequence: NOESY1D  
Solvent: cd3od  
Data collected on: Aug 4 2010



LH v CD3OD-d3 temp=25  
 Selective band center: 2.80 (ppm); width  
 : 29.9 (Hz)

exp3 NOESY1D

sw	9615.4	dn	Cl3
at	1.704	dm	mmn
np	32768		SAMPLE
fb	4000	date	Aug 4 2010
bs	32	solvent	cd3od
ss	64	file	exp
d1	1.000	SPECIAL	
nt	2024	temp	25.0
ct	2024	gain	0
TRANSMITTER			
tn	H1	pw90	not used
sfrq	599.773	FLAGS	7.250
tof	599.7	sspul	Y
tpwr	57	il	n
pw	7.250	in	n
NOESY			
mixN	0.250	hs	Y
sweppwr	41	PROCESSING	nn
swepppw	1500.000	lb	1.00
sweepshp	sech180	fn	not used
DPFGSE			
selshapeA	nada_NOE-	sp	-1208.5
SYID_013	wp		9614.8
selpwrA	-3	vs	1.9193e+06
selpwa	120387.6	sc	0
gzlv1A	3389	wc	265
gtA	0.001000	hzmm	0.97
selshapeB	nada_NOE-	is	33.57
SYID_013	rfl		1209.1
selpwrB	-3	rfp	0
selpwb	120387.6	th	27
gzlv1B	5084	ins	100.000
gtB	0.001000	ai	cdc_ph
gstabAB	0.000500		
GRADIENT			
gzlv1C	-847		
gtC	0.001000		
gstab	0.000500		
hsg1v1	5076		
hsgt	0.002000		
PRESATURATION			
satmode	n		
wet	n		



1H v CD3OD-d3 temp=25  
Selective band center: 2.80 (ppm); width: 29.9 (Hz)

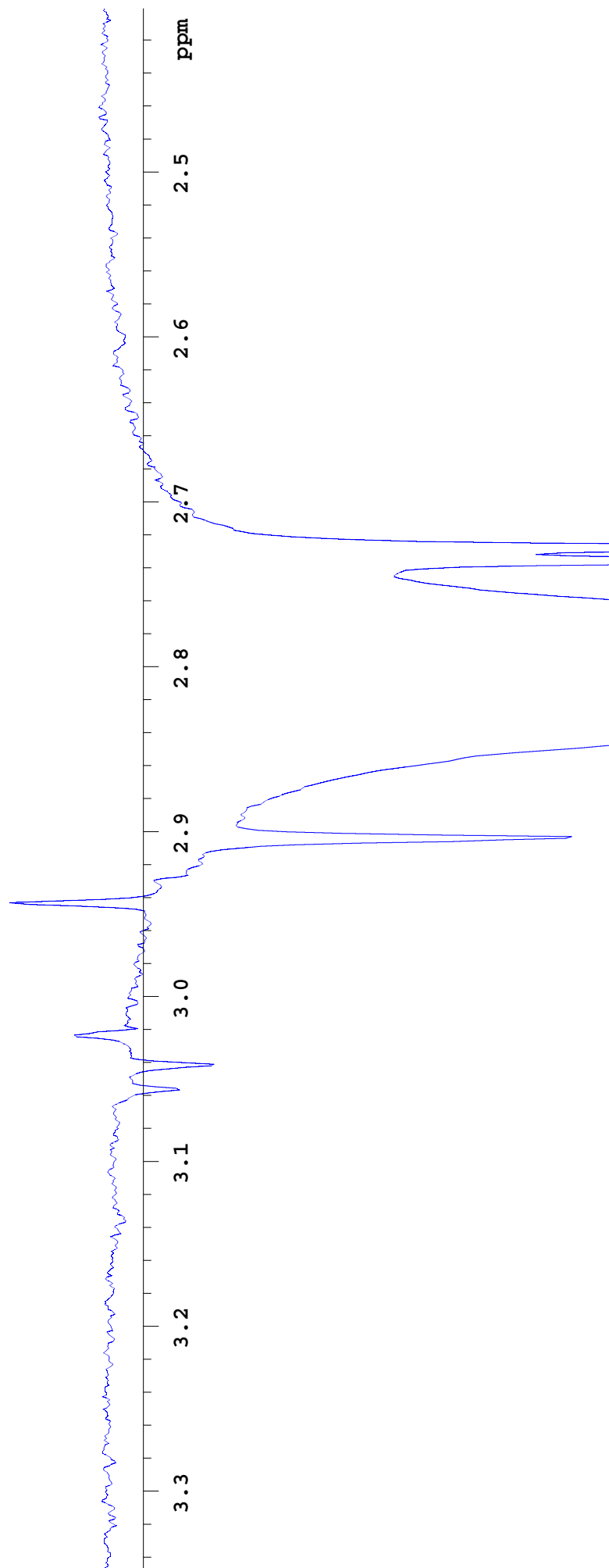
Sample Name:

Data Collected on:  
Varian-NMR-vnmrs600  
Archive directory:

Sample directory:

FidFile: NOESY1D

Pulse Sequence: NOESY1D  
Solvent: cd3od  
Data collected on: Aug 4 2010





1H v CD3OD-d3 temp=25  
Selective band center: 2.80 (ppm); width: 29.9 (Hz)

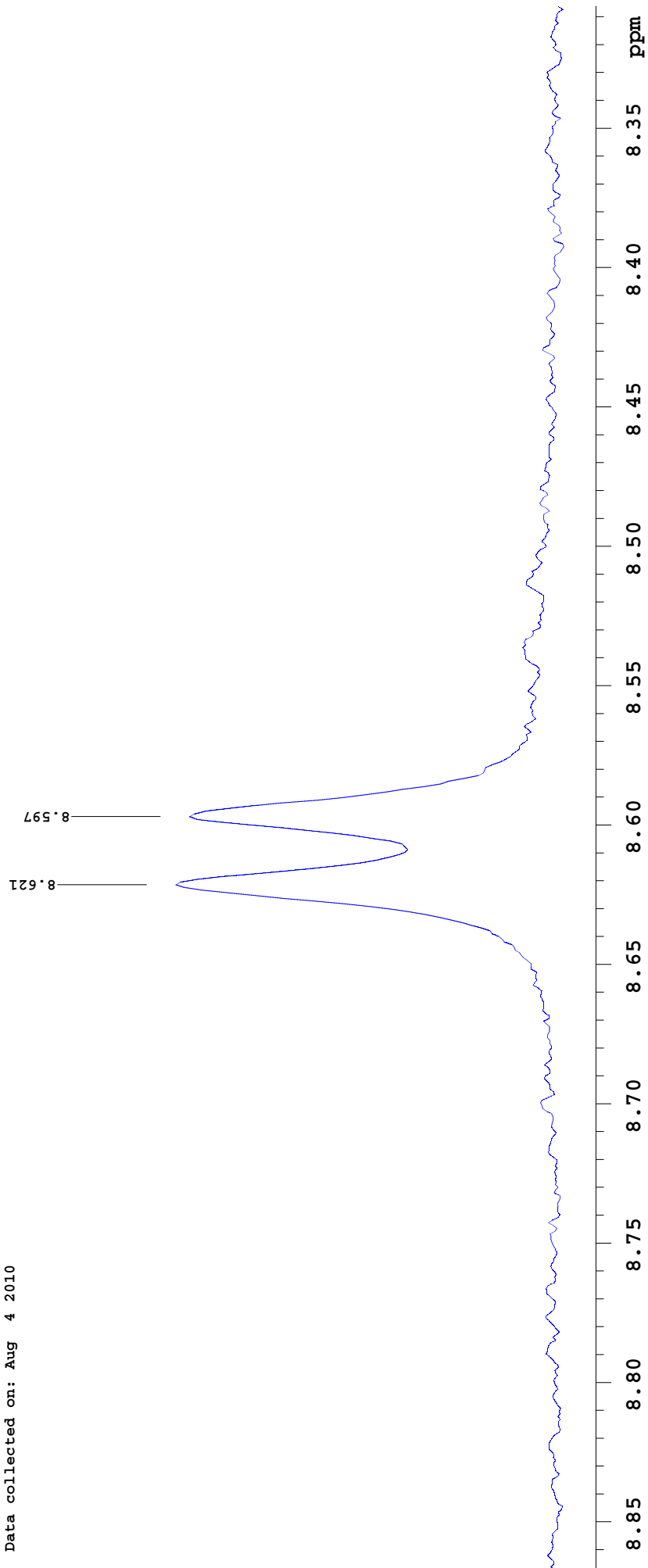
Sample Name:

Data Collected on:  
Varian-NMR-vnmrs600  
Archive directory:

Sample directory:

FidFile: NOESY1D

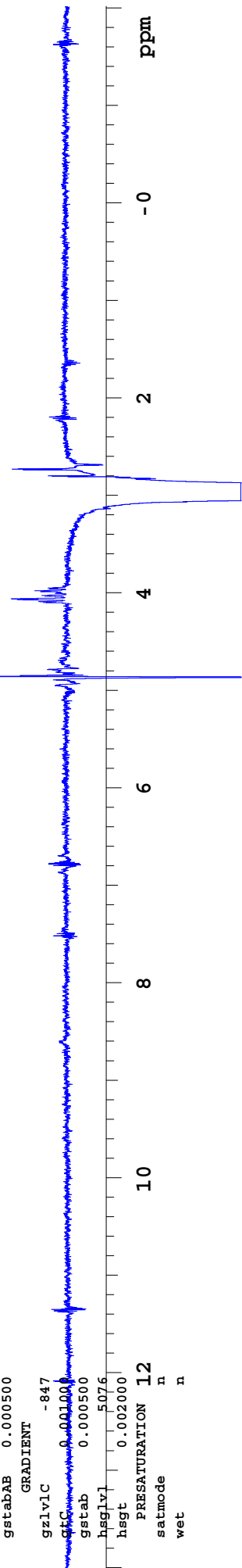
Pulse Sequence: NOESY1D  
Solvent: cd3od  
Data collected on: Aug 4 2010



H CD3OD-d3 temp=25  
 Selective band center: 2.93 (ppm); width  
 : 30.0 (Hz)

exp4 NOESY1D

sw	9615.4	dn	CL3
at	1.704	dm	mn
np	32768		SAMPLE
fb	4000	date	Aug 4 2010
bs	32	solvent	cd3od
ss	64	file	exp
d1	1.000		SPECIAL
nt	2024	temp	25.0
ct	2024	gain	0
		spn	not used
		pw90	7.250
tn	H1		FLAGS
sfrq	599.773		Y
tof	599.7	sspul	Y
tpwr	57	il	n
pw	7.250	in	n
		dp	Y
		hs	nn
mixN	0.250		
sweppwr	41		PROCESSING
sweppw	1500.000	lb	1.00
sweepshp	sech180	fn	not used
			DISPLAY
			DPFGSE
selshapeA	nada_NOE-	sp	-1208.5
	SYID_014	wp	9614.8
selpwrA	-3	vs	4.53977e+06
selpwa	120011.1	sc	0
gzlv1A	3389	wc	265
gtA	0.001000	hzmm	36.28
selshapeB	nada_NOE-	is	33.57
	SYID_014	rfl	1209.1
selpwrB	-3	rfp	0
selpwb	120011.1	th	27
gzlv1B	5084	ins	100.000
gtB	0.001000	ai	cdc
gstabAB	0.000500		ph
			GRADIENT
gzlv1C	-847		
gtC	0.001000		
gstab	0.000500		
hsg1v1	5076		
hsgt	0.002000		
			PRESATURATION 12
satmode	n		
wet	n		



H CD3OD-d3 temp=25  
Selective band center: 2.93 (ppm); width: 30.0 (Hz)

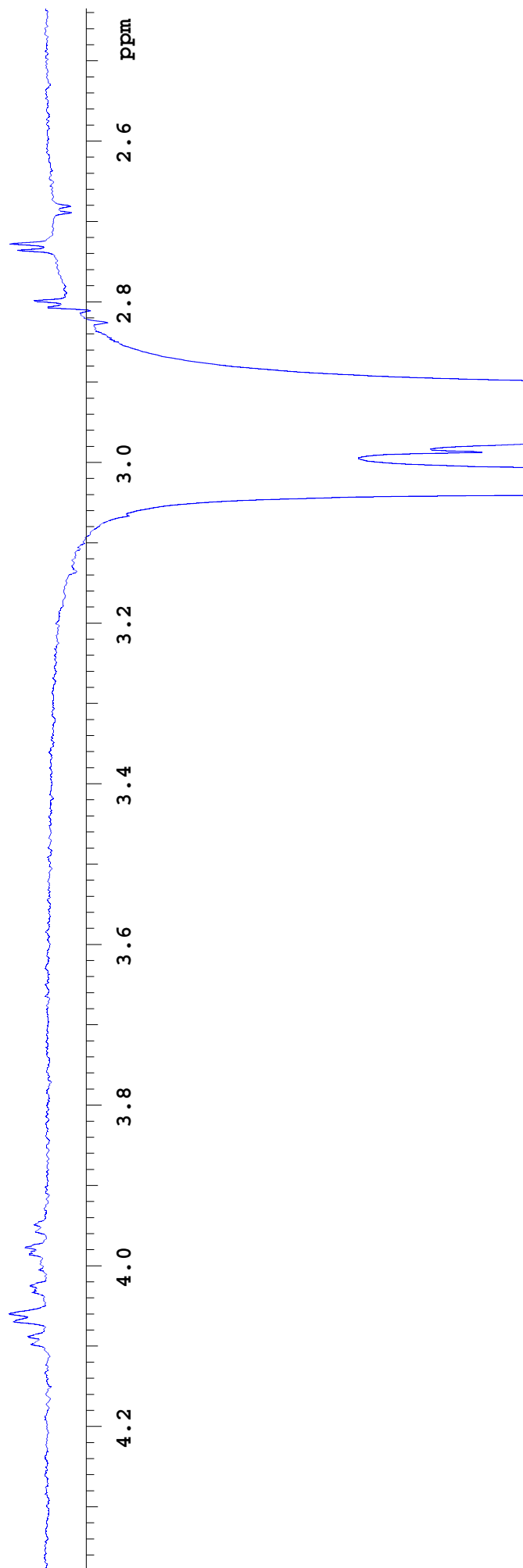
Sample Name:

Data Collected on:  
Varian-NMR-vnmrs600  
Archive directory:

Sample directory:

FidFile: NOESY1D

Pulse Sequence: NOESY1D  
Solvent: cd3od  
Data collected on: Aug 4 2010

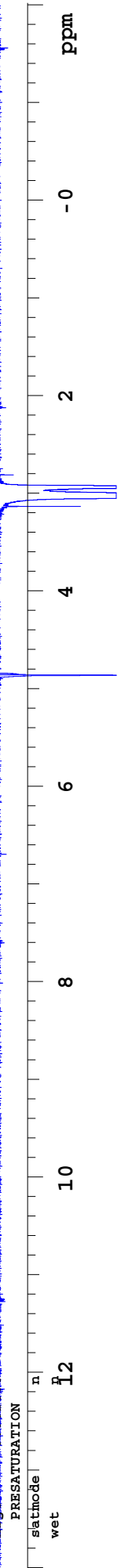


rabong1263 1H v CD3OD-d3 temp=25  
 Selective band center: 3.02 (ppm); wid  
 th: 29.9 (Hz)

exp5 NOESY1D

```

ACQUISITION      DECOUPLER
sw 9615.4 dn C13
at 1.704 dm mnn
np 32768 SAMPLE
fb 4000 date Aug 4 2010
bs 32 solvent cd3od
ss 64 file exp
d1 1.000 SPECIAL
nt 2024 temp 25.0
ct 2024 gain 0
   TRANSMITTER spin not used
tn H1 pw90 7.250
sfrq 599.773 FLAGS
tof 599.7 sspul Y
tpwr 57 il n
pw 7.250 in n
   NOESY dp Y
mixN 0.250 hs nn
sweppwr 41 PROCESSING
swepppw 1500.000 fn not used
sweepshp sech180 DISPLAY
   DPFGE sp -1208.5
selshapeA nada_NOE- wp 9614.8
SYID_015 vs 1.30508e+06
selpwra -3 sc 0
selpwa 120379.1 wc 265
gzlvla 3389 hzmm 36.28
gta 0.001000 is 33.57
selshapeB nada_NOE- rfl 1209.1
SYID_015 rfp 0
selpwrb -3 th 27
selpwB 120379.1 ins 100.000
gzlvlb 5084 ai cdc ph
gtB 0.001000
gstabAB 0.000500
GRADIENT
gzlvlc -847
gtC 0.001000
gstab 0.000500
hsglvl 5076
hsgt 0.002000
PRESATURATION
  
```



rabong1263 1H v CD3OD-d3 temp=25  
Selective band center: 3.02 (ppm); width: 29.9 (Hz)

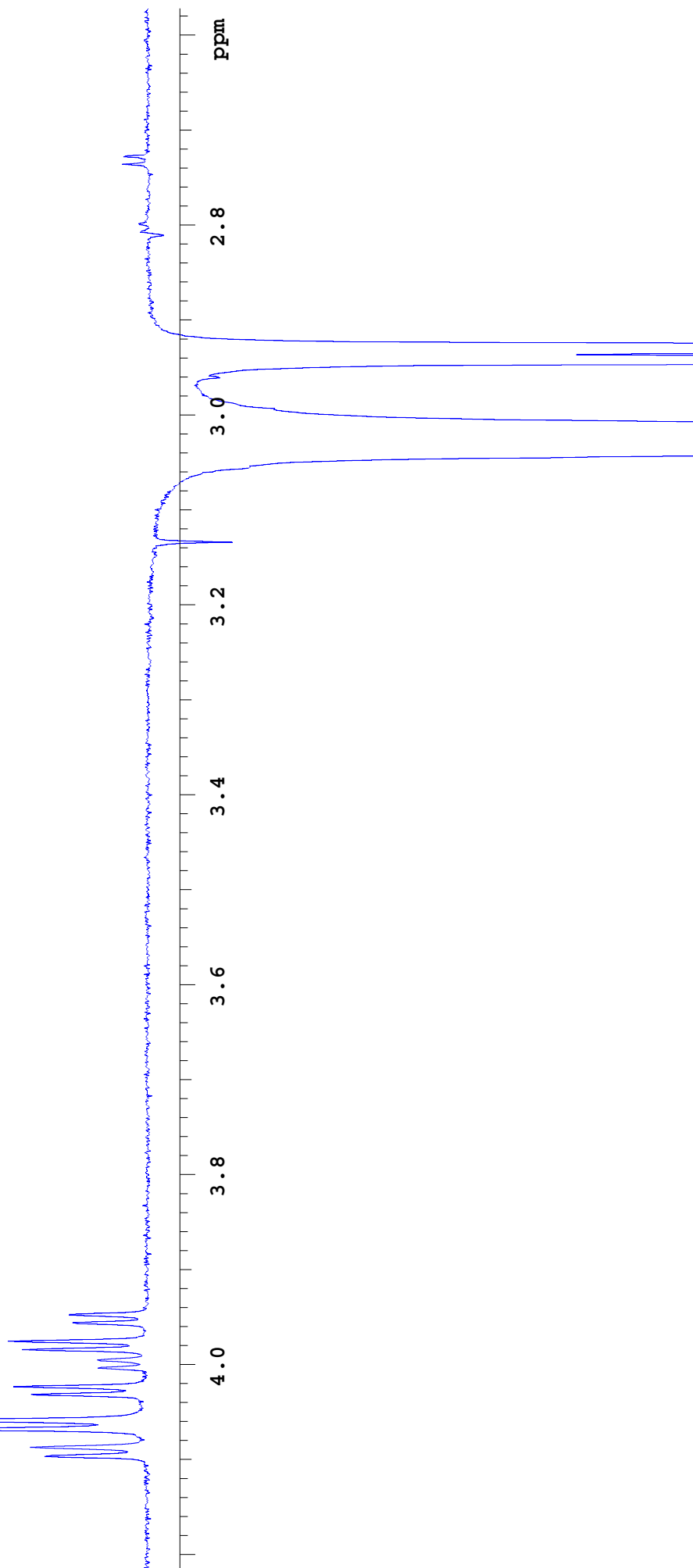
Sample Name:

Data Collected on:  
Varian-NMR-vnmrs600  
Archive directory:

Sample directory:

FidFile: NOESY1D

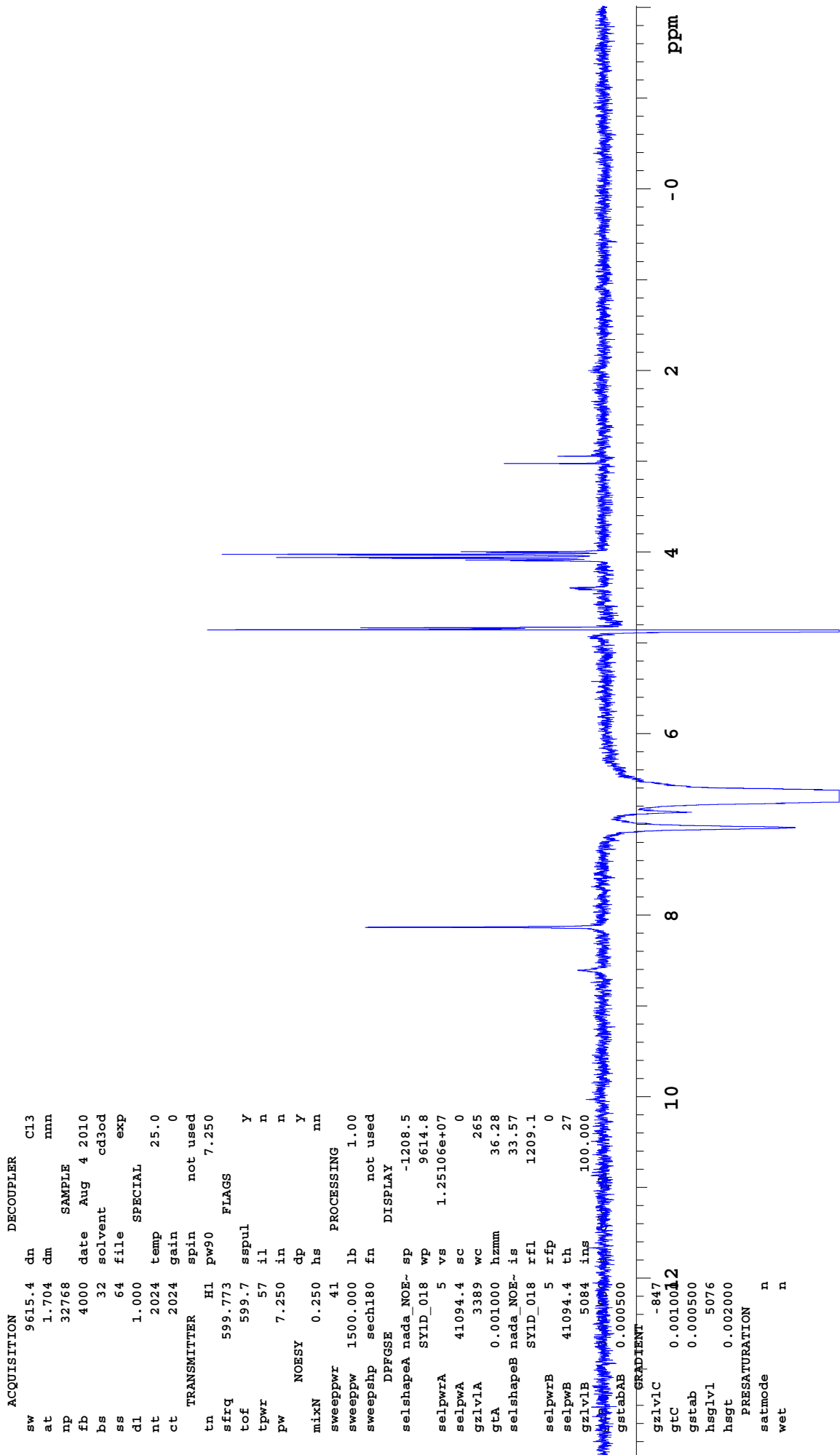
Pulse Sequence: NOESY1D  
Solvent: cd3od  
Data collected on: Aug 4 2010



rabong1263 1H v CD30D-d3 temp=25  
 Selective band center: 6.69 (ppm); wid  
 th: 87.6 (Hz)

exp8 NOESY1D

sw	9615.4	dn	C13
at	1.704	dm	mn
np	32768		SAMPLE
fb	4000	date	Aug 4 2010
bs	32	solvent	cd3od
ss	64	file	exp
d1	1.000		SPECIAL
nt	2024	temp	25.0
ct	2024	gain	0
		spn	not used
		pw90	7.250
tn	H1		FLAGS
sfrq	599.773		Y
tof	599.7	sspul	Y
tpwr	57	il	n
pw	7.250	in	n
		dp	Y
		hs	nn
mixN	0.250		nn
sweppwr	41		PROCESSING
sweppw	1500.000	lb	1.00
sweepshp	sech180	fn	not used
			DPFGSE
			DISPLAY
selshapeA	nada_NOE-	sp	-1208.5
SYID_018	wp		9614.8
selpwrA	5	vs	1.25106e+07
selpwa	41094.4	sc	0
gzlv1A	3389	wc	265
gtA	0.001000	hzmm	36.28
selshapeB	nada_NOE-	is	33.57
SYID_018	rfl		1209.1
selpwrB	5	rfp	0
selpwb	41094.4	th	27
gzlv1B	5084	ins	100.000
gstabAB	0.000500		



Selective band center: 6.69 (ppm); width: 87.6 (Hz)

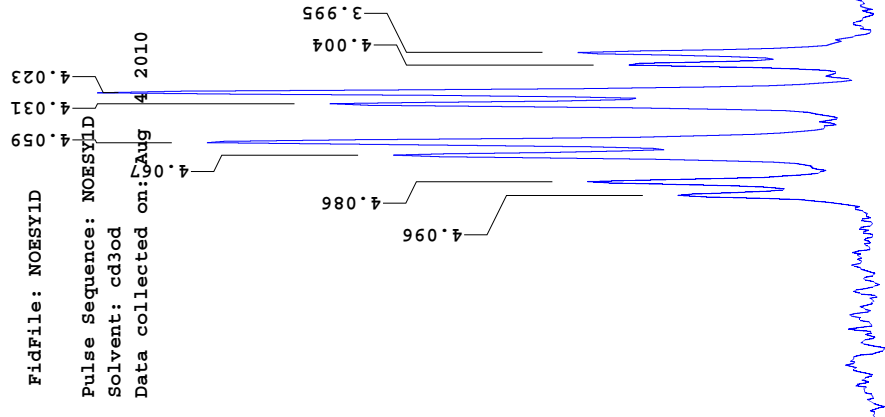
Sample Name:

Data Collected on:  
Varian-NMR-vnmrs600  
Archive directory:

Sample directory:

FidFile: NOESY1D

Pulse Sequence: NOESY1D  
Solvent: cd3od  
Data collected on: Aug 4 2010



Selective band center: 6.69 (ppm); width: 87.6 (Hz)

Sample Name:

Data Collected on:

Varian-NMR-vnmrs600

Archive directory:

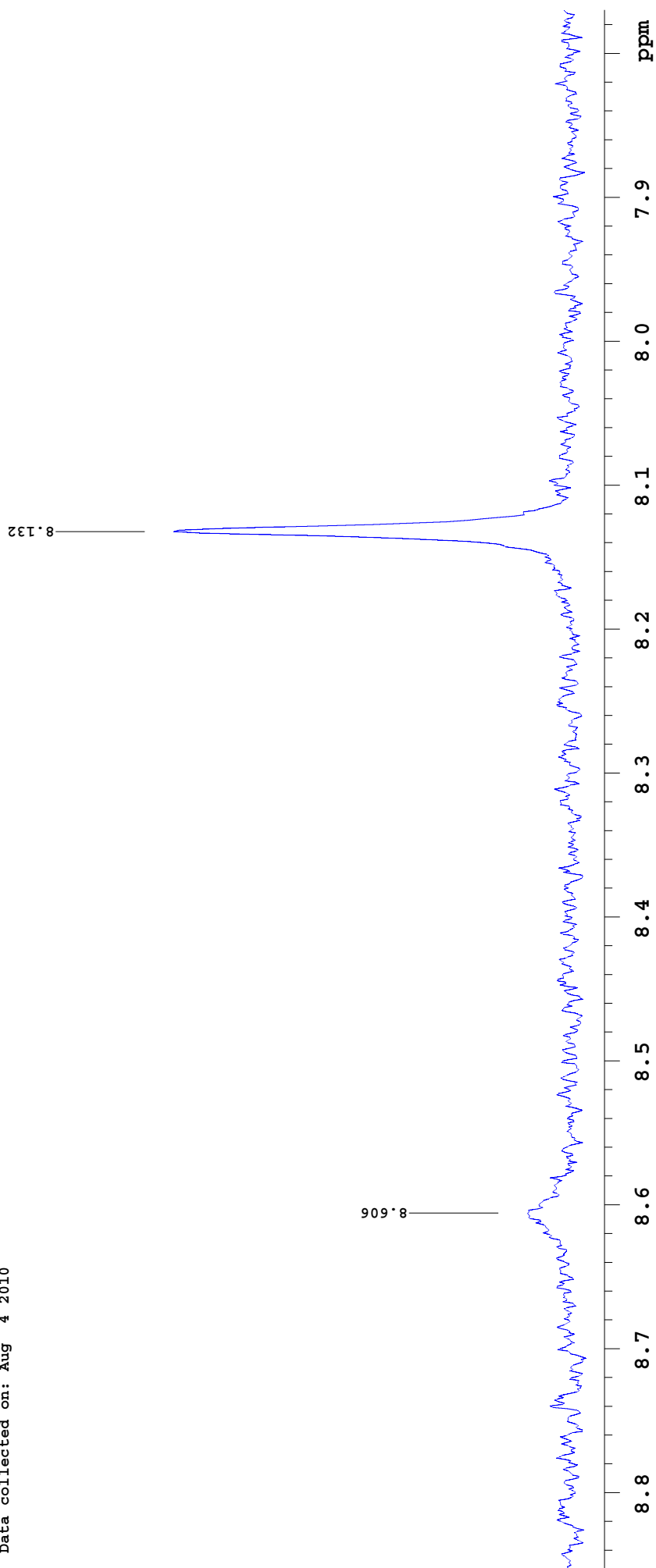
Sample directory:

FidFile: NOESY1D

Pulse Sequence: NOESY1D

Solvent: cd3od

Data collected on: Aug 4 2010

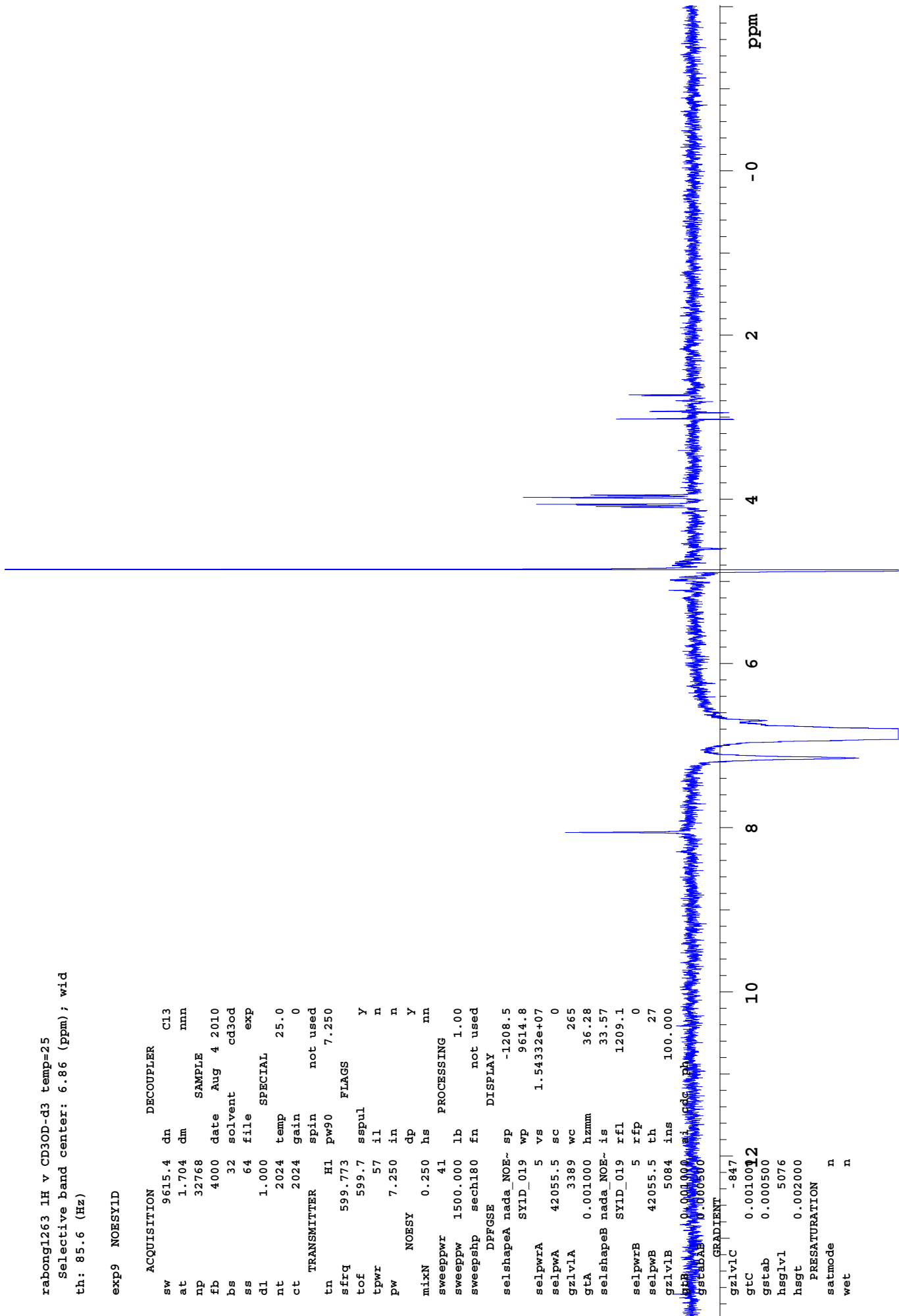




rabong1263 1H v CD3OD-d3 temp=25  
 Selective band center: 6.86 (ppm); wid  
 th: 85.6 (Hz)

exp9 NOESY1D

sw	9615.4	dn	Cl3
at	1.704	dm	mmn
np	32768		SAMPLE
fb	4000	date	Aug 4 2010
bs	32	solvent	cd3od
ss	64	file	exp
d1	1.000	SPECIAL	
nt	2024	temp	25.0
ct	2024	gain	0
		spn	not used
tn	H1	pw90	7.250
sfrq	599.773	FLAGS	
tof	599.7	sspul	Y
tpwr	57	il	n
pw	7.250	in	n
		dp	Y
mixN	0.250	hs	nn
sweepwr	41	PROCESSING	
sweeppw	1500.000	lb	1.00
sweepshp	sech180	fn	not used
		DPFGSE	DISPLAY
selshapeA	nada_NOE-	sp	-1208.5
SYID_019	wp		9614.8
selpwra	5	vs	1.54332e+07
selpwa	42055.5	sc	0
gzlvla	3389	wc	265
gtA	0.001000	hzmm	36.28
selshapeB	nada_NOE-	is	33.57
SYID_019	rfl		1209.1
selpwrb	5	rfp	0
selpwB	42055.5	th	27
gzlvLB	5084	ins	100.000
gtB	0.001000	mi	cdc
gstabAB	0.000500	ph	
		GRADIENT	-847
gzlvLC			
gtC	0.001000		12
gstab	0.000500		
hsglVL	5076		
hsgt	0.002000		
		PRESATURATION	
satmode	n		
wet	n		

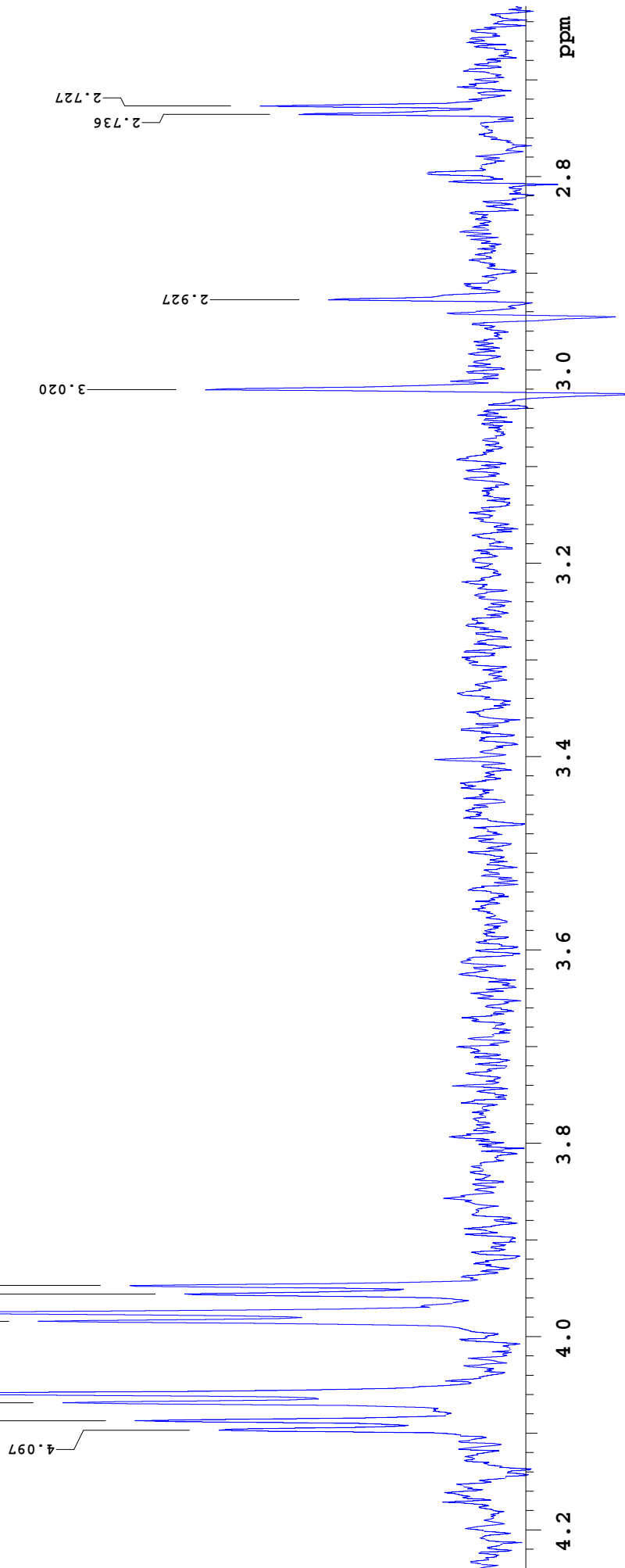


rabong1263 1H v CD3OD-d3 temp=25  
Selective band center: 6.86 (ppm); width: 85.6 (Hz)

Sample Name:

Data Collected on:  
Varian-NMR-vnmrs600  
Archive directory:

Sample directory: 0  
FidFile: NOESY1D 4 0.0000  
Pulse Sequence: NOESY1D 3 3.984  
Solvent: cd3od 3 3.975  
Data collected on: Aug 4 2016 3 3.916  
3 3.916  
3 3.916  
3 3.916



rabong1263 1H v CD3OD-d3 temp=25  
Selective band center: 6.86 (ppm); width: 85.6 (Hz)

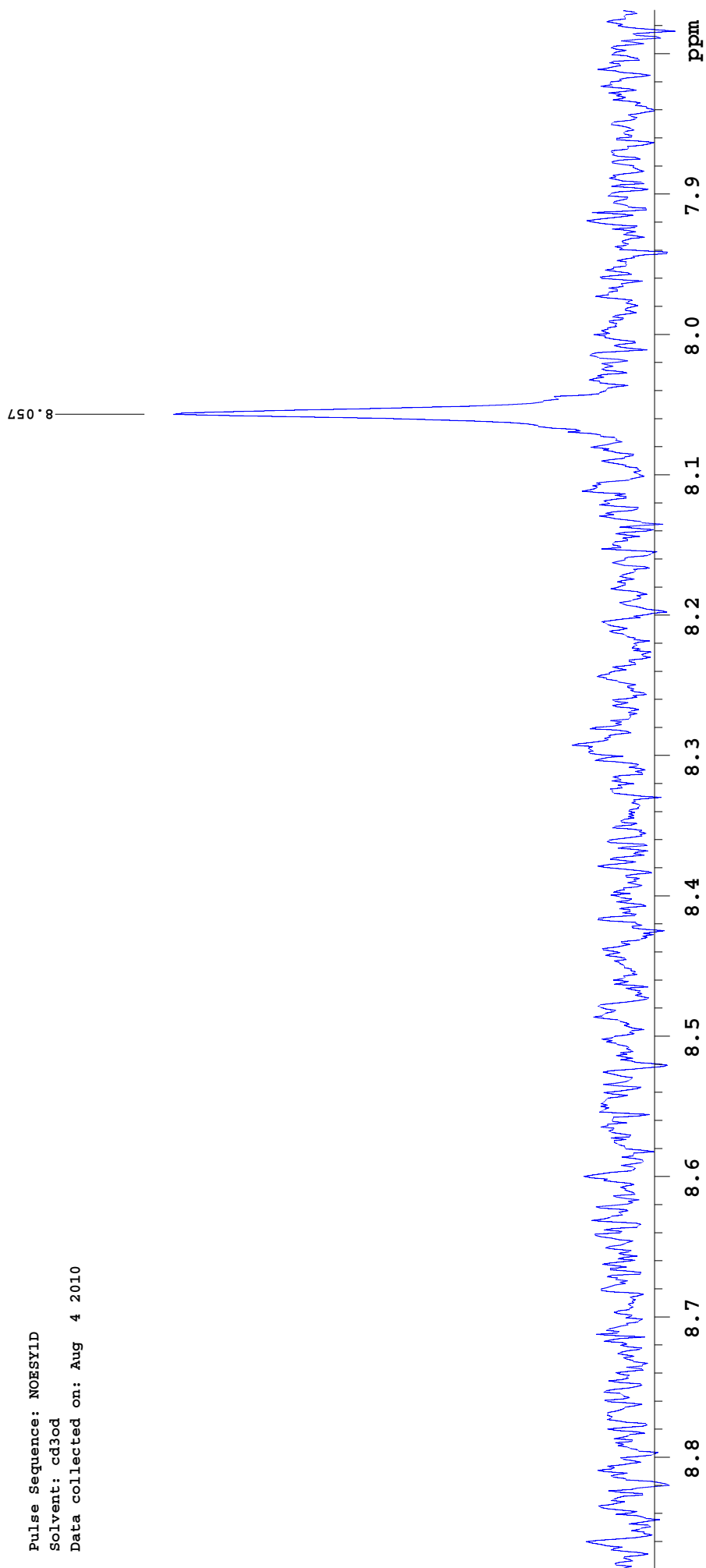
Sample Name:

Data Collected on:  
Varian-NMR-vnmrs600  
Archive directory:

Sample directory:

FidFile: NOESY1D

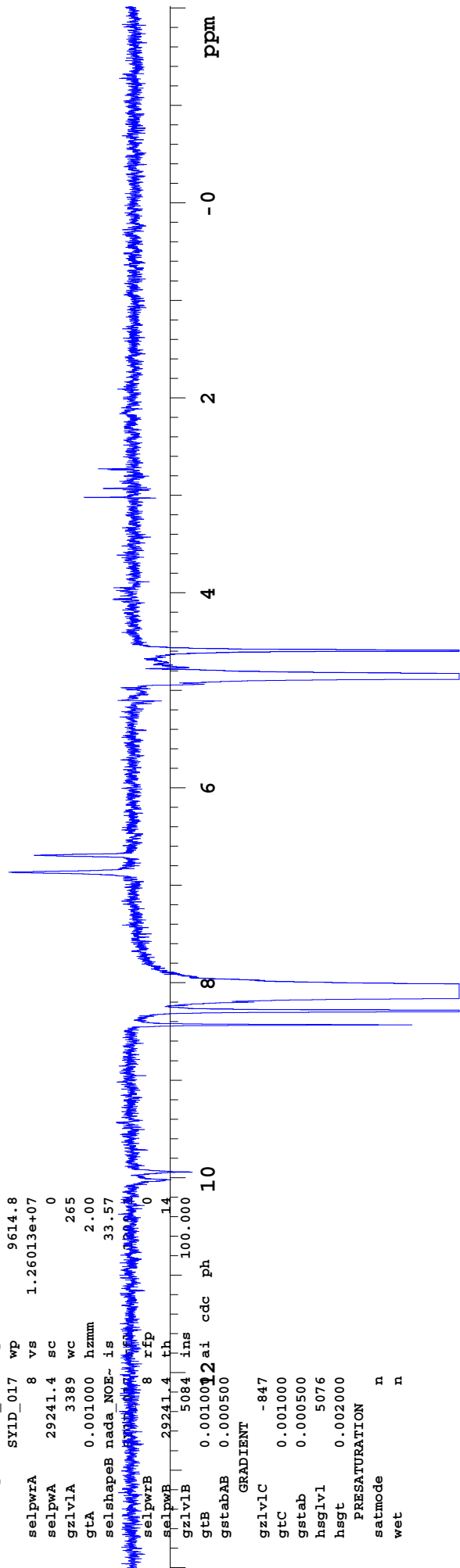
Pulse Sequence: NOESY1D  
Solvent: cd3od  
Data collected on: Aug 4 2010



rabong1263 1H v CD3OD-d3 temp=25  
 Selective band center: 8.10 (ppm); wid  
 th: 123.1 (Hz)

exp7 NOESY1D

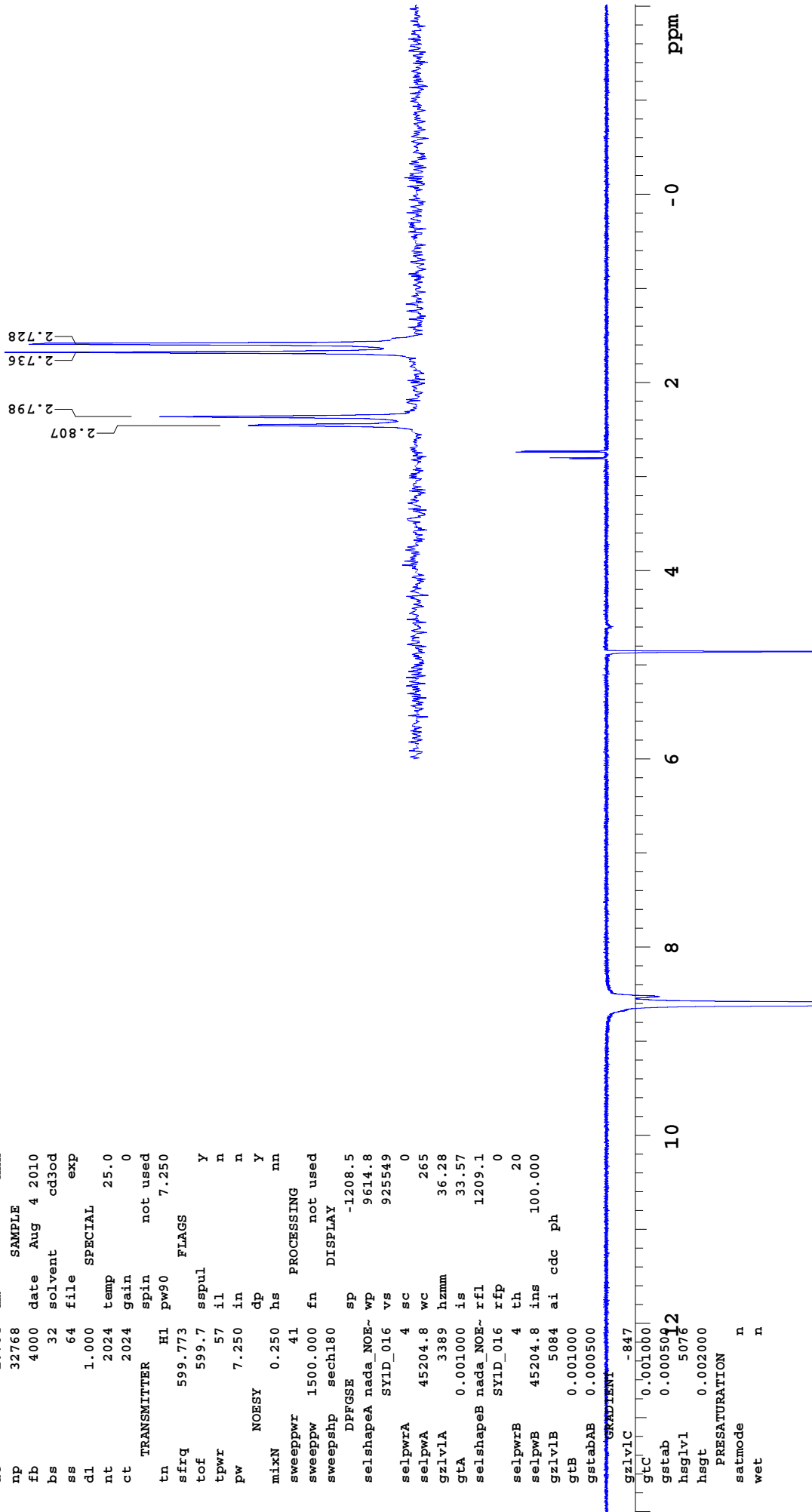
sw	9615.4	dn	C13
at	1.704	dm	mmn
np	32768		SAMPLE
fb	4000	date	Aug 4 2010
bs	32	solvent	cd3od
ss	64	file	exp
d1	1.000		SPECIAL
nt	2024	temp	25.0
ct	2024	gain	0
		spin	not used
tn	H1	pw90	7.250
sfrq	599.773		FLAGS
tof	599.7	sspul	Y
tpwr	57	il	n
pw	7.250	in	n
		dp	Y
mixN	0.250	hs	nn
sweppwr	41		PROCESSING
sweppw	1500.000	lb	1.00
sweepshp	sech180	fn	not used
			DPFGSE
selshapeA	nada_NOE-	sp	-1208.5
SYID	017	wp	9614.8
selpwrA	8	vs	1.26013e+07
selpwa	29241.4	sc	0
gzlv1A	3389	wc	265
gtA	0.001000	hzmm	2.00
selshapeB	nada_NOE-	is	33.57
selpwrB	8	rfp	0
selpwb	29241.4	th	14
gzlv1B	5084	ins	100.000
gtB	0.001000	ai	cdc
gstabAB	0.000500	ph	10
			GRADIENT
gzlv1C	-847		
gtC	0.001000		
gstab	0.000500		
hsglv1	5076		
hsgt	0.002000		
			PRESATURATION
satmode	n		
wet	n		

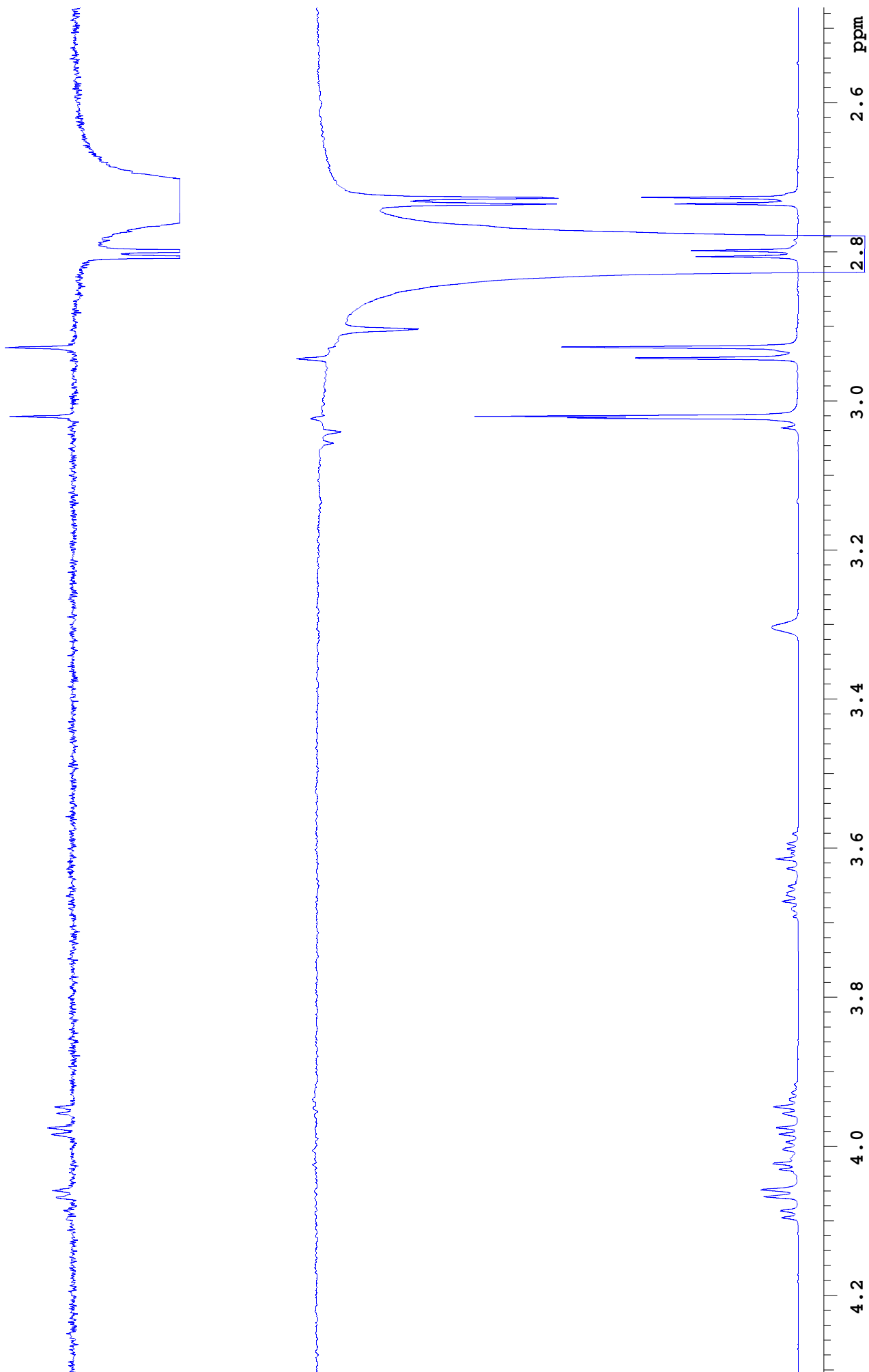


rabong1263 1H v CD30D-d3 temp=25  
 Selective band center: 8.61 (ppm); wid  
 th: 79.6 (Hz)

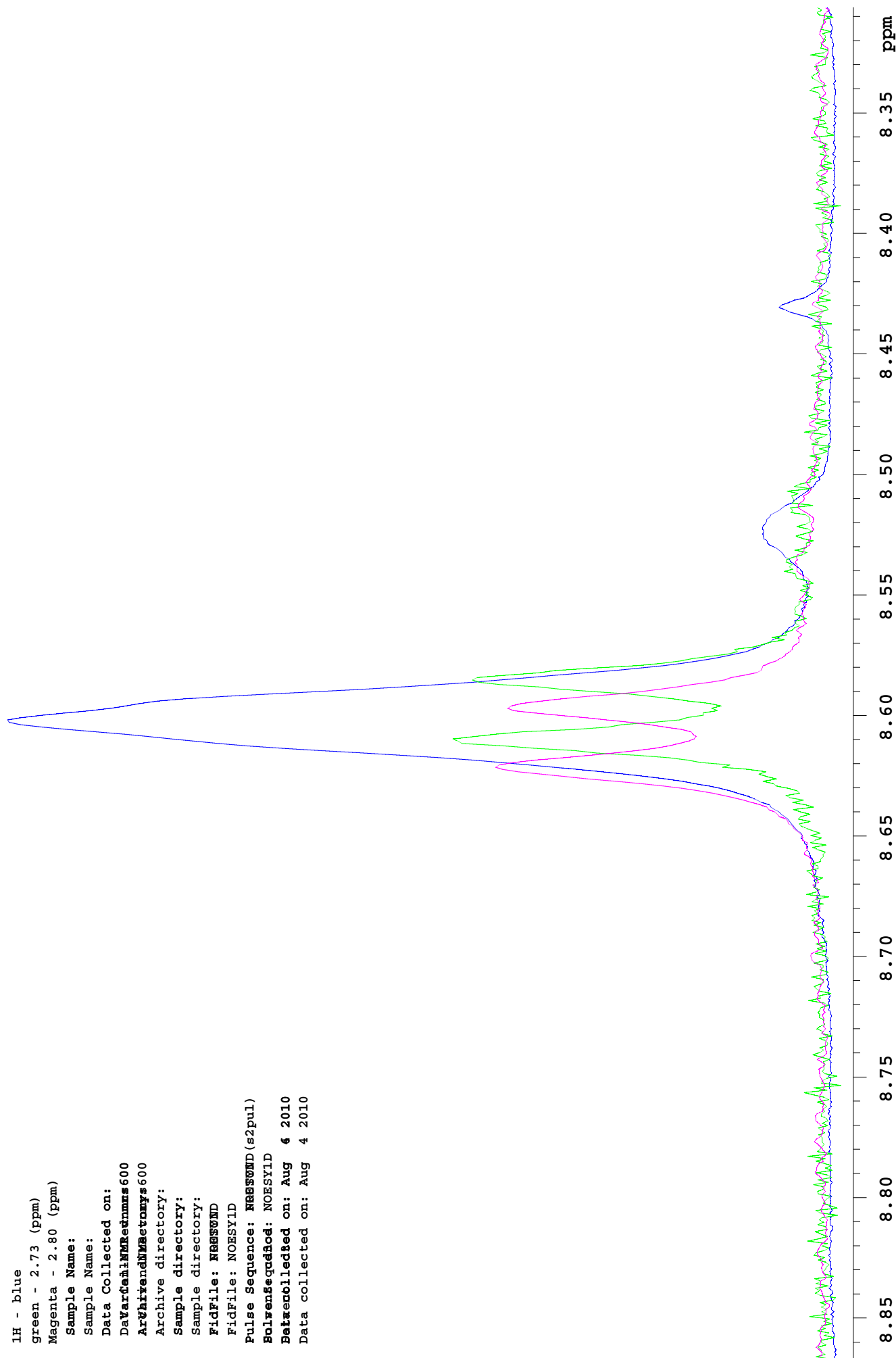
exp6 NOESY1D

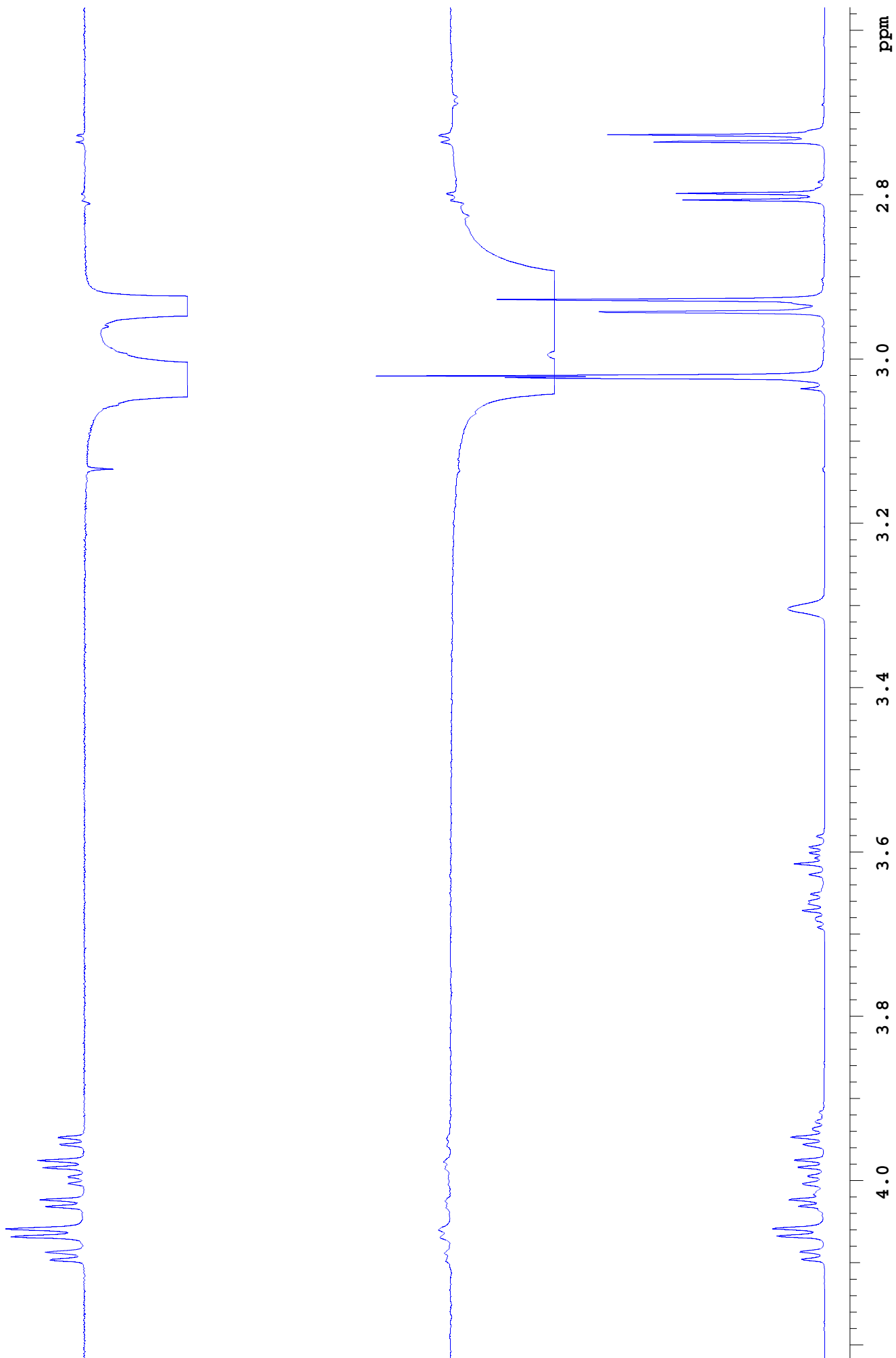
sw	9615.4	dn	C13
at	1.704	dm	mmn
np	32768		SAMPLE
fb	4000	date	Aug 4 2010
bs	32	solvent	cd3od
ss	64	file	exp
d1	1.000	SPECIAL	
nt	2024	temp	25.0
ct	2024	gain	0
TRANSMITTER			
tn	H1	pw90	7.250
sfrq	599.773	spin	not used
tof	599.7	sspul	Y
tpwr	57	il	n
pw	7.250	in	n
NOESY			
mixN	0.250	hs	nn
sweepwr	41	PROCESSING	
sweepppw	1500.000	fn	not used
sweepshp	sech180	DISPLAY	
DPFGSE			
selshapeA	nada_NOE-	wp	-1208.5
SYID_016	vs		9614.8
			925549
selpwrA	4	sc	0
selpwa	45204.8	wc	265
gzlv1A	3389	hzmm	36.28
gtA	0.001000	is	33.57
selshapeB	nada_NOE-	rfl	1209.1
SYID_016	rfp		0
selpwrB	4	th	20
selpwb	45204.8	ins	100.000
gzlv1B	5084	ai	cdc ph
gtB	0.001000		
gstabAB	0.000500		
GRADIENT			
gzlv1C	-847		
gtC	0.001000		
gstab	0.000500	12	
hsglv1	5076		
hsgt	0.002000		
PRESATURATION			
satmode	n		
wet	n		





1H - blue  
green - 2.73 (ppm)  
Magenta - 2.80 (ppm)  
Sample Name:  
Sample Name:  
Data Collected on:  
Data Collected on:  
Archive directory:  
Archive directory:  
Sample directory:  
Sample directory:  
FidFile: **NOESYD**  
FidFile: **NOESYD**  
Pulse Sequence: **NOESYD (s2pul)**  
Pulse Sequence: **NOESYD**  
Data collected on: Aug 6 2010  
Data collected on: Aug 4 2010







FK70 water 17C  
dpwgse\_water

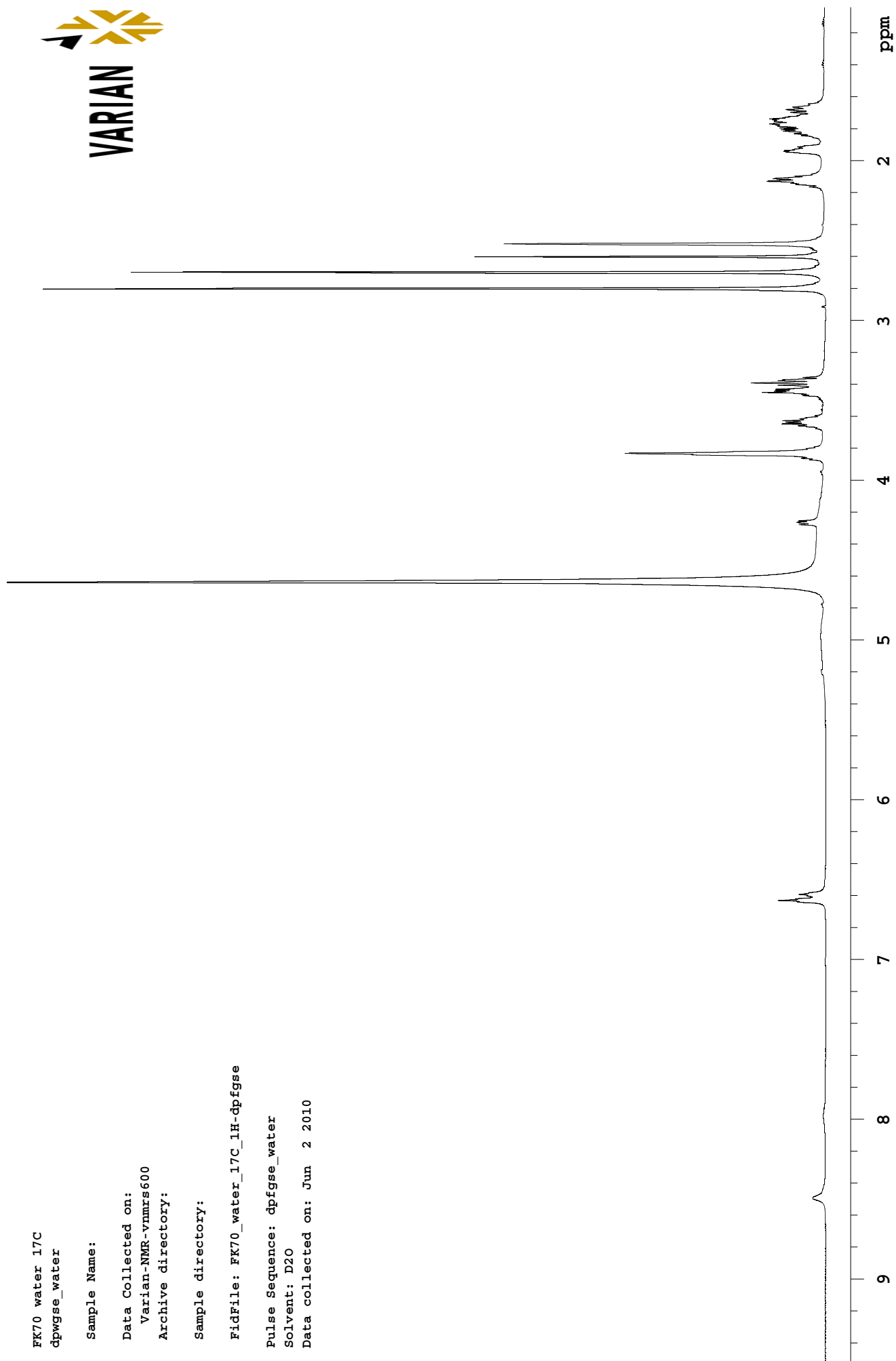
Sample Name:

Data Collected on:  
Varian-NMR-vnmrs600  
Archive directory:

Sample directory:

FidFile: FK70\_water\_17C\_1H-dpfgse

Pulse Sequence: dpfgse\_water  
Solvent: D2O  
Data collected on: Jun 2 2010



FK70 water 17C  
dpwgse\_water

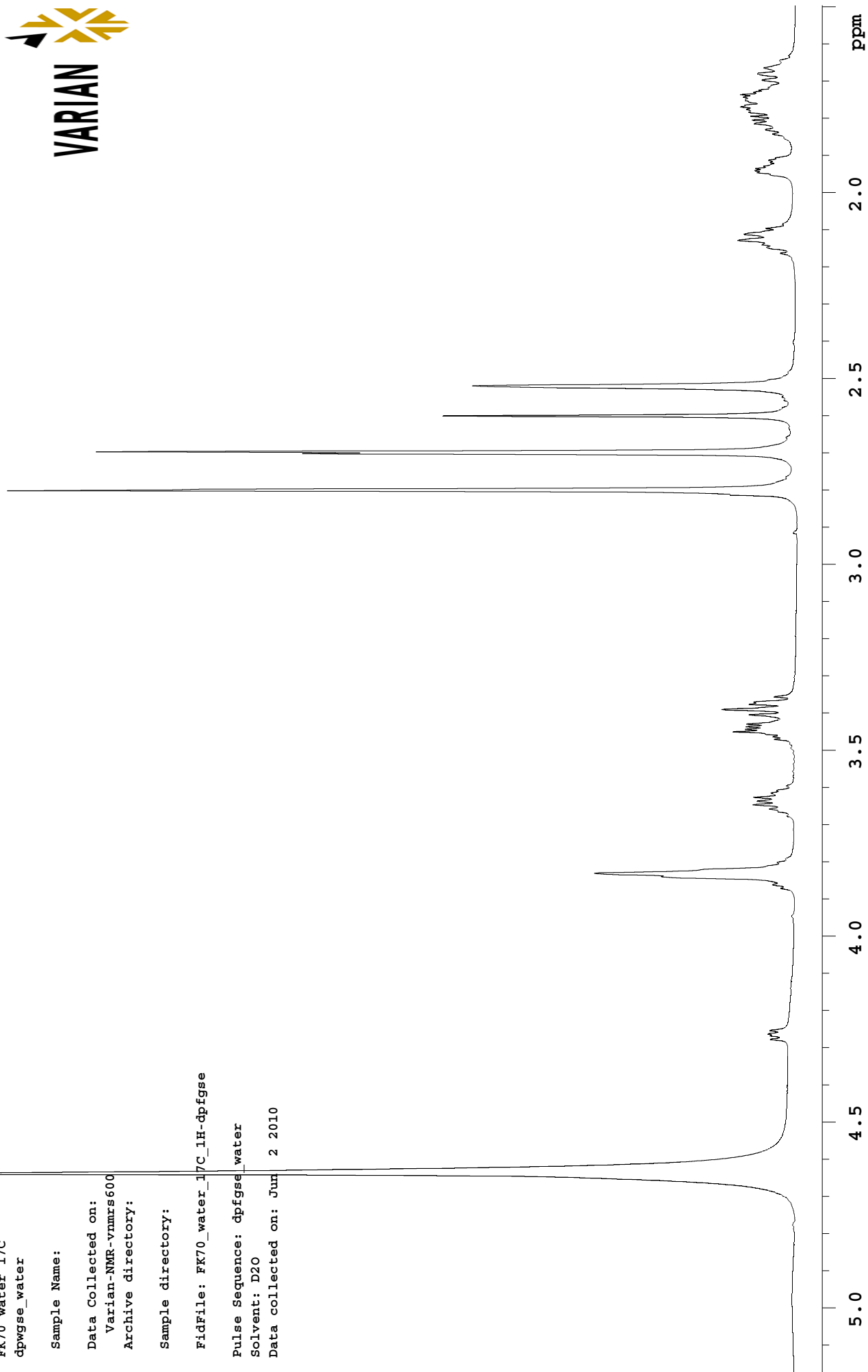
Sample Name:

Data Collected on:  
Varian-NMR-vnmrs600  
Archive directory:

Sample directory:

FidFile: FK70\_water\_17C\_1H-dpfgse

Pulse Sequence: dpfgse\_water  
Solvent: D2O  
Data collected on: Jun 2 2010



DRX-500: 1H with presaturation of JP-170 (H2O/D2O=9/1, 290K)

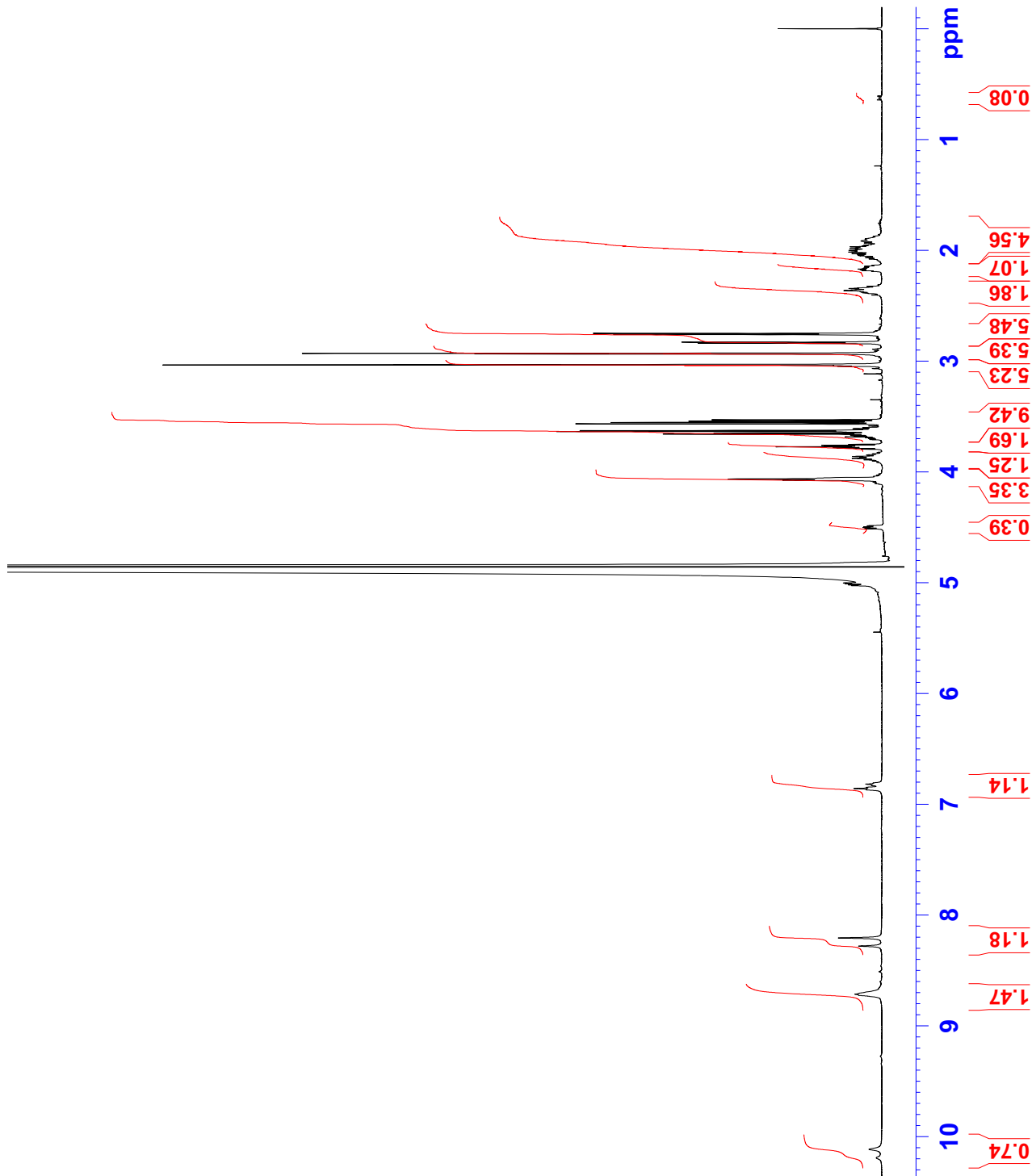


Current Data Parameters  
NAME NB\_JP-170  
EXPNO 51  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20070321  
Time\_ 15.14  
INSTRUM spect  
PROBHD 5 mm BBI 1H/2H  
PULPROG zgpr.ok  
TD 32768  
SOLVENT H2O  
NS 128  
DS 2  
SWH 10000.000 Hz  
FIDRES 0.305176 Hz  
AQ 1.6385000 sec  
RG 32  
DW 50.000 use  
DE 6.00 use  
TE 290.0 K  
D1 3.00000000 sec  
d12 0.0002000 sec  
d13 0.00000300 sec

==== CHANNEL f1 =====  
NUC1 1H  
P1 7.25 use  
PL1 0.00 dB  
PL9 55.00 dB  
SFO1 500.2523524 MHz

F2 - Processing parameters  
SI 65536  
SF 500.2499213 MHz  
WDW no  
SSB 0  
LB 0.00 Hz  
GB 0  
PC 1.00



DRX-500: 1H with presaturation of JP-170 (H2O/D2O=9/1, 290K)

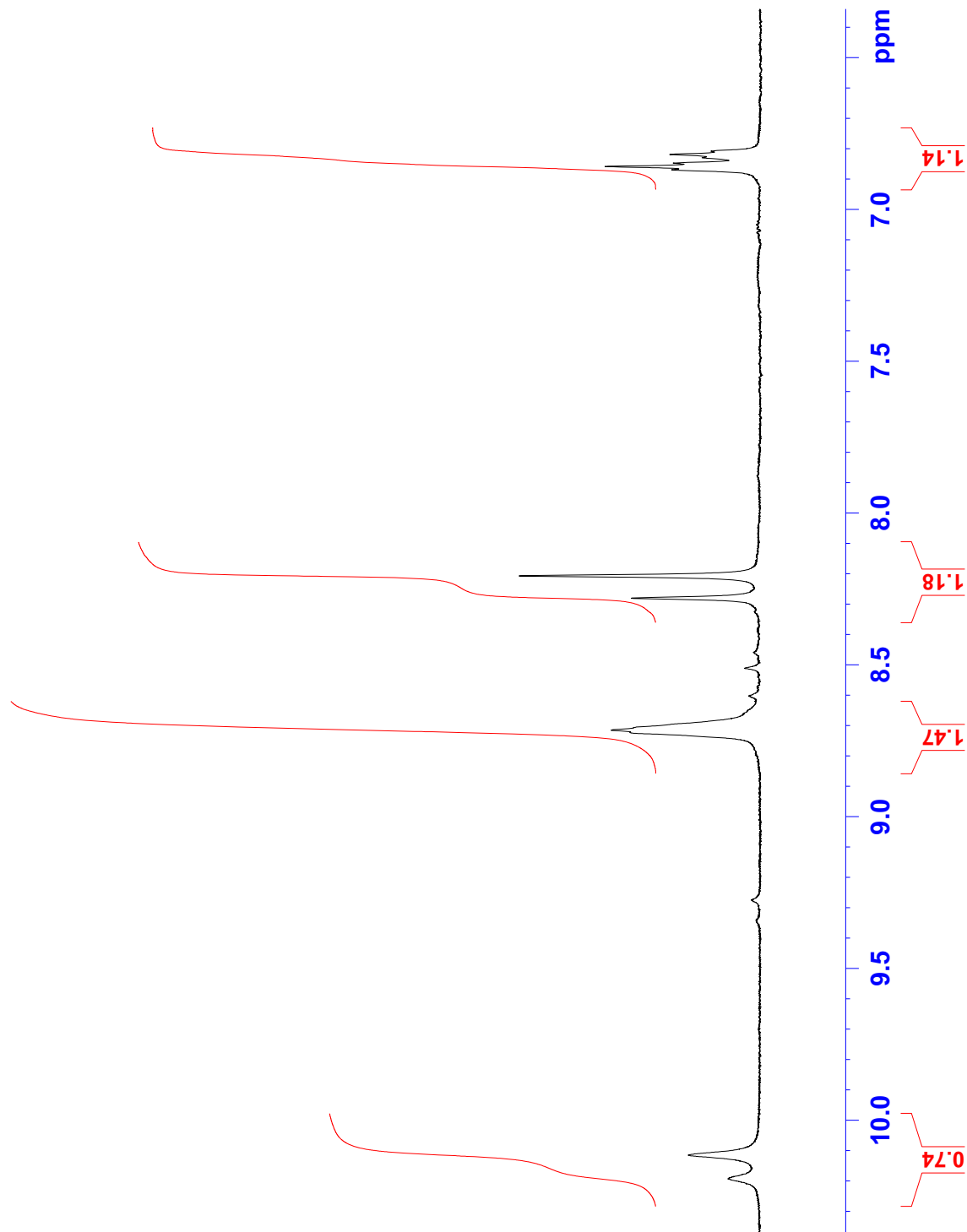


Current Data Parameters  
NAME NB\_JP-170  
EXPNO 51  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20070321  
Time\_ 15.14  
INSTRUM spect  
PROBHD 5 mm BBI 1H/2H  
PULPROG ZGPR.ok  
TD 32768  
SOLVENT H2O  
NS 128  
DS 2  
SWH 10000.000 Hz  
FIDRES 0.305176 Hz  
AQ 1.6385000 sec  
RG 32  
DW 50.000 use  
DE 6.00 use  
TE 290.0 K  
D1 3.00000000 sec  
d12 0.00002000 sec  
d13 0.00000300 sec

==== CHANNEL f1 =====  
NUC1 1H  
P1 7.25 use  
PL1 0.00 dB  
PL9 55.00 dB  
SFO1 500.2523524 MHz

F2 - Processing parameters  
SI 65536  
SF 500.2499213 MHz  
WDW no  
SSB 0  
LB 0.00 Hz  
GB 0  
PC 1.00



DRX-500: 1H with presaturation of JP-170 (H2O/D2O=9/1, 290K)

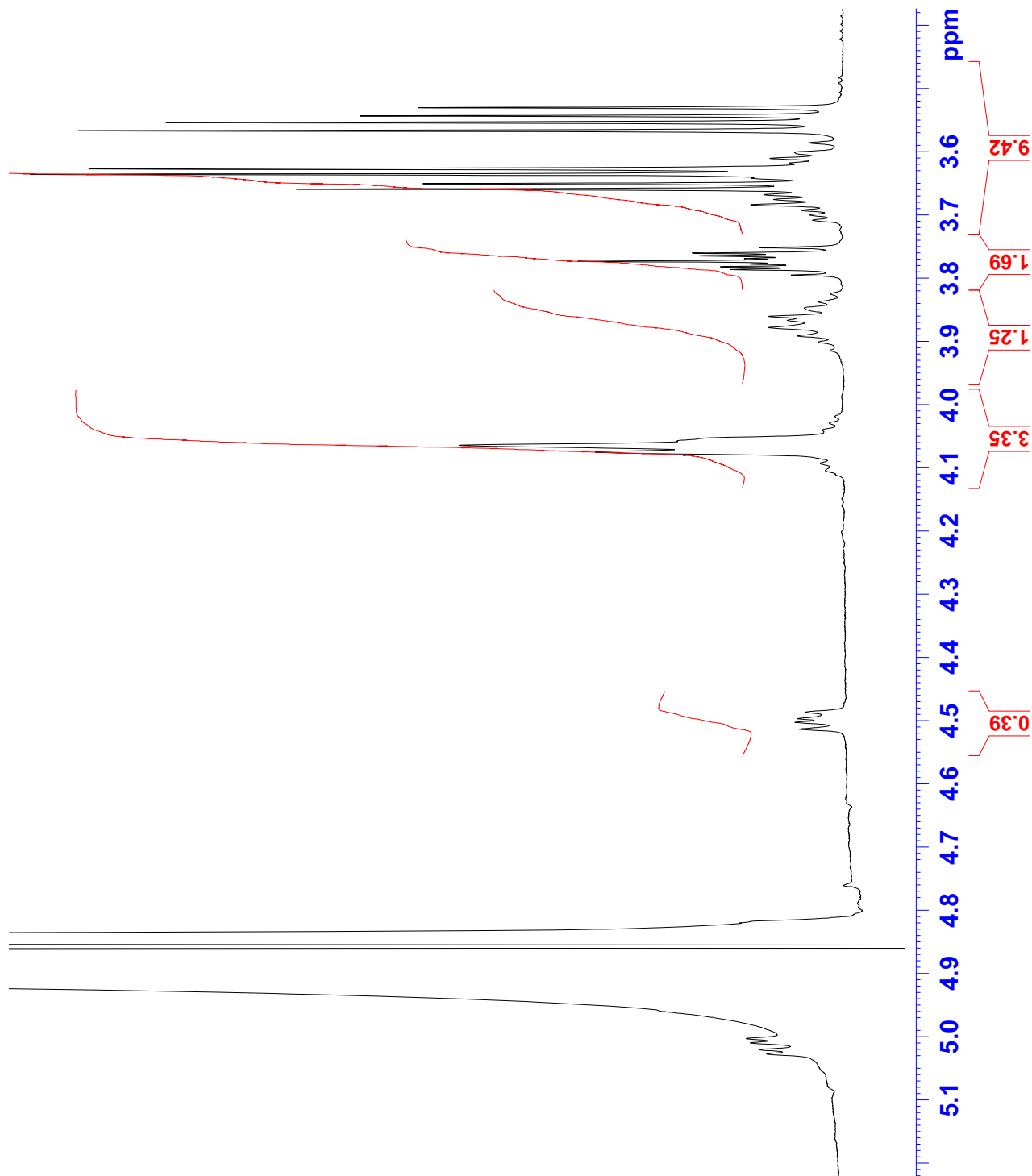


Current Data Parameters  
NAME NB\_JP-170  
EXPNO 51  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20070321  
Time\_ 15.14  
INSTRUM spect  
PROBHD 5 mm BBI 1H/2H  
PULPROG zgpr.ok  
TD 32768  
SOLVENT H2O  
NS 128  
DS 2  
SWH 10000.000 Hz  
FIDRES 0.305176 Hz  
AQ 1.6385000 sec  
RG 32  
DW 50.000 use  
DE 6.00 use  
TE 290.0 K  
D1 3.00000000 sec  
d12 0.0002000 sec  
d13 0.00000300 sec

==== CHANNEL f1 =====  
NUC1 1H  
P1 7.25 use  
PL1 0.00 dB  
PL9 55.00 dB  
SFO1 500.2523524 MHz

F2 - Processing parameters  
SI 65536  
SF 500.2499213 MHz  
WDW no  
SSB 0  
LB 0.00 Hz  
GB 0  
PC 1.00



DRX-500: 1H with presaturation of JP-170 (H2O/D2O=9/1, 290K)

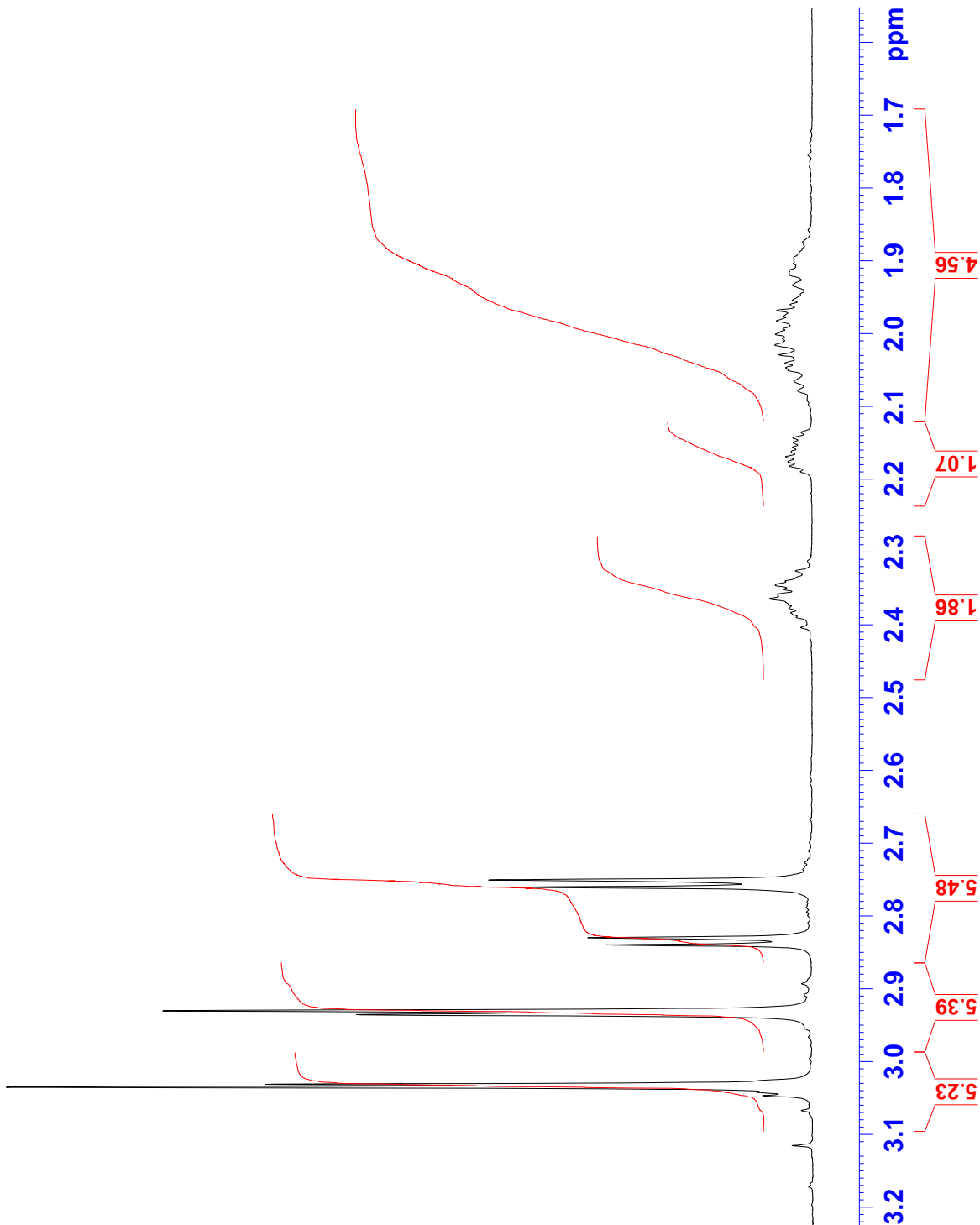


Current Data Parameters  
NAME NB\_JP-170  
EXPNO 51  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20070321  
Time\_ 15.14  
INSTRUM spect  
PROBHD 5 mm BBI 1H/2H  
PULPROG zgpgpr.ok  
TD 32768  
SOLVENT H2O  
NS 128  
DS 2  
SWH 10000.000 Hz  
FIDRES 0.305176 Hz  
AQ 1.6385000 sec  
RG 32  
DW 50.000 use  
DE 6.00 use  
TE 290.0 K  
D1 3.00000000 sec  
d12 0.00002000 sec  
d13 0.00000300 sec

==== CHANNEL f1 =====  
NUC1 1H  
P1 7.25 use  
PL1 0.00 dB  
PL9 55.00 dB  
SFO1 500.2523524 MHz

F2 - Processing parameters  
SI 65536  
SF 500.2499213 MHz  
WDW no  
SSB 0  
LB 0.00 Hz  
GB 0  
PC 1.00



DRX-500: DQF-COSY with presaturation of JP-170 (H2O/D2O=9/1, 290K)

Current Data Parameters  
 NAME NB\_JP-170  
 EXPNO 500  
 PROCNO 1

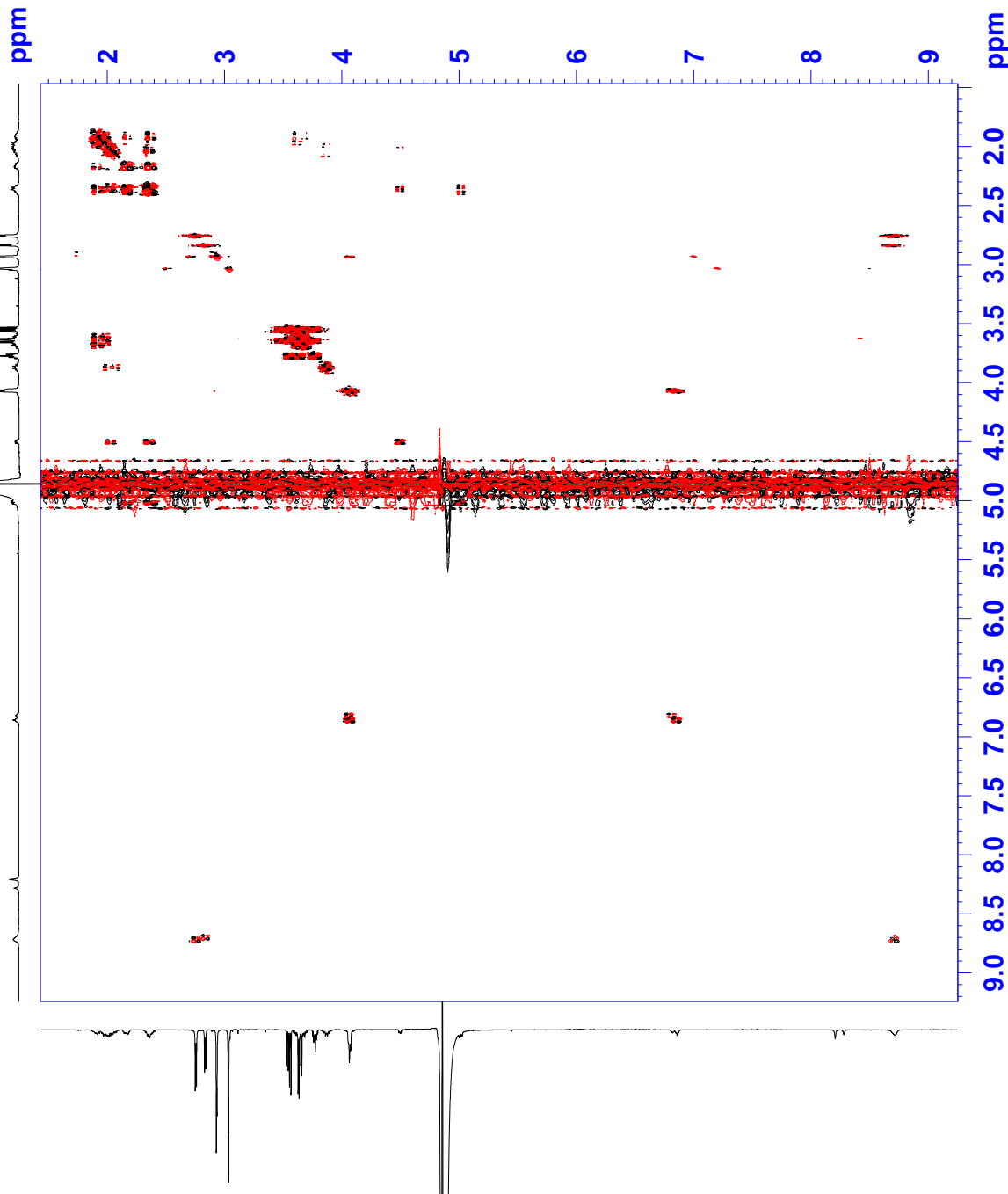
F2 - Acquisition Parameters  
 Date 500000  
 INSTRUM spect  
 PULPROG COSY\_dfstpr.ok  
 TD 4096  
 NS 8  
 SWH 6009.615 Hz  
 AQ 0.3409204 sec  
 RG 16  
 d0 0.00000300 sec  
 d11 0.03000000 sec  
 d12 0.00002000 sec  
 d13 0.00000300 sec  
 L3 256

==== CHANNEL f1 =====

F1 - Acquisition parameters  
 ND0 1  
 TD 512  
 SFO1 500.2524 MHz  
 FIDRES 11.723439 Hz  
 SW 11.999 ppm  
 FMODE undefined

F2 - Processing parameters  
 SI 4096  
 SF 500.2499213 MHz  
 WDW SINE  
 SSB 2  
 LB 0.00 Hz  
 GB 0  
 PC 1.00

F1 - Processing parameters  
 SI 1024  
 MC2 States-TpPI  
 SF 500.2499213 MHz  
 WDW SINE  
 SSB 2  
 LB 0.00 Hz  
 GB 0



DRX-500: DQF-COSY with presaturation of JP-170 (H2O/D2O=9/1, 290K)

```
Current Data Parameters
NAME      NB_JP-170
EXPNO    500
PROCNO    1

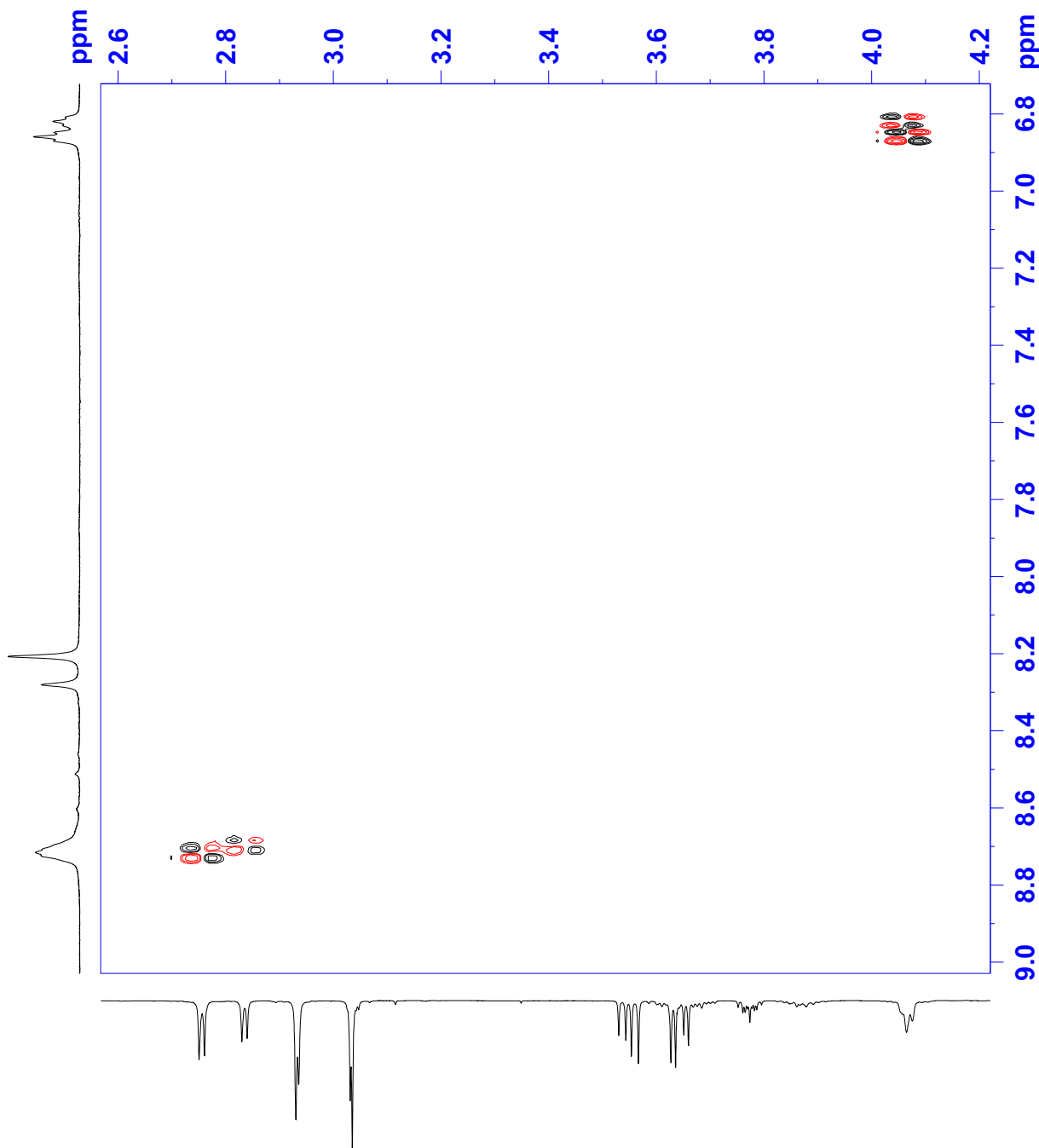
F2 - Acquisition Parameters
Date      500000
INSTRUM   spect
PULPROG   COSY_dfstpr.ok
TD        4096
NS        8
SWH       6009.615 Hz
AQ        0.3409204 sec
RG        16
d0        0.00000300 sec
d11       0.03000000 sec
d12       0.00002000 sec
d13       0.00000300 sec
l3        256

===== CHANNEL f1 =====

F1 - Acquisition parameters
ND0       1
TD        512
SFO1      500.2524 MHz
FIDRES    11.723439 Hz
SW        11.999 ppm
FnMODE    undefined

F2 - Processing parameters
SI        4096
SF        500.2499213 MHz
WDW       SINE
SSB       2
LB        0.00 Hz
GB        0
PC        1.00

F1 - Processing parameters
SI        1024
MC2       States-TpPI
SF        500.2499213 MHz
WDW       SINE
SSB       2
LB        0.00 Hz
GB        0
```





DRX-500: DQF-COSY with presaturation of JP-170 (H<sub>2</sub>O/D<sub>2</sub>O=9/1, 290K)

```

Current Data Parameters
NAME      NB_JP-170
EXPNO    500
PROCNO   1

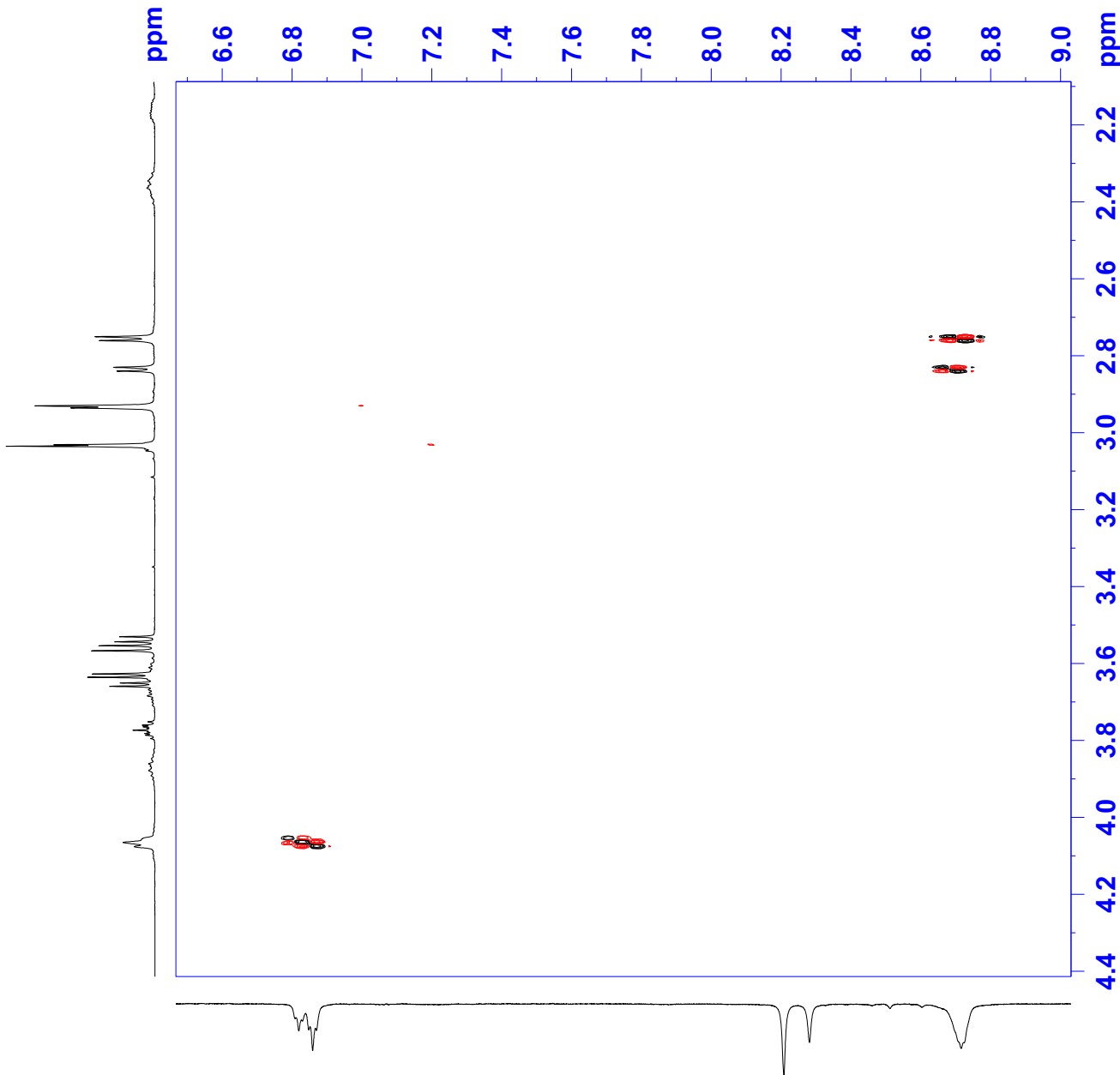
F2 - Acquisition Parameters
Date      500000
INSTRUM  spect
PULPROG  COSY_dfstpr.ok
TD        4096
NS        8
SWH       6009.615 Hz
AQ        0.3409204 sec
RG        16
d0        0.00000300 sec
d11       0.03000000 sec
d12       0.00002000 sec
d13       0.00000300 sec
l3        256

===== CHANNEL f1 =====

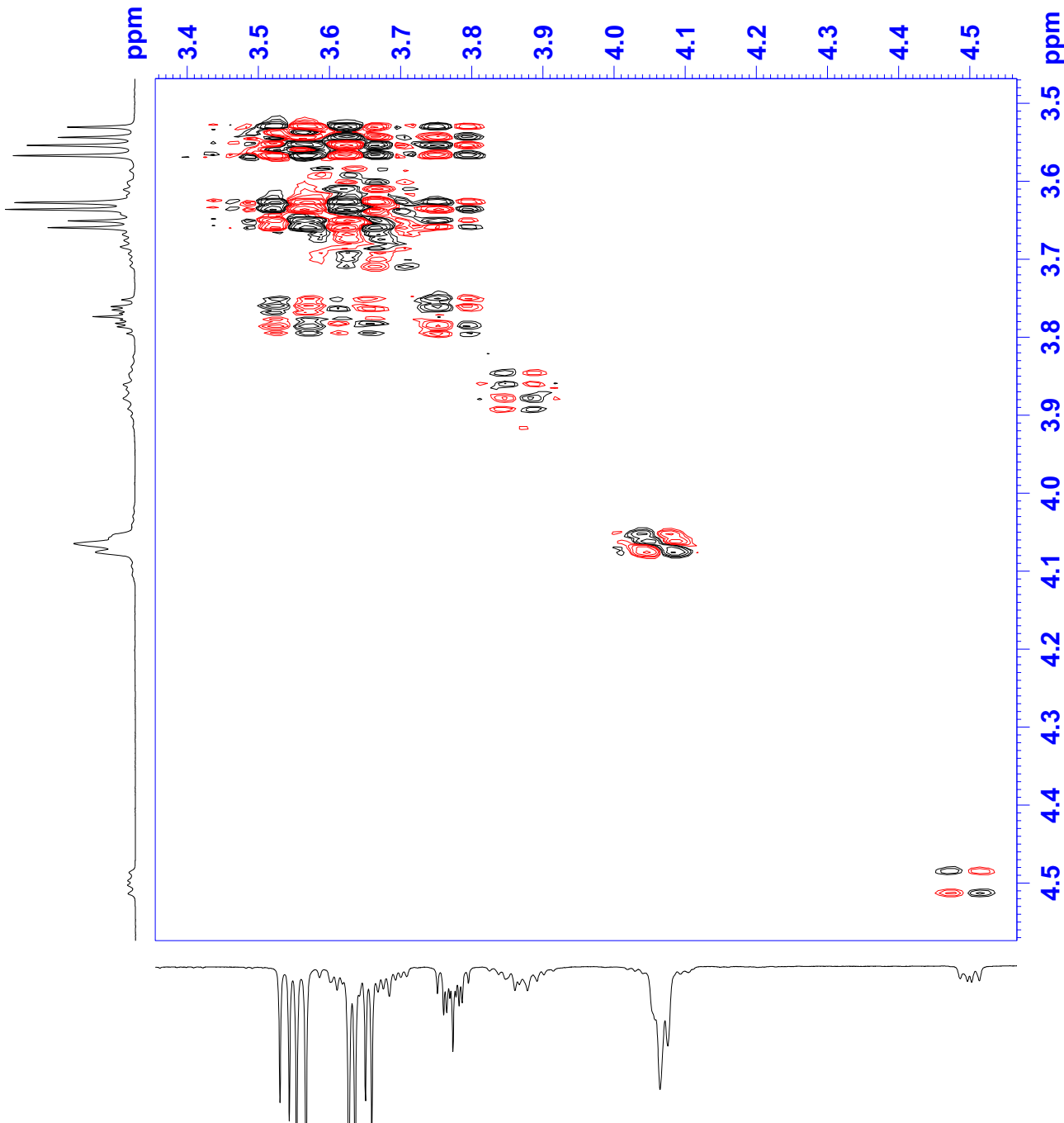
F1 - Acquisition parameters
ND0       1
TD        512
SFO1      500.2524 MHz
FIDRES    11.723439 Hz
SW        11.999 ppm
FnMODE    undefined

F2 - Processing parameters
SI        4096
SF        500.2499213 MHz
WDW       SINE
SSB       2
LB        0.00 Hz
GB        0
PC        1.00

F1 - Processing parameters
SI        1024
MC2       States-TpPI
SF        500.2499213 MHz
WDW       SINE
SSB       2
LB        0.00 Hz
GB        0
    
```



DRX-500: DQF-COSY with presaturation of JP-170 (H2O/D2O=9/1, 290K)



Current Data Parameters  
 NAME NB\_JP-170  
 EXPNO 500  
 PROCNO 1

F2 - Acquisition Parameters  
 Date 500000  
 INSTRUM spect  
 PULPROG COSY\_dfstpr.ok  
 TD 4096  
 NS 8  
 SWH 6009.615 Hz  
 AQ 0.3409204 sec  
 RG 16  
 d0 0.00000300 sec  
 d11 0.03000000 sec  
 d12 0.00002000 sec  
 d13 0.00000300 sec  
 L3 256

==== CHANNEL f1 =====

F1 - Acquisition parameters  
 ND0 1  
 TD 512  
 SFO1 500.2524 MHz  
 FIDRES 11.723439 Hz  
 SW 11.999 ppm  
 FMODE undefined

F2 - Processing parameters  
 SI 4096  
 SF 500.2499213 MHz  
 WDW SINE  
 SSB 2  
 LB 0.00 Hz  
 GB 0  
 PC 1.00

F1 - Processing parameters  
 SI 1024  
 MC2 States-TpPI  
 SF 500.2499213 MHz  
 WDW SINE  
 SSB 2  
 LB 0.00 Hz  
 GB 0

DRX-500: DQF-COSY with presaturation of JP-170 (H2O/D2O=9/1, 290K)

```
Current Data Parameters
NAME      NB_JP-170
EXPNO    500
PROCNO   1

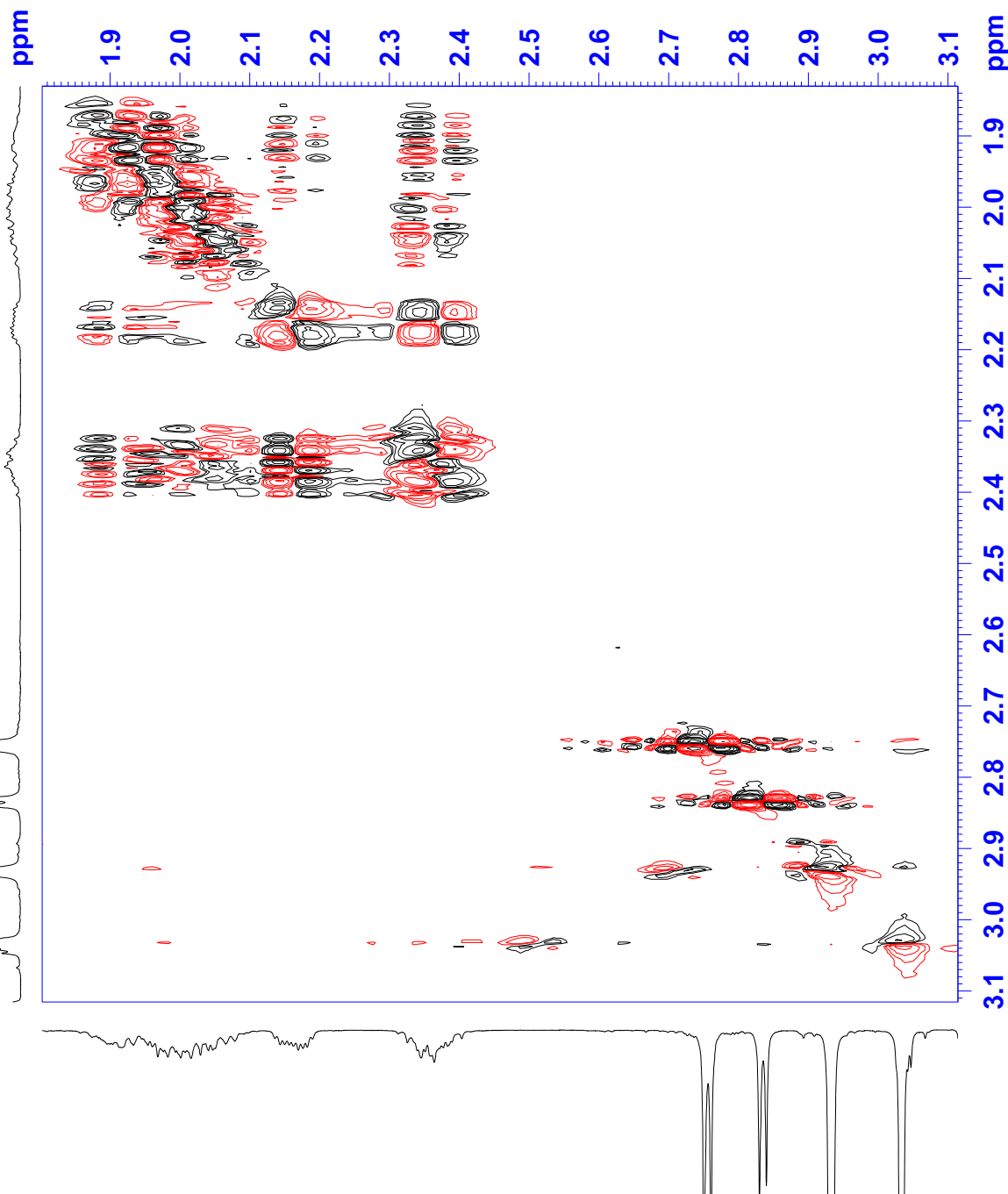
F2 - Acquisition Parameters
Date      500000
INSTRUM  spect
PULPROG  COSY_dfstpr.ok
TD        4096
NS        8
SWH       6009.615 Hz
AQ        0.3409204 sec
RG        16
d0        0.00000300 sec
d11       0.03000000 sec
d12       0.0002000 sec
d13       0.00000300 sec
l3        256

===== CHANNEL f1 =====

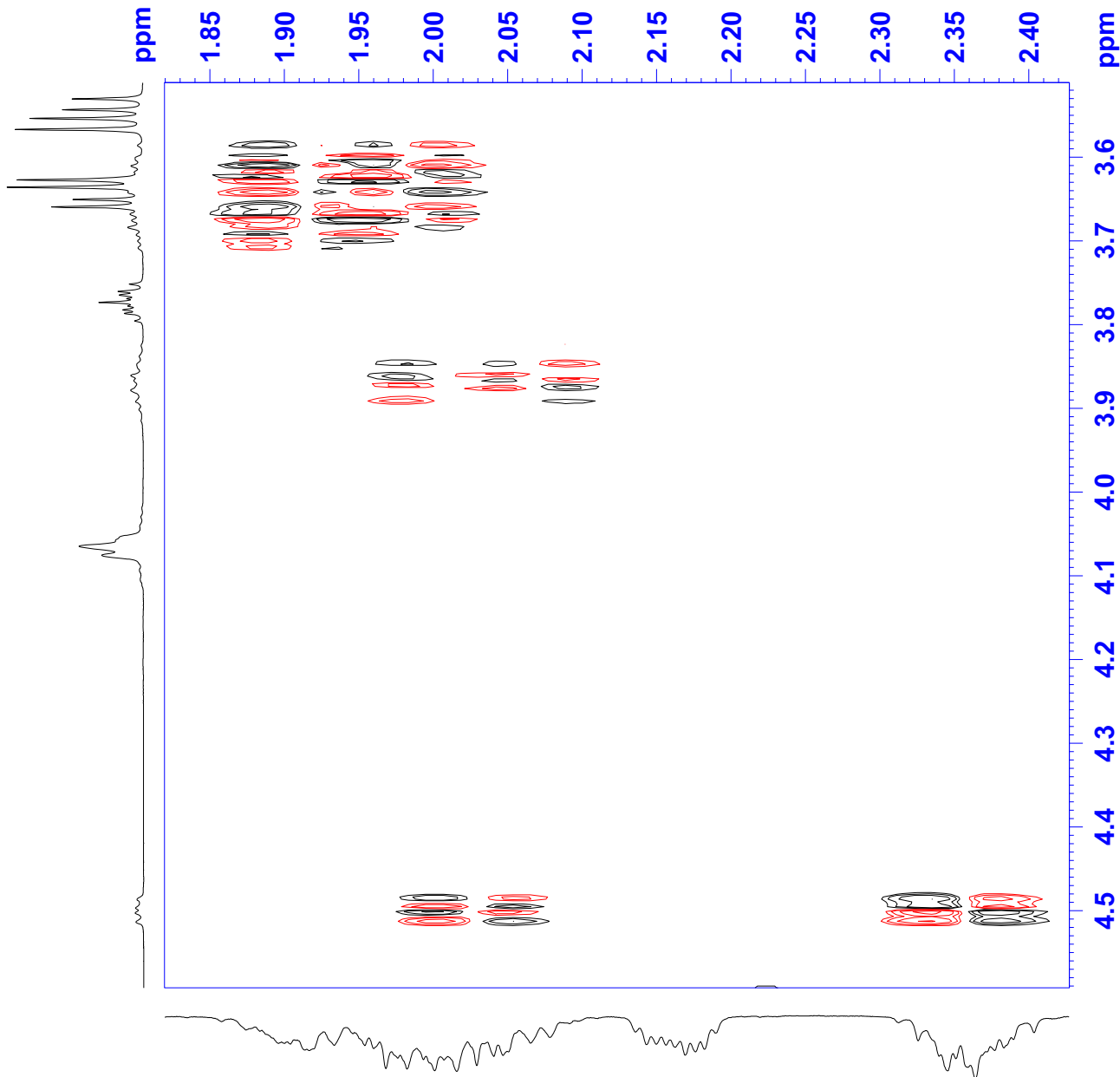
F1 - Acquisition parameters
ND0       1
TD        512
SFO1      500.2524 MHz
FIDRES    11.723439 Hz
SW        11.999 ppm
FnMODE    undefined

F2 - Processing parameters
SI        4096
SF        500.2499213 MHz
WDW       SINE
SSB       2
LB        0.00 Hz
GB        0
PC        1.00

F1 - Processing parameters
SI        1024
MC2       States-TpPI
SF        500.2499213 MHz
WDW       SINE
SSB       2
LB        0.00 Hz
GB        0
```



DRX-500: DQF-COSY with presaturation of JP-170 (H2O/D2O=9/1, 290K)



Current Data Parameters  
 NAME NB\_JP-170  
 EXPNO 500  
 PROCNO 1

F2 - Acquisition Parameters  
 Date 500000  
 INSTRUM spect  
 PULPROG COSY\_dfstpr.ok  
 TD 4096  
 NS 8  
 SWH 6009.615 Hz  
 AQ 0.3409204 sec  
 RG 16  
 d0 0.00000300 sec  
 d11 0.03000000 sec  
 d12 0.00002000 sec  
 d13 0.00000300 sec  
 l3 256

==== CHANNEL f1 =====

F1 - Acquisition parameters  
 ND0 1  
 TD 512  
 SFO1 500.2524 MHz  
 FIDRES 11.723439 Hz  
 SW 11.999 ppm  
 FMODE undefined

F2 - Processing parameters  
 SI 4096  
 SF 500.2499213 MHz  
 WDW SINE  
 SSB 2  
 LB 0.00 Hz  
 GB 0  
 PC 1.00

F1 - Processing parameters  
 SI 1024  
 MC2 States-TpPI  
 SF 500.2499213 MHz  
 WDW SINE  
 SSB 2  
 LB 0.00 Hz  
 GB 0

DRX-500: DQF-COSY with presaturation of JP-170 (H2O/D2O=9/1, 290K)

```
Current Data Parameters
NAME      NB_JP-170
EXPNO     500
PROCNO    1

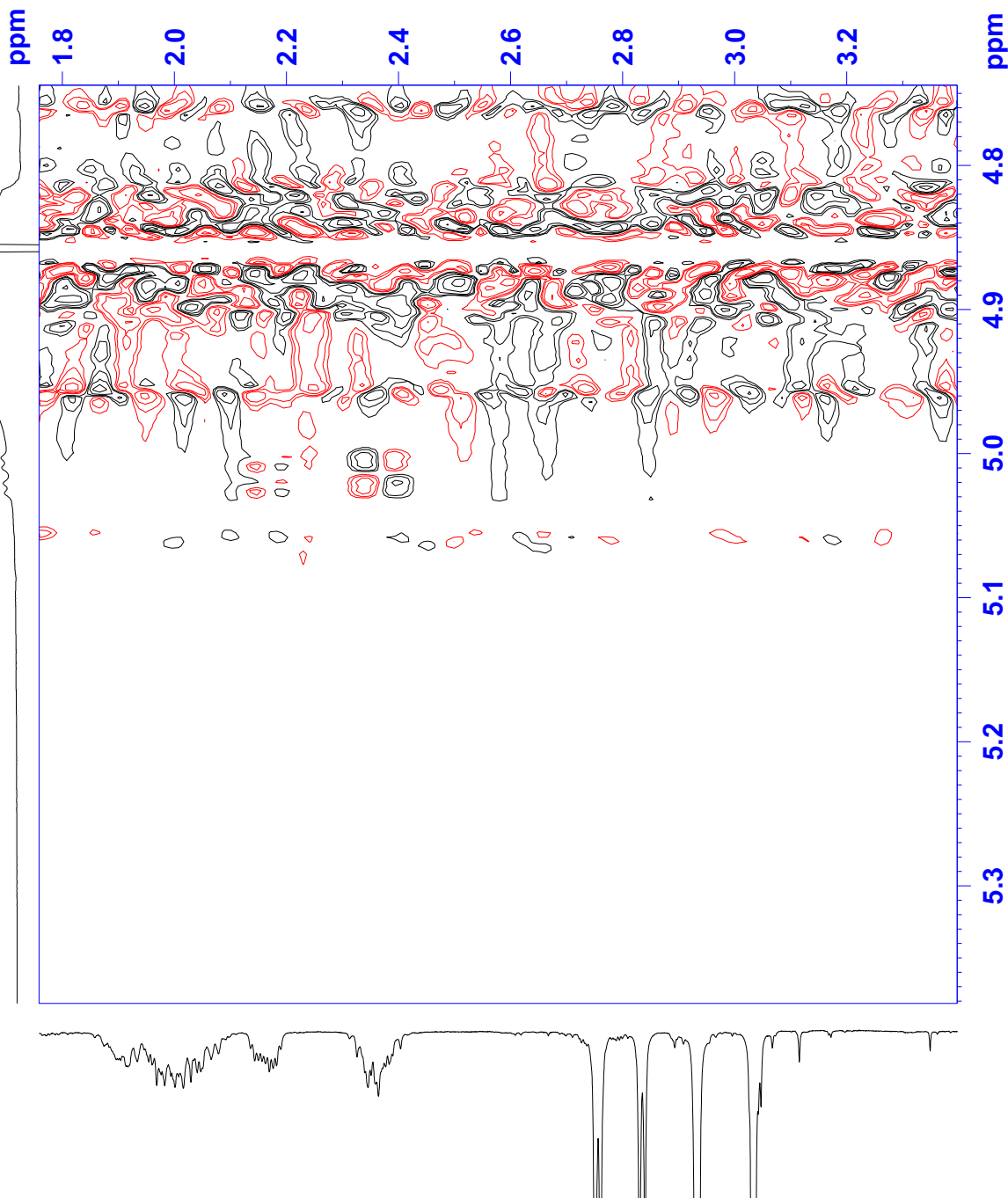
F2 - Acquisition Parameters
Date       500000
INSTRUM    spect
PULPROG    COSY_dfstpr.ok
TD          4096
NS          8
SWH         6009.615 Hz
AQ          0.3409204 sec
RG          16
d0          0.00000300 sec
d11         0.03000000 sec
d12         0.00002000 sec
d13         0.00000300 sec
l3          256

===== CHANNEL f1 =====

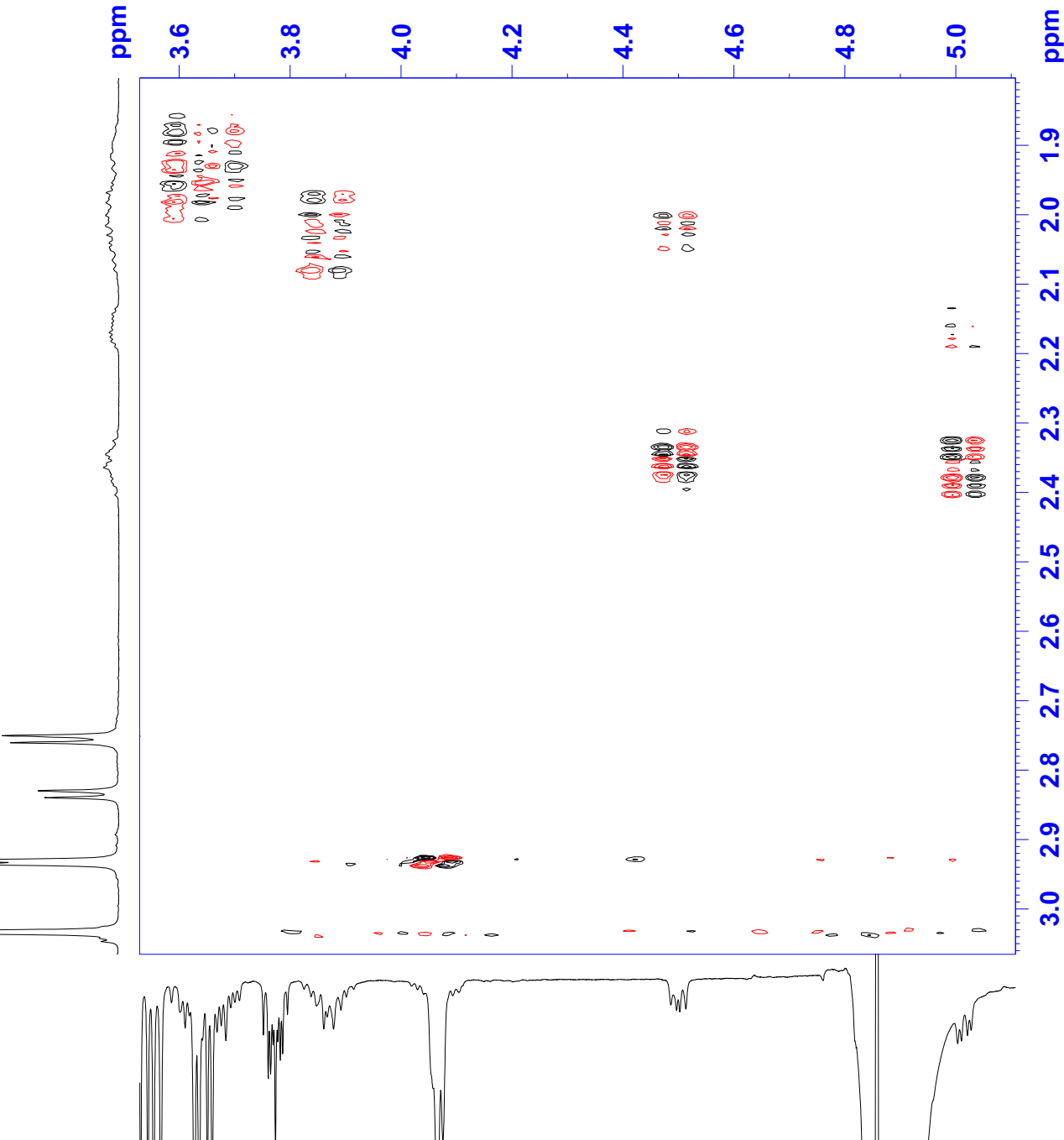
F1 - Acquisition parameters
ND0         1
TD          512
SFO1        500.2524 MHz
FIDRES      11.723439 Hz
SW          11.999 ppm
FnMODE      undefined

F2 - Processing parameters
SI          4096
SF          500.2499213 MHz
WDW         SINE
SSB         2
LB          0.00 Hz
GB          0
PC          1.00

F1 - Processing parameters
SI          1024
MC2         States-TpPI
SF          500.2499213 MHz
WDW         SINE
SSB         2
LB          0.00 Hz
GB          0
```



DRX-500: DQF-COSY with presaturation of JP-170 (H<sub>2</sub>O/D<sub>2</sub>O=9/1, 290K)



Current Data Parameters  
 NAME NB\_JP-170  
 EXPNO 500  
 PROCNO 1

F2 - Acquisition Parameters  
 Date 500000  
 INSTRUM spect  
 PULPROG COSY\_dfstpr.ok  
 TD 4096  
 NS 8  
 SWH 6009.615 Hz  
 AQ 0.3409204 sec  
 RG 16  
 d0 0.00000300 sec  
 d11 0.03000000 sec  
 d12 0.00002000 sec  
 d13 0.00000300 sec  
 L3 256

==== CHANNEL f1 =====

F1 - Acquisition parameters  
 ND0 1  
 TD 512  
 SFO1 500.2524 MHz  
 FIDRES 11.723439 Hz  
 SW 11.999 ppm  
 FMODE undefined

F2 - Processing parameters  
 SI 4096  
 SF 500.2499213 MHz  
 WDW SINE  
 SSB 2  
 LB 0.00 Hz  
 GB 0  
 PC 1.00

F1 - Processing parameters  
 SI 1024  
 MC2 States-TpPI  
 SF 500.2499213 MHz  
 WDW SINE  
 SSB 2  
 LB 0.00 Hz  
 GB 0

DRX-500: ROESY with presaturation of JP-170 (mixing time=250ms, H2O/D2O=9/1, 290K

```
Current Data Parameters
NAME      NB_JP-170
EXPNO     502
PROCNO    1

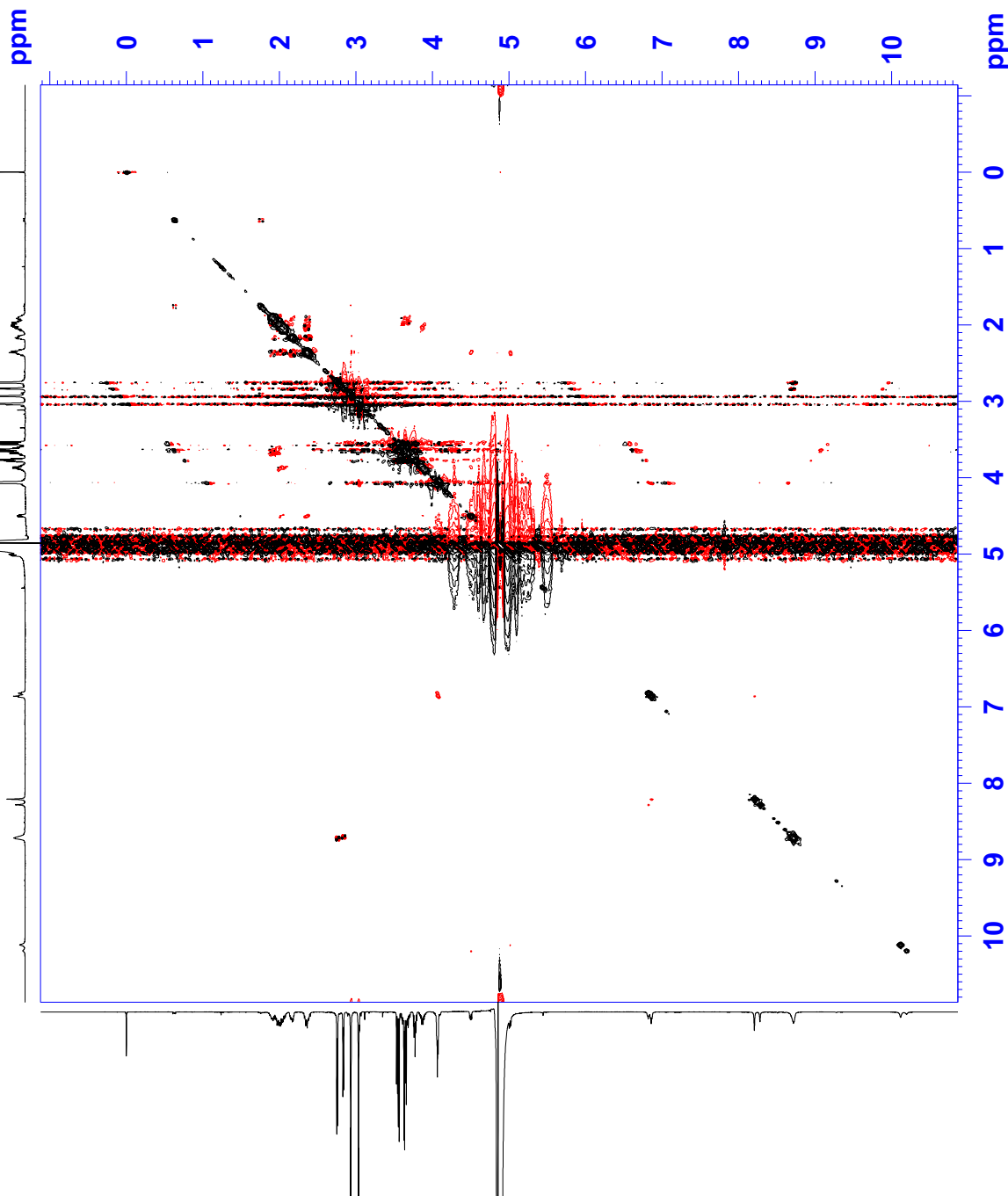
F2 - Acquisition Parameters
Date      500000
INSTRUM   spect
PULPROG   ROESY_prst.ok
TD         2048
NS         32
SWH        6009.615 Hz
AQ         0.1705268 sec
RG         32
d0         0.00000300 sec
d11        0.03000000 sec
d12        0.00002000 sec
d13        0.00000300 sec
l3         256

===== CHANNEL f1 =====

F1 - Acquisition parameters
NDO        1
TD         512
SFO1       500.2524 MHz
FIDRES     11.723439 Hz
SW         11.999 ppm
F1MODE     undefined

F2 - Processing parameters
SI         4096
SF         500.2499210 MHz
WDW        QSINE
SSB        2
LB         0.00 Hz
GB         0
PC         1.00

F1 - Processing parameters
SI         1024
MC2        States-TPPI
SF         500.2499182 MHz
WDW        QSINE
SSB        2
LB         0.00 Hz
GB         0
```



DRX-500: ROESY with presaturation of JP-170 (mixing time=250ms, H2O/D2O=9/1, 290K

```

Current Data Parameters
NAME      NB_JP-170
EXPNO     502
PROCNO    1

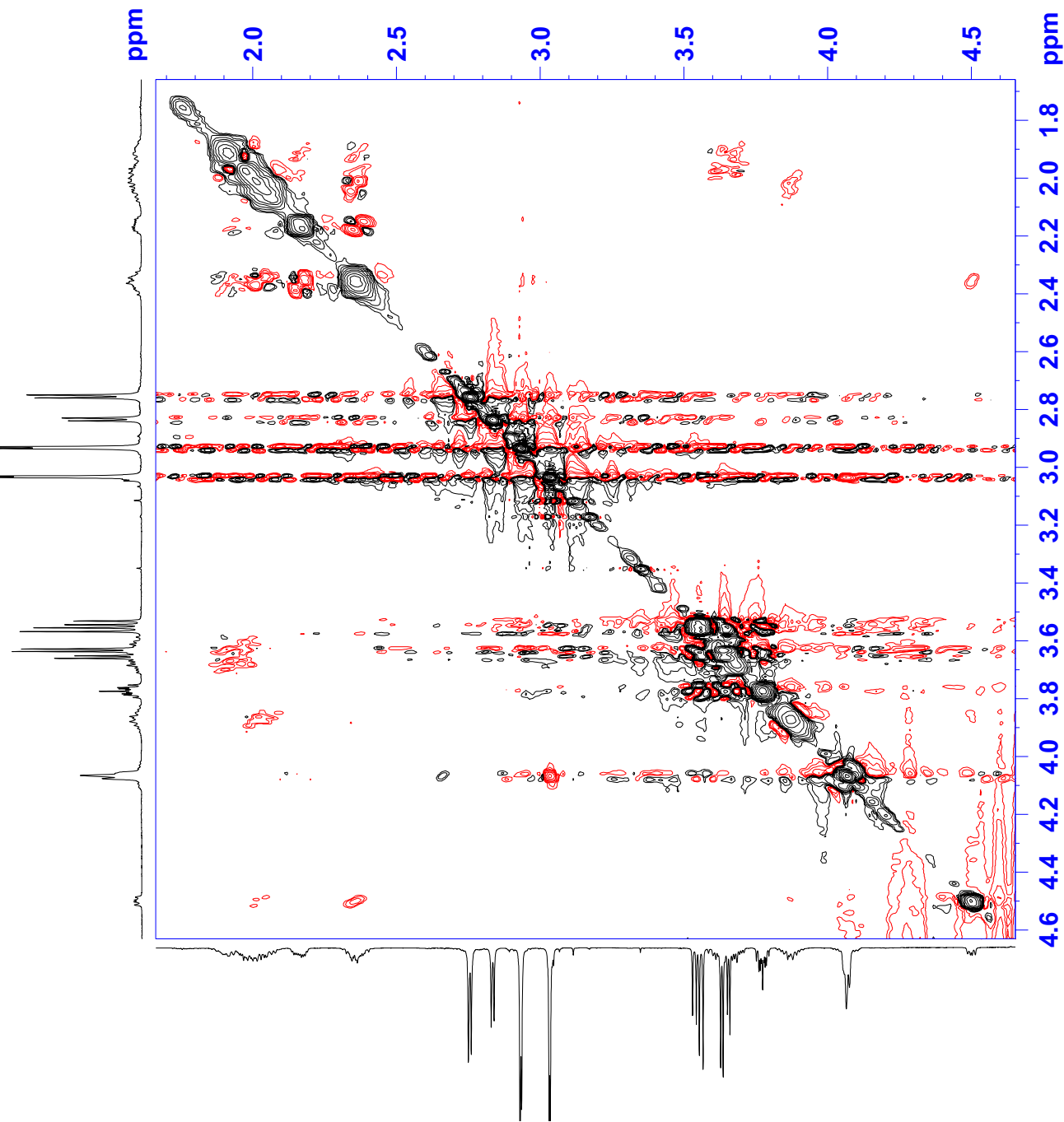
F2 - Acquisition Parameters
Date      500000
INSTRUM   spect
PULPROG   ROESY_prst.ok
TD         2048
NS         32
SWH        6009.615 Hz
AQ          0.1705268 sec
RG          32
d0          0.00000300 sec
d11         0.03000000 sec
d12         0.00002000 sec
d13         0.00000300 sec
l3          256

===== CHANNEL f1 =====

F1 - Acquisition parameters
ND0        1
TD         512
SFO1       500.2524 MHz
FIDRES     11.723439 Hz
SW         11.999 ppm
F1MODE     undefined

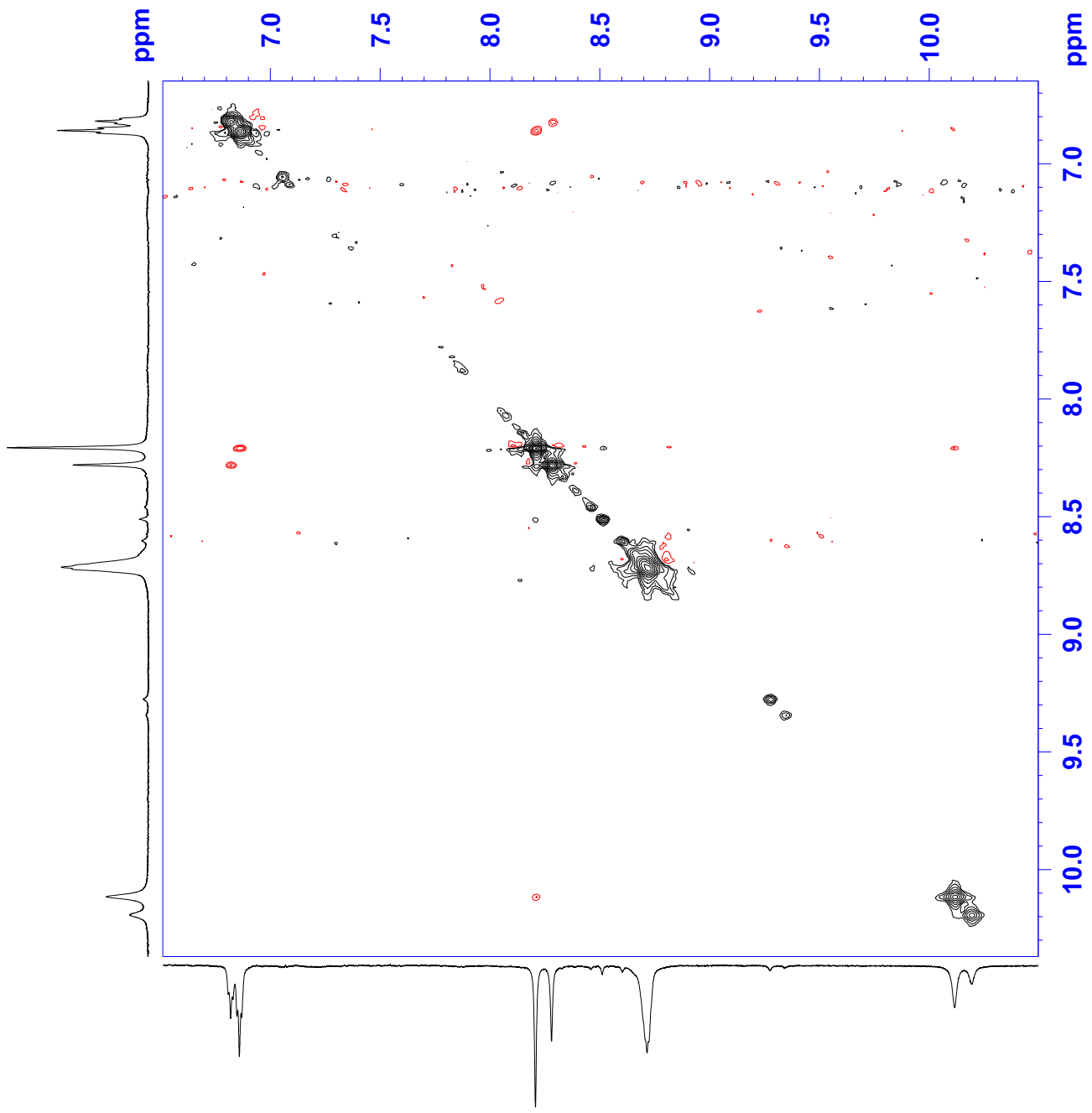
F2 - Processing parameters
SI         4096
SF         500.2499210 MHz
WDW        QSINE
SSB        2
LB         0.00 Hz
GB         0
PC         1.00

F1 - Processing parameters
SI         1024
MC2        States-TPPI
SF         500.2499182 MHz
WDW        QSINE
SSB        2
LB         0.00 Hz
GB         0
  
```





DRX-500: ROESY with presaturation of JP-170 (mixing time=250ms, H2O/D2O=9/1, 290K



Current Data Parameters  
NAME NB\_JP-170  
EXPNO 502  
PROCNO 1

F2 - Acquisition Parameters  
Date 500000  
INSTRUM spect  
PULPROG ROESY\_prst.ok  
TD 2048  
NS 32  
SWH 6009.615 Hz  
AQ 0.1705268 sec  
RG 32  
d0 0.00000300 sec  
d11 0.03000000 sec  
d12 0.00002000 sec  
d13 0.00000300 sec  
L3 256

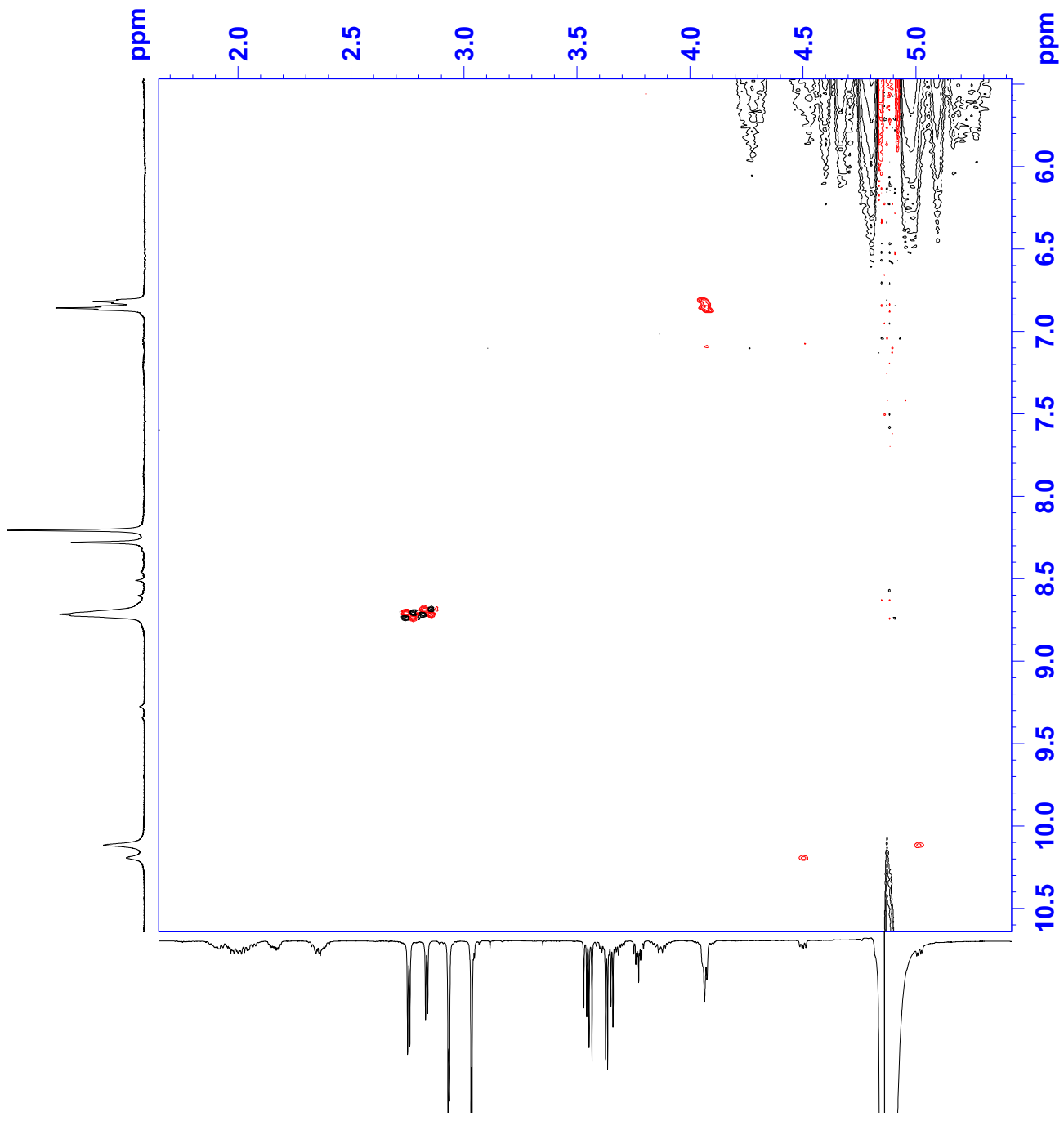
==== CHANNEL f1 =====

F1 - Acquisition parameters  
NDO 1  
TD 512  
SFO1 500.2524 MHz  
FIDRES 11.723439 Hz  
SW 11.999 ppm  
F1MODE undefined

F2 - Processing parameters  
SI 4096  
SF 500.2499210 MHz  
WDW QSINE  
SSB 2  
LB 0.00 Hz  
GB 0  
PC 1.00

F1 - Processing parameters  
SI 1024  
MC2 States-TPPI  
SF 500.2499182 MHz  
WDW QSINE  
SSB 2  
LB 0.00 Hz  
GB 0

DRX-500: ROESY with presaturation of JP-170 (mixing time=250ms, H2O/D2O=9/1, 290K



Current Data Parameters  
 NAME NB\_JP-170  
 EXPNO 502  
 PROCNO 1

F2 - Acquisition Parameters  
 Date 500000  
 INSTRUM spect  
 PULPROG ROESY\_prst.ok  
 TD 2048  
 NS 32  
 SWH 6009.615 Hz  
 AQ 0.1705268 sec  
 RG 32  
 d0 0.00000300 sec  
 d11 0.03000000 sec  
 d12 0.00002000 sec  
 d13 0.00000300 sec  
 l3 256

==== CHANNEL f1 =====

F1 - Acquisition parameters  
 NDO 1  
 TD 512  
 SFO1 500.2524 MHz  
 FIDRES 11.723439 Hz  
 SW 11.999 ppm  
 FwMODE undefined

F2 - Processing parameters  
 SI 4096  
 SF 500.2499210 MHz  
 WDW QSINE  
 SSB 2  
 LB 0.00 Hz  
 GB 0  
 PC 1.00

F1 - Processing parameters  
 SI 1024  
 MC2 States-TPPI  
 SF 500.2499182 MHz  
 WDW QSINE  
 SSB 2  
 LB 0.00 Hz  
 GB 0

DRX-500: TOCSY with presaturation of JP-170 (mixing time=100ms, H2O/D2O=9/1, 2

```
Current Data Parameters
NAME      NB_JP-170
EXPNO     501
PROCNO    1

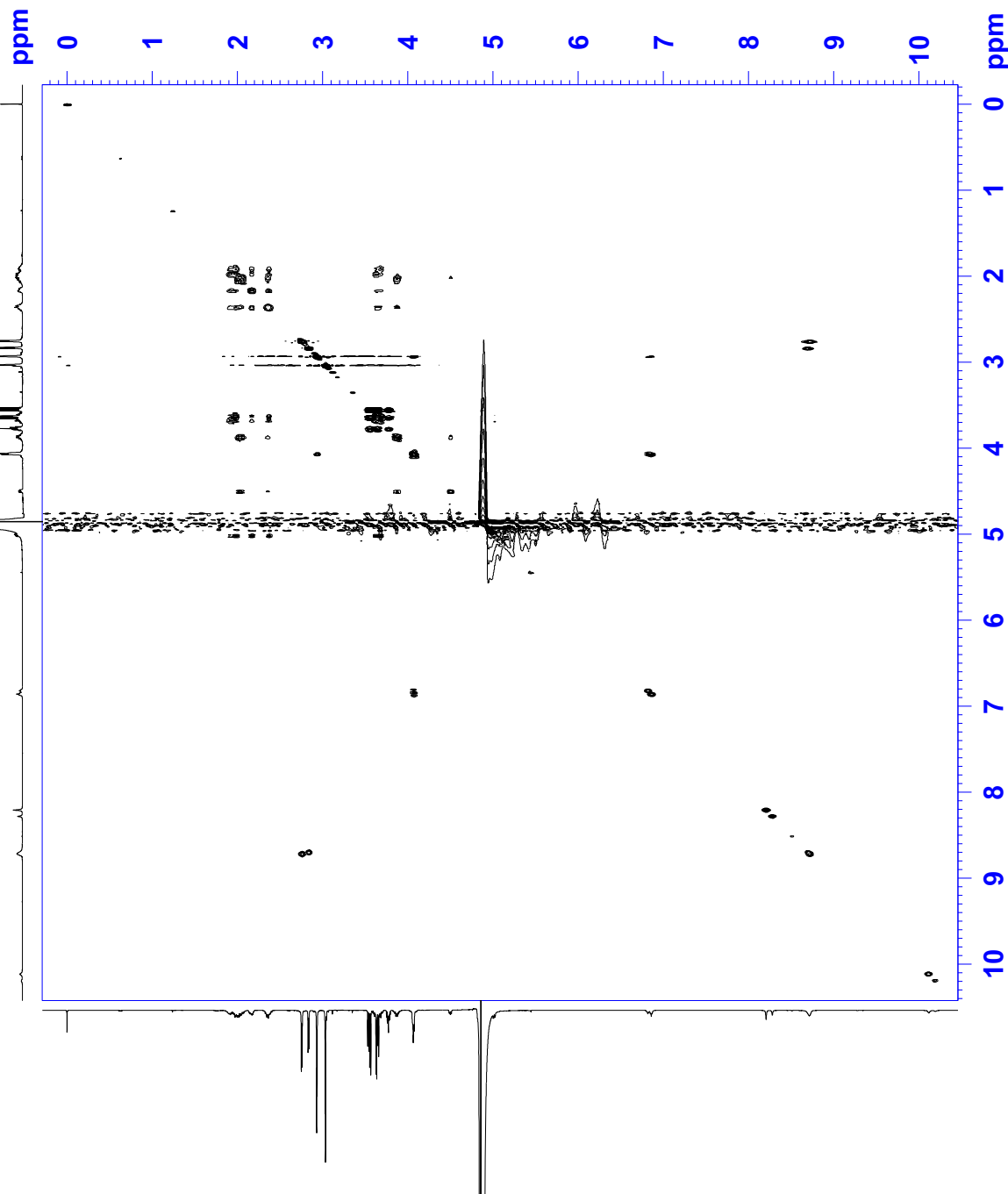
F2 - Acquisition Parameters
Date       500000
INSTRUM   spect
PULPROG   TOCSY_stpr.ok
TD         4096
NS         8
SWH        6009.615 Hz
AQ         0.3409204 sec
RG         32
d0         0.00000300 sec
d11        0.03000000 sec
d12        0.00002000 sec
d13        0.00000300 sec
FACTOR1   1073741823
l1         1073741823
l3         256
SCALEF    1073741823

===== CHANNEL f1 =====
p5         0.00 usec
p7         0.00 usec

F1 - Acquisition parameters
ND0        1
TD         512
SFO1       500.2524 MHz
FIDRES     11.723439 Hz
SW         11.999 ppm
FnmODE     undefined

F2 - Processing parameters
SI         4096
SF         500.2499244 MHz
WDW        QSINE
SSB        2
LB         0.00 Hz
GB         0
PC         1.40

F1 - Processing parameters
SI         1024
MC2        States-TPPI
SF         500.2499220 MHz
WDW        QSINE
SSB        2
LB         0.00 Hz
GB         0
```



DRX-500: TOCSY with presaturation of JP-170 (mixing time=100ms, H2O/D2O=9/1, 2

```

Current Data Parameters
NAME      NB_JP-170
EXPNO     501
PROCNO    1

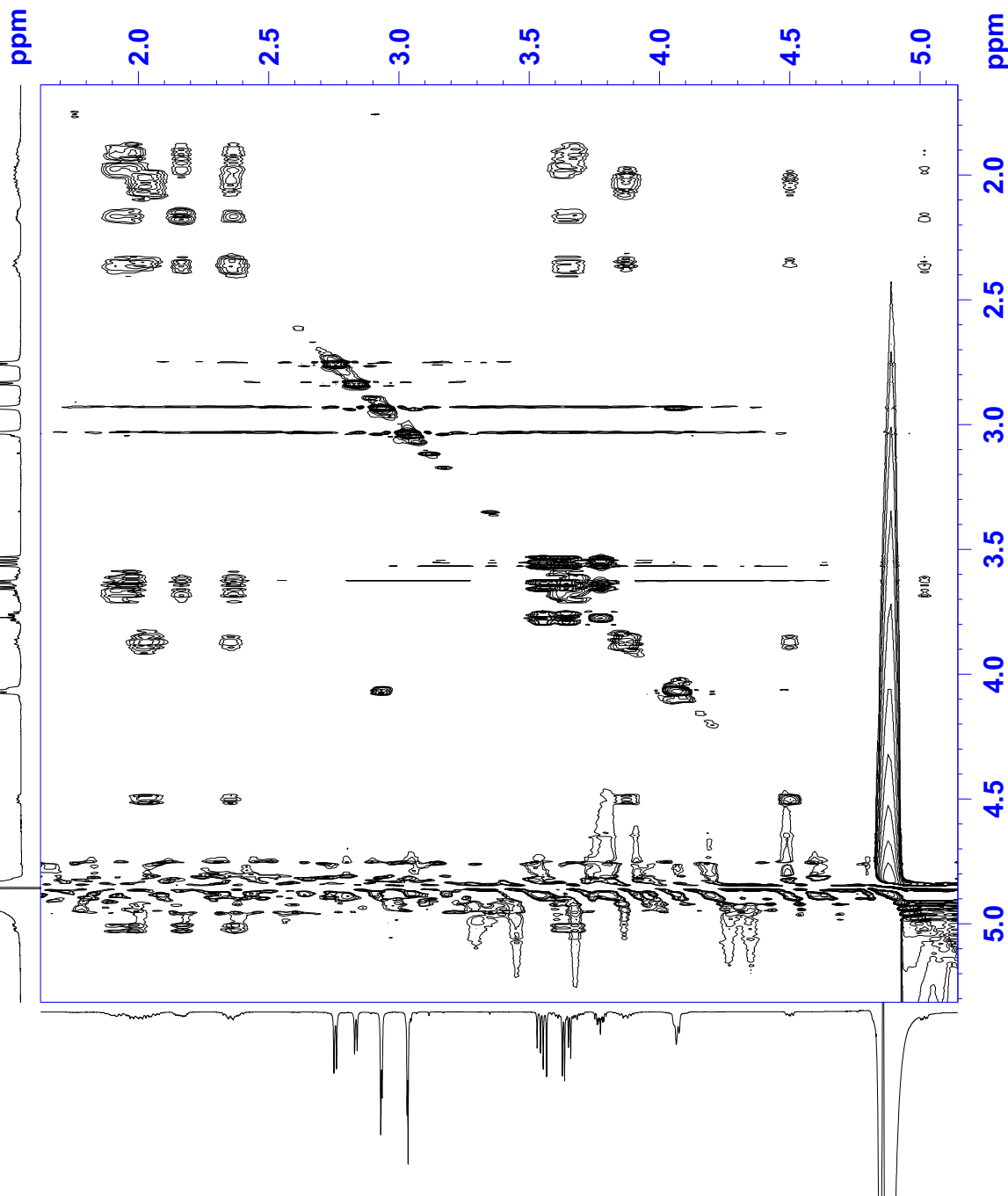
F2 - Acquisition Parameters
Date      500000
INSTRUM   spect
PULPROG   TOCSY_stpr.ok
TD         4096
NS         8
SWH        6009.615 Hz
AQ         0.3409204 sec
RG         32
d0         0.00000300 sec
d11        0.03000000 sec
d12        0.00002000 sec
d13        0.00000300 sec
FACTOR1   1073741823
f1         1073741823
f3         1073741823
SCALEF    1073741823

===== CHANNEL f1 =====
p5         0.00 usec
p7         0.00 usec

F1 - Acquisition parameters
ND0        1
TD         512
SFO1       500.2524 MHz
FIDRES     11.723439 Hz
SW         11.999 ppm
FnmODE     undefined

F2 - Processing parameters
SI         4096
SF         500.2499244 MHz
WDW        QSINE
SSB        2
LB         0.00 Hz
GB         0
PC         1.40

F1 - Processing parameters
SI         1024
MC2        States-TPPI
SF         500.2499220 MHz
WDW        QSINE
SSB        2
LB         0.00 Hz
GB         0
  
```



DRX-500: TOCSY with presaturation of JP-170 (mixing time=100ms, H2O/D2O=9/1, 2

```
Current Data Parameters
NAME      NB_JP-170
EXPNO     501
PROCNO    1

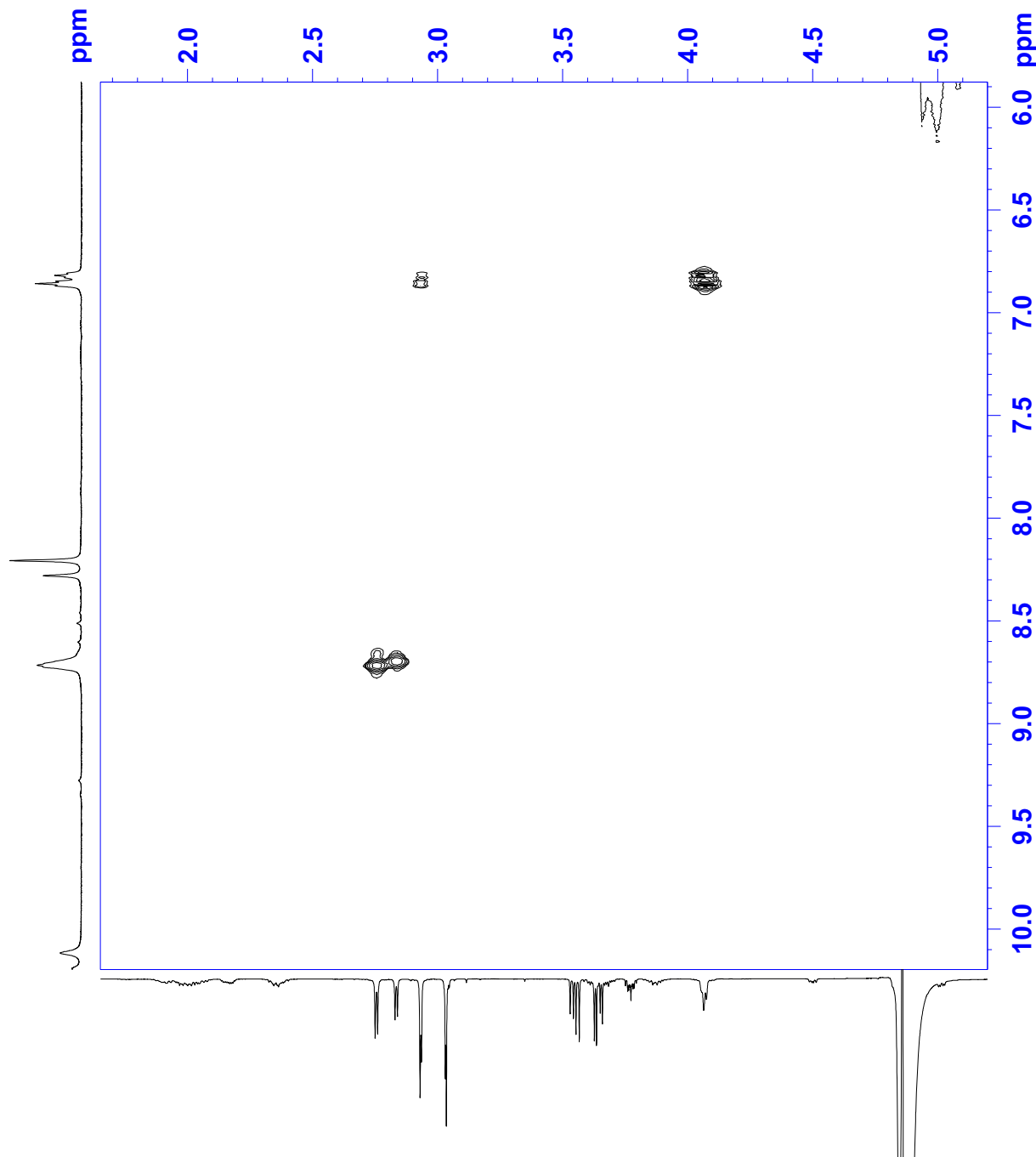
F2 - Acquisition Parameters
Date      500000
INSTRUM   spect
PULPROG   TOCSY_stpr.ok
TD         4096
NS         8
SWH        6009.615 Hz
AQ         0.3409204 sec
RG         32
d0         0.00000300 sec
d11        0.03000000 sec
d12        0.00002000 sec
d13        0.00000300 sec
FACTOR1    1073741823
l1         1073741823
l3         256
SCALEF     1073741823

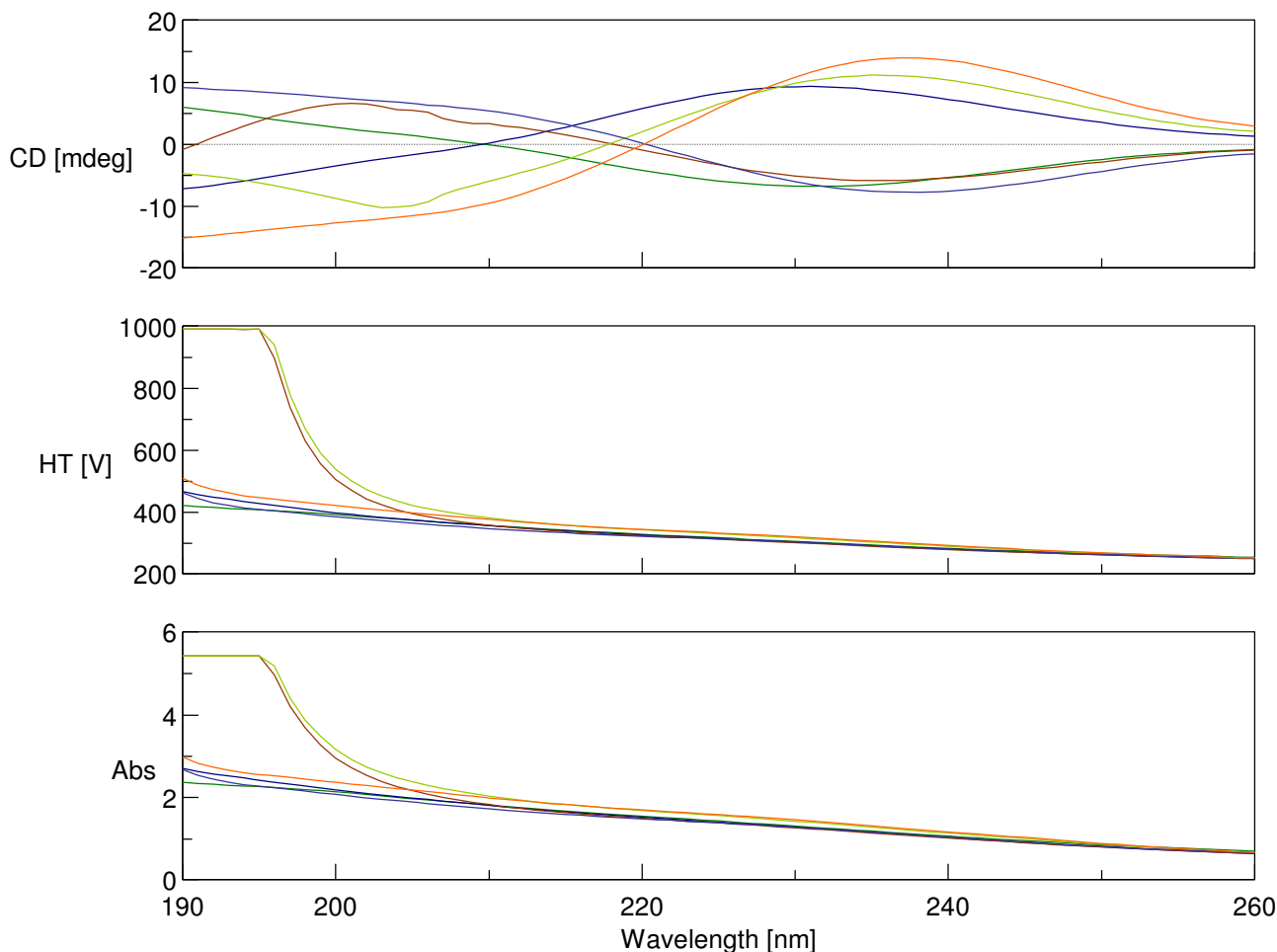
===== CHANNEL f1 =====
p5         0.00 usec
p7         0.00 usec

F1 - Acquisition parameters
ND0        1
TD         512
SFO1       500.2524 MHz
FIDRES     11.723439 Hz
SW         11.999 ppm
FnmODE     undefined

F2 - Processing parameters
SI         4096
SF         500.2499244 MHz
WDW        QSINE
SSB        2
LB         0.00 Hz
GB         0
PC         1.40

F1 - Processing parameters
SI         1024
MC2        States-TPPI
SF         500.2499220 MHz
WDW        QSINE
SSB        2
LB         0.00 Hz
GB         0
```





[Measurement Information]  
 [Comments]  
 Instrument Name FK 172  
 Sample name J-815  
 Model Name J-815  
 Comment  
 Serial No. B046961168  
 Division  
 Accessory CDF-426S  
 Company U-View  
 Accessory S/N A011561183  
 Temperature 21.99 C  
 Control Sensor Holder  
 Monitor Sensor Holder  
 Start Mode Start immediately  
 Cell Length 10 mm

FK 172.jws  
 FK 166.jws  
 FK 172.jws  
 FK 166.jws  
 FK 172.jws  
 FK 166.jws

[Detailed Information]  
 Creation date 21.12.2011 15:06

Measurement date 21.12.2011 15:03

Photometric Mode CD, HT, Abs  
 Measure Range 260 - 190 nm  
 Data pitch 1 nm  
 Sensitivity Standard  
 D.I.T. 1 sec  
 Bandwidth 1.00 nm  
 Start Mode Immediately  
 Scanning Speed 50 nm/min  
 Baseline Correction None  
 Shutter Control Auto  
 CD Detector PMT  
 PMT Voltage Auto  
 Accumulations 4  
 Concentration 100 umol/L

Data array type Linear data array \* 3  
 Horizontal axis Wavelength [nm]  
 Vertical axis(1) CD [mdeg]  
 Vertical axis(2) HT [V]  
 Vertical axis(3) Abs  
 Start 260 nm  
 End 190 nm  
 Data interval 1 nm  
 Data points 71