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 (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 ¹H- and ¹³C-NMR spectra were recorded on a Bruker AC-200 (at 200 MHz and 50 MHz, respectively) pulse Fourier-transform NMR spectrometer. Chemical shifts δ 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 DPFGSE 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 TOF²) using the matrix α-cyano-4-hydroxycinnamic acid dissolved in methanol and i-propanol. Crude residues were purified by flash chromatography using silica gel 40-63μm 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 \( \varepsilon = 78.5 \) 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 <3.5Å with a donor-hydrogen-acceptor angle of 90°<angle<180°. 

\textit{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., \textit{et al.} Gaussian 09, Revision A.1, 2009. Gaussian, Inc., Wallingford CT). Continuum solvents (water, dimethylsulfoxide, methanol (\( \varepsilon = 32.5 \) 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$_2$Cl$_2$ (15 mL) was added slowly over a period of 30mins to a triphosgene solution (3.4 g, 11.46 mmol) in CH$_2$Cl$_2$ (10 mL). After stirring further for 15mins under argon, a solution of Boc-hydrazine (3.79 g, 28.66 mmol) in CH$_2$Cl$_2$ (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$_3$ (15 mL), brine (15mL), dried over Na$_2$SO$_4$ 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$_{10}$H$_{19}$N$_3$O$_5$: C, 45.97; H, 7.33; N, 16.08. $^1$H NMR (200 MHz, CDCl$_3$): $\delta$H=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); $^{13}$C NMR (50 MHz, CDCl$_3$): $\delta$C=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$_{10}$H$_{20}$N$_4$O$_4$: C, 46.14; H, 7.74; N, 21.52. $^1$H NMR (200 MHz, CDCl$_3$): $\delta$H=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); $^{13}$C NMR (50 MHz, CDCl$_3$): $\delta$C=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 30 mins. 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 CH₂Cl₂ (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 CH₂Cl₂ (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 (2.1 g, 81%).

mp 74-75°C. Elemental analysis found: C, 50.21; H, 6.96; N, 19.43. Calc. for C₁₅H₂₇N₅O₅: C, 50.41; H, 7.61; N, 19.59. ¹H NMR (200 MHz, CDCl₃): δH=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); ¹³C NMR (50 MHz, CDCl₃): δC=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 30 mins. The white solid precipitated was filtered and washed with ethanol (10 mL) to afford 1 as a white solid (0.75 g, 71%).

*mp 201-202°C. Elemental analysis found: C, 43.54; H, 6.16; N, 22.88. Calc. for C_{13}H_{22}N_{6}O_{5}·H_{2}O: C, 43.33; H, 6.71; N, 23.32. IR (KBr) \nu_{\text{max}}/\text{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).*

*13C 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_{6}O_{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_{6}O_{5}+Na^{+}: 365.15.*
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**Table 1.** 600 MHz ($^1$H NMR) and 150 MHz ($^{13}$C NMR), respectively, chemical shifts $\delta$ of ensemble conformers 1a and 1b in d$_6$-DMSO, measured at 5mM concentration.
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 H₂O (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.
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$^{-1}$.

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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$_2$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$_2$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 $^1$H NMR chemical shift in ppm relative to TMS.
Figure 7. Relative minimum geometry from \textit{ab initio} calculations at B3LYP/6-311G\(^{++}(d,p)\) and substantiated as equilibrium conformer 1b by comparison with MD and NMR. Given in the figure is the calculated value of the \(^1\)H NMR chemical shift in ppm relative to TMS.
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.
Sample Name:

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

FidFile: FK50_DMSO_C13_17C

Pulse Sequence: CARBON (s2pul)
Solvent: dms
Data collected on: May 28 2010
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:
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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
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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
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Shifted by -0.100 sec
F1 DATA PROCESSING
Sq. sine bell 0.035 sec
Shifted by -0.028 sec
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Total time 8 min 27 sec
Sample Name: F70 dmso 37C DQCOSY

Data Collected on: 28.05.2010

Varian-NMR-vnmrs600 Archive directory:

Sample directory: Sample directory:

FidFile: F70_dmso_37C_DQCOSY_28May2010

Pulse Sequence: gDQCOSY
Solvent: dms
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

F1 (ppm)
F2 (ppm)
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
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
Sample Name: FK70
Data Collected on: May 28 2010
Varian-NMR-vnmrs600
Archive directory:

Sample directory:
FidFile: FK50_DMSO_HMBCAD_17C

Pulse Sequence: gHMBCAD
Solvent: dmsa
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

<table>
<thead>
<tr>
<th>F1 (ppm)</th>
<th>F2 (ppm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>160</td>
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<td>164</td>
<td>166</td>
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<td>170</td>
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<td>172</td>
<td></td>
</tr>
</tbody>
</table>
Sample Name: FK70
Data Collected on: Varian-NMR-vnmrs600
Archive directory:
Sample directory: FidFile: FK50_DMSO_HMBCAD_17C
Pulse Sequence: gHMBCAD
Solvent: dmsq
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
Sample Name: FK70
Data Collected on: May 28 2010
Varian-NMR-vnmrs600
Archive directory:
Sample directory: FidFile: FK50_DMSO_HMBCAD_17C

Pulse Sequence: gHMBCAD
Solvent: dmsa
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
Sample Name: FK70
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
DECOUPLED C13, 150.8356255 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
Sample Name: FK70
Data Collected on: May 28 2010
Varian-NMR-vnmrs600
Archive directory:
Sample directory: FidFile: FK50_DMSO_HSQCAD_17C
Pulse Sequence: HSQCAD
Solvent: dmsob
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
DECOUPLER C13, 150.8356295 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
Sample Name: FK70
Data Collected on: May 28 2010
Varian-NMR-vnmrs600
Archive directory: Sample directory: FidFile: FK50_DMSO_HSQCAD_17C
Pulse Sequence: HSQCAD
Solvent: dmoso
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
DECOUPLER 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
Sample Name: FK70
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 961.5 Hz
2D Width 961.5 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
Sample Name: FK70
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
Sample Name: FK70
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
<table>
<thead>
<tr>
<th>SAMPLE</th>
<th>PRESATURATION</th>
</tr>
</thead>
<tbody>
<tr>
<td>date</td>
<td>Aug 4 2010</td>
</tr>
<tr>
<td>solvent</td>
<td>cd3od wet</td>
</tr>
<tr>
<td>file</td>
<td>exp</td>
</tr>
</tbody>
</table>

**ACQUISITION**
- temp: 25.0
- sw: 9615.4
- at: 1.704
- np: 32768
- fb: 4000
- bs: 32
- ss: 2
- dl: 3.000
- nt: 4
- ct: 4

**TRANSMITTER**
- sfrq: 599.773
- tof: 599.7
- tpwr: 57
- pw: 7.250
- D:
- dn: C13
- dof: 0
- dm: mm

**DECoupler**
- rfi: 1209.1

**PLOT**
- dpwr: 47
- dmf: 35088
- ai: cdc

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

exp2 NOESY1D
$^1$H CD$_{3}$OD-d$_3$ 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
1H v CD3OD-d3 temp=25
Selective band center: 2.80 (ppm); width: 29.9 (Hz)

exp3 NOESTYD

ACQUISITION

sw 9615.4  dm  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
cg 2024  gain  0
TRANSMITTER
spin not used
tn  M1  pw90  7.250
sfrq 599.773  FLAGS
tof 599.7  sspl  y
tpwr 57  il  n
pw 7.250  in  n
NOESY
dp  y
mixN 0.250  hs  nn
sweepwr 41  PROCESSING
sweeppw 1500.000  lb  1.00
sweepbbp sech180  fn  not used

DISPLAY

sselshapeA nada_NON- sp  -120.5
SY1D_013  wp  9614.8
sselpwrA  -3  vs  1.9193e+06
sselpwA  120387.6  sc  0
gs1v0A  3389  wc  265
gtA 0.001000  hzmm  0.97
sselshapeB nada_NON- is  33.57
SY1D_013  rfl  1209.1
sselpwrB  -3  rfp  0
sselpwB  120387.6  th  27
gs1v1B  5084  ins  100.000

gtB 0.000000  st  cde ph
gstabaB 0.000500

gs1vC  -842
gtC 0.001000
gstab 0.000500
hsg1v1  5076
hsgt 0.002000
PRESATURATION
satmode  n
wet  n
$^1$H 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: Aug 4 2010
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

ACQUISITION

<table>
<thead>
<tr>
<th>sw</th>
<th>9615.4</th>
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<th>C13</th>
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<tr>
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<td>fb</td>
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<tr>
<td>bs</td>
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<tr>
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<td>file</td>
<td>exp</td>
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<tr>
<td>nt</td>
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<td>temp</td>
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<td>gain</td>
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DECOUPLER

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<tr>
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<td>in</td>
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<tr>
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<td>fn</td>
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<tr>
<td></td>
<td>not used</td>
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</tbody>
</table>

DPFSE DISPLAY

| selshapeA nada_NOE- | sp | -1208.5 |
| SY1D_014 wp         |    | 9614.8  |
| selpwA              | -3 | vs | 4.539777e+06 |
| selpwA              | 120011.1 | sc | 0 |
| gsvlvA              | 3389 | wc | 265 |
| gtvA                 | 0.001000 | hsm | 36.28 |
| selshapeB nada_NOE- | is | 33.57 |
| SY1D_014 ref | 1209.1 |
| selpwB              | -3 | rfp | 0 |
| selpwB              | 120011.1 | th | 27 |
| gsvlvB              | 5084 | ins | 100.000 |
| gtb                  | 0.001000 | aic | cdc | ph |
| gstabAB              | 0.000500 |

GRADIENT

| gsvlvC          | -847 |
| gsc             | 0.001500 |
| gstab           | 0.000500 |
| hgt             | 0.002000 |

PRESATURATION

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<tr>
<th>satmode</th>
<th>n</th>
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<tbody>
<tr>
<td>wet</td>
<td>n</td>
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</tbody>
</table>
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
dl 1.000  SPECIAL
nt 2024  temp  25.0
cg 2024  gain  0
TRANSMITTER  spin not used
tn n1 pw90  7.250
sfq 599.773  FLAGS
tof 599.7 ssqul  y
tpwr 57 il n
pw 7.250 in n
NOESY dp y
mixD 0.250 hs nn
sweepwr 41 PROCESSING
sweepw 1500.000 fn not used
sweepbp sech180  DISPLAY
DPFGSE  sp -1208.5
selshapeA nada_NOE- wp 9614.8
  SV1D_015 vs 1.30508+06
selpwrA -3 sc  0
selpwrA 120379.1 wc 265
gsl1A 3389 hzmm 36.28
gtA 0.001000 is 33.57
selshapeB nada_NOE- rfl 1209.1
  SV1D_016 rfp  0
selpwrB -3 th  27
selpwrB 120379.1 ins 100.000
gsl1B 5084 ai cdc ph
gtB 0.001000
gstabAB 0.000500
GRADIENT
gsl1c -847
gtc 0.001000
gstab 0.000500
gstgvl 5076
rabongl263 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 LH v CD3OD-d3 temp=25
Selective band center: 6.69 (ppm); wid th: 87.6 (Hz)

exp 8 NOESY1D

ACQUISITION          DECOUPLER
sw          9615.4  dn         C13
at          1.704  dn         mnn
np          32768  SAMPLE
fb          4000   date Aug 4 2010
bs          32     solvent  cd3od
ss          64     file        exp
dl          1.000  SPECIAL
nt          2024   temp        25.0
cr          2024   gain        0
TRANSMITTER     spin  not used
tn          M1     pw90     7.250
sfrq         599.773  FLAGS
tof          599.7  spupl     y
tpwr          57     il       n
pw           7.280   in      n
NOESY       dp      y
mixM          0.250  hs      nn
sweepwr       41     PROCESSING
sweeppw       1500.000  lb      1.00
sweepwpb      sec180  fn  not used
DPFGSE          DISPLAY
selshapeA nada_NOE- sp  -1208.5
  SY1D_018 wp         9614.8
selpwA          5     vs  1.25106e+07
selpwB          41094.4  sc       0
gsli1A         3389   wc       265
gtA           0.001000  hzmm    36.28
selshapeB nada_NOE- is 33.57
  SY1D_018 rfi      1209.1
selpwB          41094.4  th       27
gsli1B        5084    ins     100.000
gsttabAB      0.000500

ppm

ppm
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-vnms600
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

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
cg  2024  gain  0
TRANSMITTER
spin  not used
tn  31  pw90  7.250
sfrq  599.773  FLAGS
tof  599.7  sspsp  y
tpwr  57  il  n
pw  7.250  in  n
NOESY
dp  y
mixN  0.250  hs  nn
swepwp  41  PROCESSING
swepw  1500.000  lb  1.00
swepwdep  sech180  fn  not used
DDPGSE  DISPLAY
selshapeA  nada_MOE-  sp  -1208.5
SY1D_019  wp  9614.8
selpwrA  5  vs  1.54332e+07
selpwrA  42055.5  sc  0
gs1vLA  3389  wc  265
gtA  0.001000  hssm  36.28
selshapeB  nada_MOE-  is  33.57
SY1D_019  rfl  1209.1
selpwrB  5  xfp  0
selpwrB  42055.5  th  27
gs1vLB  5084  ins  100.000

Gradient:  0.001000 (inflated)

grad

gs1vC  -847
gtC  0.001000
gstab  0.0005000
hsq1v  5076
hsq  0.0020000
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-vmnr600
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); 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 LH v CD3OD-d3 temp=25
Selective band center: 8.10 (ppm); wid th: 123.1 (Hz)
exp7  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
dl  1.000  SPECIAL
nt  2024  temp  25.0
ci  2024  gain  0
TRANSMITTER  spin  not used
tn  N1  pw90  7.250
sfrq  599.773  FLAGS
tof  599.7  sspl  y
tpwr  57  il  n
pw  7.250  in  n
NOESY  dp  y
mixNR  0.250  hs  nn
sweepwr  41  PROCESSING
sweepw  1500.000  lb  1.000
sweepadr  sech180  fn  not used
DPFGSE  DISPLAY
selshapeA nada_NOE  sp  -1208.5
SV1D_017  wp  9614.8
selpwrA  8  vs  1.26013e+07
selpwrA  29241.4  sc  0
gszl1A  3389  wc  265
gtA  0.001000  hssm  2.00
selshapeB nada_NOE  is  33.57

DPFGSE  DISPLAY
sselwR  8  trp
sselwR  29241.4  th  14
gszl1B  5084  ins  100.000
gtB  0.001000  ai  cdc  ph
gstAB  0.000500
GRADIENT
gszl1C  -847
gtC  0.001000
gstB  0.000500
hsgvl  5076
hsrt  0.002000
PRESATURATION
satmode  n
wet  n
rabong1263 1H v CD3OD-d3 temp=25
Selective band center: 8.61 (ppm); wid th: 79.6 (Hz)

exp6  NOESY1D

ACQUISITION          DECOUPLER
sw  9615.4  dn          C13
at  1.704  dn          mn
np  32768  SAMPLE
fb  4000  date Aug 4 2010
be  32  solvent  cD3oD
ss  64  file  exp
d1  1.000  SPECIAL
nt  2024  temp  25.0
cz  2024  gain  0
TRANSMITTER          spin  not used
tn  N1  pw90  7.250
sn1q  599.773  FLAGS
tof  599.7  sspl  y
tpwr  57  il  n
pw  7.250  in  n
NOESY  dp  y
mixN  0.250  hs  nn
sweepwr  41  PROCESSING
sweeppw  1500.000  fn  not used
sweepshp  sech180  DISPLAY
DPFGSE  sp  -1208.5
se1shapeA nada_MOH-  wp  9614.8
SY1D_016  vs  925549
se1pwrA  4  sc  0
se1pwrA  45204.8  wc  265
gslv1A  3389  hzmm  36.28
gtA  0.001000  is  33.57
se1shapeB nada_MOH-  rfp  1209.1
SY1D_016  rfp  0
se1pwrB  4  th  20
se1pwrB  45204.8  ins  100.000
gslv1B  5084  ai  cdc  ph
gtB  0.001000
se1tabAB  0.000500

-847

gsc  0.500b0b1
gstb  0.000500
hsgvl  5076
hsgt  0.002000
PRESATURATION
satmode  n
wet  n
Sample Name: 
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 - blue 
green - 2.73 (ppm) 
Magenta - 2.80 (ppm) 
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 

Data collected on: Aug 6 2010 
Data collected on: Aug 4 2010
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
dpfgse_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)
DRX-500: 1H with presaturation of JP-170 (H2O/D2O=9/1, 290K)
DRX-500: 1H with presaturation of JP-170 (H2O/D2O=9/1, 290K)
DRX-500: 1H with presaturation of JP-170 (H2O/D2O=9/1, 290K)
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
d10            0.03000000 sec
d12            0.00002000 sec
d13            0.00000300 sec
l3             256

F1 - Acquisition parameters
ND0            1
TD             512
SF01           500.2524 MHz
FIDRES         11.723439 Hz
SW             11.999 ppm
PhMODE         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)
DRX-500: DQF-COSY with presaturation of JP-170 (H2O/D2O=9/1, 290K)
DRX-500: DQF-COSY with presaturation of JP-170 (H2O/D2O=9/1, 290K)
DRX-500: DQF-COSY with presaturation of JP-170 (H2O/D2O=9/1, 290K)
DRX-500: DQF-COSY with presaturation of JP-170 (H2O/D2O=9/1, 290K)
DRX-500: DQF-COSY with presaturation of JP-170 (H2O/D2O=9/1, 290K)
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_dftpr.ok
TD     4096
NS     8
SWH    6009.615 Hz
AQ     0.3409204 sec
BG     0
SW     11.999 ppm
FIDRES 11.723439 Hz
SFO1   500.2524 MHz
TD     4096
PULPROG COSY_dftpr.ok
INSTRUM spect
Date_  500000
PROCNO 1
EXPNO  500
NAME   NB_JP-170

F1 - Acquisition parameters
TD     512
SP01   500.2524 MHz
SFO1   500.2499213 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: 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 0.0300000 sec
d12 0.00002000 sec
d13 0.00000300 sec
l3 256

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

F1 - Acquisition parameters
ND0 11
TD 512
SP01 500.2524 MHz
FIDRES 11.723439 Hz
SW 11.999 ppm
FnMODE 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
F1MODE: undefined
SW: 11.999 ppm
FIDRES: 11.723439 Hz
SFO1: 500.2524 MHz
TD: 512
NS: 32
SWH: 6009.615 Hz
AQ: 0.1705268 sec
RG: 32
d0: 0.0000030 sec
d11: 0.0300000 sec
d12: 0.0000200 sec
d13: 0.0000030 sec
l3: 256

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: 500.2499210 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_pret.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
FnMODE undefined

F2 - Processing parameters
SI 4096
SF 500.249921 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_pret.ok
TD: 2048
NS: 32
SW: 6009.615 Hz
AQ: 0.1705268 sec
RG: 32
d0: 0.000000300 sec
d11: 0.03000000 sec
d12: 0.00002000 sec
d13: 0.000000300 sec
l3: 256

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

F1 - Acquisition parameters
ND0: 1
TD: 512
SP01: 500.2524 MHz
FIDRES: 11.723439 Hz
SW: 11.999 ppm
FnMODE: 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
DRX-500: TOCSY with presaturation of JP-170 (mixing time=100ms, H2O/D2O=9/1, 2
DRX-500: TOCSY with presaturation of JP-170 (mixing time=100ms, H2O/D2O=9/1, 2