

An Artificial β -Sheet that Dimerizes Through Parallel β -Sheet Interactions

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92697-2025*

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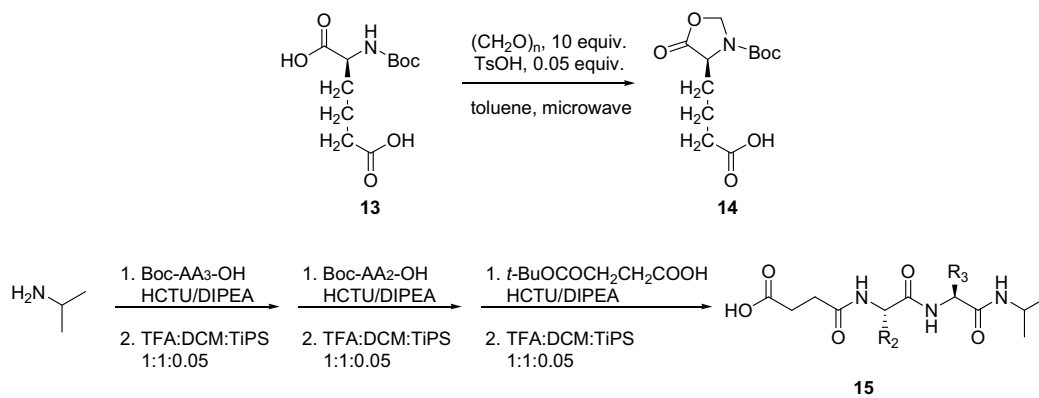
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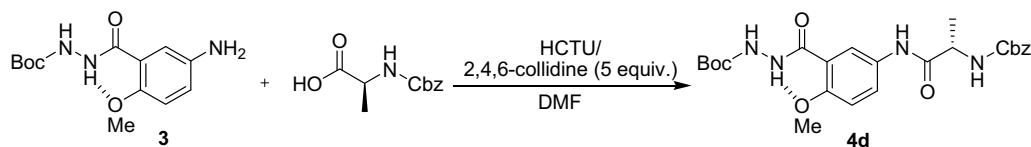
General Procedures. Commercial solvents and reagents were used without further purification, with the exception of THF, which was dried by filtration through alumina according to the procedure of Grubbs.¹ Solution-phase reactions were monitored by thin-layer chromatography (TLC) and carried out on 250 μm silica gel polyester plates on fluorescent silica gel with UV visualization. Column chromatography was performed on 40–63 μm silica gel using flash chromatography. Solvents were removed by rotary evaporation. Residual solvents were removed under vacuum (< 0.01 mmHg). Precipitated and recrystallized products were dried either under vacuum (< 0.01 mmHg) or by air suction through a filter funnel. High resolution mass spectra were obtained by electrospray ionization (ESI) on a Waters Micromass LCT Premier (instrument variation $\sigma < 5$ ppm). NMR spectra were recorded using a 500 MHz Bruker AVANCETM, 600 MHz Bruker AVANCETM spectrometers and Varian 800 MHz Unity InovaTM spectrometer. Chemical shifts are reported in parts per million (ppm) on the δ scale. ¹H spectra NMR were referenced with TMS ($\delta = 0.00$ ppm) and ¹³C NMR NMR spectra were referenced either with TMS ($\delta = 0.00$ ppm) or with DMSO-d₆ ($\delta = 39.53$ ppm).

¹ Pangborn, A. B.; Giardello, M. A.; Grubbs, R. H.; Rosen, R. K.; Trimmers, F. J. *Organometallics* **1996**, *15*, 1518-1520.

Synthetic Scheme (continued)



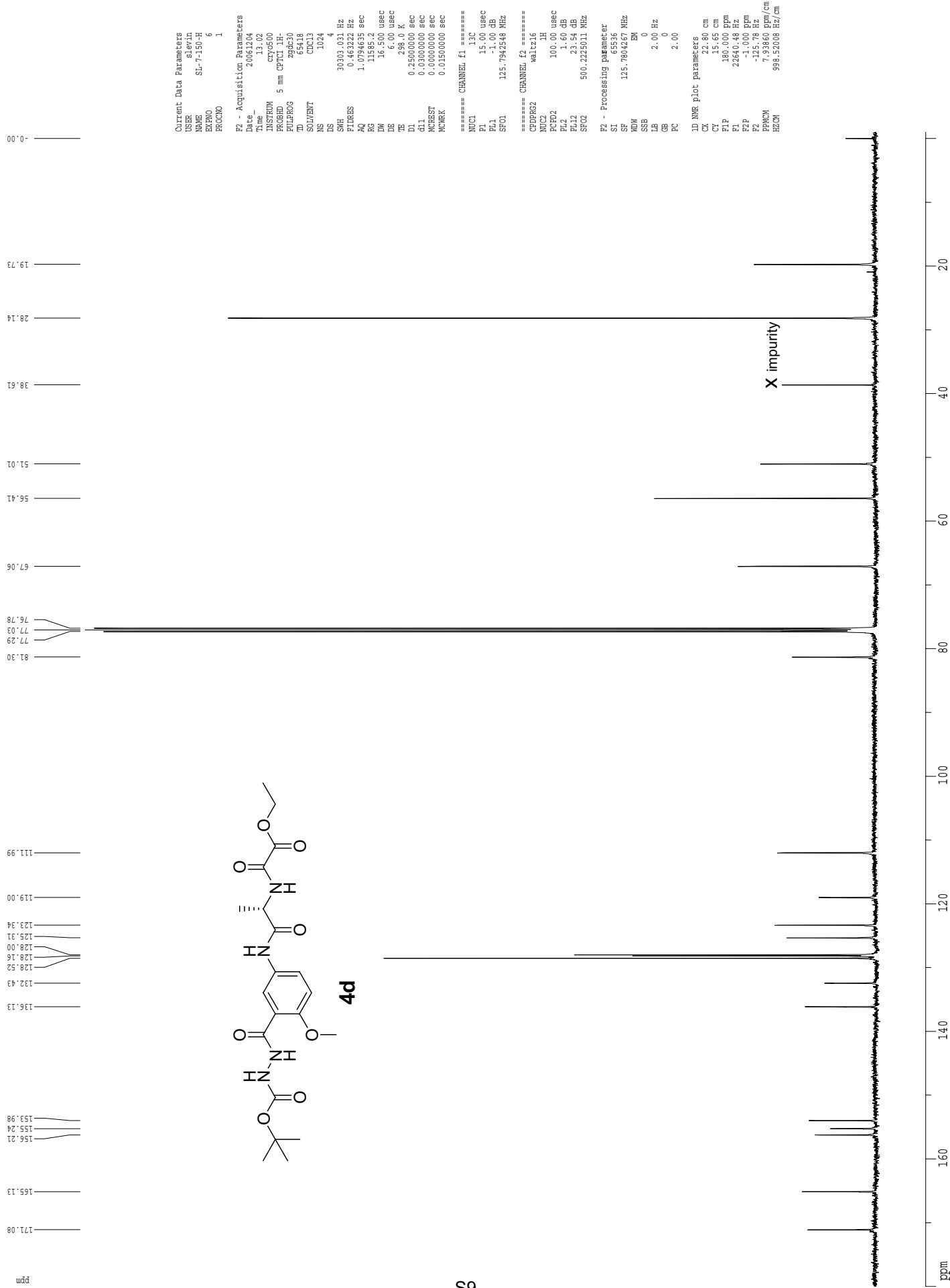
Representative synthetic procedures for the synthesis of the
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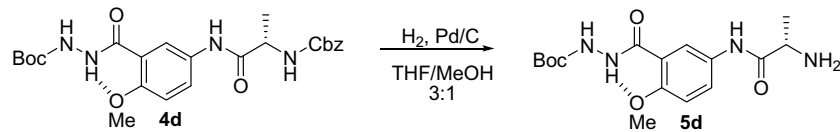


Amide 4d. A 500-mL, three-necked, round-bottomed flask equipped with a nitrogen inlet adapter, a glass stopper, a rubber septum, and a magnetic stirring bar was charged with aniline **3**² (2.7 g, 9.5 mmol) and DMF (100 mL). The apparatus was evacuated and flushed with nitrogen (3 times). A solution of Cbz-Ala-OH (2.4 g, 10.8 mmol) and HCTU (4.7 g, 11.4 mmol) in DMF (100 mL) was added to the stirred solution through syringe, followed by 2,4,6-collidine (6.3 mL, 48 mmol). The pale yellow solution was left under nitrogen for 24 h, then concentrated under vacuum. The residue was dissolved in dichloromethane (200 mL), and the solution was washed 1 M HCl (3 \times ca. 100 mL), saturated aqueous NaHCO₃ (3 \times ca. 100 mL), water (3 \times ca. 100 mL), dried over MgSO₄, filtered and concentrated to give 4.8 g (98%) of **4d** as a white solid. The compound was used without further purification.

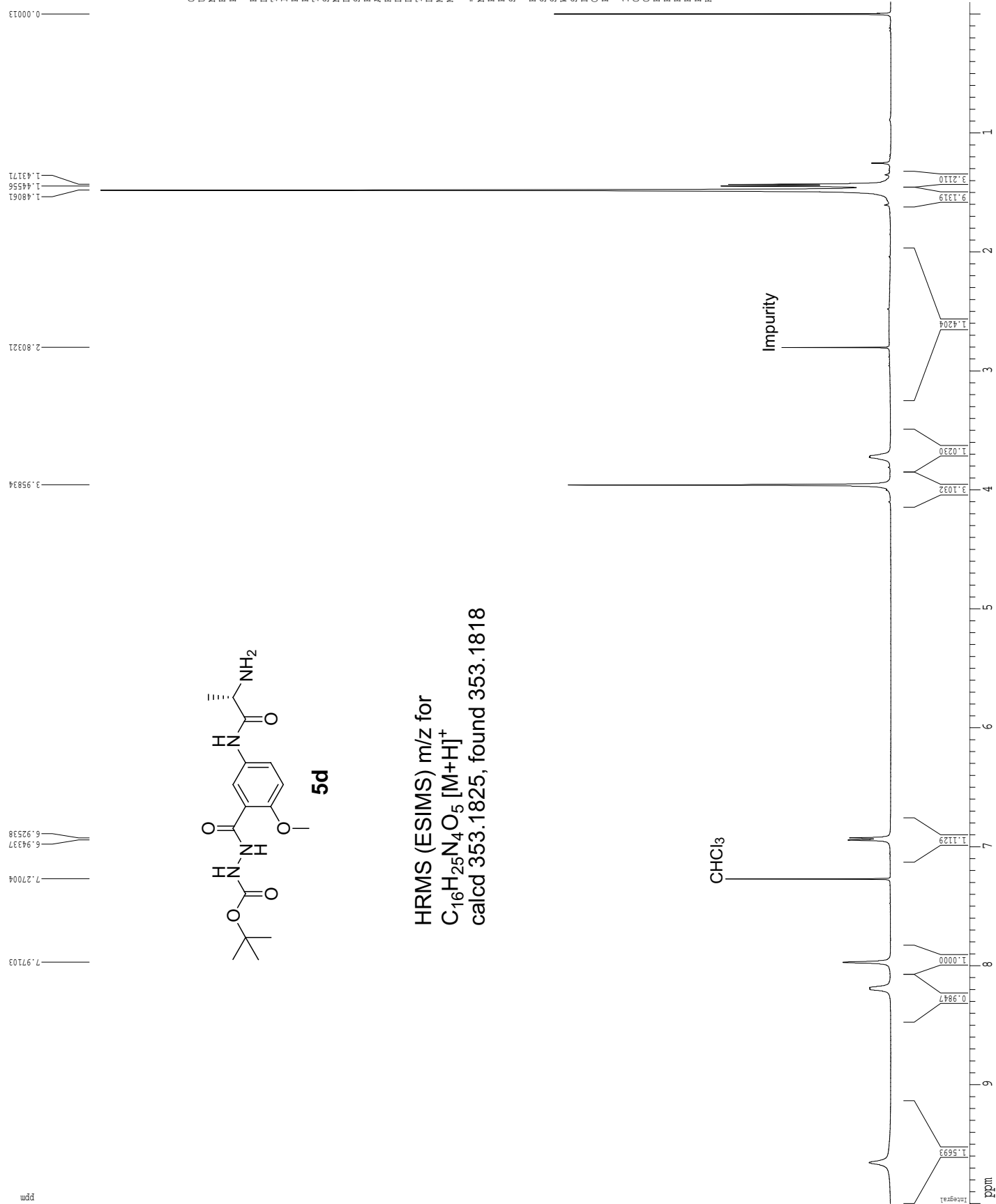
² Tsai, J. H.; Waldman, A-S.; Nowick, J. S. *Bioorg. Med. Chem.*, **1999**, *7*, 29-38.

125 MHz ¹³C NMR Spectrum in CDCl₃





Amine 5d. A 500-mL, three-necked, round-bottomed flask equipped with a nitrogen inlet adapter, a glass stopper, a gas stopper, a gas inlet adapter fitted with a hydrogen balloon, and a magnetic stirring bar was charged with 250 mL of tetrahydrofuran, 100 mL of methanol, and amide **4d** (4.6 g, 9.5 mmol). 10% Pd/C (0.5 g) was added to the reaction mixture under the nitrogen flow. The flask was evacuated and filled with hydrogen and then maintained under the hydrogen atmosphere for 4.5 h. The reaction mixture was filtered through celite, the celite was washed with ethyl acetate (100 mL), and the combined solution was concentrated under vacuum yielding 3.6 g (109%) of amine **5d** as a fluffy white solid, which was used without further purification. An analytical sample was further dried under high vacuum.

500 MHz ¹H NMR Spectrum in CDCl₃

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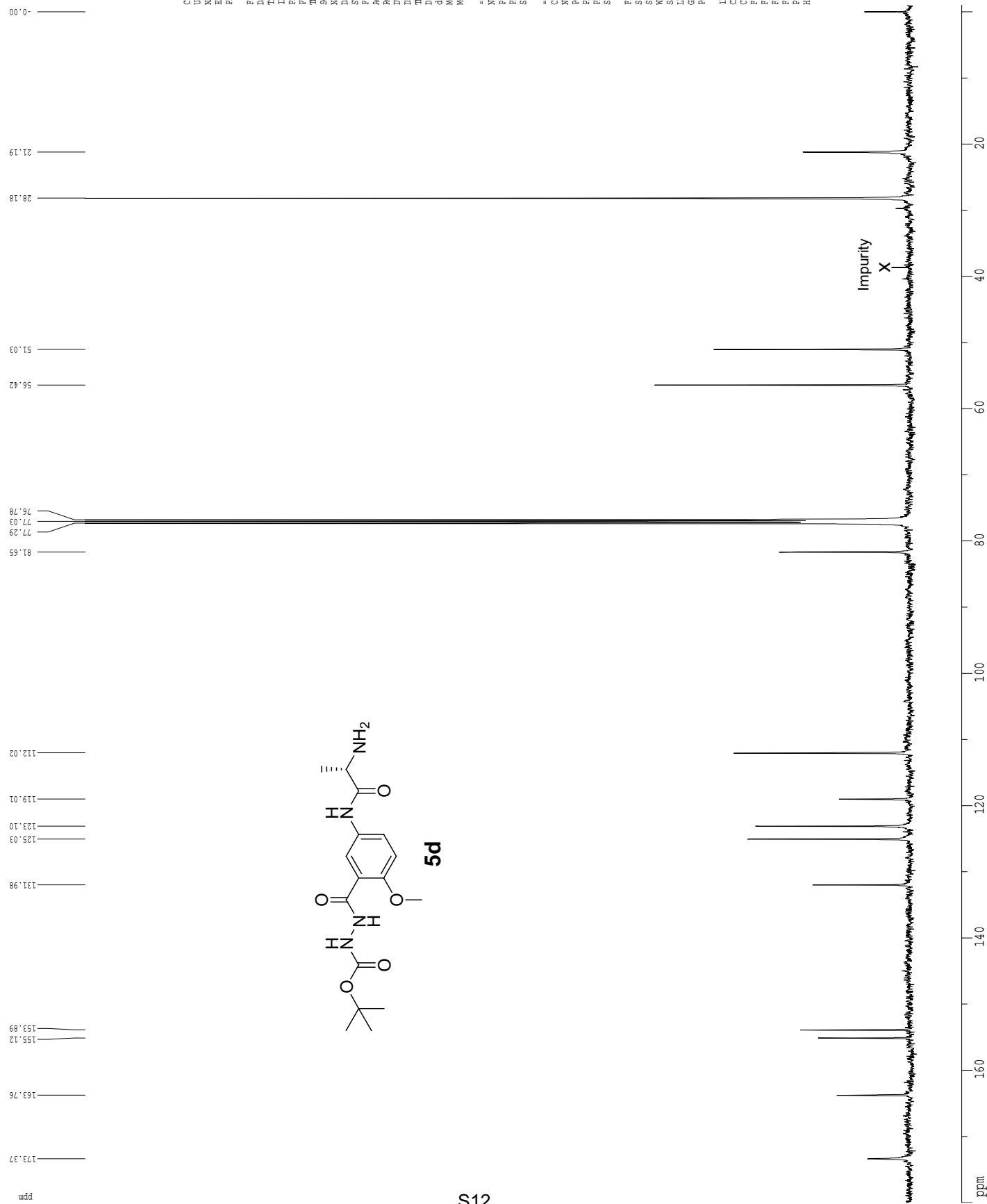
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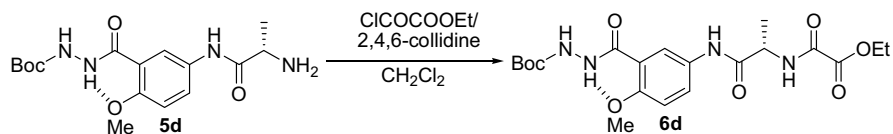
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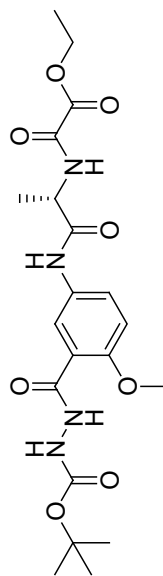
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 HZCN 221.58871 Hz/cm

HRMS (ESIMS) m/z for
 $C_{16}H_{25}N_4O_5 [M+H]^+$
 calcd 353.1825, found 353.1818

125 MHz C13 NMR Spectrum in CDCl₃



Ester 6d. A solution of the amide **5d** (3.30 g, 9.40 mmol) and 2,4,6-collidine (2.50 mL, 19.0 mmol) in dichloromethane (250 mL) was cooled to 0° C with an ice-bath. Ethyl chloroformate (1.05 mL, 9.40 mmol) was slowly added to the stirred solution over 15 min. The solution was left stirred for an extra 15 minutes and washed 1 M HCl (ca. 250 mL), saturated aqueous NaHCO₃ (ca. 250 mL), and water (ca. 250 mL). The solution was dried over MgSO₄, filtered and concentrated to give 4.07 g (96%) of **6d** as a white solid, which was used without further purification. An analytical sample was recrystallized from the ethanol.

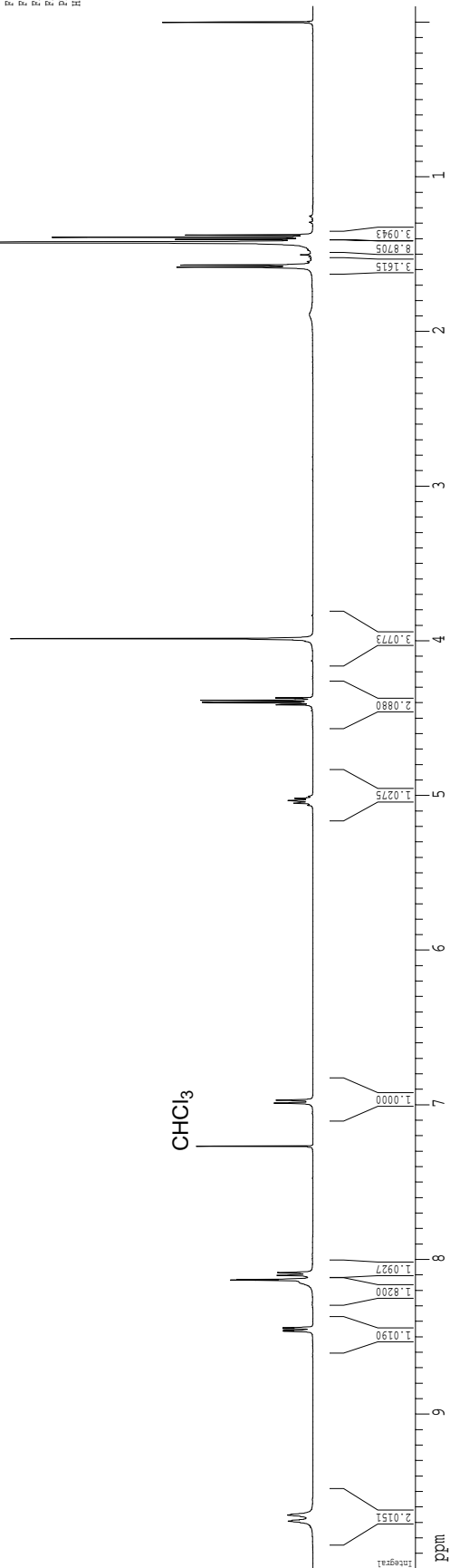
500 MHz ¹H NMR Spectrum in CDCl₃**6d**

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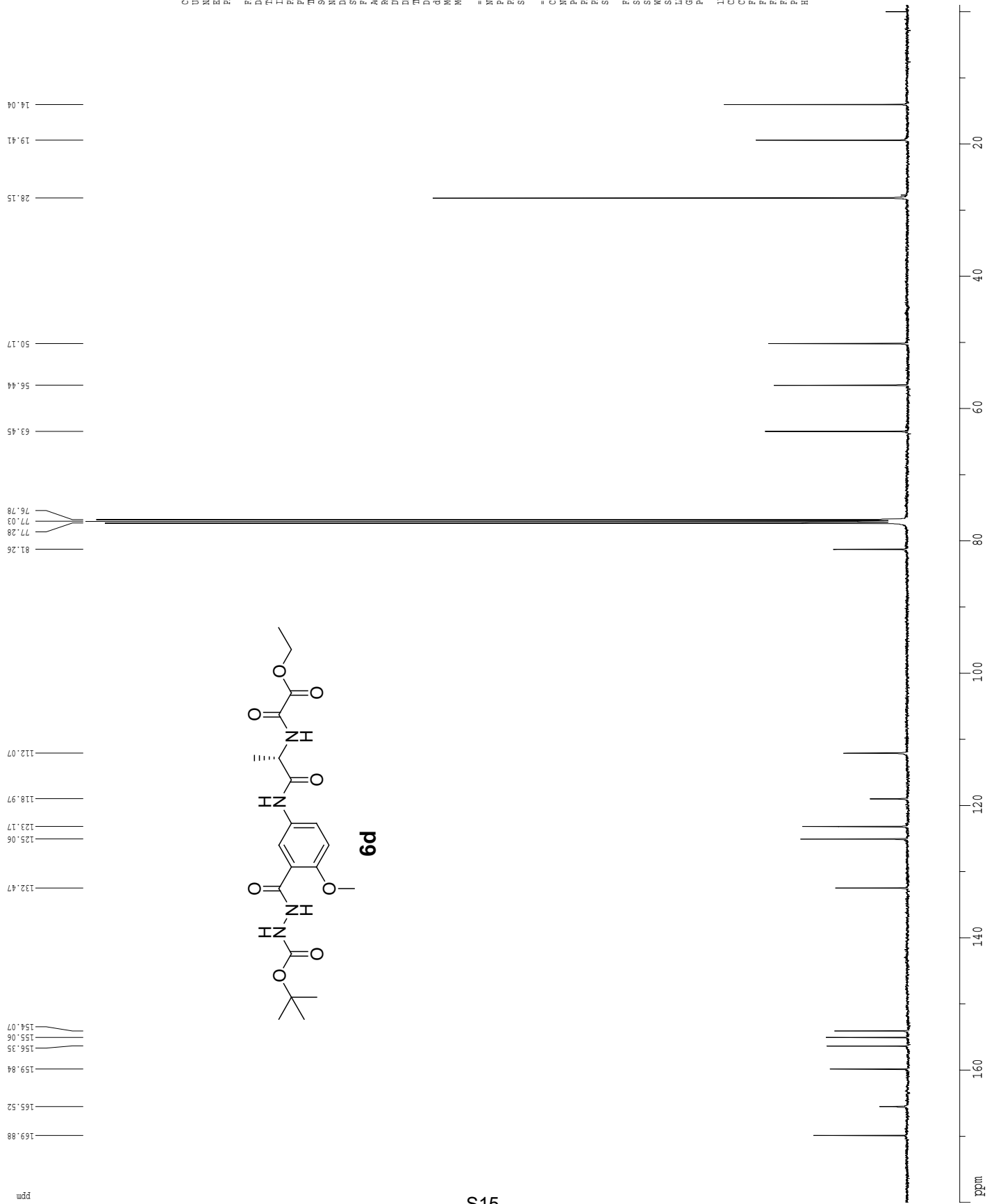
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S14



125 MHz ¹³C NMR spectrum in CDCl₃



```

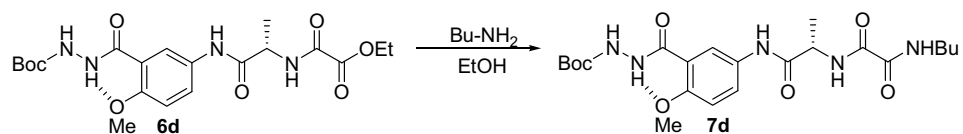
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F3P          -12.578 Hz
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HZCN         998.52008 Hz/cm
    
```



Amide 7d. Butylamine (5.0 mL, 54 mmol) was added in one portion to a solution of the ester **6d** (4.07 g, 9.00 mmol) in ethanol (150 mL). After 10 minutes a white precipitate formed. The precipitate was filtered and dried to yield 3.70 g (86%) of amide **7d** as a white solid.

500 MHz ¹H NMR R Spectrum in CDCl₃



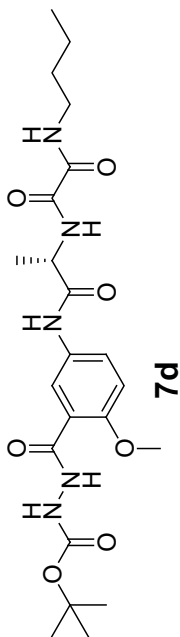
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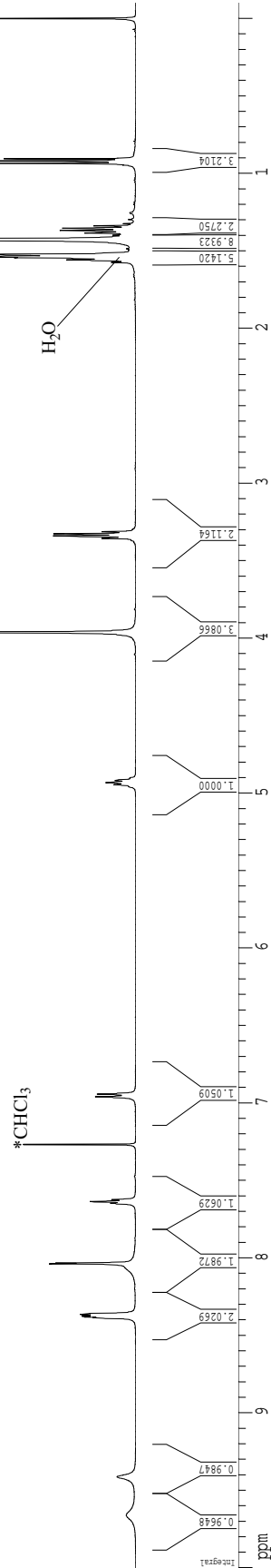
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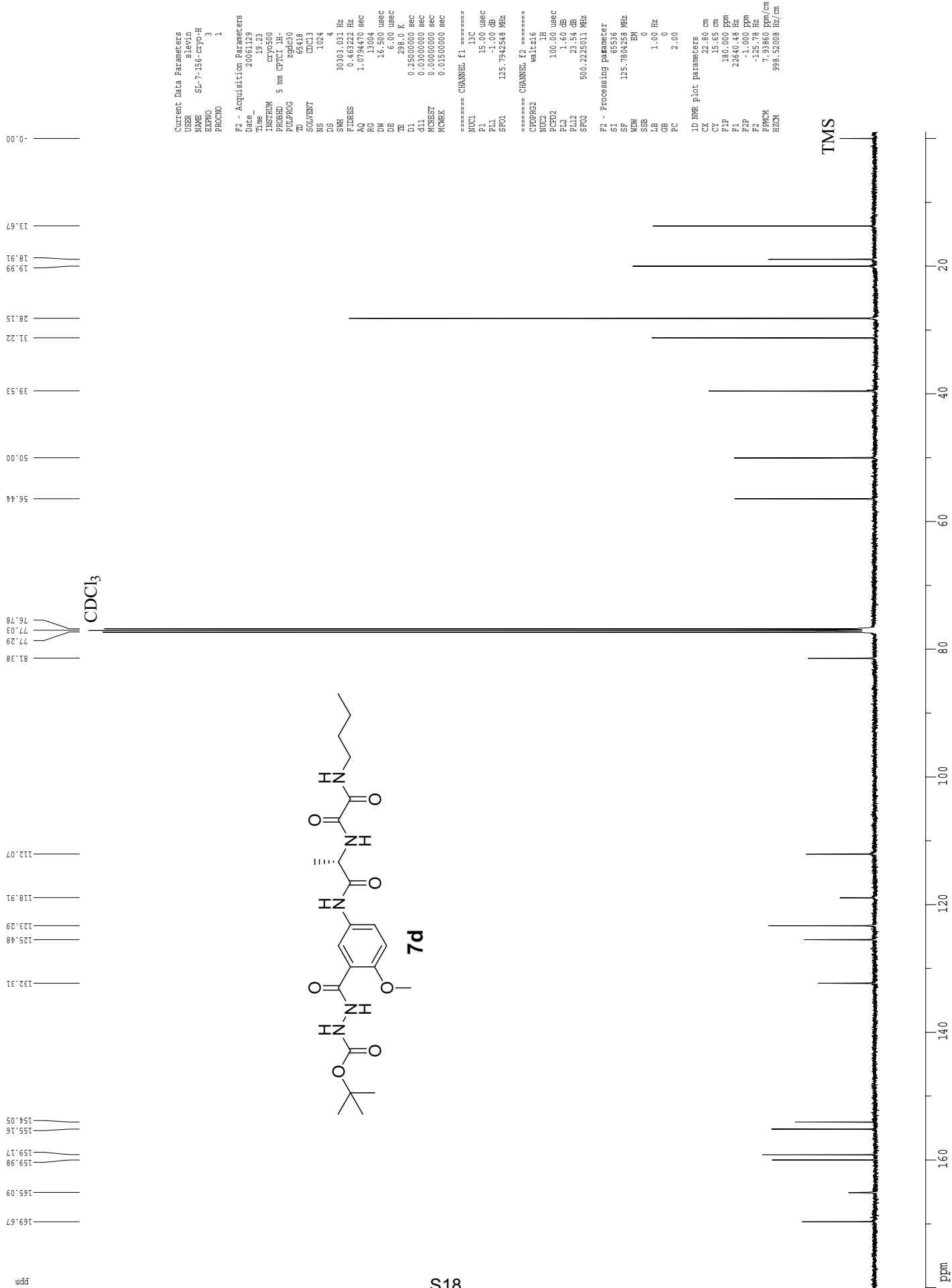
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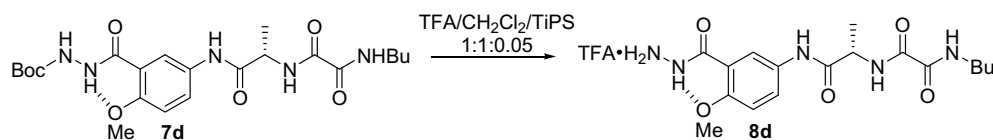


HRMS (ESIMS) m/z for
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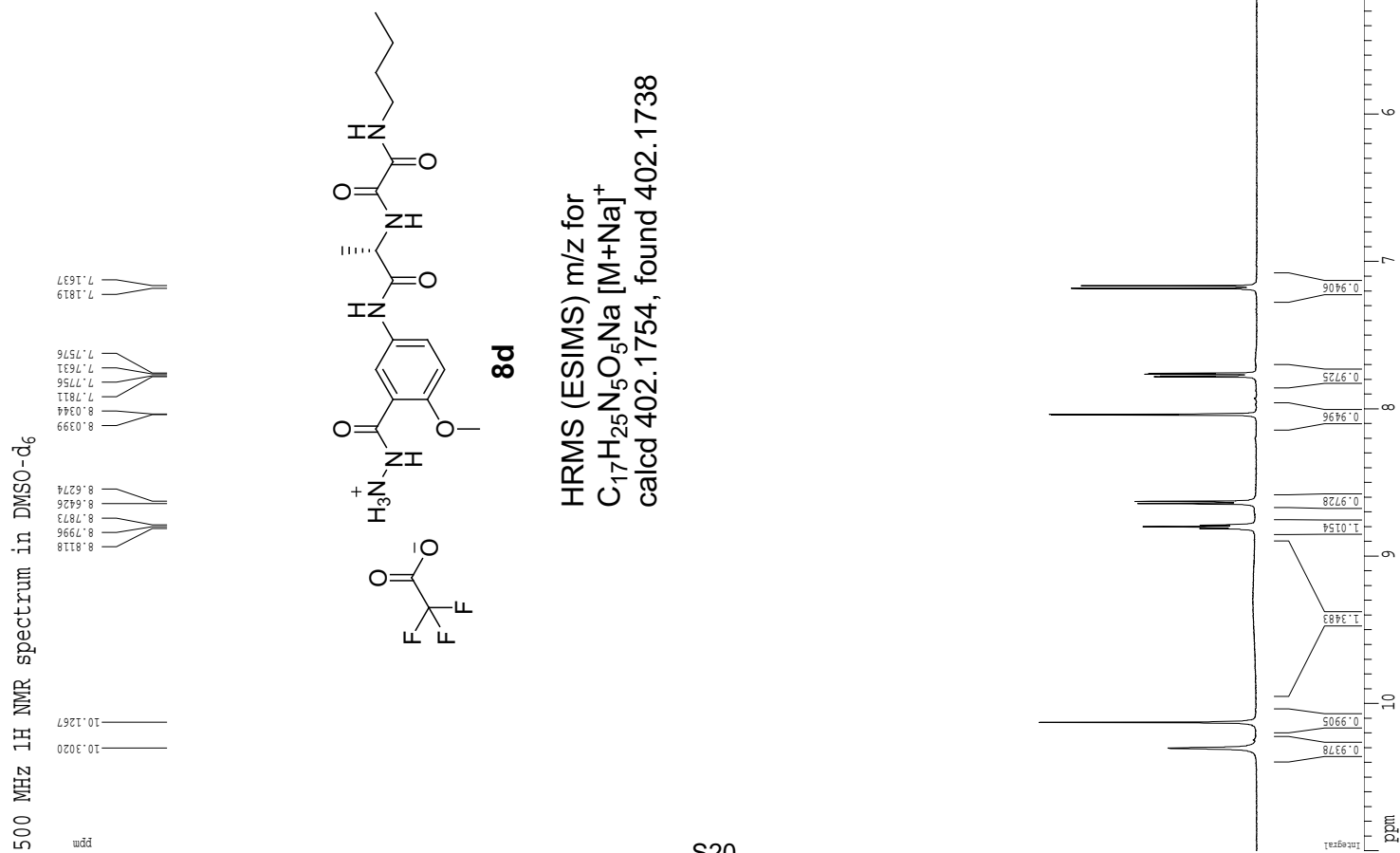


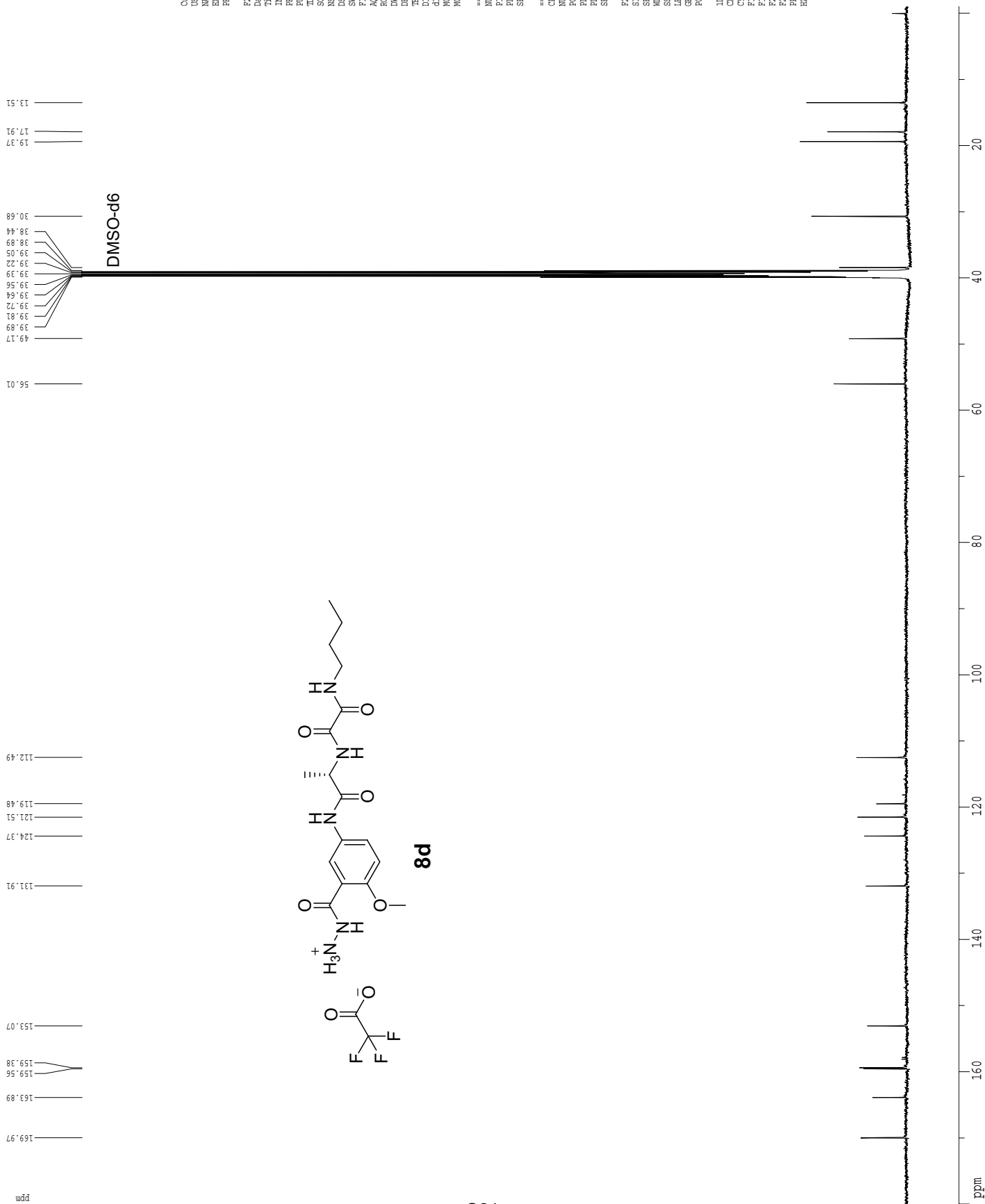
125MHz z13CNM R Spectrum in CDCl₃





Salt 8d. Amide **7d** (3.70 g, 7.37 mmol) was dissolved in a mixture of dichloromethane (100 mL), trifluoroacetic acid (100 mL) and trisopropylsilane (0.5 mL). After 0.5 h, the solution was concentrated and the residue triturated with the diethyl ether to yield 3.55 g (92%) of salt **8d** as a white powder.



125 MHz ¹³C spectrum in DMSO-d₆

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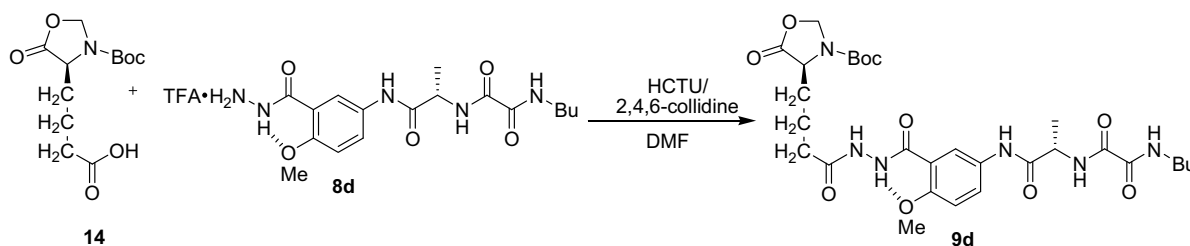
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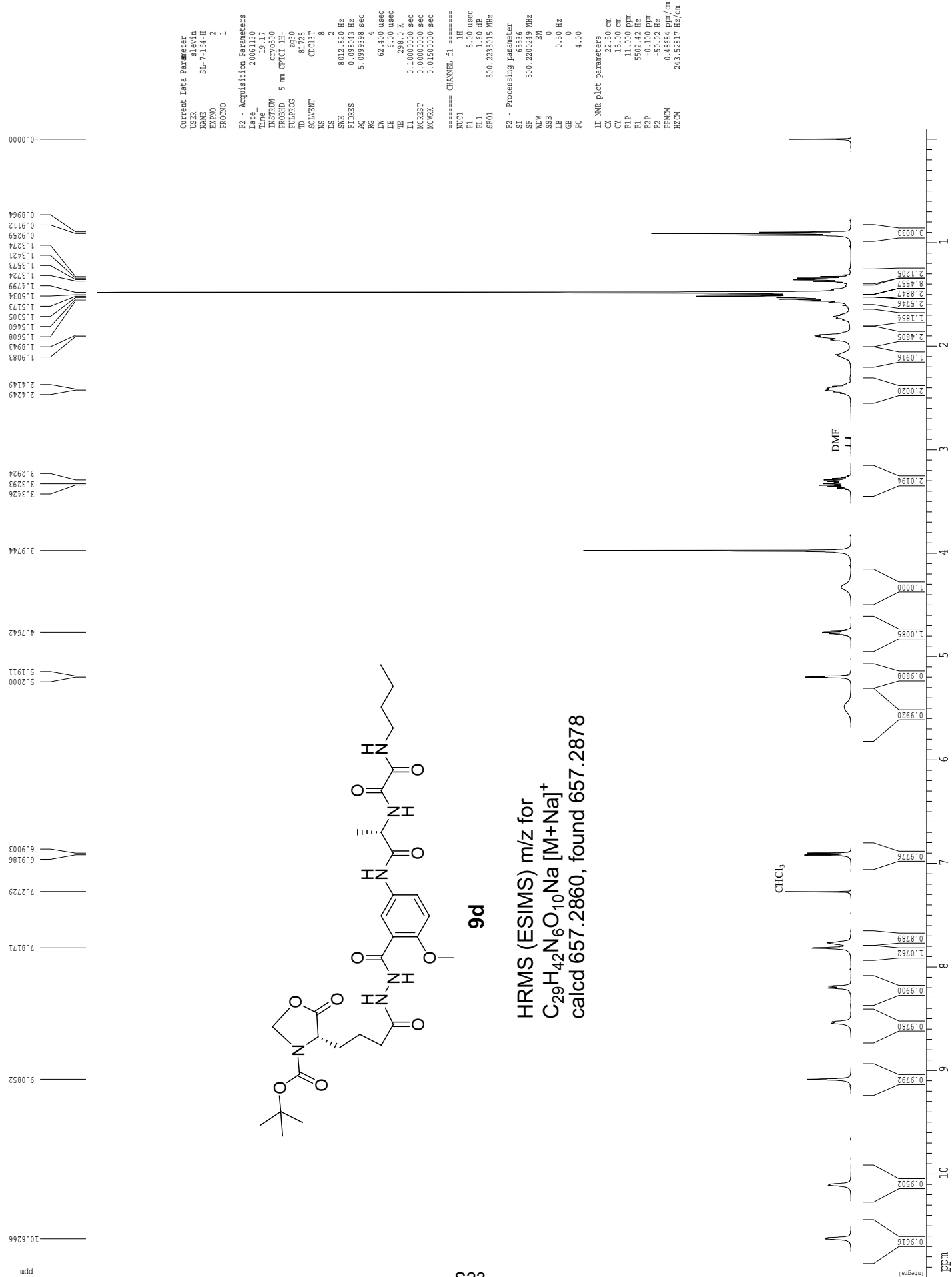


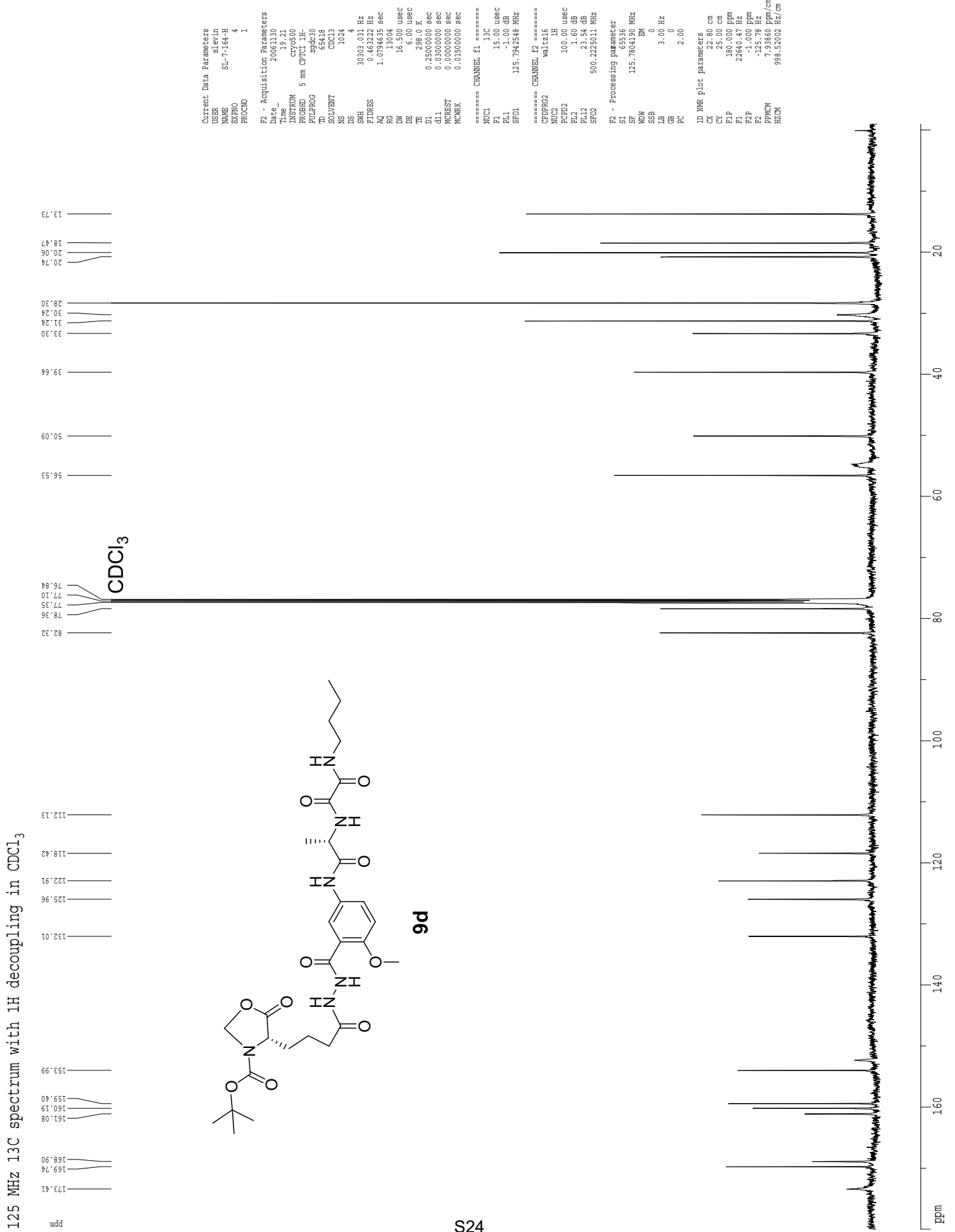
Oxazolidinone 9d. A solution of oxazolidinone **14**^{3,4} (1.7 g, 6.1 mmol), HCTU (2.8 g, 6.7 mmol), and 2,4,6-collidine (2.0 mL, 15.2 mmol) in dimethylformamide (50 mL) was added to a solution of **8d** (3.0 g, 6.1 mmol) and 2,4,6-collidine (2.0 mL, 15 mmol) in dimethylformamide (50 mL). After 6 h, the reaction mixture, was poured into 700 mL ice-water, and the resulting precipitate was filtered and washed with water (200 mL). Upon drying, 3.20 g (83%) of reasonably pure (90% purity) compound **9d** was isolated. Further purification was achieved using column chromatography (4:1 chloroform:*i*-Pr-OH) yielding 2.1 g (54%)⁵ of pure **9d** as a white solid.

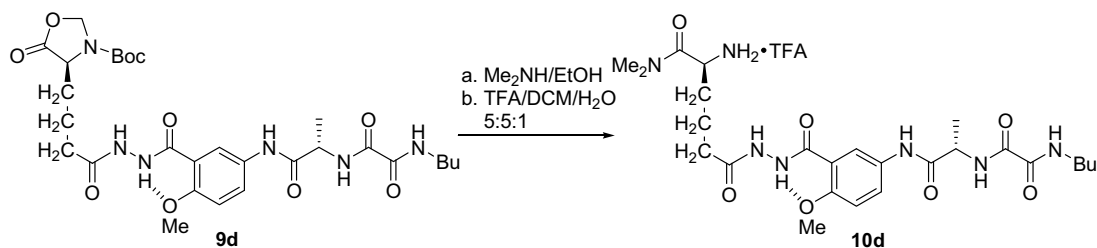
³ Olsen, R. K.; Ramasamy, K. *J. Org. Chem.* **1985**, *50*, 2264-2271.

⁴ **14** was synthesized according to the procedure: Tantry, S. J.; Kantaraju.; Suresh Babu, V. V. *Tetrahedron Lett.* **2002**, *43*, 9461-9462.

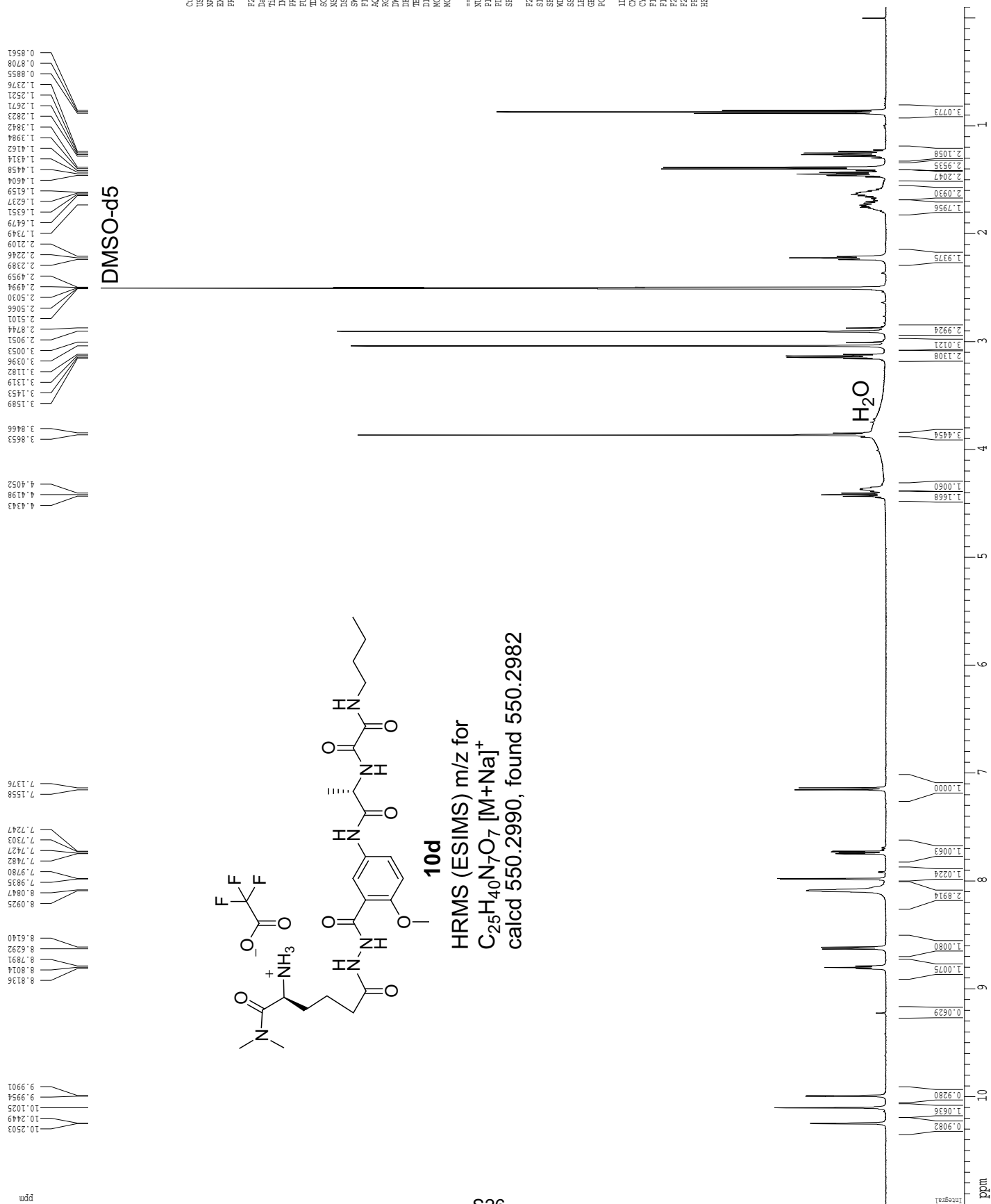
⁵ The low yield is due to compound loss while trying to purify **9d** with different solvent system.

500 MHz ¹H NMR Spectrum in CDCl₃



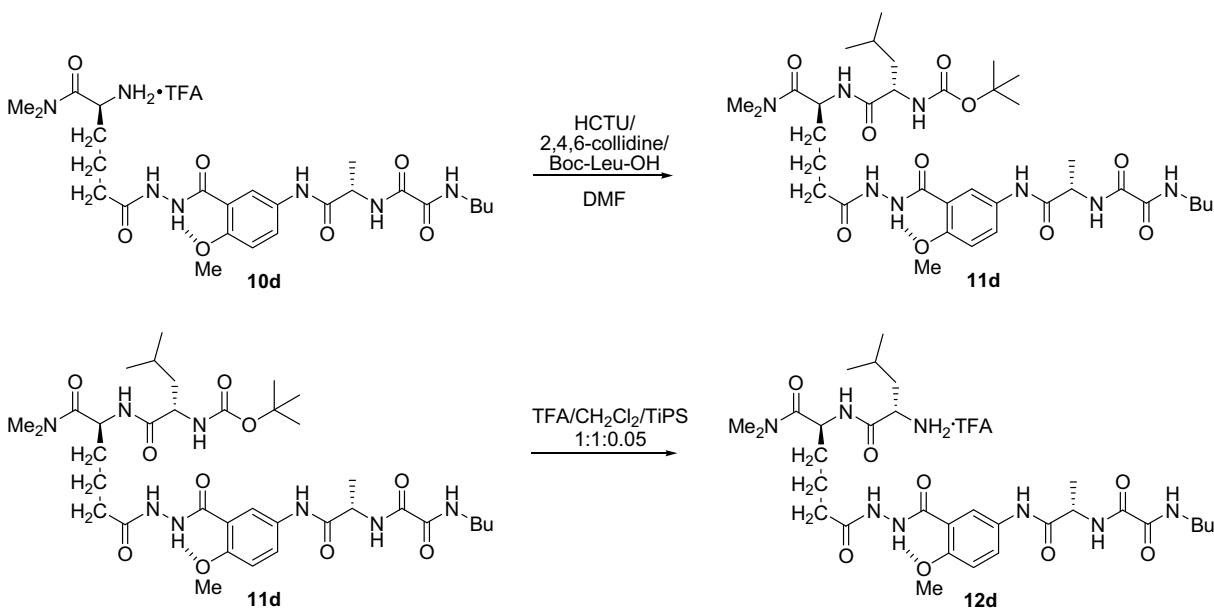


Salt 10d. A 5.6 M solution of dimethylamine in ethanol (15 mL, 84 mmol) was added to a stirred mixture of **9d** (1.5 g, 2.2 mmol) and ethanol (100 mL). The mixture was warmed to form a homogeneous solution, and the solution was stirred for 0.5 h and then concentrated under vacuum. The white residue was dissolved in a deprotection cocktail (100 mL, 5:5:1 TFA:DCM:H₂O) and the resulting solution was left to react for 1 h. The solution was concentrated under vacuum and the residue was triturated with diethyl ether to afford 1.59 g (101%) of **10d** as a white powder, which was used in the next step without purification. An analytical sample was purified by RP-HPLC (C₁₈ column, gradient 20% CH₃CN - 90% H₂O to 90% CH₃CN - 10% H₂O).

500 MHz ¹H NMR spectrum in DMSO-d₆

125 MHz ¹³C NMR Spectrum in DMSO-d₆



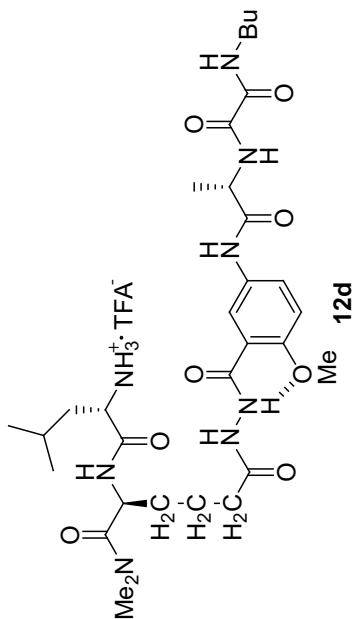


Salt 12d. A solution of **10d** (0.52 g, 0.80 mmol), HCTU (0.39 g, 0.94 mmol), and 2,4,6-collidine (1.0 mL, 7.6 mmol) in DMF (50 mL) was stirred at room temperature for 1.5 h and then concentrated under vacuum to form a brown oil. The oil was triturated with water and dried under vacuum. Purification by column chromatography (9:1 chloroform-isopropanol) yielded 0.33 g (55%) of **11d** as a white solid, which was deprotected for 0.5 h with cleavage cocktail (100 mL, 1:1:0.05 TFA-CH₂Cl₂-triisopropylsilane). The solution was concentrated under vacuum and the residue triturated with diethyl ether to afford 0.25 g (76%) of **12d** as a white solid. The compound was used in the next step without further purification.

500 MHz 1H Spectrum in DMSO-d6



DMSO-d5



HRMS (ESIMS) m/z for
 $C_{31}H_{51}N_8O_8 [M+H]^+$
 calcd 663.3830, found 663.3820

S29

```

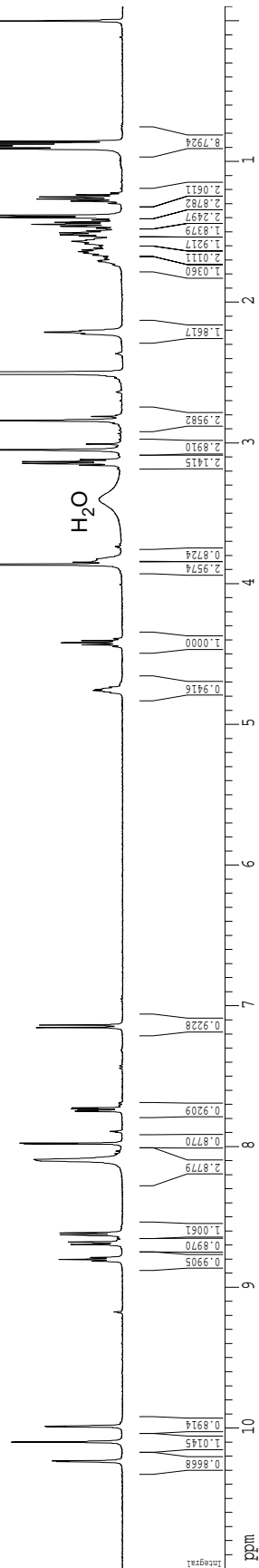
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EXPNO        1
PROCNO       1

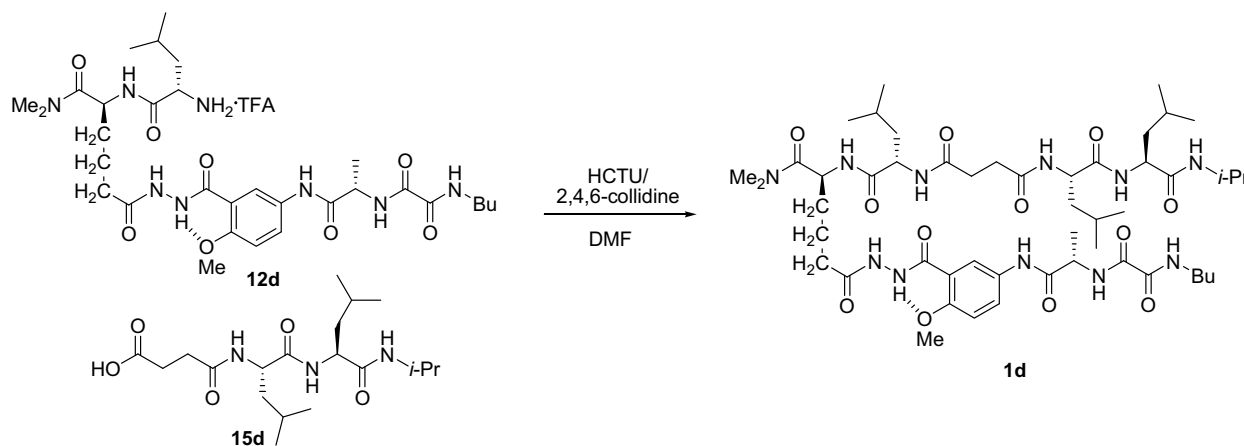
F2 - Acquisition Parameters
Date_         20070106
Time_        17.52
INSTRUM      cryco50
PROBHD       5 mm CPTCI 1H
PULPROG      zg30
TD           81728
SOLVENT      DMSO
NS           8
DS           2
SWH          8012.823 Hz
AQ           0.18883 Hz
RG           5.0990776 sec
FIDRES       62.400 usec
AQRES        298.0 K
DE           6.00 usec
TE           6.00 usec
D1           0.10000000 sec
MCREST       0.00000000 sec
MCWRK       0.01500000 sec

===== CHANNEL f1 =====
NUC1          1H
P1           8.00 usec
PD1          1.60 dB
SFO1         500.2335015 MHz

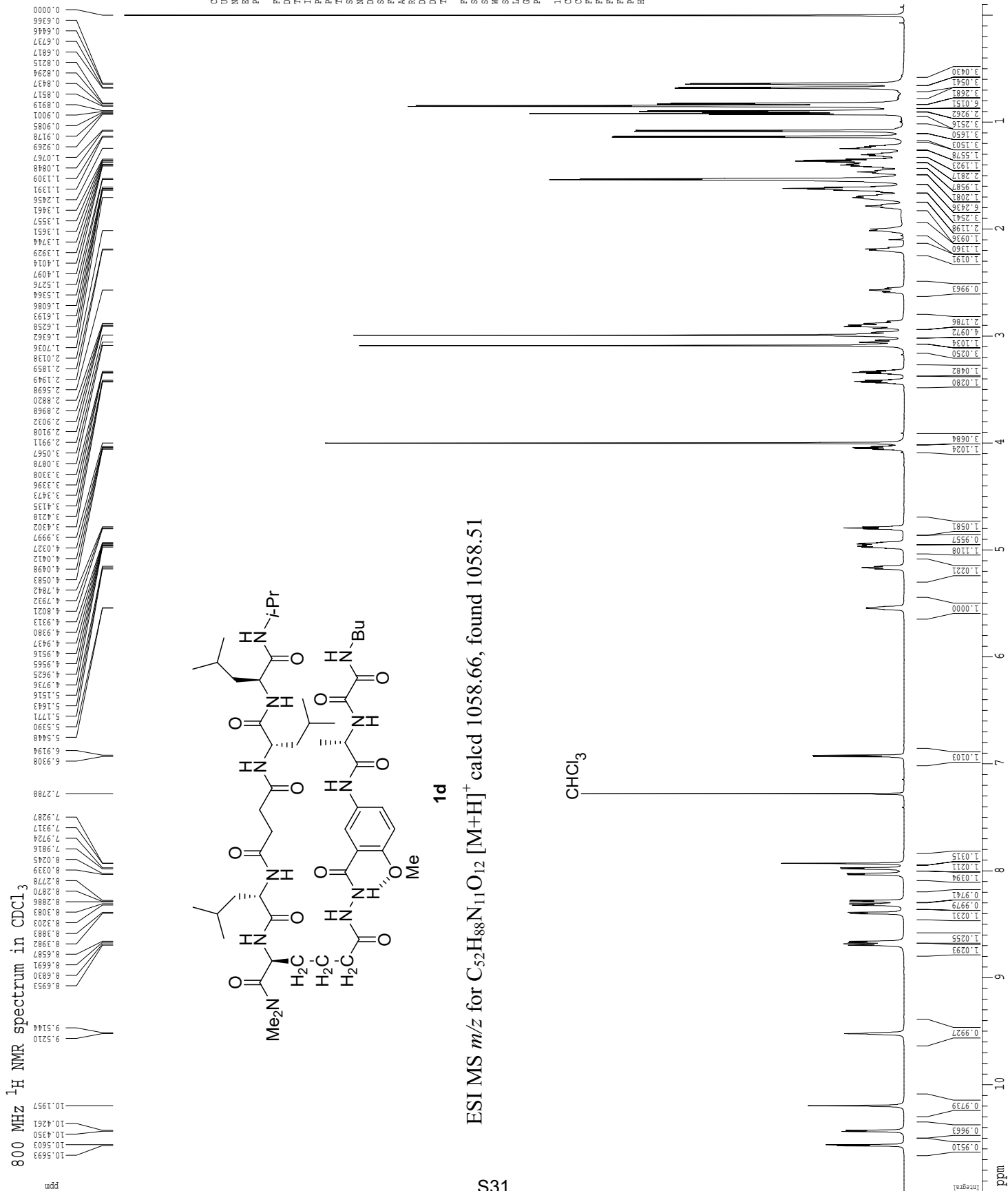
F2 - Processing parameter
SI           65536
SF          500.2200117 MHz
WDW          EM
SSB          0
LB           0.30 Hz
GB           0
PC           4.00

JD NMR Plot parameters
CT          22.80 cm
SI          1500.00 cm
F1P         5502.43 Hz
F2P         -0.1000 ppm
F2          -50.02 Hz
PPMCH      0.48684 ppm/cm
HZCN       243.52815 Hz/cm
    
```

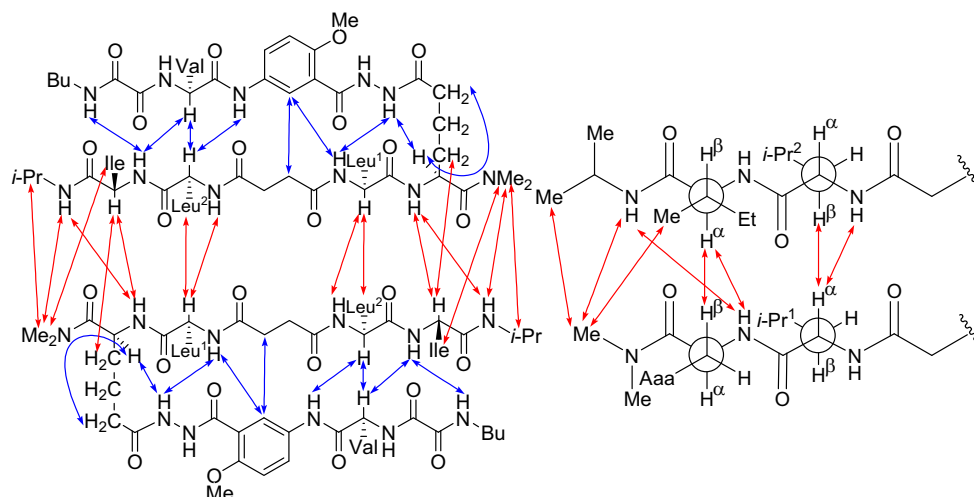




Artificial β -sheet 1d. A mixture of **12d** (0.070 g, 0.090 mmol), **15** (0.035 g, 0.091 mmol) and 2,4,6-collidine (0.12 mL, 0.91 mmol) in dimethylformamide (10 mL) was allowed to react for 3.5 h at room temperature. The solution was concentrated under vacuum and residue was partitioned between dichloromethane (50 mL) and water (50 mL). The water layer was washed extra dichloromethane (50 mL). The organic layers were combined and concentrated to give 0.060g (64%) of **1d** as a white powder, which was further purified by the recrystallization from acetonitrile (2 times), to yield 0.030 g (32%) of **1d** as a white powder.



Spectroscopic DATA for the compound **1a**
(10 mM, CDCl₃ 268K)



Key NOEs assigned as *intermolecular* are represented with red arrows
Key NOEs assigned as *intramolecular* are represented with blue arrows

Key data for amino acids.

Amino acid	H _α Shift ppm	NH Shift ppm	³ J _{NHα} Hz
Aaa	5.15	8.57	8.4
R ₁ = Leu ¹	5.51	8.52	7.7
R ₂ = Leu ²	5.09	8.24	9.7
R ₃ = Ile	4.73	8.70	10.1
R ₄ = Val	4.49	8.05	9.4

Amino adipic acid (Aaa) δ proton resonances.

pro-R: 2.92 ppm, t, (*overlap*)

pro-S: 2.18 ppm, td, (*J*₁ = 11.5 Hz; *J*₂ = 7.0 Hz)

anisotropy = 0.74 ppm

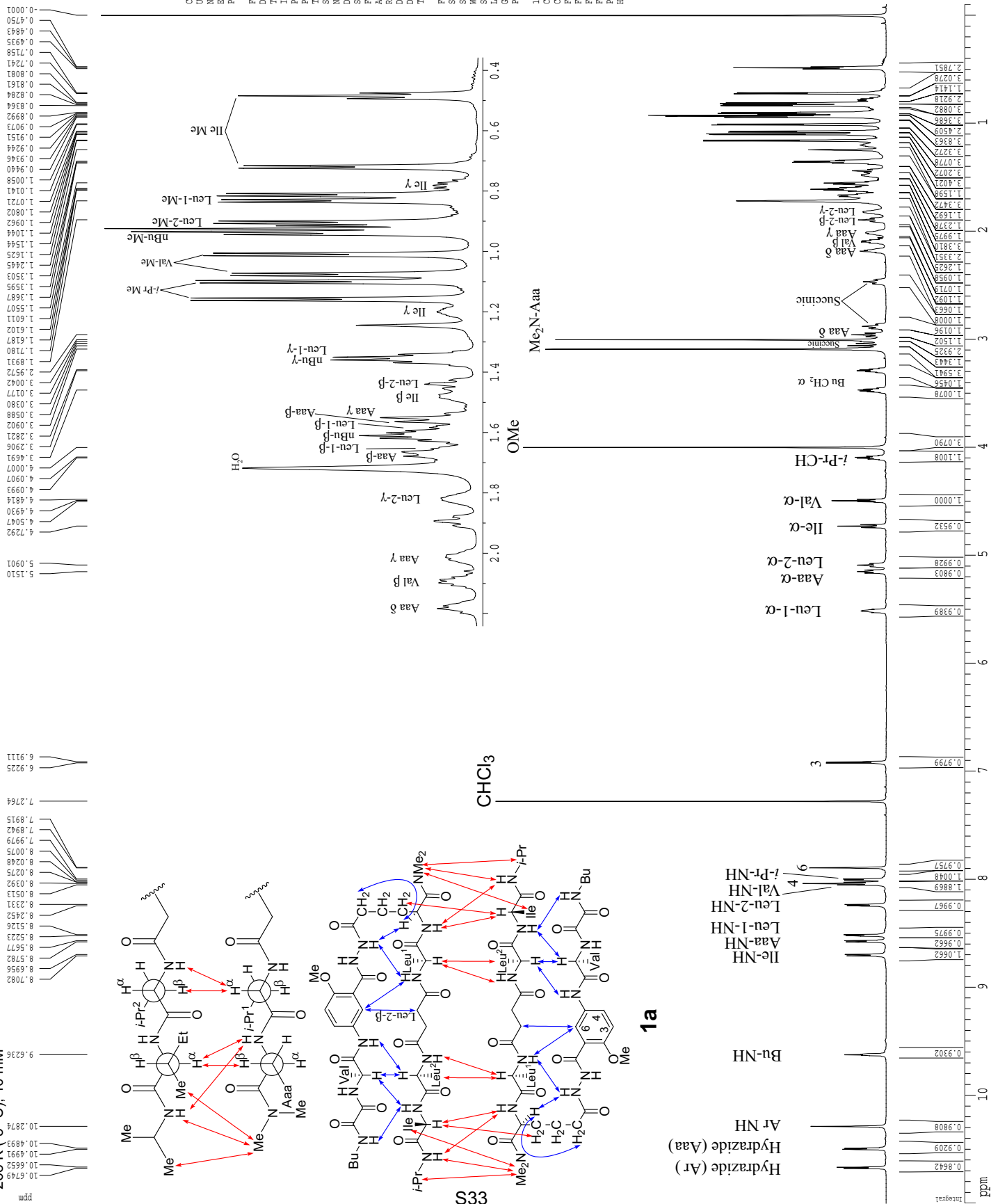
Key data for other NH protons.

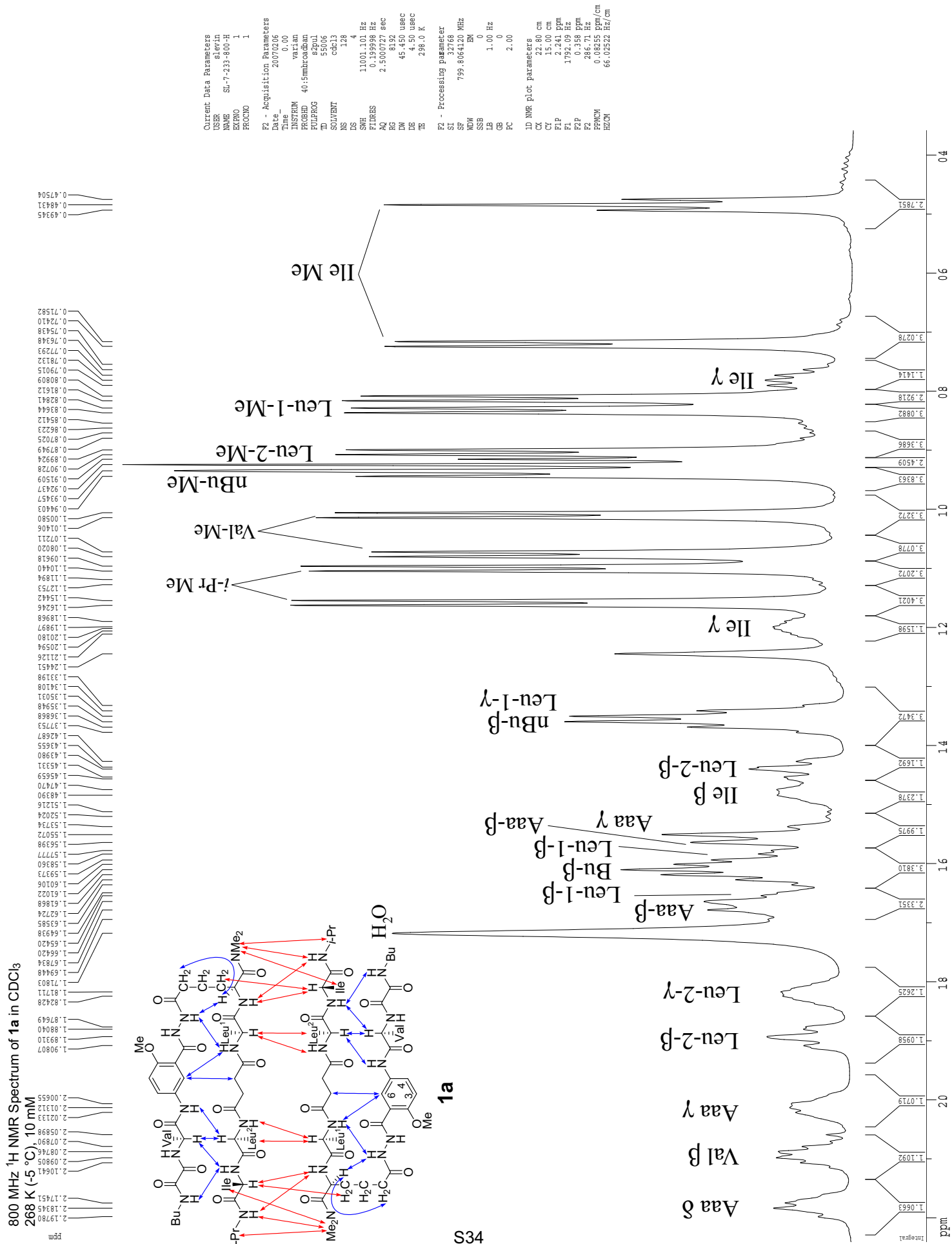
Proton	NH Shift ppm	<i>J</i> Hz
Ar-NH	10.29	-
Hydrazide Ar	10.67	7.7
Hydrazide Aaa	10.49	7.7
Bu-NH	9.62	5.5
<i>i</i> -Pr-NH	8.00	8.1

ESI MS *m/z* for C₅₂H₈₈N₁₁O₁₂ [M+H]⁺ calcd 1058.66, found 1058.51.

800 MHz ¹H NMR Spectrum of **1a** in CDCl₃

268 K (-5 °C), 10 mM





Supporting Information

Current Data Parameters
 USER slevin
 NAME SL-7-233-800-H
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters

Date_ 20070206
 Time 0.00
 INSTRUM varian
 PROBHD 40:5mmroadban
 PULPROG zgpg30
 TD 4096
 SOLVENT cdcl3
 NS 8
 DS 64
 SWH 11001.101 Hz
 FIDRES 2.685816 Hz
 AQ 0.1843700 sec
 RG 4096
 DW 45.450 usec
 DE 231.43 usec
 TE 268.5 K

F1 - Acquisition Parameters

ND0 1
 TD 512
 SFO1 799.8107 MHz
 FIDRES 21.486525 Hz
 SW 13.755 ppm
 FhMODE undefined

F2 - Processing parameters

SI 2048
 SF 799.8064119 MHz
 WDW SINE
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.40

F1 - Processing parameters

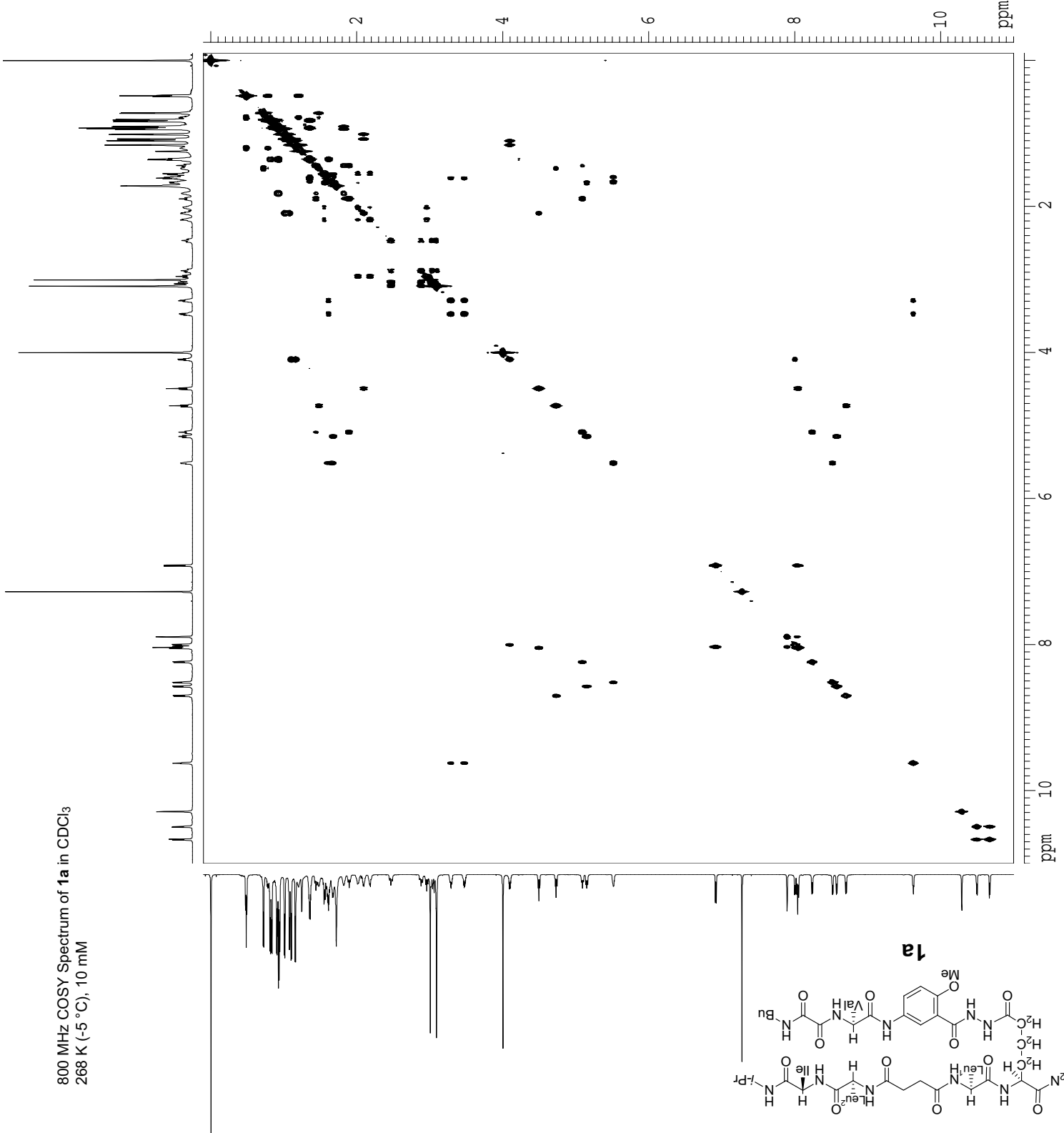
SI 512
 MC2 QF
 SF 799.8064119 MHz
 WDW SINE
 SSB 0
 LB 0.00 Hz
 GB 0

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2D NMR plot parameters

CX2 15.00 cm
 CX1 15.00 cm
 F2PLO 11.000 ppm
 F2LO 8797.87 Hz
 F2PHI -0.100 ppm
 F2HI -79.98 Hz
 F1PLO 11.000 ppm
 F1LO 8797.87 Hz
 F1PHI -0.100 ppm
 F1HI -79.98 Hz
 F2PPMCM 0.74000 ppm/cm
 F2HZCM 591.85669 Hz/cm
 F1PPMCM 0.74000 ppm/cm
 F1HZCM 591.85669 Hz/cm

800 MHz COSY Spectrum of **1a** in CDCl₃
 268 K (-5 °C), 10 mM



Current Data Parameters
 USER slevin
 NAME SL-7-233-800-H
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters

Date_ 20070206
 Time 0.00
 INSTRUM varian
 PROBHD 40:5mmroadban
 PULPROG gcpsy
 TD 4096
 SOLVENT cdc13
 NS 8
 DS 64
 SWH 11001.101 Hz
 FIDRES 2.685816 Hz
 AQ 0.1843700 sec
 RG 4096
 DW 45.450 usec
 DE 231.43 usec
 TE 268.5 K

F1 - Acquisition parameters

ND0 1
 TD 512
 SF01 799.8107 MHz
 FIDRES 21.486525 Hz
 SW 13.755 ppm
 F1MODE undefined

F2 - Processing parameters

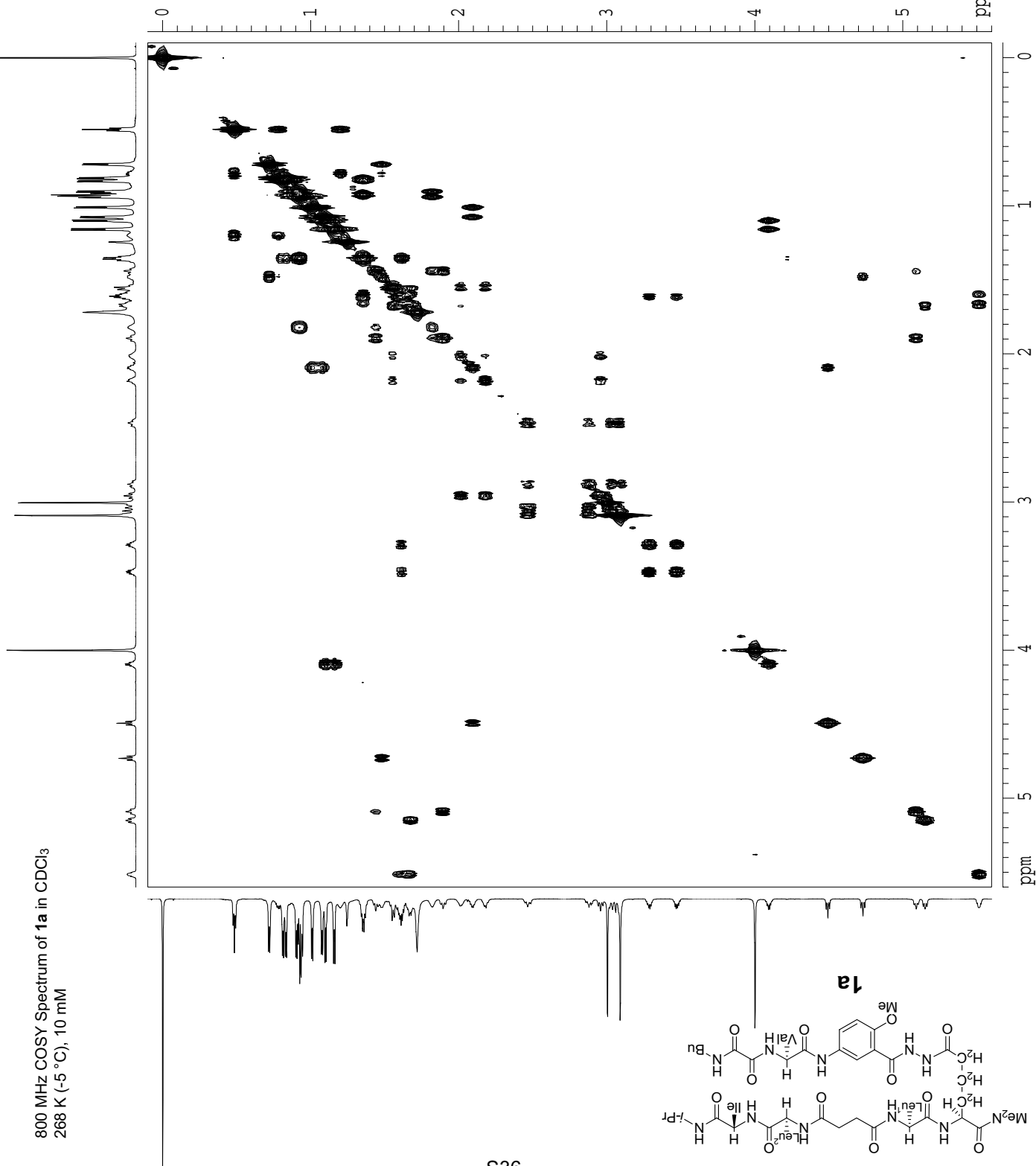
SI 2048
 SF 799.8064119 MHz
 WDW SINE
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.40

F1 - Processing parameters

SI 512
 MC2 QF
 SF 799.8064119 MHz
 WDW SINE
 SSB 0
 LB 0.00 Hz
 GB 0

2D NMR plot parameters

CX2 15.00 cm
 CX1 15.00 cm
 F2PLO 5.600 ppm
 F2LO 4478.92 Hz
 F2PHI -0.100 ppm
 F2HI -79.98 Hz
 F1PLO 5.600 ppm
 F1LO 4478.92 Hz
 F1PHI -0.100 ppm
 F1HI -79.98 Hz
 F2PWC 0.38000 ppm/cm
 F2ZCM 303.92645 Hz/cm
 F1PWC 0.38000 ppm/cm
 F1ZCM 303.92645 Hz/cm



Current Data Parameters
 USER slevin
 NAME SL-7-233-800-H
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters

Date_ 20070206
 Time_ 0.00
 INSTRUM varian
 PROBHD 40:5mm broadband
 PULPROG gcosy
 TD 4096
 SOLVENT cdcl3
 NS 8
 DS 64
 SWH 11001.101 Hz
 FIDRES 2.685816 Hz
 AQ 0.1843700 sec
 RG 4096
 DW 45.450 usec
 DE 231.43 usec
 TE 268.5 K

F1 - Acquisition parameters

ND0 1
 TD 512
 SF01 799.8107 MHz
 FIDRES 21.486525 Hz
 SW 13.755 ppm
 FMODE undefined

F2 - Processing parameters

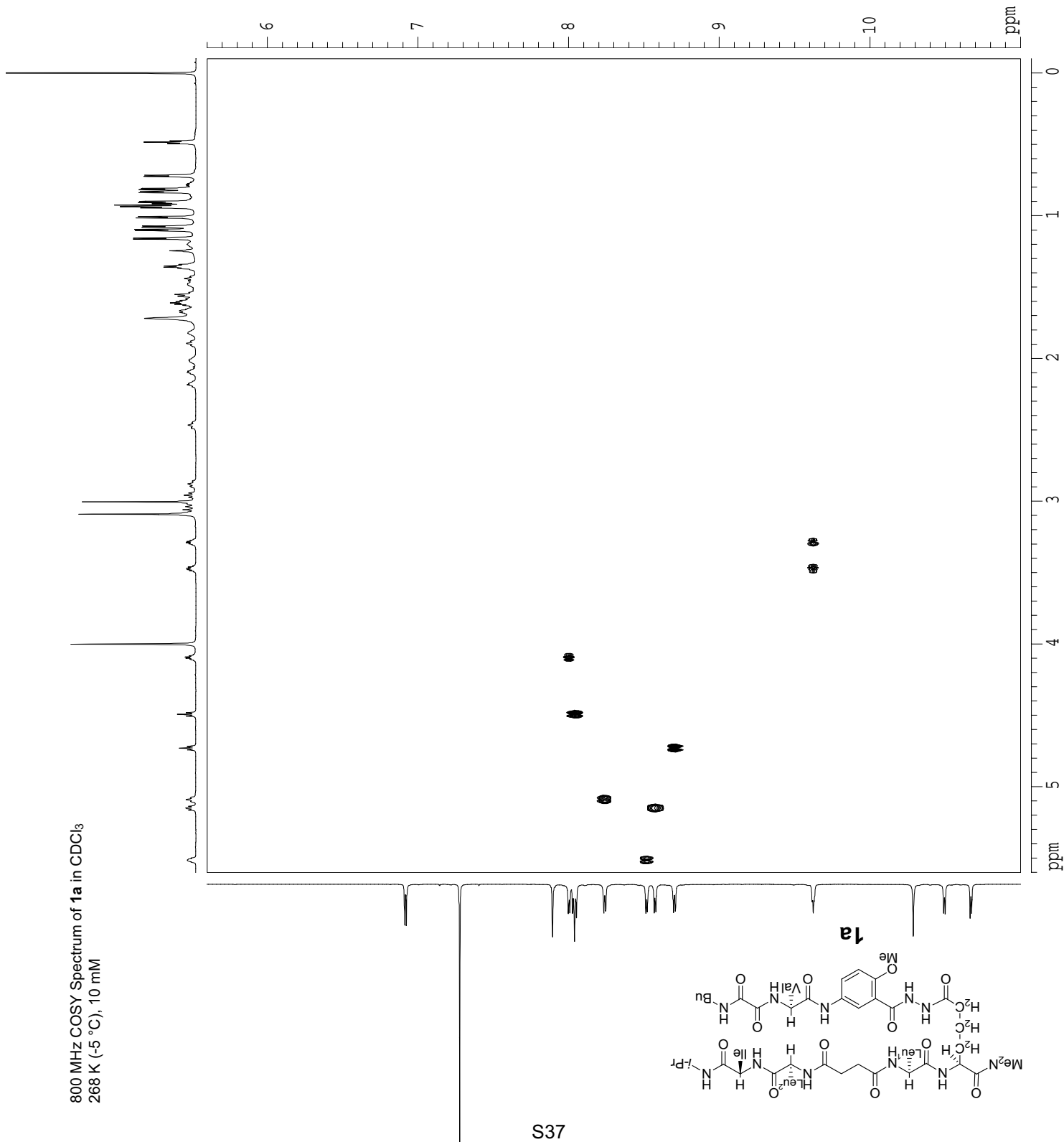
SI 2048
 SF 799.8064119 MHz
 WDW SINE
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.40

F1 - Processing parameters

SI 512
 MC2 QF
 SF 799.8064119 MHz
 WDW SINE
 SSB 0
 LB 0.00 Hz
 GB 0

2D NMR plot parameters

CX2 15.00 cm
 CX1 15.00 cm
 F2PLO 5.602 ppm
 F2LO 4480.61 Hz
 F2PHI -0.100 ppm
 F2HI -79.98 Hz
 F1PLO 11.000 ppm
 F1LO 8797.87 Hz
 F1PHI 5.600 ppm
 F1HI 4478.92 Hz
 F2PFCM 0.38014 ppm/cm
 F2HZCM 304.03955 Hz/cm
 F1PFCM 0.36000 ppm/cm
 F1HZCM 287.93030 Hz/cm



Current Data Parameters
 USER slevin
 NAME SL-7-233-800-H
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters

Date_ 20070206
 Time_ 0.00
 INSTRUM varian
 PROBHD 40:5mmbroadban
 PULPROG gpcsy
 TD 4096
 SOLVENT cdcl3
 NS 8
 DS 64
 SWH 11001.101 Hz
 FIDRES 2.685816 Hz
 AQ 0.1843700 sec
 RG 4096
 DW 45.450 usec
 DE 231.43 usec
 TE 268.5 K

F1 - Acquisition parameters

ND0 1
 TD 512
 SFO1 799.8107 MHz
 FIDRES 21.486525 Hz
 SW 13.755 ppm
 FMODE undefined

F2 - Processing parameters

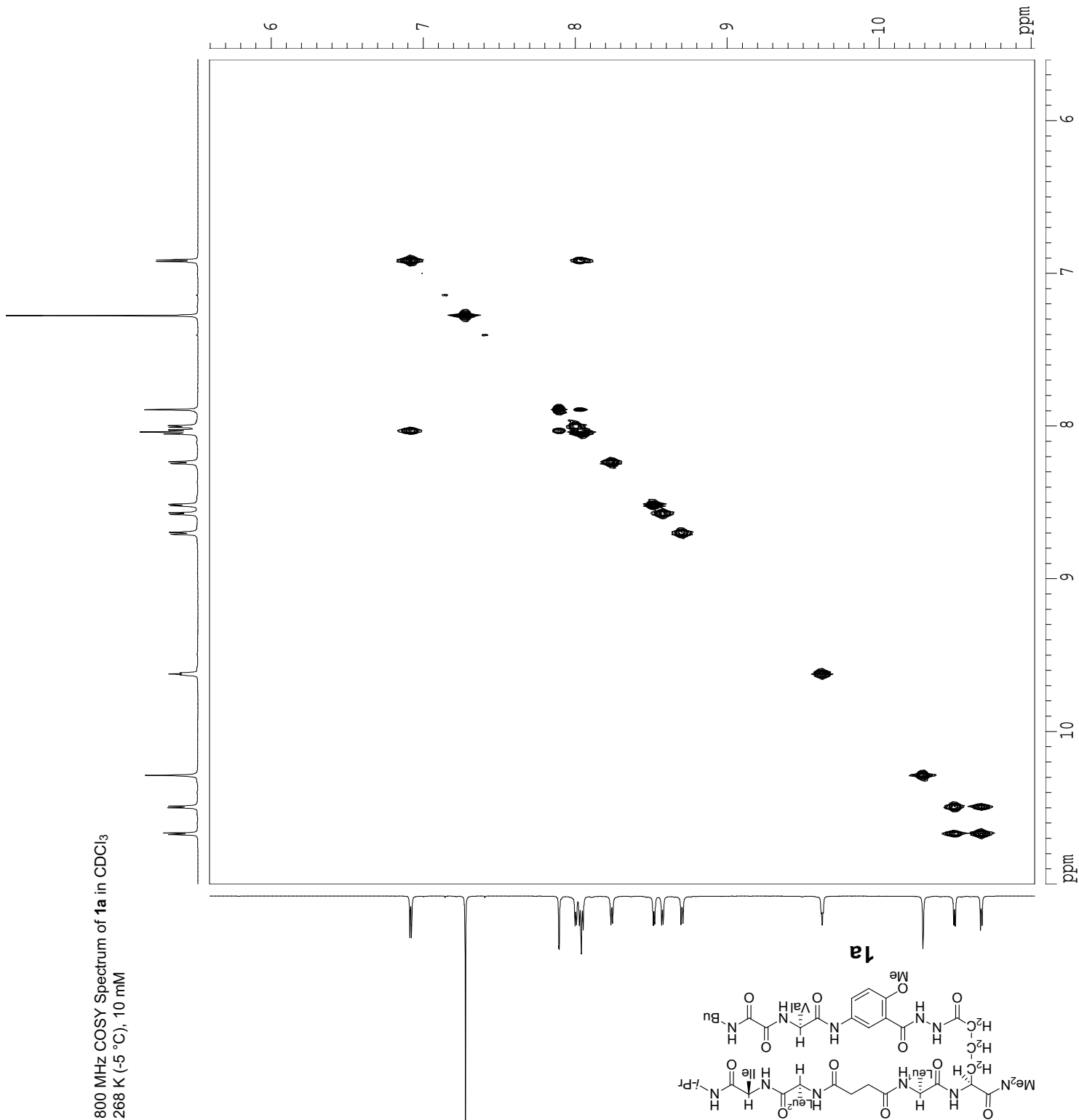
SI 2048
 SF 799.8064119 MHz
 WDW SINE
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.40

F1 - Processing parameters

SI 512
 MC2 QF
 SF 799.8064119 MHz
 WDW SINE
 SSB 0
 LB 0.00 Hz
 GB 0

2D NMR plot parameters

CX2 15.00 cm
 CX1 15.00 cm
 F2PLO 11.000 ppm
 F2LO 8797.87 Hz
 F2PHI 5.600 ppm
 F2HI 4478.92 Hz
 F1PLO 11.022 ppm
 F1LO 8815.52 Hz
 F1PHI 5.595 ppm
 F1HI 4475.24 Hz
 F2PWCW 0.36000 ppm/cm
 F2HZCW 287.93030 Hz/cm
 F1PWCW 0.36178 ppm/cm
 F1HZCW 289.35184 Hz/cm



Current Data Parameters
 USER slewin
 NAME SL-7-233-800-H
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters

Date_ 20070206
 Time_ 0:00
 INSTRUM varian
 PROBHD 40:5mm broadband
 PULPROG gcosy
 TD 4096
 SOLVENT cdc13
 NS 8
 DS 64
 SWH 11001.101 Hz
 FIDRES 2.685816 Hz
 AQ 0.1843700 sec
 RG 4096
 DW 45.450 usec
 DE 231.43 usec
 TE 268.5 K

F1 - Acquisition parameters

ND0 1
 TD 512
 SF01 799.8107 MHz
 FIDRES 21.486525 Hz
 SW 13.755 ppm
 F1MODE undefined

F2 - Processing parameters

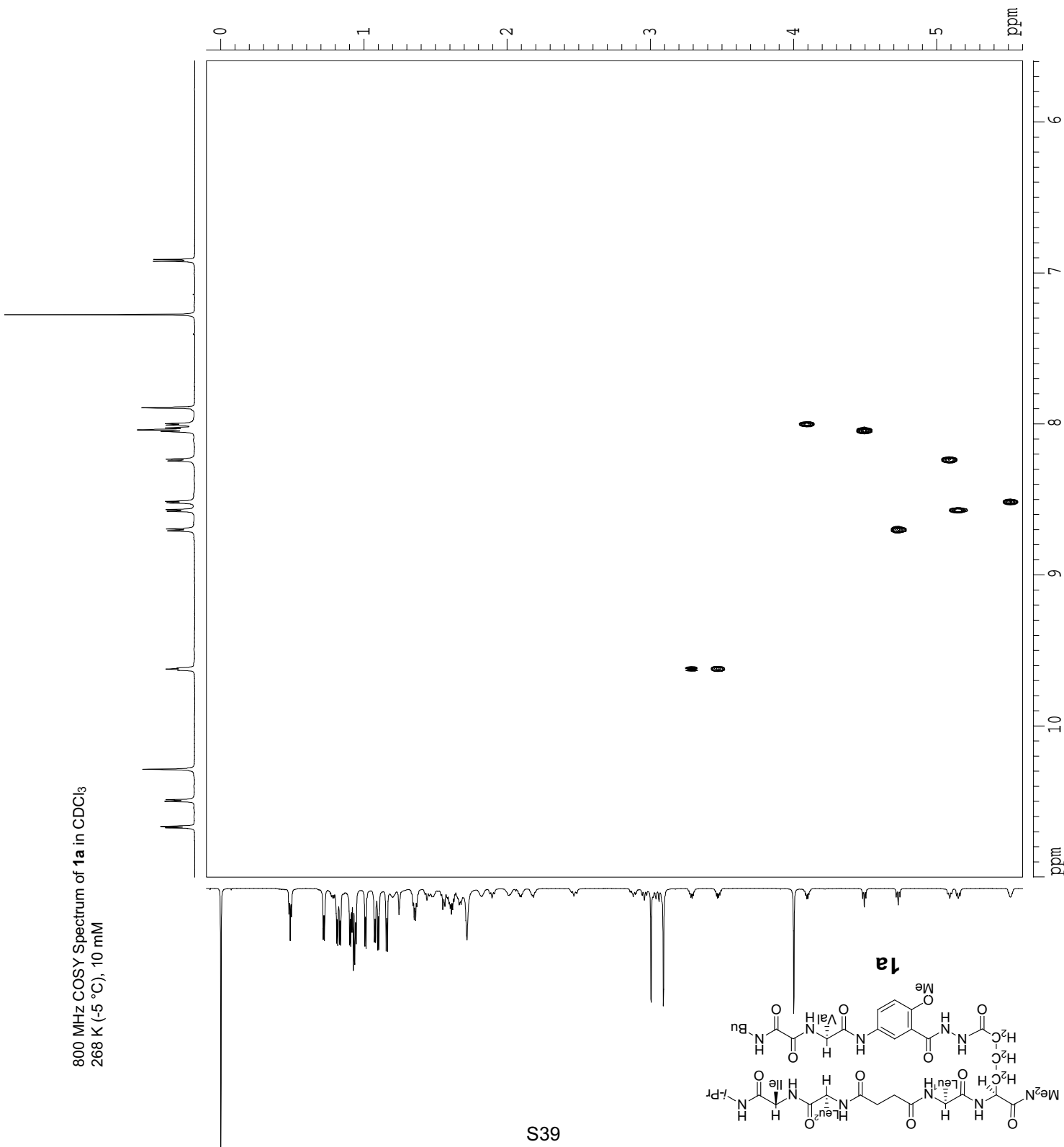
SI 2048
 SF 799.8064119 MHz
 SINE SINE
 WDW 0
 LB 0.00 Hz
 GB 0
 PC 1.40

F1 - Processing parameters

SI 512
 MC2 QF
 SF 799.8064119 MHz
 WDW SINE
 SSB 0
 LB 0.00 Hz
 GB 0

2D NMR plot parameters

CX2 15.00 cm
 CX1 15.00 cm
 F2PLO 11.002 ppm
 F2LO 8799.40 Hz
 F2PHI 5.595 ppm
 F2HI 4475.24 Hz
 F1PLO 5.600 ppm
 F1LO 4478.92 Hz
 F1PHI -0.100 ppm
 F1HI -79.98 Hz
 F2PPMCM 0.36043 ppm/cm
 F2HZCM 288.27753 Hz/cm
 F1PPMCM 0.38000 ppm/cm
 F1HZCM 303.92645 Hz/cm



Current Data Parameters
 USER slevin
 NAME SL-7-233-800-H
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters

Date_ 20070206
 Time 0.00
 INSTRUM varian
 PROBHD 40:5mmBroadban
 PULPROG gcosy
 TD 4096
 SOLVENT cdcl3
 NS 8
 DS 64
 SWH 11001.101 Hz
 FIDRES 2.685816 Hz
 AQ 0.1843700 sec
 RG 4096
 DW 45.450 usec
 DE 231.43 usec
 TE 268.5 K

F1 - Acquisition parameters

ND0 1
 TD 512
 SF01 799.8107 MHz
 FIDRES 21.486525 Hz
 SW 13.755 ppm
 F1MODE undefined

F2 - Processing parameters

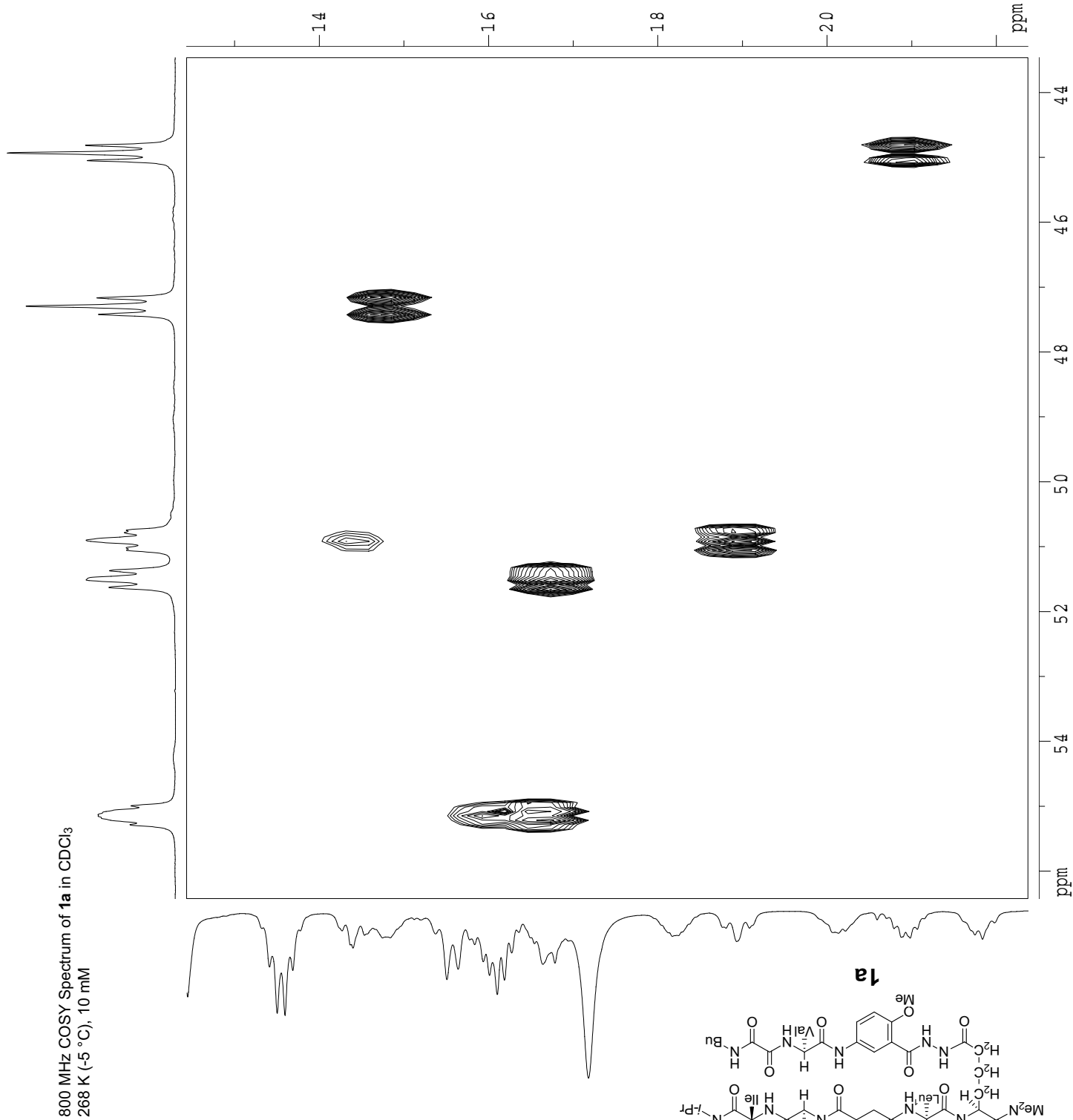
SI 2048
 SF 799.8064119 MHz
 WDW SINE
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.40

F1 - Processing parameters

SI 512
 MC2 QF
 SF 799.8064119 MHz
 WDW SINE
 SSB 0
 LB 0.00 Hz
 GB 0

2D NMR plot parameters

CX2 15.00 cm
 CX1 15.00 cm
 F2PLO 5.642 ppm
 F2LO 4512.84 Hz
 F2PHI 4.346 ppm
 F2HI 3476.12 Hz
 F1PLO 2.237 ppm
 F1LO 1789.43 Hz
 F1PHI 1.243 ppm
 F1HI 994.42 Hz
 F2PPMCM 0.08641 ppm/cm
 F2HZCM 69.11499 Hz/cm
 F1PPMCM 0.06627 ppm/cm
 F1HZCM 53.00010 Hz/cm



Supporting Information

Current Data Parameters
 USER slevin
 NAME SL-7-233-800-H
 EXPNO 3
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20070206
 Time 0.00
 INSTRUM varian
 PROBHD 40:5mmrroadbn
 PULPROG wgtocsy_bn
 TD 4096
 SOLVENT CDCl3
 NS 16
 DS 64
 SWH 11001.101 Hz
 FIDRES 2.685816 Hz
 AQ 0.1862132 sec
 RG 287.4
 DW 45.450 usec
 DE 6.00 usec
 TE 268.5 K

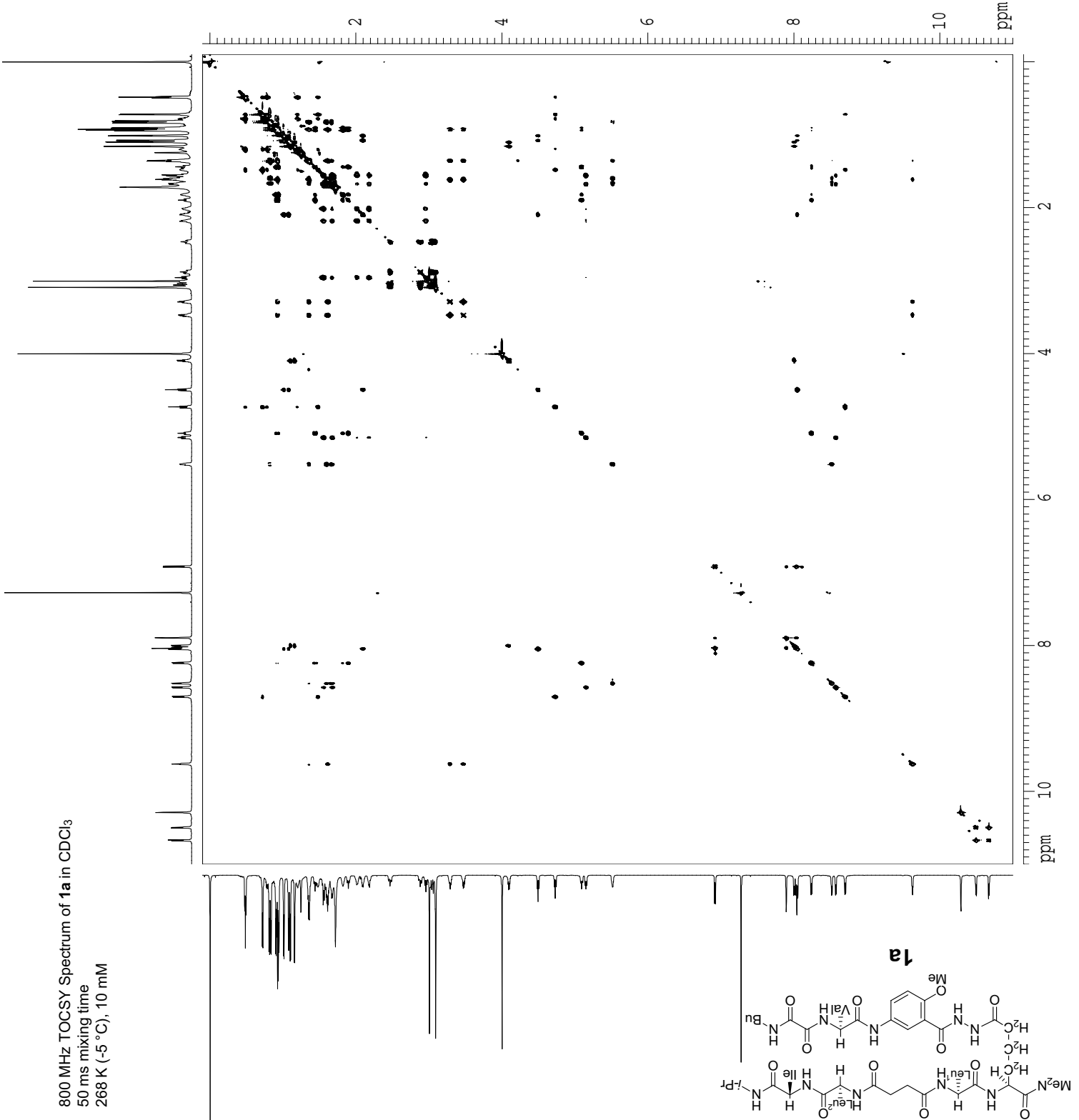
F1 - Acquisition Parameters
 ND0 1
 TD 1024
 SFO1 799.8107 MHz
 FIDRES 10.743262 Hz
 SW 13.755 ppm
 PrMODE undefined

F2 - Processing parameters
 SI 2048
 SF 799.8064119 MHz
 WDW QSINE
 SSB 2
 LB 0.00 Hz
 GB 0
 PC 1.40

F1 - Processing parameters
 SI 1024
 MC2 States
 SF 799.8064119 MHz
 WDW QSINE
 SSB 2
 LB 0.00 Hz
 GB 0

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2D NMR plot parameters
 CX2 15.00 cm
 CX1 15.00 cm
 F2PLO 11.000 ppm
 F2LO 8797.87 Hz
 F2PHI -0.100 ppm
 F2HI -79.98 Hz
 F1PLO 11.000 ppm
 F1LO 8797.87 Hz
 F1PHI -0.100 ppm
 F1HI -79.98 Hz
 F2PPMCM 0.74000 ppm/cm
 F1PPMCM 591.85669 Hz/cm
 F1HZCM 0.74000 ppm/cm
 F1HZCM 591.85669 Hz/cm



800 MHz TOCSY Spectrum of **1a** in CDCl₃
 50 ms mixing time
 268 K (-5 °C), 10 mM

Supporting Information

S. Levin and J. S. Nowick

Current Data Parameters
 USER slevin
 NAME SL-7-233-800-H
 EXPNO 3
 PROCNO 1

F2 - Acquisition Parameters

Date_ 20070206
 Time_ 0.00
 INSTRUM varian
 PROBHD 40:5mmBroadban
 PULPROG wgtocsy_bn
 TD 4096
 SOLVENT CDCl3
 NS 16
 DS 64
 SWH 11001.101 Hz
 FIDRES 2.685816 Hz
 AQ 0.1862132 sec
 RG 287.4
 DW 45.450 usec
 DE 6.00 usec
 TE 268.5 K

F1 - Acquisition Parameters

ND0 1
 TD 1024
 SFO1 799.8107 MHz
 FIDRES 10.743262 Hz
 SW 13.755 ppm
 FmMODE undefined

F2 - Processing parameters

SI 2048
 SF 799.8064119 MHz
 WDW QSI
 SSB 2
 LB 0.00 Hz
 GB 0
 PC 1.40

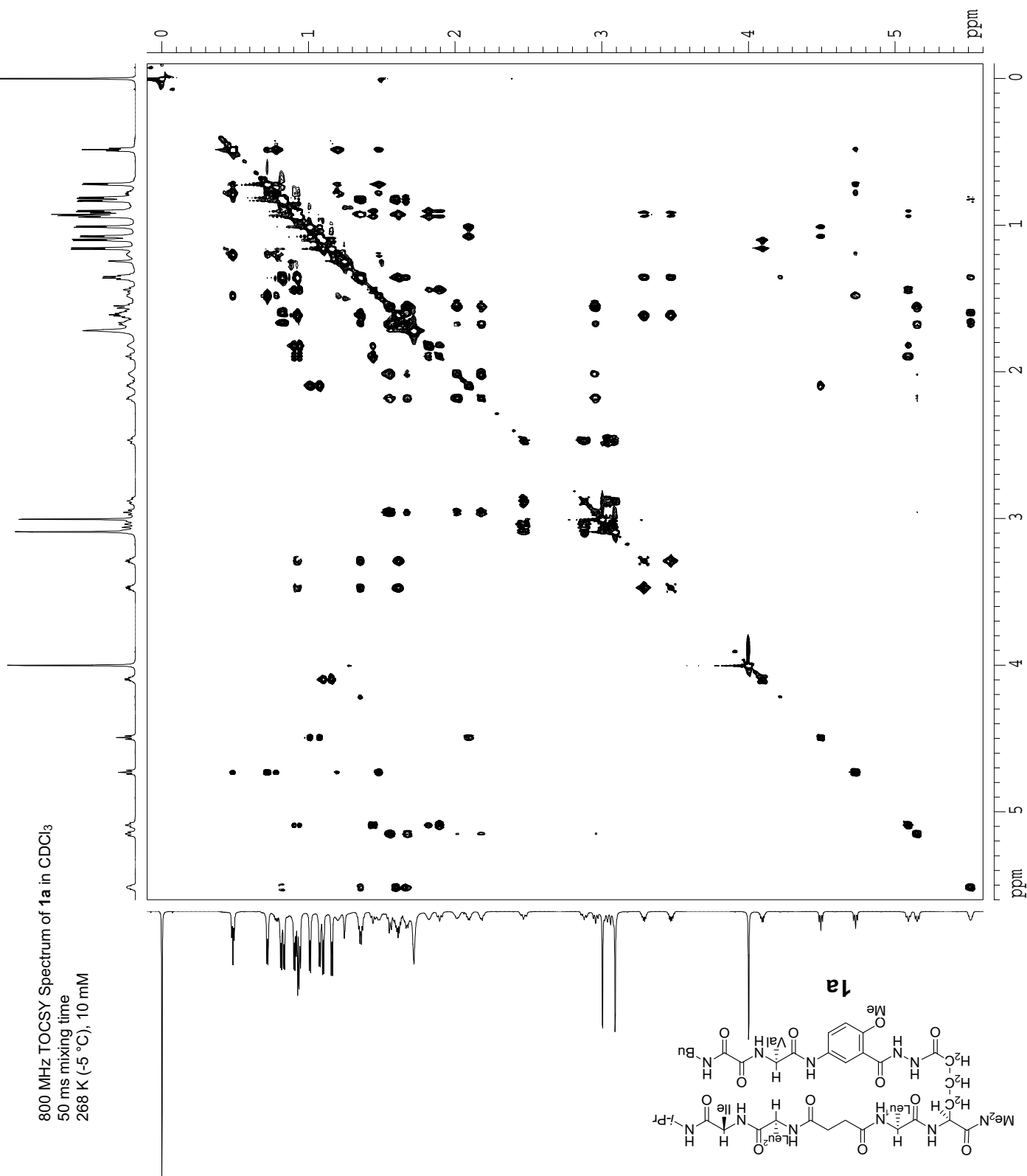
F1 - Processing parameters

SI 1024
 MC2 States
 SF 799.8064119 MHz
 WDW QSI
 SSB 2
 LB 0.00 Hz
 GB 0

2D NMR plot parameters

CX2 15.00 cm
 CX1 15.00 cm
 F2FLO 5.600 ppm
 F2LO 4478.92 Hz
 F2PHI -0.100 ppm
 F2HI -79.98 Hz
 F1FLO 5.600 ppm
 F1LO 4478.92 Hz
 F1PHI -0.100 ppm
 F1HI -79.98 Hz
 F2PPMCM 0.38000 ppm/cm
 F2HZCM 303.92645 Hz/cm
 F1PPMCM 0.38000 ppm/cm
 F1HZCM 303.92645 Hz/cm

800 MHz TOCSY Spectrum of **1a** in CDCl₃
 50 ms mixing time
 268 K (-5 °C), 10 mM



Supporting Information

Current Data Parameters
 USER slevin
 NAME SL-7-233-800-H
 EXPNO 3
 PROCNO 1

F2 - Acquisition Parameters

Date_ 20070206
 Time_ 0.00
 INSTRUM varian
 PROBHD 40:5mm broadband
 PULPROG wgtocsy_bn
 TD 4096
 SOLVENT CDCl3
 NS 16
 DS 64
 SWH 11001.101 Hz
 FIDRES 2.685816 Hz
 AQ 0.1862132 sec
 RG 287.4
 DW 45.450 usec
 DE 6.00 usec
 TE 268.5 K

F1 - Acquisition Parameters

ND0 1
 TD 1024
 SF01 799.8107 MHz
 FIDRES 10.743262 Hz
 SW 13.755 ppm
 F1MODE undefined

F2 - Processing parameters

SI 2048
 SF 799.8064119 MHz
 WDW QSI
 SSB 2
 LB 0.00 Hz
 GB 0
 PC 1.40

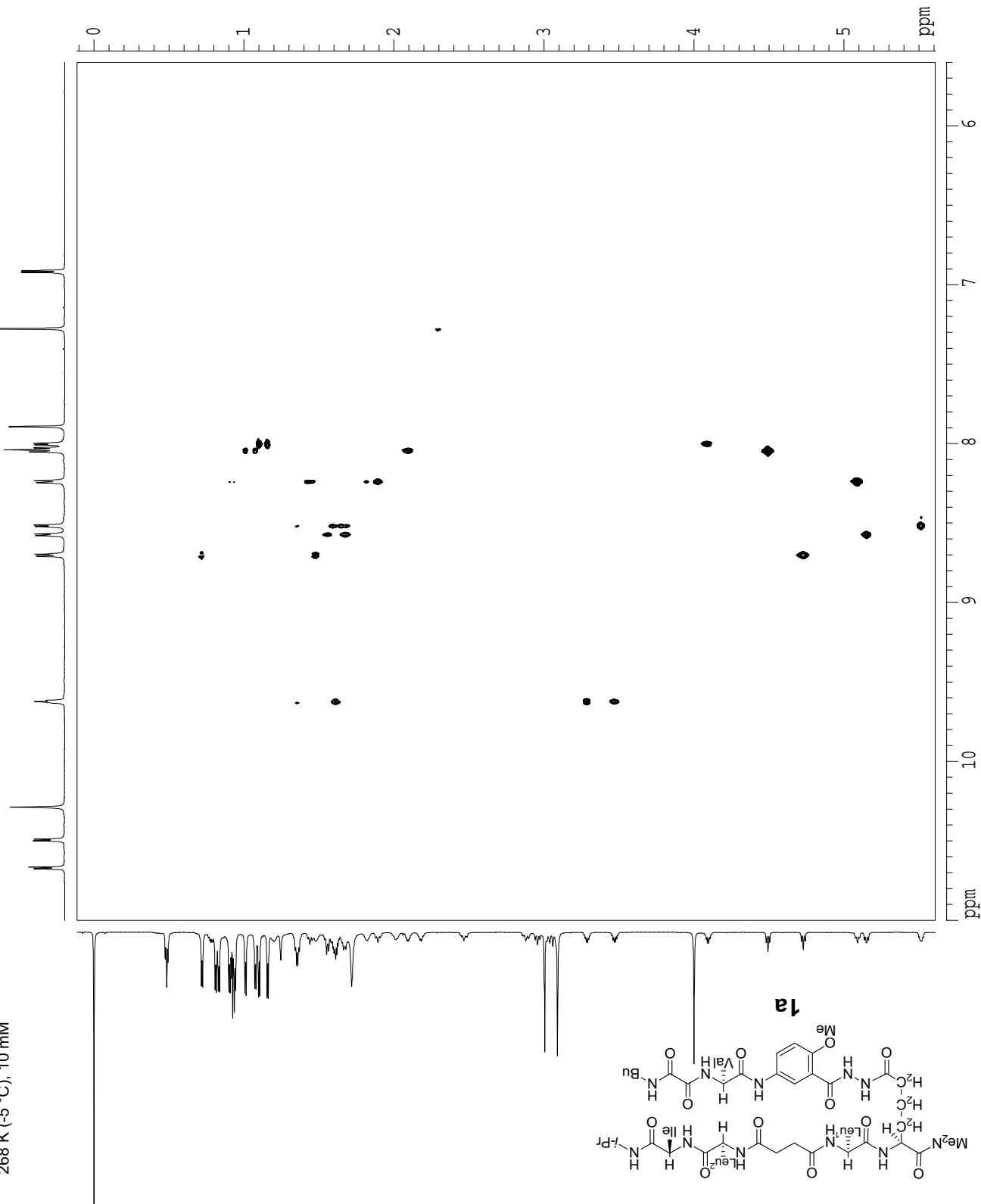
F1 - Processing parameters

SI 1024
 MC2 States
 SF 799.8064119 MHz
 WDW QSI
 SSB 2
 LB 0.00 Hz
 GB 0

2D NMR plot parameters

CX2 15.00 cm
 CX1 15.00 cm
 F2PLO 11.000 ppm
 F2LO 8797.87 Hz
 F2PHI 5.600 ppm
 F2HI 4478.92 Hz
 F1PLO 5.609 ppm
 F1LO 4485.98 Hz
 F1PHI -0.113 ppm
 F1HI -90.64 Hz
 F2PPMCM 0.36000 ppm/cm
 F2HZCM 287.93030 Hz/cm
 F1PPMCM 0.38148 ppm/cm
 F1HZCM 305.10861 Hz/cm

800 MHz TOCSY Spectrum of **1a** in CDCl₃
 50 ms mixing time
 268 K (-5 °C), 10 mM



Supporting Information

Current Data Parameters
 USER slevin
 NAME SL-7-233-800-H
 EXPNO 3
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20070206
 Time 0:00
 INSTRUM varian
 PROBHD 40:5mm broadband
 PULPROG wgtocsy_bn
 TD 4096
 SOLVENT CDCl3
 NS 16
 DS 64
 SWH 11001.101 Hz
 FIDRES 2.685816 Hz
 AQ 0.1862132 sec
 RG 287.4
 DW 45.450 usec
 DE 6.00 usec
 TE 268.5 K

F1 - Acquisition Parameters
 ND0 1
 TD 1024
 SF01 799.8107 MHz
 FIDRES 10.743262 Hz
 SW 13.755 ppm
 F1MODE undefined

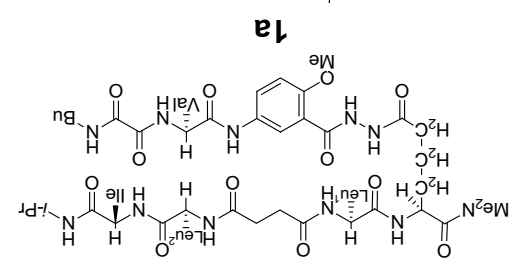
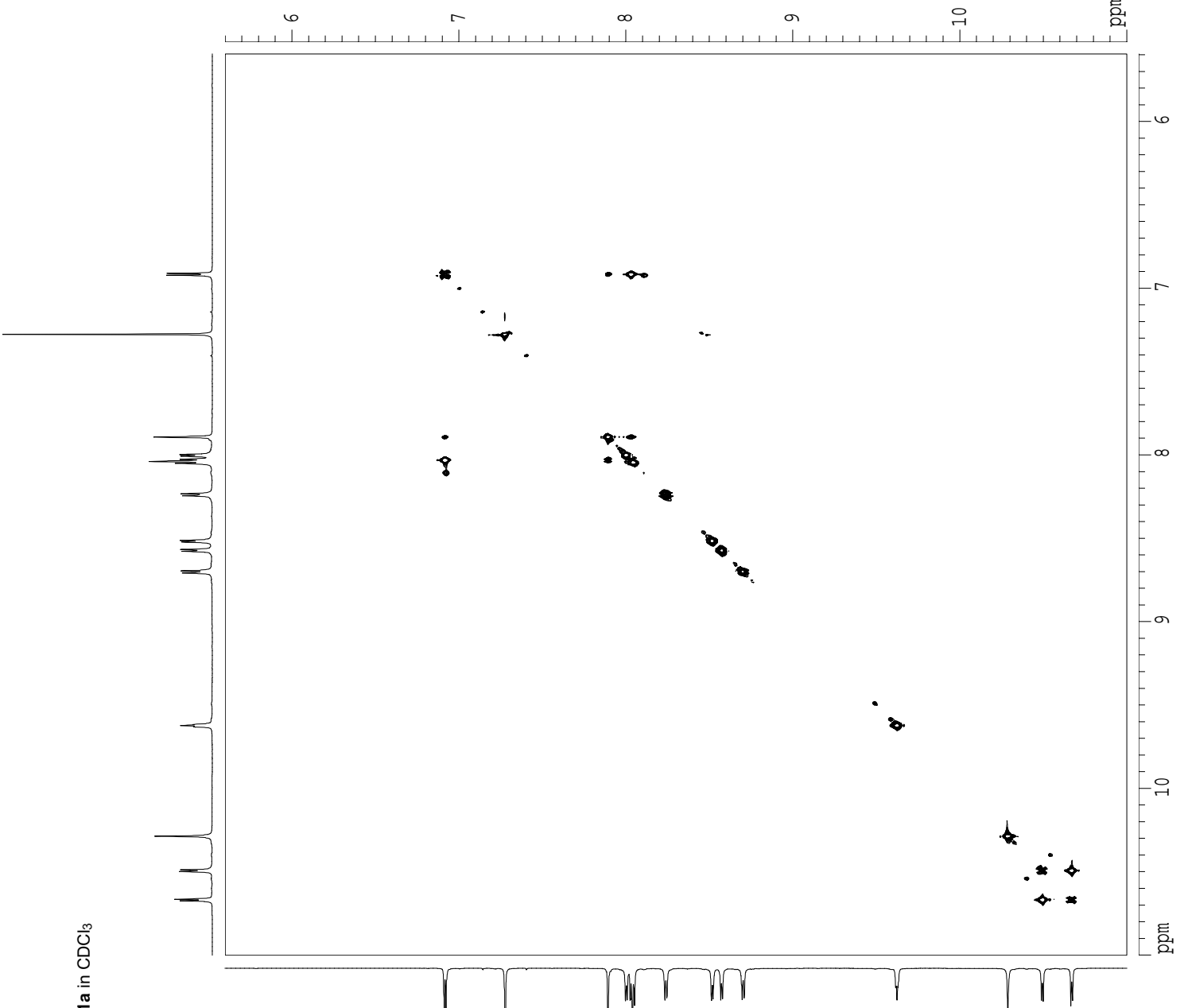
F2 - Processing parameters
 SI 2048
 SF 799.8064119 MHz
 WDW QSI
 SSB 2
 LB 0.00 Hz
 GB 0
 PC 1.40

F1 - Processing parameters
 SI 1024
 MC2 States
 SF 799.8064119 MHz
 WDW QSI
 SSB 2
 LB 0.00 Hz
 GB 0

2D NMR plot parameters
 CX2 15.00 cm
 CX1 15.00 cm
 F2PLO 11.002 ppm
 F2LO 8799.40 Hz
 F2PHI 5.595 ppm
 F2HI 4475.24 Hz
 F1PLO 11.000 ppm
 F1LO 8797.87 Hz
 F1PHI 5.600 ppm
 F1HI 4478.92 Hz
 F2PDMC 0.36043 ppm/cm
 F2HZCM 288.27753 Hz/cm
 F1PDMC 0.36000 ppm/cm
 F1HZCM 287.93030 Hz/cm

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800 MHz TOCSY Spectrum of **1a** in CDCl₃
 50 ms mixing time
 268 K (-5 °C), 10 mM



Supporting Information

Current Data Parameters
 USER sievin
 NAME SL-7-233-800-H
 EXPNO 3
 PROCNO 1

F2 - Acquisition Parameters

Date_ 20070206
 Time_ 0.00
 INSTRUM varian
 PROBHD 40:5mmBroadban
 PULPROG wgtocsy_bn
 TD 4096
 SOLVENT CDCl3
 NS 16
 DS 64
 SWH 11001.101 Hz
 FIDRES 2.685816 Hz
 AQC 0.1862132 sec
 RG 287.4
 DW 45.450 usec
 DE 6.00 usec
 TE 268.5 K

F1 - Acquisition parameters

ND0 1
 TD 1024
 SF01 799.8107 MHz
 FIDRES 10.743262 Hz
 SW 13.755 ppm
 FMODE undefined

F2 - Processing parameters

SI 2048
 SF 799.8064119 MHz
 WDW QSINE
 SSB 2
 LB 0.00 Hz
 GB 0
 PC 1.40

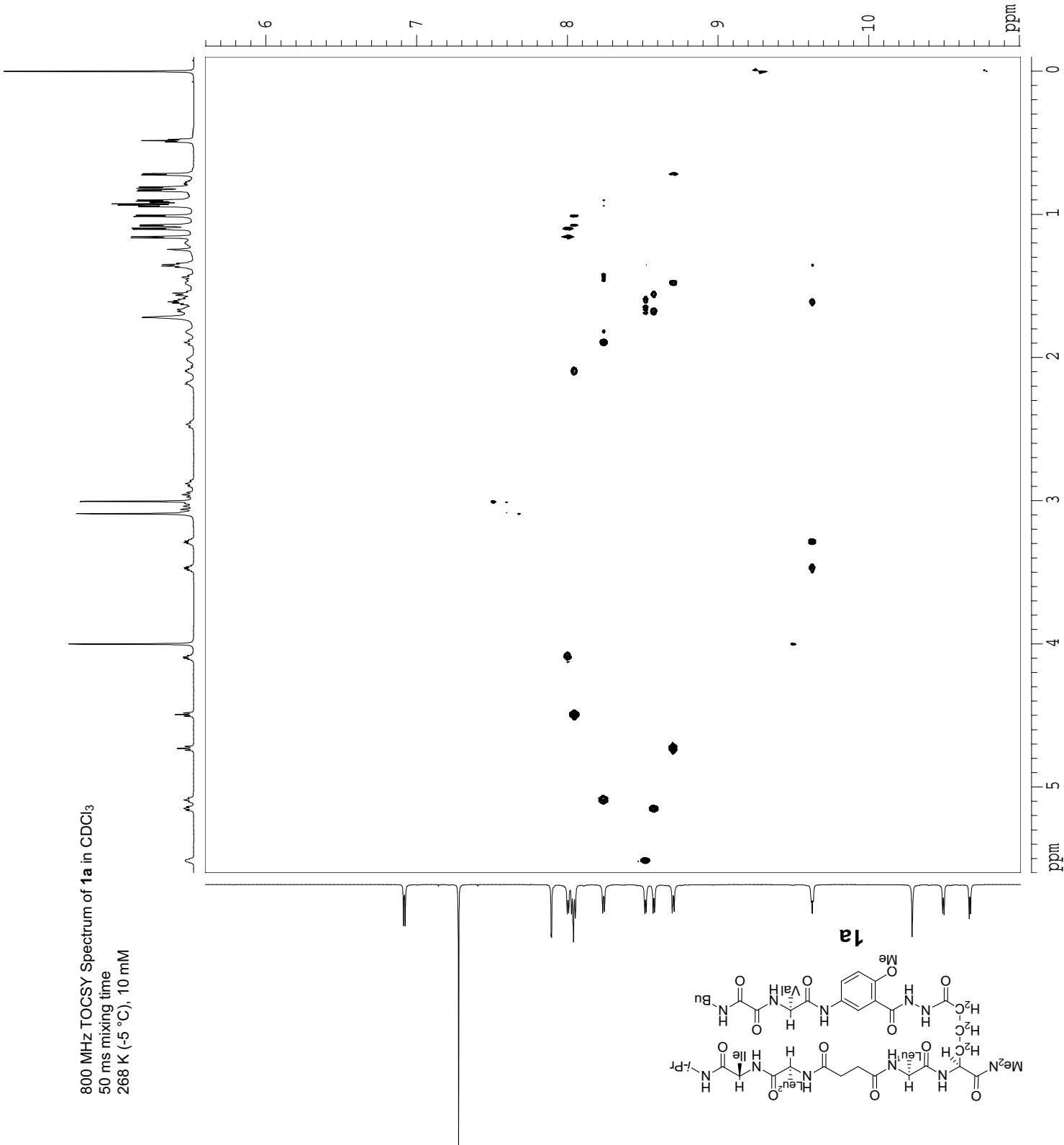
F1 - Processing parameters

SI 1024
 MC2 States
 SF 799.8064119 MHz
 WDW QSINE
 SSB 2
 LB 0.00 Hz
 GB 0

S. Levin and J. S. Nowick

2D NMR plot parameters

CX2 15.00 cm
 CX1 15.00 cm
 F2PLO 5.600 ppm
 F2LO 4478.92 Hz
 F2PHI -0.100 ppm
 F2HI -79.98 Hz
 F1PLO 11.009 ppm
 F1LO 8804.78 Hz
 F1PHI 5.595 ppm
 F1HI 4475.24 Hz
 F2PPCM 0.38000 ppm/cm
 F2HZCM 303.92645 Hz/cm
 F1PPCM 0.36088 ppm/cm
 F1HZCM 288.63562 Hz/cm



800 MHz TOCSY Spectrum of **1a** in CDCl₃
 50 ms mixing time
 268 K (-5 °C), 10 mM

Supporting Information

Current Data Parameters

USER slevin
 NAME SL-7-233-800-H
 EXPNO 3
 PROCNO 1

F2 - Acquisition Parameters

Date_ 20070206
 Time_ 0.00
 INSTRUM varian
 PROBHD 40-5mm broadband
 PULPROG wgtocsy_bn
 TD 4096
 SOLVENT CDCl3
 NS 16
 DS 64
 SWH 11001.101 Hz
 FIDRES 2.685816 Hz
 AQ 0.1862132 sec
 RG 287.4
 DW 45.450 usec
 DE 6.00 usec
 TE 268.5 K

F1 - Acquisition Parameters

ND0 1
 TD 1024
 SFO1 799.8107 MHz
 FIDRES 10.743262 Hz
 SW 13.755 ppm
 FMODE undefined

F2 - Processing parameters

SI 2048
 SF 799.8064119 MHz
 WDW QSI
 SSB 2
 LB 0.00 Hz
 GB 0
 PC 1.40

F1 - Processing parameters

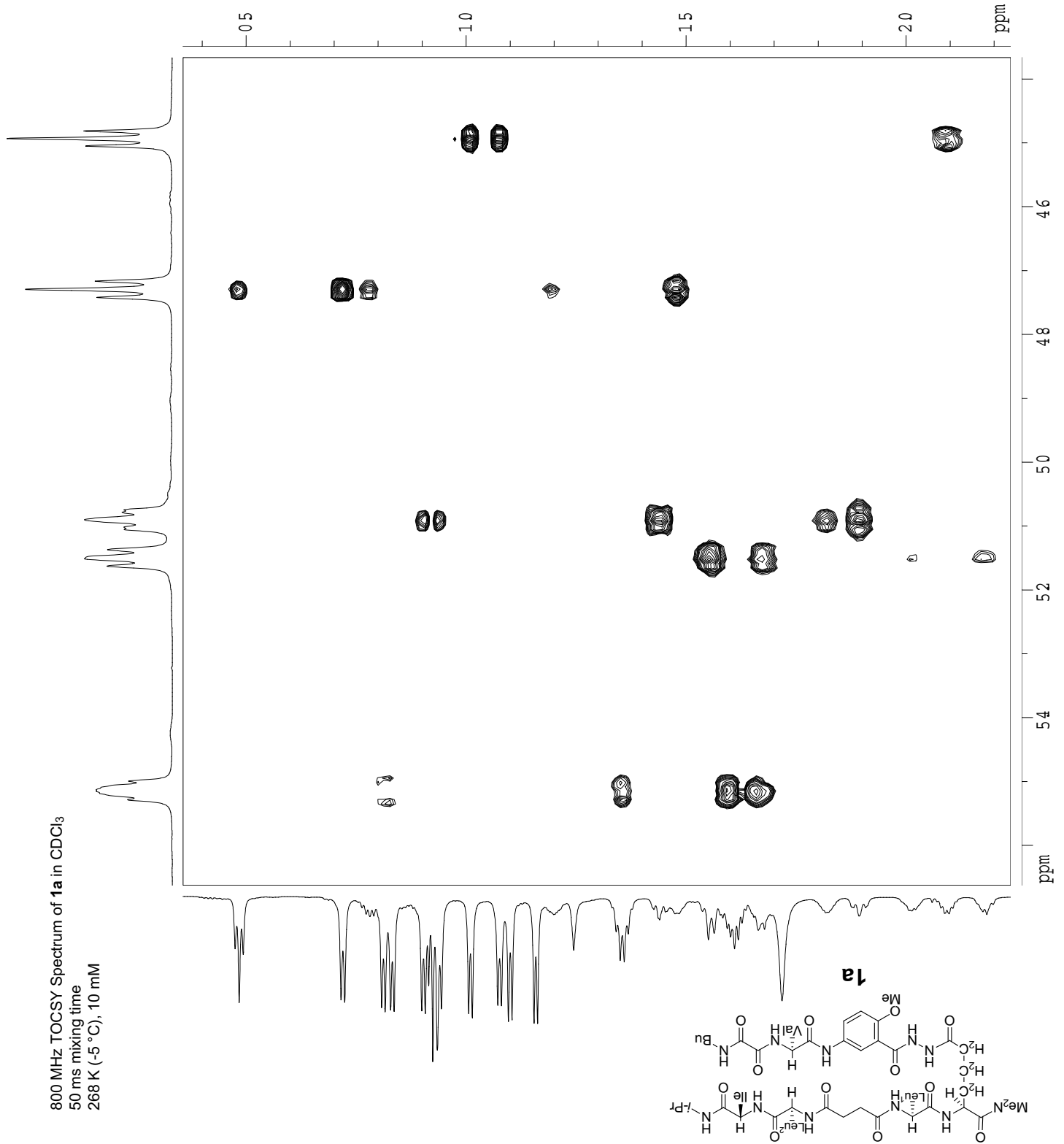
SI 1024
 MC2 States
 SF 799.8064119 MHz
 WDW QSI
 SSB 2
 LB 0.00 Hz
 GB 0

S. Levin and J. S. Nowick

2D NMR plot parameters

CX2 15.00 cm
 CX1 15.00 cm
 F2PLO 5.663 ppm
 F2LO 4528.96 Hz
 F2PHI 4.366 ppm
 F2HI 3492.23 Hz
 F1PLO 2.237 ppm
 F1LO 1789.43 Hz
 F1PHI 0.357 ppm
 F1HI 285.37 Hz
 F2PFCM 0.08641 ppm/cm
 F2H2CM 69.11497 Hz/cm
 F1PFCM 0.12537 ppm/cm
 F1H2CM 100.27044 Hz/cm

800 MHz TOCSY Spectrum of **1a** in CDCl₃
 50 ms mixing time
 268 K (-5 °C), 10 mM



Current Data Parameters
 USER slevin
 NAME SL-7-233-800-H
 EXPNO 4
 PROCNO 1

F2 - Acquisition Parameters

Date_ 20070206
 Time 0.00
 INSTRUM varian
 PROBHD 40:5mmbroadban
 PULPROG noesyh2o_pfg_800_pln
 TD 4096
 SOLVENT CDCl3
 NS 16
 DS 64
 SWH 11001.101 Hz
 FIDRES 2.685816 Hz
 AQ 0.1862132 sec
 RG 128
 DW 45.450 usec
 DE 6.00 usec
 TE 288.5 K

F1 - Acquisition Parameters

ND0 1
 TD 1024
 SF01 799.8107 MHz
 FIDRES 10.743262 Hz
 SW 13.755 ppm
 FhMODE undefined

F2 - Processing parameters

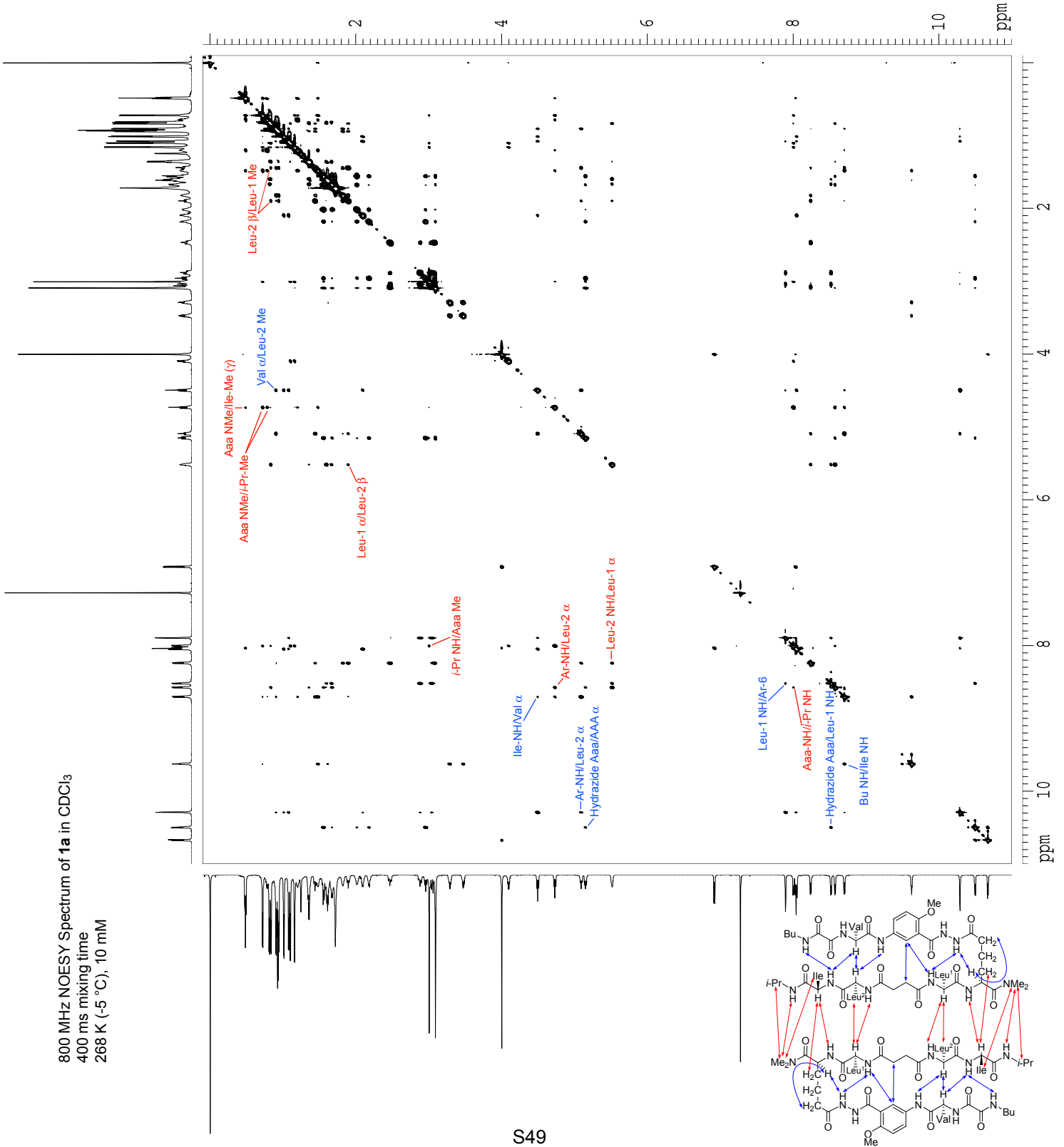
SI 2048
 SF 799.8064119 MHz
 WDW QSI
 SSB 2
 LB 0.00 Hz
 GB 0
 PC 1.40

F1 - Processing parameters

SI 1024
 MC2 States
 SF 799.8064119 MHz
 WDW QSI
 SSB 2
 LB 0.00 Hz
 GB 0

2D NMR plot parameters

CX2 15.00 cm
 CX1 15.00 cm
 F2PLO 11.000 ppm
 F2LO 8797.87 Hz
 F2PHI -0.100 ppm
 F2HI -79.98 Hz
 F1PLO 11.000 ppm
 F1LO 8797.87 Hz
 F1PHI -0.100 ppm
 F1HI -79.98 Hz
 F2PPMCM 0.74000 ppm/cm
 F2HZCM 591.85669 Hz/cm
 F1PPMCM 0.74000 ppm/cm
 F1HZCM 591.85669 Hz/cm



Current Data Parameters
 USER slevin
 NAME SL-7-233-800-H
 EXPNO 4
 PROCNO 1

F2 - Acquisition Parameters

Date 20070206
 Time_ 0.00
 INSTRUM varian
 PROBHD 40:5mm broadband
 PULPROG noesyh2o_pfg_800_pln
 TD 4096
 SOLVENT CDCl₃
 NS 16
 DS 64
 SWH 11001.101 Hz
 FIDRES 2.685816 Hz
 AQ 0.1862132 sec
 RG 128
 DW 45.450 usec
 DE 6.00 usec
 TE 268.5 K

F1 - Acquisition Parameters

ND0 1
 TD 1024
 SF01 799.8107 MHz
 FIDRES 10.743262 Hz
 SW 13.755 ppm
 FhMODE undefined

F2 - Processing parameters

SI 2048
 SF 799.8064119 MHz
 WDW QSI
 SSB 2
 LB 0.00 Hz
 GB 0
 PC 1.40

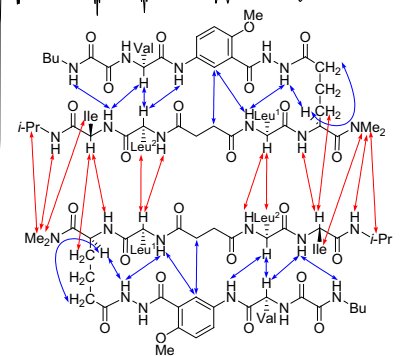
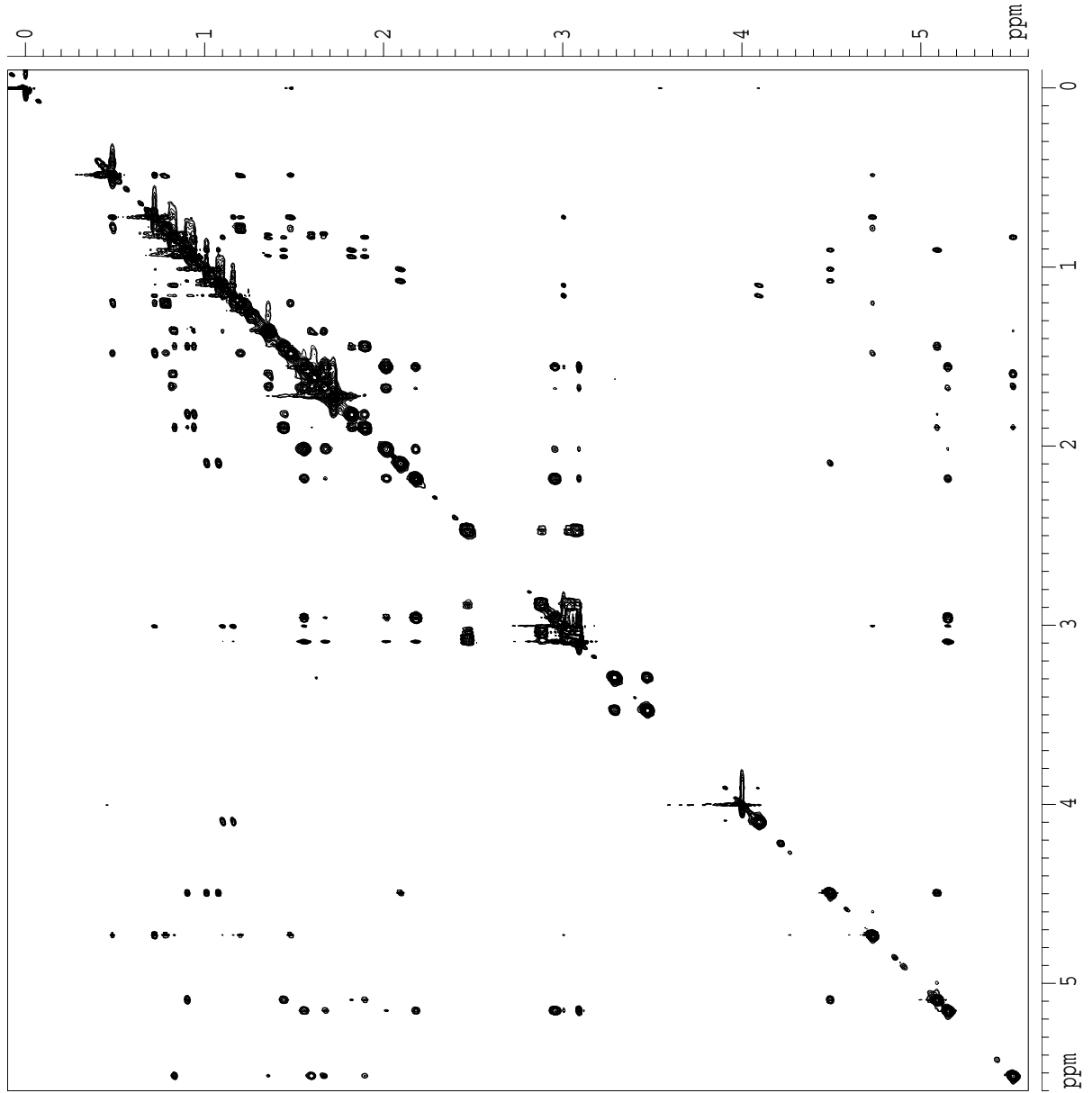
F1 - Processing parameters

SI 2048
 MC2 States
 SF 799.8064119 MHz
 WDW QSI
 SSB 2
 LB 0.00 Hz
 GB 0

2D NMR plot parameters

CX2 15.00 cm
 CX1 15.00 cm
 F2PLO 5.600 ppm
 F2LO 4478.92 Hz
 F2PHI -0.100 ppm
 F2HI -79.98 Hz
 F1PLO 5.600 ppm
 F1LO 4478.92 Hz
 F1PHI -0.100 ppm
 F1HI -79.98 Hz
 F2PPMCM 0.38000 ppm/cm
 F2HZCM 303.92645 Hz/cm
 F1PPMCM 0.38000 ppm/cm
 F1HZCM 303.92645 Hz/cm

800 MHz NOESY Spectrum of **1a** in CDCl₃
 400 ms mixing time
 268 K (-5 °C), 10 mM



Supporting Information

Current Data Parameters

USER slevin
 NAME SL-7-233-800-H
 EXPNO 4
 PROCNO 1

F2 - Acquisition Parameters

Date_ 20070206
 Time 0.00
 INSTRUM varian
 PROBDH 40:5mm broadband
 PULPROG noesyh2o_pfg_800_pln

TD 4096
 SOLVENT CDCl3
 NS 16
 DS 64

SWH 11001.101 Hz
 FIDRES 2.685816 Hz
 AQ 0.1862132 sec
 RG 128
 DW 45.450 usec
 DE 6.00 usec
 TE 268.5 K

F1 - Acquisition Parameters

ND0 1
 TD 1024
 SF01 799.8107 MHz
 FIDRES 10.743262 Hz
 SW 13.755 ppm
 F1MODE undefined

F2 - Processing parameters

SI 2048
 SF 799.8064119 MHz
 WDW QSI
 SSB 2
 LB 0.00 Hz
 GB 0
 PC 1.40

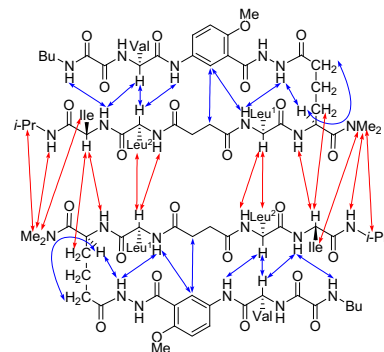
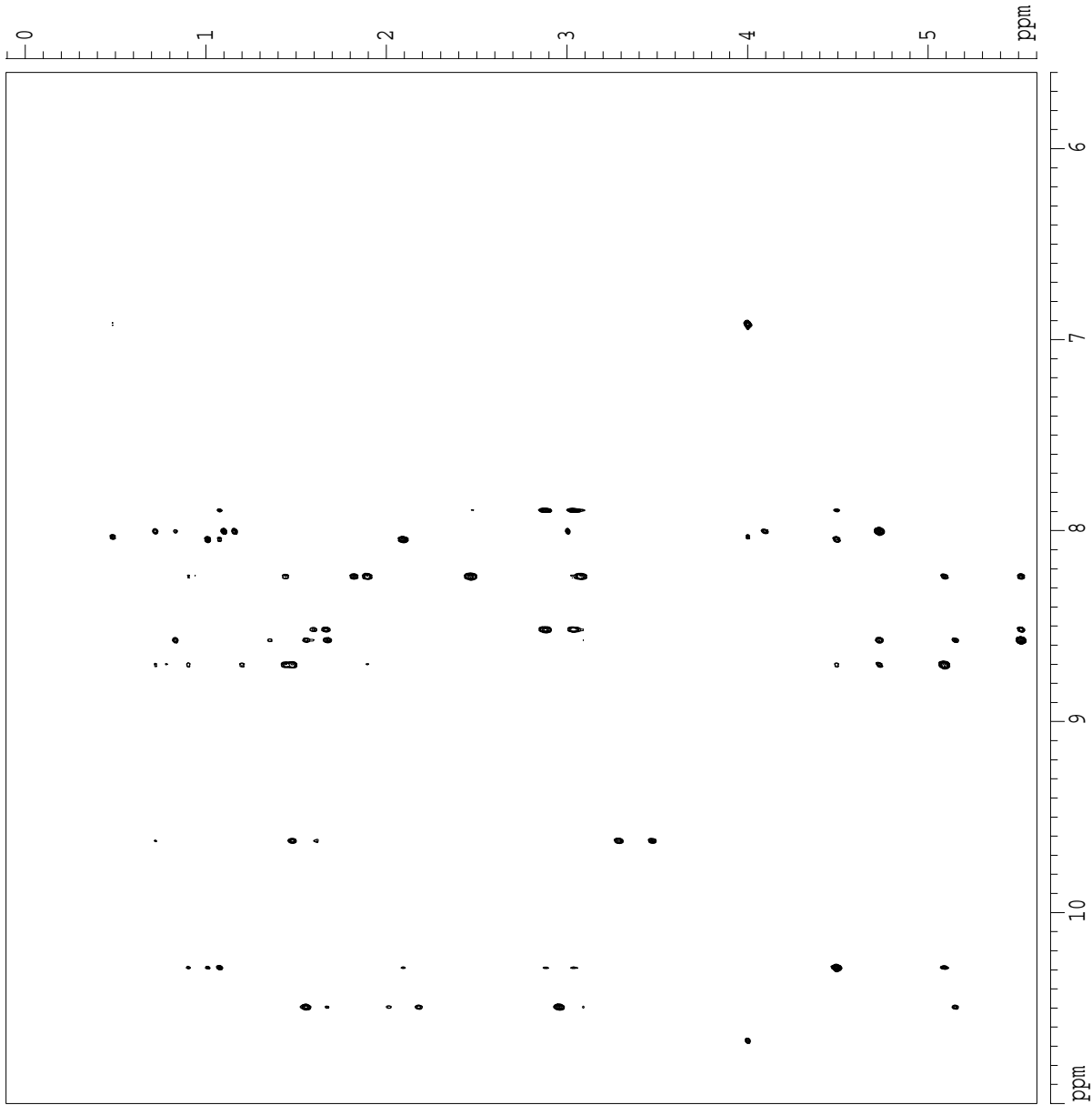
F1 - Processing parameters

SI 2048
 MC2 States
 SF 799.8064119 MHz
 WDW QSI
 SSB 2
 LB 0.00 Hz
 GB 0

2D NMR plot parameters

CX2 15.00 cm
 CX1 15.00 cm
 F2PLO 11.000 ppm
 F2LO 8797.87 Hz
 F2PHI 5.600 ppm
 F2HI 4478.92 Hz
 F1PLO 5.602 ppm
 F1LO 4480.61 Hz
 F1PHI -0.107 ppm
 F1HI -85.27 Hz
 F2PPMCM 0.36000 ppm/cm
 F2HZCM 287.93030 Hz/cm
 F1PPMCM 0.38058 ppm/cm
 F1HZCM 304.39243 Hz/cm

800 MHz NOESY Spectrum of **1a** in CDCl₃
 400 ms mixing time
 268 K (-5 °C), 10 mM



Supporting Information

S. Levin and J. S. Nowick

Current Data Parameters
 USER slevin
 NAME SL-7-233-800-H
 EXPNO 4
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20070206
 Time 0.00
 INSTRUM varian
 PROBHD 40:5mmBroadban
 PULPROG noesyh2o_pfg_800_p1n
 TD 4096
 SOLVENT CDCl3
 NS 16
 DS 64
 SWH 11001.101 Hz
 FIDRES 2.685816 Hz
 AQ 0.1862132 sec
 RG 128
 DW 45.450 usec
 DE 6.00 usec
 TE 288.5 K

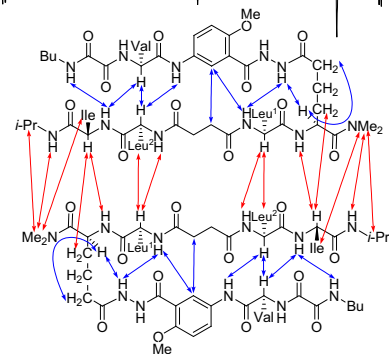
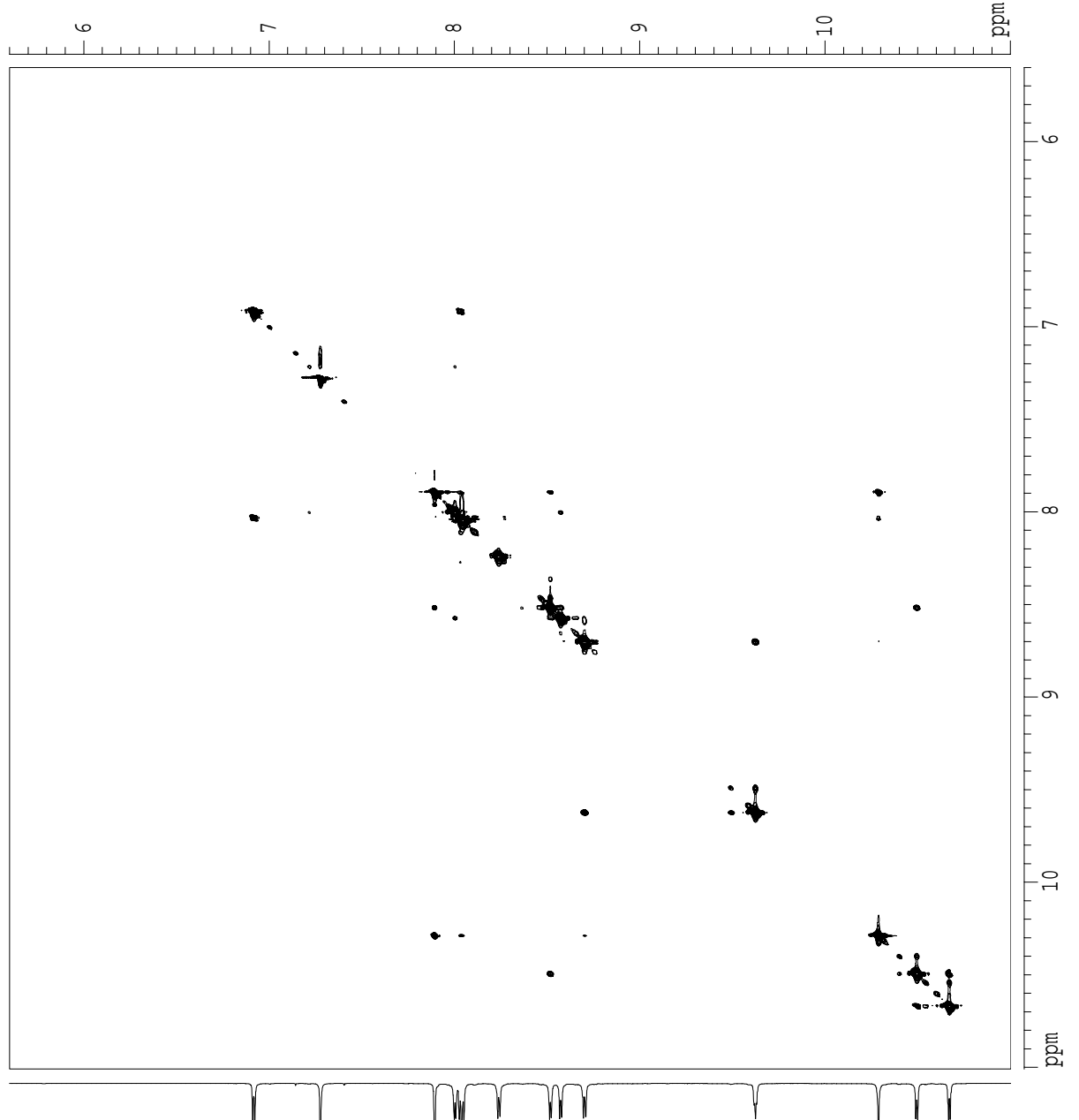
F1 - Acquisition parameters
 ND0 1
 TD 1024
 SF01 799.8107 MHz
 FIDRES 10.743262 Hz
 SW 13.755 ppm
 FMODE undefined

F2 - Processing parameters
 SI 2048
 SF 799.8064119 MHz
 WDW QSI
 SSB 2
 LB 0.00 Hz
 GB 0
 PC 1.40

F1 - Processing parameters
 SI 2048
 MC2 States
 SF 799.8064119 MHz
 WDW QSI
 SSB 2
 LB 0.00 Hz
 GB 0

2D NMR plot parameters
 CX2 15.00 cm
 CX1 15.00 cm
 F2PLO 11.009 ppm
 F2LO 8804.78 Hz
 F2PHI 5.600 ppm
 F2HI 4478.92 Hz
 F1PLO 11.002 ppm
 F1LO 8799.40 Hz
 F1PHI 5.600 ppm
 F1HI 4478.92 Hz
 F2PPMCM 0.36058 ppm/cm
 F2HZCM 288.39066 Hz/cm
 F1PPMCM 0.36013 ppm/cm
 F1HZCM 288.03253 Hz/cm

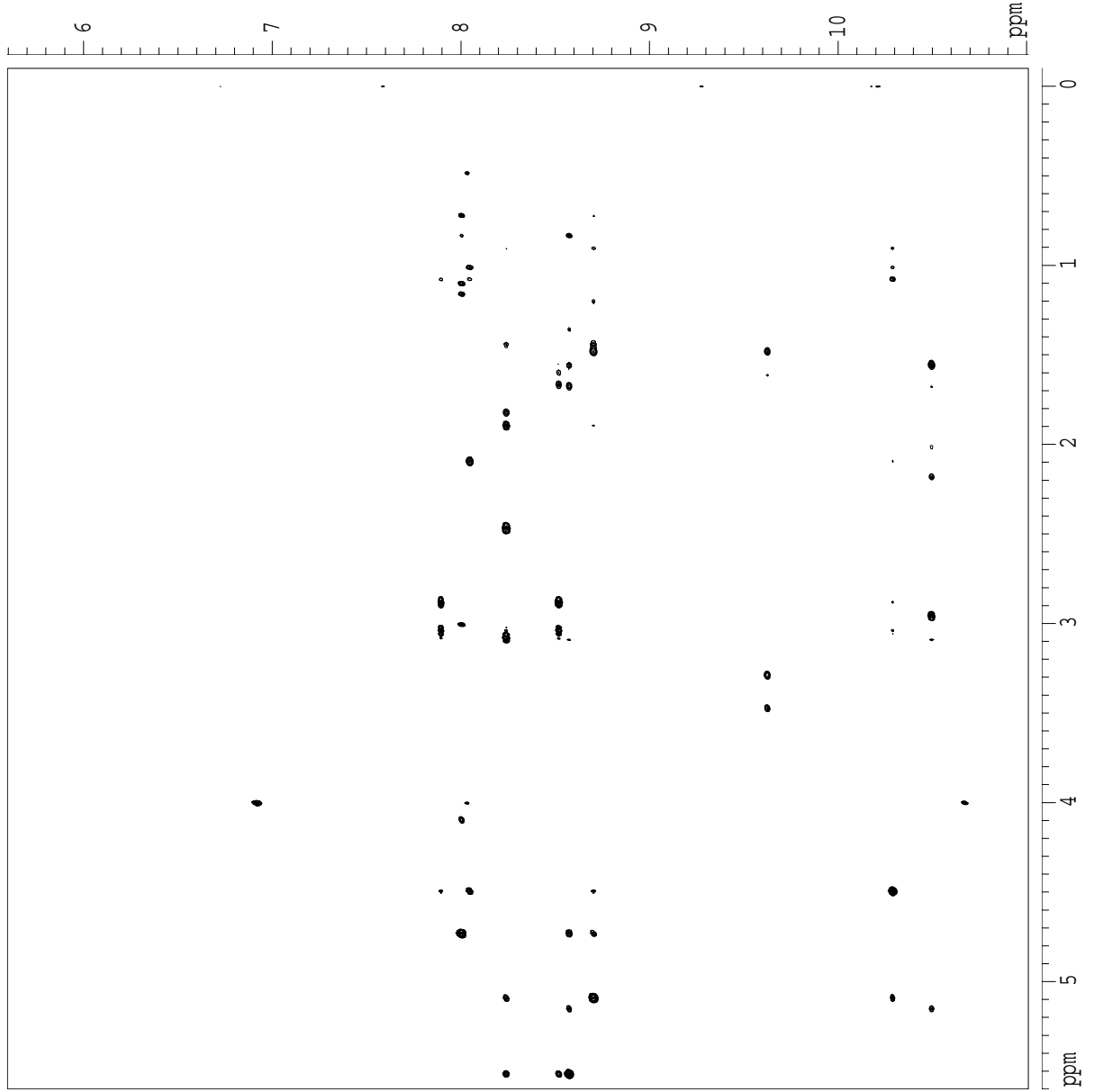
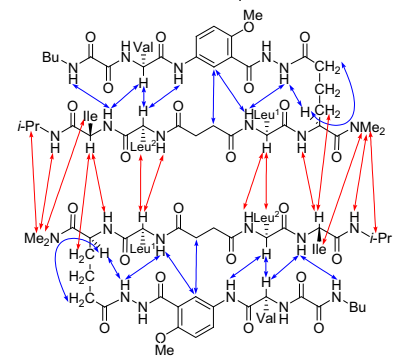
800 MHz NOESY Spectrum of **1a** in CDCl₃
 400 ms mixing time
 268 K (-5 °C), 10 mM



Supporting Information

S. Levin and J. S. Nowick

800 MHz NOESY Spectrum of **1a** in CDCl₃
 400 ms mixing time
 268 K (-5 °C), 10 mM



Current Data Parameters
 USER slevin
 NAME SL-7-233-800-H
 EXPNO 4
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20070206
 Time 0.00
 INSTRUM varian
 PROBHD 40:5mmBroadban
 PULPROG noesyh2o_pfg_800_p1n
 TD 4096
 SOLVENT CDCl3
 NS 16
 DS 64
 SWH 11001.101 Hz
 FIDRES 2.685816 Hz
 AQ 0.1862132 sec
 RG 128
 DW 45.450 usec
 DE 6.00 usec
 TE 268.5 K

F1 - Acquisition Parameters
 ND0 1
 TD 1024
 SF01 799.8107 MHz
 FIDRES 10.743262 Hz
 SW 13.755 ppm
 F1MODE undefined

F2 - Processing parameters
 SI 2048
 SF 799.8064119 MHz
 WDW QSI
 SSB 2
 LB 0.00 Hz
 GB 0
 PC 1.40

F1 - Processing parameters
 SI 2048
 MC2 States
 SF 799.8064119 MHz
 WDW QSI
 SSB 2
 LB 0.00 Hz
 GB 0

2D NMR plot parameters
 CX2 15.00 cm
 CX1 15.00 cm
 F2PLO 5.600 ppm
 F2LO 4478.92 Hz
 F2PHI -0.100 ppm
 F2HI -79.98 Hz
 F1PLO 11.009 ppm
 F1LO 8804.78 Hz
 F1PHI 5.595 ppm
 F1HI 4475.24 Hz
 F2PPMCM 0.38000 ppm/cm
 F2HZCM 303.92645 Hz/cm
 F1PPMCM 0.36088 ppm/cm
 F1HZCM 288.63562 Hz/cm

Supporting Information

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Current Data Parameters
 USER slevin
 NAME SL-7-233-800-H
 EXPNO 4
 PROCNO 1

F2 - Acquisition Parameters

Date_ 20070206
 Time_ 0.00
 INSTRUM varian
 PROBHD 40:5mm broadband
 PULPROG noesyh2o_pfg_800_pln
 TD 4096
 SOLVENT CDCl3
 NS 16
 DS 64
 SMH 11001.101 Hz
 FIDRES 2.685816 Hz
 AQ 0.1862132 sec
 RG 128
 DW 45.450 usec
 DE 6.00 usec
 TE 268.5 K

F1 - Acquisition Parameters

ND0 1
 TD 1024
 SFO1 799.8107 MHz
 FIDRES 10.743262 Hz
 SW 13.755 ppm
 F1MODE undefined

F2 - Processing parameters

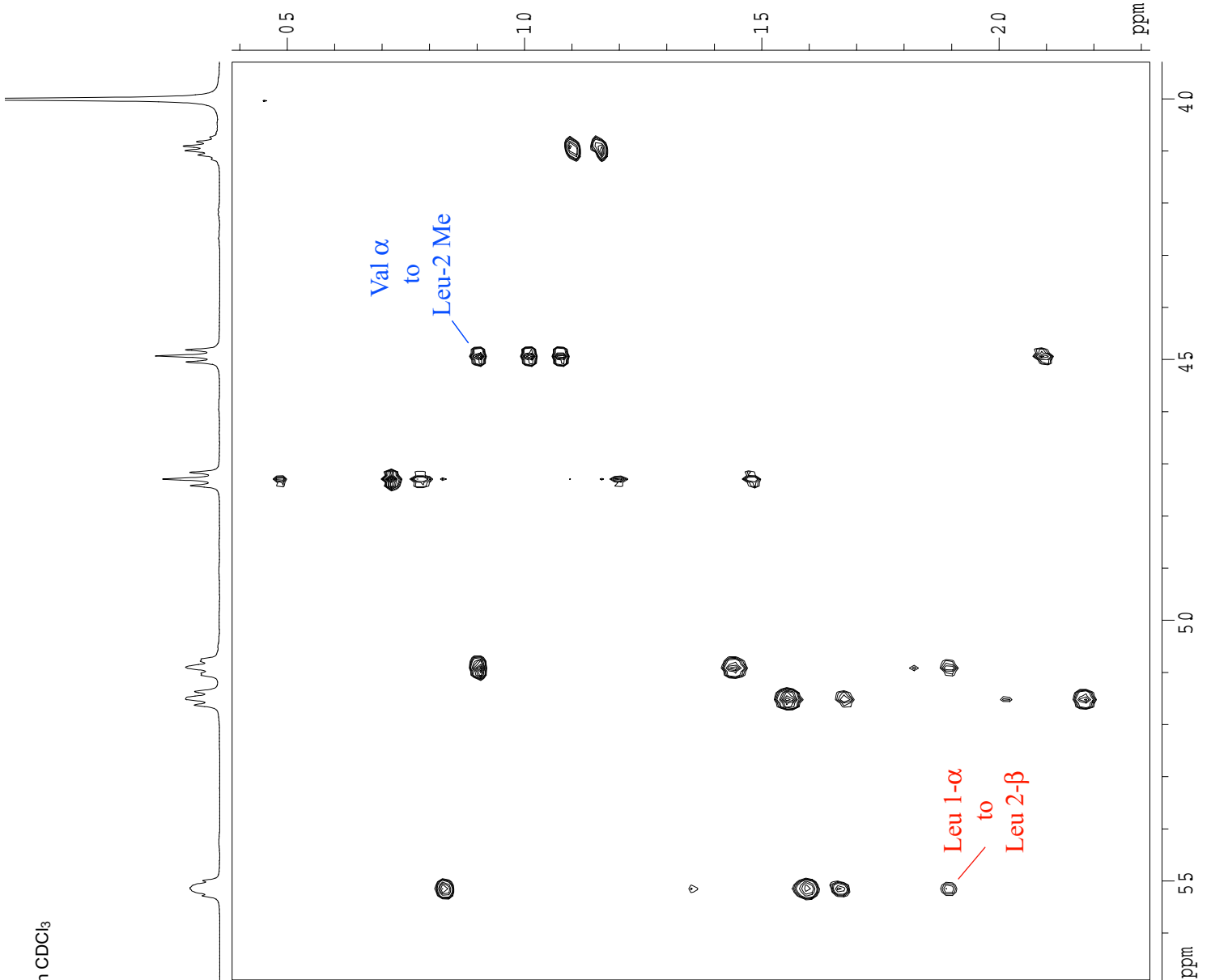
SI 2048
 SF 799.8064119 MHz
 WDW QSI
 SSB 2
 LB 0.00 Hz
 GB 0
 PC 1.40

F1 - Processing parameters

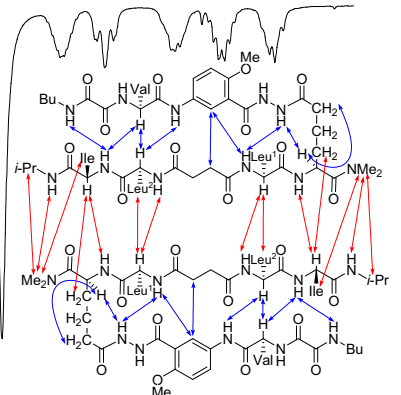
SI 1024
 MC2 States
 SF 799.8064119 MHz
 WDW QSI
 SSB 2
 LB 0.00 Hz
 GB 0

2D NMR plot parameters

CX2 15.00 cm
 CX1 15.00 cm
 F2PLO 5.689 ppm
 F2LO 4550.44 Hz
 F2PHI 3.930 ppm
 F2HI 3143.08 Hz
 F1PLO 2.318 ppm
 F1LO 1853.89 Hz
 F1PHI 0.384 ppm
 F1HI 306.86 Hz
 F2P1MCM 0.11731 ppm/cm
 F2H1MCM 93.82449 Hz/cm
 F1P1MCM 0.12895 ppm/cm
 F1H1MCM 103.13531 Hz/cm



800 MHz NOESY Spectrum of **1a** in CDCl₃
 400 ms mixing time
 268 K (-5 °C), 10 mM



Supporting Information

Current Data Parameters
 USER slewin
 NAME SL-7-233-800-H
 EXPNO 4
 PROCNO 1

F2 - Acquisition Parameters

Date_ 20070206
 Time_ 0.00
 INSTRUM varian
 PROBD 40:5mmbroadban
 PULPROG noesyh2o_pfg_800_pln
 TD 4096
 SOLVENT CDCl3
 NS 16
 DS 64
 SWH 11001.101 Hz
 FIDRES 2.685816 Hz
 AQ 0.1862132 sec
 RG 128
 DM 45.450 usec
 DE 6.00 usec
 TE 268.5 K

F1 - Acquisition parameters

ND0 1
 TD 1024
 SF01 799.8107 MHz
 FIDRES 10.743262 Hz
 SW 13.755 ppm
 FMODE undefined

F2 - Processing parameters

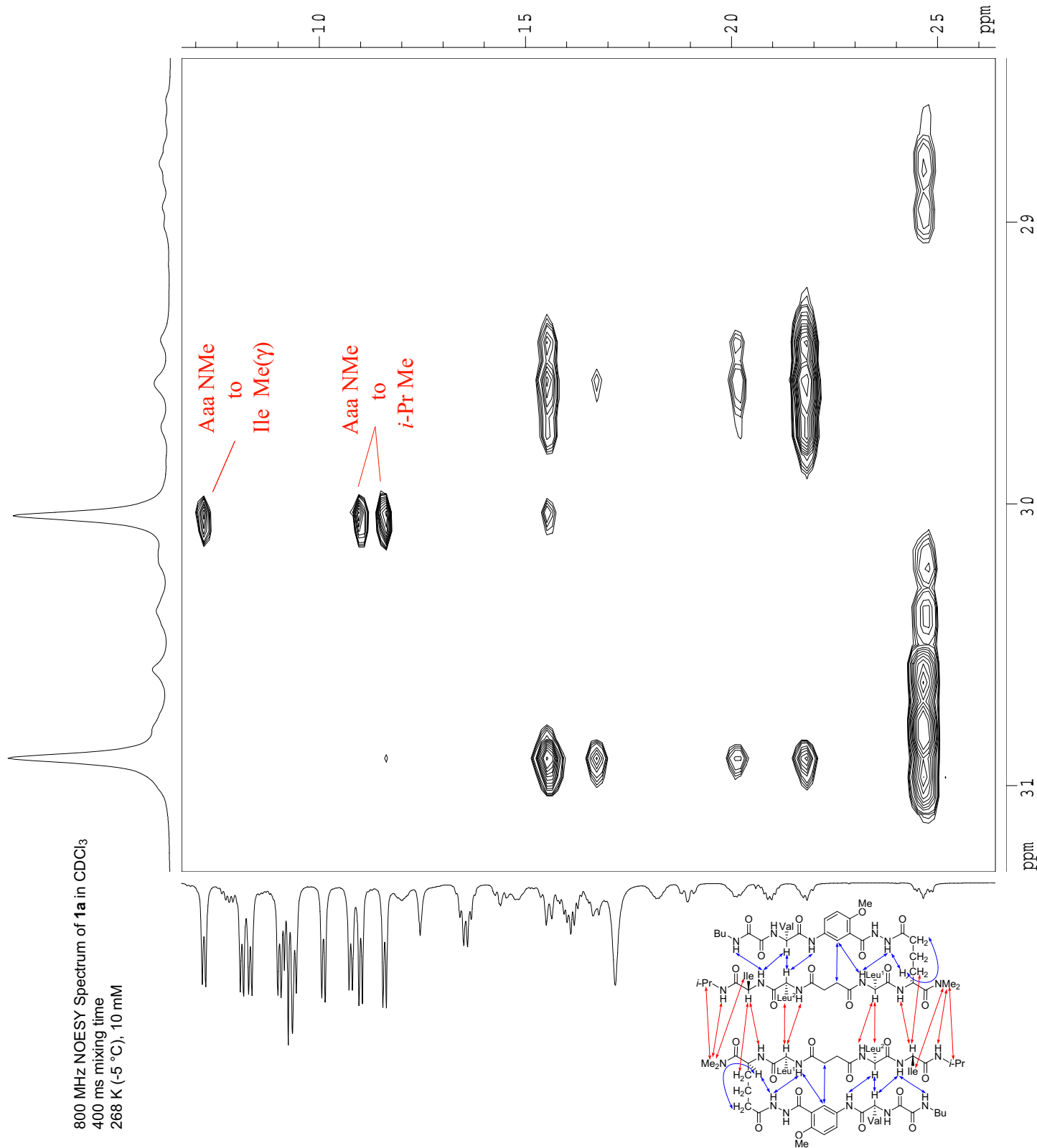
SI 2048
 SF 799.8064119 MHz
 WDM QSINE
 SSB 2
 LB 0.00 Hz
 GB 0
 PC 1.40

F1 - Processing parameters

SI 1024
 MC2 States
 SF 799.8064119 MHz
 WDM QSINE
 SSB 2
 LB 0.00 Hz
 GB 0

2D NMR plot parameters

CX2 15.00 cm
 CX1 15.00 cm
 F2PLO 3.131 ppm
 F2LO 2503.85 Hz
 F2PHI 2.842 ppm
 F2HI 2272.87 Hz
 F1PLO 2.640 ppm
 F1LO 2111.72 Hz
 F1PHI 0.666 ppm
 F1HI 532.46 Hz
 F2PFCM 0.01925 ppm/cm
 F2HZCM 15.39867 Hz/cm
 F1PFCM 0.13164 ppm/cm
 F1HZCM 105.28397 Hz/cm



800 MHz NOESY Spectrum of **1a** in CDCl₃
 400 ms mixing time
 268 K (-5 °C), 10 mM

Supporting Information

Current Data Parameters
 USER slevin
 NAME SL-7-233-800-H
 EXNO 4
 PROCNO 1

F2 - Acquisition Parameters

Date_ 20070206
 Time_ 0.00
 INSTRUM varian
 PROBHD 40:5mm broadband
 PULPROG noesyh2o_pfg_800_pln
 TD 4096

SOLVENT CDCl3
 NS 16
 DS 64
 SWH 11001.101 Hz
 FIDRES 2.685816 Hz
 AQ 0.1862132 sec
 RG 128
 DW 45.450 usec
 DE 6.00 usec
 TE 268.5 K

F1 - Acquisition parameters

ND0 1
 TD 1024
 SF01 799.8107 MHz
 FIDRES 10.743262 Hz
 SW 13.755 ppm
 FwMODE undefined

F2 - Processing parameters

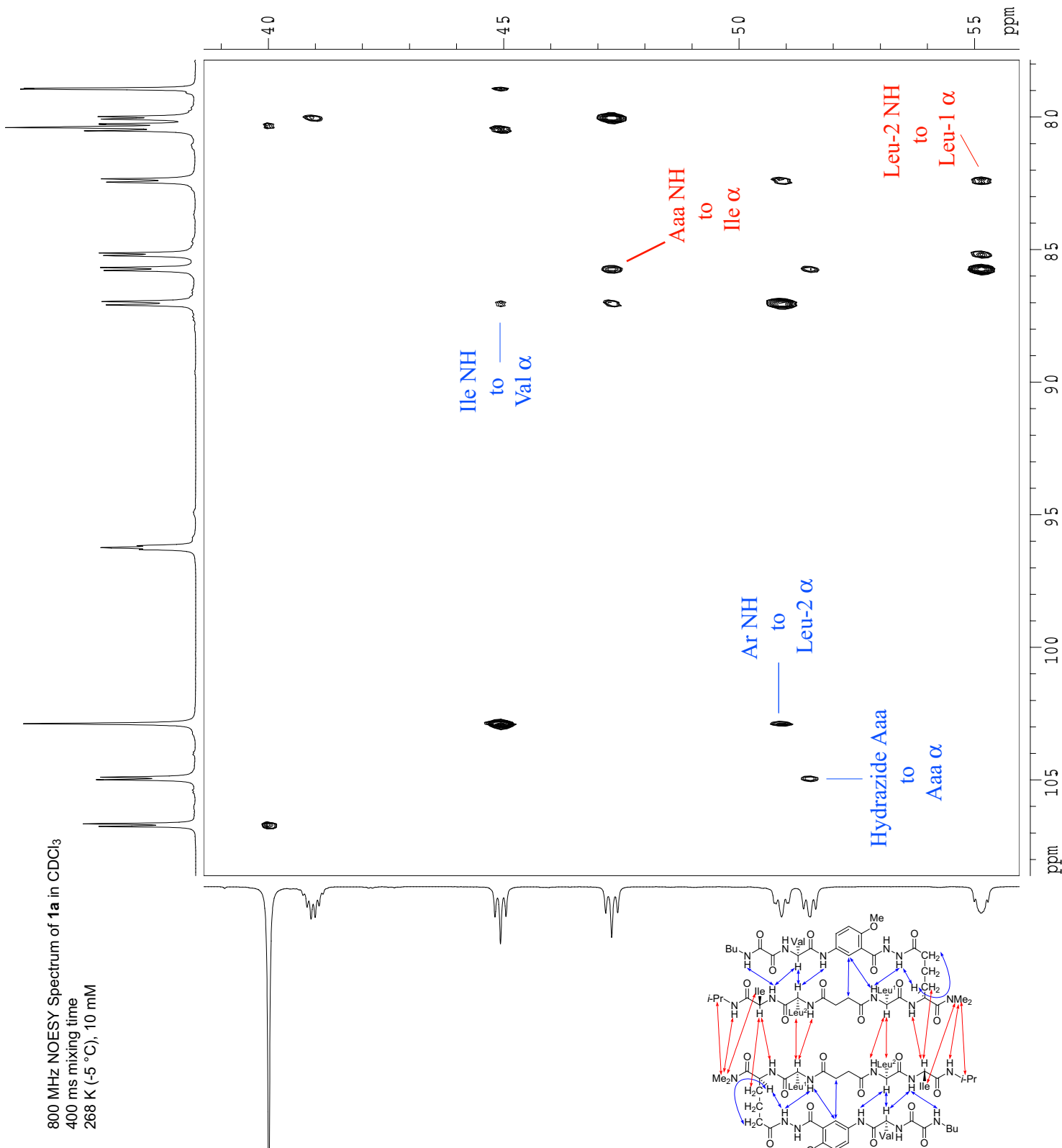
SI 2048
 SF 799.8064119 MHz
 WDW QSI
 SSB 2
 LB 0.00 Hz
 GB 0
 PC 1.40

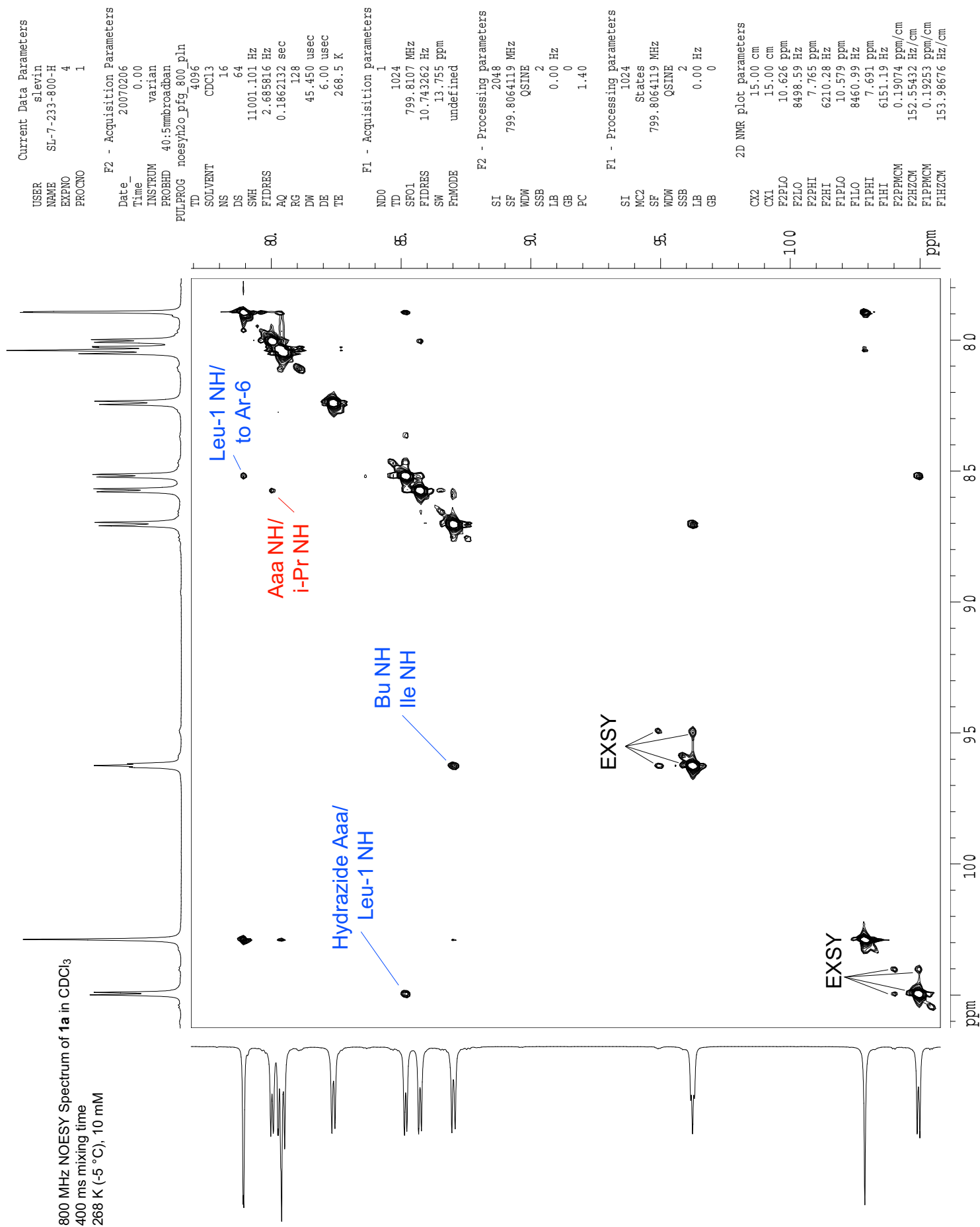
F1 - Processing parameters

SI 1024
 MC2 States
 SF 799.8064119 MHz
 WDW QSI
 SSB 2
 LB 0.00 Hz
 GB 0

2D NMR plot parameters

CX2 15.00 cm
 CX1 15.00 cm
 F2PLO 10.861 ppm
 F2LO 8686.60 Hz
 F2PHI 7.785 ppm
 F2FI 6226.39 Hz
 F1PLO 5.595 ppm
 F1LO 4475.24 Hz
 F1PHI 3.863 ppm
 F1FI 3089.36 Hz
 F2PPCM 0.20507 ppm/cm
 F2HZCM 164.01379 Hz/cm
 F1PPCM 0.11552 ppm/cm
 F1HZCM 92.39206 Hz/cm





800 MHz NOESY Spectrum of **1a** in CDCl₃
 400 ms mixing time
 268 K (-5 °C), 10 mM

Supporting Information

Current Data Parameters
 USER slevin
 NAME SL-7-233-800-H
 EXPNO 4
 PROCNO 1

F2 - Acquisition Parameters

Date_ 20070206
 Time_ 0.00
 INSTRUM varian
 PROBHD 40:5mm broadband
 PULPROG noesyh2o_pfg_800_pln
 TD 4096

SOLVENT CDCl₃
 NS 16
 DS 64
 SWH 11001.101 Hz
 FIDRES 2.685816 Hz
 AQ 0.1862132 sec
 RG 128
 DW 45.450 usec
 DE 6.00 usec
 TE 268.5 K

F1 - Acquisition parameters

ND0 1
 TD 1024
 SFO1 799.8107 MHz
 FIDRES 10.743262 Hz
 SW 13.755 ppm
 FwMODE undefined

F2 - Processing parameters

SI 2048
 SF 799.8064119 MHz
 WDW QSINE
 SSB 2
 LB 0.00 Hz
 GB 0
 PC 1.40

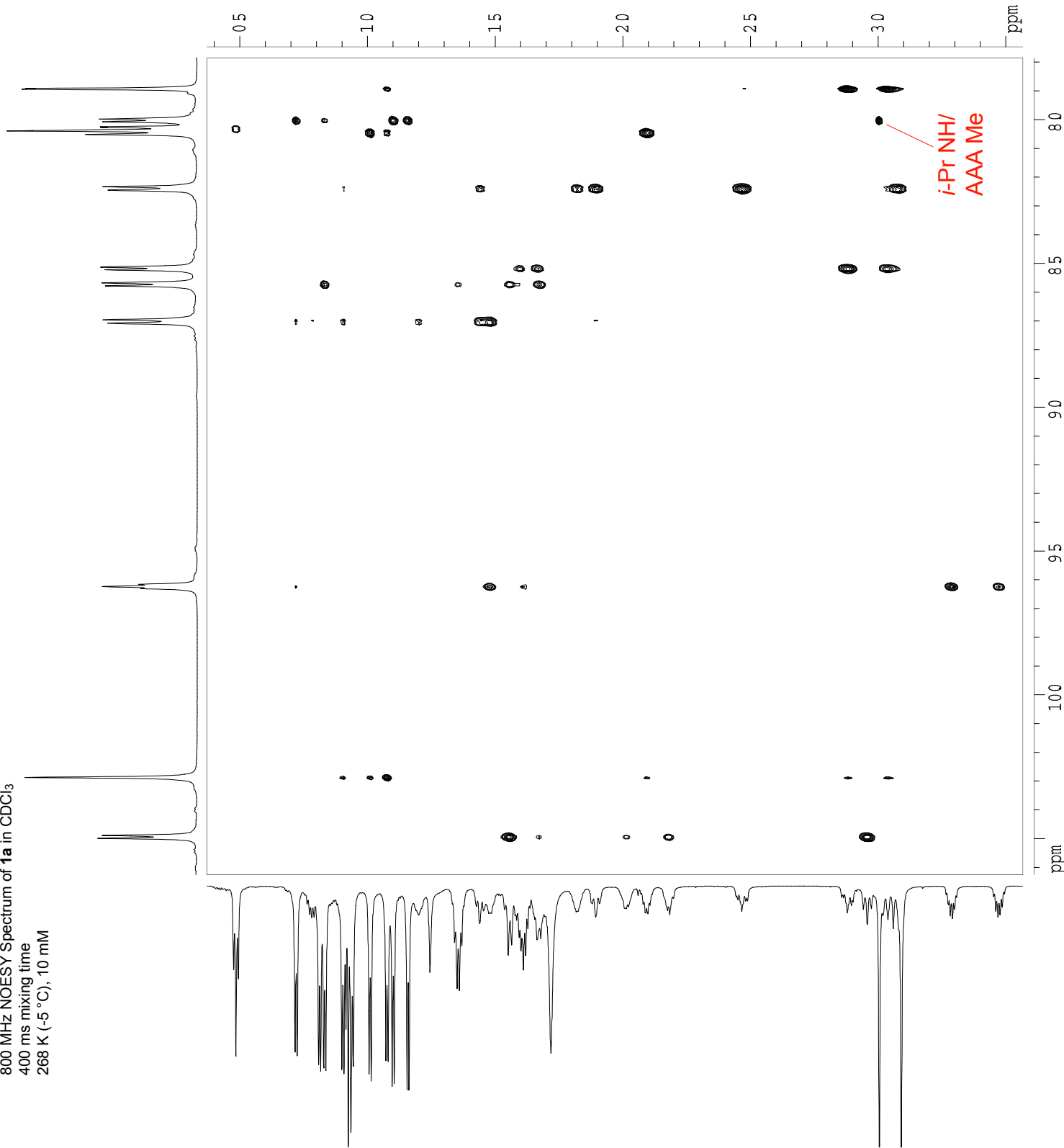
F1 - Processing parameters

SI 1024
 MC2 States
 SF 799.8064119 MHz
 WDW QSINE
 SSB 2
 LB 0.00 Hz
 GB 0

2D NMR plot parameters

CX2 15.00 cm
 CX1 15.00 cm
 F2PLO 10.626 ppm
 F2LO 8498.59 Hz
 F2PHI 7.785 ppm
 F2HI 6226.39 Hz
 F1PLO 3.567 ppm
 F1LO 2853.01 Hz
 F1PHI 0.370 ppm
 F1HI 296.11 Hz
 F2PPMCM 0.18940 ppm/cm
 F2HZCM 151.47998 Hz/cm
 F1PPMCM 0.21313 ppm/cm
 F1HZCM 170.45975 Hz/cm

S. Levin and J. S. Nowick



Supporting Information

S. Levin and J. S. Nowick

Current Data Parameters
 USER slevin
 NAME SL-7-233-800-H
 EXPNO 4
 PROCNO 1

F2 - Acquisition Parameters
 Date 20070206
 Time 0.00
 INSTRUM varian
 PROBHD 40:5mmrbroadban
 PULPROG noesyh2o_pfg_800_pln
 TD 4096

SOLVENT CDCl3
 NS 16
 DS 64
 SWH 11001.101 Hz
 FIDRES 2.685816 Hz
 AQ 0.1862132 sec
 RG 128
 DW 45.450 usec
 DE 6.00 usec
 TE 268.5 K

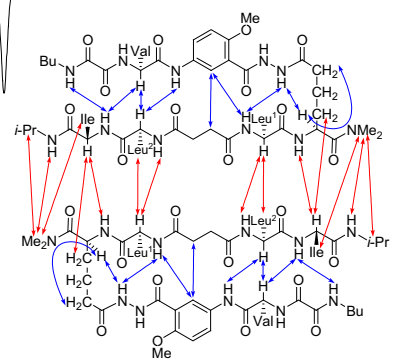
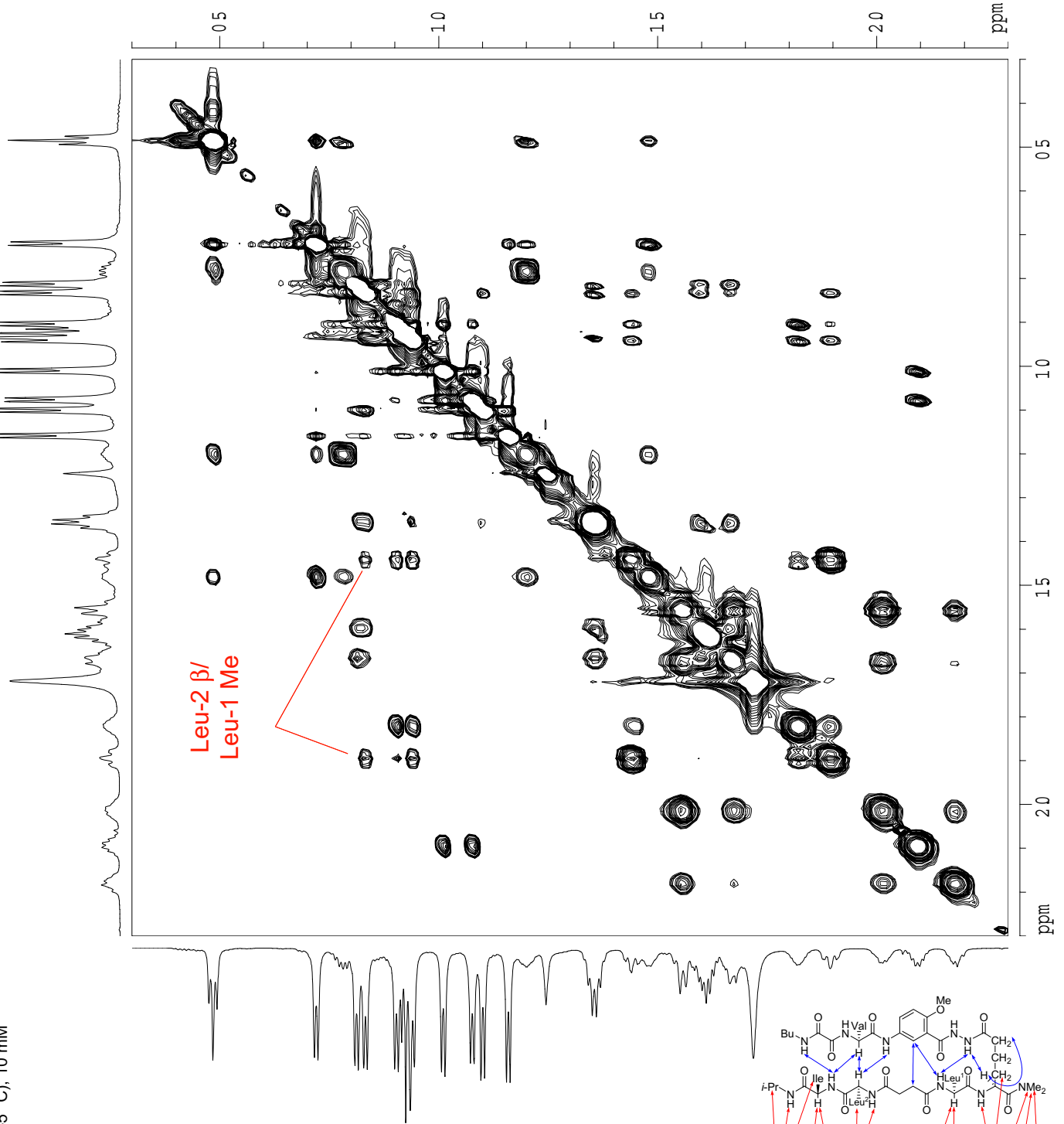
F1 - Acquisition parameters
 ND0 1
 TD 1024
 SF01 799.8107 MHz
 FIDRES 10.743262 Hz
 SW 13.755 ppm
 FMODE undefined

F2 - Processing parameters
 SI 2048
 SF 799.8064119 MHz
 WDM QSINE
 SSB 2
 LB 0.00 Hz
 GB 0
 PC 1.40

F1 - Processing parameters
 SI 1024
 MC2 States
 SF 799.8064119 MHz
 WDM QSINE
 SSB 2
 LB 0.00 Hz
 GB 0

2D NMR plot parameters
 CX2 15.00 cm
 CX1 15.00 cm
 F2PLO 2.300 ppm
 F2LO 1839.55 Hz
 F2PHI 0.300 ppm
 F2HI 239.94 Hz
 F1PLO 2.300 ppm
 F1LO 1839.55 Hz
 F1PHI 0.300 ppm
 F1HI 239.94 Hz
 F2PPMCM 0.13333 ppm/cm
 F2HZCM 106.64085 Hz/cm
 F1PPMCM 0.13333 ppm/cm
 F1HZCM 106.64085 Hz/cm

800 MHz NOESY Spectrum of **1a** in CDCl₃
 400 ms mixing time
 268 K (-5 °C), 10 mM



Current Data Parameters

USER slevin
 NAME SL-7-233-800-H
 EXPNO 4
 PROCNO 1

F2 - Acquisition Parameters

Date_ 20070206
 Time_ 0.00
 INSTRUM varian
 PROBHD 40:5mm broadband
 PULPROG noesyh2o_pfg 800_pln
 TD 4096
 SOLVENT CDCl3
 NS 16
 DS 64
 SWH 11001.101 Hz
 FIDRES 2.685816 Hz
 AQ 0.1862132 sec
 RG 128
 DW 45.450 usec
 DE 6.00 usec
 TE 268.5 K

F1 - Acquisition parameters

ND0 1
 TD 1024
 SFO1 799.8107 MHz
 FIDRES 10.743262 Hz
 SW 13.755 ppm
 F1MODE undefined

F2 - Processing parameters

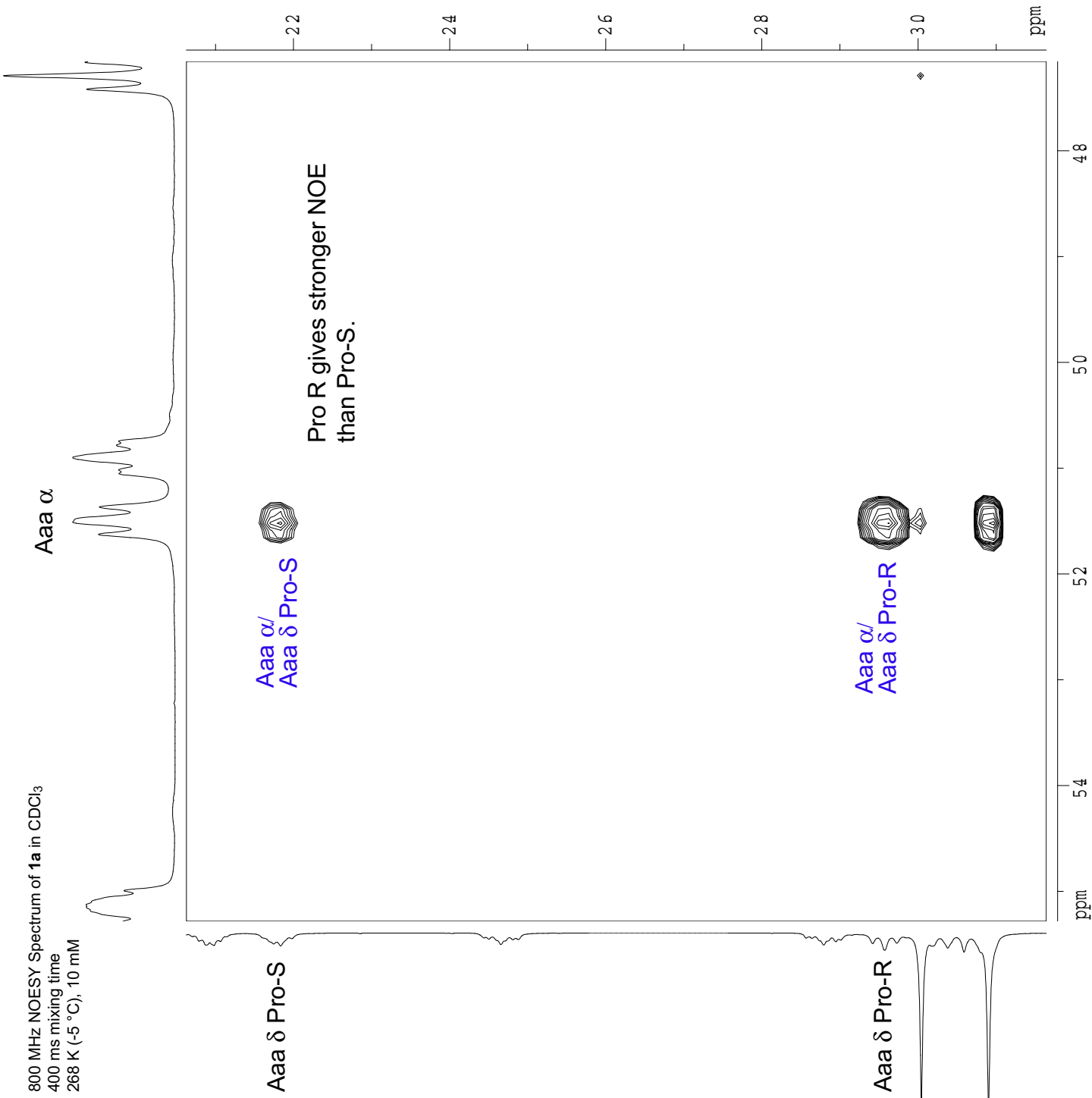
SI 2048
 SF 799.8064119 MHz
 WDW QSINE
 SSB 2
 LB 0.00 Hz
 GB 0
 PC 1.40

F1 - Processing parameters

SI 1024
 MC2 States
 SF 799.8064119 MHz
 WDW QSINE
 SSB 2
 LB 0.00 Hz
 GB 0

2D NMR plot parameters

CX2 15.00 cm
 CX1 15.00 cm
 F2PLO 5.528 ppm
 F2LO 4421.52 Hz
 F2PHI 4.716 ppm
 F2HI 3771.56 Hz
 F1PLO 3.164 ppm
 F1LO 2530.71 Hz
 F1PHI 2.063 ppm
 F1HI 1649.76 Hz
 F2PNCM 0.05418 ppm/cm
 F2HZCM 43.33116 Hz/cm
 F1PNCM 0.07343 ppm/cm
 F1HZCM 58.72982 Hz/cm



Current Data Parameters
 USER slevin
 NAME SL-7-233-800-H
 EXPNO 4
 PROCNO 1

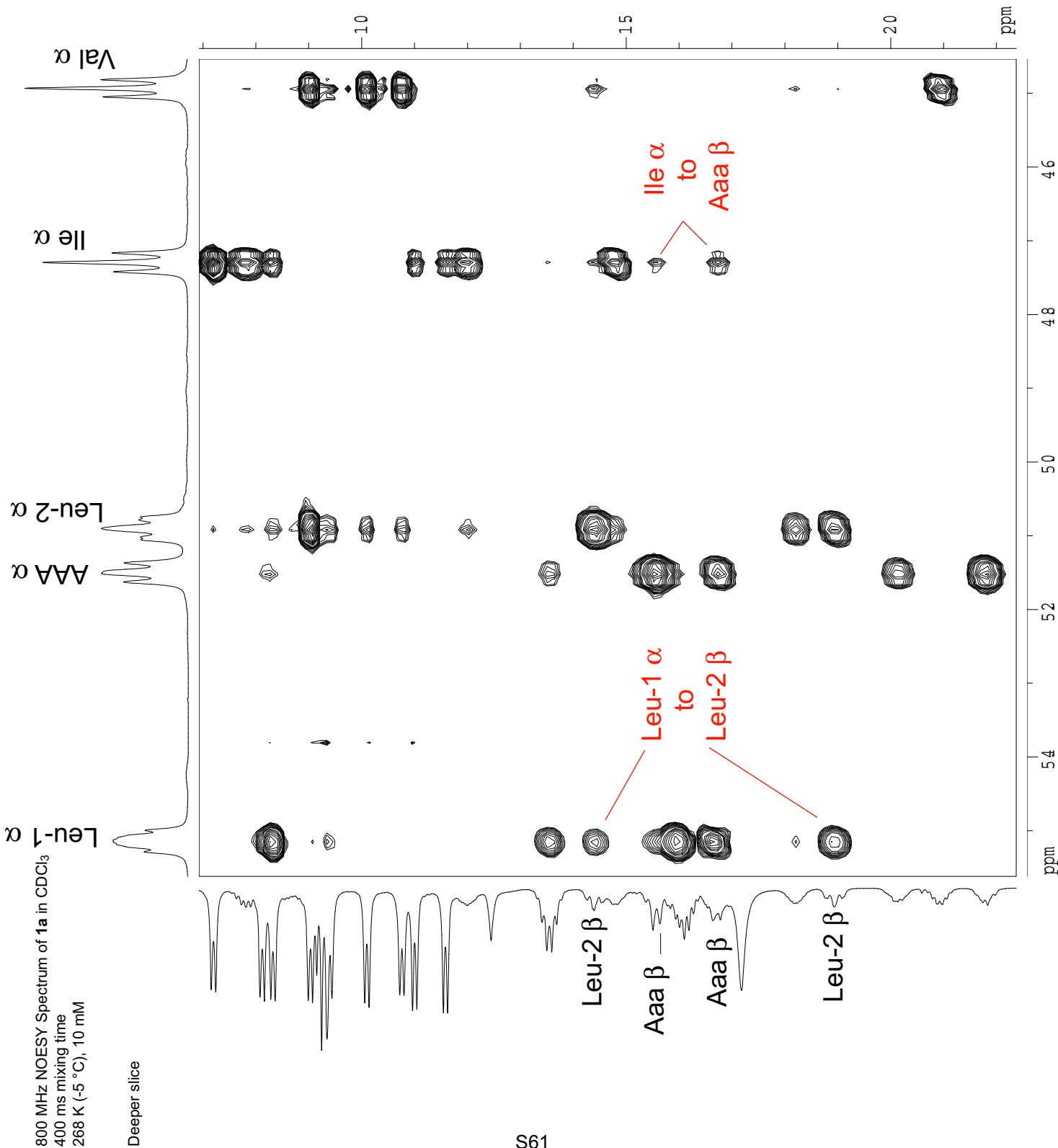
F2 - Acquisition Parameters
 Date_ 20070206
 Time_ 0.00
 INSTRUM varian
 PROBHD 40:5mmbroadban
 PULPROG noesyh2o_pfg_800_pln
 TD 4096
 SOLVENT CDCl3
 NS 16
 DS 64
 SWH 11001.101 Hz
 FIDRES 2.683816 Hz
 AQ 0.1862132 sec
 RG 128
 DW 45.450 usec
 DE 6.00 usec
 TE 288.5 K

F1 - Acquisition parameters
 ND0 1
 TD 1024
 SF01 799.8107 MHz
 FIDRES 10.743262 Hz
 SW 13.755 ppm
 FMODE undefined

F2 - Processing parameters
 SI 2048
 SF 799.8064119 MHz
 WDM QSIINE
 SSB 2
 LB 0.00 Hz
 GB 0
 PC 1.40

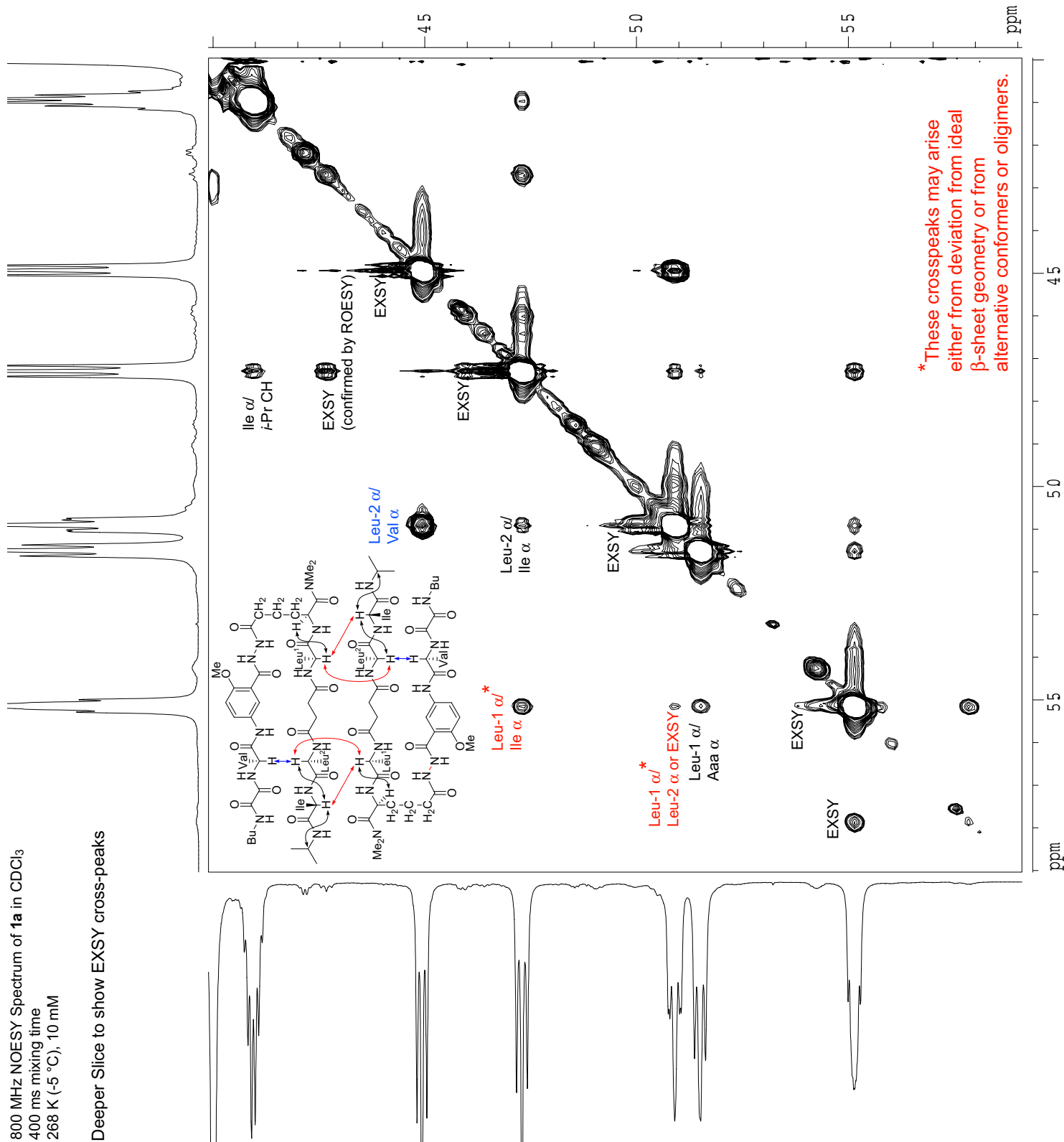
F1 - Processing parameters
 SI 1024
 MC2 States
 SF 799.8064119 MHz
 WDM QSIINE
 SSB 2
 LB 0.00 Hz
 GB 0

2D NMR plot parameters
 CX2 15.00 cm
 CX1 15.00 cm
 F2PLO 5.562 ppm
 F2LO 4448.38 Hz
 F2PHI 4.454 ppm
 F2HI 3562.06 Hz
 F1PLO 2.237 ppm
 F1LO 1789.43 Hz
 F1PHI 0.693 ppm
 F1HI 553.95 Hz
 F2PPMCM 0.07388 ppm/cm
 F2HZCM 59.08795 Hz/cm
 F1PPMCM 0.10298 ppm/cm
 F1HZCM 82.36501 Hz/cm



800 MHz NOESY Spectrum of **1a** in CDCl₃
 400 ms mixing time
 268 K (-5 °C), 10 mM

Deeper Slice to show EXSY cross-peaks



Supporting Information

Current Data Parameters
 USER slevin
 NAME SL-7-233-800-H
 EXPNO 4
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20070206
 Time_ 0.00
 INSTRUM varian
 PROBHD 40:5mm broadband
 PULPROG noesyh2o_pfg_800_pln

TD 4096
 SOLVENT CDCl3
 NS 16
 DS 64
 SWH 11001.101 Hz
 FIDRES 2.685816 Hz
 AQ 0.1862132 sec
 RG 128
 DW 45.450 usec
 DE 6.00 usec
 TE 268.5 K

F1 - Acquisition parameters
 NDO 1
 TD 1024
 SFO1 799.8107 MHz
 FIDRES 10.743262 Hz
 SW 13.755 ppm
 FreqMODE undefined

F2 - Processing parameters
 SI 2048
 SF 799.8064119 MHz
 WDW QSI
 SSB 2
 LB 0.00 Hz
 GB 0
 PC 1.40

F1 - Processing parameters
 SI 1024
 MC2 States
 SF 799.8064119 MHz
 WDW QSI
 SSB 2
 LB 0.00 Hz
 GB 0

2D NMR plot parameters
 CX2 15.00 cm
 CX1 15.00 cm
 F2PLO 5.904 ppm
 F2LO 4721.66 Hz
 F2PHI 3.996 ppm
 F2HI 3196.12 Hz
 F1PLO 5.910 ppm
 F1LO 4727.03 Hz
 F1PHI 3.989 ppm
 F1HI 3190.74 Hz
 F2PPMCM 0.12716 ppm/cm
 F2HZCM 101.70288 Hz/cm
 F1PPMCM 0.12805 ppm/cm
 F1HZCM 102.41909 Hz/cm

Supporting Information

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Current Data Parameter
 USER slevin
 NAME SL-7-233-600N-H
 EXNO 9
 PROCNO 1

F2 - Acquisition Parameter

Date 20070201
 Time 0.54
 INSTRUM av600
 PROBHD 5 mm TBI 1H/13
 PULPROG roesyph.2.prd
 TD 1912
 SOLVENT CDCl3
 NS 32
 DS 16
 SWH 7211.539 Hz
 FIDRES 3.771725 Hz
 AQ 0.1326153 sec
 RG 1150
 DW 69.333 usec
 DE 6.00 usec
 TE 268.0 K
 d0 0.00006033 sec
 D1 2.00000000 sec
 d8 0.25000000 sec
 d12 0.00002000 sec
 INO 0.00013885 sec
 L4 500
 STICNT 128

***** CHANNEL f1 *****

MUCL 1H
 P1 8.00 usec
 P25 250.00 usec
 PL1 -1.00 dB
 PL27 22.70 dB
 SF01 600.1335408 MHz

F1 - Acquisition parameter

ND0 1
 TD 256
 SF01 600.1335 MHz
 FIDRES 28.132877 Hz
 SW 12.001 ppm
 FwMODE States-TPII

F2 - Processing parameter

SI 1024
 SF 600.1300226 MHz
 WDM QSIINE
 SSB 2
 LB 0.00 Hz
 GB 0
 PC 1.40

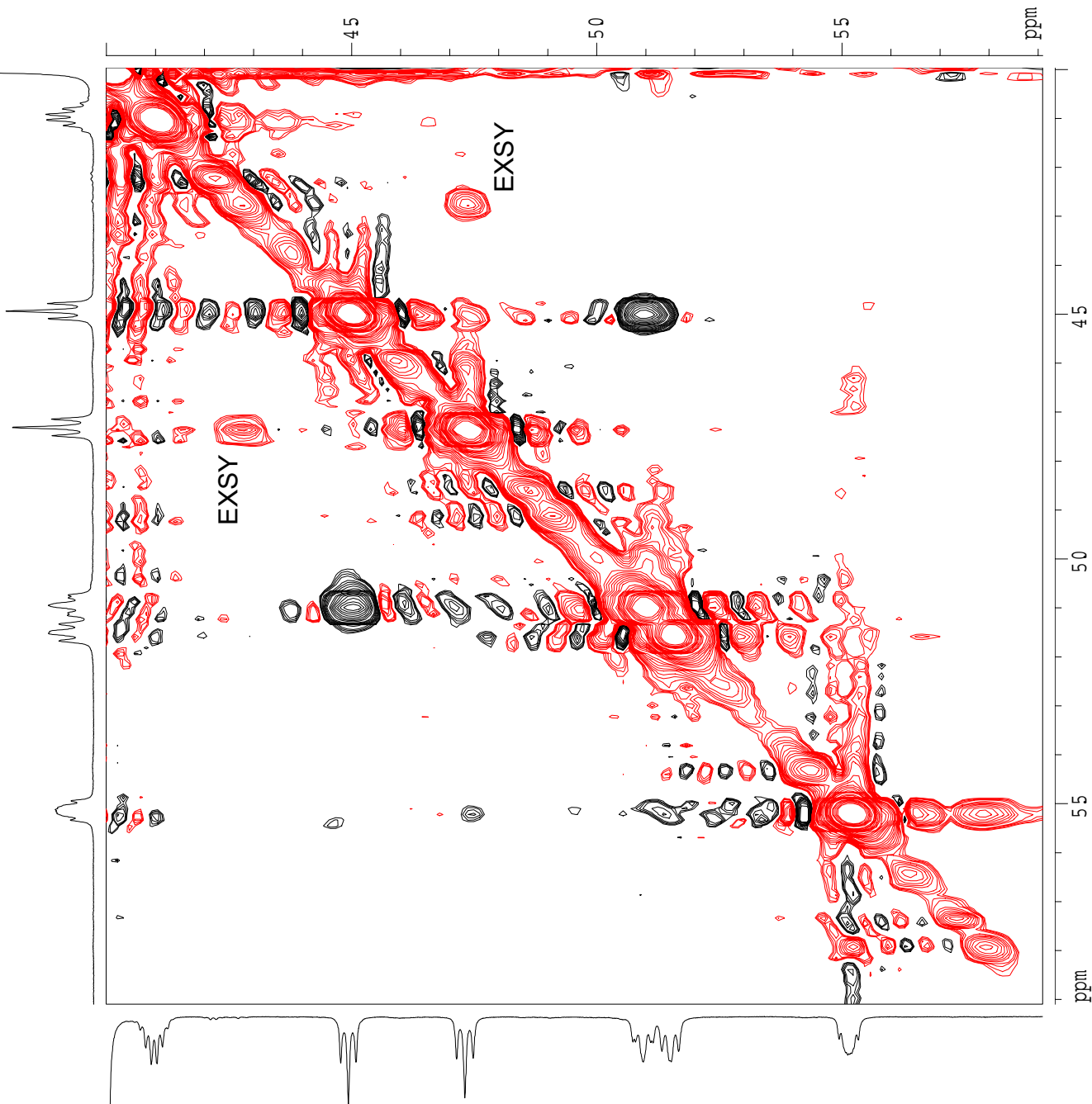
F1 - Processing parameter

SI 1024
 MC2 States-TPII
 SF 600.1300226 MHz
 WDM QSIINE
 SSB 2
 LB 0.00 Hz
 GB 0

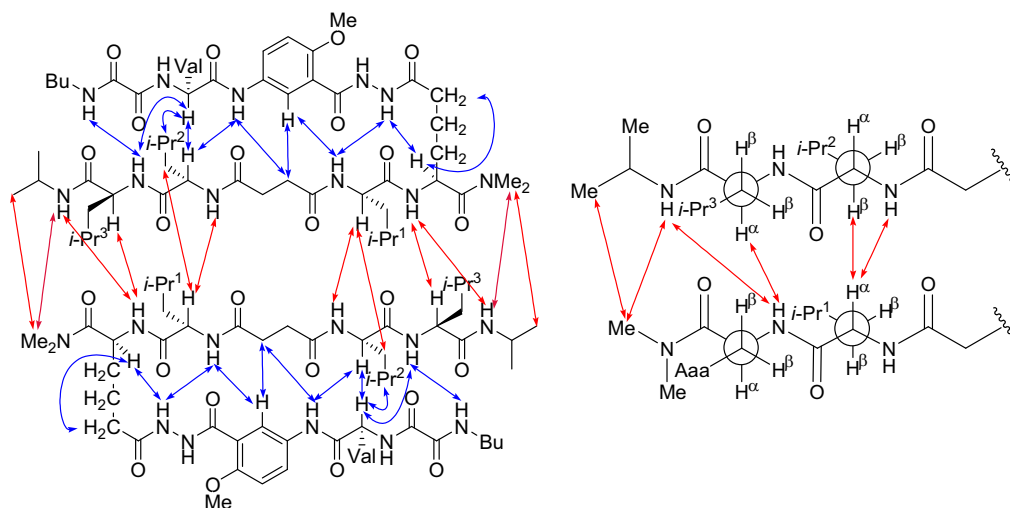
2D NMR plot parameter

CX2 15.00 cm
 CX1 15.00 cm
 F2PLO 5.909 ppm
 F2LO 3546.36 Hz
 F2PHI 3.997 ppm
 F2HI 2398.43 Hz
 F1PLO 5.909 ppm
 F1LO 3546.33 Hz
 F1PHI 3.999 ppm
 F1HI 2399.51 Hz
 F2PMCM 0.12752 ppm/cm
 F2HCM 76.52869 Hz/cm
 F1PMCM 0.12735 ppm/cm
 F1HCM 76.42765 Hz/cm

600 MHz ROESY Spectrum of **1a** in CDCl₃
 250 ms spin-locking time
 268 K (-5 °C), 10 mM



Spectroscopic DATA for the compound **1b**
(6 mM, CDCl₃ 268K)



Key NOEs assigned as *intermolecular* are represented with red arrows

Key NOEs assigned as *intramolecular* are represented with blue arrows

Key data for amino acids.

Amino acid	H _α Shift ppm	NH Shift ppm	³ J _{NHα} Hz
Aaa	5.16	8.67	9.1
R ₁ = Leu ¹	5.53	8.47	8.0
R ₂ = Leu ²	5.02	8.25	9.7
R ₃ = Leu ³	5.01	8.68	10.4
R ₄ = Val	4.46	8.04	8.7

Amino adipic acid (Aaa) δ proton resonances.

pro-R: 2.92 ppm, t, (*overlap*)

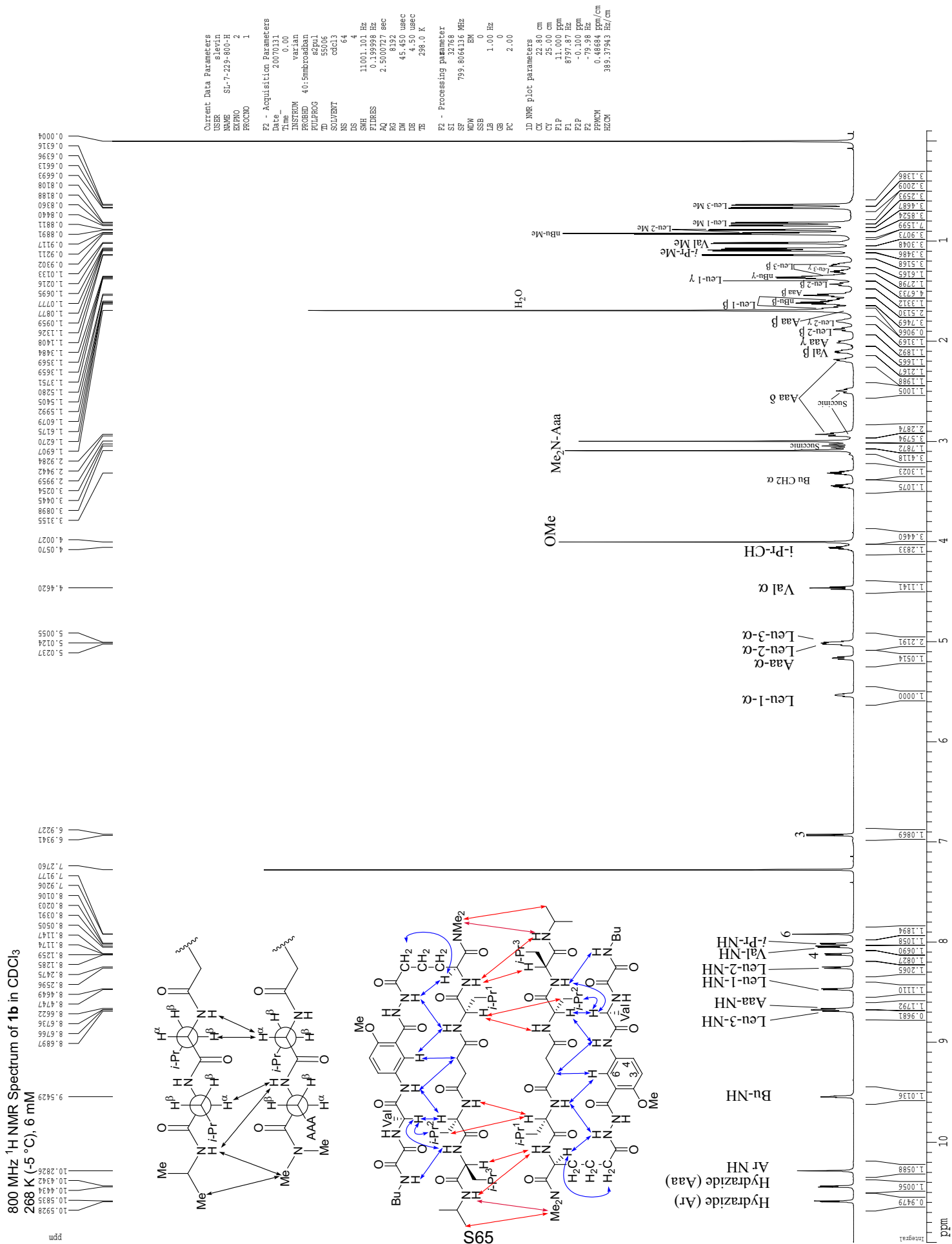
pro-S: 2.18 ppm, td, (*J*₁ = 11.5 Hz; *J*₂ = 7.0 Hz)

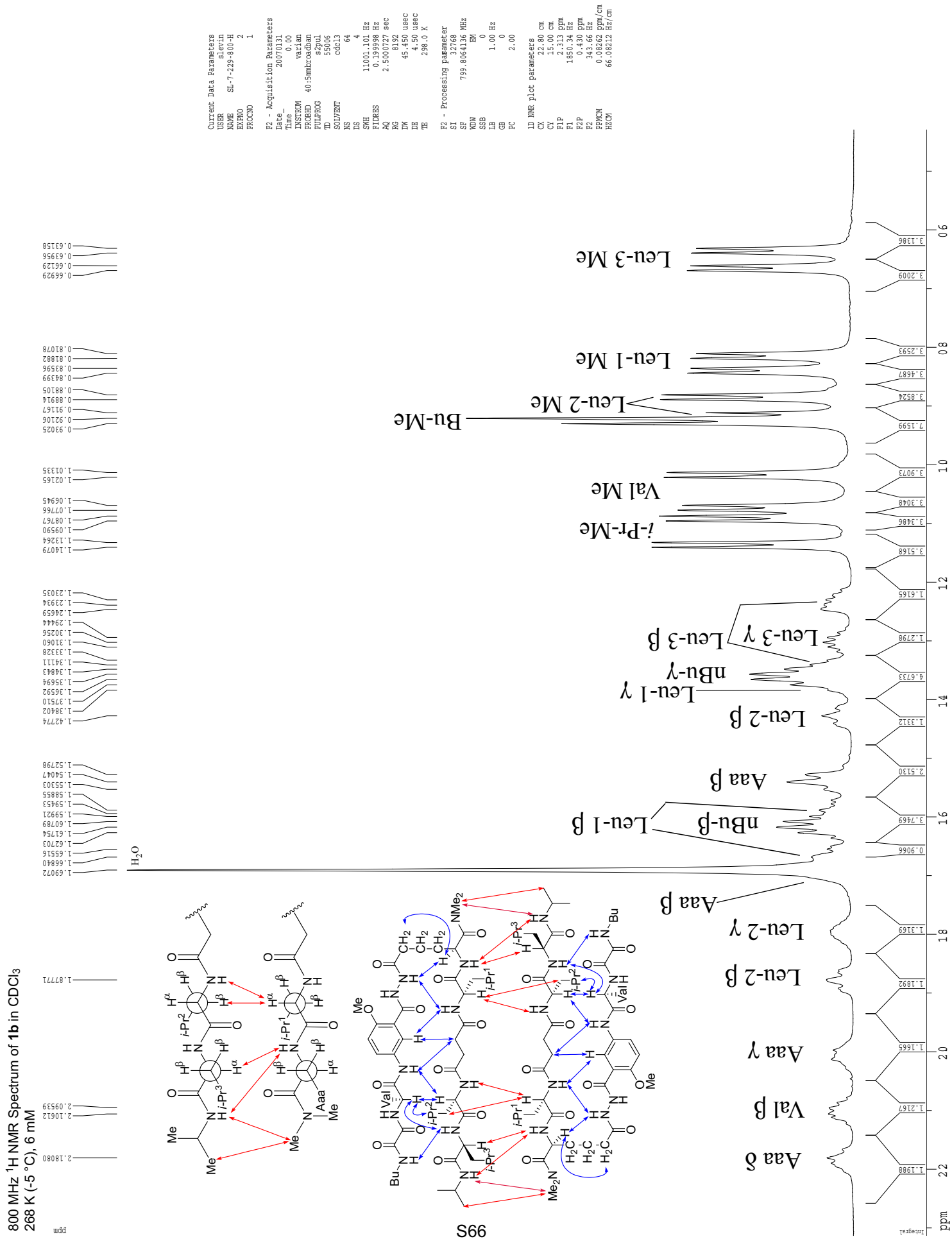
anisotropy = 0.74ppm

Key data for other NH protons.

Proton	NH Shift ppm	<i>J</i> Hz
Ar-NH	10.28	-
Hydrazide Ar	10.59	7.4
Hydrazide Aaa	10.44	7.4
Bu-NH	9.54	5.9
<i>i</i> -Pr-NH	8.03	7.7

ESI MS *m/z* for C₅₂H₈₈N₁₁O₁₂ [M+H]⁺ calcd 1058.66, found 1058.51.





Supporting Information

Current Data Parameters
 USER slevin
 NAME SL-7-229-800-H
 EXPNO 3
 PROCNO 1

F2 - Acquisition Parameters

Date_ 20070130
 Time 0.00
 INSTRUM varian
 PROBHD 40:5mm broadband
 PULPROG gpcsy
 TD 4096
 SOLVENT cdcl3
 NS 8
 DS 64
 SWH 11001.101 Hz
 FIDRES 2.685816 Hz
 AQ 0.1843700 sec
 RG 4096
 DW 45.450 usec
 DE 231.43 usec
 TE 288.5 K

F1 - Acquisition Parameters

ND0 1
 TD 512
 SFO1 799.8107 MHz
 FIDRES 21.486525 Hz
 SW 13.755 ppm
 FRMODE undefined

F2 - Processing parameters

SI 2048
 SF 799.8064136 MHz
 WDW SINE
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.40

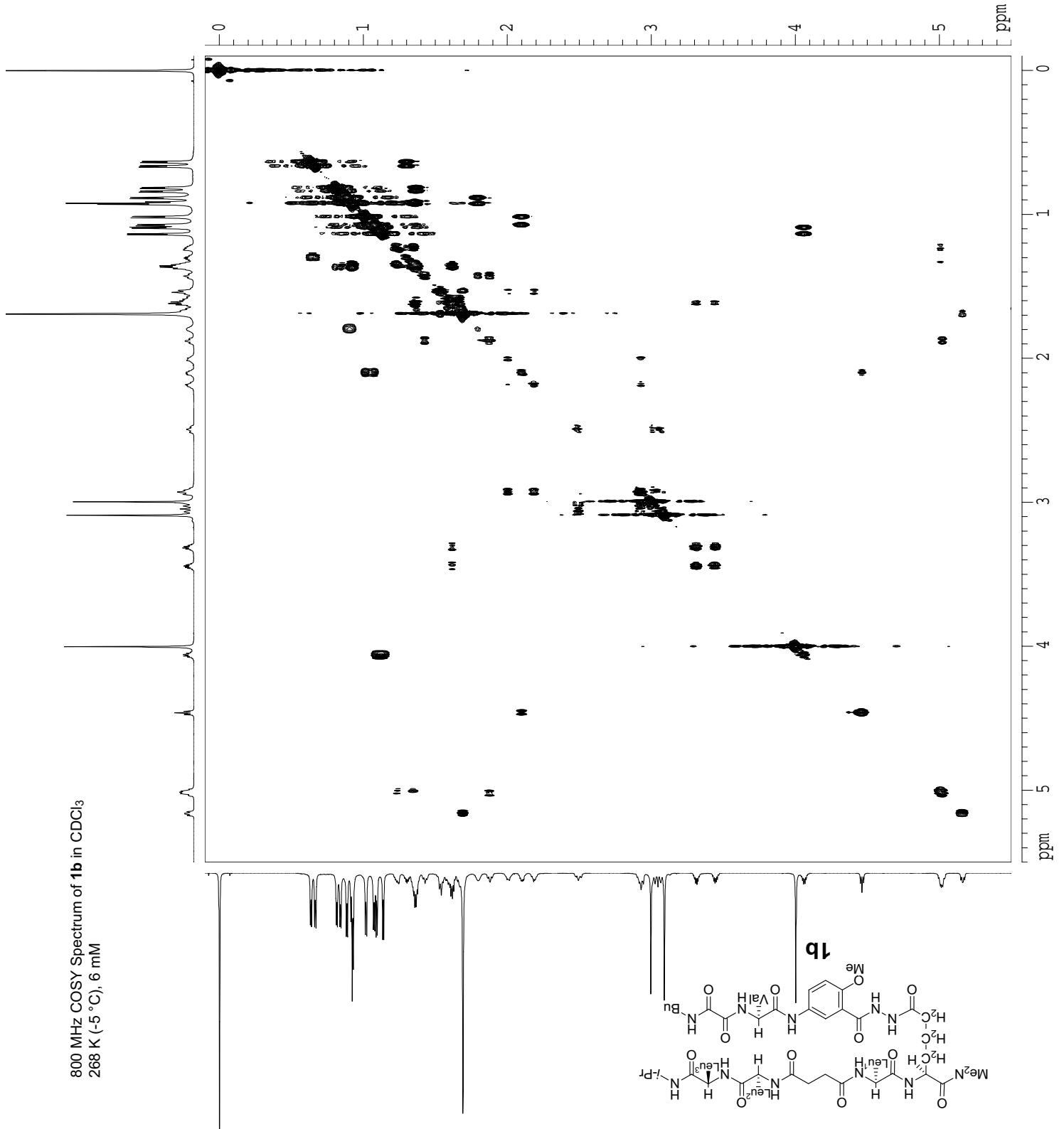
F1 - Processing parameters

SI 1024
 MC2 QF
 SF 799.8064136 MHz
 WDW SINE
 SSB 0
 LB 0.00 Hz
 GB 0

2D NMR plot parameters

CX2 15.00 cm
 CX1 15.00 cm
 F2PLO 5.500 ppm
 F2LO 4398.94 Hz
 F2PHI -0.100 ppm
 F2HI -79.98 Hz
 F1PLO 5.500 ppm
 F1LO 4398.94 Hz
 F1PHI -0.100 ppm
 F1HI -79.98 Hz
 F2PPMCM 0.37333 ppm/cm
 F2HZCM 298.59439 Hz/cm
 F1PPMCM 0.37333 ppm/cm
 F1HZCM 298.59439 Hz/cm

800 MHz COSY Spectrum of **1b** in CDCl₃
 288 K (-5 °C), 6 mM



Supporting Information

Current Data Parameters

USER slevin
 NAME SL-7-229-800-H
 EXPNO 3
 PROCNO 1

F2 - Acquisition Parameters

Date_ 20070130
 Time_ 0.00
 INSTRUM varian
 PROBHD 40:5mmrbroadban
 PULPROG gcosy
 TD 4096
 SOLVENT cdcl3
 NS 8
 DS 64
 SWH 11001.101 Hz
 FIDRES 2.685816 Hz
 AQ 0.1843700 sec
 RG 4096
 DW 45.450 usec
 DE 231.43 usec
 TE 268.5 K

F1 - Acquisition parameters

ND0 1
 TD 512
 SFO1 799.8107 MHz
 FIDRES 21.486525 Hz
 SW 13.755 ppm
 F1MODE undefined

F2 - Processing parameters

SI 2048
 SF 799.8064136 MHz
 WDW SINE
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.40

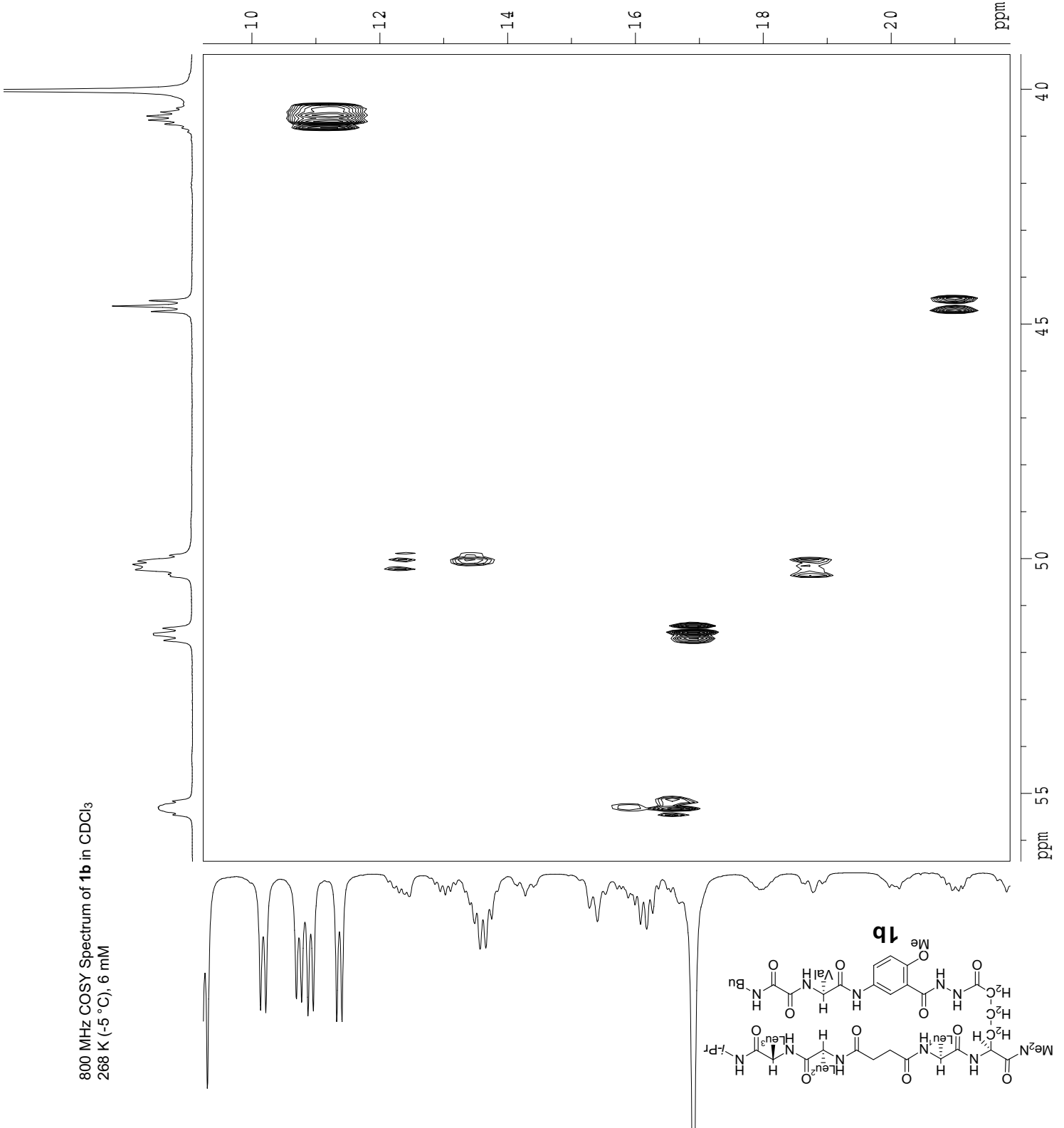
F1 - Processing parameters

SI 1024
 MC2 QF
 SF 799.8064136 MHz
 WDW SINE
 SSB 0
 LB 0.00 Hz
 GB 0

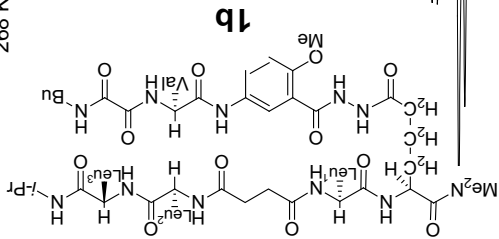
2D NMR plot parameters

CX2 15.00 cm
 CX1 15.00 cm
 F2PLO 5.645 ppm
 F2LO 4514.86 Hz
 F2PHI 3.926 ppm
 F2HI 3139.72 Hz
 F1PLO 2.186 ppm
 F1LO 1748.47 Hz
 F1PHI 0.923 ppm
 F1HI 738.60 Hz
 F2PPMCM 0.11462 ppm/cm
 F2HZCM 91.67583 Hz/cm
 F1PPMCM 0.08418 ppm/cm
 F1HZCM 67.32444 Hz/cm

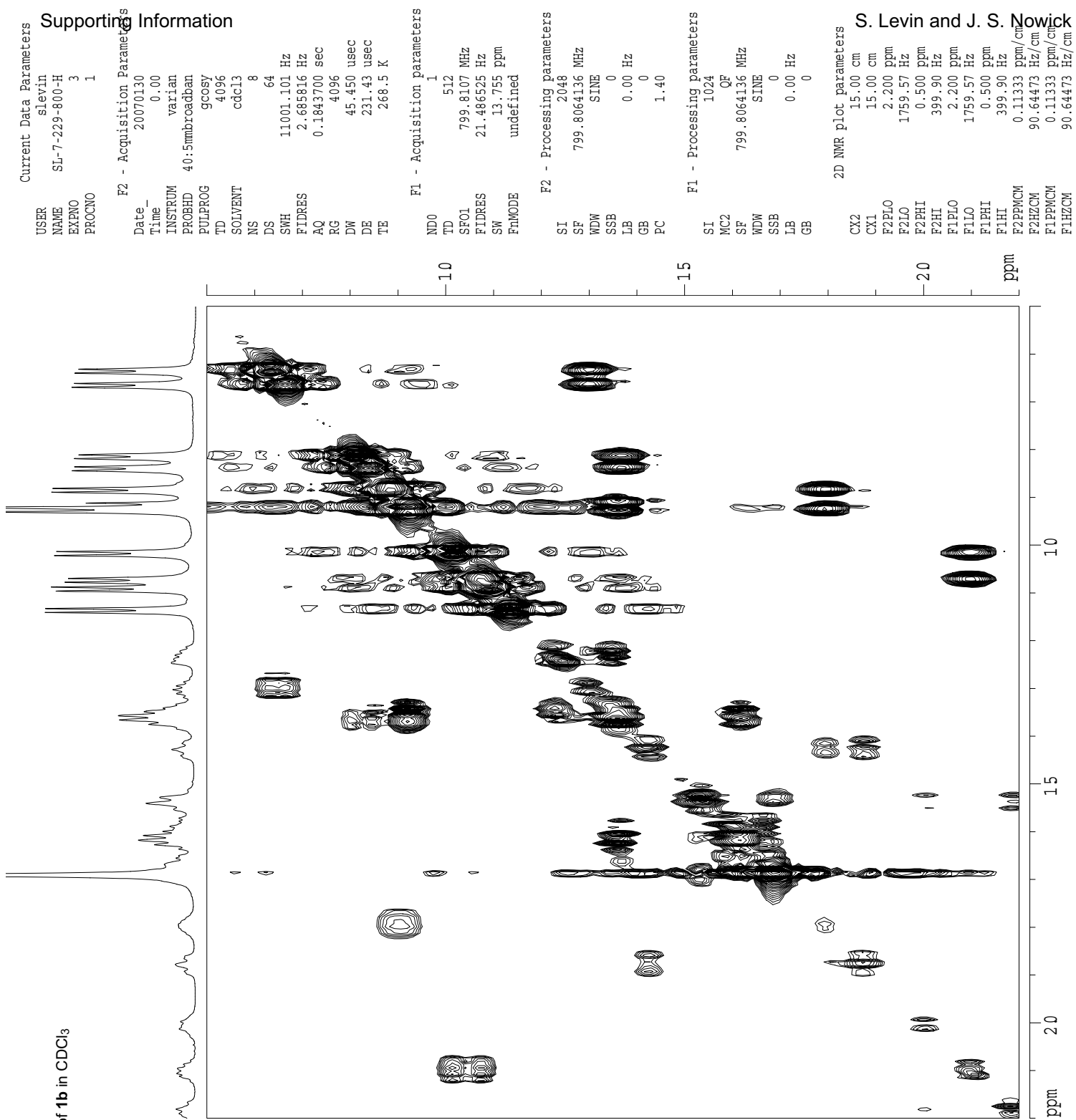
800 MHz COSY Spectrum of **1b** in CDCl₃
 268 K (-5 °C), 6 mM



800 MHz COSY Spectrum of **1b** in CDCl₃
 268 K (-5 °C), 6 mM



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Supporting Information

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Current Data Parameters
 USER slewin
 NAME SL-7-229-800-H
 EXPNO 3
 PROCNO 1

F2 - Acquisition Parameters

Date_ 20070130
 Time_ 0.00
 INSTRUM varian
 PROBHD 40:5mm broadband
 PULPROG gcosy
 TD 4096
 SOLVENT cdc13
 NS 8
 DS 64
 SWH 11001.101 Hz
 FIDRES 2.685816 Hz
 AQ 0.1843700 sec
 RG 4096
 DW 45.450 usec
 DE 231.43 usec
 TE 268.5 K

F1 - Acquisition parameters

ND0 1
 TD 512
 SFO1 799.8107 MHz
 FIDRES 21.486525 Hz
 SW 13.755 ppm
 FhMODE undefined

F2 - Processing parameters

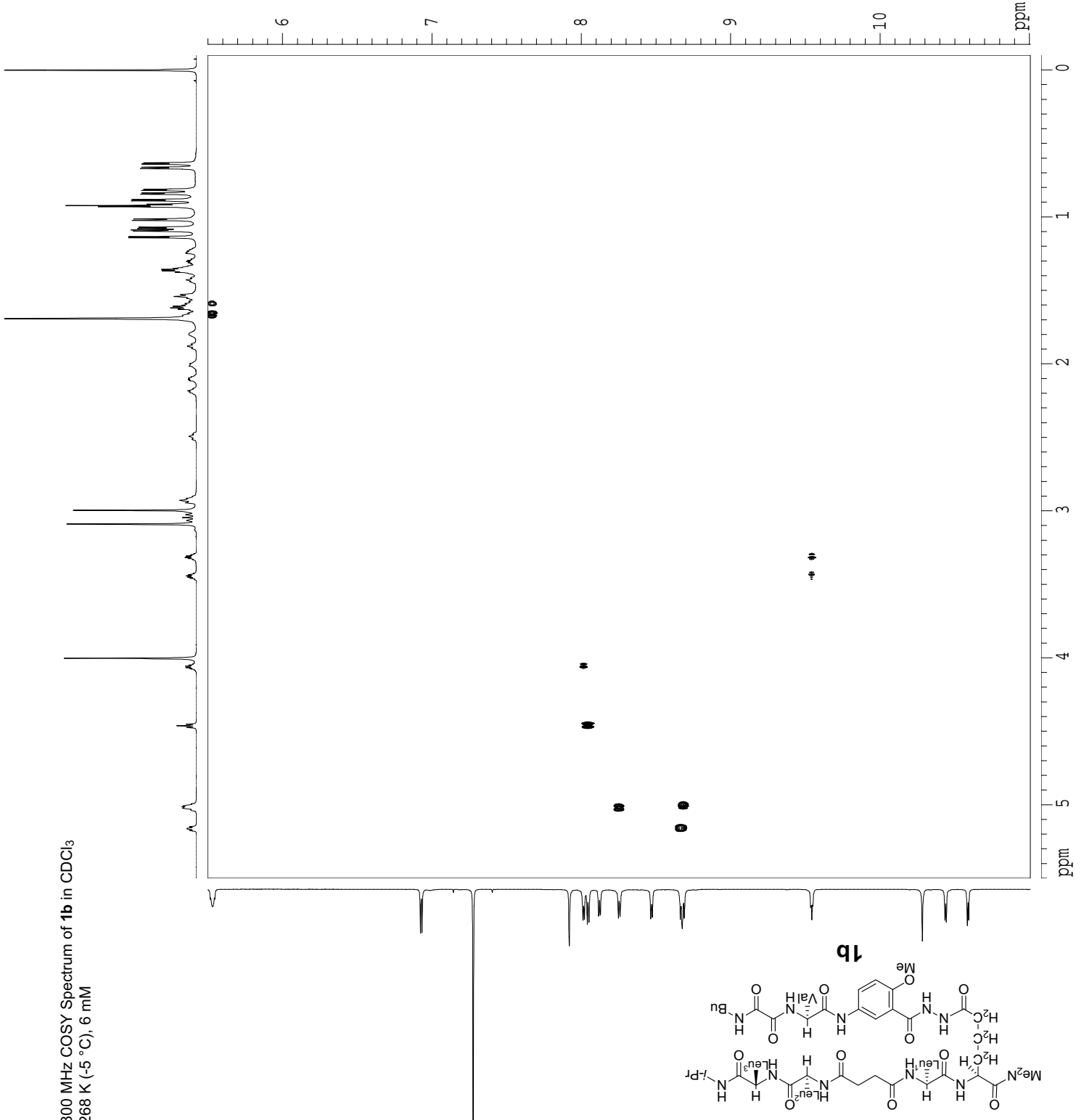
SI 2048
 SF 799.8064136 MHz
 WDW SINE
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.40

F1 - Processing parameters

SI 1024
 MC2 OF
 SF 799.8064136 MHz
 WDW SINE
 SSB 0
 LB 0.00 Hz
 GB 0

2D NMR plot parameters

CX2 15.00 cm
 CX1 15.00 cm
 F2FLO 5.500 ppm
 F2LO 4398.94 Hz
 F2PHI -0.100 ppm
 F2HI -79.98 Hz
 F1FLO 11.007 ppm
 F1LO 8803.10 Hz
 F1PHI 5.499 ppm
 F1HI 4398.36 Hz
 F2PpMCM 0.37333 ppm/cm
 F2HzCM 298.59439 Hz/cm
 F1PpMCM 0.36715 ppm/cm
 F1HzCM 293.64917 Hz/cm



800 MHz COSY Spectrum of **1b** in CDCl₃
 268 K (-5 °C), 6 mM

Current Data Parameters
 USER slevin
 NAME SL-7-229-800-H
 EXPNO 3
 PROCNO 1

F2 - Acquisition Parameters

Date 20070130
 Time 0.00
 INSTRUM varian
 PROBHD 40:5mm broadband
 PULPROG gcpsy
 TD 4096
 SOLVENT cdcl3
 NS 8
 DS 64
 SWH 11001.101 Hz
 FIDRES 2.685816 Hz
 AQ 0.1843700 sec
 RG 4096
 DW 45.450 usec
 DE 231.43 usec
 TE 268.5 K

F1 - Acquisition Parameters

ND0 1
 TD 512
 SF01 799.8107 MHz
 FIDRES 21.486525 Hz
 SW 13.755 ppm
 F1MODE undefined

F2 - Processing parameters

SI 2048
 SF 799.8064136 MHz
 WDW SINE
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.40

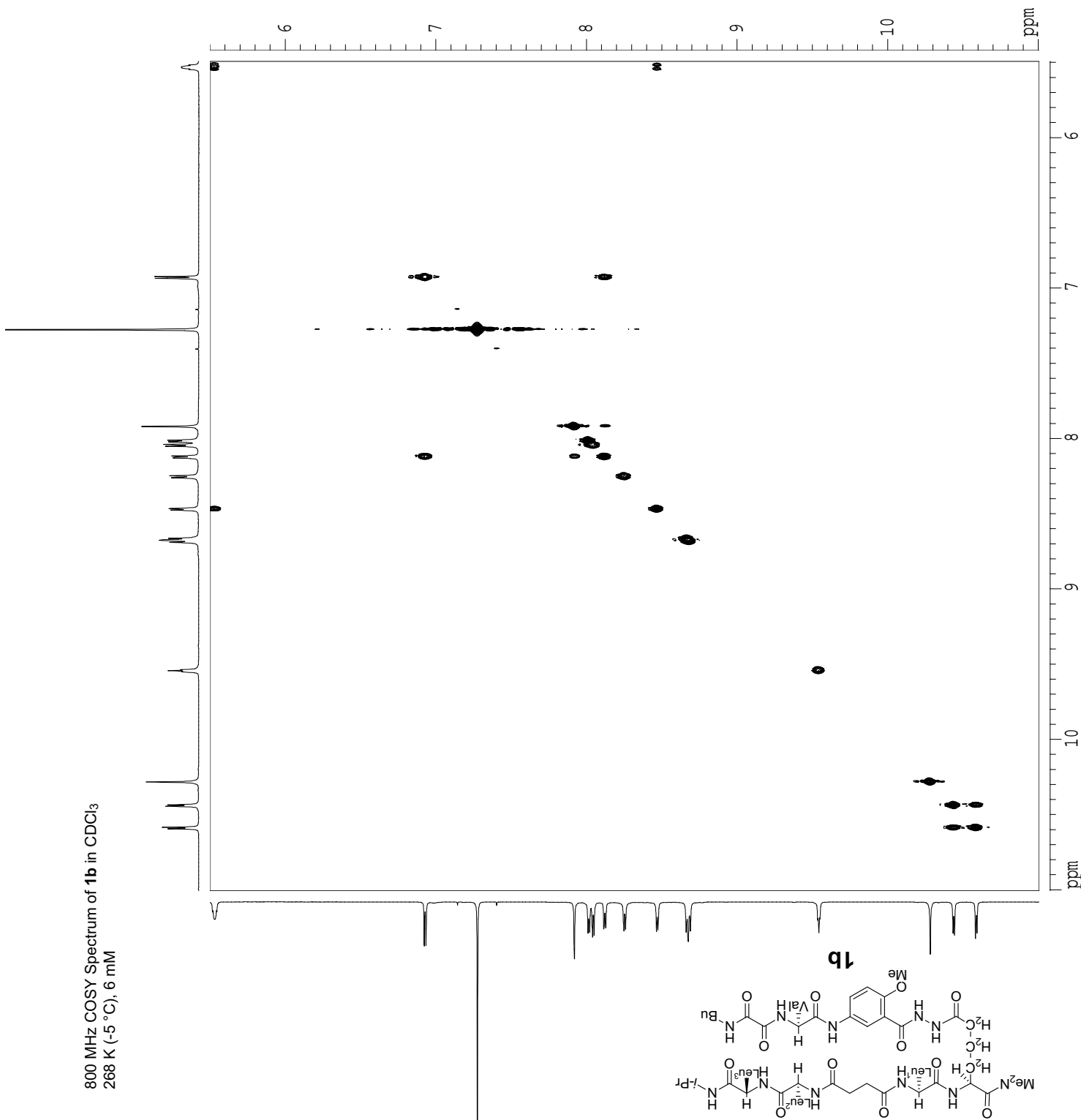
F1 - Processing parameters

SI 1024
 MC2 QF
 SF 799.8064136 MHz
 WDW SINE
 SSB 0
 LB 0.00 Hz
 GB 0

2D NMR plot parameters

CX2 15.00 cm
 CX1 15.00 cm
 F2PLO 11.007 ppm
 F2LO 8803.10 Hz
 F2PHI 5.493 ppm
 F2HI 4392.99 Hz
 F1PLO 11.007 ppm
 F1LO 8803.10 Hz
 F1PHI 5.500 ppm
 F1HI 4398.94 Hz
 F2PPMCM 0.36760 ppm/cm
 F2HZCM 294.00726 Hz/cm
 F1PPMCM 0.36710 ppm/cm
 F1HZCM 293.61072 Hz/cm

800 MHz COSY Spectrum of **1b** in CDCl₃
 268 K (-5 °C), 6 mM



Supporting Information

Current Data Parameters

USER slevin
 NAME SL-7-229-800-H
 EXPNO 3
 PROCNO 1

F2 - Acquisition Parameters

Date_ 20070130
 Time_ 0.00
 INSTRUM varian
 PROBHD 40:5mm broadband
 PULPROG gcosy
 TD 4096
 SOLVENT cdcl3
 NS 8
 DS 64
 SWH 11001.101 Hz
 FIDRES 2.685816 Hz
 AQ 0.1843700 sec
 RG 4096
 DW 45.450 usec
 DE 231.43 usec
 TE 268.5 K

F1 - Acquisition parameters

ND0 1
 TD 512
 SF01 799.8107 MHz
 FIDRES 21.486525 Hz
 SW 13.755 ppm
 FhMODE undefined

F2 - Processing parameters

SI 2048
 SF 799.8064136 MHz
 WDW SINE
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.40

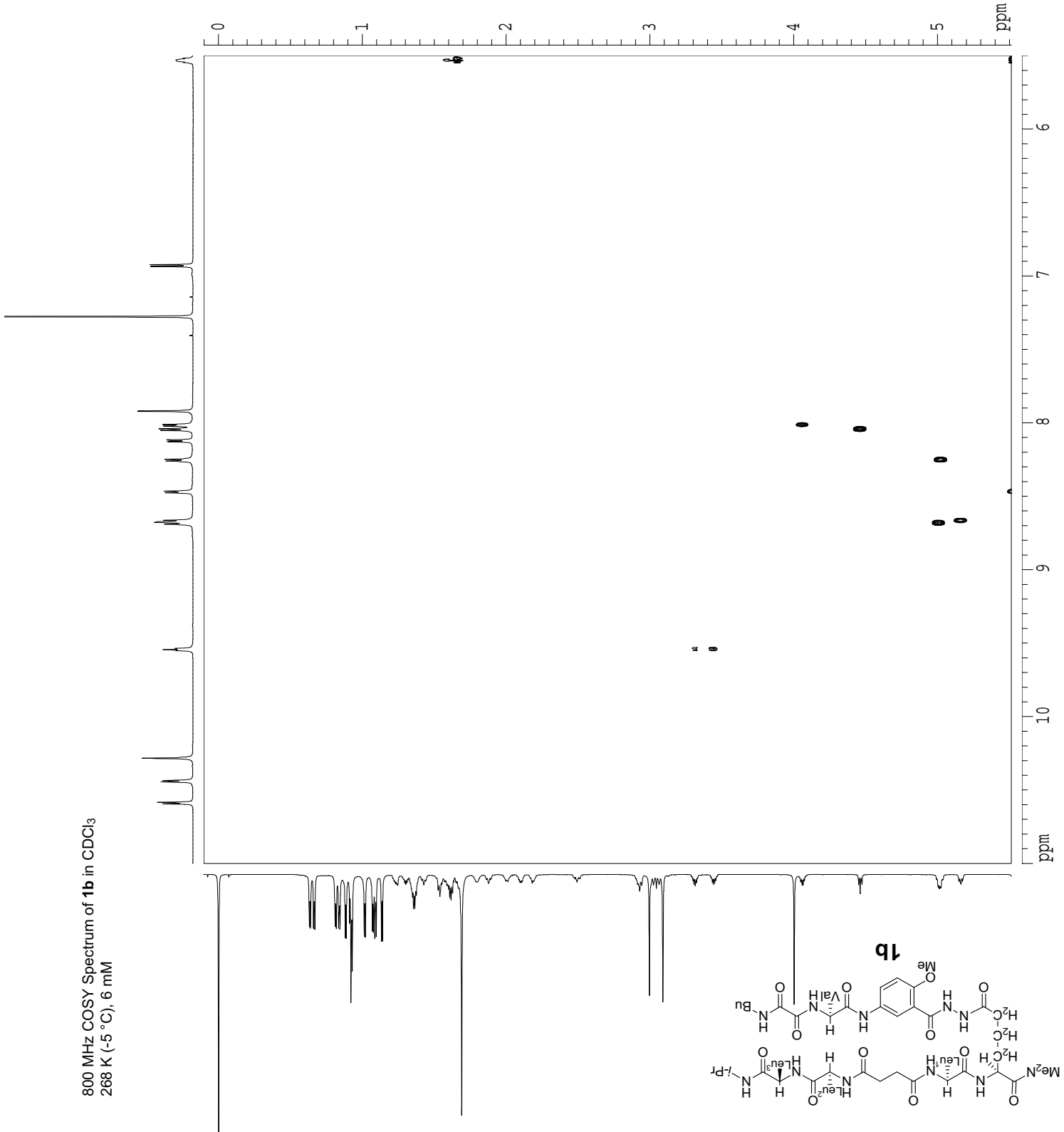
F1 - Processing parameters

SI 1024
 MC2 OF
 SF 799.8064136 MHz
 WDW SINE
 SSB 0
 LB 0.00 Hz
 GB 0

2D NMR plot parameters

CX2 15.00 cm
 CX1 15.00 cm
 F2PLO 11.000 ppm
 F2LO 8797.87 Hz
 F2PHI 5.500 ppm
 F2HI 4398.94 Hz
 F1PLO 5.513 ppm
 F1LO 4409.10 Hz
 F1PHI -0.102 ppm
 F1HI -81.58 Hz
 F2PPMCM 0.36667 ppm/cm
 F2HZCM 293.26236 Hz/cm
 F1PPMCM 0.37431 ppm/cm
 F1HZCM 299.37891 Hz/cm

800 MHz COSY Spectrum of **1b** in CDCl₃
 268 K (-5 °C), 6 mM



Supporting Information

Current Data Parameters
 USER slevin
 NAME SL-7-229-800-H
 EXPNO 3
 PROCNO 1

F2 - Acquisition Parameters

Date_ 20070130
 Time 0.00
 INSTRUM varian
 PROBHD 40:5mmbroadban
 PULPROG gcpsy
 TD 4096
 SOLVENT cdc13
 NS 8
 DS 64
 SWH 11001.101 Hz
 FIDRES 2.685816 Hz
 AQ 0.1843700 sec
 RG 4096
 DW 45.450 usec
 DE 231.43 usec
 TE 268.5 K

F1 - Acquisition Parameters

ND0 1
 TD 512
 SF01 799.8107 MHz
 FIDRES 21.486525 Hz
 SW 13.755 ppm
 F1MODE undefined

F2 - Processing Parameters

SI 2048
 SF 799.8064136 MHz
 WDW SINE
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.40

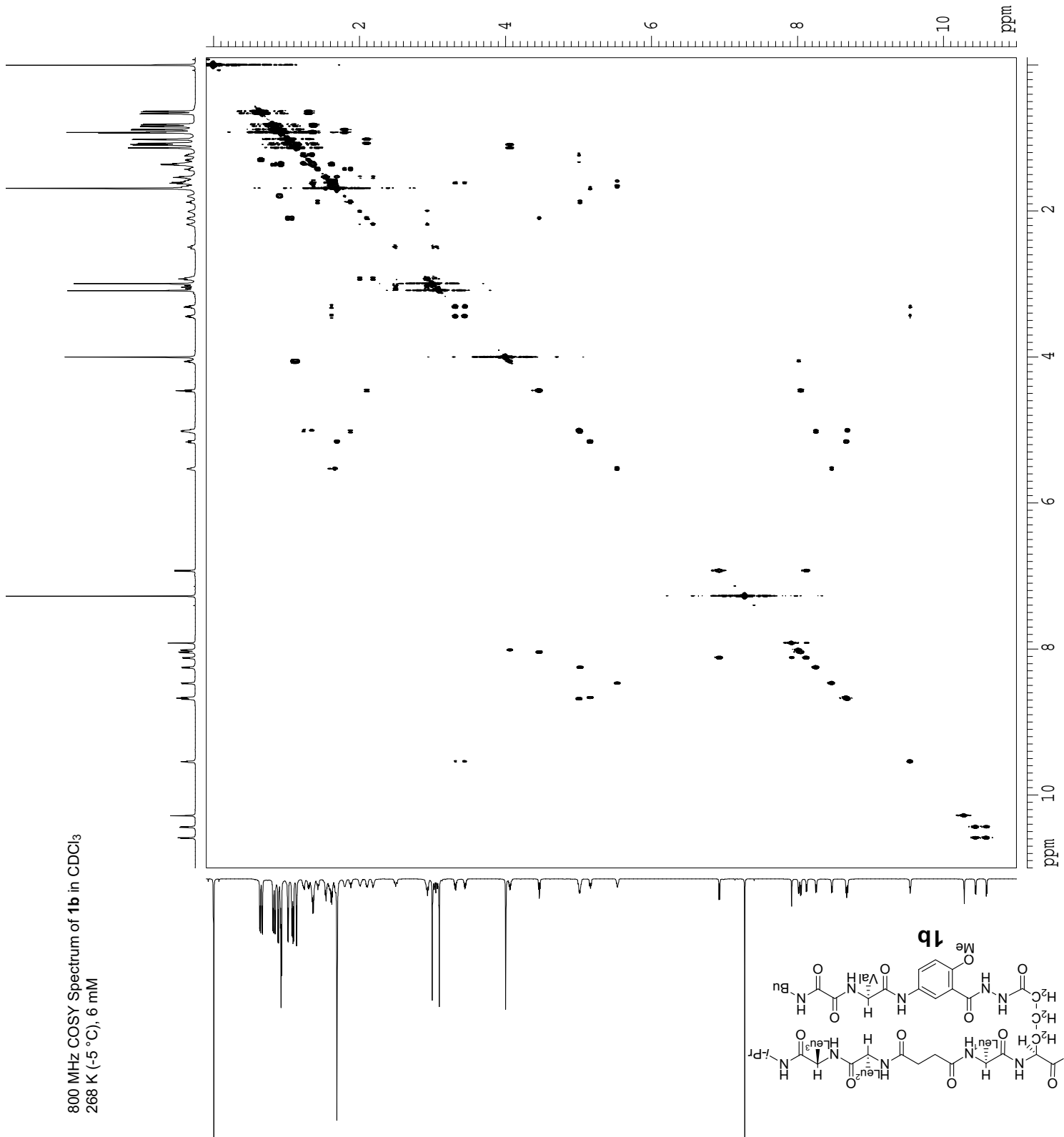
F1 - Processing Parameters

SI 1024
 MC2 QF
 SF 799.8064136 MHz
 WDW SINE
 SSB 0
 LB 0.00 Hz
 GB 0

2D NMR plot parameters

CX2 15.00 cm
 CX1 15.00 cm
 F2PLO 11.000 ppm
 F2LO 8797.87 Hz
 F2PHI -0.100 ppm
 F2HI -79.98 Hz
 F1PLO 11.000 ppm
 F1LO 8797.87 Hz
 F1PHI -0.100 ppm
 F1HI -79.98 Hz
 F2PPMCM 0.74000 ppm/cm
 F2HZCM 591.85669 Hz/cm
 F1PPMCM 0.74000 ppm/cm
 F1HZCM 591.85669 Hz/cm

800 MHz COSY Spectrum of **1b** in CDCl₃
 268 K (-5 °C), 6 mM



Supporting Information

Current Data Parameters
 USER slevin
 NAME SL-7-229-800-H
 EXPNO 4
 PROCNO 1

F2 - Acquisition Parameters

Date_ 20070131
 Time_ 0.00
 INSTRUM varian
 PROBHD 40:5mmbroadban
 PULPROG wgtocsy_bn
 TD 4096
 SOLVENT CDCl3
 NS 16
 DS 64
 SWH 11001.101 Hz
 FIDRES 2.685816 Hz
 AQ 0.1862132 sec
 RG 287.4
 DW 45.450 usec
 DE 6.00 usec
 TE 268.5 K

F1 - Acquisition Parameters

ND0 1
 TD 1024
 SF01 799.8107 MHz
 FIDRES 10.743262 Hz
 SW 13.755 ppm
 FMODE undefined

F2 - Processing Parameters

SI 2048
 SF 799.8064136 MHz
 WDW QSINE
 SSB 2
 LB 0.00 Hz
 GB 0
 PC 1.40

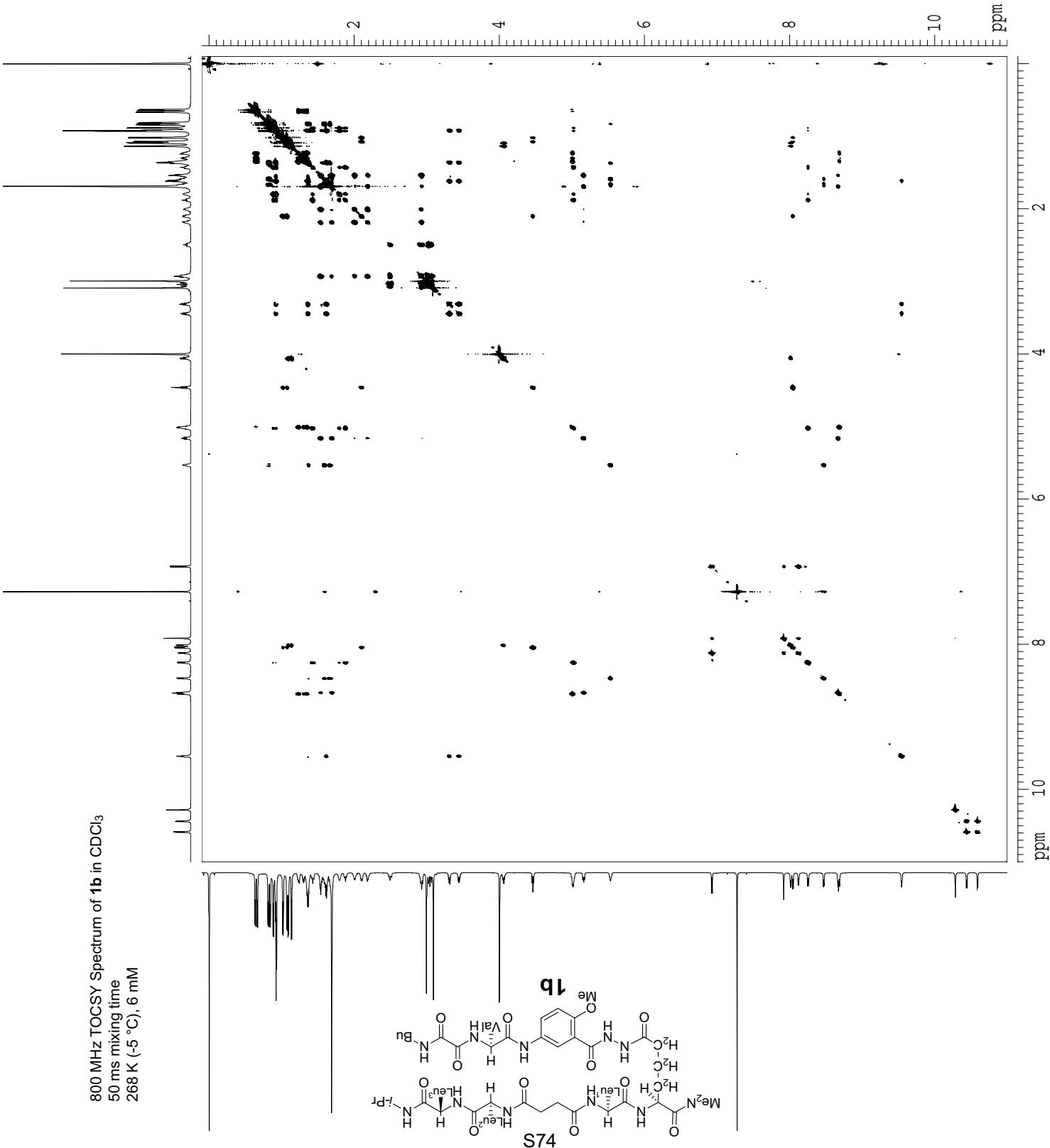
F1 - Processing Parameters

SI 1024
 MC2 States
 SF 799.8064136 MHz
 WDW QSINE
 SSB 2
 LB 0.00 Hz
 GB 0

2D NMR plot parameters

CX2 15.00 cm
 CX1 15.00 cm
 F2PLO 11.000 ppm
 F2LO 8797.87 Hz
 F2PHI -0.100 ppm
 F2HI -79.98 Hz
 F1PLO 11.000 ppm
 F1LO 8797.87 Hz
 F1PHI -0.100 ppm
 F1HI -79.98 Hz
 F2PQCM 0.74000 ppm/cm
 F2HZCM 591.85669 Hz/cm
 F1PQCM 0.74000 ppm/cm
 F1HZCM 591.85669 Hz/cm

800 MHz TOCSY Spectrum of **1b** in CDCl₃
 50 ms mixing time
 268 K (-5 °C), 6 mM



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Supporting Information

Current Data Parameters
 USER slevin
 NAME SL-7-229-800-H
 EXPNO 4
 PROCNO 1

F2 - Acquisition Parameters

Date 20070131
 Time 0.00
 INSTRUM varian
 PROBHD 40:5mmbroadban
 PULPROG wgtocsy_bn
 TD 4096
 SOLVENT CDCl3
 NS 16
 DS 64
 SWH 11001.101 Hz
 FIDRES 2.685816 Hz
 AQ 0.1862132 sec
 RG 287.4
 DW 45.450 usec
 DE 6.00 usec
 TE 268.5 K

F1 - Acquisition Parameters

ND0 1
 TD 1024
 SF01 799.8107 MHz
 FIDRES 10.743262 Hz
 SW 13.755 ppm
 FMODE undefined

F2 - Processing parameters

SI 2048
 SF 799.8064136 MHz
 WDW QSI
 SSB 2
 LB 0.00 Hz
 GB 0
 PC 1.40

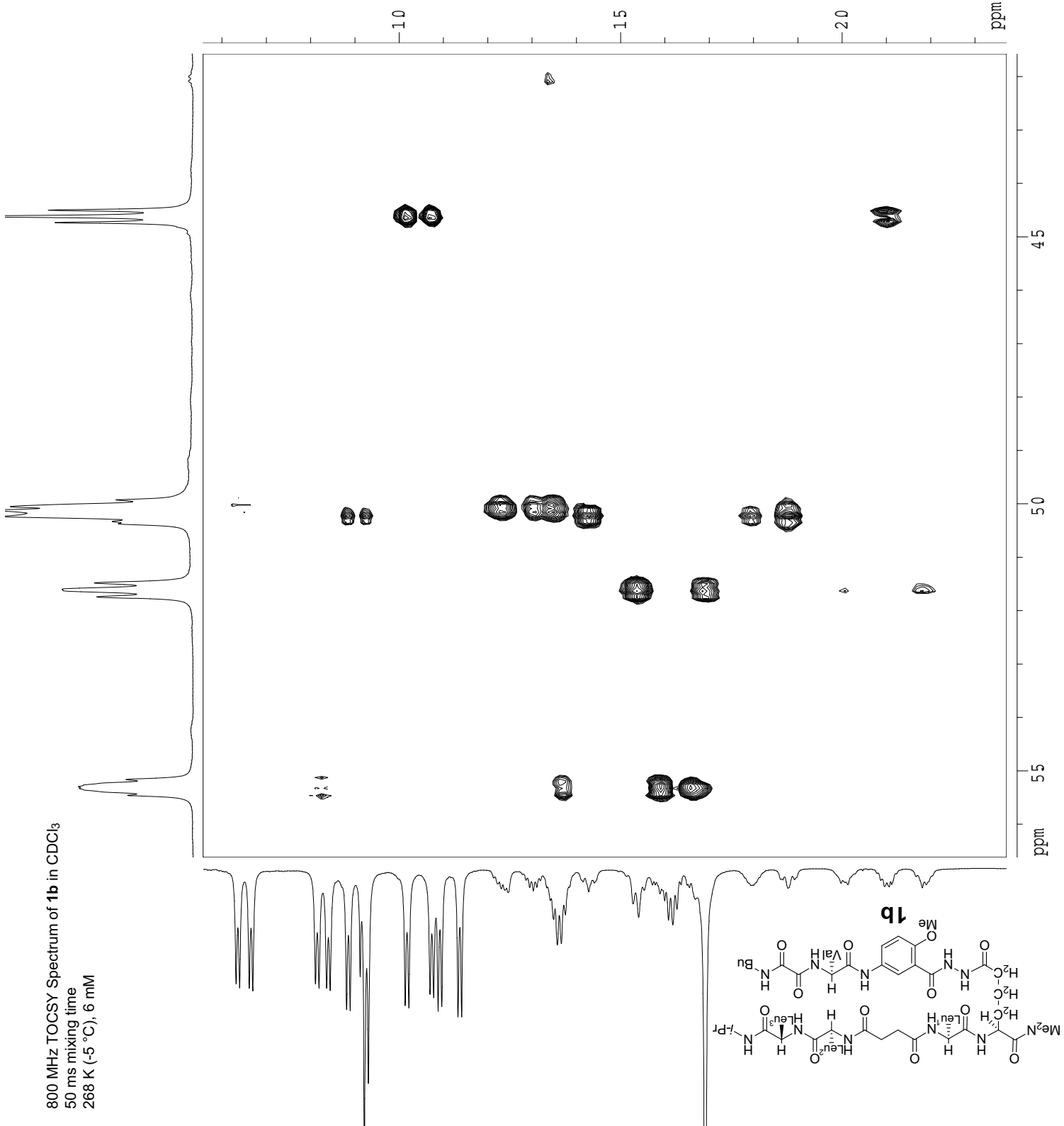
F1 - Processing parameters

SI 1024
 MC2 States
 SF 799.8064136 MHz
 WDW QSI
 SSB 2
 LB 0.00 Hz
 GB 0

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2D NMR plot parameters

CX2 15.00 cm
 CX1 15.00 cm
 F2PLO 5.662 ppm
 F2LO 4528.29 Hz
 F2PHI 4.157 ppm
 F2HI 3325.04 Hz
 F1PLO 2.371 ppm
 F1LO 1896.19 Hz
 F1PHI 0.557 ppm
 F1HI 445.85 Hz
 F2PPMCM 0.10029 ppm/cm
 F2HZCM 80.21635 Hz/cm
 F1PPMCM 0.12089 ppm/cm
 F1HZCM 96.68935 Hz/cm



Supporting Information

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Current Data Parameters
 USER sievin
 NAME SL-7-229-800-H
 EXPNO 4
 PROCNO 1

F2 - Acquisition Parameters

Date_ 20070131
 Time 0.00
 INSTRUM varian
 PROBHD 40:5mm broadband
 PULPROG wgtocsy bn
 TD 4096
 SOLVENT CDCl3
 NS 16
 DS 64
 SWH 11001.101 Hz
 FIDRES 2.685816 Hz
 AQ 0.1862132 sec
 RG 287.4
 DW 45.450 usec
 DE 6.00 usec
 TE 268.5 K

F1 - Acquisition parameters

ND0 1
 TD 1024
 SF01 799.8107 MHz
 FIDRES 10.743262 Hz
 SW 13.755 ppm
 F1MODE undefined

F2 - Processing parameters

SI 2048
 SF 799.8064136 MHz
 WDW QSINE
 SSB 2
 LB 0.00 Hz
 GB 0
 PC 1.40

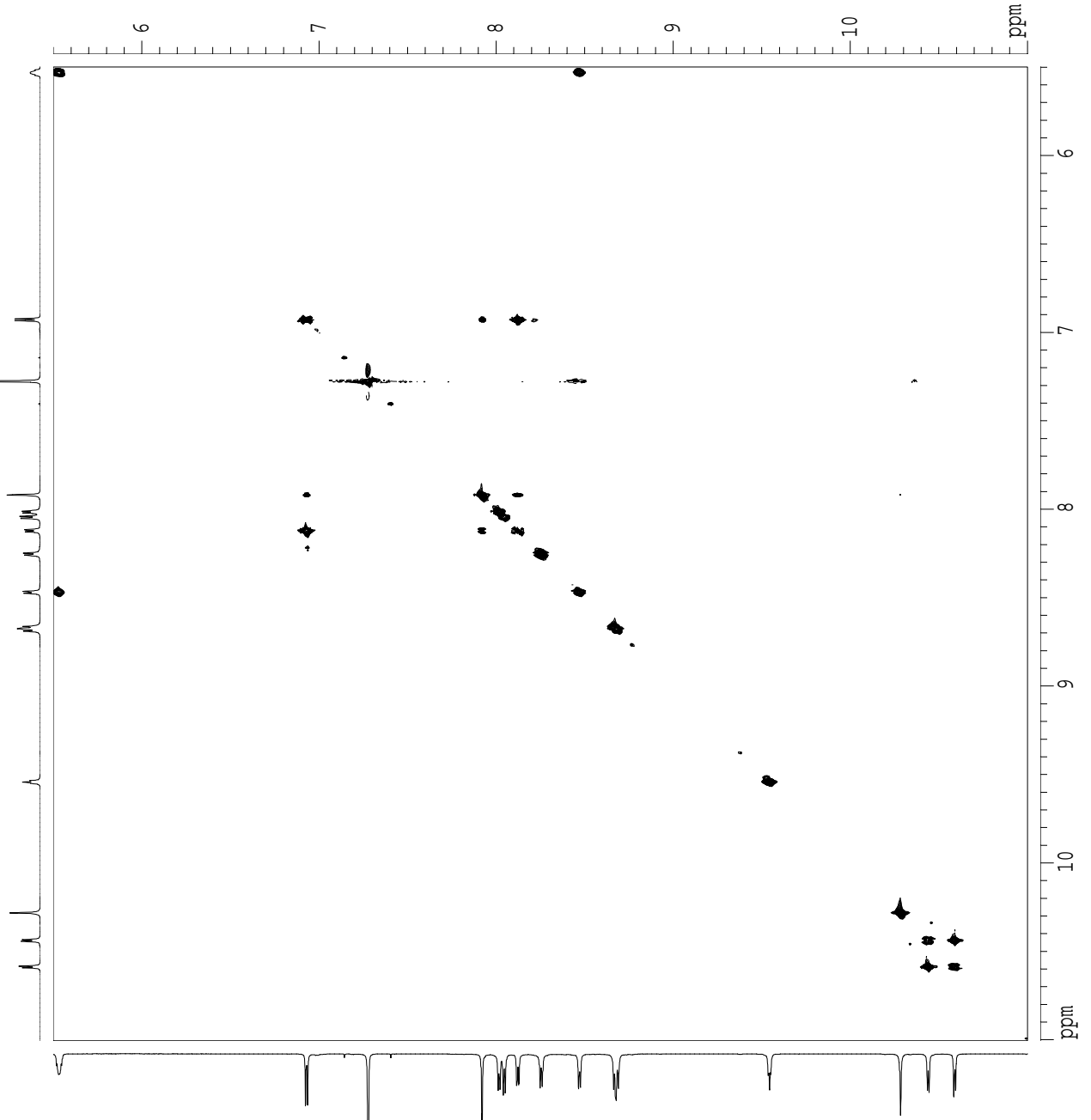
F1 - Processing parameters

SI 1024
 MC2 States
 SF 799.8064136 MHz
 WDW QSINE
 SSB 2
 LB 0.00 Hz
 GB 0

2D NMR plot parameters

CX2 15.00 cm
 CX1 15.00 cm
 F2PLO 11.007 ppm
 F2LO 8803.10 Hz
 F2PHI 5.499 ppm
 F2HI 4398.36 Hz
 F1PLO 11.000 ppm
 F1LO 8797.87 Hz
 F1PHI 5.500 ppm
 F1HI 4398.94 Hz
 F2PVMCM 0.36715 ppm/cm
 F2HZCM 293.64917 Hz/cm
 F1PVMCM 0.36667 ppm/cm
 F1HZCM 293.26236 Hz/cm

800 MHz TOCSY Spectrum of **1b** in CDCl₃
 50 ms mixing time
 268 K (-5 °C), 6 mM



Supporting Information

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Current Data Parameters
 USER slevin
 NAME SL-7-229-800-H
 EXPNO 4
 PROCNO 1

F2 - Acquisition Parameters

Date_ 20070131
 Time 0.00
 INSTRUM varian
 PROBHD 40:5mm broadband
 PULPROG wgtocsy_bn
 TD 4096
 SOLVENT CDCl3
 NS 16
 DS 64
 SWH 11001.101 Hz
 FIDRES 2.685816 Hz
 AQ 0.1862132 sec
 RG 287.4
 DW 45.450 usec
 DE 6.00 usec
 TE 268.5 K

F1 - Acquisition Parameters

ND0 1
 TD 1024
 SF01 799.8107 MHz
 FIDRES 10.743262 Hz
 SW 13.755 ppm
 F1MODE undefined

F2 - Processing Parameters

SI 2048
 SF 799.8064136 MHz
 WDW QSSINE
 SSB 2
 LB 0.00 Hz
 GB 0
 PC 1.40

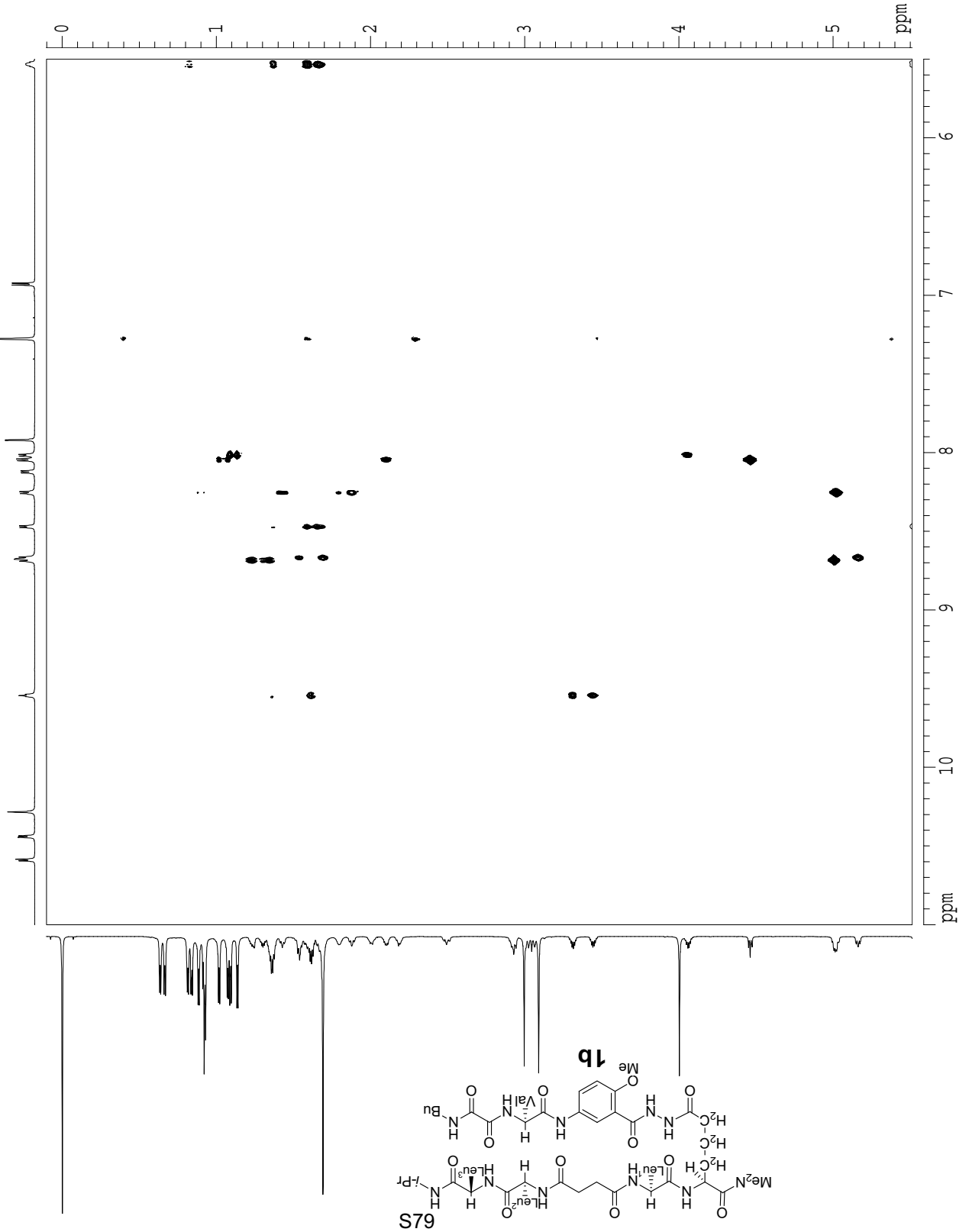
F1 - Processing Parameters

SI 1024
 MC2 States
 SF 799.8064136 MHz
 WDW QSSINE
 SSB 2
 LB 0.00 Hz
 GB 0

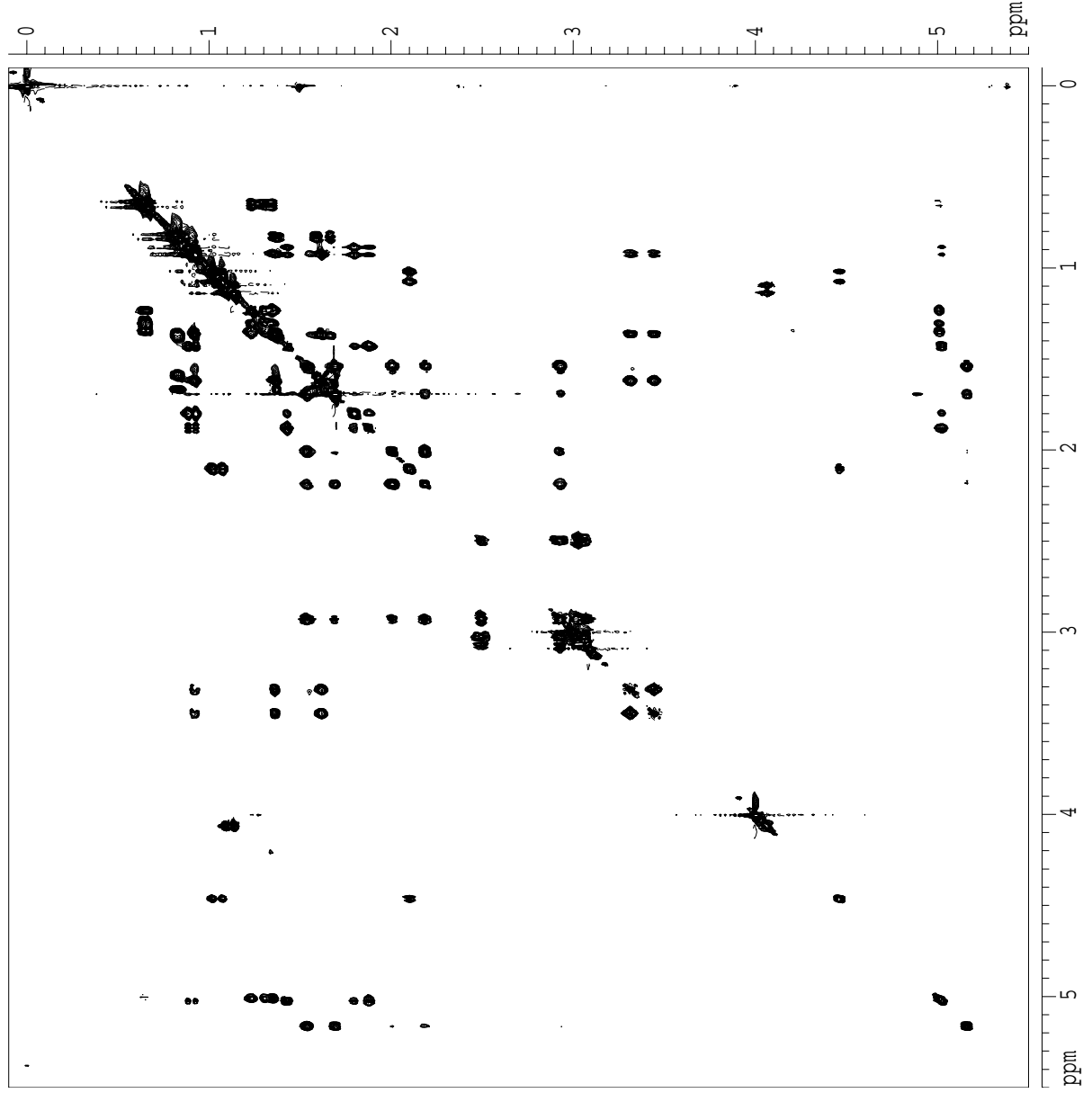
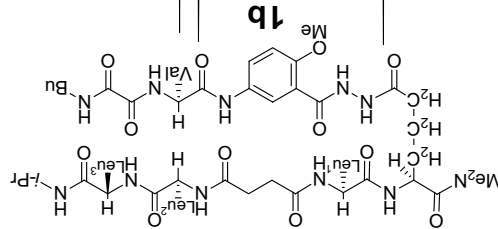
2D NMR plot parameters

CX2 15.00 cm
 CX1 15.00 cm
 F2PLO 11.000 ppm
 F2LO 8797.87 Hz
 F2PHI 5.500 ppm
 F2HI 4398.94 Hz
 F1PLO 5.513 ppm
 F1LO 4409.10 Hz
 F1PHI -0.102 ppm
 F1HI -81.58 Hz
 F2PPMCM 0.36667 ppm/cm
 F2HZCM 293.26236 Hz/cm
 F1PPMCM 0.37431 ppm/cm
 F1HZCM 299.37891 Hz/cm

800 MHz TOCSY Spectrum of **1b** in CDCl₃
 50 ms mixing time
 268 K (-5 °C), 6 mM



800 MHz TOCSY Spectrum of **1b** in CDCl₃
 50 ms mixing time
 268 K (-5 °C), 6 mM



Supporting Information

Current Data Parameters
 USER slevin
 NAME SL-7-229-800-H
 EXPNO 4
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20070131
 Time_ 0.00
 INSTRUM varian
 PROBHD 40:5mm broadband
 PULPROG wgtocpsy_bn
 TD 4096
 SOLVENT CDC13
 NS 16
 DS 64
 SWH 11001.101 Hz
 FIDRES 2.685816 Hz
 AQ 0.1862132 sec
 RG 287.4
 DW 45.450 usec
 DE 6.00 usec
 TE 268.5 K

F1 - Acquisition parameters
 ND0 1
 TD 1024
 SFO1 799.8107 MHz
 FIDRES 10.743262 Hz
 SW 13.755 ppm
 F1MODE undefined

F2 - Processing parameters
 SI 2048
 SF 799.8064136 MHz
 WDW QSI
 SSB 2
 LB 0.00 Hz
 GB 0
 PC 1.40

F1 - Processing parameters
 SI 1024
 MC2 States
 SF 799.8064136 MHz
 WDW QSI
 SSB 2
 LB 0.00 Hz
 GB 0

2D NMR plot parameters
 CX2 15.00 cm
 CX1 15.00 cm
 F2PLO 5.500 ppm
 F2LO 4398.94 Hz
 F2PHI -0.100 ppm
 F2HI -79.98 Hz
 F1PLO 5.500 ppm
 F1LO 4398.94 Hz
 F1PHI -0.100 ppm
 F1HI -79.98 Hz
 F2PFCM 0.37333 ppm/cm
 F2HZCM 298.59439 Hz/cm
 F1PFCM 0.37333 ppm/cm
 F1HZCM 298.59439 Hz/cm

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Supporting Information

Current Data Parameters
 USER slevin
 NAME SL-7-229-800-H
 EXPNO 5
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20070131
 Time_ 0.00
 INSTRUM varian
 PROBHD 40:5mm broadband
 PULPROG noesyh2o_pfg_800_pln
 TD 4096
 SOLVENT CDCl3
 NS 16
 DS 64
 SWH 11001.101 Hz
 FLDRES 2.685816 Hz
 AQ 0.1862132 sec
 RG 128
 DW 45.450 usec
 DE 6.00 usec
 TE 268.5 K

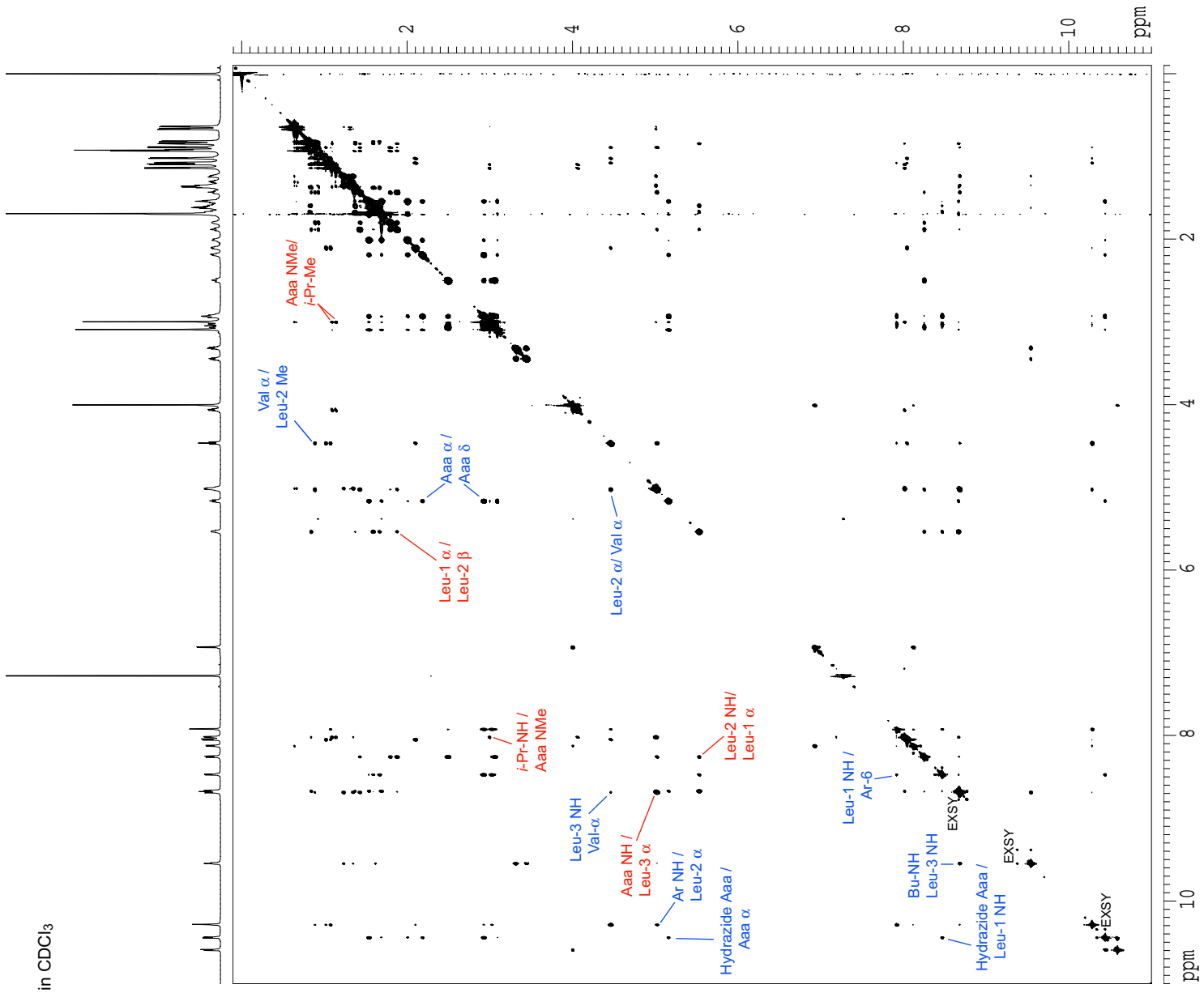
F1 - Acquisition parameters
 ND0 1
 TD 1024
 SF01 799.8107 MHz
 FLDRES 10.743262 Hz
 SW 13.755 ppm
 FMODE undefined

F2 - Processing parameters
 SI 2048
 SF 799.8064136 MHz
 MDW QSINE
 SSB 2
 LB 0.00 Hz
 GB 0
 PC 1.40

F1 - Processing parameters
 SI 1024
 MC2 States
 SF 799.8064136 MHz
 MDW QSINE
 SSB 2
 LB 0.00 Hz
 GB 0

2D NMR plot parameters
 CX2 15.00 cm
 CX1 15.00 cm
 F2PLO 11.001 ppm
 F2LO 8798.73 Hz
 F2PHI -0.101 ppm
 F2HI -80.58 Hz
 F1PLO 11.001 ppm
 F1LO 8798.73 Hz
 F1PHI -0.107 ppm
 F1HI -85.95 Hz
 F2PPMCM 0.74012 ppm/cm
 F2HZCM 591.95374 Hz/cm
 F1PPMCM 0.74057 ppm/cm
 F1HZCM 592.31183 Hz/cm

800 MHz NOESY Spectrum of **1b** in CDCl₃
 400 ms mixing time
 268 K (-5 °C), 6 mM



800 MHz NOESY Spectrum of **1b** in CDCl₃
 400 ms mixing time
 268 K (-5 °C), 6 mM

Supporting Information

Current Data Parameters
 USER slewin
 NAME SL-7-229-800-H
 EXPNO 5
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20070131
 Time 0.00
 INSTRUM varian
 PROBHD 40:5mm broadband
 PULPROG noesyh2o_pfg_800_pln
 TD 4096
 SOLVENT CDCl3
 NS 16
 DS 64
 SWH 11001.101 Hz
 FIDRES 2.685816 Hz
 AQ 0.1862132 sec
 RG 128
 DW 45.450 usec
 DE 6.00 usec
 TE 268.5 K

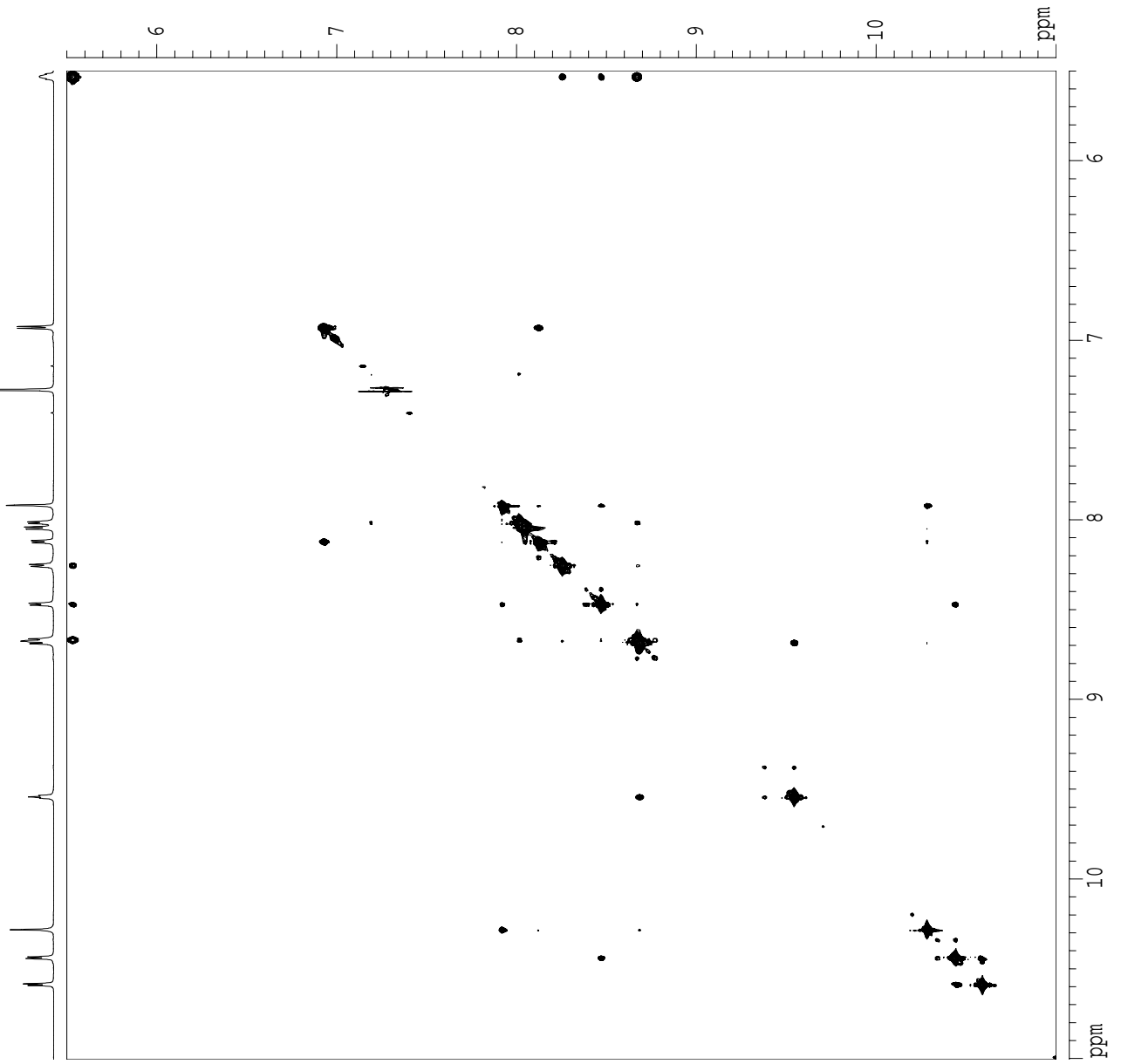
F1 - Acquisition Parameters
 ND0 1
 TD 1024
 SFO1 799.8107 MHz
 FIDRES 10.743262 Hz
 SW 13.755 ppm
 FmODE undefined

F2 - Processing parameters
 SI 2048
 SF 799.8064136 MHz
 WDW QSIINE
 SSB 2
 LB 0.00 Hz
 GB 0
 PC 1.40

F1 - Processing parameters
 SI 1024
 MC2 States
 SF 799.8064136 MHz
 WDW QSIINE
 SSB 2
 LB 0.00 Hz
 GB 0

2D NMR plot parameters
 CX2 15.00 cm
 CX1 15.00 cm
 F2PLO 11.007 ppm
 F2LO 8803.10 Hz
 F2PHI 5.499 ppm
 F2HI 4398.36 Hz
 F1PLO 11.000 ppm
 F1LO 8797.87 Hz
 F1PHI 5.500 ppm
 F1HI 4398.94 Hz
 F2PPMCM 0.36715 ppm/cm
 F2HZCM 293.64917 Hz/cm
 F1PPMCM 0.36667 ppm/cm
 F1HZCM 293.26236 Hz/cm

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Supporting Information

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Current Data Parameters
 USER slevin
 NAME SL-7-229-800-H
 EXENO 5
 PROCNO 1

F2 - Acquisition Parameters

Date 20070131
 Time_ 0.00
 INSTRUM varian
 PROBD 40:5mmroadban
 PULPROG noesyh2o_pfg_800_pln
 TD 4096
 SOLVENT CDCl3
 NS 16
 DS 64
 SWH 11001.101 Hz
 FIDRES 2.685816 Hz
 AQ 0.1862132 sec
 RG 128
 DW 45.450 usec
 DE 6.00 usec
 TE 268.5 K

F1 - Acquisition Parameters

ND0 1
 TD 1024
 SF01 799.8107 MHz
 FIDRES 10.743262 Hz
 SW 13.755 ppm
 FnmODE undefined

F2 - Processing parameters

SI 2048
 SF 799.8064136 MHz
 WDW QSINE
 SSB 2
 LB 0.00 Hz
 GB 0
 PC 1.40

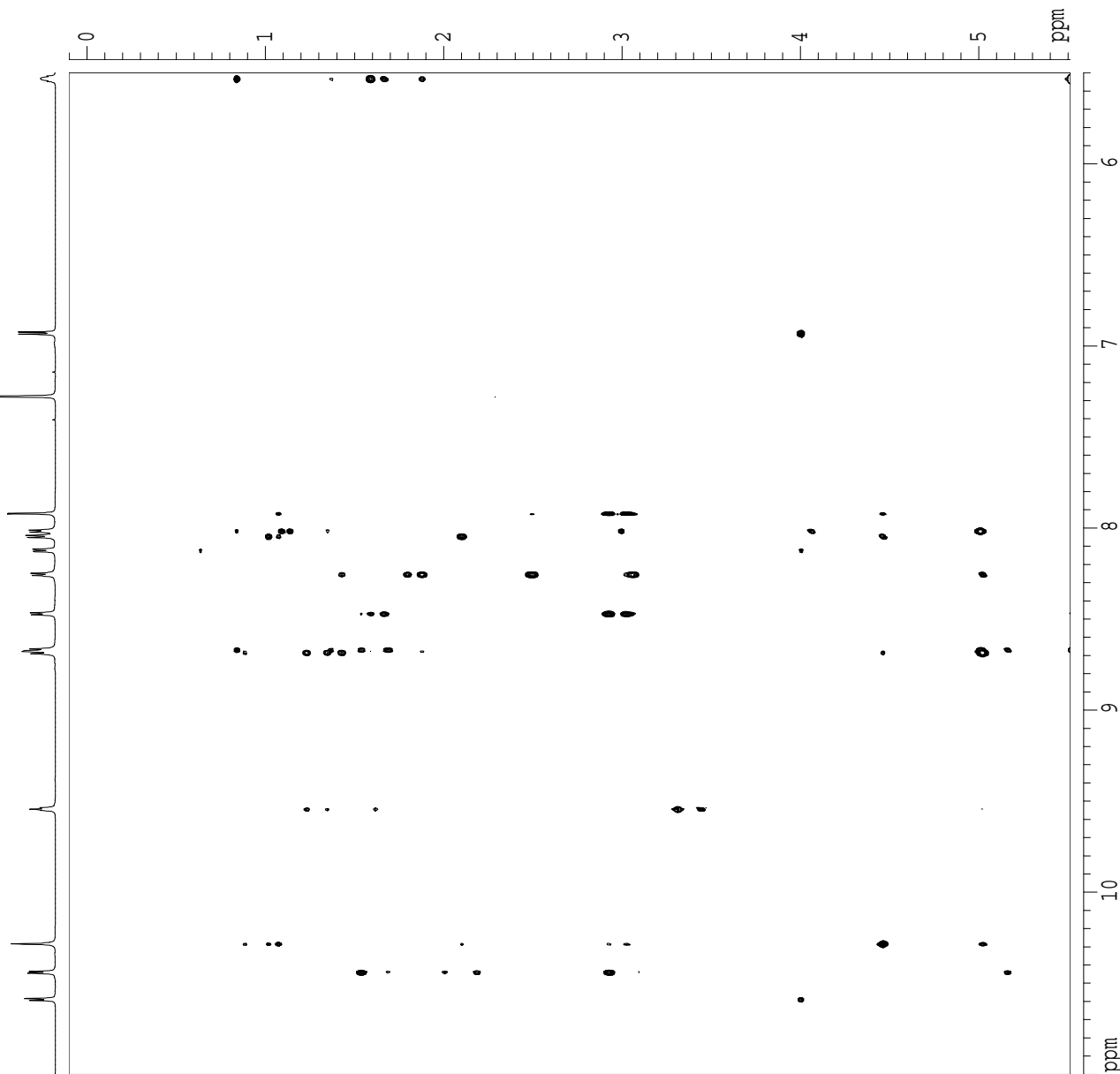
F1 - Processing parameters

SI 1024
 MC2 States
 SF 799.8064136 MHz
 WDW QSINE
 SSB 2
 LB 0.00 Hz
 GB 0

2D NMR plot parameters

CX2 15.00 cm
 CX1 15.00 cm
 F2FLO 11.000 ppm
 F2LO 8797.87 Hz
 F2PHI 5.500 ppm
 F2HI 4398.94 Hz
 F1FLO 5.513 ppm
 F1LO 4409.10 Hz
 F1PHI -0.102 ppm
 F1HI -81.58 Hz
 F2PPMCM 0.36667 ppm/cm
 F2HZCM 293.26236 Hz/cm
 F1PPMCM 0.37431 ppm/cm
 F1HZCM 299.37891 Hz/cm

800 MHz NOESY Spectrum of **1b** in CDCl₃
 400 ms mixing time
 268 K (-5 °C), 6 mM



Current Data Parameters
 USER slevin
 NAME SL-7-229-800-H
 EXPNO 5
 PROCNO 1

F2 - Acquisition Parameters

Date 20070131
 Time 0.00
 INSTRUM varian
 PROBHD 40:5mmbroadban
 PULPROG noesyh2_pfg_800_pln
 TD 4096

SOLVENT CDCl3
 NS 16
 DS 64

SWH 11001.101 Hz
 FIDRES 2.685816 Hz
 AQ 0.1862132 sec

RG 128
 DW 45.450 usec
 DE 6.00 usec
 TE 268.5 K

F1 - Acquisition Parameters

ND0 1
 TD 1024
 SF01 799.8107 MHz
 FIDRES 10.743262 Hz
 SW 13.755 ppm
 FhMODE undefined

F2 - Processing parameters

SI 2048
 SF 799.8064136 MHz
 WDW QSINE
 SSB 2
 LB 0.00 Hz
 GB 0
 PC 1.40

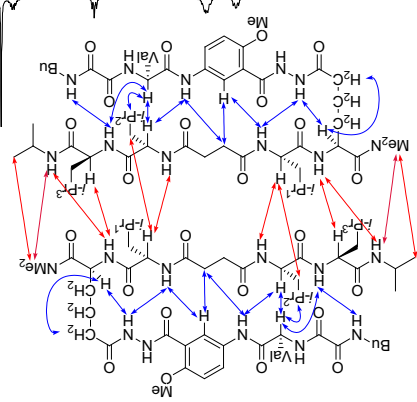
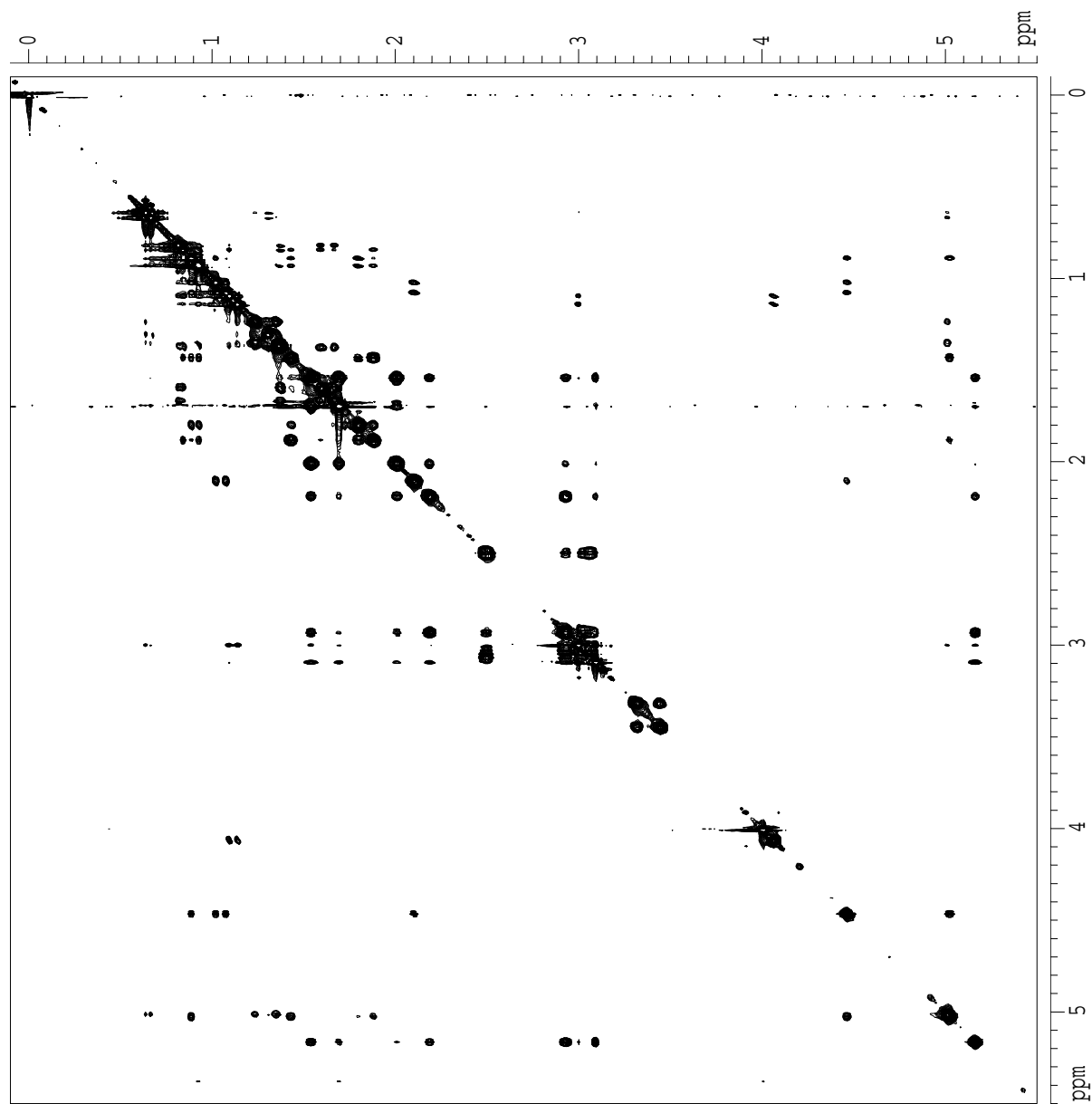
F1 - Processing parameters

SI 1024
 MC2 States
 SF 799.8064136 MHz
 WDW QSINE
 SSB 2
 LB 0.00 Hz
 GB 0

2D NMR plot parameters

CX2 15.00 cm
 CX1 15.00 cm
 F2PFO 5.500 ppm
 F2LO 4398.94 Hz
 F2PHI -0.100 ppm
 F2HI -79.98 Hz
 F1PFO 5.500 ppm
 F1LO 4398.94 Hz
 F1PHI -0.100 ppm
 F1HI -79.98 Hz
 F2PPMCM 0.37333 ppm/cm
 F2HZCM 298.59439 Hz/cm
 F1PPMCM 0.37333 ppm/cm
 F1HZCM 298.59439 Hz/cm

800 MHz NOESY Spectrum of **1b** in CDCl₃
 400 ms mixing time
 268 K (-5 °C), 6 mM



Supporting Information

Current Data Parameters
 USER slevin
 NAME SL-7-229-800-H
 EXPNO 5
 PROCNO 1

F2 - Acquisition Parameters

Date_ 20070131
 Time_ 0.00
 INSTRUM varian
 PROBHD 40:5mm broadband
 PULPROG noesyhzo_prg_800.pln
 TD 4096
 SOLVENT CDCl3
 NS 16
 DS 64
 SWH 11001.101 Hz
 FIDRES 2.685816 Hz
 AQ 0.1862132 sec
 RG 128
 DW 45.450 usec
 DE 6.00 usec
 TE 268.5 K

F1 - Acquisition parameters

ND0 1
 TD 1024
 SFO1 799.8107 MHz
 FIDRES 10.743262 Hz
 SW 13.755 ppm
 FMODE undefined

F2 - Processing parameters

SI 2048
 SF 799.8064136 MHz
 WDW QSINE
 SSB 2
 LB 0.00 Hz
 GB 0
 PC 1.40

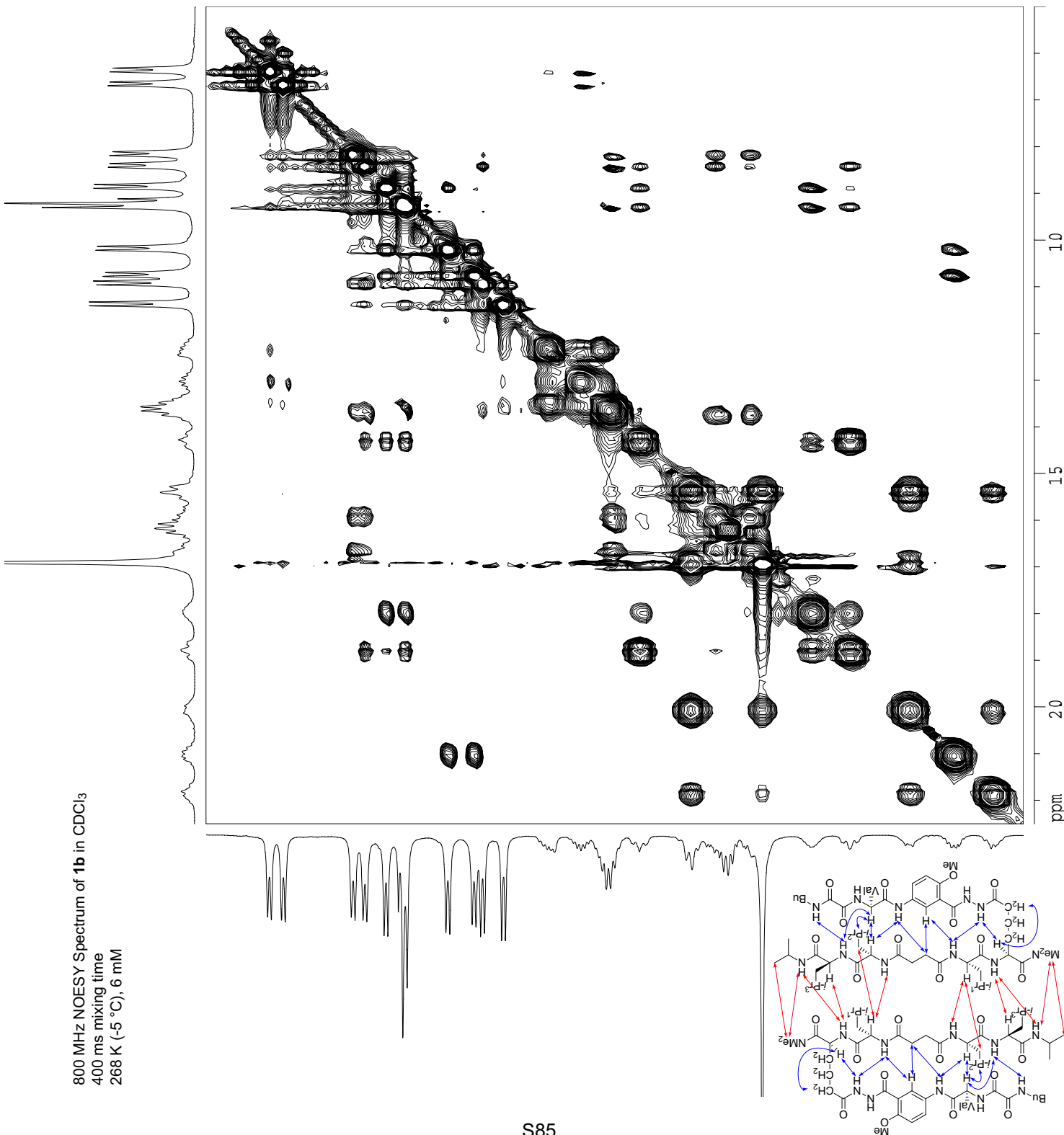
F1 - Processing parameters

SI 1024
 MC2 States
 SF 799.8064136 MHz
 WDW QSINE
 SSB 2
 LB 0.00 Hz
 GB 0

2D NMR plot parameters

CX2 15.00 cm
 CX1 15.00 cm
 F2PLO 2.250 ppm
 F2LO 1799.56 Hz
 F2PHI 0.500 ppm
 F2HI 399.90 Hz
 F1PLO 2.250 ppm
 F1LO 1799.56 Hz
 F1PHI 0.500 ppm
 F1HI 399.90 Hz
 F2PPMCM 0.11667 ppm/cm
 F2HZCM 93.31075 Hz/cm
 F1PPMCM 0.11667 ppm/cm
 F1HZCM 93.31075 Hz/cm

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800 MHz NOESY Spectrum of **1b** in CDCl₃
 400 ms mixing time
 268 K (-5 °C), 6 mM

800 MHz NOESY Spectrum of **1b** in CDCl₃
 400 ms mixing time
 268 K (-5 °C), 6 mM

Supporting Information

Current Data Parameters
 USER sievin
 NAME SL-7-229-800-H
 EXPNO 5
 PROCNO 1

F2 - Acquisition Parameters

Date_ 20070131
 Time_ 0.00
 INSTRUM varian
 PROBHD 40:5mm broadband
 PULPROG noesyh2o_pfg_800_pln
 TD 4096
 SOLVENT CDCl₃
 NS 16
 DS 64
 SWH 11001.101 Hz
 FIDRES 2.685816 Hz
 AQ 0.1862132 sec
 RG 128
 DW 45.450 usec
 DE 6.00 usec
 TE 268.5 K

F1 - Acquisition Parameters

ND0 1
 TD 1024
 SFO1 799.8107 MHz
 FIDRES 10.743262 Hz
 SW 13.755 ppm
 FwMODE undefined

F2 - Processing Parameters

SI 2048
 SF 799.8064136 MHz
 WDW QSINE
 SSB 2
 LB 0.00 Hz
 GB 0
 PC 1.40

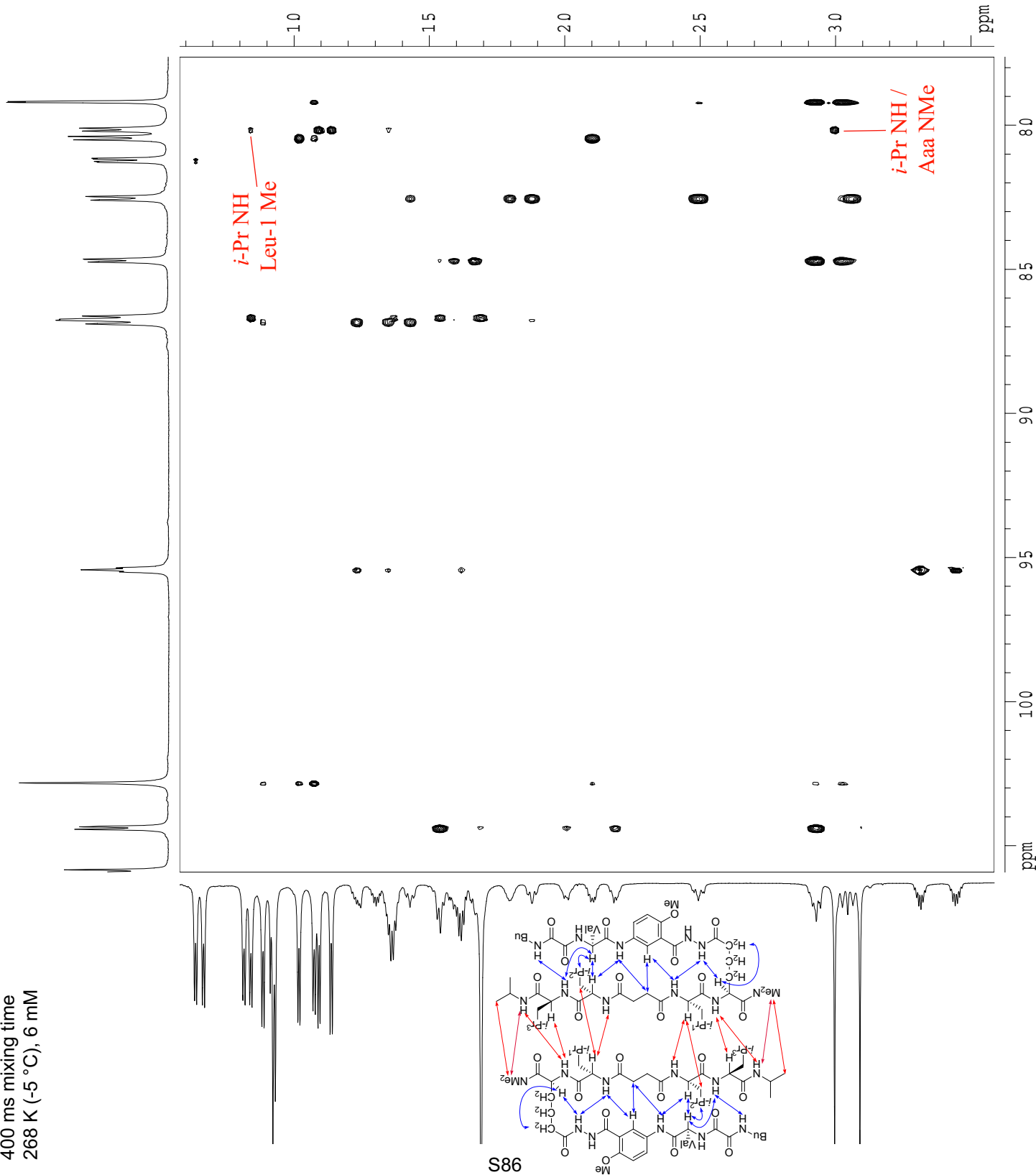
F1 - Processing Parameters

SI 1024
 MC2 States
 SF 799.8064136 MHz
 WDW QSINE
 SSB 2
 LB 0.00 Hz
 GB 0

2D NMR plot parameters

CX2 15.00 cm
 CX1 15.00 cm
 F2PLO 10.591 ppm
 F2LO 8471.06 Hz
 F2PHI 7.764 ppm
 F2HI 6209.60 Hz
 F1PLO 3.586 ppm
 F1LO 2868.45 Hz
 F1PHI 0.578 ppm
 F1HI 461.96 Hz
 F2PPMCM 0.18850 ppm/cm
 F2HZCM 150.76378 Hz/cm
 F1PPMCM 0.20059 ppm/cm
 F1HZCM 160.43269 Hz/cm

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Supporting Information

800 MHz NOESY Spectrum of **1b** in CDCl₃
 400 ms mixing time
 268 K (-5 °C), 6 mM

Current Data Parameters
 USER slevin
 NAME SL-7-229-800-H
 EXPNO 5
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20070131
 Time 0.00
 INSTRUM varian
 PROBHD 40:5mmroadban
 PULPROG noesyh2o_pfg_800.pln
 TD 4096

SOLVENT CDCl₃
 NS 16
 DS 64
 SWH 11001.101 Hz
 FIDRES 2.685816 Hz
 AQ 0.1862132 sec
 RG 128
 DW 45.450 usec
 DE 6.00 usec
 TE 268.5 K

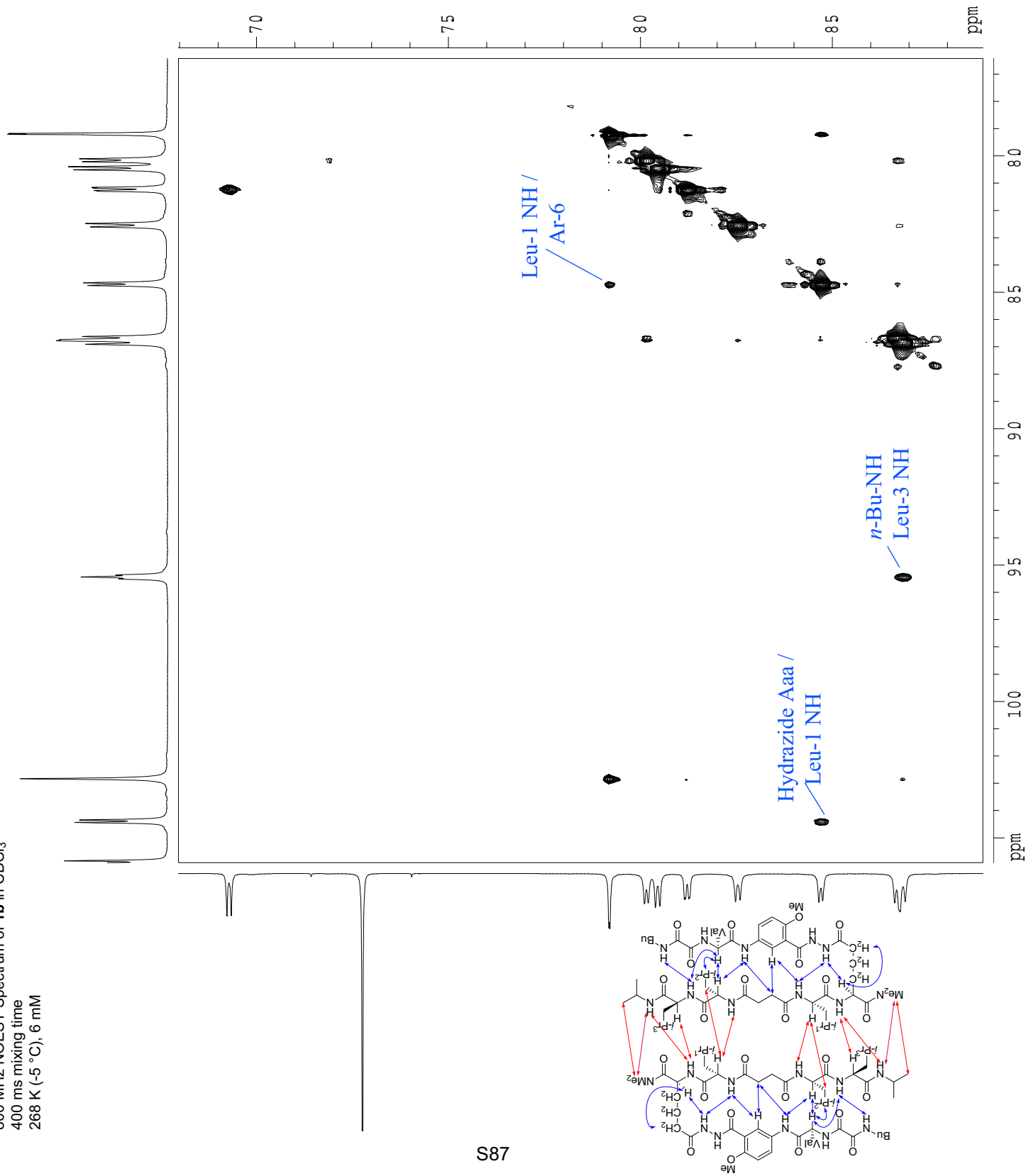
F1 - Acquisition Parameters
 ND0 1
 TD 1024
 SF01 799.8107 MHz
 FIDRES 10.743262 Hz
 SW 13.755 ppm
 F1MODE undefined

F2 - Processing parameters
 SI 2048
 SF 799.8064136 MHz
 WDM QSINE
 SSB 2
 LB 0.00 Hz
 GB 0
 PC 1.40

F1 - Processing parameters
 SI 1024
 MC2 States
 SF 799.8064136 MHz
 WDM QSINE
 SSB 2
 LB 0.00 Hz
 GB 0

2D NMR plot parameters
 CX2 15.00 cm
 CX1 15.00 cm
 F2PLO 10.591 ppm
 F2LO 8471.06 Hz
 F2PHI 7.643 ppm
 F2HI 6112.91 Hz
 F1PLO 8.892 ppm
 F1LO 7112.04 Hz
 F1PHI 6.797 ppm
 F1HI 5436.09 Hz
 F2PPMCM 0.19656 ppm/cm
 F2HZCM 157.20972 Hz/cm
 F1PPMCM 0.13970 ppm/cm
 F1HZCM 111.72990 Hz/cm

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800 MHz NOESY Spectrum of **1b** in CDCl₃
 400 ms mixing time
 268 K (-5 °C), 6 mM

Supporting Information

Current Data Parameters
 USER sleivin
 NAME SL-7-229-800-H
 EXPNO 5
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20070131
 Time 0.00
 INSTRUM varian
 PROBHD 40:5mmbroacdban
 PULPROG noesyh2o_pfg_800_pln
 TD 4096
 SOLVENT CDCl₃
 NS 16
 DS 64
 SWH 11001.101 Hz
 FIDRES 2.685816 Hz
 AQ 0.1862132 sec
 RG 128
 DW 45.450 usec
 DE 6.00 usec
 TE 268.5 K

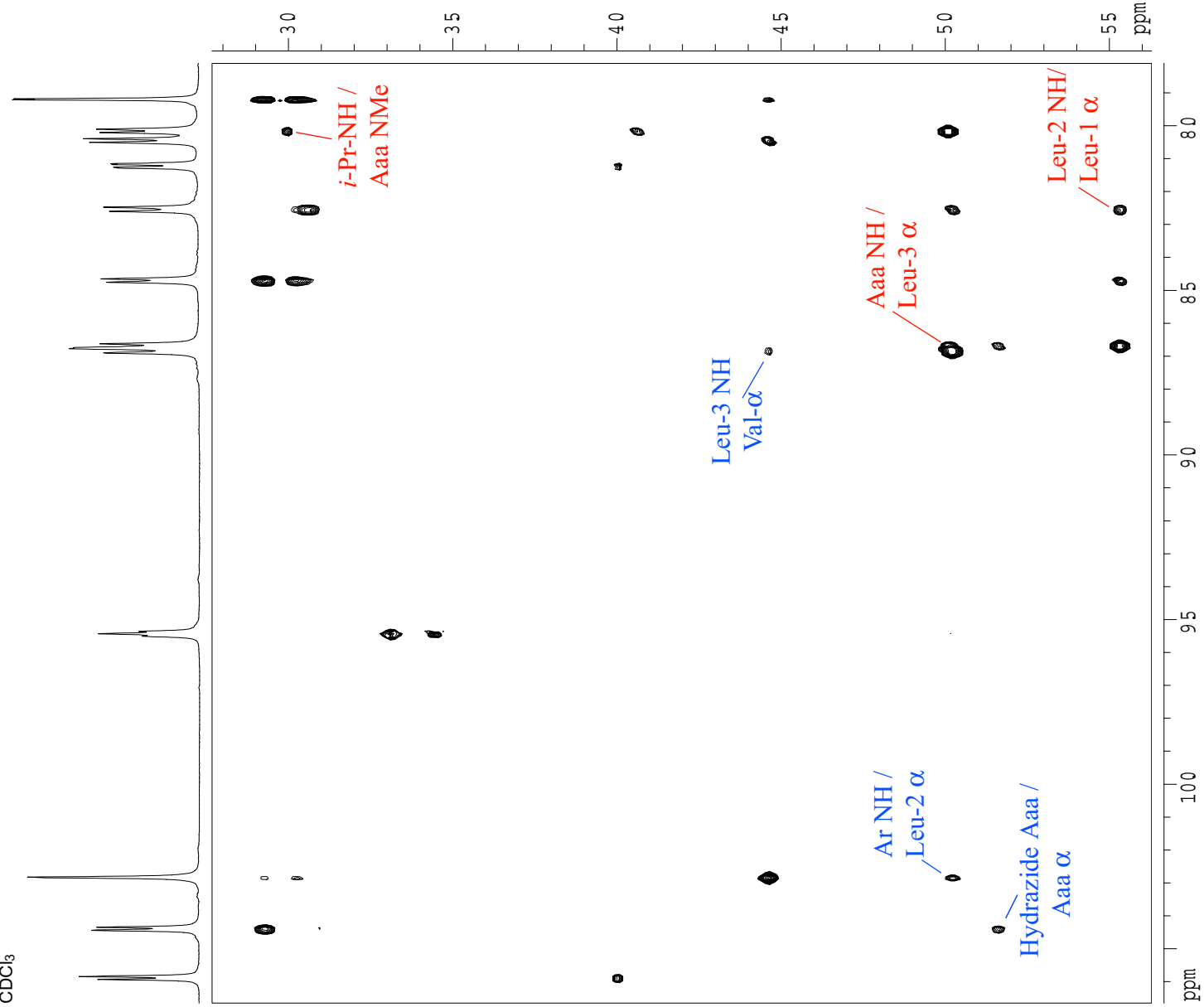
F1 - Acquisition parameters
 ND0 1
 TD 1024
 SF01 799.8107 MHz
 FIDRES 10.743262 Hz
 SW 13.755 ppm
 FMODE undefined

F2 - Processing parameters
 SI 2048
 SF 799.8064136 MHz
 WDW QSI
 SSB 2
 LB 0.00 Hz
 GB 0
 PC 1.40

F1 - Processing parameters
 SI 1024
 MC2 States
 SF 799.8064136 MHz
 WDW QSI
 SSB 2
 LB 0.00 Hz
 GB 0

2D NMR plot parameters
 CX2 15.00 cm
 CX1 15.00 cm
 F2PLO 10.665 ppm
 F2LO 8530.15 Hz
 F2PHI 7.811 ppm
 F2HI 6247.20 Hz
 F1PLO 5.628 ppm
 F1LO 4501.42 Hz
 F1PHI 2.767 ppm
 F1HI 2213.11 Hz
 F2PPMCM 0.19029 ppm/cm
 F2HZCM 152.19621 Hz/cm
 F1PPMCM 0.19074 ppm/cm
 F1HZCM 152.55431 Hz/cm

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Supporting Information

Current Data Parameters
 USER slevin
 NAME SL-7-229-800-H
 EXPNO 5
 PROCNO 1

F2 - Acquisition Parameters

Date 20070131
 Time 0.00
 INSTRUM varian
 PROBHD 40:5mm broadband
 PULPROG noesyh2o_pfg_800_pln
 TD 4096
 SOLVENT CDCl3
 NS 16
 DS 64
 SWH 11001.101 Hz
 FIDRES 2.685816 Hz
 AQC 0.1862132 sec
 RG 128
 DW 45.450 usec
 DE 6.00 usec
 TE 268.5 K

F1 - Acquisition parameters

ND0 1
 TD 1024
 SF01 799.8107 MHz
 FIDRES 10.743262 Hz
 SW 13.755 ppm
 FwMODE undefined

F2 - Processing parameters

SI 2048
 SF 799.8064136 MHz
 WDW QSI
 SSB 2
 LB 0.00 Hz
 GB 0
 PC 1.40

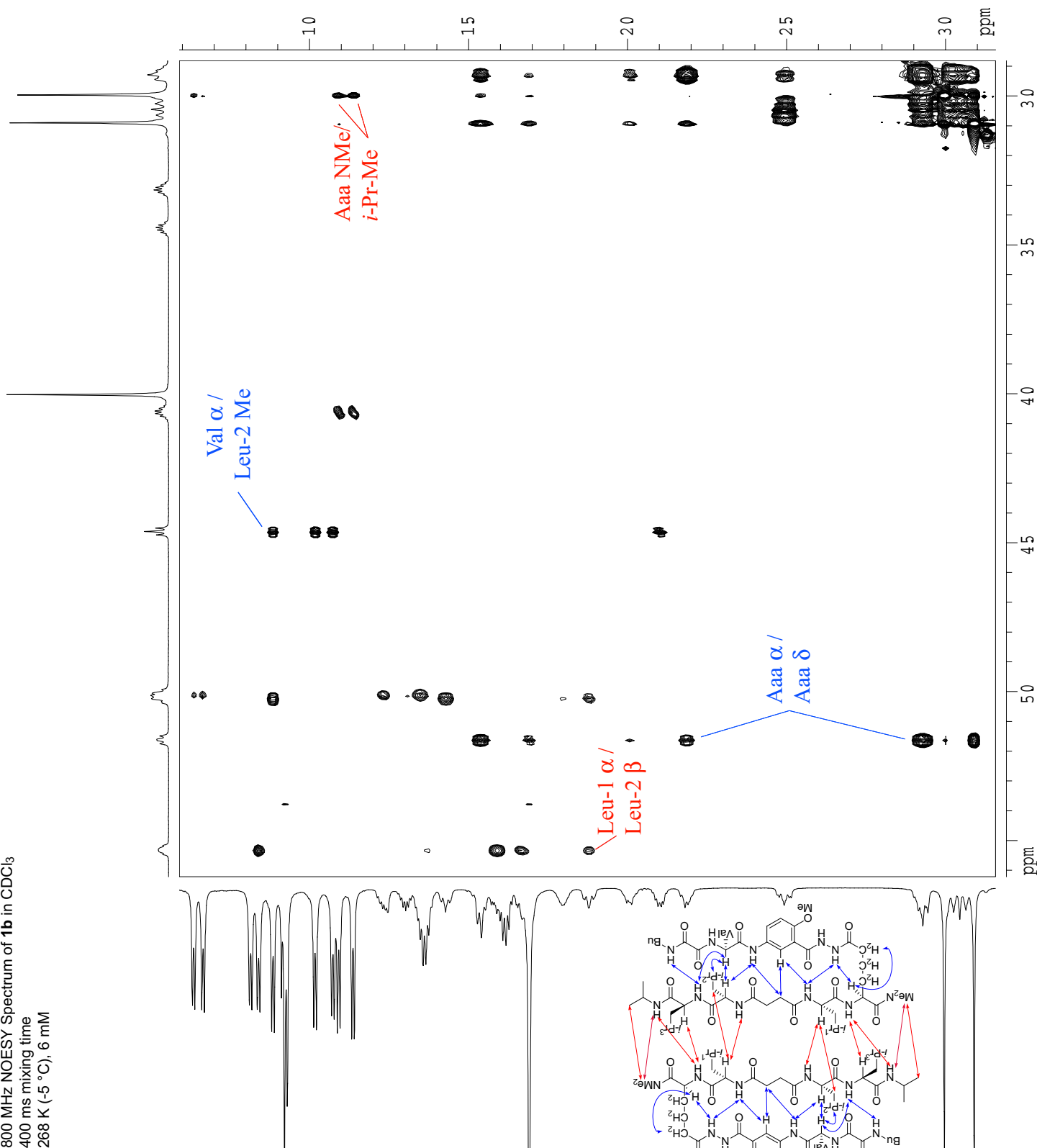
F1 - Processing parameters

SI 1024
 MC2 States
 SF 799.8064136 MHz
 WDW QSI
 SSB 2
 LB 0.00 Hz
 GB 0

2D NMR plot parameters

CX2 15.00 cm
 CX1 15.00 cm
 F2PLO 5.621 ppm
 F2LO 4496.05 Hz
 F2PHI 2.881 ppm
 F2HI 2304.43 Hz
 F1PLO 3.157 ppm
 F1LO 2524.66 Hz
 F1PHI 0.591 ppm
 F1HI 472.70 Hz
 F2PPMCM 0.18268 ppm/cm
 F2HZCM 146.10835 Hz/cm
 F1PPMCM 0.17104 ppm/cm
 F1HZCM 136.79753 Hz/cm

800 MHz NOESY Spectrum of **1b** in CDCl₃
 400 ms mixing time
 268 K (-5 °C), 6 mM



Supporting Information

800 MHz NOESY Spectrum of **1b** in CDCl₃
 400 ms mixing time
 268 K (-5 °C), 6 mM

Current Data Parameters
 USER slewin
 NAME SL-7-229-800-H
 EXPNO 5
 PROCNO 1

F2 - Acquisition Parameters

Date_ 20070131
 Time_ 0.00
 INSTRUM varian
 PROBHD 40:5mm broadband
 PULPROG noesyh2o_pig_800_pln
 TD 4096

SOLVENT CDCl₃

NS 16
 DS 64
 SWH 11001.101 Hz
 FIDRES 2.685816 Hz
 AQ 0.1862132 sec
 RG 128
 DW 45.450 usec
 DE 6.00 usec
 TE 288.5 K

F1 - Acquisition Parameters

ND0 1
 TD 1024
 SFO1 799.8107 MHz
 FIDRES 10.743262 Hz
 SW 13.755 ppm
 FMODE undefined

F2 - Processing parameters

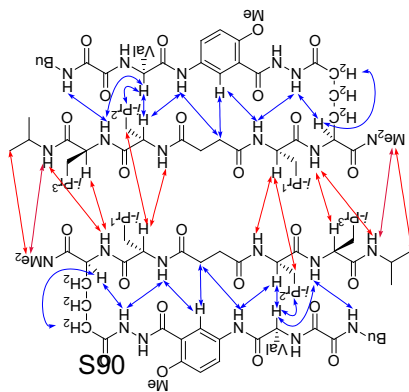
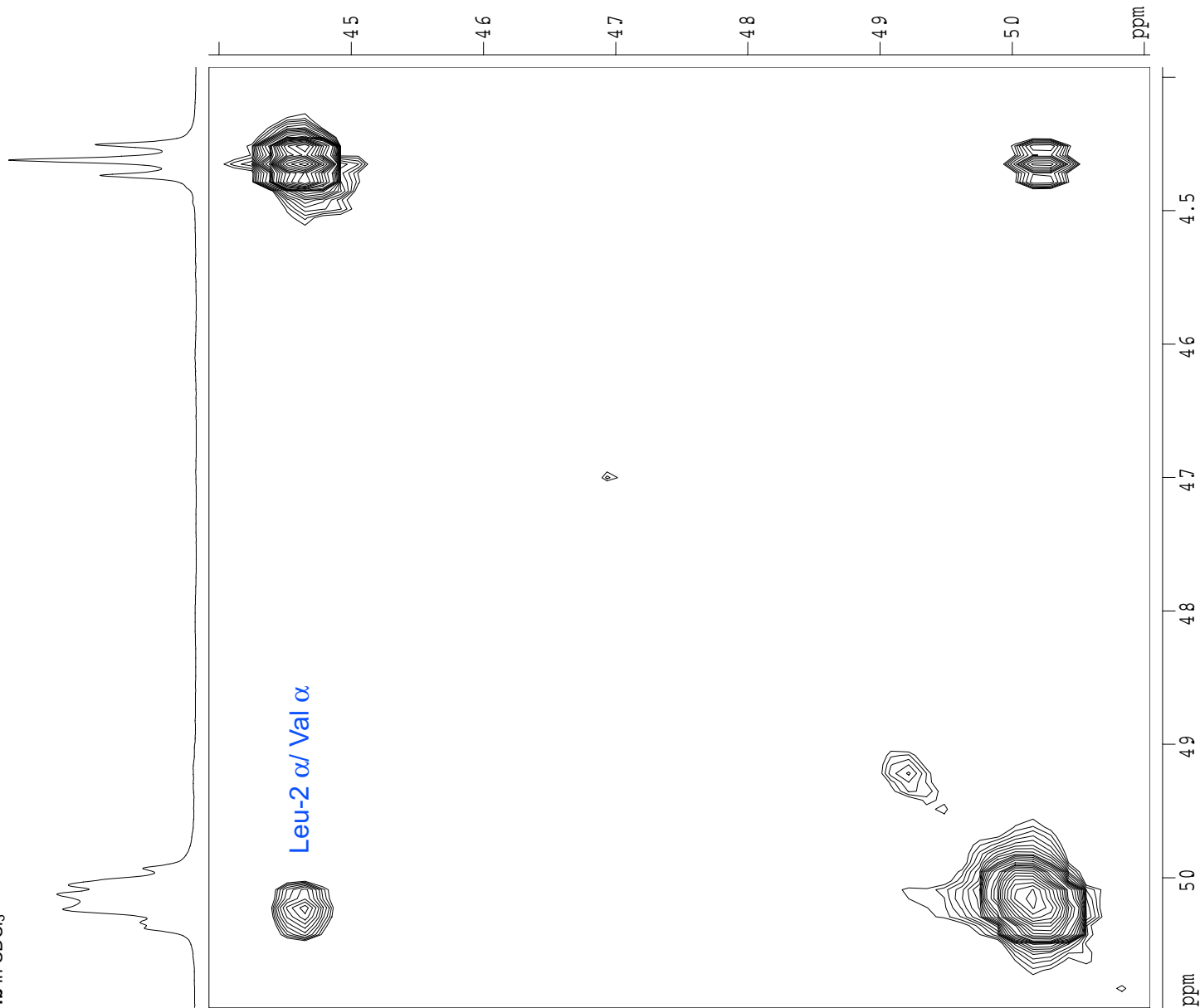
SI 2048
 SF 799.8064136 MHz
 WDW QSI
 SSB 2
 LB 0.00 Hz
 GB 0
 PC 1.40

F1 - Processing parameters

SI 1024
 MC2 States
 SF 799.8064136 MHz
 WDW QSI
 SSB 2
 LB 0.00 Hz
 GB 0

2D NMR plot parameters

CX2 15.00 cm
 CX1 15.00 cm
 F2PLO 5.098 ppm
 F2LO 4077.06 Hz
 F2PHI 4.392 ppm
 F2HI 3513.04 Hz
 F1PLO 5.104 ppm
 F1LO 4082.44 Hz
 F1PHI 4.392 ppm
 F1HI 3513.04 Hz
 F2PMCM 0.04701 ppm/cm
 F2HZCM 37.60142 Hz/cm
 F1PMCM 0.04746 ppm/cm
 F1HZCM 37.95954 Hz/cm



Supporting Information

Current Data Parameters

USER slevin
 NAME SL-7-229-800-H
 EXPNO 5
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20070131
 Time 0.00
 INSTRUM varian
 PROBHD 40:5mmrbroadban
 PULPROG noesyh2o_pfg_800_p1n
 TD 4096

SOLVENT CDCl3
 NS 16
 DS 64
 SWH 11001.101 Hz
 FIDRES 2.685816 Hz
 AQ 0.1862132 sec
 RG 128
 DW 45.450 usec
 DE 6.00 usec
 TE 268.5 K

F1 - Acquisition Parameters
 ND0 1
 TD 1024
 SF01 799.8107 MHz
 FIDRES 10.743262 Hz
 SW 13.755 ppm
 PRMODE undefined

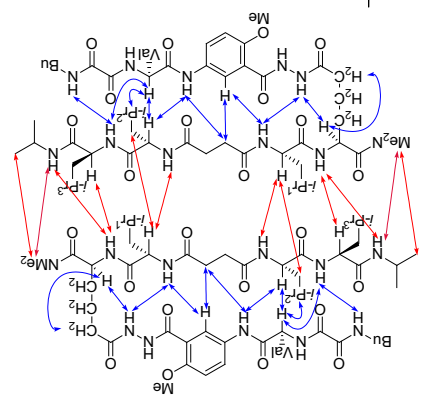
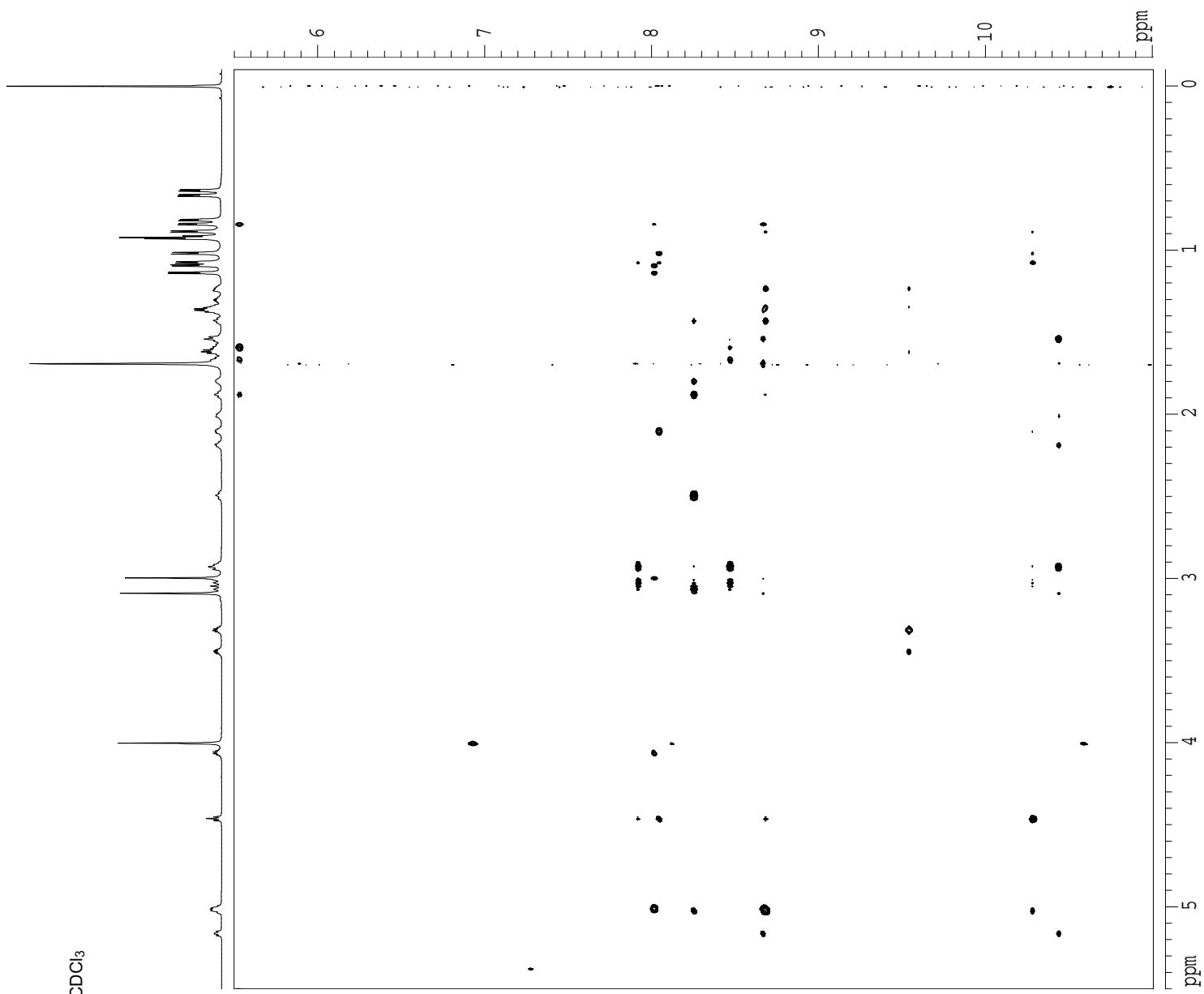
F2 - Processing parameters
 SI 2048
 SF 799.8064136 MHz
 WDW QSINE
 SSB 2
 LB 0.00 Hz
 GB 0
 PC 1.40

F1 - Processing parameters
 SI 1024
 MC2 States
 SF 799.8064136 MHz
 WDW QSINE
 SSB 2
 LB 0.00 Hz
 GB 0

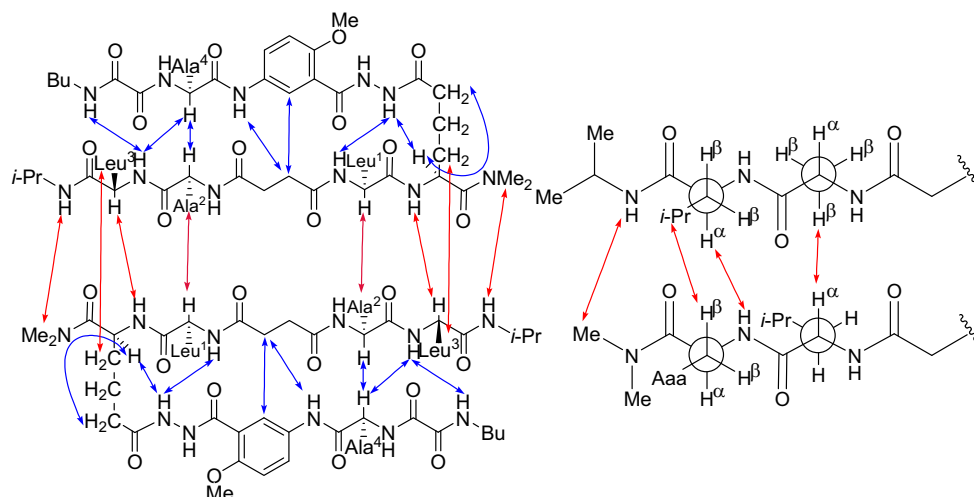
2D NMR plot parameters
 CX2 15.00 cm
 CX1 15.00 cm
 F2PLO 5.500 ppm
 F2LO 4398.94 Hz
 F2PHI -0.100 ppm
 F2HI -79.98 Hz
 F1PLO 11.007 ppm
 F1LO 8803.10 Hz
 F1PHI 5.499 ppm
 F1HI 4398.36 Hz
 F2PPMCM 0.37333 ppm/cm
 F2HZCM 298.59439 Hz/cm
 F1PPMCM 0.36715 ppm/cm
 F1HZCM 293.64917 Hz/cm

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800 MHz NOESY Spectrum of **1b** in CDCl₃
 400 ms mixing time
 268 K (-5 °C), 6 mM



Spectroscopic DATA for the compound **1c**
(8 mM, CDCl₃ 268K)



Key NOEs assigned as *intermolecular* are represented with red arrows
Key NOEs assigned as *intramolecular* are represented with blue arrows

Key data for amino acids.

Amino acid	H _α Shift ppm	NH Shift ppm	³ J _{NHα} Hz
Aaa	5.17	8.37	broad
R ₁ = Leu ¹	5.53	8.40	broad
R ₂ = Ala ²	5.06	8.42	broad
R ₃ = Leu ³	5.01	8.60	8.4
R ₄ = Ala ⁴	4.68	8.00	broad

Amino adipic acid (Aaa) δ proton resonances.

pro-R: 2.94 ppm, t, (*J* = 12.2 Hz)

pro-S: 2.19 ppm, td, (*J*₁ = 11.4 Hz; *J*₂ = 7.0 Hz)

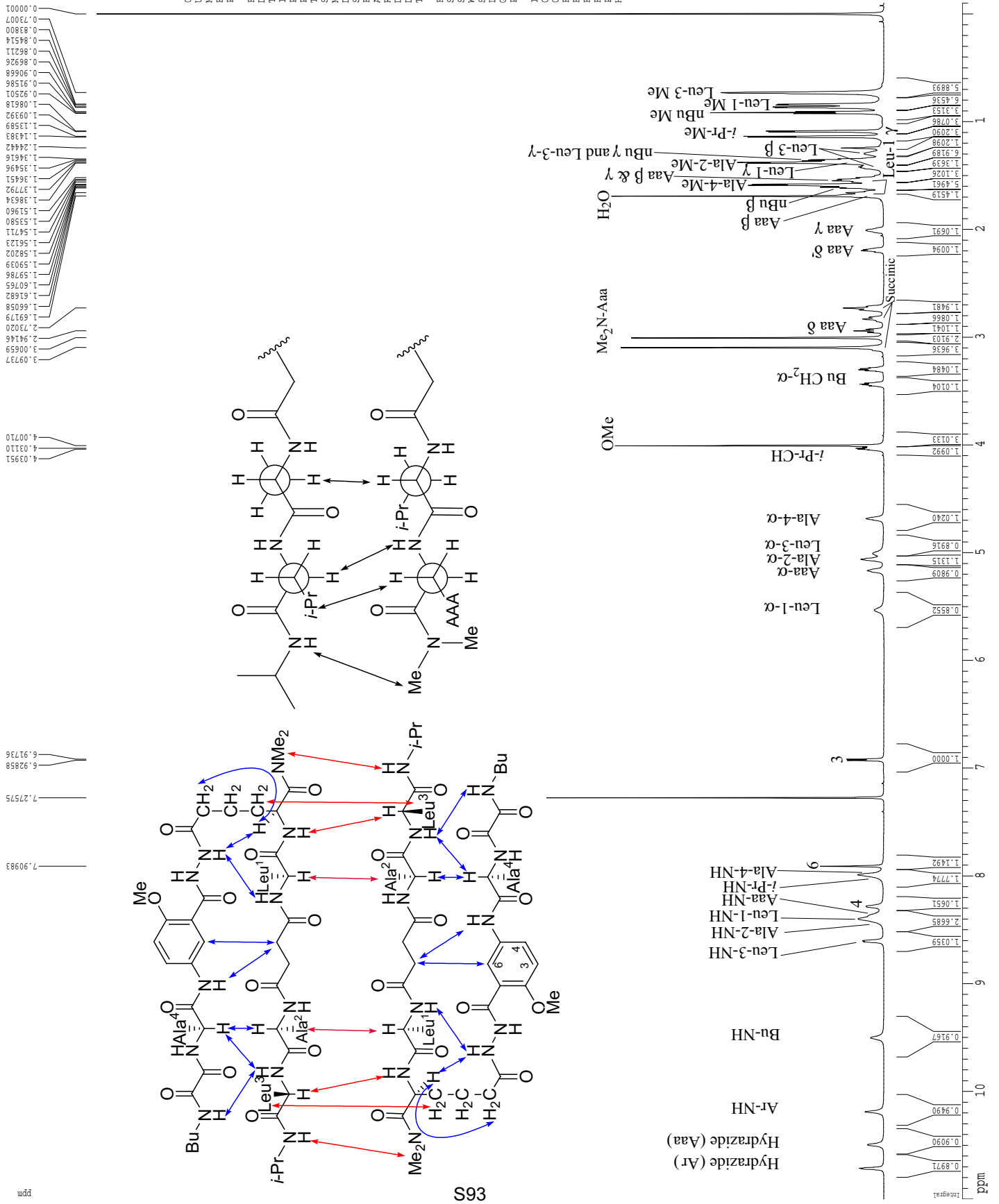
anisotropy = 0.75ppm

Key data for other NH protons.

Proton	NH Shift ppm	<i>J</i> Hz
Ar-NH	10.19	-
Hydrazide Ar	10.71	broad
Hydrazide Aaa	10.50	broad
Bu-NH	9.50	broad
<i>i</i> -Pr-NH	8.00	broad

ESI MS *m/z* for C₄₇H₇₈N₁₁O₁₂ [M+H]⁺ calcd 988.58, found 988.45.

800 MHz ¹H NMR Spectrum of **1c** in CDCl₃
268 K (-5 °C), 8 mM



Current Data Parameters
USER slevin
NAME SL-7-213-800-H
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters

Date_ 20070122
Time_ 0.00
INSTRUM varian
PROBHD 40:5mmrbroadban
PULPROG gpcosy
TD 4096
SOLVENT cdcl3
NS 8
DS 64
SWH 11001.101 Hz
FIDRES 2.685816 Hz
AQ 0.1843700 sec
RG 4096
DW 45.450 usec
DE 231.43 usec
TE 268.5 K

F1 - Acquisition parameters

ND0 1
TD 512
SF01 799.8107 MHz
FIDRES 21.486525 Hz
SW 13.755 ppm
FRMODE undefined

F2 - Processing parameters

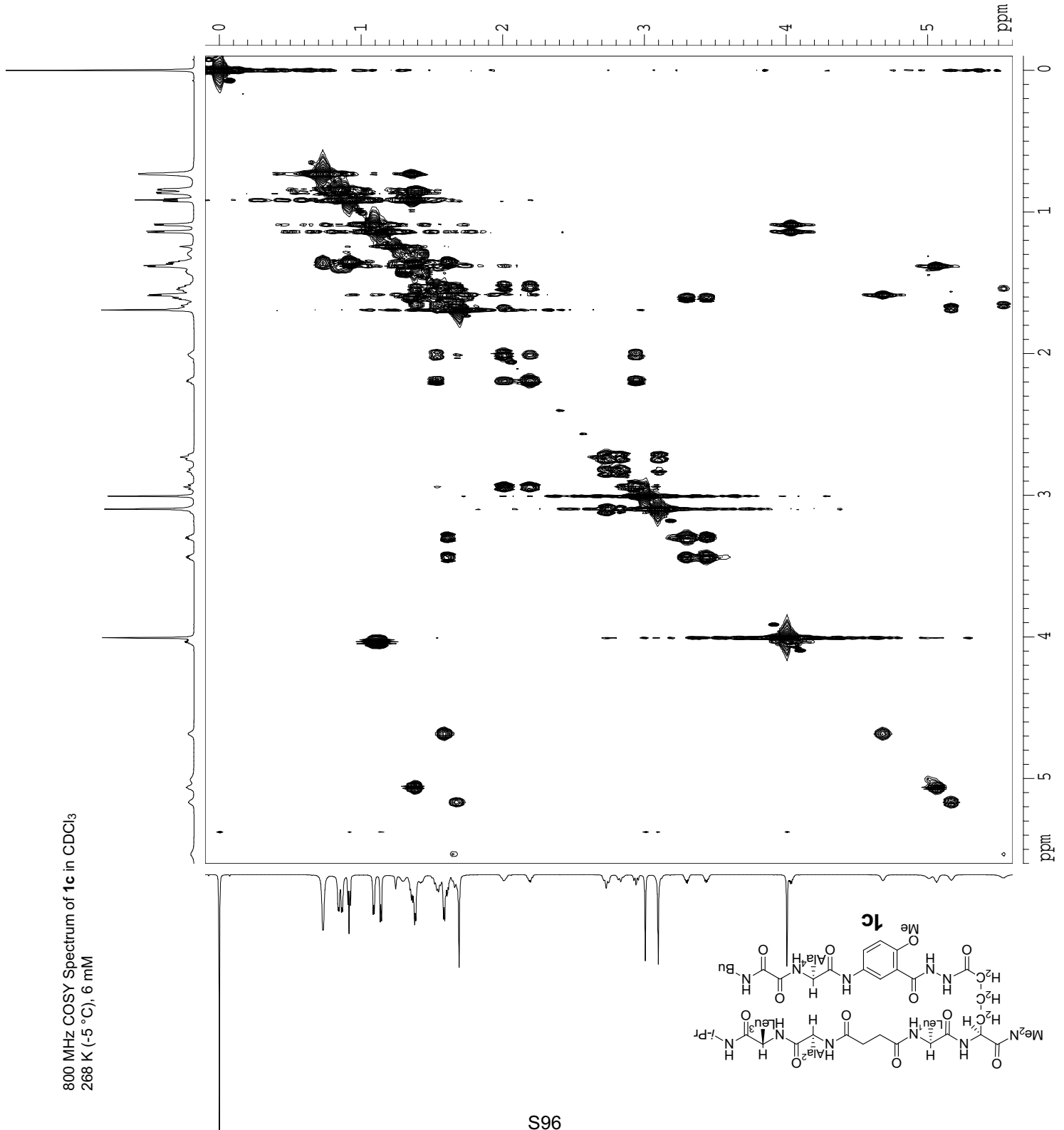
SI 2048
SF 799.8064140 MHz
WDW SINE
SSB 0
LB 0.00 Hz
GB 0
PC 1.40

F1 - Processing parameters

SI 512
MC2 OF
SF 799.8064140 MHz
WDW SINE
SSB 0
LB 0.00 Hz
GB 0

2D NMR plot parameters

CX2 15.00 cm
CX1 15.00 cm
F2PLO 5.600 ppm
F2LO 4478.92 Hz
F2PHI -0.100 ppm
F2HI -79.98 Hz
F1PLO 5.600 ppm
F1LO 4478.92 Hz
F1PHI -0.100 ppm
F1HI -79.98 Hz
F2PNCM 0.38000 ppm/cm
F2ZCM 303.92645 Hz/cm
F1PNCM 0.38000 ppm/cm
F1ZCM 303.92645 Hz/cm



Current Data Parameters
 USER slevin
 NAME SL-7-213-800-H
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters

Date_ 20070122
 Time_ 0.00
 INSTRUM varian
 PROBHD 40:5mmrbroadban
 PULPROG gcosy
 TD 4096
 SOLVENT cdcl3
 NS 8
 DS 64
 SWH 11001.101 Hz
 FIDRES 2.685816 Hz
 AQ 0.1843700 sec
 RG 4096
 DW 45.450 usec
 DE 231.43 usec
 TE 268.5 K

F1 - Acquisition parameters

ND0 1
 TD 512
 SF01 799.8107 MHz
 FIDRES 21.486525 Hz
 SW 13.755 ppm
 FnmODE undefined

F2 - Processing parameters

SI 2048
 SF 799.8064140 MHz
 WDW SINE
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.40

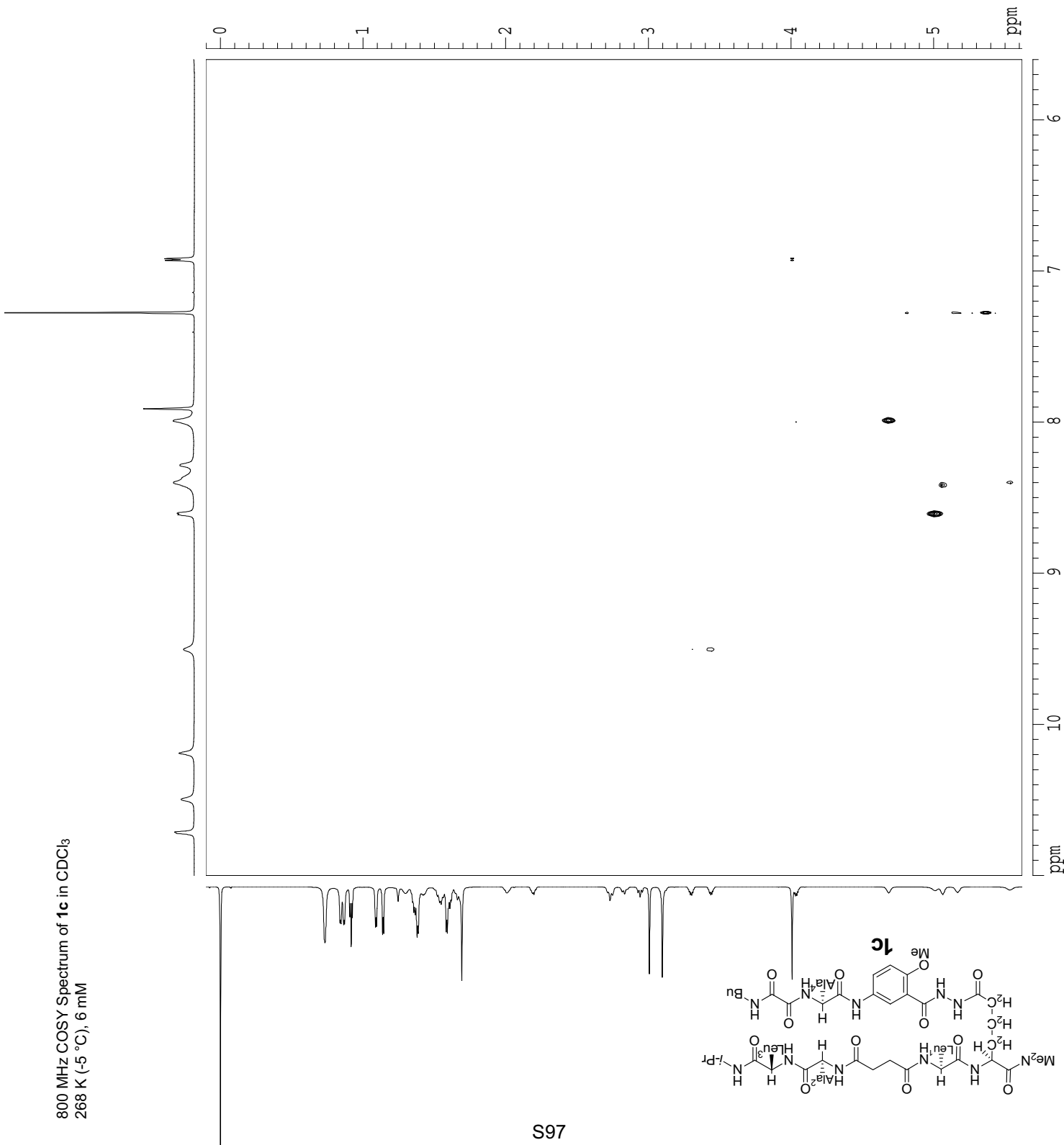
F1 - Processing parameters

SI 512
 MC2 QF
 SF 799.8064140 MHz
 WDW SINE
 SSB 0
 LB 0.00 Hz
 GB 0

2D NMR plot parameters

CX2 15.00 cm
 CX1 15.00 cm
 F2PLO 11.000 ppm
 F2LLO 8797.87 Hz
 F2PHI 5.600 ppm
 F2HTI 4478.92 Hz
 F1PLO 5.620 ppm
 F1LLO 4494.71 Hz
 F1PHI -0.102 ppm
 F1HTI -81.92 Hz
 F2PPMCM 0.36000 ppm/cm
 F2HZCM 287.93030 Hz/cm
 F1PPMCM 0.38148 ppm/cm
 F1HZCM 305.10861 Hz/cm

800 MHz COSY Spectrum of **1c** in CDCl₃
 268 K (-5 °C), 6 mM



Current Data Parameters
 USER slewin
 NAME SL-7-213-800-H
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters

Date 20070122
 Time 0.00
 INSTRUM varian
 PROBD 40.5mm broadband
 PULPROG gcpsy
 TD 4096
 SOLVENT cdcl3
 NS 8
 DS 64
 SWH 11001.101 Hz
 FIDRES 2.685816 Hz
 AQ 0.1843700 sec
 RG 4096
 DW 45.450 usec
 DE 231.43 usec
 TE 268.5 K

F1 - Acquisition parameters

ND0 1
 TD 512
 SF01 799.8107 MHz
 FIDRES 21.486525 Hz
 SW 13.755 ppm
 FMODE undefined

F2 - Processing parameters

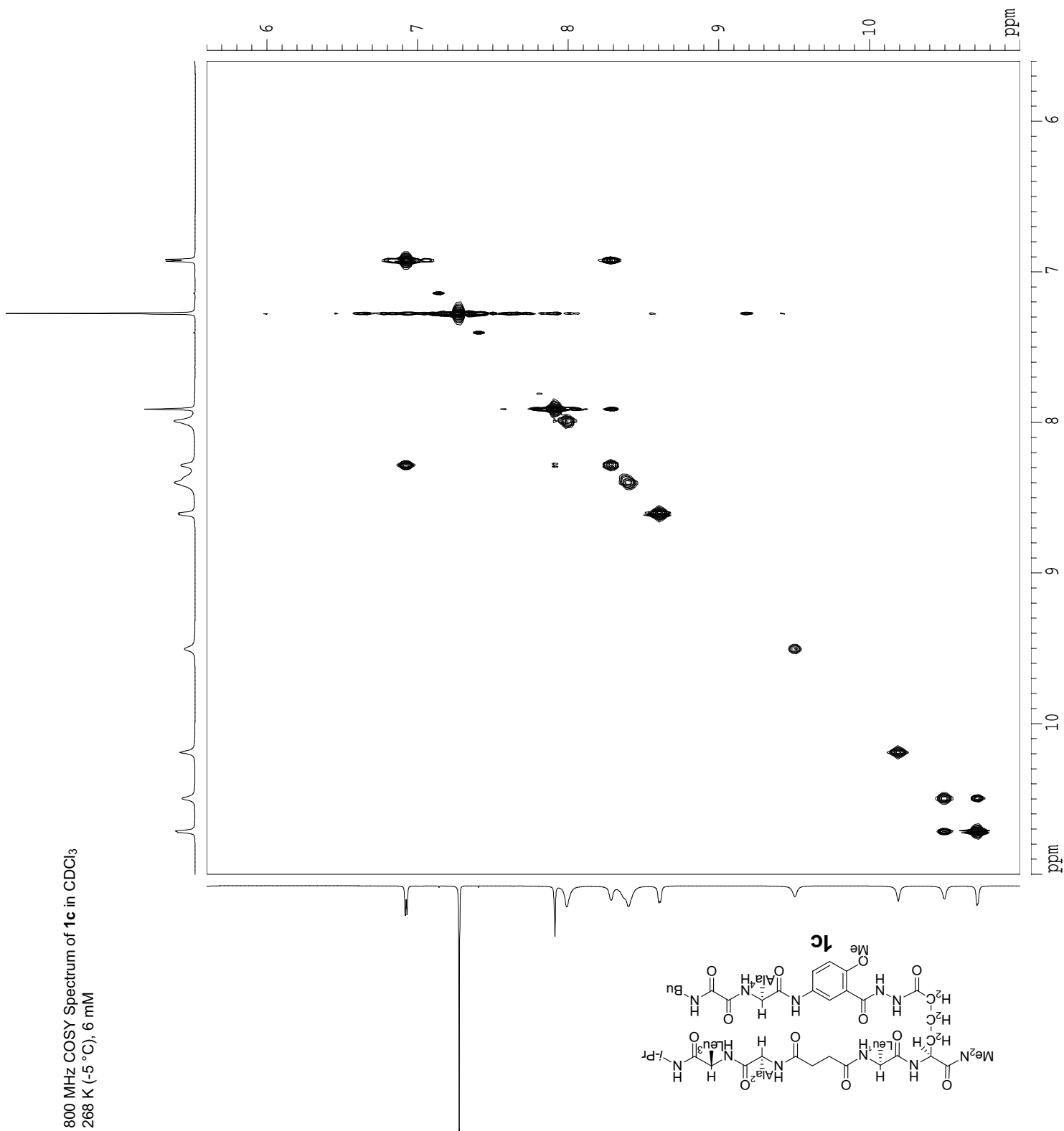
SI 2048
 SF 799.8064140 MHz
 WDW SINE
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.40

F1 - Processing parameters

SI 512
 MC2 QF
 SF 799.8064140 MHz
 WDW SINE
 SSB 0
 LB 0.00 Hz
 GB 0

2D NMR plot parameters

CX2 15.00 cm
 CX1 15.00 cm
 F2PLO 11.000 ppm
 F2LO 8797.87 Hz
 F2PHI 5.600 ppm
 F2HI 4478.92 Hz
 F1PLO 11.000 ppm
 F1LO 8797.87 Hz
 F1PHI 5.600 ppm
 F1HI 4478.92 Hz
 F2PPMCW 0.36000 ppm/cm
 F2HZCM 287.93030 Hz/cm
 F1PPMCW 0.36000 ppm/cm
 F1HZCM 287.93030 Hz/cm



Supporting Information

S. Levin and J. S. Nowick

Current Data Parameters
 USER slevin
 NAME SL-7-213-800-H
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters

Date_ 20070122
 Time_ 0.00
 INSTRUM varian
 PROBHD 40:5mmrbroadban
 PULPROG gcosy
 TD 4096
 SOLVENT cdcl3
 NS 8
 DS 64
 SWH 11001.101 Hz
 FIDRES 2.685816 Hz
 AQ 0.1843700 sec
 RG 4096
 DW 45.450 usec
 DE 231.43 usec
 TE 268.5 K

F1 - Acquisition Parameters

ND0 1
 TD 512
 SFO1 799.8107 MHz
 FIDRES 21.486525 Hz
 SW 13.755 ppm
 F1MODE undefined

F2 - Processing parameters

SI 2048
 SF 799.8064140 MHz
 WDW SINE
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.40

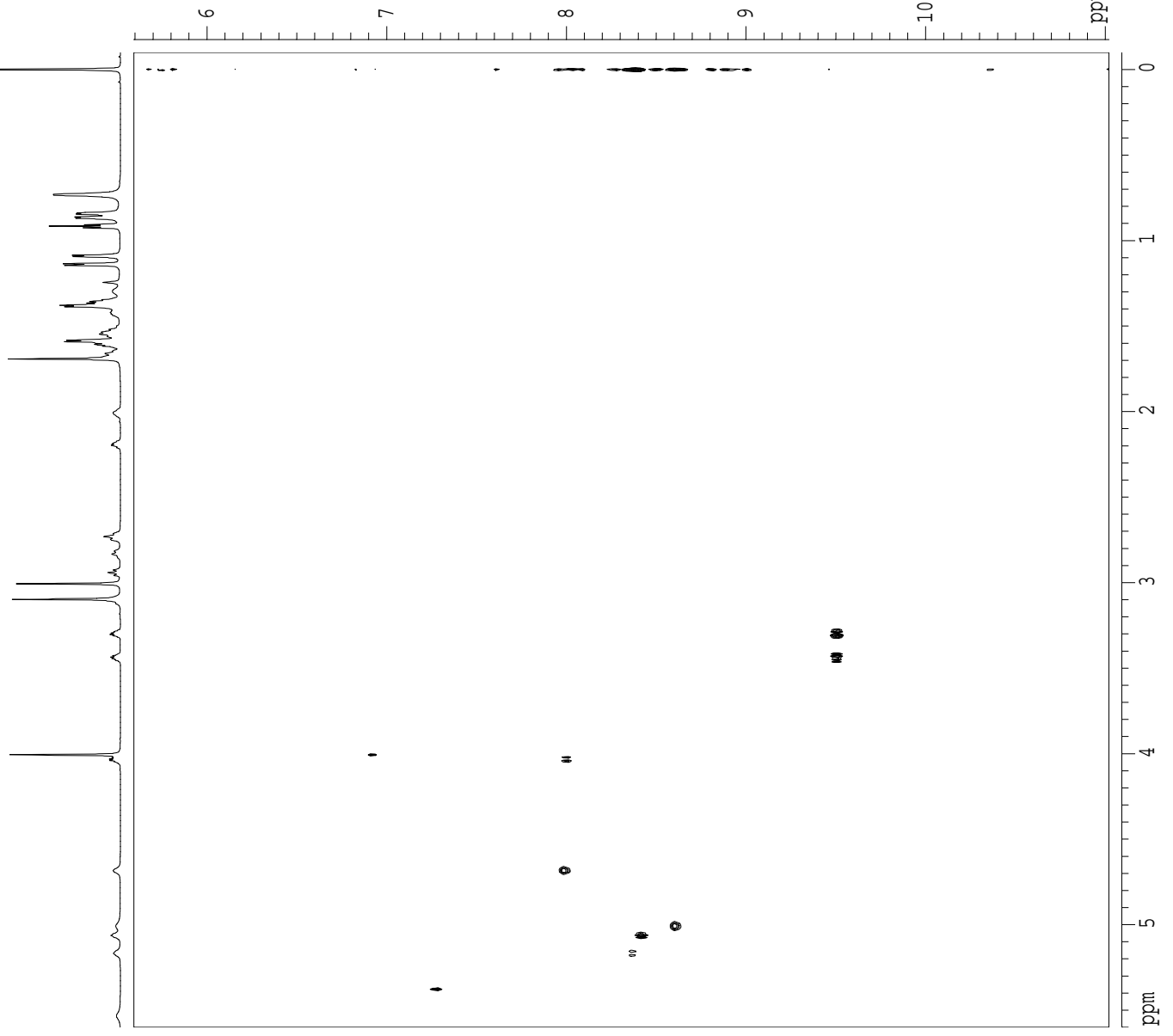
F1 - Processing parameters

SI 512
 MC2 OF
 SF 799.8064140 MHz
 WDW SINE
 SSB 0
 LB 0.00 Hz
 GB 0

2D NMR plot parameters

CX2 15.00 cm
 CX1 15.00 cm
 F2PLO 5.600 ppm
 F2LO 4478.92 Hz
 F2PHI -0.100 ppm
 F2HI -79.98 Hz
 F1PLO 11.020 ppm
 F1LO 8813.50 Hz
 F1PHI 5.593 ppm
 F1HI 4473.23 Hz
 F2PMCM 0.38000 ppm/cm
 F2HZCM 303.92645 Hz/cm
 F1PMCM 0.36178 ppm/cm
 F1HZCM 289.35184 Hz/cm

800 MHz COSY Spectrum of **1c** in CDCl₃
 268 K (-5 °C), 6 mM



Supporting Information

S. Levin and J. S. Nowick

Current Data Parameters
 USER slevin
 NAME SL-7-213-800-H
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters

Date_ 20070122
 Time 0.00
 INSTRUM varian
 PROBHD 40:5mm broadband
 PULPROG gpcsy
 TD 4096
 SOLVENT cdc13
 NS 8
 DS 64
 SWH 11001.101 Hz
 FIDRES 2.685816 Hz
 AQ 0.1843700 sec
 RG 4096
 DW 45.450 usec
 DE 231.43 usec
 TE 268.5 K

F1 - Acquisition Parameters

ND0 1
 TD 512
 SFO1 799.8107 MHz
 FIDRES 21.486525 Hz
 SW 13.755 ppm
 F1MODE undefined

F2 - Processing parameters

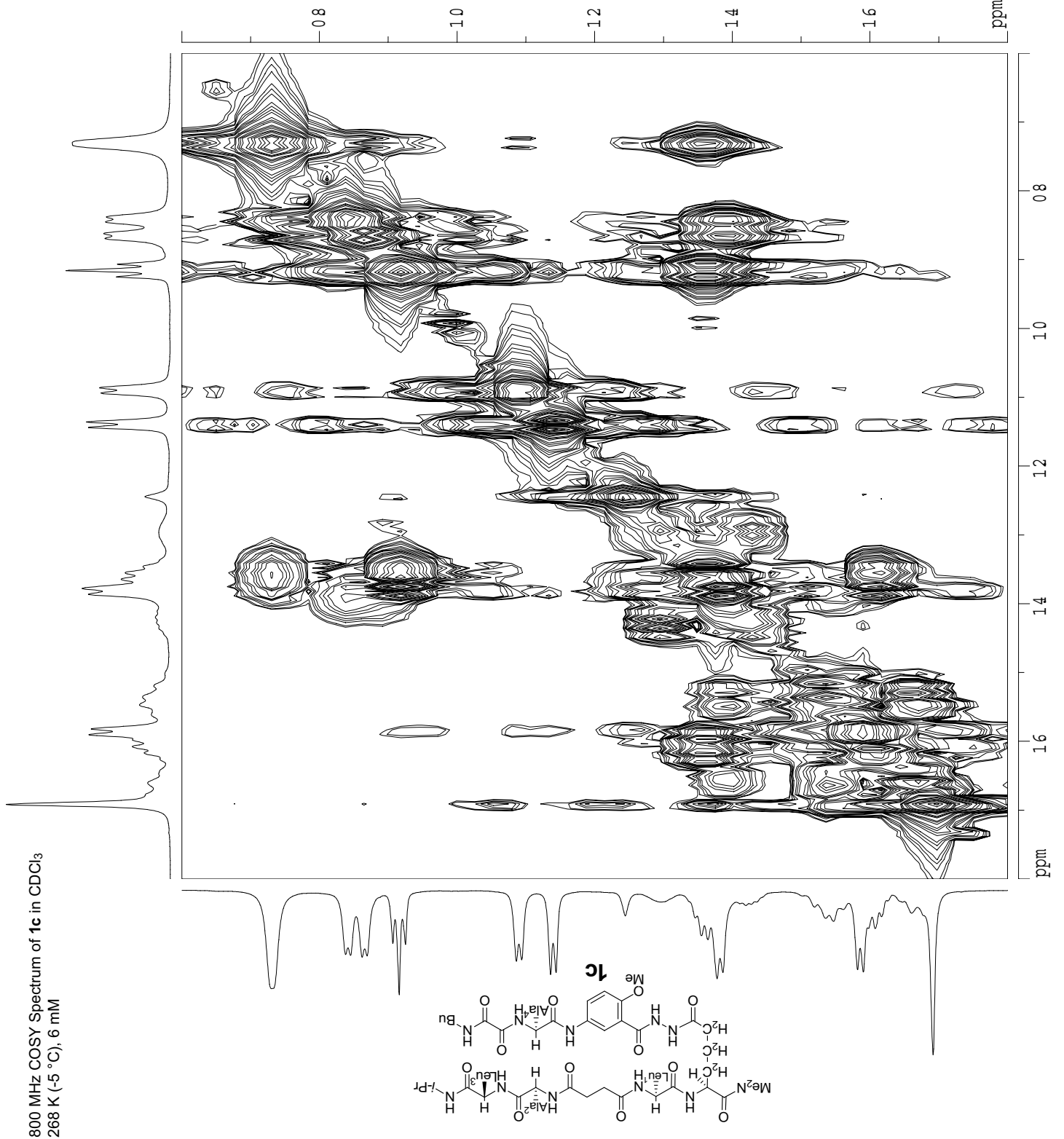
SI 2048
 SF 799.8064140 MHz
 WDW SINE
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.40

F1 - Processing parameters

SI 512
 MC2 QF
 SF 799.8064140 MHz
 WDW SINE
 SSB 0
 LB 0.00 Hz
 GB 0

2D NMR plot parameters

CX2 15.00 cm
 CX1 15.00 cm
 F2PLO 1.800 ppm
 F2LO 1439.65 Hz
 F2PHI 0.600 ppm
 F2HI 479.88 Hz
 F1PLO 1.800 ppm
 F1LO 1439.65 Hz
 F1PHI 0.600 ppm
 F1HI 479.88 Hz
 F2PFCM 0.08000 ppm/cm
 F2HZCM 63.98452 Hz/cm
 F1PFCM 0.08000 ppm/cm
 F1HZCM 63.98452 Hz/cm



800 MHz COSY Spectrum of **1c** in CDCl₃
 268 K (-5 °C), 6 mM

Supporting Information

S. Levin and J. S. Nowick

Current Data Parameters
 USER slewin
 NAME SL-7-213-800-H
 EXPNO 3
 PROCNO 1

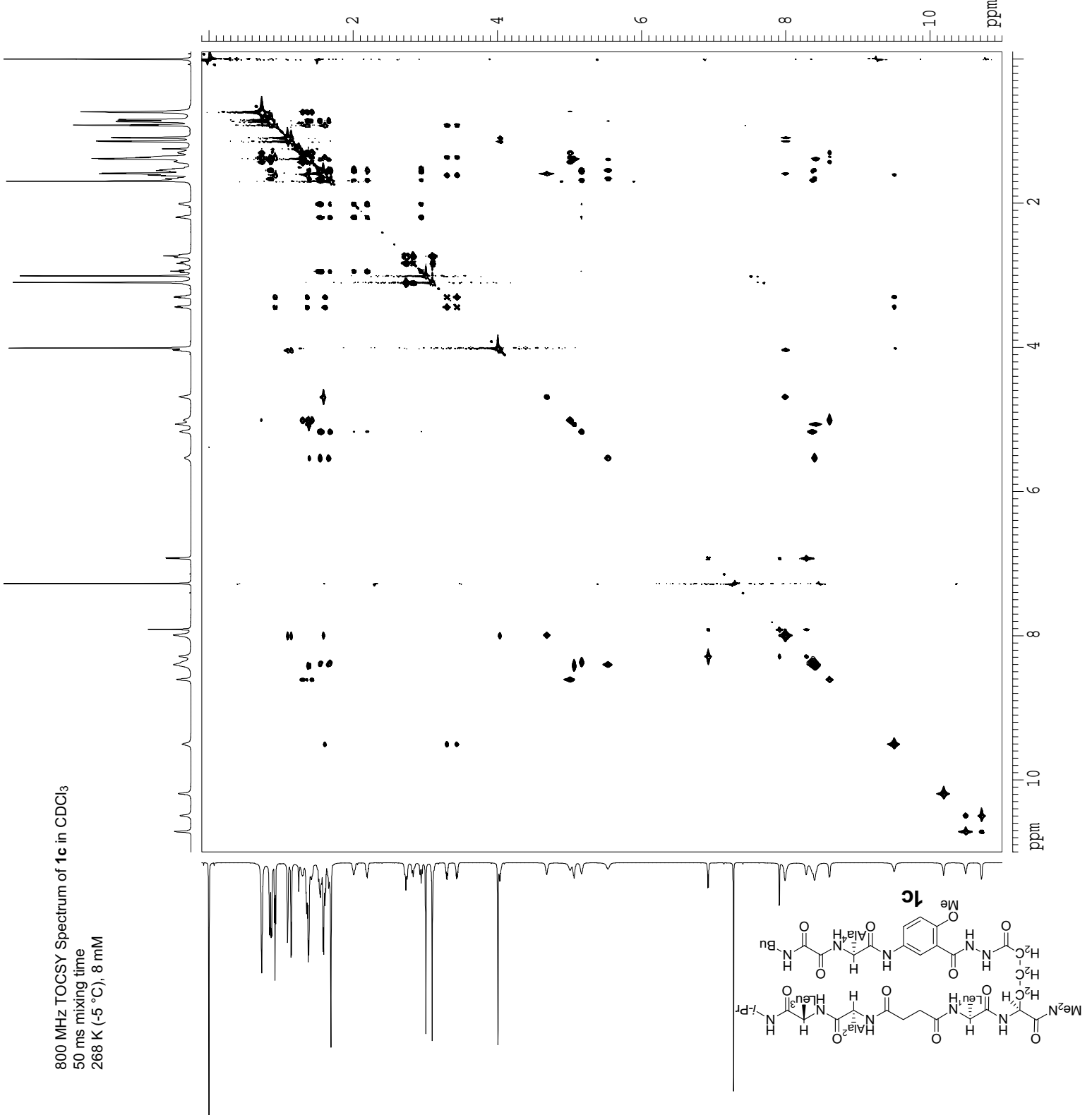
F2 - Acquisition Parameters
 Date_ 20070122
 Time 0.00
 INSTRUM varian
 PROBHD 40:5mmBroadban
 PULPROG wgtocsy.bn
 TD 4096
 SOLVENT CDCl3
 NS 16
 DS 64
 SWH 11001.101 Hz
 FIDRES 2.685816 Hz
 AQ 0.1862132 sec
 RG 287.4
 DW 45.450 usec
 DE 6.00 usec
 TE 288.5 K

F1 - Acquisition Parameters
 ND0 1
 TD 1024
 SFO1 799.8107 MHz
 FIDRES 10.743262 Hz
 SW 13.755 ppm
 FwMODE undefined

F2 - Processing parameters
 SI 2048
 SF 799.8064126 MHz
 WDW QSI
 SSB 2
 LB 0.00 Hz
 GB 0
 PC 1.40

F1 - Processing parameters
 SI 2048
 MC2 States
 SF 799.8064126 MHz
 WDW QSI
 SSB 2
 LB 0.00 Hz
 GB 0

2D NMR plot parameters
 CX2 15.00 cm
 CX1 15.00 cm
 F2PLO 11.000 ppm
 F2LO 8797.87 Hz
 F2PHI -0.100 ppm
 F2HI -79.98 Hz
 F1PLO 11.001 ppm
 F1LO 8798.73 Hz
 F1PHI -0.101 ppm
 F1HI -80.57 Hz
 F2PPMCM 0.74000 ppm/cm
 F2HZCM 591.85669 Hz/cm
 F1PPMCM 0.74012 ppm/cm
 F1HZCM 591.95367 Hz/cm



800 MHz TOCSY Spectrum of **1c** in CDCl₃
 50 ms mixing time
 288 K (-5 °C), 8 mM

Current Data Parameters

USER slevin
 NAME SL-7-213-800-H
 EXPNO 3
 PROCNO 1

F2 - Acquisition Parameters

Date_ 20070122
 Time_ 0.00
 INSTRUM varian
 PROBHD 40:5mmrbroadban
 PULPROG wgtocpsy bn
 TD 4096
 SOLVENT CDCl3
 NS 16
 DS 64
 SWH 11001.101 Hz
 FIDRES 2.685816 Hz
 AQ 0.1862132 sec
 RG 287.4
 DW 45.450 usec
 DE 6.00 usec
 TE 268.5 K

F1 - Acquisition parameters

ND0 1
 TD 1024
 SF01 799.8107 MHz
 FIDRES 10.743262 Hz
 SW 13.755 ppm
 F1MODE undefined

F2 - Processing parameters

SI 2048
 SF 799.8064126 MHz
 WDW QSI
 SSB 2
 LB 0.00 Hz
 GB 0
 PC 1.40

F1 - Processing parameters

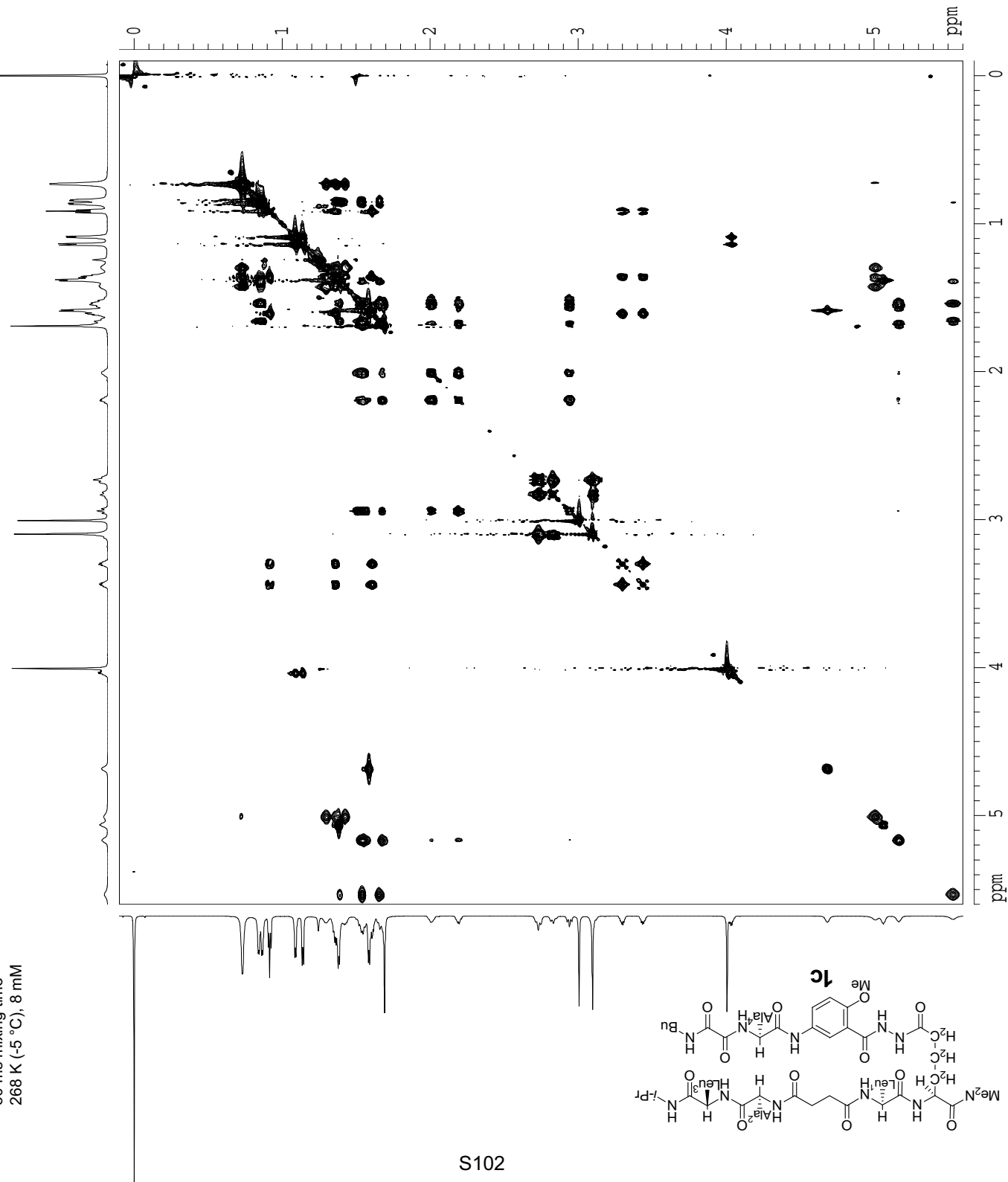
SI 2048
 MC2 States
 SF 799.8064126 MHz
 WDW QSI
 SSB 2
 LB 0.00 Hz
 GB 0

2D NMR plot parameters

CX2 15.00 cm
 CX1 15.00 cm
 F2PLO 5.600 ppm
 F2LO 4478.92 Hz
 F2PHI -0.100 ppm
 F2HI -79.98 Hz
 F1PLO 5.600 ppm
 F1LO 4478.92 Hz
 F1PHI -0.100 ppm
 F1HI -79.98 Hz
 F2PVMCM 0.38000 ppm/cm
 F2HZCM 303.92645 Hz/cm
 F1PVMCM 0.38000 ppm/cm
 F1HZCM 303.92645 Hz/cm

800 MHz TOCSY Spectrum of **1c** in CDCl₃

50 ms mixing time
 268 K (-5 °C), 8 mM



Current Data Parameters
 USER slewin
 NAME SL-7-213-800-H
 EXPNO 3
 PROCNO 1

F2 - Acquisition Parameters

Date 20070122
 Time 0.00
 INSTRUM varian
 PROBHD 40:5mm broadband
 PULPROG wgtocsy_bn
 TD 4096
 SOLVENT CDCl3
 NS 16
 DS 64
 SWH 11001.101 Hz
 FIDRES 2.685816 Hz
 AQ 0.1862132 sec
 RG 287.4
 DW 45.450 usec
 DE 6.00 usec
 TE 268.5 K

F1 - Acquisition parameters

ND0 1
 TD 1024
 SFO1 799.8107 MHz
 FIDRES 10.743262 Hz
 SW 13.755 ppm
 FMODE undefined

F2 - Processing parameters

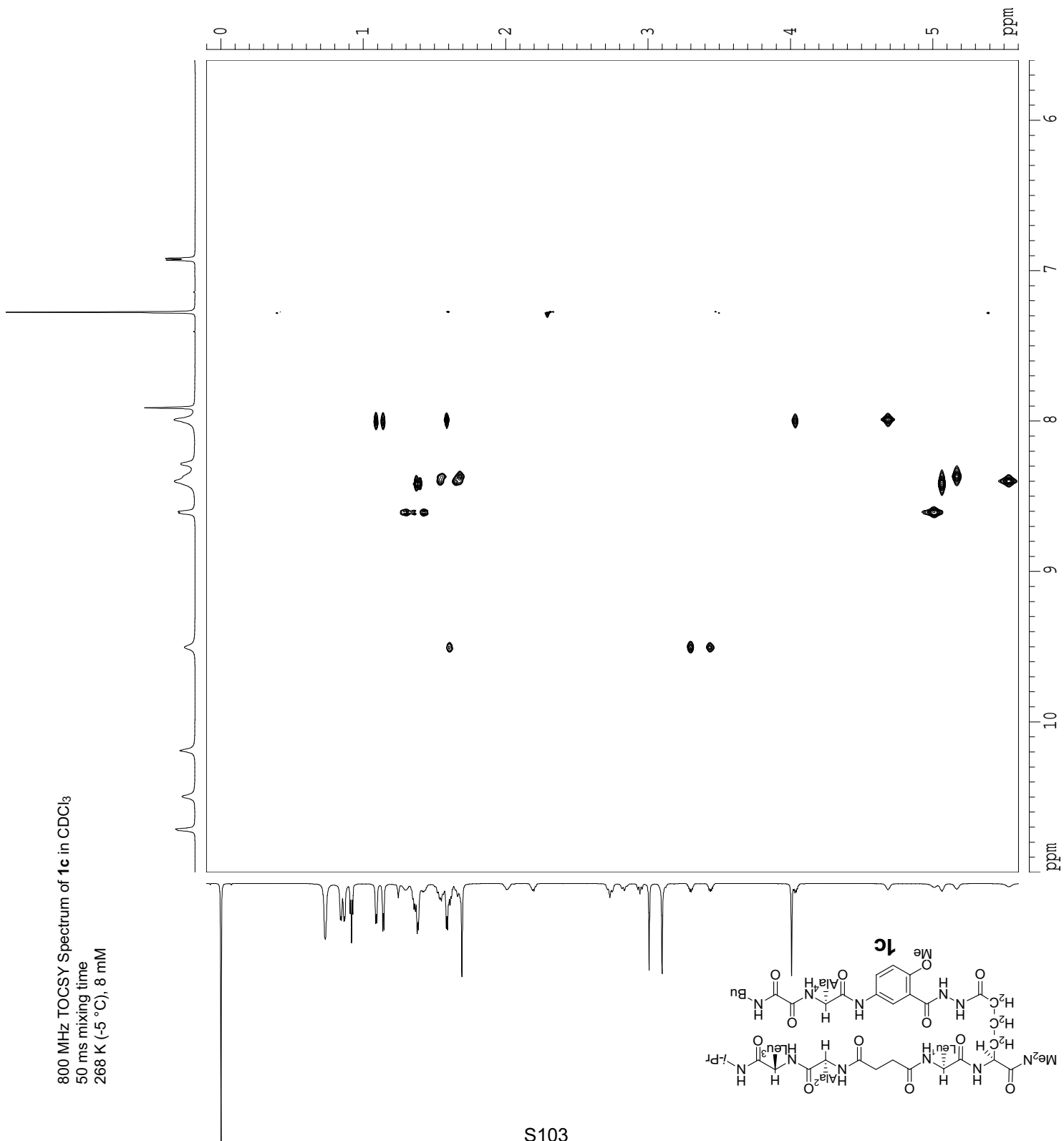
SI 2048
 SF 799.8064126 MHz
 WDW QSI
 SSB 2
 LB 0.00 Hz
 GB 0
 PC 1.40

F1 - Processing parameters

SI 2048
 MC2 States
 SF 799.8064126 MHz
 WDW QSI
 SSB 2
 LB 0.00 Hz
 GB 0

2D NMR plot parameters

CX2 15.00 cm
 CX1 15.00 cm
 F2PLO 11.000 ppm
 F2LO 8797.87 Hz
 F2PHI 5.600 ppm
 F2HI 4478.92 Hz
 F1PLO 5.601 ppm
 F1LO 4479.94 Hz
 F1PHI -0.101 ppm
 F1HI -80.57 Hz
 F2PPMCM 0.36000 ppm/cm
 F2HZCM 287.93030 Hz/cm
 F1PPMCM 0.38013 ppm/cm
 F1HZCM 304.03430 Hz/cm



800 MHz TOCSY Spectrum of **1c** in CDCl₃
 50 ms mixing time
 268 K (-5 °C), 8 mM

Current Data Parameters
 USER slevin
 NAME SL-7-213-800-H
 EXPNO 3
 PROCNO 1

F2 - Acquisition Parameters

Date 20070122
 Time_ 0.00
 INSTRUM varian
 PROBHD 40:5mmBroadban
 PULPROG wgtocsy_bn
 TD 4096
 SOLVENT CDCl3
 NS 16
 DS 64
 SWH 11001.101 Hz
 FIDRES 2.685816 Hz
 AQ 0.1862132 sec
 RG 287.4
 DW 45.450 usec
 DE 6.00 usec
 TE 268.5 K

F1 - Acquisition parameters

ND0 1
 TD 1024
 SF01 799.8107 MHz
 FIDRES 10.743262 Hz
 SW 13.755 ppm
 FhMODE undefined

F2 - Processing parameters

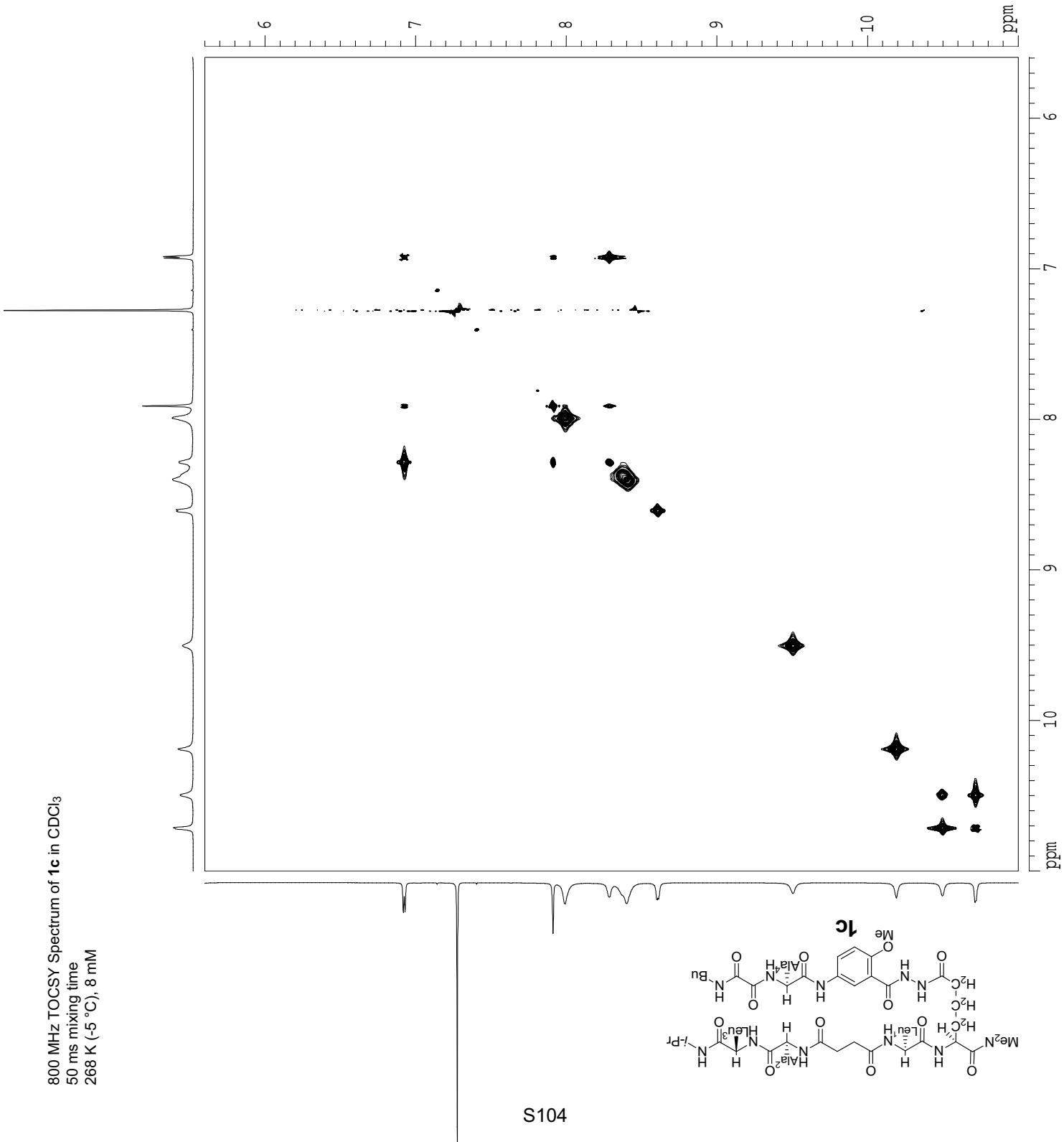
SI 2048
 SF 799.8064126 MHz
 WDW QSI
 SSB 2
 LB 0.00 Hz
 GB 0
 PC 1.40

F1 - Processing parameters

SI 2048
 MC2 States
 SF 799.8064126 MHz
 WDW QSI
 SSB 2
 LB 0.00 Hz
 GB 0

2D NMR plot parameters

CX2 15.00 cm
 CX1 15.00 cm
 F2PLO 11.001 ppm
 F2LO 8798.73 Hz
 F2PHI 5.595 ppm
 F2HI 4474.57 Hz
 F1PLO 11.000 ppm
 F1LO 8797.87 Hz
 F1PHI 5.600 ppm
 F1HI 4478.92 Hz
 F2PPMCM 0.36043 ppm/cm
 F2HZCM 288.27753 Hz/cm
 F1PPMCM 0.36000 ppm/cm
 F1HZCM 287.93030 Hz/cm



800 MHz TOCSY Spectrum of **1c** in CDCl₃
 50 ms mixing time
 268 K (-5 °C), 8 mM

Current Data Parameters
 USER slevin
 NAME SL-7-213-800-H
 EXPNO 3
 PROCNO 1

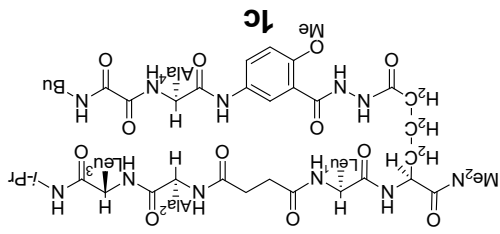
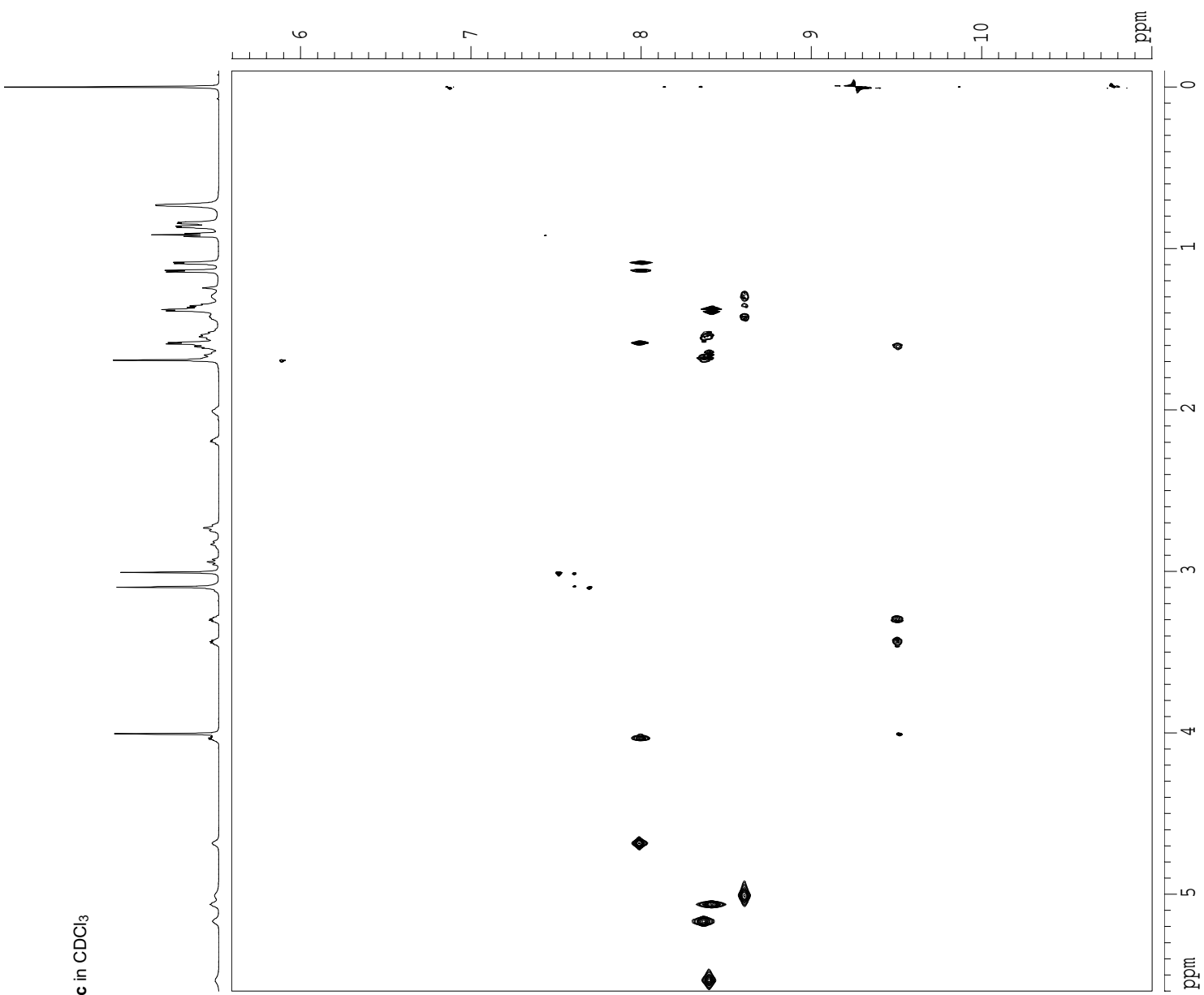
F2 - Acquisition Parameters
 Date_ 20070122
 Time 0.00
 INSTRUM varian
 PROBHD 40:5mmBroadban
 PULPROG wgtocpsy_bn
 TD 4096
 SOLVENT CDCl3
 NS 16
 DS 64
 SWH 11001.101 Hz
 FIDRES 2.685816 Hz
 AQ 0.1862132 sec
 RG 287.4
 DW 45.450 usec
 DE 6.00 usec
 TE 268.5 K

F1 - Acquisition parameters
 ND0 1
 TD 1024
 SF01 799.8107 MHz
 FIDRES 10.743262 Hz
 SW 13.755 ppm
 FMODE undefined

F2 - Processing parameters
 SI 2048
 SF 799.8064126 MHz
 WDW QSI
 SSB 2
 LB 0.00 Hz
 GB 0
 PC 1.40

F1 - Processing parameters
 SI 2048
 MC2 States
 SF 799.8064126 MHz
 WDW QSI
 SSB 2
 LB 0.00 Hz
 GB 0

2D NMR plot parameters
 CX2 15.00 cm
 CX1 15.00 cm
 F2PLO 5.600 ppm
 F2LO 4478.92 Hz
 F2PHI -0.100 ppm
 F2HI -79.98 Hz
 F1PLO 11.001 ppm
 F1LO 8798.73 Hz
 F1PHI 5.595 ppm
 F1HI 4474.57 Hz
 F2PWCW 0.38000 ppm/cm
 F2HZCW 303.92645 Hz/cm
 F1PWCW 0.36043 ppm/cm
 F1HZCW 288.27753 Hz/cm



800 MHz TOCSY Spectrum of **1c** in CDCl₃
 50 ms mixing time
 268 K (-5 °C), 8 mm

Supporting Information

S. Levin and J. S. Nowick

Current Data Parameters
 USER slevin
 NAME SL-7-213-800-H
 EXPNO 4
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20070122
 Time 0:00
 INSTRUM varian
 PROBHD 40:5mmbroadban
 PULPROG noesy2o_pfg_800_pln
 TD 4096

SOLVENT CDCl3
 NS 16
 DS 64
 SWH 11001.101 Hz
 FIDRES 2.685816 Hz
 AQ 0.1862132 sec
 RG 128
 DW 45.450 usec
 DE 6.00 usec
 TE 268.5 K

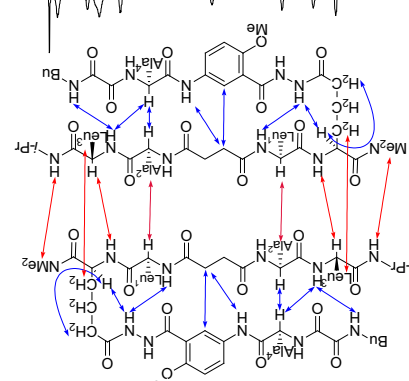
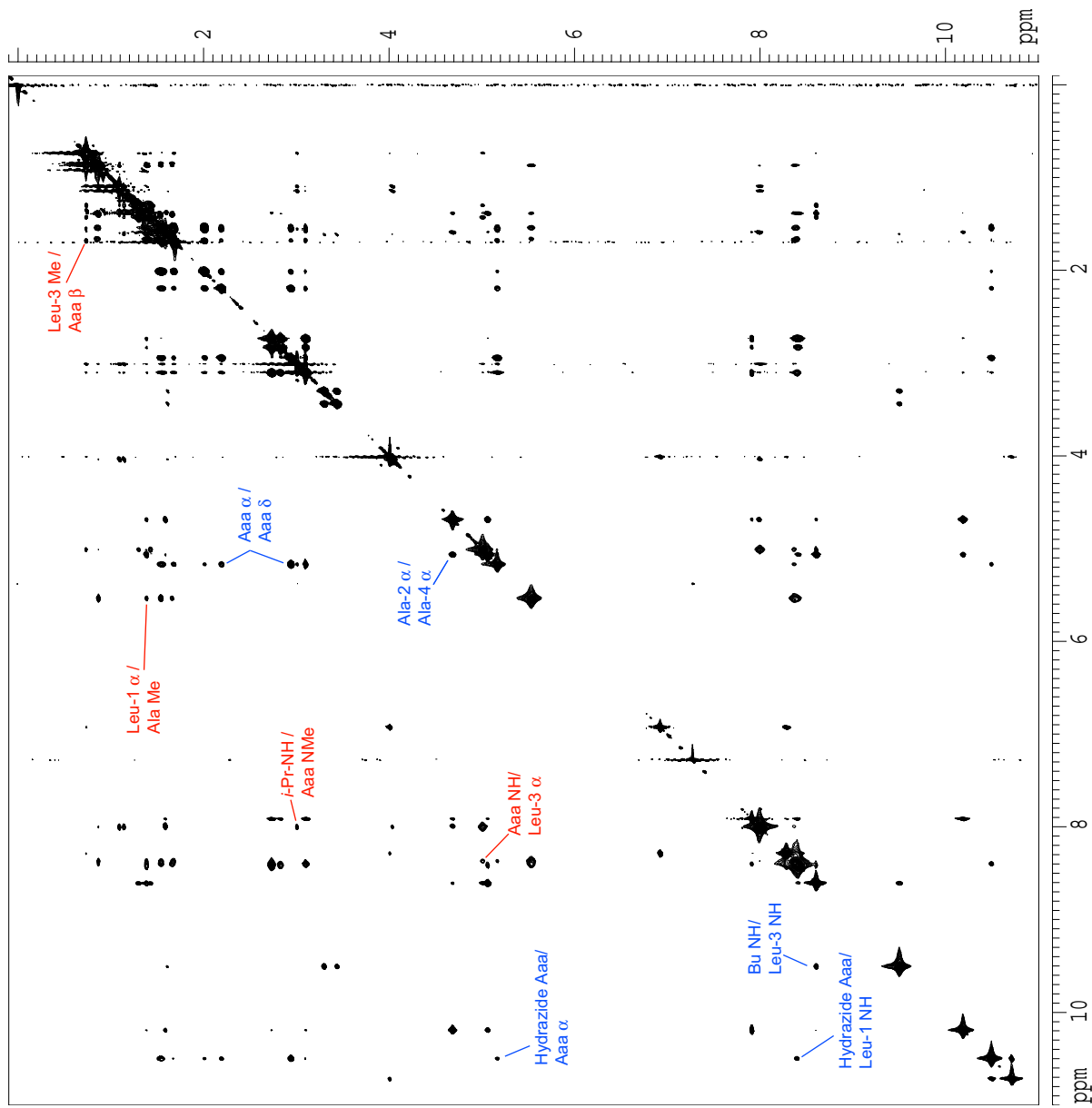
F1 - Acquisition Parameters
 ND0 1
 TD 1024
 SF01 799.8107 MHz
 FIDRES 10.743262 Hz
 SW 13.755 ppm
 F1MODE undefined

F2 - Processing parameters
 SI 2048
 SF 799.8064140 MHz
 WDM QSINE
 SSB 2
 LB 0.00 Hz
 GB 0
 PC 1.40

F1 - Processing parameters
 SI 1024
 MC2 States
 SF 799.8064140 MHz
 WDM QSINE
 SSB 2
 LB 0.00 Hz
 GB 0

2D NMR plot parameters
 CX2 15.00 cm
 CX1 15.00 cm
 F2PLO 11.001 ppm
 F2LO 8798.73 Hz
 F2PHI -0.101 ppm
 F2HI -80.57 Hz
 F1PLO 11.008 ppm
 F1LO 8804.10 Hz
 F1PHI -0.101 ppm
 F1HI -80.57 Hz
 F2PFCM 0.74012 ppm/cm
 F2H2CM 591.95367 Hz/cm
 F1PFCM 0.74057 ppm/cm
 F1H2CM 592.31183 Hz/cm

800 MHz NOESY Spectrum of **1c** in CDCl₃
 400 ms mixing time
 268 K (-5 °C), 8 mM



Current Data Parameters
 USER slevin
 NAME SL-7-213-800-H
 EXPNO 4
 PROCNO 1

F2 - Acquisition Parameters

Date_ 20070122
 Time 0.00
 INSTRUM varian
 PROBHD 40:5mmbroadban
 PULPROG noesyh2o_pfg_800_pln
 TD 4096
 SOLVENT CDCl3
 NS 16
 DS 64
 SWH 11001.101 Hz
 FIDRES 2.685816 Hz
 AQ 0.1862132 sec
 RG 128
 DW 45.450 usec
 DE 6.00 usec
 TE 288.5 K

F1 - Acquisition Parameters

ND0 1
 TD 1024
 SF01 799.8107 MHz
 FIDRES 10.743262 Hz
 SW 13.755 ppm
 FwMODE undefined

F2 - Processing parameters

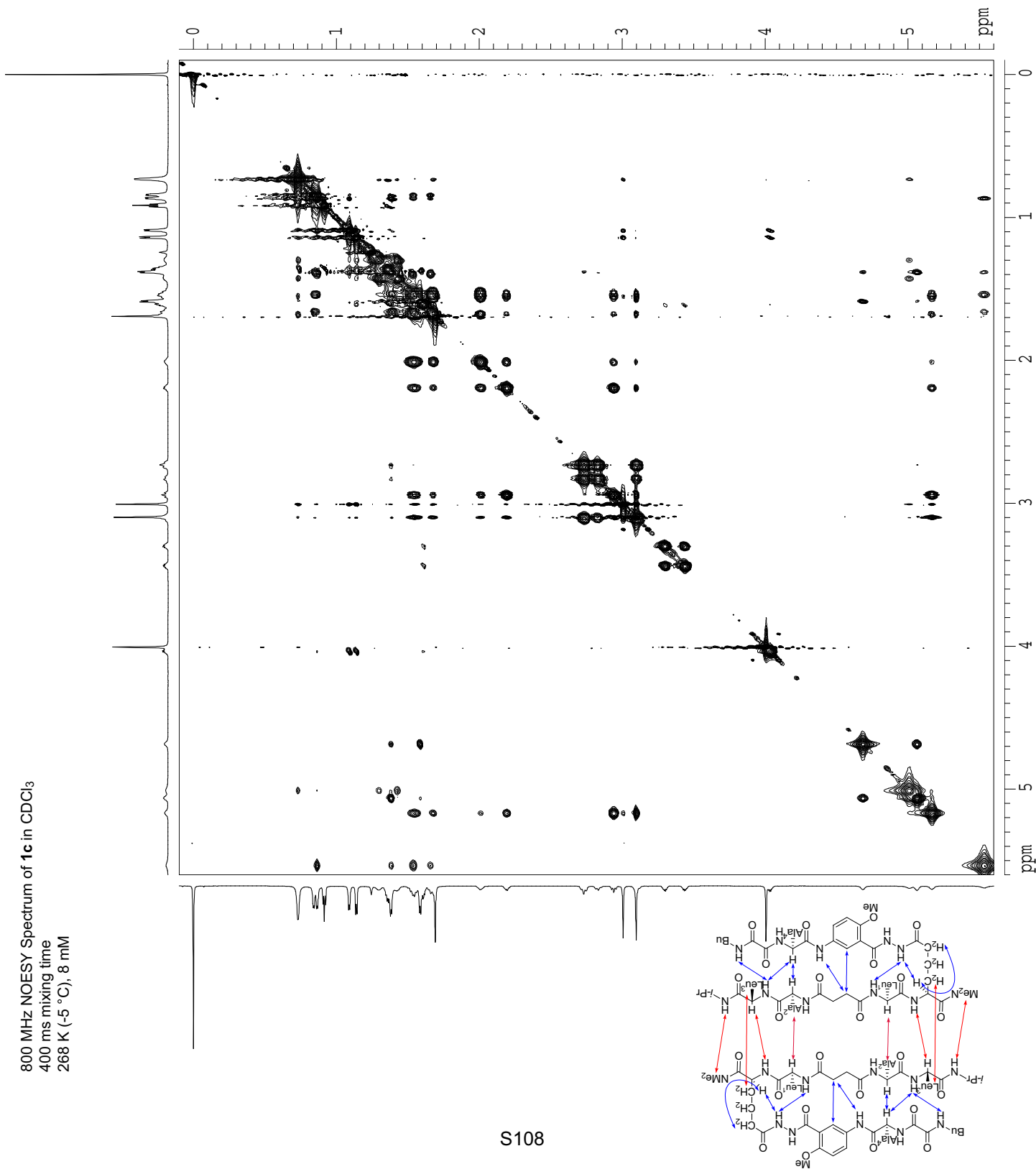
SI 2048
 SF 799.8064140 MHz
 WDM QSIGNE
 SSB 2
 LB 0.00 Hz
 GB 0
 PC 1.40

F1 - Processing parameters

SI 1024
 MC2 States
 SF 799.8064140 MHz
 WDM QSIGNE
 SSB 2
 LB 0.00 Hz
 GB 0

2D NMR plot parameters

CX2 15.00 cm
 CX1 15.00 cm
 F2PLO 5.600 ppm
 F2LO 4478.92 Hz
 F2PHI -0.100 ppm
 F2HI -79.98 Hz
 F1PLO 5.600 ppm
 F1LO 4478.92 Hz
 F1PHI -0.100 ppm
 F1HI -79.98 Hz
 F2PPMCM 0.38000 ppm/cm
 F2HZCM 303.92645 Hz/cm
 F1PPMCM 0.38000 ppm/cm
 F1HZCM 303.92645 Hz/cm



Supporting Information

Current Data Parameters
 USER slevin
 NAME SL-7-213-800-H
 EXPNO 4
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20070122
 Time_ 0.00
 INSTRUM varian
 PROBHD 40:5mm broadband
 PULPROG noesyh2o_pfg_800_pln
 TD 4096
 SOLVENT CDCl3
 NS 16
 DS 64
 SWH 11001.101 Hz
 FIDRES 2.685816 Hz
 AQ 0.1862132 sec
 RG 128
 DW 45.450 usec
 DE 6.00 usec
 TE 268.5 K

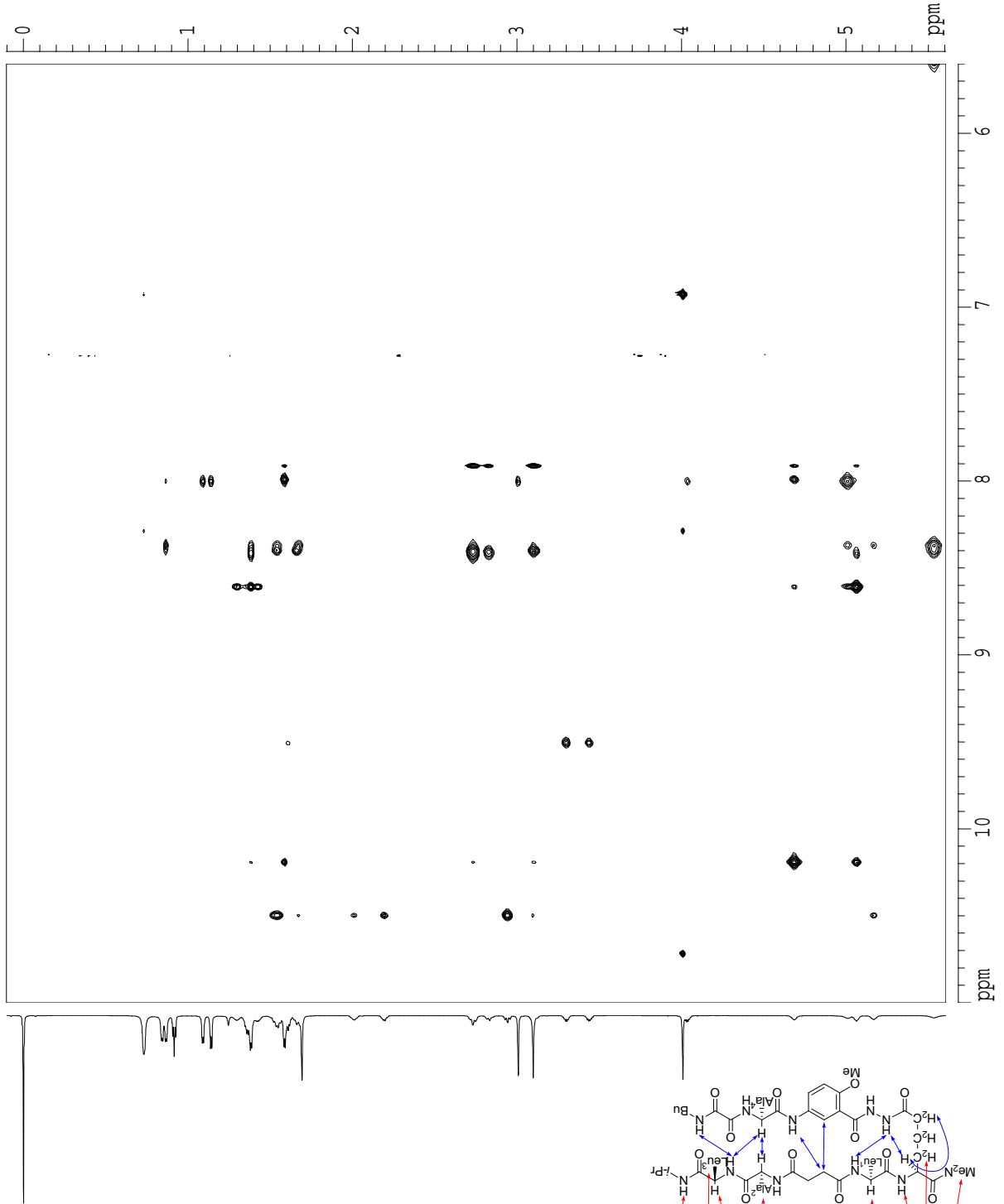
F1 - Acquisition Parameters
 ND0 1
 TD 1024
 SF01 799.8107 MHz
 FIDRES 10.743262 Hz
 SW 13.755 ppm
 FMODE undefined

F2 - Processing parameters
 SI 2048
 SF 799.8064140 MHz
 WDW QSI
 SSB 2
 LB 0.00 Hz
 GB 0
 PC 1.40

F1 - Processing parameters
 SI 1024
 MC2 States
 SF 799.8064140 MHz
 WDW QSI
 SSB 2
 LB 0.00 Hz
 GB 0

2D NMR plot parameters
 CX2 15.00 cm
 CX1 15.00 cm
 F2PLO 11.000 ppm
 F2LO 8797.87 Hz
 F2PHI 5.600 ppm
 F2HI 4478.92 Hz
 F1PLO 5.606 ppm
 F1LO 4483.97 Hz
 F1PHI -0.102 ppm
 F1HI -81.92 Hz
 F2PEMCM 0.36000 ppm/cm
 F2HZCM 287.93030 Hz/cm
 F1PEMCM 0.38058 ppm/cm
 F1HZCM 304.39243 Hz/cm

800 MHz NOESY Spectrum of **1c** in CDCl₃
 400 ms mixing time
 268 K (-5 °C), 8 mM



Current Data Parameters
 USER slevin
 NAME SL-7-213-800-H
 EXPNO 4
 PROCNO 1

F2 - Acquisition Parameters

Date 20070122
 Time 0.00
 INSTRUM varian
 PROBHD 40:5mmbroadban
 PULPROG noesyh2o_pfg_800_pln
 TD 4096
 SOLVENT CDCl3
 NS 16
 DS 64
 SWH 11001.101 Hz
 FIDRES 2.685816 Hz
 AQ 0.1862132 sec
 RG 128
 DW 45.450 usec
 DE 6.00 usec
 TE 268.5 K

F1 - Acquisition Parameters

ND0 1
 TD 1024
 SF01 799.8107 MHz
 FIDRES 10.743262 Hz
 SW 13.755 ppm
 F1MODE undefined

F2 - Processing parameters

SI 2048
 SF 799.8064140 MHz
 WDM QSIINE
 SSB 2
 LB 0.00 Hz
 GB 0
 PC 1.40

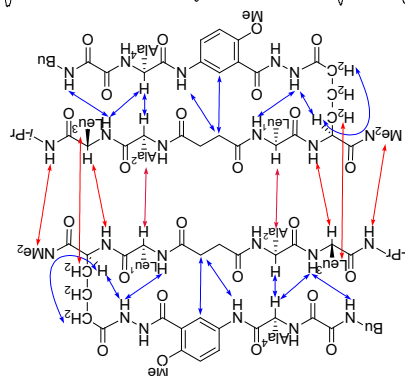
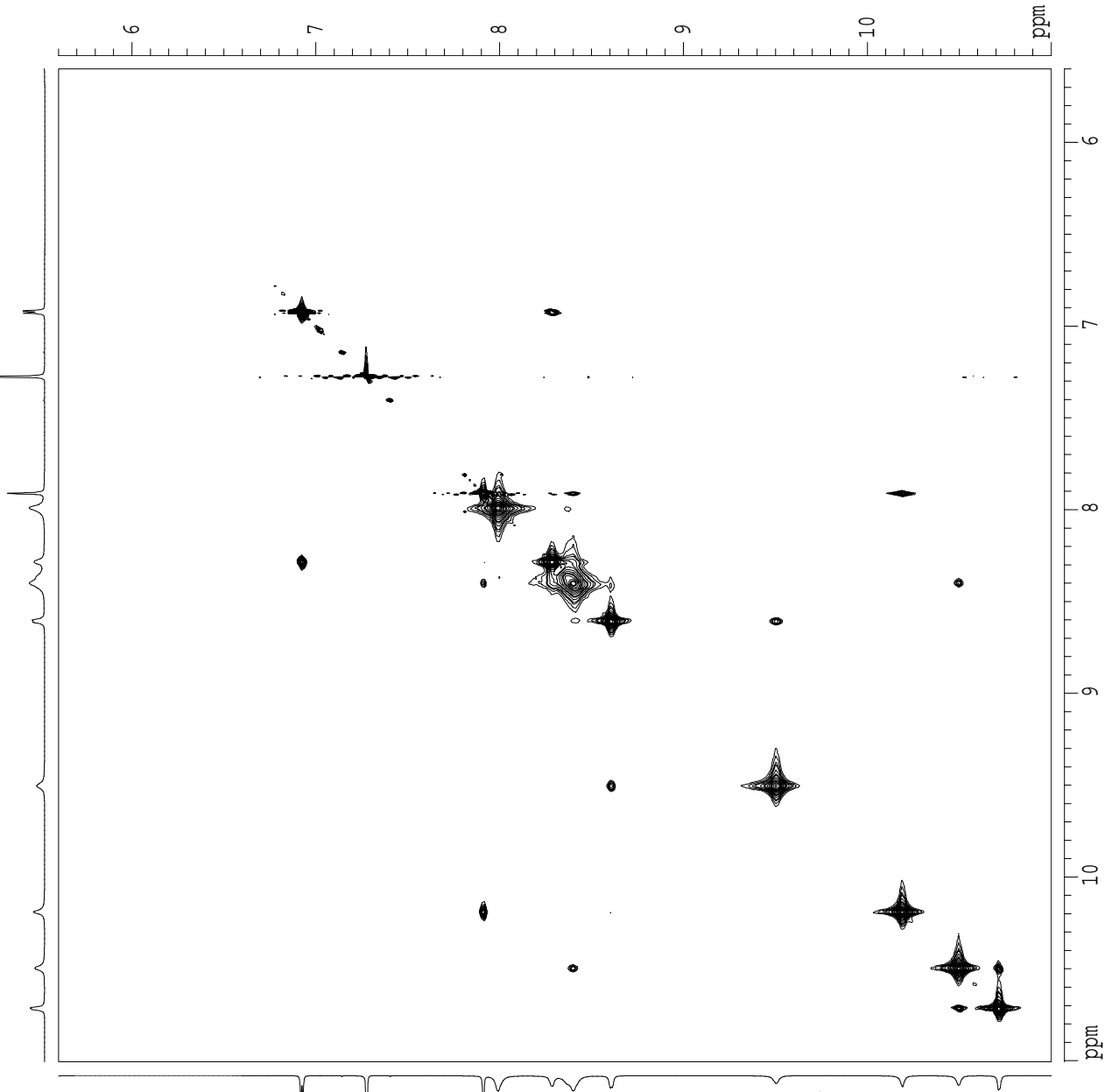
F1 - Processing parameters

SI 1024
 MC2 States
 SF 799.8064140 MHz
 WDM QSIINE
 SSB 2
 LB 0.00 Hz
 GB 0

2D NMR plot parameters

CX2 15.00 cm
 CX1 15.00 cm
 F2PLO 11.006 ppm
 F2LO 8802.76 Hz
 F2PHI 5.600 ppm
 F2HI 4478.60 Hz
 F1PLO 11.000 ppm
 F1LO 8797.87 Hz
 F1PHI 5.600 ppm
 F1HI 4478.92 Hz
 F2PPMCM 0.36043 ppm/cm
 F2HZCM 288.27753 Hz/cm
 F1PPMCM 0.36000 ppm/cm
 F1HZCM 287.93030 Hz/cm

800 MHz NOESY Spectrum of **1c** in CDCl₃
 400 ms mixing time
 268 K (-5 °C), 8 mM



Supporting Information

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Current Data Parameters
 USER slevin
 NAME SL-7-213-800-H
 EXPNO 4
 PROCNO 1

F2 - Acquisition Parameters

Date_ 20070122
 Time 0.00
 INSTRUM varian
 PROBDH 40:5mmrbroadban
 PULPROG noesyh2o_pfg_800_pln
 TD 4096
 SOLVENT CDCl3
 NS 16
 DS 64
 SMH 11001.101 Hz
 FIDRES 2.685816 Hz
 AQ 0.1862132 sec
 RG 128
 DW 45.450 usec
 DE 6.00 usec
 TE 268.5 K

F1 - Acquisition Parameters

ND0 1
 TD 1024
 SFO1 799.8107 MHz
 FIDRES 10.743262 Hz
 SW 13.755 ppm
 FmMODE undefined

F2 - Processing Parameters

SI 2048
 SF 799.8064140 MHz
 WDW QSINE
 SSB 2
 LB 0.00 Hz
 GB 0
 PC 1.40

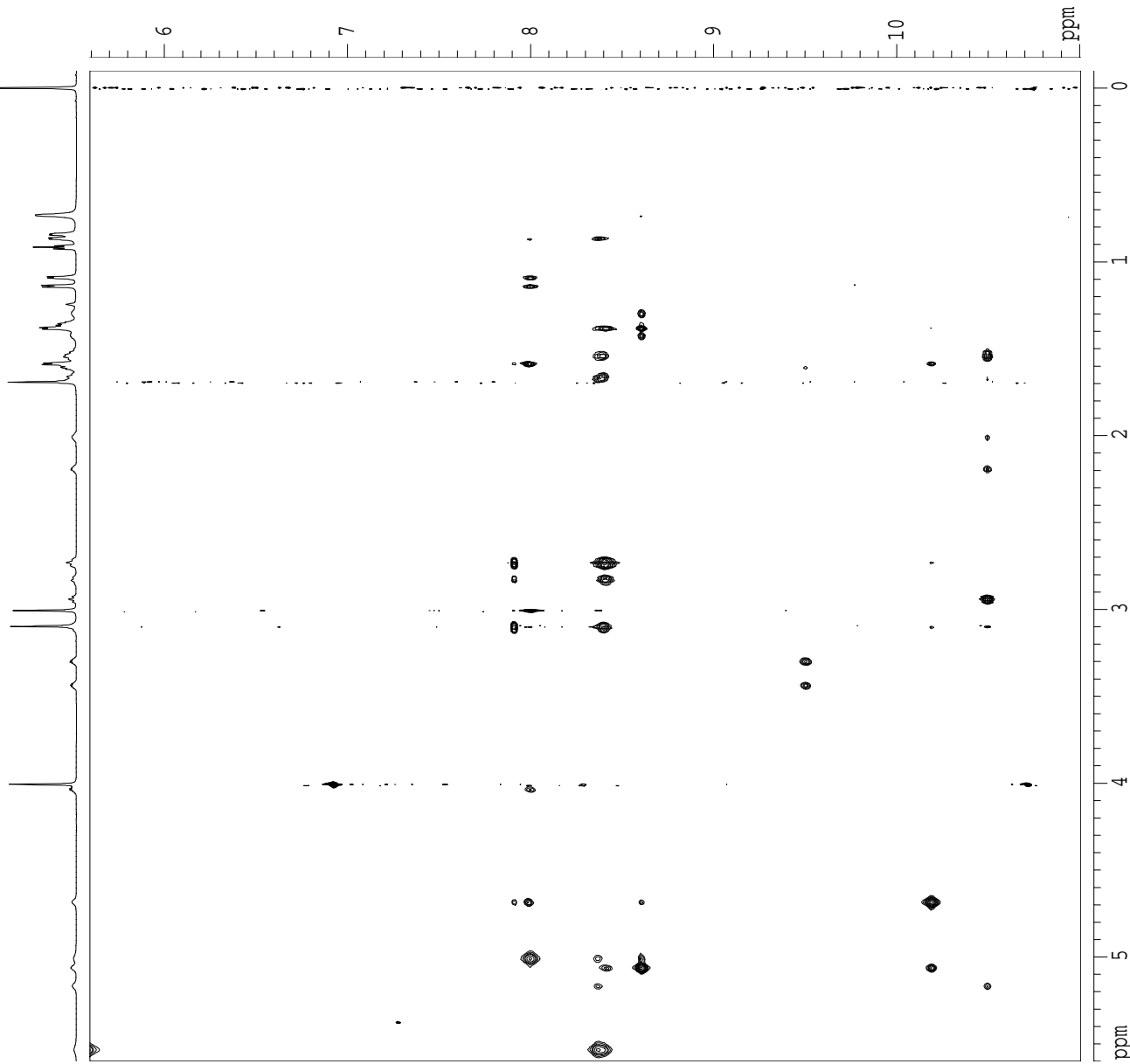
F1 - Processing Parameters

SI 1024
 MC2 States
 SF 799.8064140 MHz
 WDW QSINE
 SSB 2
 LB 0.00 Hz
 GB 0

2D NMR plot parameters

CX2 15.00 cm
 CX1 15.00 cm
 F2PLO 5.600 ppm
 F2LO 4478.92 Hz
 F2PHI -0.100 ppm
 F2HI -79.98 Hz
 F1PLO 11.006 ppm
 F1LO 8802.76 Hz
 F1PHI 5.593 ppm
 F1HI 4473.23 Hz
 F2PPMCM 0.38000 ppm/cm
 F2HZCM 303.92645 Hz/cm
 F1PPMCM 0.36088 ppm/cm
 F1HZCM 288.63562 Hz/cm

800 MHz NOESY Spectrum of **1c** in CDCl₃
 400 ms mixing time
 268 K (-5 °C), 8 mM



Current Data Parameters
 USER slewin
 NAME SL-7-213-800-H
 EXPNO 4
 PROCNO 1

F2 - Acquisition Parameters

Date_ 20070122
 Time 0.00
 INSTRUM varian
 PROBHD 40:5mmrbroadban
 PULPROG noesyh2o_pfg_800_pln
 TD 4096
 SOLVENT CDCl3
 NS 16
 DS 64
 SWH 11001.101 Hz
 FIDRES 2.685816 Hz
 AQ 0.1862132 sec
 RG 128
 DW 45.450 usec
 DE 6.00 usec
 TE 268.5 K

F1 - Acquisition Parameters

ND0 1
 TD 1024
 SFO1 799.8107 MHz
 FIDRES 10.743262 Hz
 SW 13.755 ppm
 F1MODE undefined

F2 - Processing parameters

SI 2048
 SF 799.8064140 MHz
 MDW QSINE
 SSB 2
 LB 0.00 Hz
 GB 0
 PC 1.40

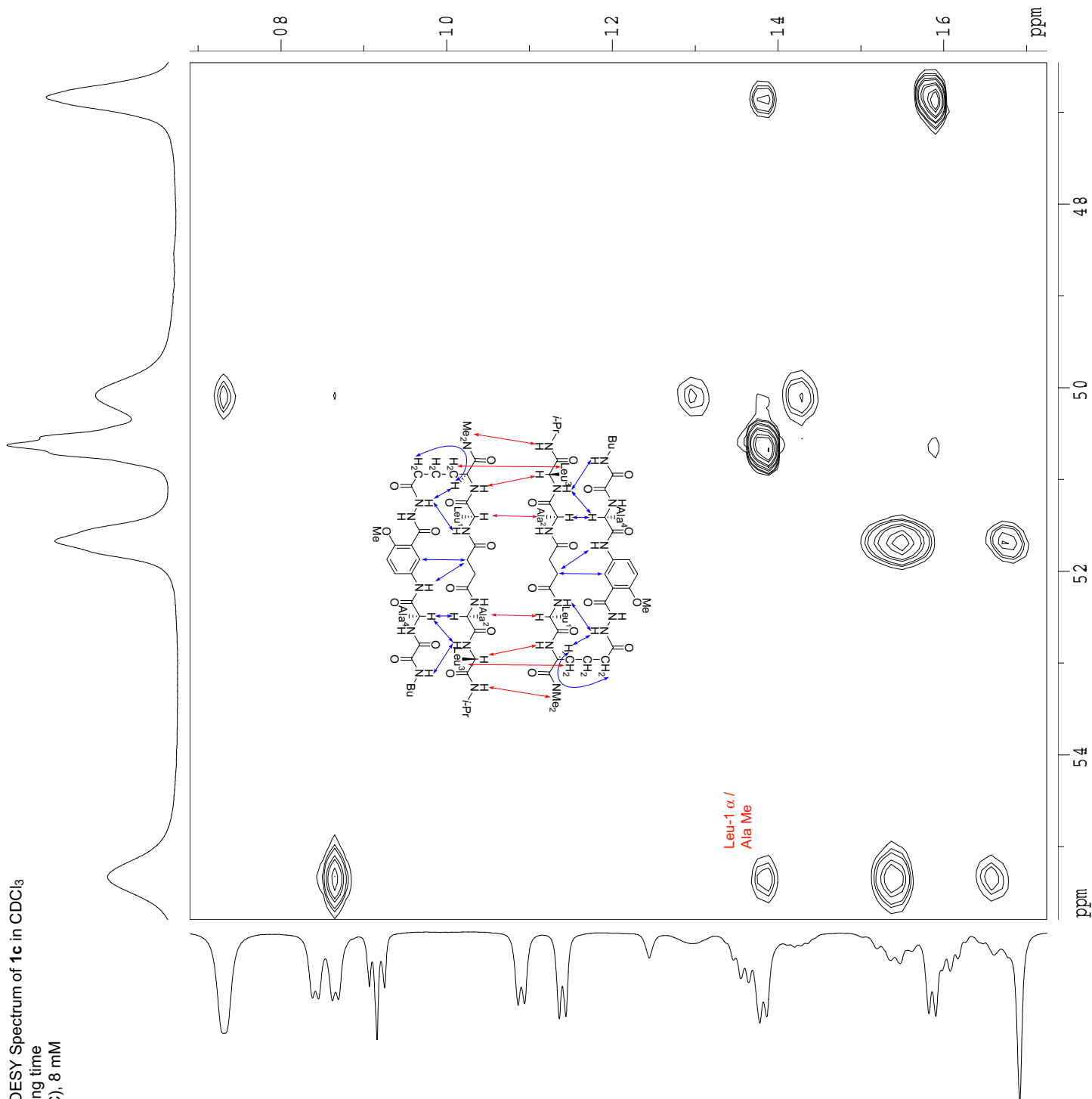
F1 - Processing parameters

SI 1024
 MC2 States
 SF 799.8064140 MHz
 MDW QSINE
 SSB 2
 LB 0.00 Hz
 GB 0

2D NMR plot parameters

CX2 15.00 cm
 CX1 15.00 cm
 F2PLO 5.579 ppm
 F2LO 4462.48 Hz
 F2PHI 4.646 ppm
 F2HI 3715.83 Hz
 F1PLO 1.724 ppm
 F1LO 1379.17 Hz
 F1PHI 0.690 ppm
 F1HI 551.93 Hz
 F2PPMCM 0.06224 ppm/cm
 F2HZCM 49.77710 Hz/cm
 F1PPMCM 0.06895 ppm/cm
 F1HZCM 55.14874 Hz/cm

800 MHz NOESY Spectrum of **1c** in CDCl₃
 400 ms mixing time
 268 K (-5 °C), 8 mM



Supporting Information

Current Data Parameters
 USER slewin
 NAME SL-7-213-800-H
 EXPNO 4
 PROCNO 1

F2 - Acquisition Parameters

Date_ 20070122
 Time_ 0.00
 INSTRUM varian
 PROBHD 40:5mmBroadban
 PULPROG noesyh2o_pfg_800_pln
 TD 4096
 SOLVENT CDCl3
 NS 16
 DS 64
 SWH 11001.101 Hz
 FIDRES 2.685816 Hz
 AQ 0.1862132 sec
 RG 128
 DW 45.450 usec
 DE 6.00 usec
 TE 288.5 K

F1 - Acquisition Parameters

ND0 1
 TD 1024
 SF01 799.8107 MHz
 FIDRES 10.743262 Hz
 SW 13.755 ppm
 FMODE undefined

F2 - Processing parameters

SI 2048
 SF 799.8064140 MHz
 WDW QSIGNE
 SSB 2
 LB 0.00 Hz
 GB 0
 PC 1.40

F1 - Processing parameters

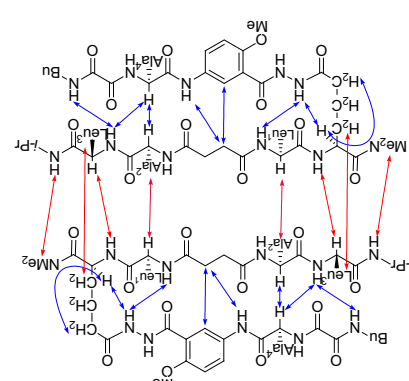
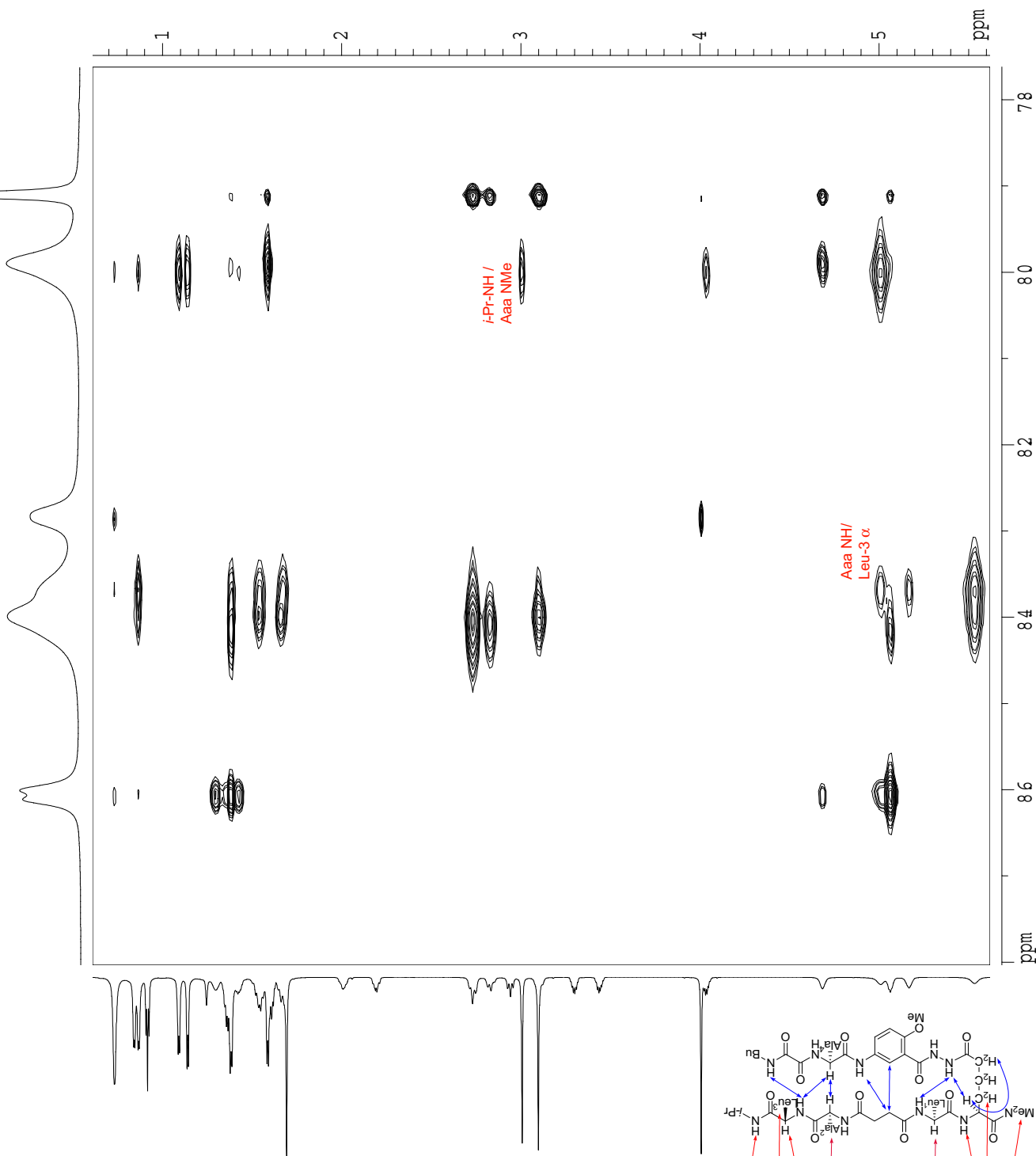
SI 1024
 MC2 States
 SF 799.8064140 MHz
 WDW QSIGNE
 SSB 2
 LB 0.00 Hz
 GB 0

2D NMR plot parameters

CX2 15.00 cm
 CX1 15.00 cm
 F2PLO 8.803 ppm
 F2LO 7040.86 Hz
 F2PHI 7.762 ppm
 F2HI 6208.26 Hz
 F1PLO 5.620 ppm
 F1LO 4494.71 Hz
 F1PHI 0.609 ppm
 F1HI 487.48 Hz
 F2PMCM 0.06940 ppm/cm
 F2HZCM 55.50684 Hz/cm
 F1PMCM 0.33402 ppm/cm
 F1HZCM 267.14911 Hz/cm

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800 MHz NOESY Spectrum of **1c** in CDCl₃
 400 ms mixing time
 268 K (-5 °C), 8 mM



Current Data Parameters
 USER slevin
 NAME SL-7-213-800-H
 EXPNO 4
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20070122
 Time 0.00
 INSTRUM varian
 PROBHD 40:5mmbrdabban
 PULPROG noesyh2o_pfg_800_p1n
 TD 4096

SOLVENT CDCl3
 NS 16
 DS 64
 SWH 11001.101 Hz
 FIDRES 2.685816 Hz
 AQ 0.1862132 sec
 RG 128
 DW 45.450 usec
 DE 6.00 usec
 TE 268.5 K

F1 - Acquisition parameters
 NDO 1
 TD 1024
 SFO1 799.8107 MHz
 FIDRES 10.743262 Hz
 SW 13.755 ppm
 FMODE undefined

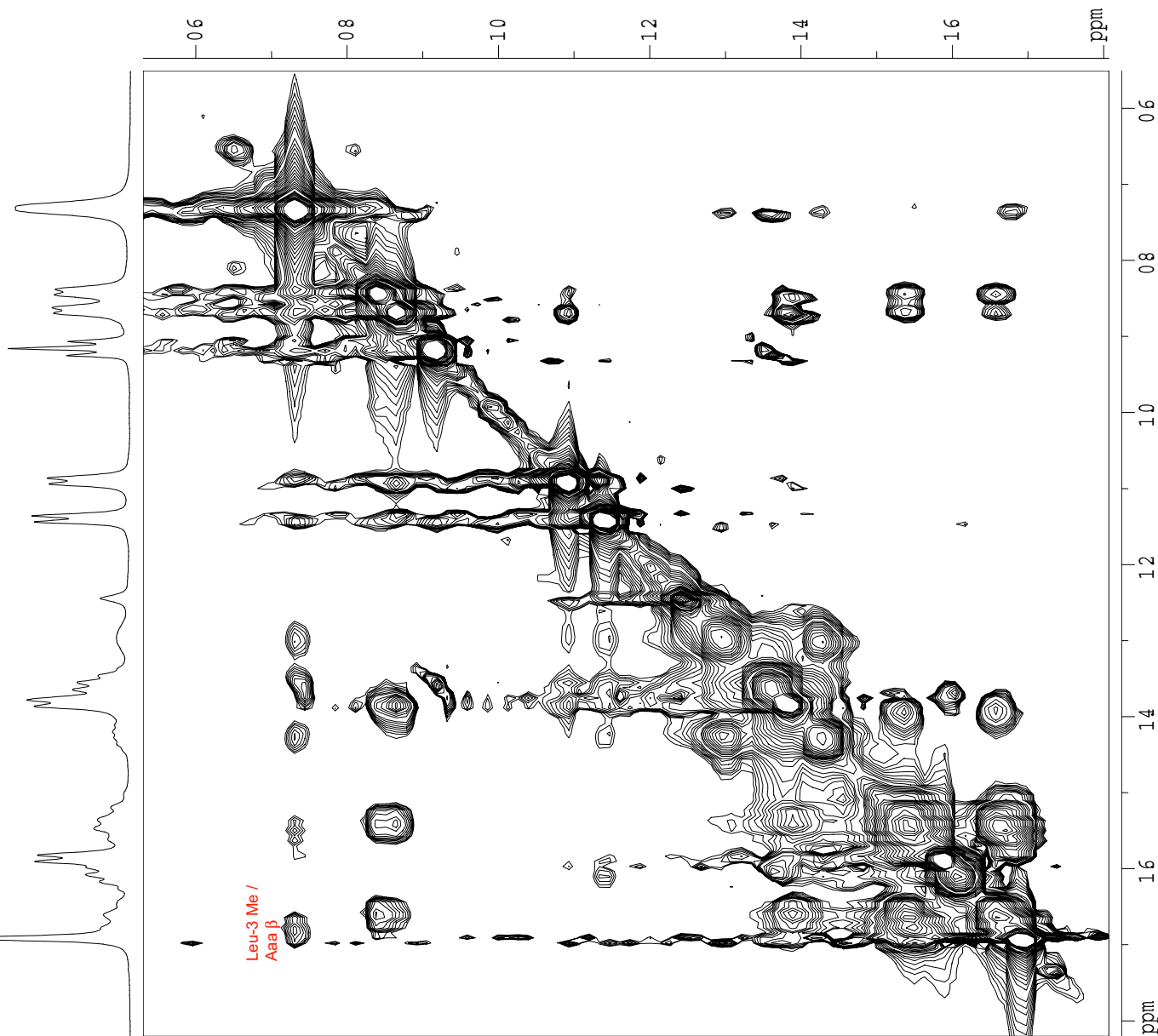
F2 - Processing parameters
 SI 2048
 SF 799.8064140 MHz
 WDW QSINE
 SSB 2
 LB 0.00 Hz
 GB 0
 PC 1.40

F1 - Processing parameters
 SI 1024
 MC2 States
 SF 799.8064140 MHz
 WDW QSINE
 SSB 2
 LB 0.00 Hz
 GB 0

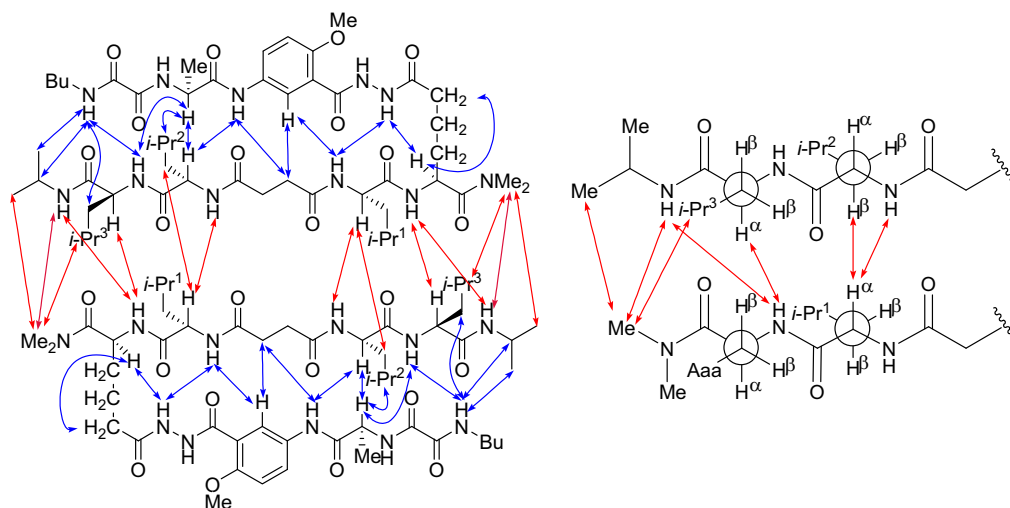
2D NMR plot parameters

CX2 15.00 cm
 CX1 15.00 cm
 F2PLO 1.820 ppm
 F2LO 1455.71 Hz
 F2PHI 0.551 ppm
 F2HI 440.47 Hz
 F1PLO 1.807 ppm
 F1LO 1444.97 Hz
 F1PHI 0.531 ppm
 F1HI 424.36 Hz
 F2PPMCM 0.08462 ppm/cm
 F2HZCM 67.68256 Hz/cm
 F1PPMCM 0.08507 ppm/cm
 F1HZCM 68.04066 Hz/cm

800 MHz NOESY Spectrum of **1c** in CDCl₃
 400 ms mixing time
 268 K (-5 °C), 8 mM



Spectroscopic DATA for the compound **1d**
(20 mM, CDCl₃ 268K)



Key NOEs assigned as *intermolecular* are represented with red arrows
Key NOEs assigned as *intramolecular* are represented with blue arrows

Key data for amino acids.

Amino acid	H _α Shift ppm	NH Shift ppm	³ J _{NHα} Hz
Aaa	5.16	8.67	8.7
R ₁ = Leu ¹	5.54	8.39	8.0
R ₂ = Leu ²	4.94	8.31	9.2
R ₃ = Leu ³	4.97	8.69	10.0
R ₄ = Ala	4.79	7.98	7.4

Amino adipic acid (Aaa) δ proton resonances.

pro-R: 2.91 ppm, t, (*overlap*)

pro-S: 2.19 ppm, td, (*J*₁ = 11.5 Hz; *J*₂ = 7.0 Hz)

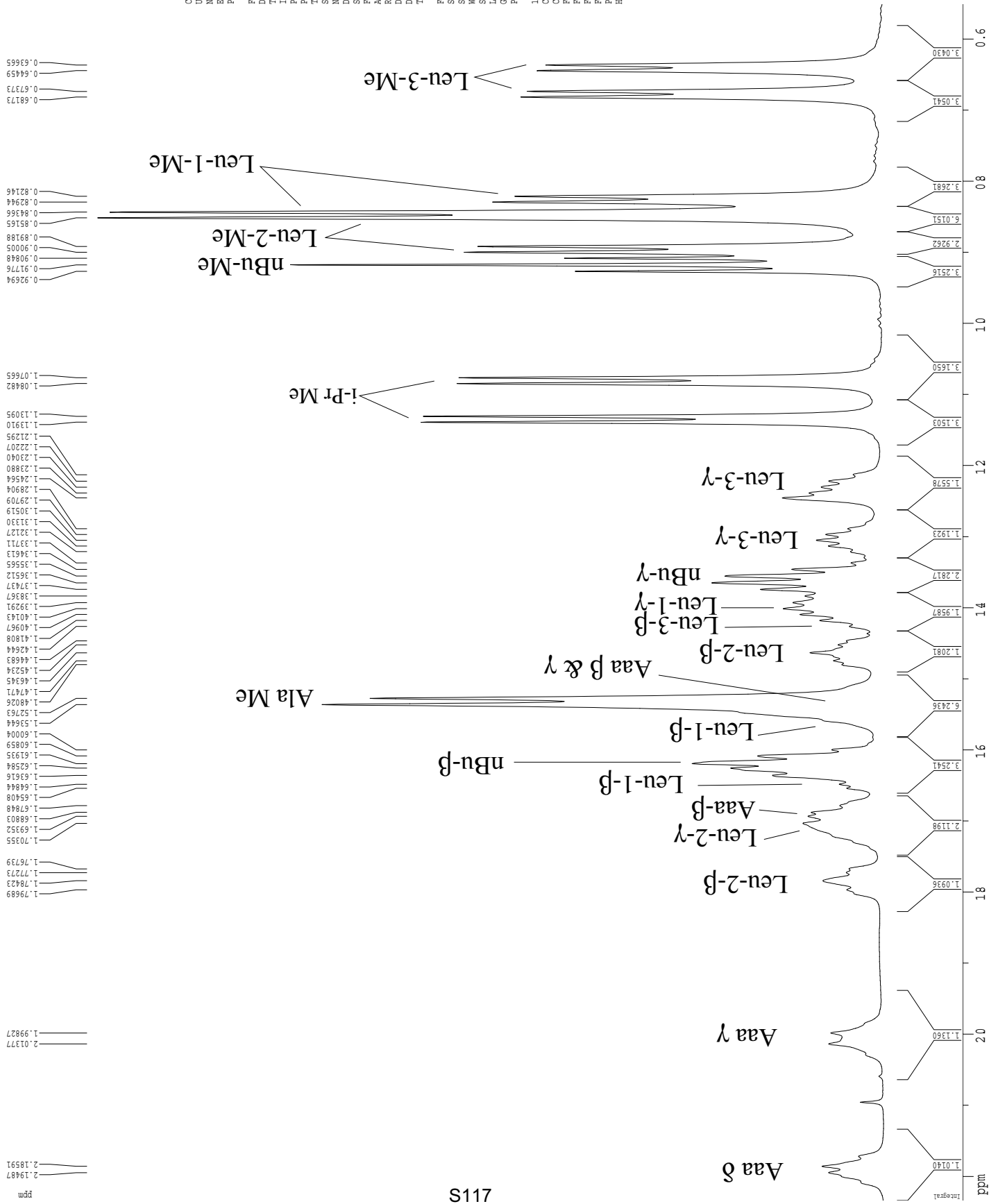
anisotropy = 0.72ppm

Key data for other NH protons.

Proton	NH Shift ppm	<i>J</i> Hz
Ar-NH	10.20	-
Hydrazide Ar	10.57	7.4
Hydrazide Aaa	10.43	7.4
Bu-NH	9.62	broad
<i>i</i> -Pr-NH	8.03	7.4

ESI MS *m/z* for C₅₀H₈₄N₁₁O₁₂ [M+H]⁺ calcd 1030.63, found 1030.50.

800 MHz ¹H NMR Spectrum of **1d** in CDCl₃
268 K (-5 °C), 20 mM



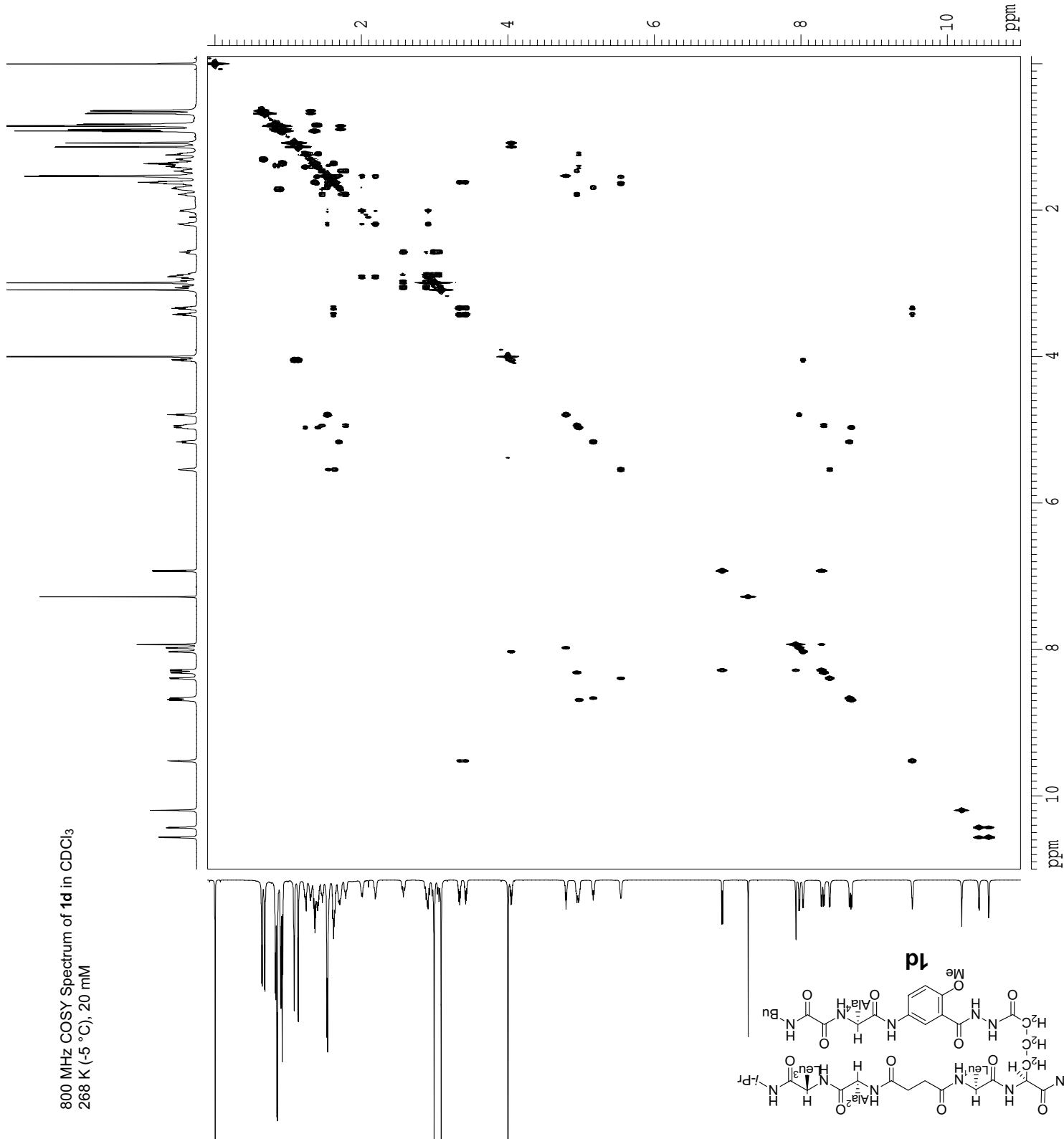
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 USER slevin
 NAME SL-7-20-800-H
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20070117
 Time 0.00
 INSTRUM varian
 PROBHD 40:5mmbrdcaan
 PULPROG zgpg30
 TD 65506
 SFO 500.135
 SOLVENT cdcl3
 NS 32
 DS 4
 SWH 11001.101 Hz
 FIDRES 0.199998 Hz
 AQ 2.5000727 sec
 RG 8192
 DW 45.450 usec
 DE 4.50 usec
 TE 268.5 K

F2 - Processing parameter
 SI 32768
 SF 799.8064113 MHz
 EN
 GB 0
 CB 0
 SC 0
 PC 2.00

1D NMR plot parameters
 CX 22.80 cm
 CY 15.00 cm
 F1P 2.234 ppm
 F1 1786.71 Hz
 F2P 0.551 ppm
 F2 441.08 Hz
 PPMCM 0.07379 ppm/cm
 HZCM 59.03900 Hz/cm

800 MHz COSY Spectrum of **1d** in CDCl₃
 268 K (-5 °C), 20 mM



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Supporting Information

Current Data Parameters
 USER slevin
 NAME SL-7-202-800-H
 EXPNO 3
 PROCNO 1

F2 - Acquisition Parameters

Date_ 20070117
 Time 0.00
 INSTRUM varian
 PROBHD 40:5mmrbroadban
 PULPROG gcosy
 TD 4096
 SOLVENT cdcl3
 NS 4
 DS 64
 SWH 11001.101 Hz
 FIDRES 2.685816 Hz
 AQ 0.1843700 sec
 RG 4096
 DW 45.450 usec
 DE 231.43 usec
 TE 268.5 K

F1 - Acquisition Parameters

ND0 1
 TD 512
 SFO1 799.8107 MHz
 FIDRES 21.486525 Hz
 SW 13.755 ppm
 F1MODE undefined

F2 - Processing parameters

SI 2048
 SF 799.8064113 MHz
 WDW SINE
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.40

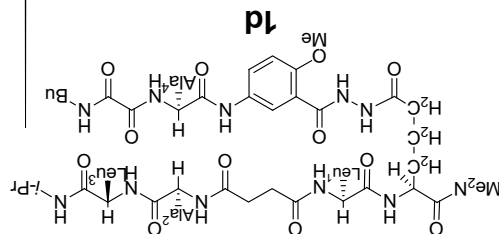
F1 - Processing parameters

SI 512
 MC2 QF
 SF 799.8064113 MHz
 WDW SINE
 SSB 0
 LB 0.00 Hz
 GB 0

2D NMR plot parameters

CX2 15.00 cm
 CX1 15.00 cm
 F2PLO 11.000 ppm
 F2LO 8797.87 Hz
 F2PHI -0.100 ppm
 F2HI -79.98 Hz
 F1PLO 11.000 ppm
 F1LO 8797.87 Hz
 F1PHI -0.100 ppm
 F1HI -79.98 Hz
 F2PPMCM 0.74000 ppm/cm
 F2HZCM 591.85669 Hz/cm
 F1PPMCM 0.74000 ppm/cm
 F1HZCM 591.85669 Hz/cm

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Current Data Parameters
 USER slevin
 NAME SL-7-202-800-H
 EXPNO 3
 PROCNO 1

F2 - Acquisition Parameters

Date_ 20070117
 Time 0.00
 INSTRUM varian
 PROBHD 40:5mm broadband
 PULPROG gcpsy
 TD 4096
 SOLVENT cdcl3
 NS 4
 DS 64
 SWH 11001.101 Hz
 FIDRES 2.685816 Hz
 AQ 0.1843700 sec
 RG 4096
 DW 45.450 usec
 DE 231.43 usec
 TE 268.5 K

F1 - Acquisition parameters

ND0 1
 TD 512
 SF01 799.8107 MHz
 FIDRES 21.486525 Hz
 SW 13.755 ppm
 F1MODE undefined

F2 - Processing parameters

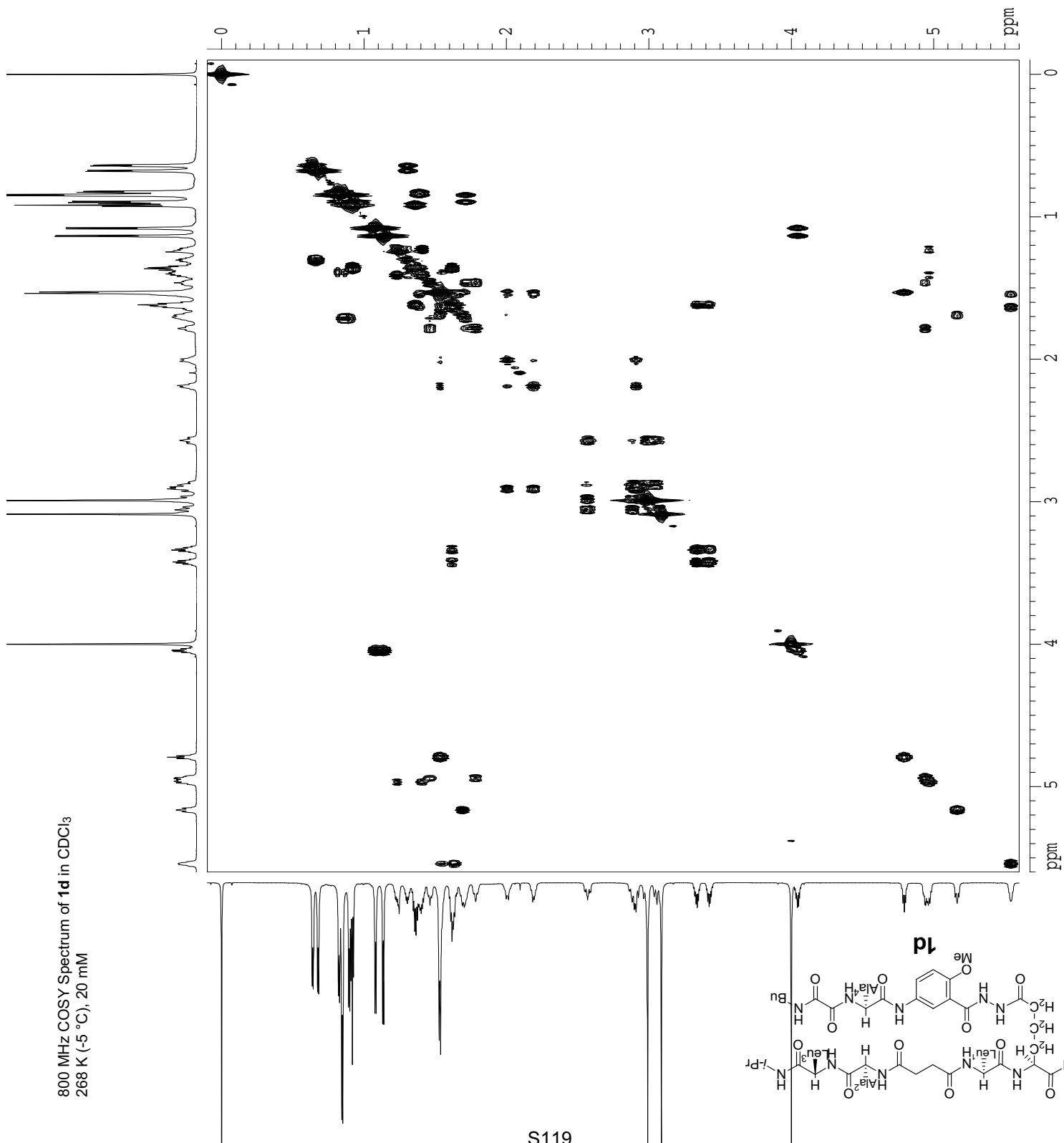
SI 2048
 SF 799.8064113 MHz
 SINE
 WDW 0
 LB 0.00 Hz
 GB 0
 PC 1.40

F1 - Processing parameters

SI 512
 MC2 QF
 SF 799.8064113 MHz
 SINE
 WDW 0
 LB 0.00 Hz
 GB 0

2D NMR plot parameters

CX2 15.00 cm
 CX1 15.00 cm
 F2PLO 5.600 ppm
 F2LO 4478.92 Hz
 F2PHI -0.100 ppm
 F2HT -79.98 Hz
 F1PLO 5.600 ppm
 F1LO 4478.92 Hz
 F1PHI -0.100 ppm
 F1HT -79.98 Hz
 F2PPMCW 0.38000 ppm/cm
 F2HZCM 303.92645 Hz/cm
 F1PPMCW 0.38000 ppm/cm
 F1HZCM 303.92645 Hz/cm



800 MHz COSY Spectrum of **1d** in CDCl₃
 268 K (-5 °C), 20 mM

Supporting Information

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Current Data Parameters
 USER slewin
 NAME SL-7-202-800-H
 EXPNO 3
 PROCNO 1

F2 - Acquisition Parameters

Date 20070117
 Time 0.00
 INSTRUM varian
 PROBHD 40:5mmBroadban
 PULPROG gcosy
 TD 4096
 SOLVENT cdcl3
 NS 4
 DS 64
 SWH 11001.101 Hz
 FIDRES 2.685816 Hz
 AQ 0.1843700 sec
 RG 4096
 DW 45.450 usec
 DE 231.43 usec
 TE 268.5 K

F1 - Acquisition Parameters

ND0 1
 TD 512
 SFO1 799.8107 MHz
 FIDRES 21.486525 Hz
 SW 13.755 ppm
 F1MODE undefined

F2 - Processing parameters

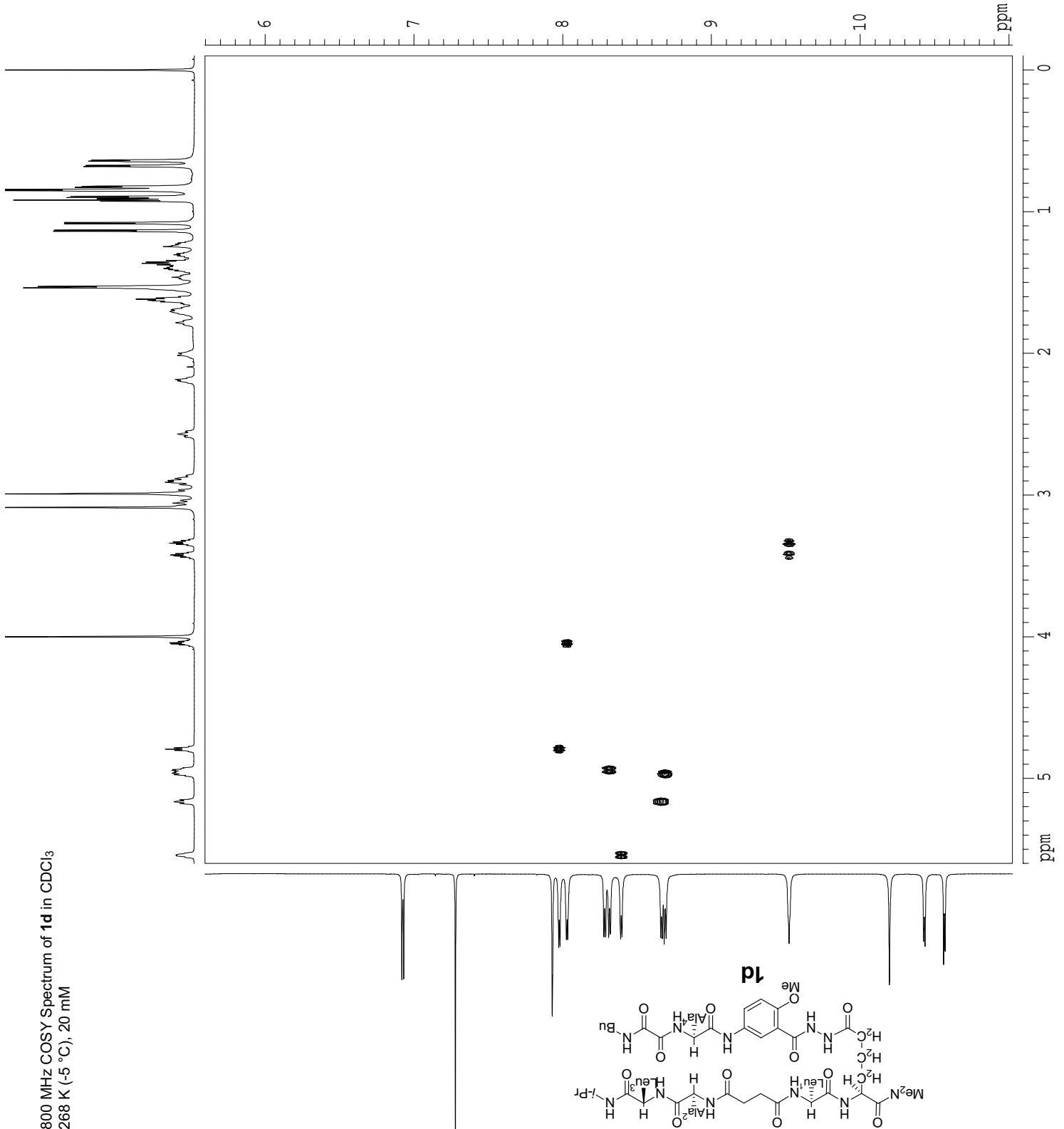
SI 2048
 SF 799.8064113 MHz
 WDW SINE
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.40

F1 - Processing parameters

SI 512
 MC2 OF
 SF 799.8064113 MHz
 WDW SINE
 SSB 0
 LB 0.00 Hz
 GB 0

2D NMR plot parameters

CX2 15.00 cm
 CX1 15.00 cm
 F2PLO 5.600 ppm
 F2LO 4478.92 Hz
 F2PHI -0.100 ppm
 F2HI -79.98 Hz
 F1PLO 11.023 ppm
 F1LO 8816.19 Hz
 F1PHI 5.596 ppm
 F1HI 4475.91 Hz
 F2PPMCM 0.38000 ppm/cm
 F2HZCM 303.92645 Hz/cm
 F1PPMCM 0.36178 ppm/cm
 F1HZCM 289.35184 Hz/cm



Current Data Parameters
 USER slevin
 NAME SL-7-202-800-H
 EXNO 3
 PROCNO 1

F2 - Acquisition Parameters

Date_ 20070117
 Time_ 0.00
 INSTRUM varian
 PROBHD 40:5mmbroadban
 PULPROG gcosy
 TD 4096
 SOLVENT cdcl3
 NS 4
 DS 64
 SWH 11001.101 Hz
 FIDRES 2.685816 Hz
 AQ 0.1843700 sec
 RG 4096
 DW 45.450 usec
 DE 231.43 usec
 TE 268.5 K

F1 - Acquisition Parameters

ND0 1
 TD 512
 SF01 799.8107 MHz
 FIDRES 21.486525 Hz
 SW 13.755 ppm
 F1MODE undefined

F2 - Processing parameters

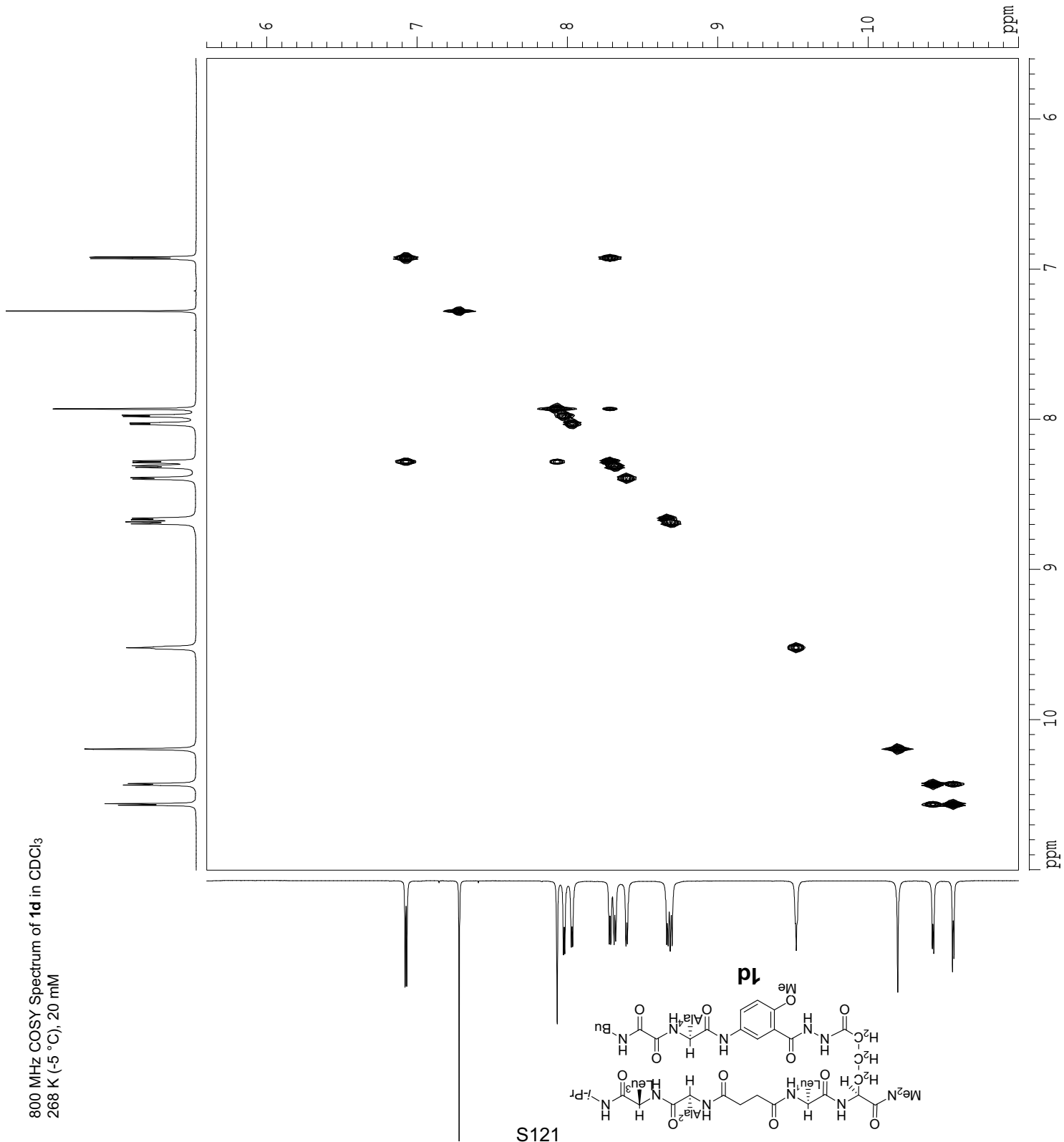
SI 2048
 SF 799.8064113 MHz
 SINE
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.40

F1 - Processing parameters

SI 512
 MC2 QF
 SF 799.8064113 MHz
 SINE
 SSB 0
 LB 0.00 Hz
 GB 0

2D NMR plot parameters

CX2 15.00 cm
 CX1 15.00 cm
 F2FLO 11.003 ppm
 F2LO 8800.08 Hz
 F2PHI 5.596 ppm
 F2HI 4475.91 Hz
 F1FLO 11.000 ppm
 F1LO 8797.87 Hz
 F1PHI 5.600 ppm
 F1HI 4478.92 Hz
 F2PPMCM 0.36043 ppm/cm
 F2HZCM 288.27753 Hz/cm
 F1PPMCM 0.36000 ppm/cm
 F1HZCM 287.93030 Hz/cm



800 MHz COSY Spectrum of **1d** in CDCl₃
 268 K (-5 °C), 20 mM

Supporting Information

Current Data Parameters
 USER slevin
 NAME SL-7-202-800-H
 EXPNO 3
 PROCNO 1

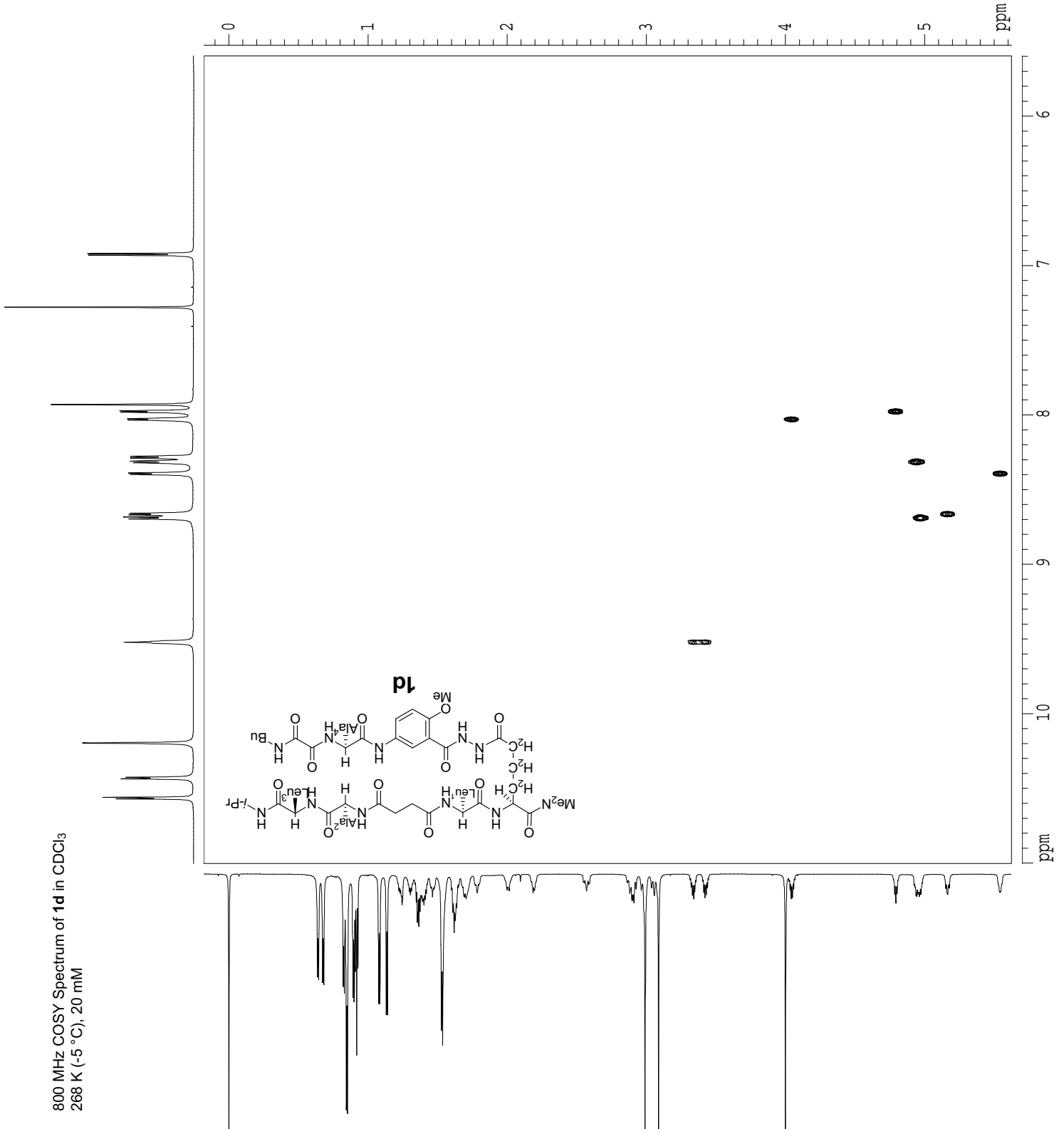
F2 - Acquisition Parameters
 Date_ 20070117
 Time_ 0.00
 INSTRUM varian
 PROBDH 40:5mmbroadban
 PULPROG gocsy
 TD 4096
 SOLVENT cdc13
 NS 4
 DS 64
 SWH 11001.101 Hz
 FIDRES 2.685816 Hz
 AQ 0.1843700 sec
 RG 4096
 DW 45.450 usec
 DE 231.43 usec
 TE 268.5 K

F1 - Acquisition Parameters
 ND0 1
 TD 512
 SFO1 799.8107 MHz
 FIDRES 21.486525 Hz
 SW 13.755 ppm
 F1MODE undefined

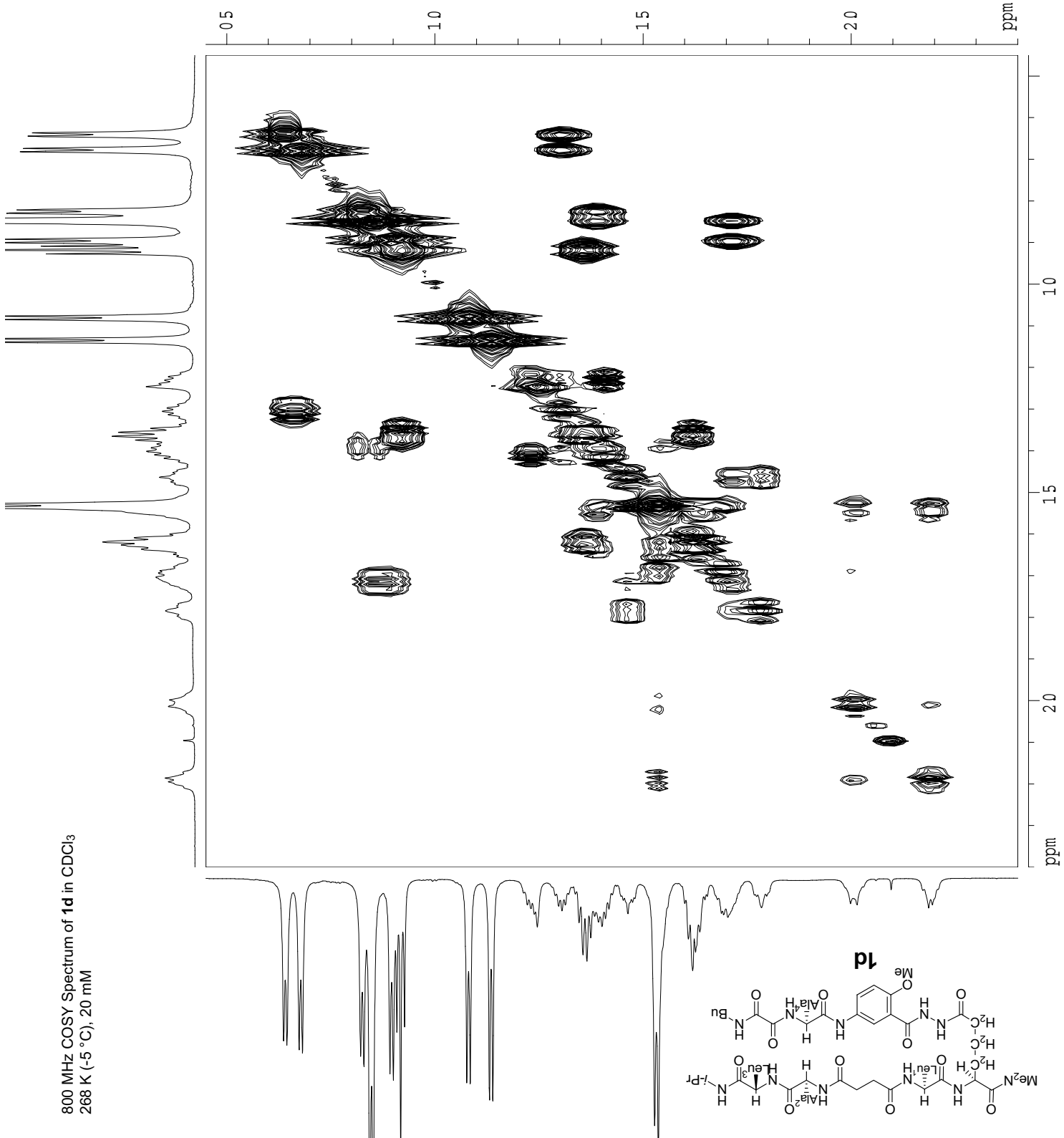
F2 - Processing parameters
 SI 2048
 SF 799.8064113 MHz
 WDW SINE
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.40

F1 - Processing parameters
 SI 512
 MC2 QF
 SF 799.8064113 MHz
 WDW SINE
 SSB 0
 LB 0.00 Hz
 GB 0

S. Levin and J. S. Nowick
 2D NMR plot parameters
 CX2 15.00 cm
 CX1 15.00 cm
 F2PLO 11.003 ppm
 F2LO 8800.08 Hz
 F2PHI 5.596 ppm
 F2HI 4475.91 Hz
 F1PLO 5.623 ppm
 F1LO 4497.40 Hz
 F1PHI -0.180 ppm
 F1HI -143.69 Hz
 F2PPMCM 0.36043 ppm/cm
 F1PPMCM 288.27753 Hz/cm
 F1HZCM 0.38685 ppm/cm
 F1HZCM 309.40594 Hz/cm



800 MHz COSY Spectrum of **1d** in CDCl₃
268 K (-5 °C), 20 mM



Supporting Information

Current Data Parameters
 USER slewin
 NAME SL-7-202-800-H
 EXPNO 3
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20070117
 Time_ 0.00
 INSTRUM varian
 PROBHD 40:5mm broadband
 PULPROG gcpsy
 TD 4096
 SOLVENT cdcl3
 NS 4
 DS 64
 SWH 11001.101 Hz
 FIDRES 2.685816 Hz
 AQC 0.1843700 sec
 RG 4096
 DW 45.450 usec
 DE 231.43 usec
 TE 268.5 K

F1 - Acquisition parameters
 ND0 1
 TD 512
 SF01 799.8107 MHz
 FIDRES 21.486525 Hz
 SW 13.755 ppm
 FMODE undefined

F2 - Processing parameters
 SI 2048
 SF 799.8064113 MHz
 WDW SINE
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.40

F1 - Processing parameters
 SI 512
 MC2 QF
 SF 799.8064113 MHz
 WDW SINE
 SSB 0
 LB 0.00 Hz
 GB 0

2D NMR plot parameters
 CX2 15.00 cm
 CX1 15.00 cm
 F2PLO 2.400 ppm
 F2LO 1919.54 Hz
 F2PHI 0.450 ppm
 F2HI 359.91 Hz
 F1PLO 2.400 ppm
 F1LO 1919.54 Hz
 F1PHI 0.450 ppm
 F1HI 359.91 Hz
 F2PPMCM 0.13000 ppm/cm
 F2HZCM 103.97483 Hz/cm
 F1PPMCM 0.13000 ppm/cm
 F1HZCM 103.97483 Hz/cm

Supporting Information

S. Levin and J. S. Nowick

Current Data Parameters
 USER slevin
 NAME SL-7-202-800-H
 EXPNO 4
 PROCNO 1

F2 - Acquisition Parameters

Date_ 20070117
 Time 0.00
 INSTRUM varian
 PROBHD 40.5mm broadband
 PULPROG wgtocsy.bn
 TD 4096
 SOLVENT CDCl3
 NS 16
 DS 64
 SWH 11001.101 Hz
 FIDRES 2.685816 Hz
 AQ 0.1862132 sec
 RG 287.4
 DW 45.450 usec
 DE 6.00 usec
 TE 268.5 K

F1 - Acquisition Parameters

ND0 1
 TD 512
 SF01 799.8107 MHz
 FIDRES 21.486525 Hz
 SW 13.755 ppm
 F1MODE undefined

F2 - Processing parameters

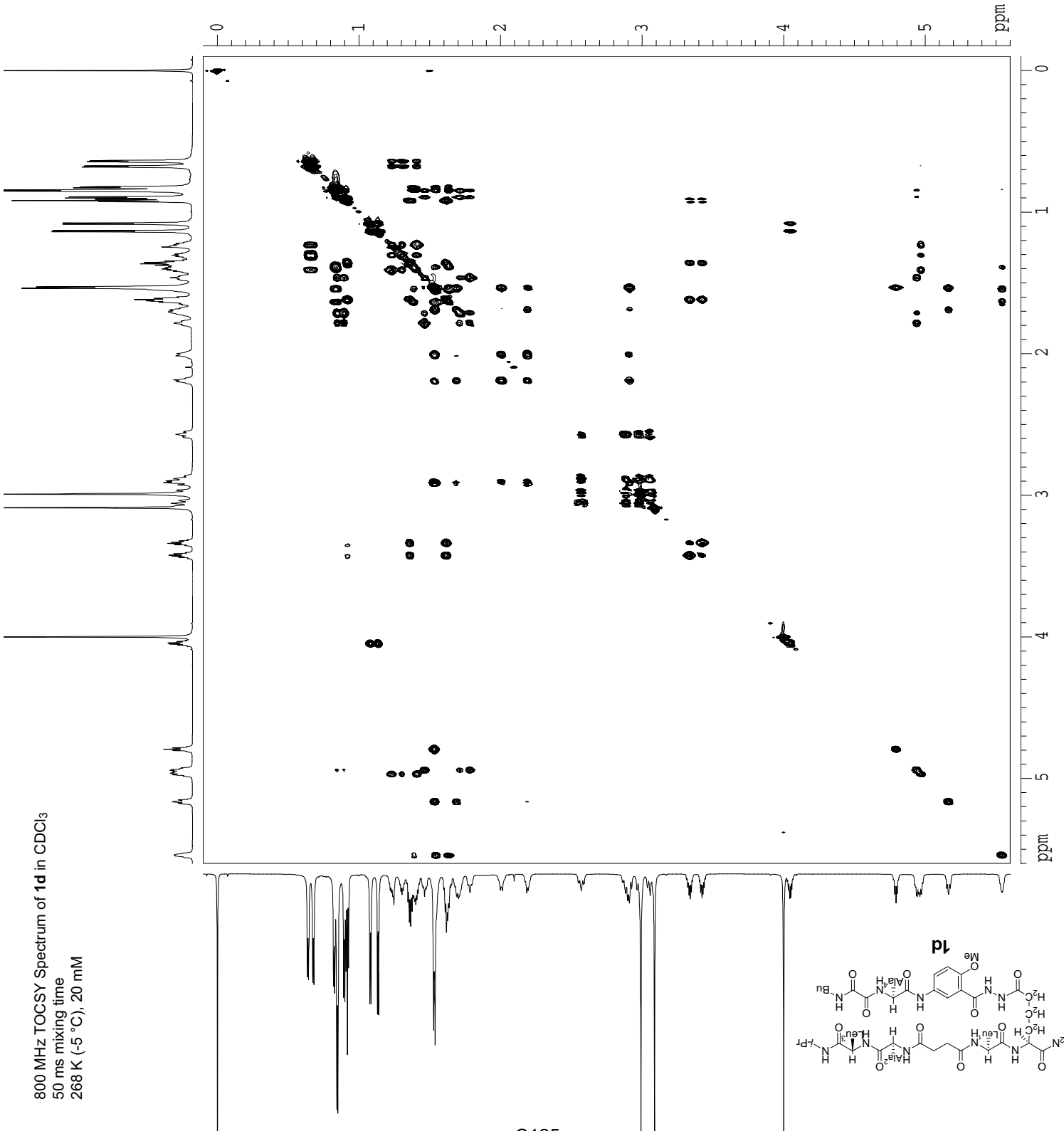
SI 2048
 SF 799.8064113 MHz
 WDW QSI
 SSB 2
 LB 0.00 Hz
 GB 0
 PC 1.40

F1 - Processing parameters

SI 1024
 MC2 States
 SF 799.8064113 MHz
 WDW QSI
 SSB 2
 LB 0.00 Hz
 GB 0

2D NMR plot parameters

CX2 15.00 cm
 CX1 15.00 cm
 F2PLO 5.600 ppm
 F2LO 4478.92 Hz
 F2PHI -0.100 ppm
 F2HI -79.98 Hz
 F1PLO 5.600 ppm
 F1LO 4478.92 Hz
 F1PHI -0.100 ppm
 F1HI -79.98 Hz
 F2PPMCM 0.38000 ppm/cm
 F2HZCM 303.92645 Hz/cm
 F1PPMCM 0.38000 ppm/cm
 F1HZCM 303.92645 Hz/cm



Supporting Information

S. Levin and J. S. Nowick

Current Data Parameters
 USER slevin
 NAME SL-7-202-800-H
 EXPNO 4
 PROCNO 1

F2 - Acquisition Parameters

Date 20070117
 Time 0.00
 INSTRUM varian
 PROBHD 40:5mmrbroadban
 PULPROG wgtocsy_bn
 TD 4096
 SOLVENT CDCl3
 NS 16
 DS 64
 SWH 11001.101 Hz
 FIDRES 2.685816 Hz
 AQ 0.1862132 sec
 RG 287.4
 DW 45.450 usec
 DE 6.00 usec
 TE 268.5 K

F1 - Acquisition Parameters

ND0 1
 TD 512
 SFO1 799.8107 MHz
 FIDRES 21.486525 Hz
 SW 13.755 ppm
 F1MODE undefined

F2 - Processing parameters

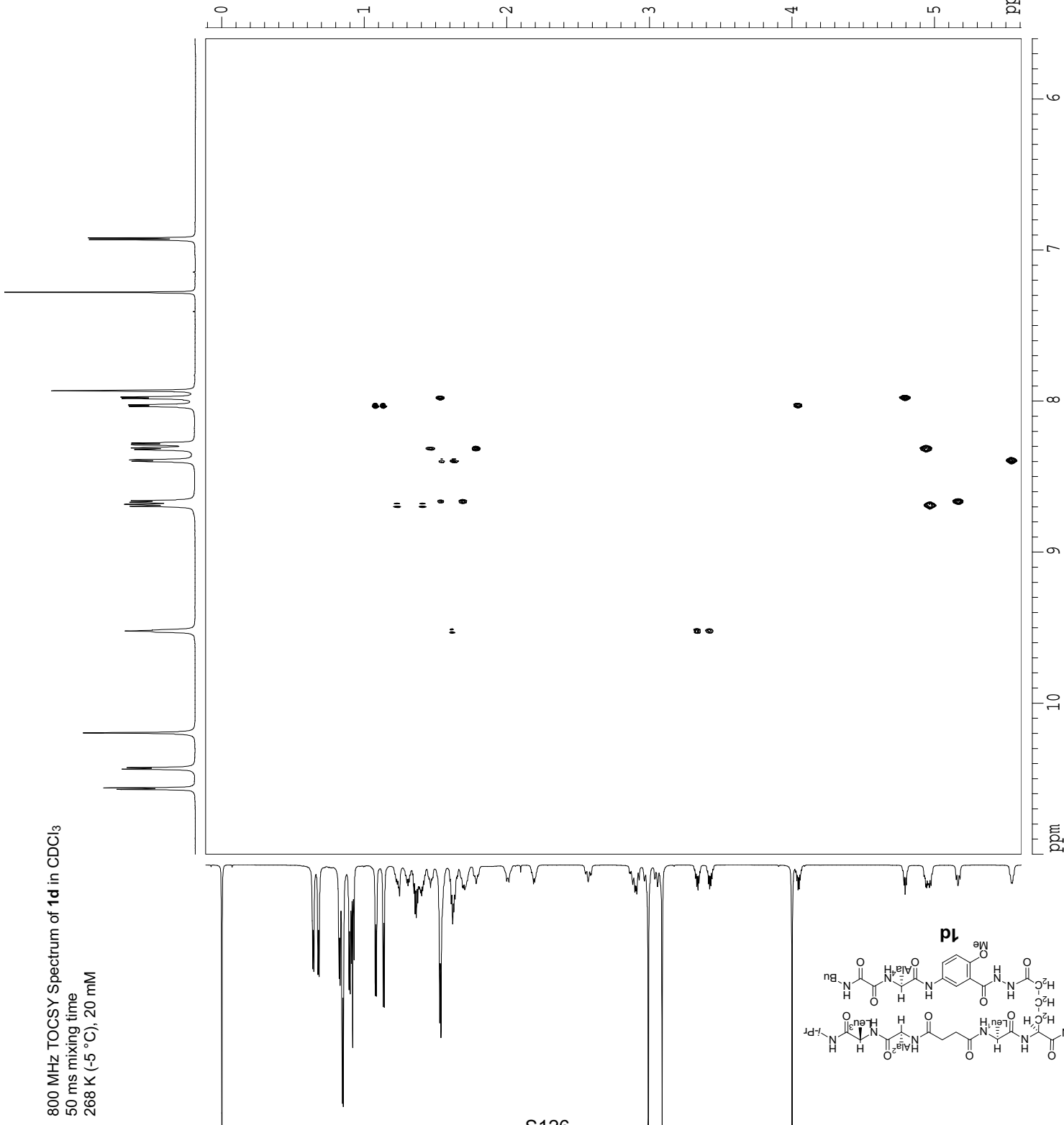
SI 2048
 SF 799.8064113 MHz
 WDW QSI
 SSB 2
 LB 0.00 Hz
 GB 0
 PC 1.40

F1 - Processing parameters

SI 1024
 MC2 States
 SF 799.8064113 MHz
 WDW QSI
 SSB 2
 LB 0.00 Hz
 GB 0

2D NMR plot parameters

CX2 15.00 cm
 CX1 15.00 cm
 F2PLO 11.000 ppm
 F2LO 8797.87 Hz
 F2PHI 5.600 ppm
 F2HI 4478.92 Hz
 F1LO 5.610 ppm
 F1PHI 4486.66 Hz
 F1HI -0.112 ppm
 F1H1 -89.97 Hz
 F2PWC1 0.36000 ppm/cm
 F2H2C1 287.93030 Hz/cm
 F1PWC1 0.38148 ppm/cm
 F1H2C1 305.10861 Hz/cm



Supporting Information

S. Levin and J. S. Nowick

Current Data Parameters

USER slevin
 NAME SL-7-202-800-H
 EXPNO 4
 PROCNO 1

F2 - Acquisition Parameters

Date_ 20070117
 Time_ 0.00
 INSTRUM varian
 PROBHD 40:5mmrbroadban
 PULPROG wgtocsy_bn
 TD 4096
 SOLVENT CDCl3
 NS 16
 DS 64
 SWH 11001.101 Hz
 FIDRES 2.685816 Hz
 AQ 0.1862132 sec
 RG 287.4
 DW 45.450 usec
 DE 6.00 usec
 TE 268.5 K

F1 - Acquisition parameters

ND0 1
 TD 512
 SF01 799.8107 MHz
 FIDRES 21.486525 Hz
 SW 13.755 ppm
 F1MODE undefined

F2 - Processing parameters

SI 2048
 SF 799.8064113 MHz
 WDW QSI
 SSB 2
 LB 0.00 Hz
 GB 0
 PC 1.40

F1 - Processing parameters

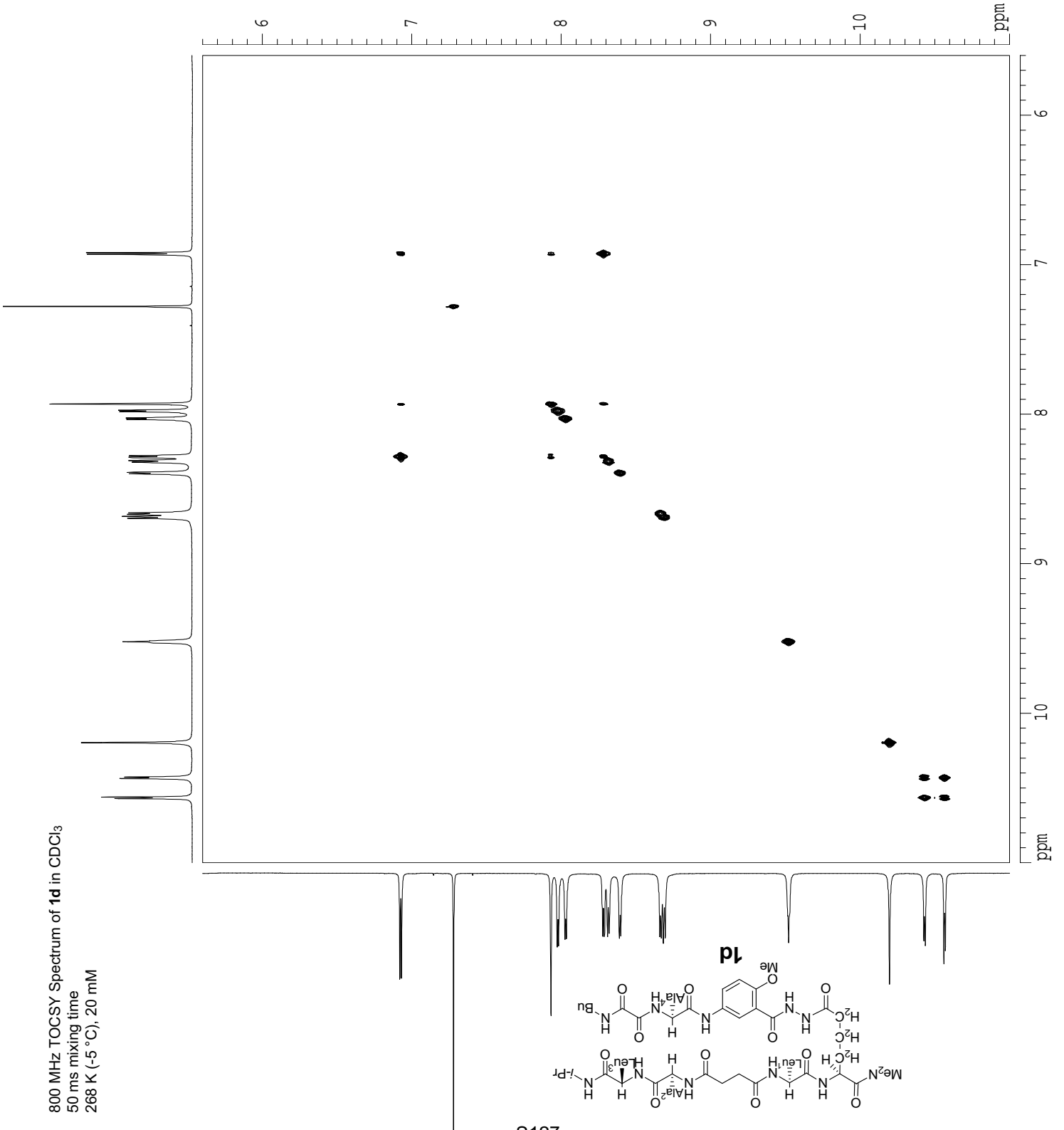
SI 1024
 MC2 States
 SF 799.8064113 MHz
 WDW QSI
 SSB 2
 LB 0.00 Hz
 GB 0

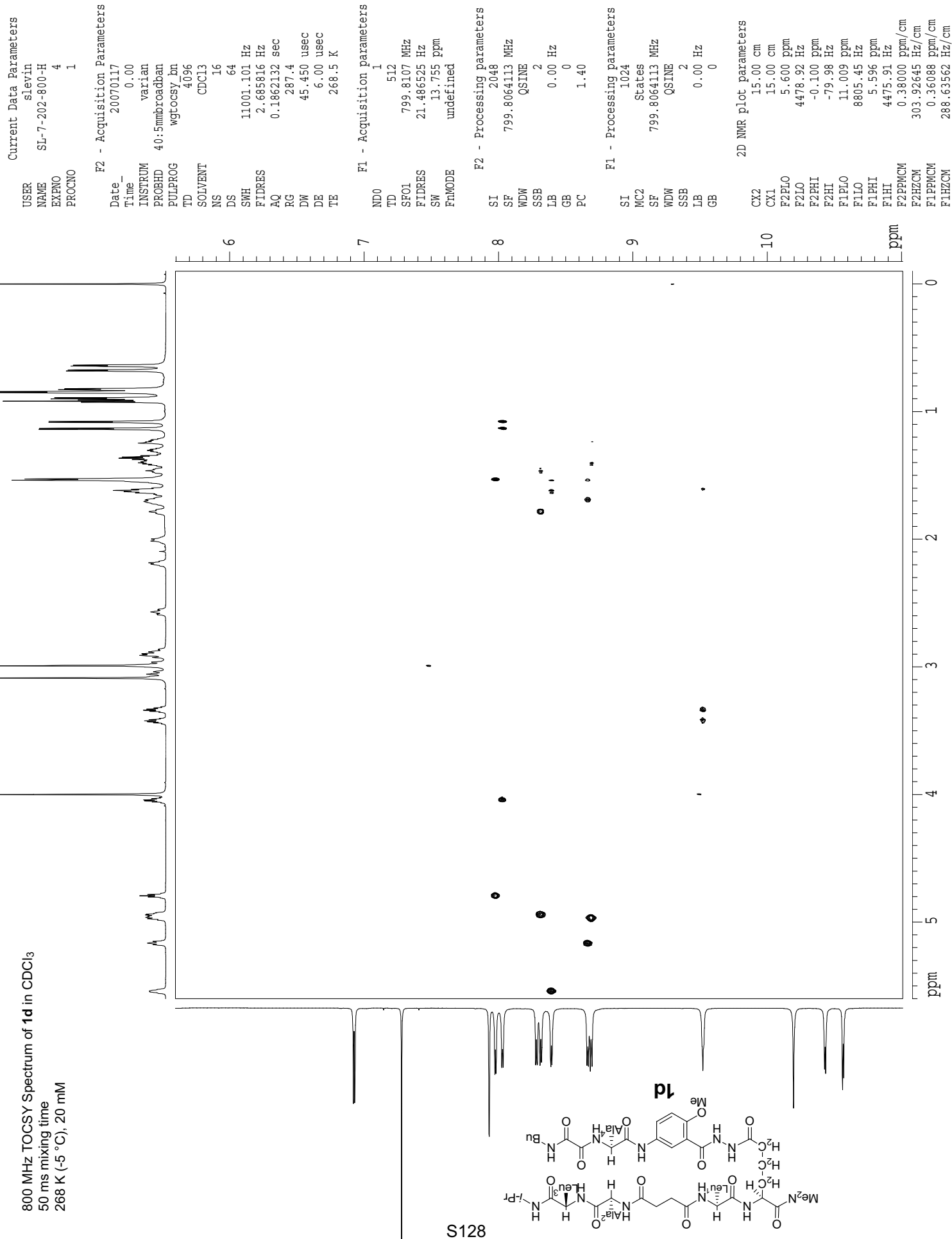
2D NMR plot parameters

CX2 15.00 cm
 CX1 15.00 cm
 F2PLO 11.000 ppm
 F2LO 8797.87 Hz
 F2PHI 5.600 ppm
 F2HI 4478.92 Hz
 F1PLO 11.000 ppm
 F1LO 8797.87 Hz
 F1PHI 5.600 ppm
 F1HI 4478.92 Hz
 F2PPMCM 0.36000 ppm/cm
 F2HZCM 287.93030 Hz/cm
 F1PPMCM 0.36000 ppm/cm
 F1HZCM 287.93030 Hz/cm

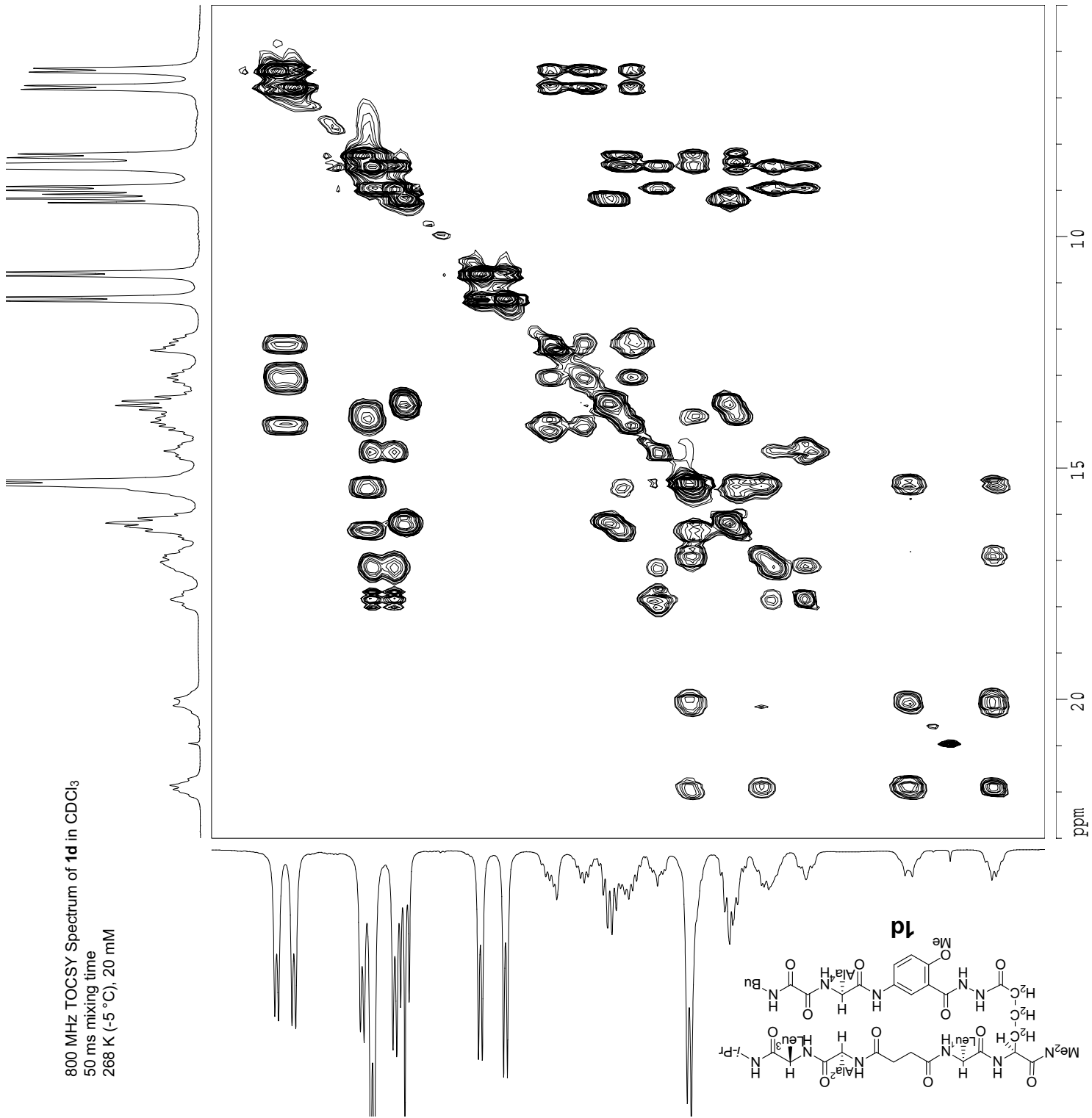
800 MHz TOCSY Spectrum of **1d** in CDCl₃

50 ms mixing time
 268 K (-5 °C), 20 mM





800 MHz TOCSY Spectrum of **1d** in CDCl₃
 50 ms mixing time
 268 K (-5 °C), 20 mM



Current Data Parameters
 USER slewin
 NAME SL-7-202-800-H
 EXPNO 4
 PROCNO 1

F2 - Acquisition Parameters

Date_ 20070117
 Time_ 0.00
 INSTRUM varian
 PROBHD 40:5mm broadband
 PULPROG wgtocsy_bn
 TD 4096
 SOLVENT CDCl3
 NS 16
 DS 64
 SWH 11001.101 Hz
 FIDRES 2.685816 Hz
 AQ 0.1862132 sec
 RG 287.4
 DW 45.450 usec
 DE 6.00 usec
 TE 268.5 K

F1 - Acquisition Parameters

ND0 1
 TD 512
 SF01 799.8107 MHz
 FIDRES 21.486525 Hz
 SW 13.755 ppm
 FwMODE undefined

F2 - Processing parameters

SI 2048
 SF 799.8064113 MHz
 WDW QSSINE
 SSB 2
 LB 0.00 Hz
 GB 0
 PC 1.40

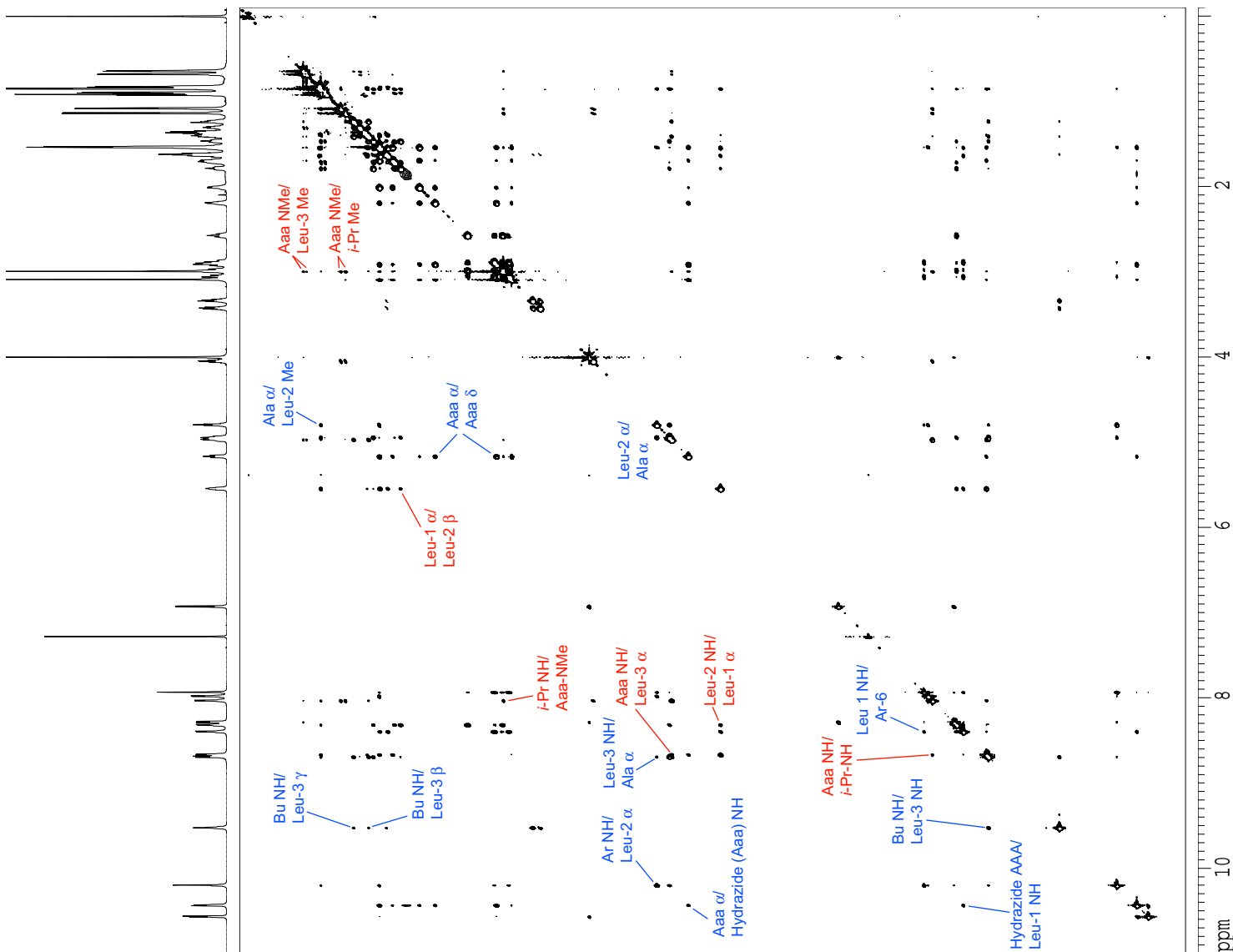
F1 - Processing parameters

SI 1024
 MC2 States
 SF 799.8064113 MHz
 WDW QSSINE
 SSB 2
 LB 0.00 Hz
 GB 0

2D NMR plot parameters

S. Levin and J. S. Nowick
 CX2 15.00 cm
 CX1 15.00 cm
 F2FLO 2.300 ppm
 F2LO 1839.55 Hz
 F2PHI 0.500 ppm
 F2HI 399.90 Hz
 F1FLO 2.300 ppm
 F1LO 1839.55 Hz
 F1PHI 0.500 ppm
 F1HI 399.90 Hz
 F2PPMCM 0.12000 ppm/cm
 F2HZCM 95.97677 Hz/cm
 F1PPMCM 0.12000 ppm/cm
 F1HZCM 95.97677 Hz/cm

800 MHz NOESY Spectrum of **1d** in CDCl₃
400 ms mixing time
268 K (-5 °C), 20 mM



Current Data Parameters
USER slevin
NAME SL-7-202-800-H
EXPNO 5
PROCNO 1

F2 - Acquisition Parameters
Date_ 20070117
Time 0.00
INSTRUM varian
PROBHD 40:5mmrbroadban
PULPROG noesyh2o_pfg 800 p1p2
TD 4096
SOLVENT CDCl3
NS 16
DS 64
SWH 11001.101 Hz
FIDRES 2.685816 Hz
AQ 0.1862132 sec
RG 128
DW 45.450 usec
DE 6.00 usec
TE 268.5 K

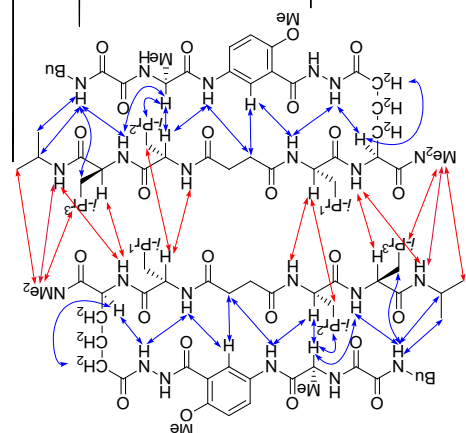
F1 - Acquisition Parameters
ND0 1
TD 1024
SF01 799.8107 MHz
FIDRES 10.743262 Hz
SW 13.755 ppm
FMODE undefined

F2 - Processing parameters
SI 4096
SF 799.8064113 MHz
WDW QSSINE
SSB 2
LB 0.00 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 2048
MC2 States
SF 799.8064113 MHz
WDW QSSINE
SSB 2
LB 0.00 Hz
GB 0

2D NMR plot parameters
CX2 15.00 cm
CX1 15.00 cm
F2PLO 10.734 ppm
F2LO 8585.21 Hz
F2PHI 7.789 ppm
F2PHI 6229.75 Hz
F1PLO 5.771 ppm
F1LO 4615.58 Hz
F1PHI 3.890 ppm
F1HI 3111.52 Hz
F2PPMCM 0.19634 ppm/cm
F2HZCM 157.03067 Hz/cm
F1PPMCM 0.12537 ppm/cm
F1HZCM 100.27044 Hz/cm

S. Levin and J. M. Swick



800 MHz NOESY Spectrum of **1d** in CDCl₃
 400 ms mixing time
 268 K (-5 °C), 20 mM

Current Data Parameters
 USER slevin
 NAME SL-7-202-800-H
 EXPNO 5
 PROCNO 1

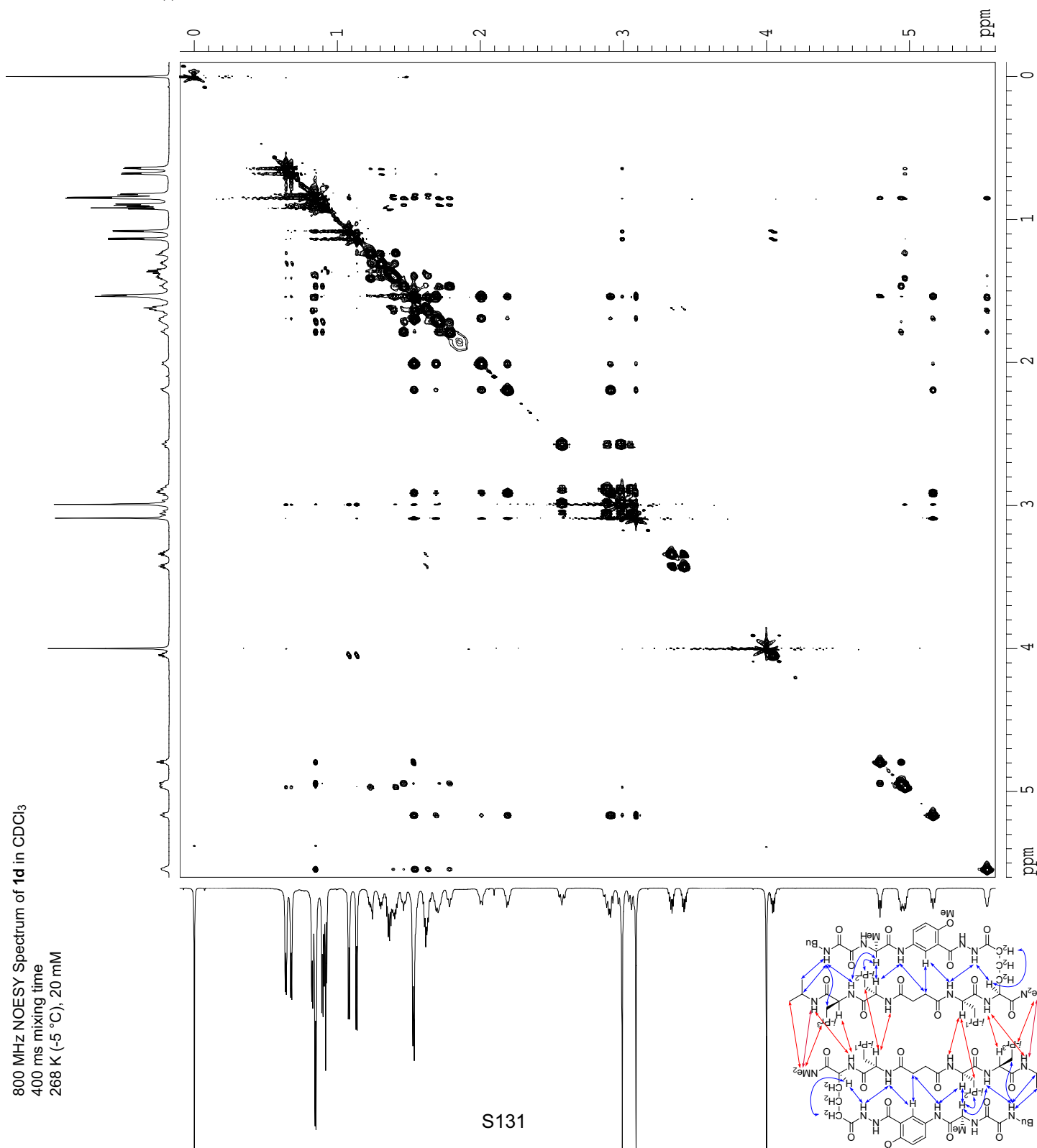
F2 - Acquisition Parameters
 Date_ 20070117
 Time_ 0.00
 INSTRUM varian
 PROBHD 40:5mmrbroadban
 PULPROG noesyh2o_pfg_800_pln
 TD 4096
 SOLVENT CDCl3
 NS 16
 DS 64
 SWH 11001.101 Hz
 FIDRES 2.685816 Hz
 AQ 0.1862132 sec
 RG 128
 DW 45.450 usec
 DE 6.00 usec
 TE 268.5 K

F1 - Acquisition parameters
 ND0 1
 TD 1024
 SF01 799.8107 MHz
 FIDRES 10.743262 Hz
 SW 13.755 ppm
 FRMODE undefined

F2 - Processing parameters
 SI 4096
 SF 799.8064113 MHz
 WDW QSIINE
 SSB 2
 LB 0.00 Hz
 GB 0
 PC 1.40

F1 - Processing parameters
 SI 2048
 MC2 States
 SF 799.8064113 MHz
 WDW QSIINE
 SSB 2
 LB 0.00 Hz
 GB 0

2D NMR plot parameters
 CX2 15.00 cm
 CX1 15.00 cm
 F2PLO 5.600 ppm
 F2LO 4478.92 Hz
 F2PHI -0.100 ppm
 F2HI -79.98 Hz
 F1PLO 5.600 ppm
 F1LO 4478.92 Hz
 F1PHI -0.100 ppm
 F1HI -79.98 Hz
 F2PPMCM 0.38000 ppm/cm
 F2HZCM 303.92645 Hz/cm
 F1PPMCM 0.38000 ppm/cm
 F1HZCM 303.92645 Hz/cm



Supporting Information

S. Levin and J. S. Nowick

Current Data Parameters
 USER slevin
 NAME SL-7-202-800-H
 EXPNO 5
 PROCNO 1

F2 - Acquisition Parameters

Date 20070117
 Time 0.00
 INSTRUM varian
 PROBHD 40:5mm broadband
 PULPROG noesyh2o_pfg_800_pln
 TD 4096
 SOLVENT CDCl3
 NS 16
 DS 64
 SWH 11001.101 Hz
 FIDRES 2.685816 Hz
 AQ 0.1862132 sec
 RG 128
 DW 45.450 usec
 DE 6.00 usec
 TE 268.5 K

F1 - Acquisition Parameters

ND0 1
 TD 1024
 SFO1 799.8107 MHz
 FIDRES 10.743262 Hz
 SW 13.755 ppm
 FRMODE undefined

F2 - Processing parameters

SI 4096
 SF 799.8064113 MHz
 WDW QSI
 SSB 2
 LB 0.00 Hz
 GB 0
 PC 1.40

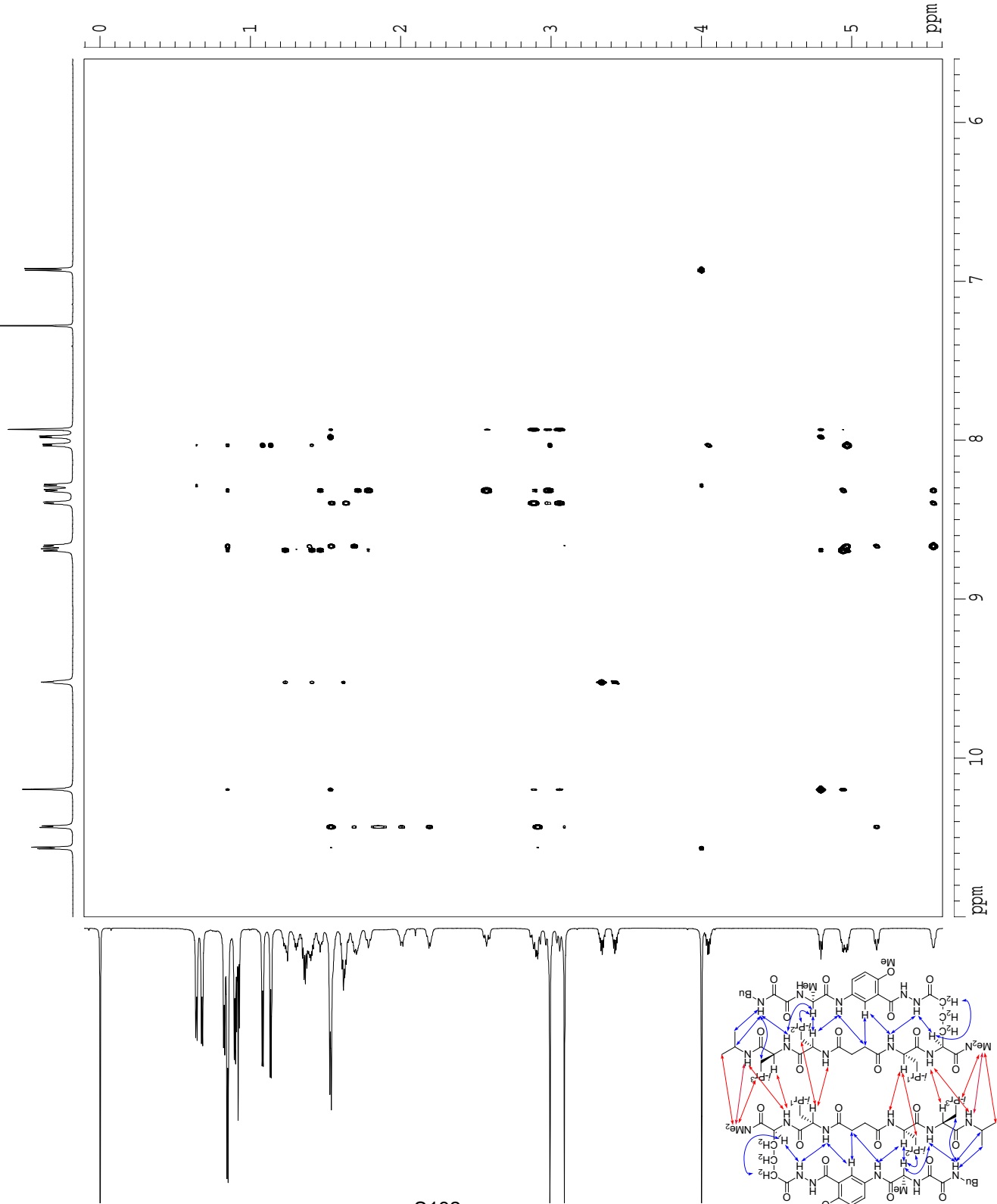
F1 - Processing parameters

SI 2048
 MC2 States
 SF 799.8064113 MHz
 WDW QSI
 SSB 2
 LB 0.00 Hz
 GB 0

2D NMR plot parameters

CX2 15.00 cm
 CX1 15.00 cm
 F2PLO 11.000 ppm
 F2LO 8797.87 Hz
 F2PHI 5.600 ppm
 F2HI 4478.92 Hz
 F1PLO 5.603 ppm
 F1LO 4481.28 Hz
 F1PHI -0.106 ppm
 F1HI -84.60 Hz
 F2PPMCM 0.36000 ppm/cm
 F2HZCM 287.93030 Hz/cm
 F1PPMCM 0.38058 ppm/cm
 F1HZCM 304.39243 Hz/cm

800 MHz NOESY Spectrum of **1d** in CDCl₃
 400 ms mixing time
 268 K (-5 °C), 20 mM



Current Data Parameters
 USER slevin
 NAME SL-7-202-800-H
 EXPNO 5
 PROCNO 1

F2 - Acquisition Parameters

Date_ 20070117
 Time 0.00
 INSTRUM varian
 PROBDH 40:5mmbrdaban
 PULPROG noesyh2o_pfg_800_pln
 TD 4096
 SOLVENT CDCl3
 NS 16
 DS 64
 SWH 11001.101 Hz
 FIDRES 2.685816 Hz
 AQ 0.1862132 sec
 RG 128
 DW 45.450 usec
 DE 6.00 usec
 TE 288.5 K

F1 - Acquisition Parameters

ND0 1
 TD 1024
 SFO1 799.8107 MHz
 FIDRES 10.743262 Hz
 SW 13.755 ppm
 FMODE undefined

F2 - Processing parameters

SI 4096
 SF 799.8064113 MHz
 WDW QSI
 SSB 2
 LB 0.00 Hz
 GB 0
 PC 1.40

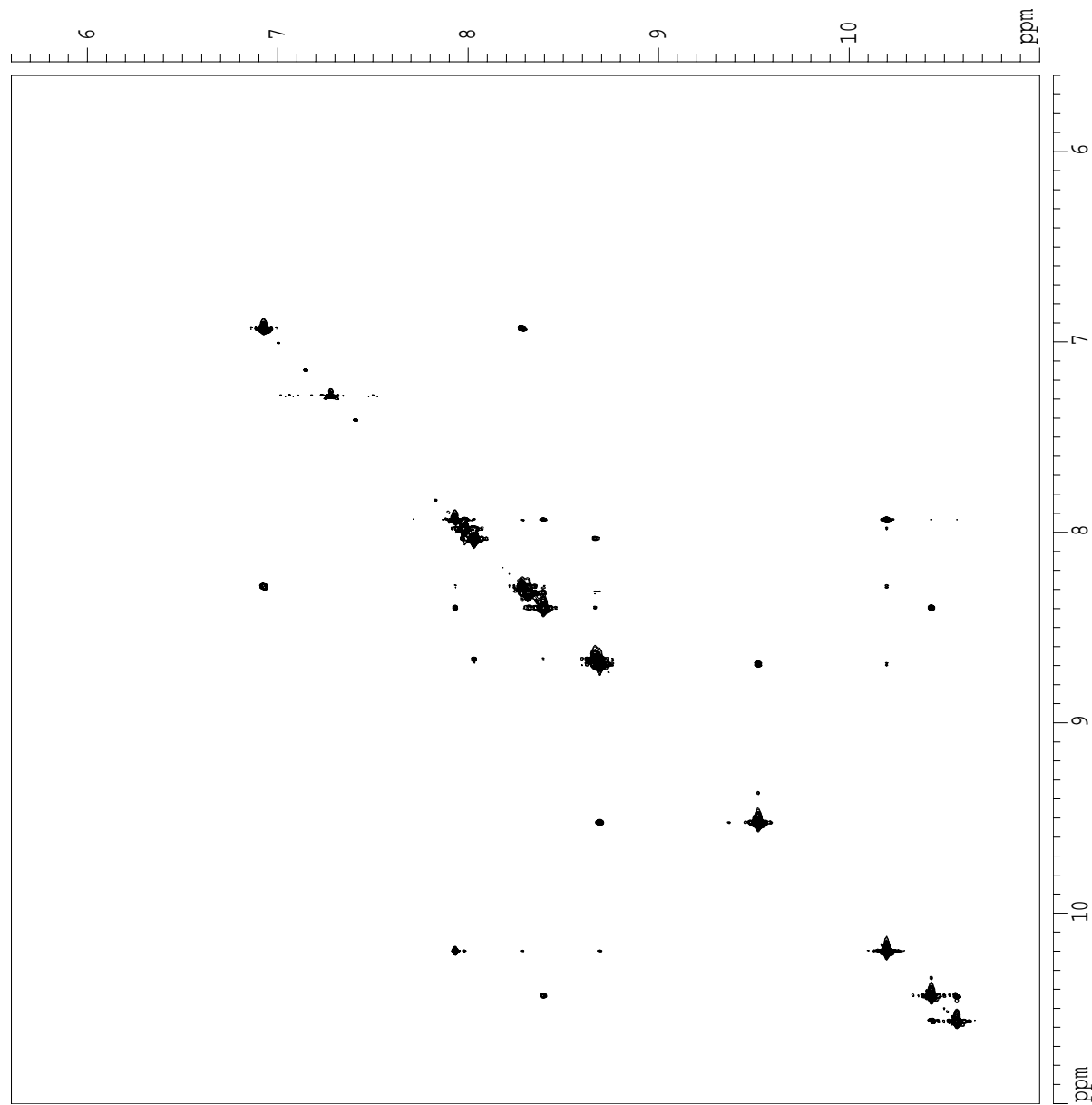
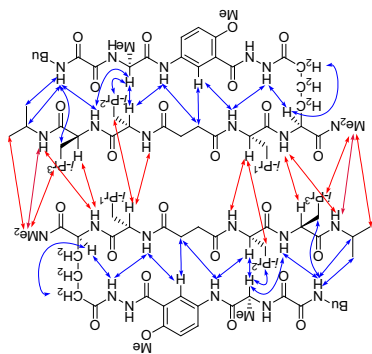
F1 - Processing parameters

SI 2048
 MC2 States
 SF 799.8064113 MHz
 WDW QSI
 SSB 2
 LB 0.00 Hz
 GB 0

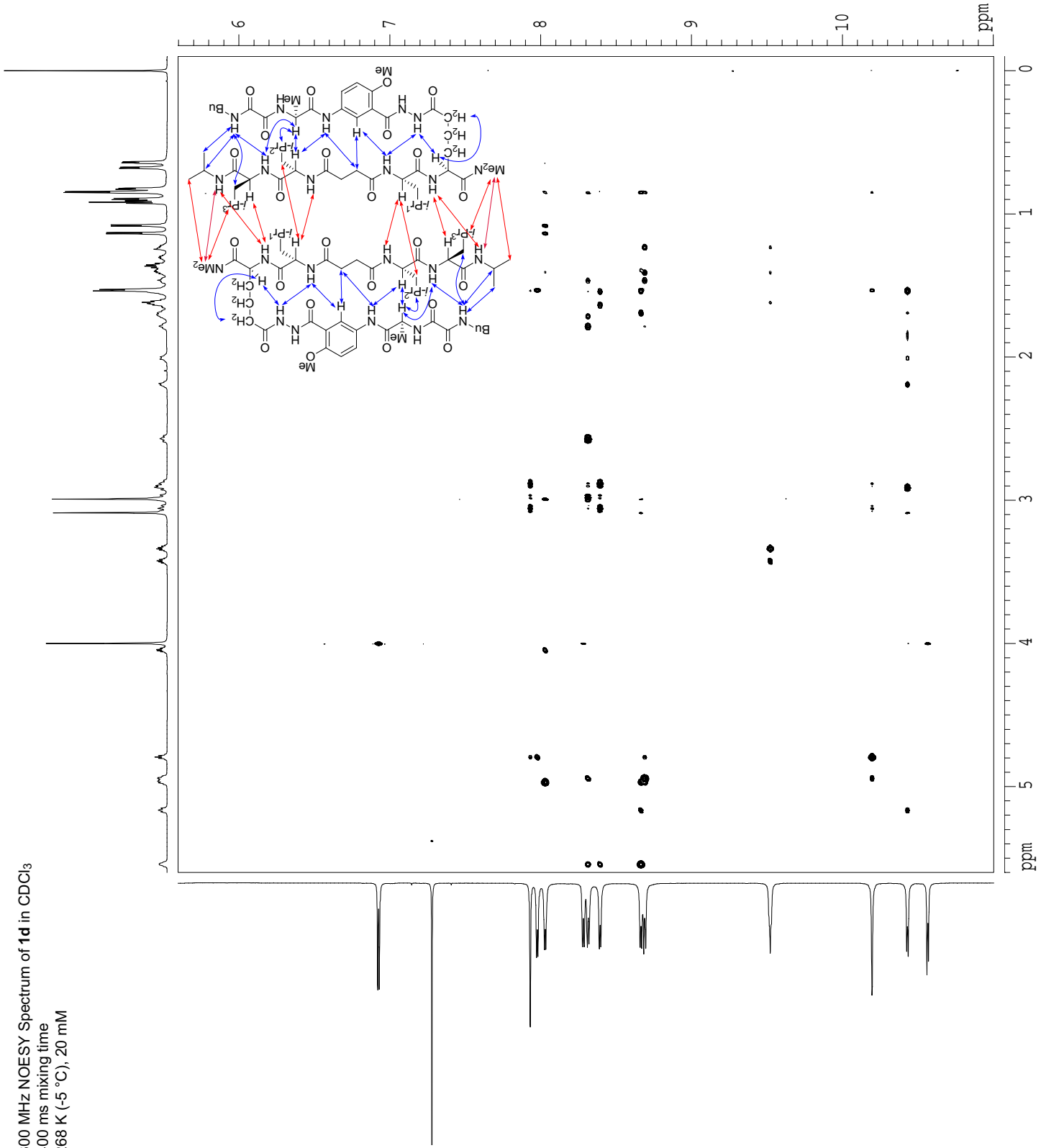
2D NMR plot parameters

CX2 15.00 cm
 CX1 15.00 cm
 F2PLO 11.003 ppm
 F2LO 8800.08 Hz
 F2PHI 5.600 ppm
 F2HI 4478.60 Hz
 F1PLO 11.000 ppm
 F1LO 8797.87 Hz
 F1PHI 5.600 ppm
 F1HI 4478.92 Hz
 F2PMMCM 0.36021 ppm/cm
 F2HZCM 288.09848 Hz/cm
 F1PMMCM 0.36000 ppm/cm
 F1HZCM 287.993030 Hz/cm

800 MHz NOESY Spectrum of **1d** in CDCl₃
 400 ms mixing time
 268 K (-5 °C), 20 mM



800 MHz NOESY Spectrum of **1d** in CDCl₃
 400 ms mixing time
 268 K (-5 °C), 20 mM



Current Data Parameters
 USER slevin
 NAME SL-7-202-800-H
 EXPNO 5
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20070117
 Time 0.00
 INSTRUM varian
 PROBHD 40:5mmroadban
 PULPROG noesyh2o_pfg_800_p1n
 TD 4096
 SOLVENT CDCl3
 NS 16
 DS 64
 SWH 11001.101 Hz
 FIDRES 2.685816 Hz
 AQ 0.1862132 sec
 RG 128
 DW 45.450 usec
 DE 6.00 usec
 TE 268.5 K

F1 - Acquisition parameters
 ND0 1
 TD 1024
 SF01 799.8107 MHz
 FIDRES 10.743262 Hz
 SW 13.755 ppm
 FwMODE undefined

F2 - Processing parameters
 SI 4096
 SF 799.8064113 MHz
 WDW QSI
 SSB 2
 LB 0.00 Hz
 GB 0
 PC 1.40

F1 - Processing parameters
 SI 2048
 MC2 States
 SF 799.8064113 MHz
 WDW QSI
 SSB 2
 LB 0.00 Hz
 GB 0

2D NMR plot parameters
 CX2 15.00 cm
 CX1 15.00 cm
 F2PLO 5.600 ppm
 F2LO 4478.92 Hz
 F2PHI -0.100 ppm
 F2HT -79.98 Hz
 F1PLO 11.003 ppm
 F1LO 8800.08 Hz
 F1PHI 5.596 ppm
 F1HT 4475.91 Hz
 F2PPMCM 0.38000 ppm/cm
 F2HZCM 303.92645 Hz/cm
 F1PPMCM 0.36043 ppm/cm
 F1HZCM 288.27753 Hz/cm

800 MHz NOESY Spectrum of **1d** in CDCl₃
 400 ms mixing time
 268 K (-5 °C), 20 mM

Supporting Information

Current Data Parameters
 USER sleivin
 NAME SL-7-202-800-H
 EXPNO 5
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20070117
 Time 0.00
 INSTRUM varian
 PROBHD 40:5mm broadband
 PULPROG noesyh2o_prg_800_pln
 TD 4096
 SOLVENT CDCl₃
 NS 16
 DS 64
 SWH 11001.101 Hz
 FIDRES 2.685816 Hz
 AQ 0.1862132 sec
 RG 128
 DW 45.450 usec
 DE 6.00 usec
 TE 268.5 K

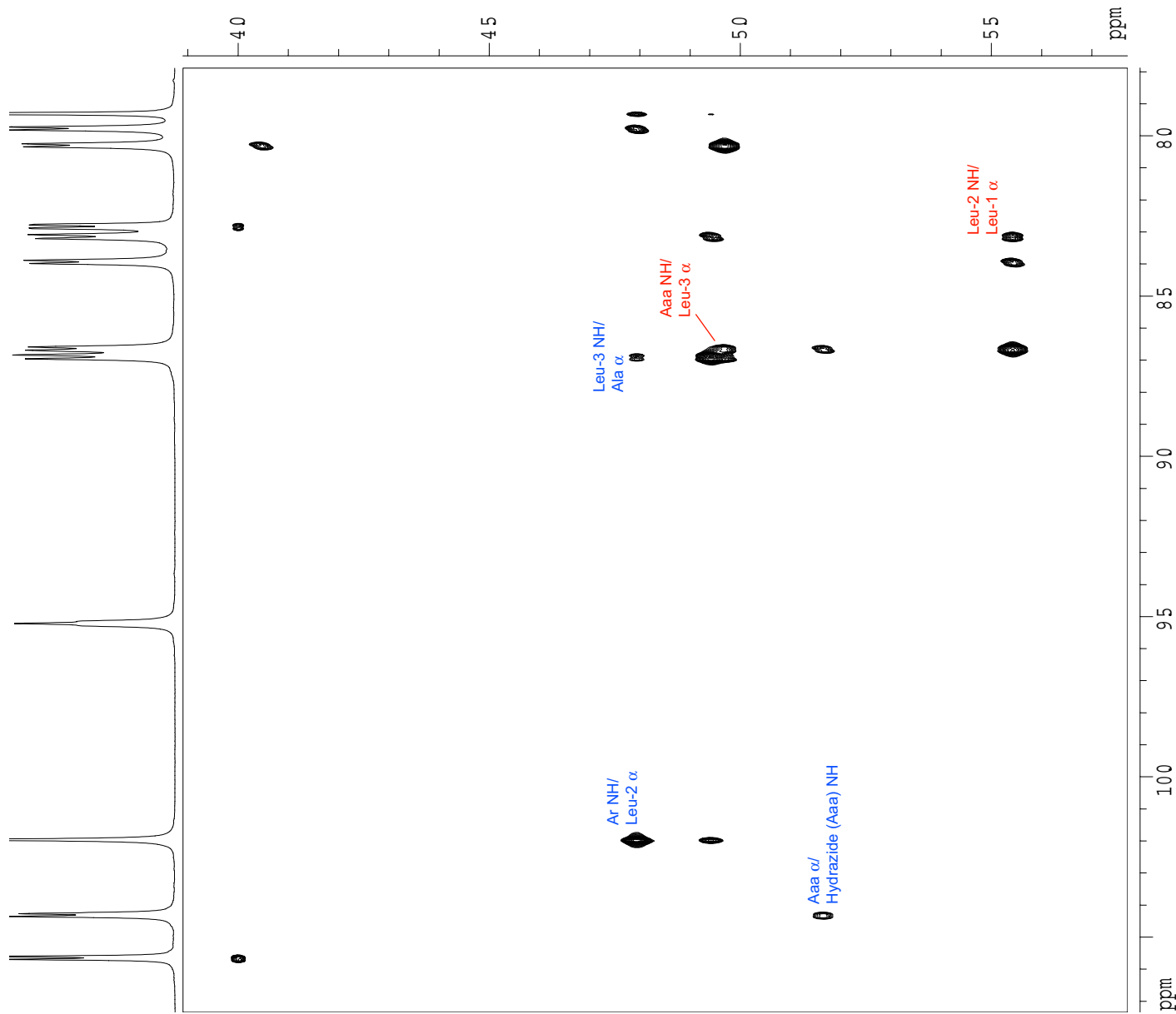
F1 - Acquisition Parameters
 ND0 1
 TD 1024
 SF01 799.8107 MHz
 FIDRES 10.743262 Hz
 SW 13.755 ppm
 FmMODE undefined

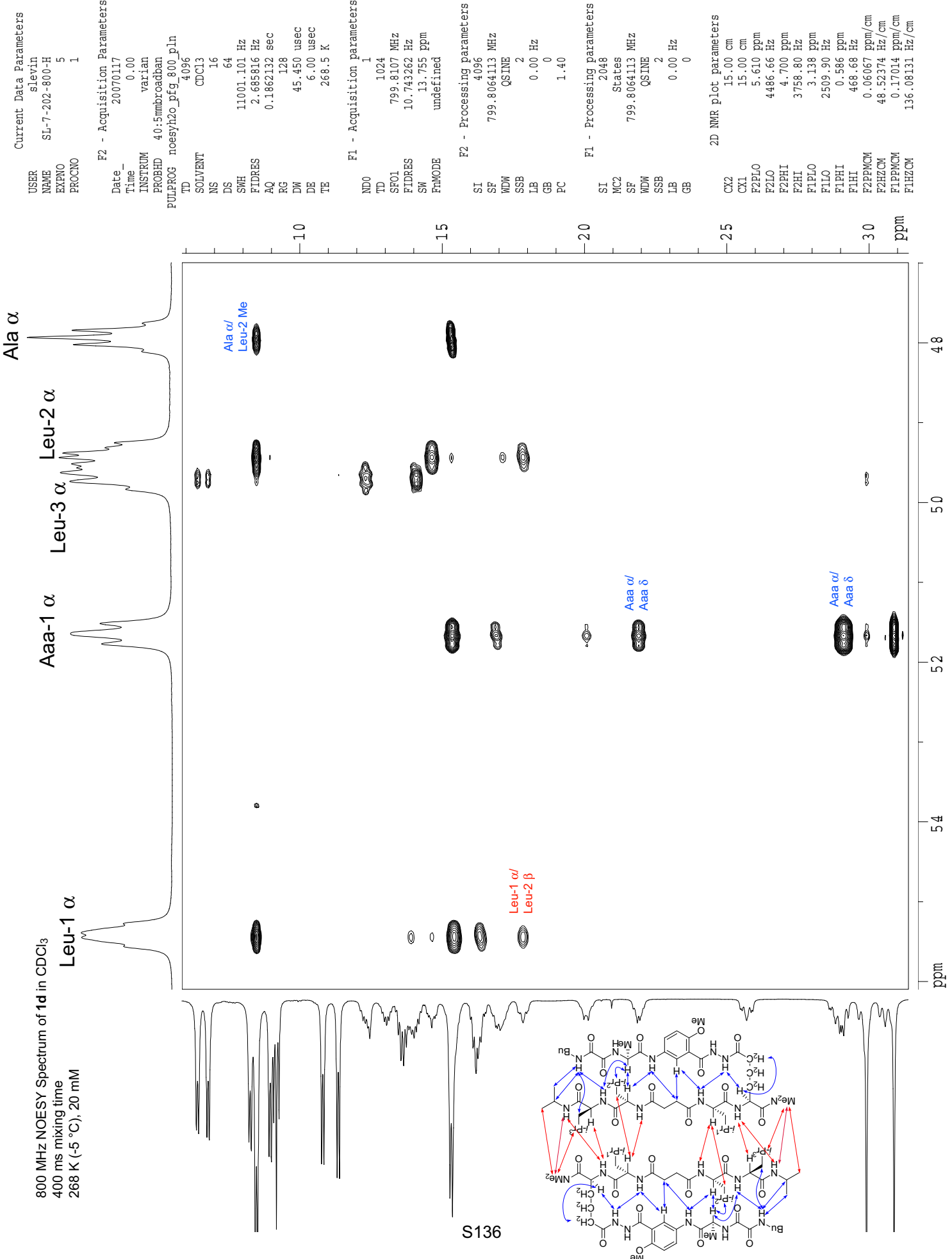
F2 - Processing parameters
 SI 4096
 SF 799.8064113 MHz
 MDW QSIINE
 SSB 2
 LB 0.00 Hz
 GB 0
 PC 1.40

F1 - Processing parameters
 SI 2048
 MC2 States
 SF 799.8064113 MHz
 MDW QSIINE
 SSB 2
 LB 0.00 Hz
 GB 0

2D NMR plot parameters
 CX2 15.00 cm
 CX1 15.00 cm
 F2PLO 10.734 ppm
 F2LO 8585.21 Hz
 F2PHI 7.789 ppm
 F2ZHI 6229.75 Hz
 F1PLO 5.771 ppm
 F1LO 4615.58 Hz
 F1PHI 3.890 ppm
 F1ZHI 3111.52 Hz
 F2PMMCM 0.19634 ppm/cm
 F2HZCM 157.03067 Hz/cm
 F1PMMCM 0.12537 ppm/cm
 F1HZCM 100.27044 Hz/cm

S. Levin and J. S. Nowick





Supporting Information

Current Data Parameters

USER slewin
 NAME SL-7-202-800-H
 EXPNO 5
 PROCNO 1

F2 - Acquisition Parameters

Date_ 20070117
 Time 0.00
 INSTRUM varian
 PROBHD 40:5mmroadban
 PULPROG noesyh2o_pfg_800_pln
 TD 4096
 SOLVENT CDCl3
 NS 16
 DS 64
 SWH 11001.101 Hz
 FIDRES 2.685816 Hz
 AQ 0.1862132 sec
 RG 128
 DW 45.450 usec
 DE 6.00 usec
 TE 268.5 K

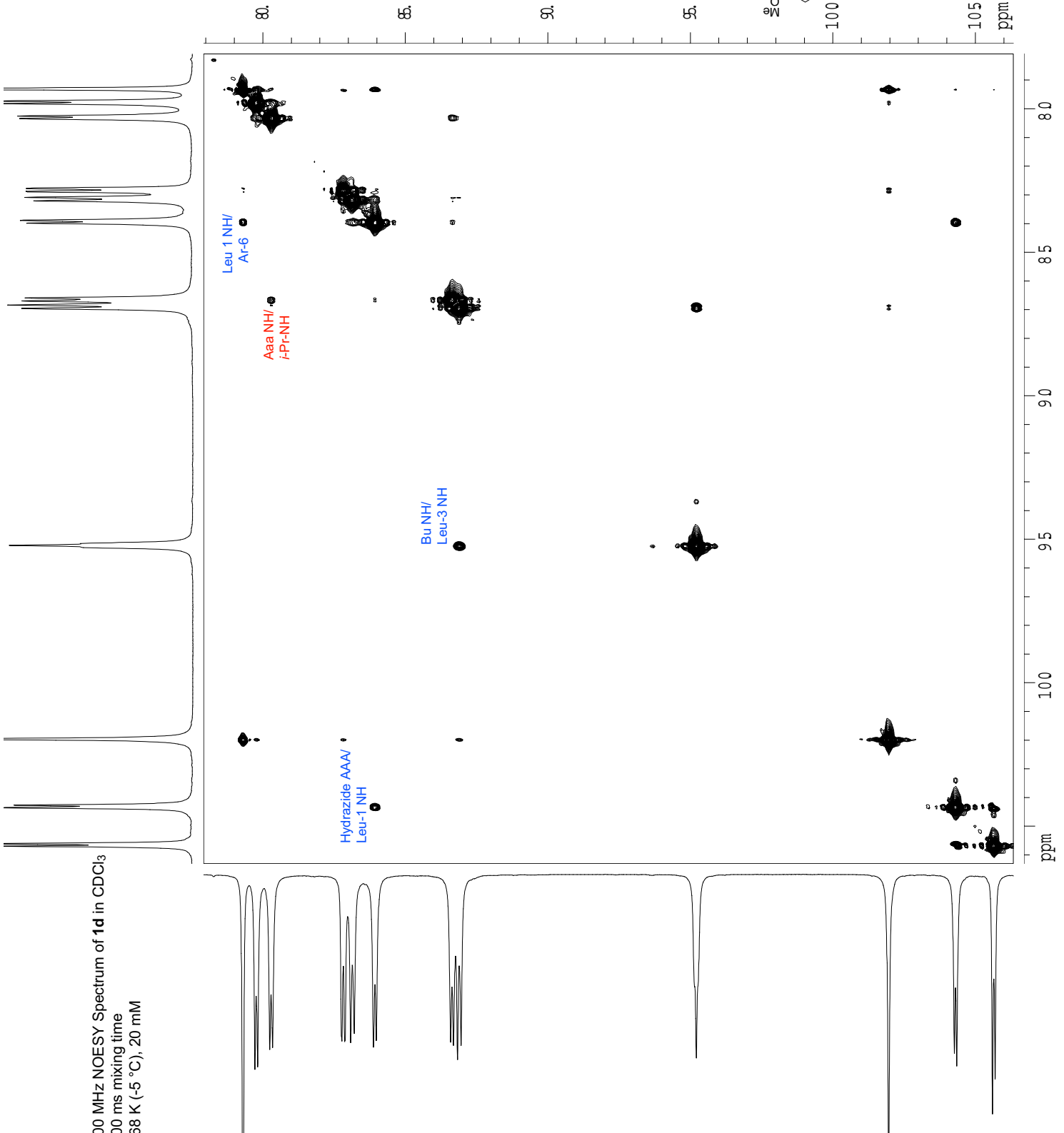
F1 - Acquisition parameters

ND0 1
 TD 1024
 SF01 799.8107 MHz
 FIDRES 10.743262 Hz
 SW 13.755 ppm
 F1MODE undefined

F2 - Processing parameters

SI 4096
 SF 799.8064113 MHz
 WDW QSI
 SSB 2
 LB 0.00 Hz
 GB 0
 PC 1.40

800 MHz NOESY Spectrum of **1d** in CDCl₃
 400 ms mixing time
 268 K (-5 °C), 20 mM



S. Levin and J. S. Nowick

800 MHz NOESY Spectrum of **1d** in CDCl₃
 400 ms mixing time
 268 K (-5 °C), 20 mM

Supporting Information

Current Data Parameters
 USER sLevin
 NAME SL-7-202-800-H
 EXPNO 5
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20070117
 Time 0:00
 INSTRUM varian
 PROBHD 40:5mmrbroadban
 PULPROG noesyh2o_pfg_800_pln
 TD 4096
 SOLVENT CDCl₃
 NS 16
 DS 64
 SWH 11001.101 Hz
 FIDRES 2.685816 Hz
 AQ 0.1862132 sec
 RG 128
 DW 45.450 usec
 DE 6.00 usec
 TE 268.5 K

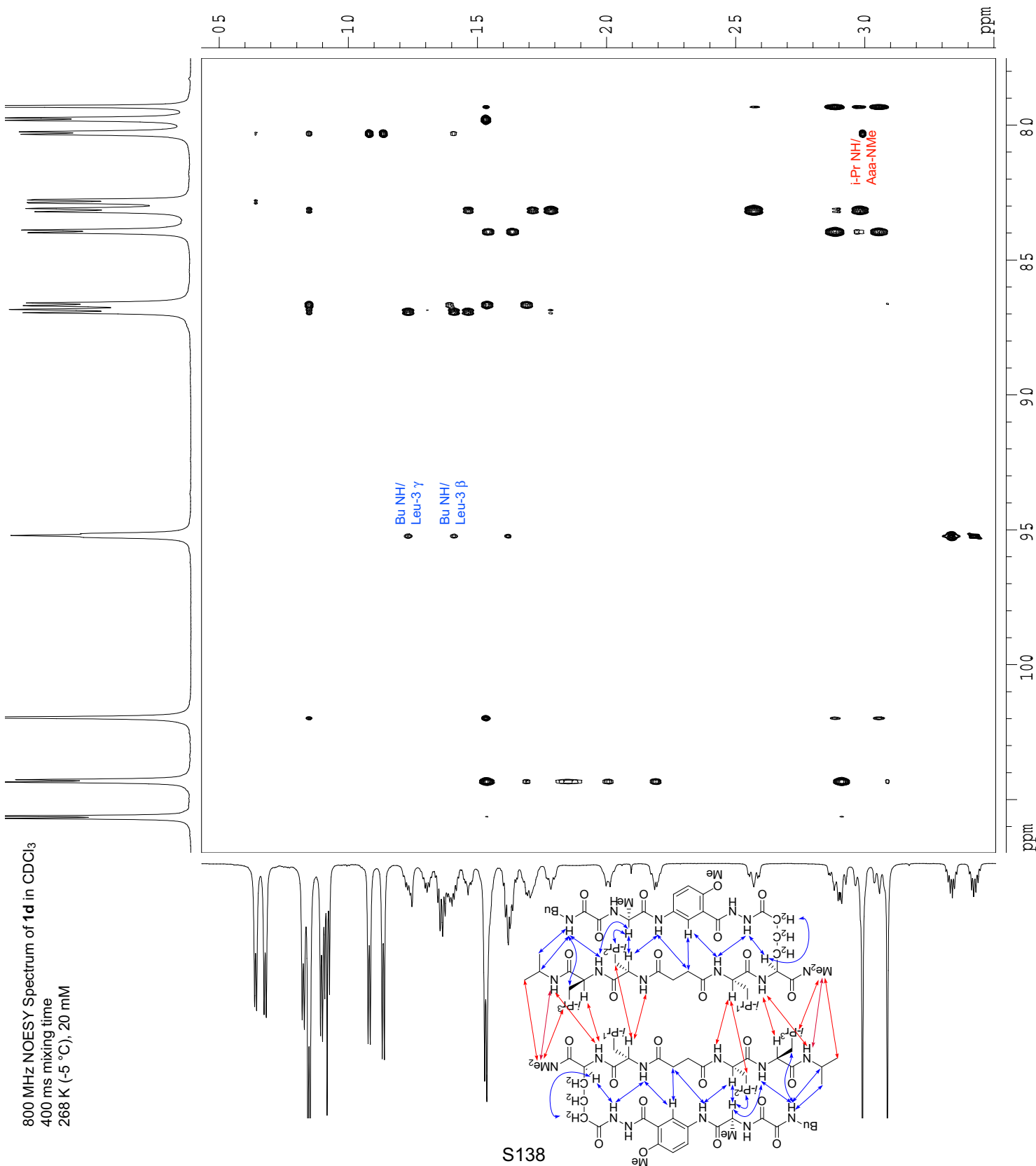
F1 - Acquisition Parameters
 ND0 1
 TD 1024
 SF01 799.8107 MHz
 FIDRES 10.743262 Hz
 SW 13.765 ppm
 FreqMODE undefined

F2 - Processing parameters
 SI 4096
 SF 799.8064113 MHz
 WDM QSINE
 SSB 2
 LB 0.00 Hz
 GB 0
 PC 1.40

F1 - Processing parameters
 SI 2048
 MC2 States
 SF 799.8064113 MHz
 WDM QSINE
 SSB 2
 LB 0.00 Hz
 GB 0

2D NMR plot parameters
 CX2 15.00 cm
 CX1 15.00 cm
 F2PLO 10.697 ppm
 F2LO 8555.67 Hz
 F2PHI 7.752 ppm
 F2HI 6200.21 Hz
 F1PLO 3.508 ppm
 F1LO 2805.34 Hz
 F1PHI 0.432 ppm
 F1HI 345.13 Hz
 F2PPMCM 0.19634 ppm/cm
 F2HZCM 157.03067 Hz/cm
 F1PPMCM 0.20507 ppm/cm
 F1HZCM 164.01379 Hz/cm

S. Levin and J. Nowick



Supporting Information

Current Data Parameters
 USER slevin
 NAME SL-7-202-800-H
 EXPNO 5
 PROCNO 1

F2 - Acquisition Parameters

Date_ 20070117
 Time 0.00
 INSTRUM varian
 PROBDH 40:5mmbroadban
 PULPROG noesyh2o_pfg_800_pln
 TD 4096

SOLVENT CDCL3
 NS 16
 DS 64
 SMH 11001.101 Hz
 FIDRES 2.685816 Hz
 AQ 0.1862132 sec
 RG 128
 DW 45.450 usec
 DE 6.00 usec
 TE 268.5 K

F1 - Acquisition Parameters

ND0 1
 TD 1024
 SFO1 799.8107 MHz
 FIDRES 10.743262 Hz
 SW 13.755 ppm
 FwMODE undefined

F2 - Processing Parameters

SI 4096
 SF 799.8064113 MHz
 WDW QSINE
 SSB 2
 LB 0.00 Hz
 GB 0
 PC 1.40

F1 - Processing Parameters

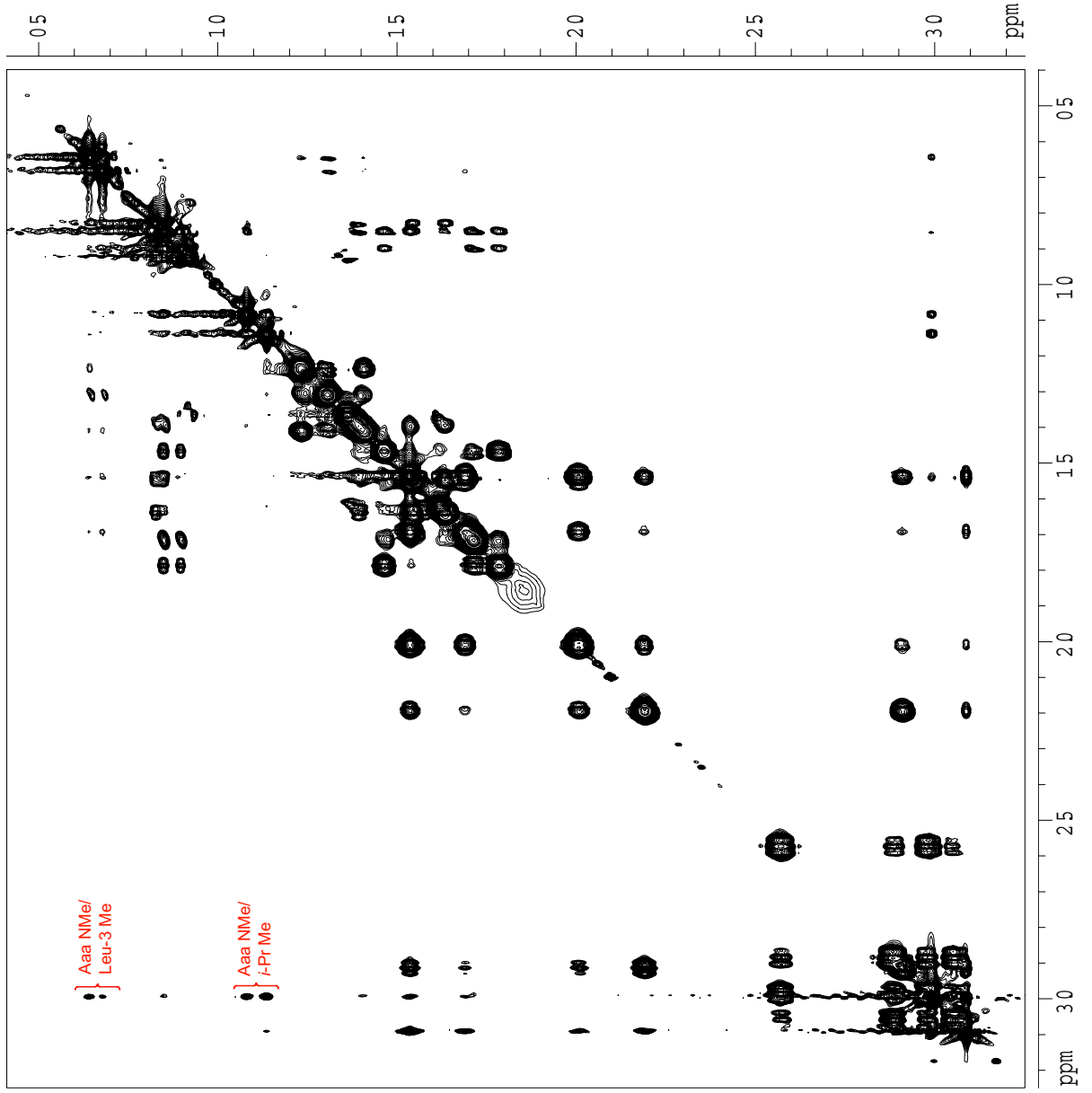
SI 2048
 MC2 States
 SF 799.8064113 MHz
 WDW QSINE
 SSB 2
 LB 0.00 Hz
 GB 0

2D NMR plot parameters

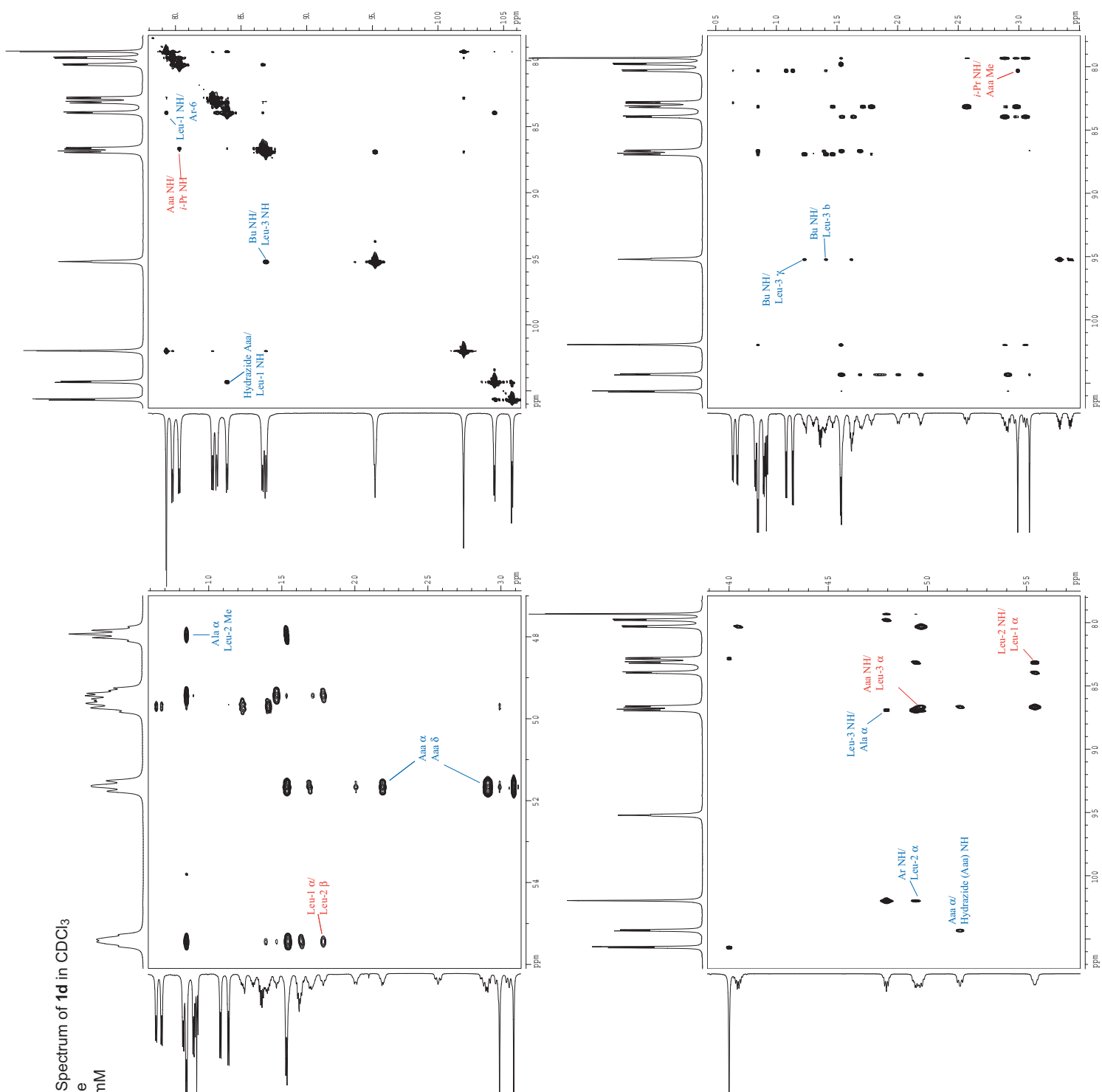
CX2 15.00 cm
 CX1 15.00 cm
 F2PLO 3.249 ppm
 F2LO 2598.53 Hz
 F2PHI 0.398 ppm
 F2HI 318.27 Hz
 F1PLO 3.252 ppm
 F1LO 2601.21 Hz
 F1PHI 0.411 ppm
 F1HI 329.01 Hz
 F2PPMCM 0.19007 ppm/cm
 F2HZCM 152.01715 Hz/cm
 F1PPMCM 0.18940 ppm/cm
 F1HZCM 151.47998 Hz/cm

S. Levin and J. S. Nowick

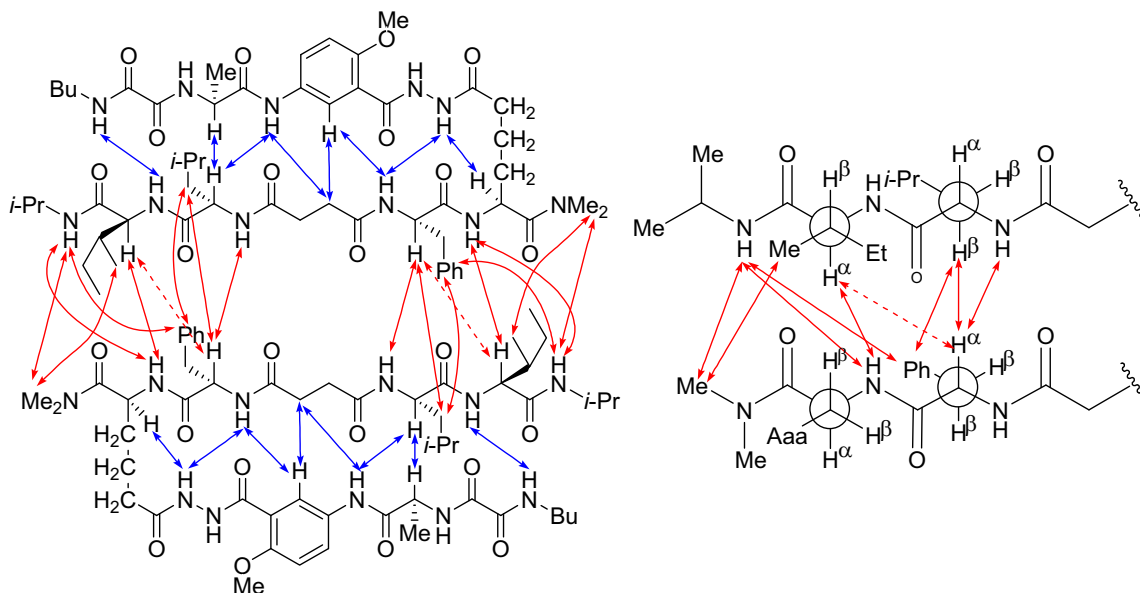
800 MHz NOESY Spectrum of **1d** in CDCl₃
 400 ms mixing time
 268 K (-5 °C), 20 mM



800 MHz NOESY Spectrum of **1d** in CDCl₃
400 ms mixing time
268 K (-5 °C), 20 mM



Spectroscopic DATA for the compound **1e**
(1 mM, CDCl₃ 268K)



Key NOEs assigned as *intermolecular* are represented with red arrows

Key NOEs assigned as *intramolecular* are represented with blue arrows

Dashed arrow represents an NOE that may arise from deviation from ideal β -sheet geometry or from an alternative conformer or oligomer.

Key data for amino acids.

Amino acid	H _α Shift ppm	NH Shift ppm	³ J _{NHα} Hz
Aaa	4.83	8.01	8.0
R ₁ = Phe	5.94	8.66	7.7
R ₂ = Leu	5.06	8.23	9.7
R ₃ = Ile	4.72	8.78	9.7
R ₄ = Ala	4.81	7.93	overlap

Aminoacidic acid (Aaa) δ proton resonances.

pro-R: 2.80 ppm, t, (*overlap*)

pro-S: 2.14 ppm, td, ($J_1 = 11.9$ Hz; $J_2 = 7.0$ Hz)

anisotropy = 0.66ppm

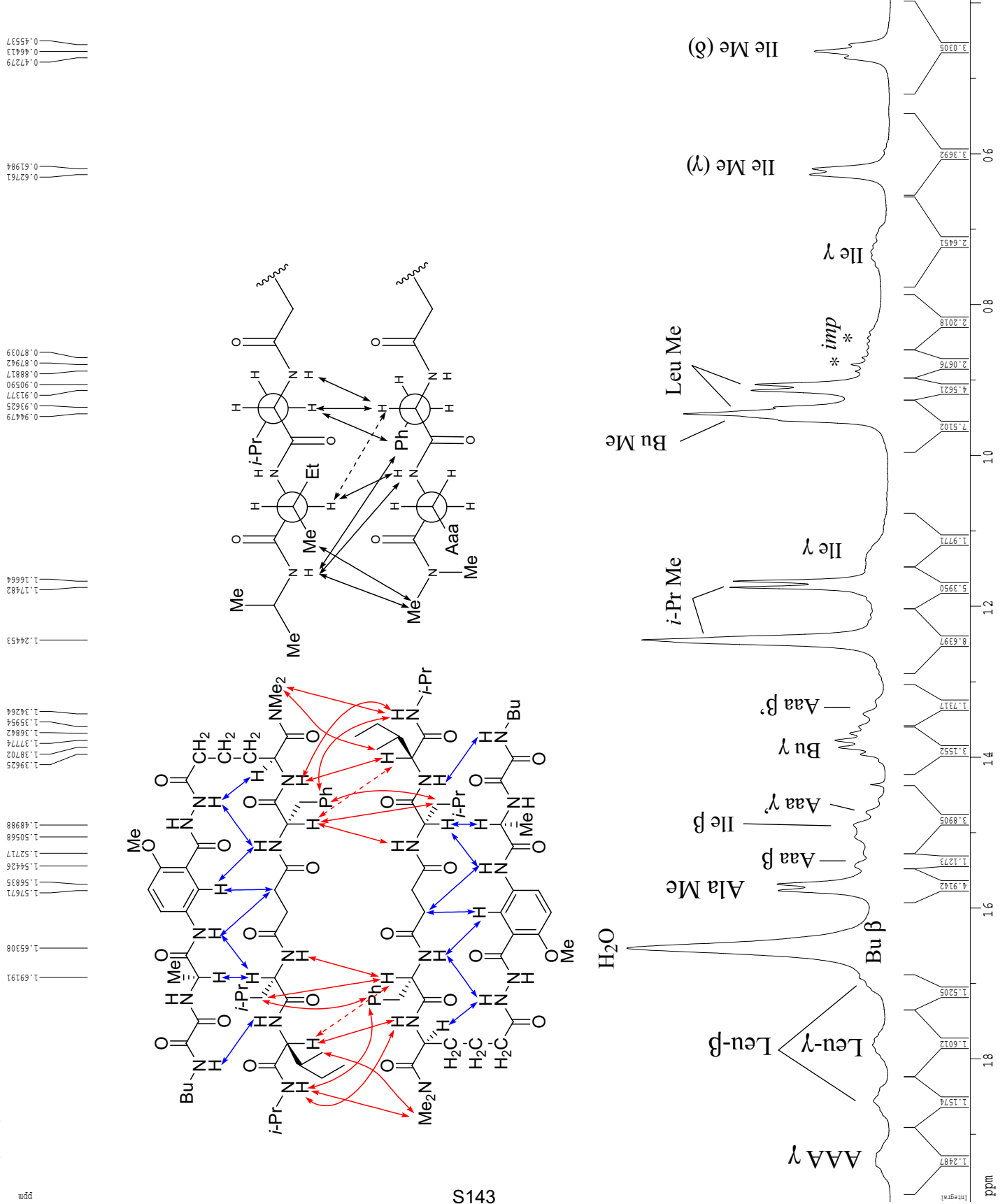
Key data for other NH protons.

Proton	NH Shift ppm	J Hz
Ar-NH	10.20	-
Hydrazide Ar	10.69	7.4
Hydrazide Aaa	10.63	7.4
Bu-NH	9.65	broad
<i>i</i> -Pr-NH	8.06	7.7

ESI MS m/z for C₅₃H₈₂N₁₁O₁₂ [M+H]⁺ calcd 1064.61, found 1064.48.

800 MHz ¹H NMR Spectrum of **1e** in CDCl₃
268 K (-5 °C), 1 mM

Current Data Parameters
 USER slevin
 NAME SL-7-137-800-H
 EXPNO 2
 PROCNO 1
 F2 - Acquisition Parameters
 Date_ 20061109
 Time 0.00
 INSTRUM varian
 PROBHD 40:5mmhruoban
 PULPROG zgpg30
 TD 65506
 SFO 800.132416
 SOLVENT cdcl3
 NS 128
 DS 4
 SWH 11001.101 Hz
 FIDRES 0.199998 Hz
 AQ 2.5000727 sec
 RG 8192
 DW 45.450 usec
 DE 4.50 usec
 TE 268.5 K
 F2 - Processing parameter
 SI 32768
 SF 799.8064116 MHz
 ACQ 0.00
 LB 1.0 Hz
 GB 0
 PC 2.00
 1D NMR plot parameters
 CX 22.80 cm
 CY 5.00 cm
 F1P 1.990 ppm
 F1 1591.24 Hz
 F2P 0.392 ppm
 F2 313.47 Hz
 PPMCM 0.07007 ppm/cm
 HZCM 56.04266 Hz/cm



Current Data Parameters
 USER slevin
 NAME SL-7-137-800-H
 EXPNO 3
 PROCNO 1

F2 - Acquisition Parameters

Date_ 20061108
 Time_ 0.00
 INSTRUM varian
 PROBHD 40:5mmbroadban
 PULPROG gcosy
 TD 4096
 SOLVENT cdc13
 NS 16
 DS 64
 SWH 11001.101 Hz
 FIDRES 2.685816 Hz
 AQ 0.1843700 sec
 RG 4096
 DW 45.450 usec
 DE 231.43 usec
 TE 268.5 K

F1 - Acquisition parameters

ND0 1
 TD 512
 SF01 799.8107 MHz
 FIDRES 21.486525 Hz
 SW 13.755 ppm
 F1MODE undefined

F2 - Processing parameters

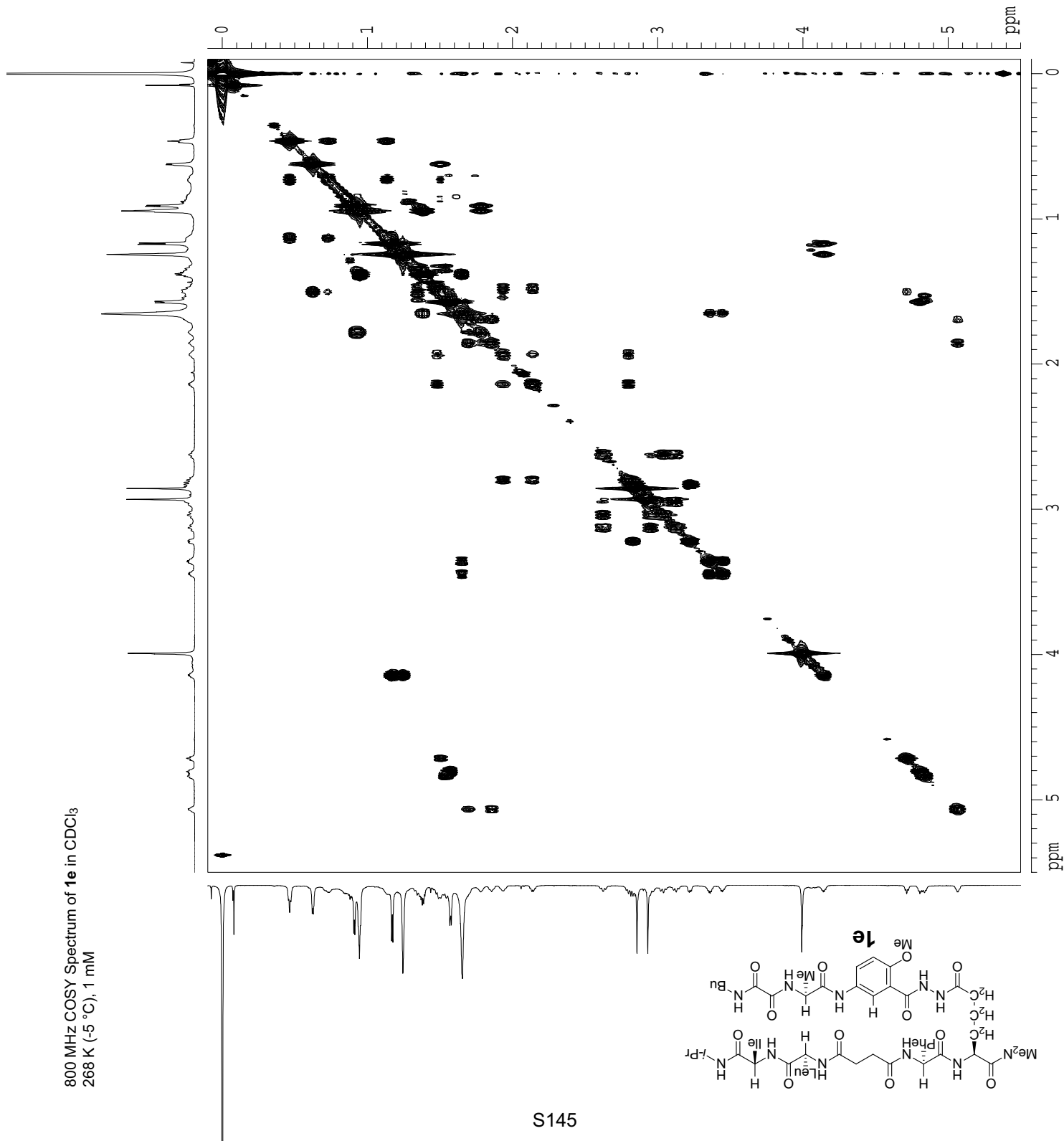
SI 4096
 SF 799.8064116 MHz
 WDW SINE
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.40

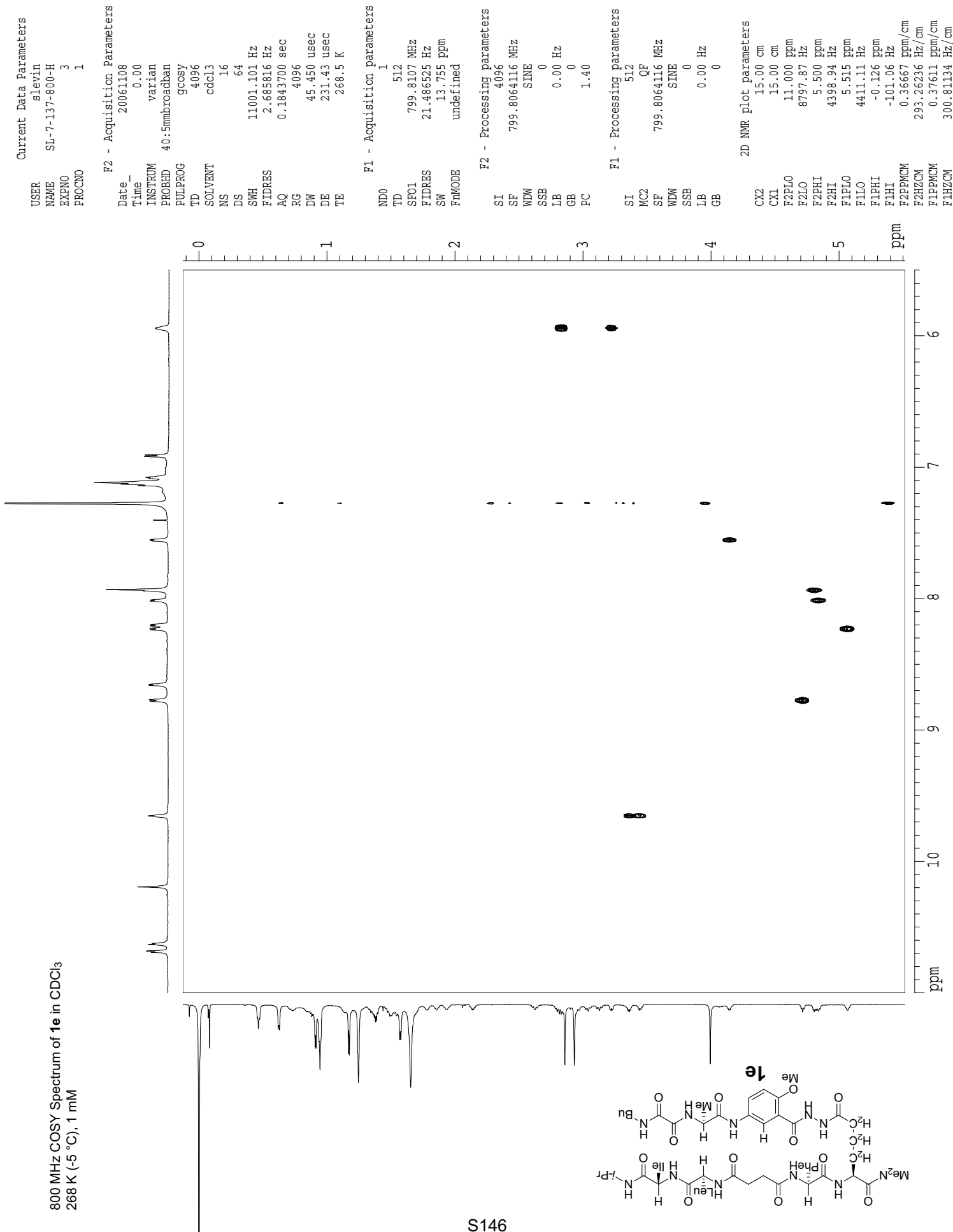
F1 - Processing parameters

SI 512
 MC2 QF
 SF 799.8064116 MHz
 WDW SINE
 SSB 0
 LB 0.00 Hz
 GB 0

2D NMR plot parameters

CX2 15.00 cm
 CX1 15.00 cm
 F2PLO 5.500 ppm
 F2LO 4398.94 Hz
 F2PHI -0.100 ppm
 F2HI -79.98 Hz
 F1PLO 5.500 ppm
 F1LO 4398.94 Hz
 F1PHI -0.100 ppm
 F1HI -79.98 Hz
 F2PPMCM 0.37333 ppm/cm
 F2HZCM 298.59439 Hz/cm
 F1PPMCM 0.37333 ppm/cm
 F1HZCM 298.59439 Hz/cm





Current Data Parameters
 USER slevin
 NAME SL-7-137-800-H
 EXPNO 3
 PROCNO 1

F2 - Acquisition Parameters

Date_ 20061108
 Time_ 0.00
 INSTRUM varian
 PROBHD 40:5mmrbroadban
 PULPROG gcosy
 TD 4096
 SOLVENT cdcl3
 NS 16
 DS 64
 SWH 11001.101 Hz
 FIDRES 2.685816 Hz
 AQ 0.1843700 sec
 RG 4096
 DW 45.450 usec
 DE 231.43 usec
 TE 268.5 K

F1 - Acquisition Parameters

ND0 1
 TD 512
 SF01 799.8107 MHz
 FIDRES 21.486525 Hz
 SW 13.755 ppm
 FMODE undefined

F2 - Processing parameters

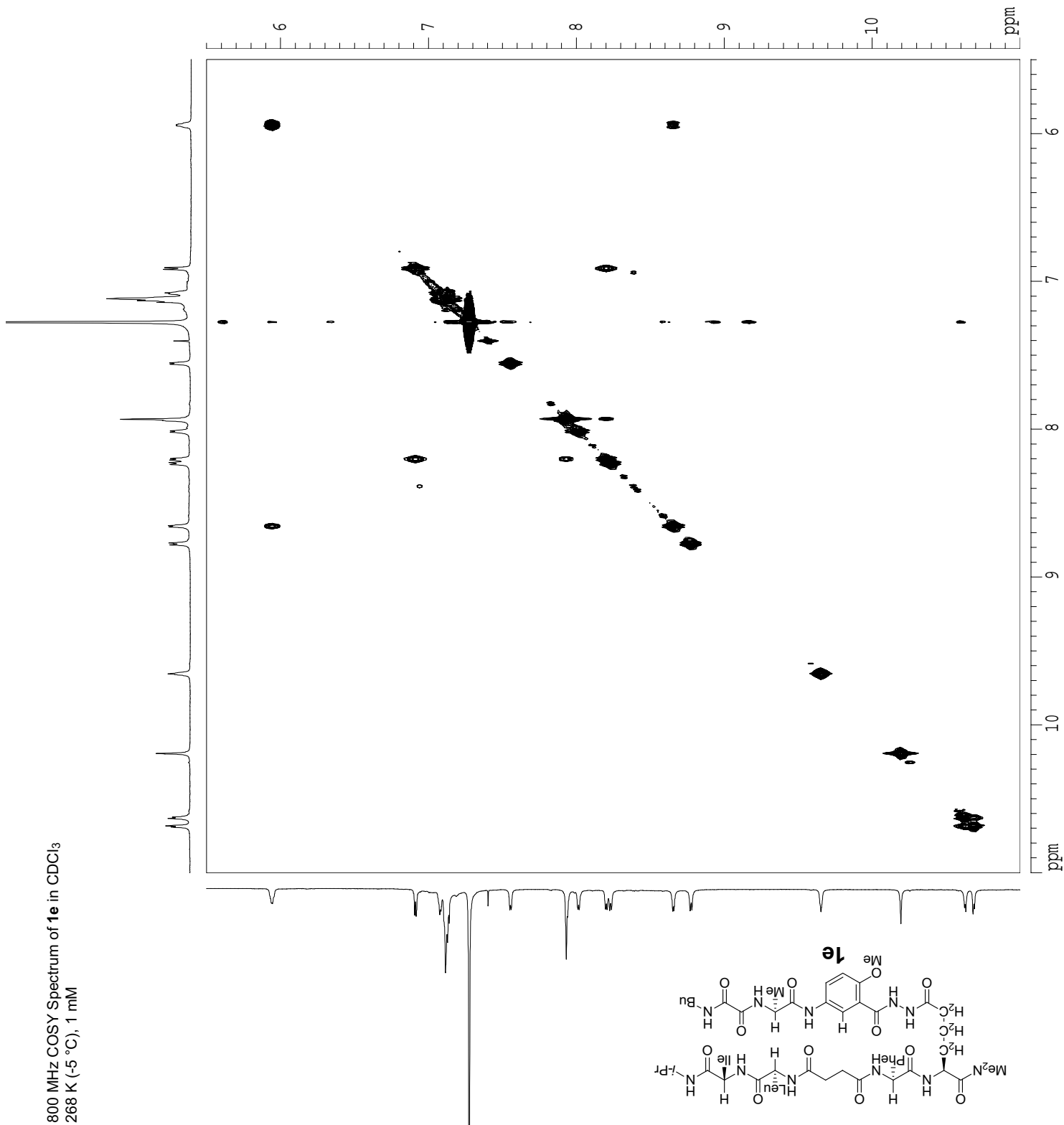
SI 4096
 SF 799.8064116 MHz
 WDW SINE
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.40

F1 - Processing parameters

SI 512
 MC2 OF
 SF 799.8064116 MHz
 WDW SINE
 SSB 0
 LB 0.00 Hz
 GB 0

2D NMR plot parameters

CX2 15.00 cm
 CX1 15.00 cm
 F2PLO 11.002 ppm
 F2LO 8799.73 Hz
 F2PHI 5.498 ppm
 F2HI 4397.68 Hz
 F1PLO 11.000 ppm
 F1LO 8797.87 Hz
 F1PHI 5.500 ppm
 F1HI 4398.94 Hz
 F2P2MCM 0.36693 ppm/cm
 F2HZCM 293.47009 Hz/cm
 F1P2MCM 0.36667 ppm/cm
 F1HZCM 293.26236 Hz/cm



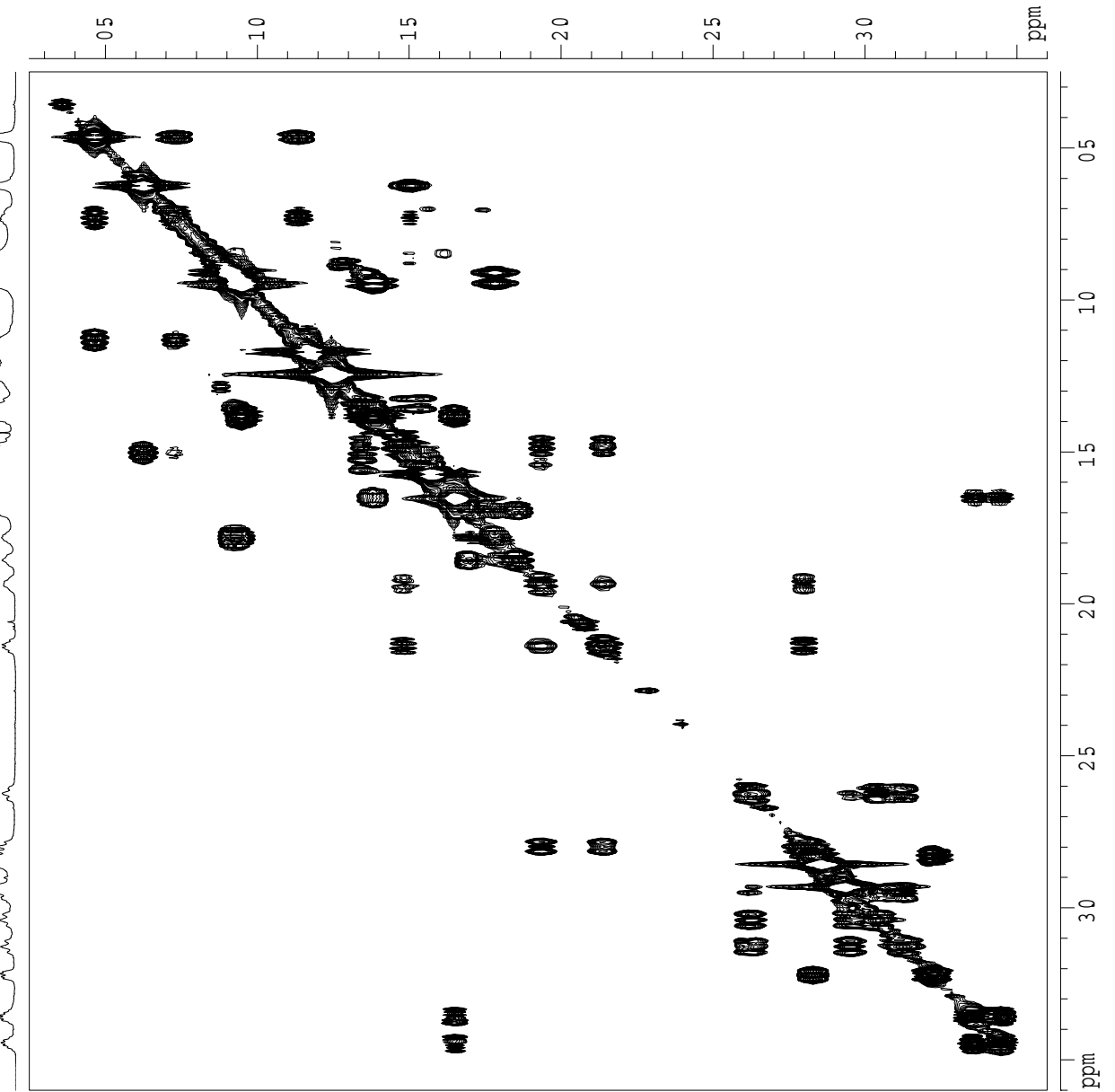
Supporting Information

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Current Data Parameters
 USER slevin
 NAME SL-7-137-800-H
 EXPNO 3
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20061108
 Time_ 0.00
 INSTRUM varian
 PROBHD 40:5mm broadband
 PULPROG gcosy
 TD 4096
 SOLVENT cdcl3
 NS 16
 DS 64
 SWH 11001.101 Hz
 FIDRES 2.685816 Hz
 AQ 0.1843700 sec
 RG 4096
 DW 45.450 usec
 DE 231.43 usec
 TE 268.5 K

F1 - Acquisition Parameters
 ND0 1
 TD 512
 SFO1 799.8107 MHz
 FIDRES 21.486525 Hz
 SW 13.755 ppm
 FMODE undefined

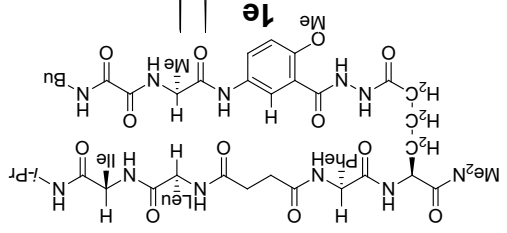


F2 - Processing parameters
 SI 4096
 SF 799.8064116 MHz
 WDW SINE
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.40

F1 - Processing parameters
 SI 512
 MC2 QF
 SF 799.8064116 MHz
 WDW SINE
 SSB 0
 LB 0.00 Hz
 GB 0

2D NMR plot parameters
 CX2 15.00 cm
 CX1 15.00 cm
 F2PLO 3.600 ppm
 F2LO 2879.30 Hz
 F2PHI 0.250 ppm
 F2HI 199.95 Hz
 F1PLO 3.600 ppm
 F1LO 2879.30 Hz
 F1PHI 0.250 ppm
 F1HI 199.75 Hz
 F2PFCM 0.22333 ppm/cm
 F2HZCM 178.62343 Hz/cm
 F1PFCM 0.22335 ppm/cm
 F1HZCM 178.63680 Hz/cm

800 MHz COSY Spectrum of **1e** in CDCl₃
 268 K (-5 °C), 1 mM



Supporting Information

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Current Data Parameters
 USER slevin
 NAME SL-7-137-800-H
 EXPNO 4
 PROCNO 1

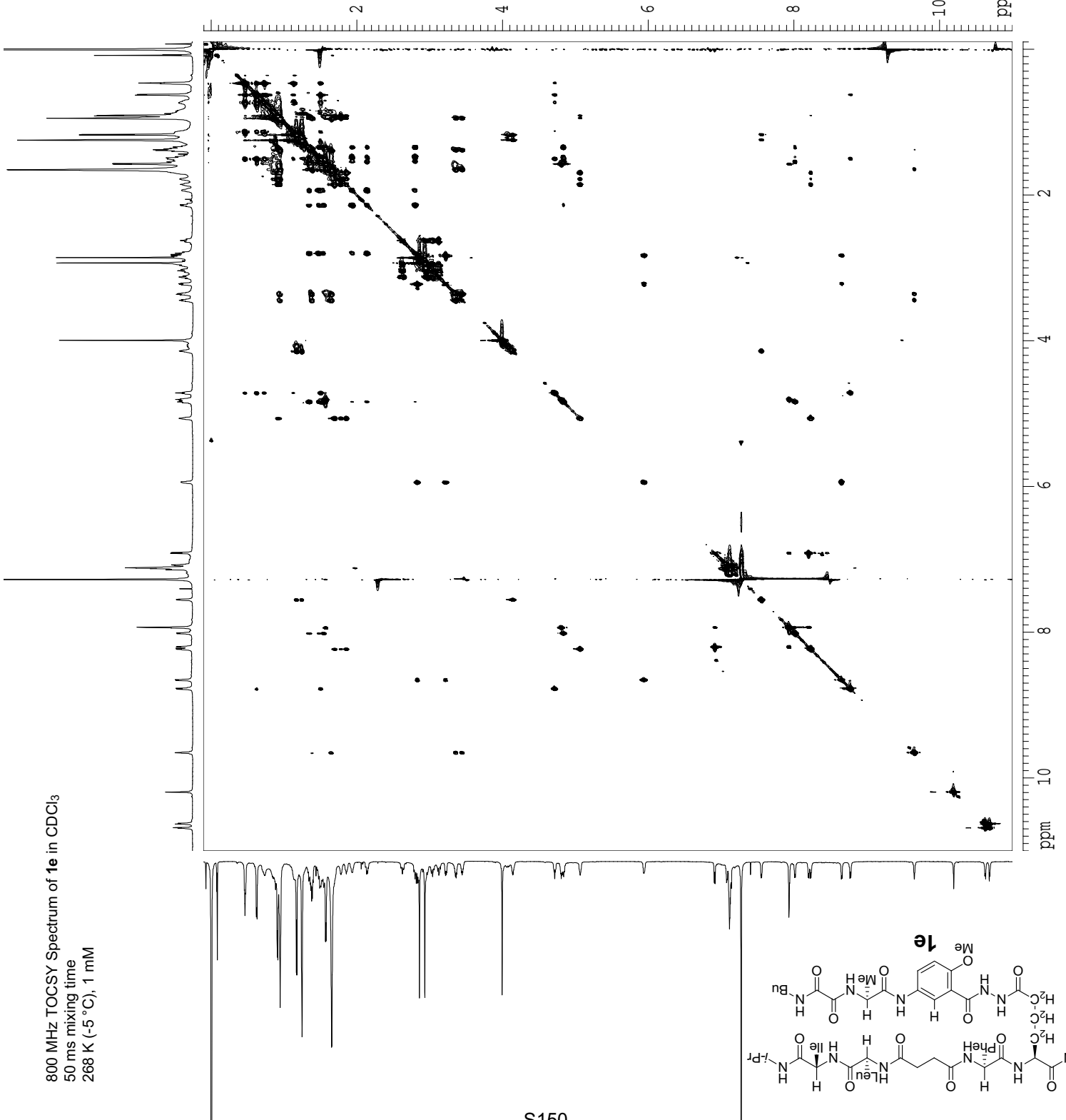
F2 - Acquisition Parameters
 Date_ 20061108
 Time 0.00
 INSTRUM varian
 PROBHD 40:5mmbroadban
 PULPROG wgtocsy_bn
 TD 4096
 SOLVENT CDCl3
 NS 16
 DS 64
 SWH 11001.101 Hz
 FIDRES 2.685816 Hz
 AQ 0.1862132 sec
 RG 287.4
 DW 45.450 usec
 DE 6.00 usec
 TE 268.5 K

F1 - Acquisition parameters
 ND0 1
 TD 512
 SFO1 799.8107 MHz
 FIDRES 21.486525 Hz
 SW 13.755 ppm
 FwMODE undefined

F2 - Processing parameters
 SI 2048
 SF 799.8064116 MHz
 WDW QSIINE
 SSB 2
 LB 0.00 Hz
 GB 0
 PC 1.40

F1 - Processing parameters
 SI 2048
 MC2 States
 SF 799.8064116 MHz
 WDW QSIINE
 SSB 2
 LB 0.00 Hz
 GB 0

2D NMR plot parameters
 CX2 15.00 cm
 CX1 15.00 cm
 F2PLO 11.002 ppm
 F2LLO 8799.73 Hz
 F2PHI -0.106 ppm
 F2HI -84.95 Hz
 F1PLO 11.002 ppm
 F1LLO 8799.73 Hz
 F1PHI -0.106 ppm
 F1HI -84.95 Hz
 F2PPMCM 0.74057 ppm/cm
 F2HZCM 592.31183 Hz/cm
 F1PPMCM 0.74057 ppm/cm
 F1HZCM 592.31183 Hz/cm



Current Data Parameters

USER slevin
 NAME SL-7-137-800-H
 EXPNO 4
 PROCNO 1

F2 - Acquisition Parameters

Date_ 20061108
 Time_ 0.00
 INSTRUM varian
 PROBHD 40:5mmbroadban
 PULPROG wgtocpsy_bn
 TD 4096
 SOLVENT CDC13
 NS 16
 DS 64
 SWH 11001.101 Hz
 FIDRES 2.685816 Hz
 AQ 0.1862132 sec
 RG 287.4
 DW 45.450 usec
 DE 6.00 usec
 TE 268.5 K

F1 - Acquisition parameters

ND0 1
 TD 512
 SF01 799.8107 MHz
 FIDRES 21.486525 Hz
 SW 13.755 ppm
 FnmODE undefined

F2 - Processing parameters

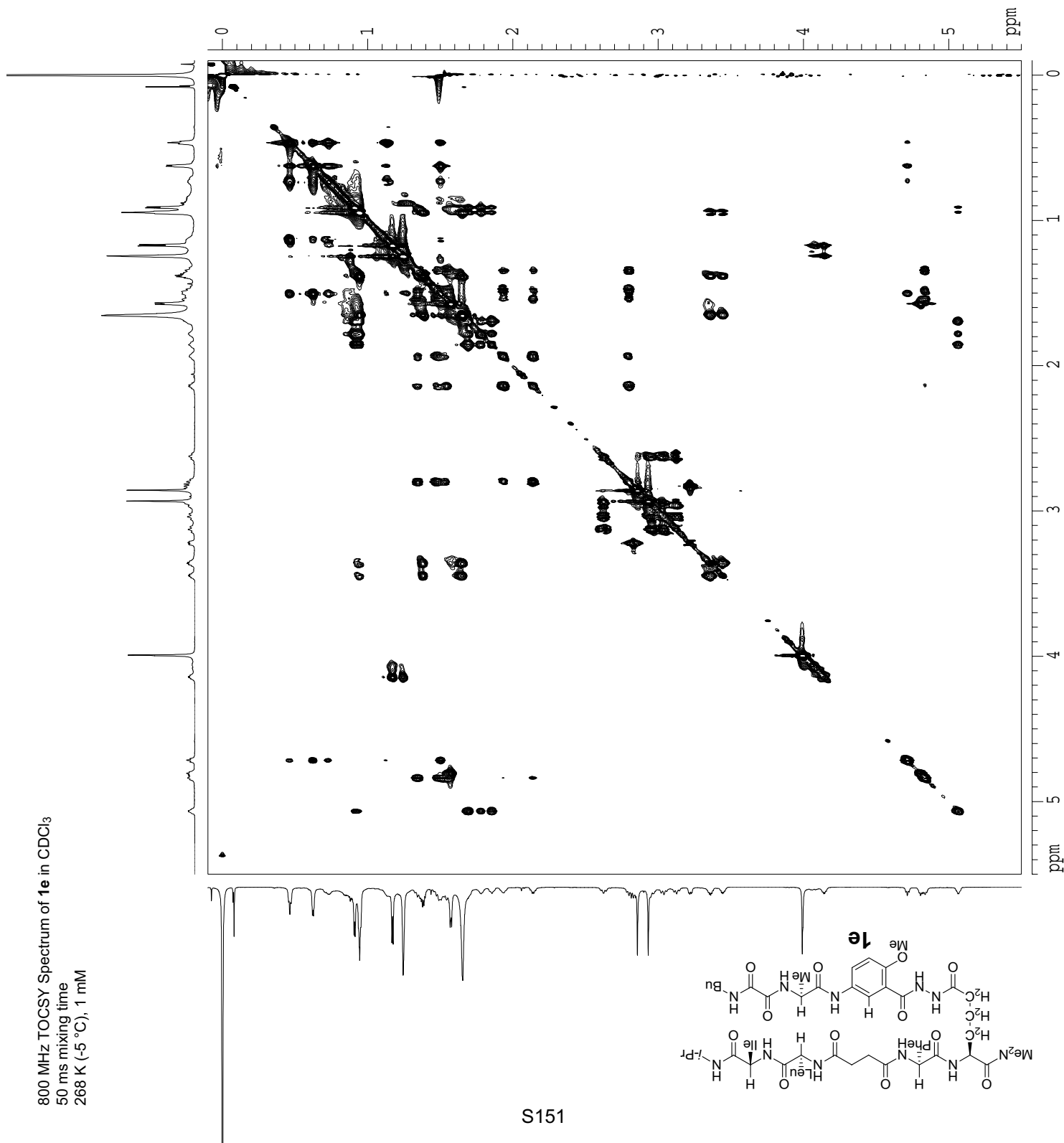
SI 2048
 SF 799.8064116 MHz
 WDW QSSINE
 SSB 2
 LB 0.00 Hz
 GB 0
 PC 1.40

F1 - Processing parameters

SI 2048
 MC2 States
 SF 799.8064116 MHz
 WDW QSSINE
 SSB 2
 LB 0.00 Hz
 GB 0

2D NMR plot parameters

CX2 15.00 cm
 CX1 15.00 cm
 F2FLO 5.500 ppm
 F2LO 4398.94 Hz
 F2PHI -0.100 ppm
 F2HI -79.98 Hz
 F1FLO 5.500 ppm
 F1LO 4398.94 Hz
 F1PHI -0.100 ppm
 F1HI -79.98 Hz
 F2PPMCM 0.37333 ppm/cm
 F2HZCM 298.59439 Hz/cm
 F1PPMCM 0.37333 ppm/cm
 F1HZCM 298.59439 Hz/cm



Current Data Parameters
 USER slevin
 NAME SL-7-137-800-H
 EXPNO 4
 PROCNO 1

F2 - Acquisition Parameters

Date_ 20061108
 Time 0.00
 INSTRUM varian
 PROBHD 40-5mm broadband
 PULPROG wgtocsy_bn
 TD 4096
 SOLVENT CDCl₃
 NS 16
 DS 64
 SWH 11001.101 Hz
 FIDRES 2.685816 Hz
 AQ 0.1862132 sec
 RG 287.4
 DW 45.450 usec
 DE 6.00 usec
 TE 268.5 K

F1 - Acquisition parameters

ND0 1
 TD 512
 SF01 799.8107 MHz
 FIDRES 21.486525 Hz
 SW 13.755 ppm
 FwMODE undefined

F2 - Processing parameters

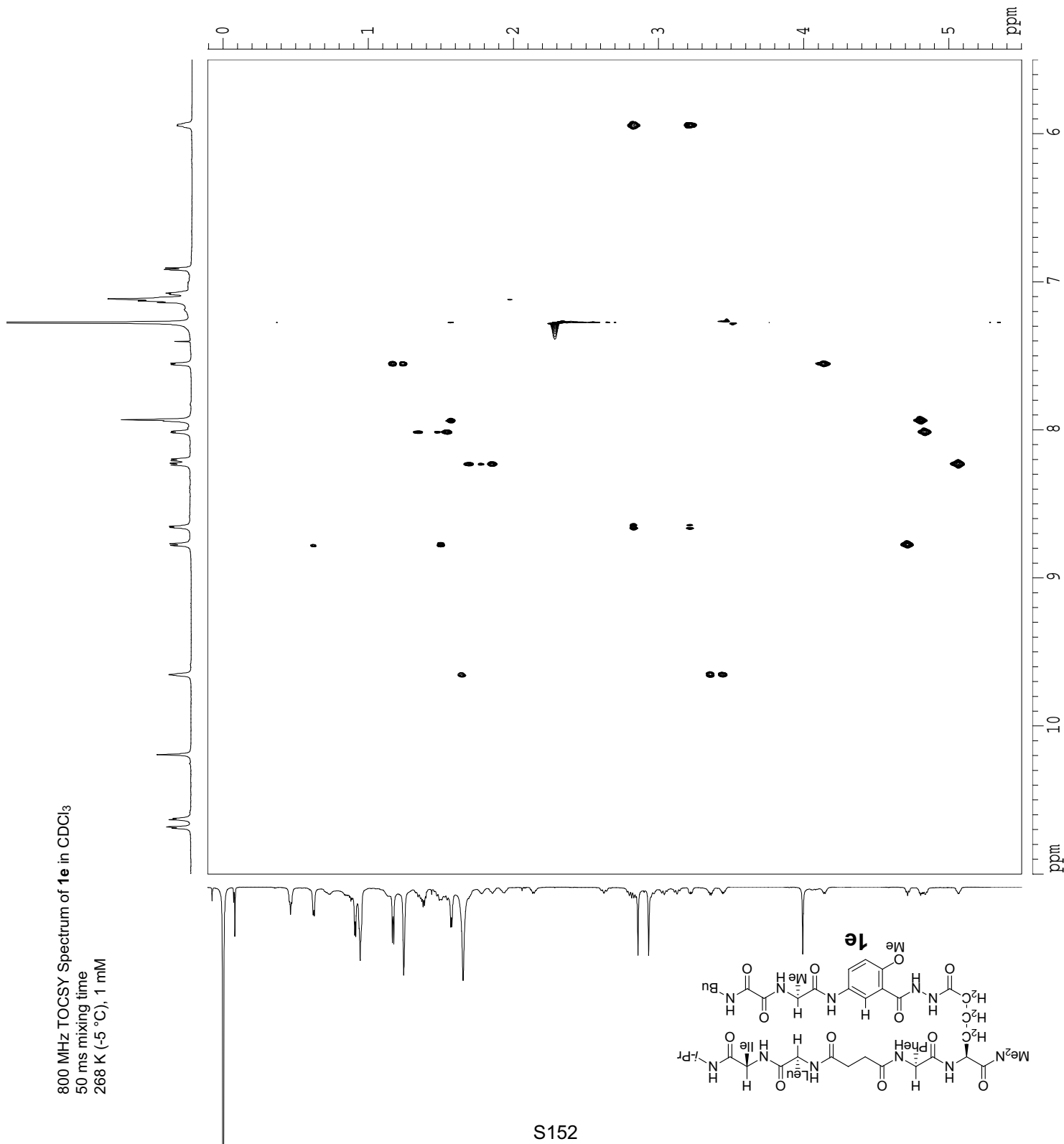
SI 2048
 SF 799.8064116 MHz
 WDW QSI
 SSB 2
 LB 0.00 Hz
 GB 0
 PC 1.40

F1 - Processing parameters

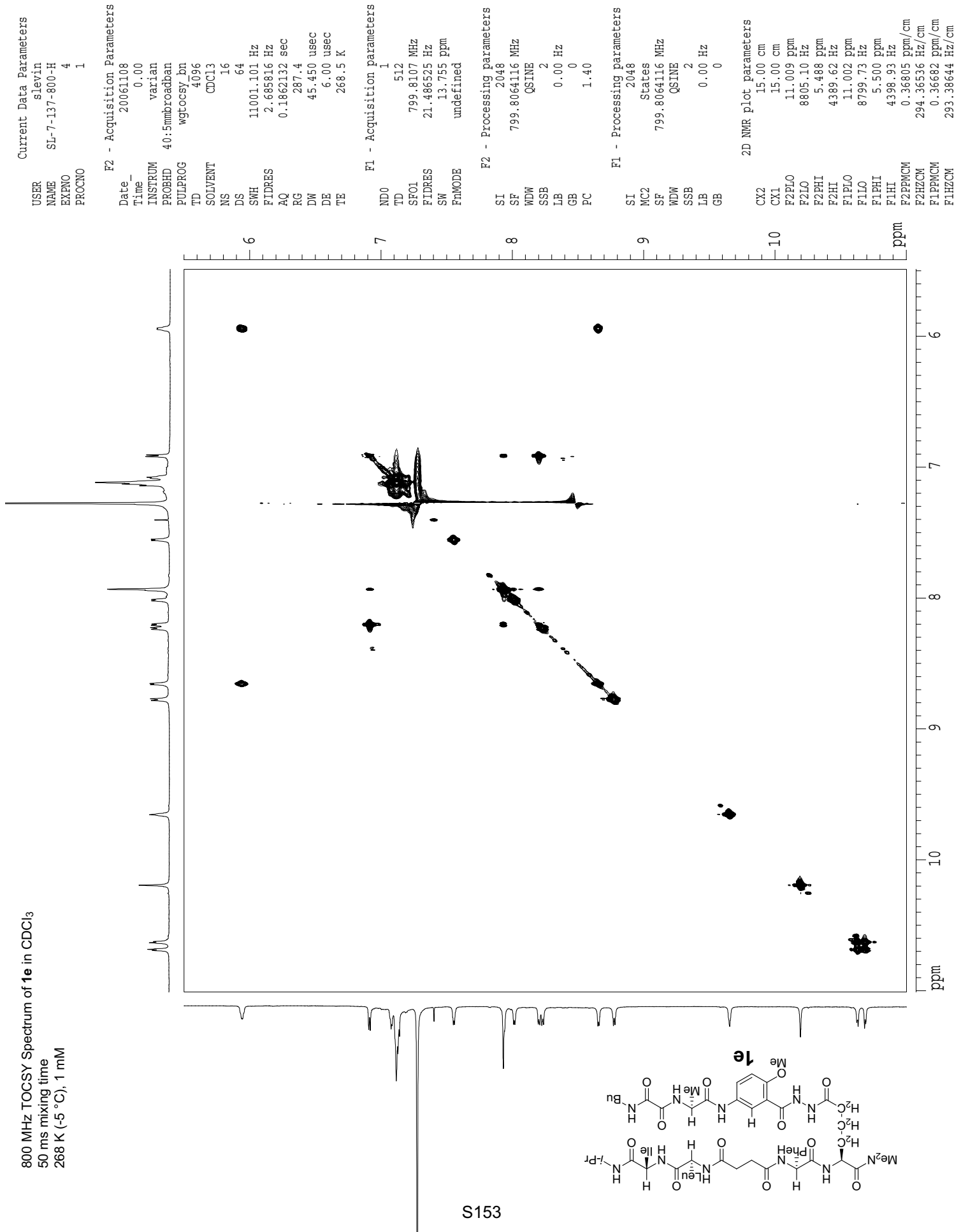
SI 2048
 MC2 States
 SF 799.8064116 MHz
 WDW QSI
 SSB 2
 LB 0.00 Hz
 GB 0

2D NMR plot parameters

CX2 15.00 cm
 CX1 15.00 cm
 F2PLO 11.000 ppm
 F2LO 8797.87 Hz
 F2PHI 5.500 ppm
 F2HI 4398.94 Hz
 F1PLO 5.502 ppm
 F1LO 4400.37 Hz
 F1PHI -0.106 ppm
 F1HI -84.95 Hz
 F2PPMCM 0.36667 ppm/cm
 F2HZCM 293.26236 Hz/cm
 F1PPMCM 0.37387 ppm/cm
 F1HZCM 299.02078 Hz/cm



800 MHz TOCSY Spectrum of **1e** in CDCl₃
 50 ms mixing time
 268 K (-5 °C), 1 mM



Current Data Parameters
 USER slevin
 NAME SL-7-137-800-H
 EXPNO 4
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20061108
 Time 0.00
 INSTRUM varian
 PROBHD 40:5mmbroadban
 PULPROG wgtocsy bt
 TD 4096
 SOLVENT CDCl3
 NS 16
 DS 64
 SWH 11001.101 Hz
 FIDRES 2.685816 Hz
 AQ 0.1862132 sec
 RG 287.4
 DW 45.450 usec
 DE 6.00 usec
 TE 268.5 K

F1 - Acquisition parameters
 ND0 1
 TD 512
 SF01 799.8107 MHz
 FIDRES 21.486525 Hz
 SW 13.755 ppm
 F1MODE undefined

F2 - Processing parameters
 SI 2048
 SF 799.8064116 MHz
 WDW QSINE
 SSB 2
 LB 0.00 Hz
 GB 0
 PC 1.40

F1 - Processing parameters
 SI 2048
 MC2 States
 SF 799.8064116 MHz
 WDW QSINE
 SSB 2
 LB 0.00 Hz
 GB 0

2D NMR plot parameters
 CX2 15.00 cm
 CX1 15.00 cm
 F2PLO 11.009 ppm
 F2LO 8805.10 Hz
 F2PHI 5.488 ppm
 F2HI 4389.62 Hz
 F1PLO 11.002 ppm
 F1LO 8799.73 Hz
 F1PHI 5.500 ppm
 F1HI 4398.93 Hz
 F2PPMCM 0.36805 ppm/cm
 F2HZCM 294.36536 Hz/cm
 F1PPMCM 0.36682 ppm/cm
 F1HZCM 293.38644 Hz/cm

Supporting Information

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Current Data Parameters
 USER slevin
 NAME SL-7-137-800-H
 EXPNO 4
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20061108
 Time 0.00
 INSTRUM varian
 PROBHD 40.5mmroadban
 PULPROG wgtocsy_bn
 TD 4096
 SOLVENT CDCl3
 NS 16
 DS 64
 SWH 11001.101 Hz
 FIDRES 2.685816 Hz
 AQ 0.1862132 sec
 RG 287.4
 DW 45.450 usec
 DE 6.00 usec
 TE 268.5 K

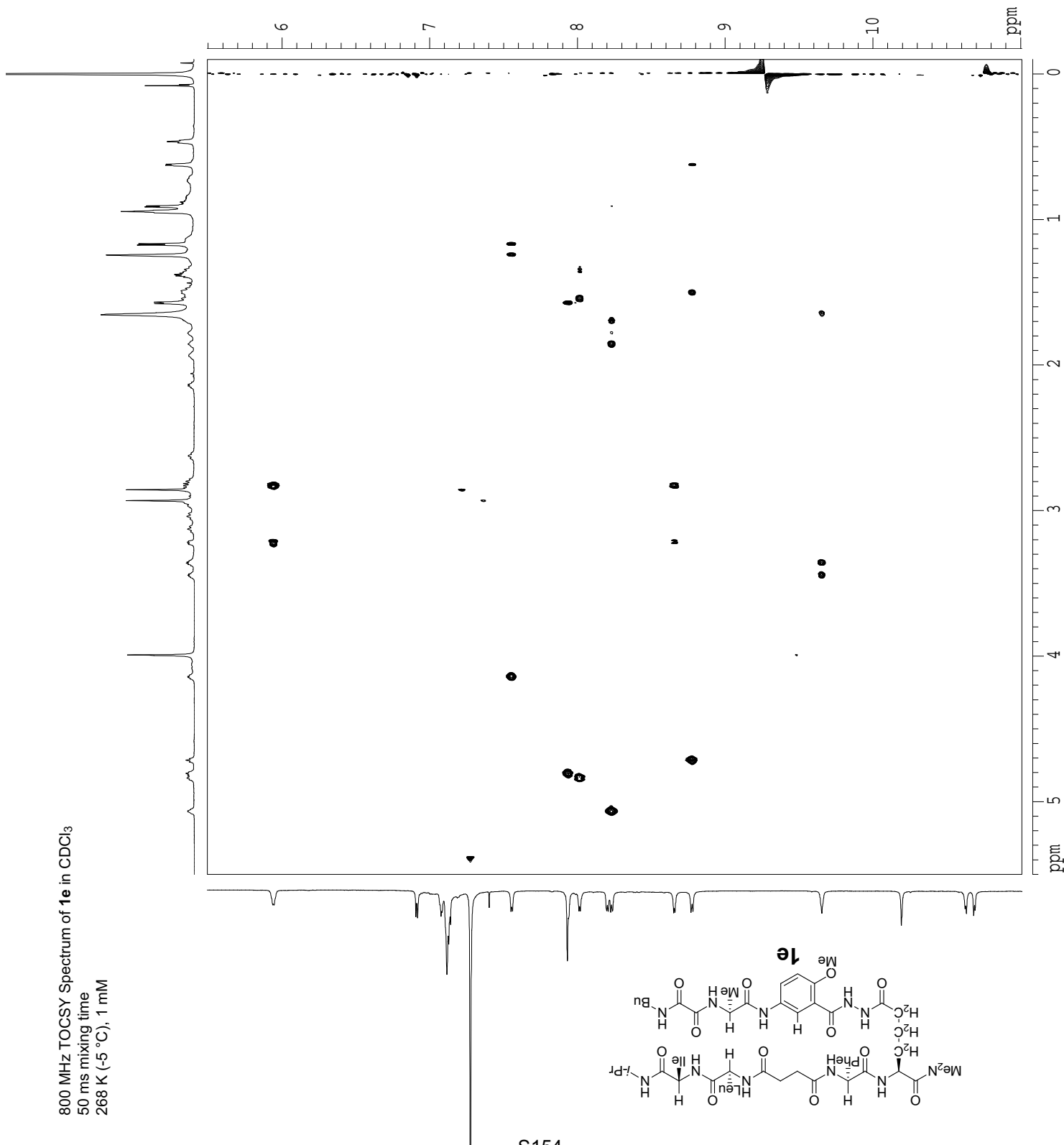
F1 - Acquisition Parameters
 ND0 1
 TD 512
 SF01 799.8107 MHz
 FIDRES 21.486525 Hz
 SW 13.755 ppm
 F1MODE undefined

F2 - Processing parameters
 SI 2048
 SF 799.8064116 MHz
 WDW QSI
 SSB 2
 LB 0.00 Hz
 GB 0
 PC 1.40

F1 - Processing parameters
 SI 2048
 MC2 States
 SF 799.8064116 MHz
 WDW QSI
 SSB 2
 LB 0.00 Hz
 GB 0

2D NMR plot parameters
 CX2 15.00 cm
 CX1 15.00 cm
 F2PLO 5.500 ppm
 F2LO 4398.94 Hz
 F2PHI -0.100 ppm
 F2HI -79.98 Hz
 F1PLO 11.009 ppm
 F1LO 8805.10 Hz
 F1PHI 5.495 ppm
 F1HI 4394.99 Hz
 F2PPMCM 0.37333 ppm/cm
 F2HZCM 298.59439 Hz/cm
 F1PPMCM 0.36760 ppm/cm
 F1HZCM 294.00726 Hz/cm

800 MHz TOCSY Spectrum of **1e** in CDCl₃
 50 ms mixing time
 268 K (-5 °C), 1 mM



Supporting Information

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Current Data Parameters
 USER slevin
 NAME SL-7-137-800-H
 EXPNO 4
 PROCNO 1

F2 - Acquisition Parameters

Date_ 20061108
 Time_ 0.00
 INSTRUM varian
 PROBHD 40:5mmbroadban
 PULPROG wgtocsy_bn
 TD 4096
 SOLVENT CDCl3
 NS 16
 DS 64
 SWH 11001.101 Hz
 FIDRES 2.685816 Hz
 AQ 0.1862132 sec
 RG 287.4
 DW 45.450 usec
 DE 6.00 usec
 TE 268.5 K

F1 - Acquisition parameters

ND0 1
 TD 512
 SFO1 799.8107 MHz
 FIDRES 21.486525 Hz
 SW 13.755 ppm
 F1MODE undefined

F2 - Processing parameters

SI 2048
 SF 799.8064116 MHz
 WDW QSTINE
 SSB 2
 LB 0.00 Hz
 GB 0
 PC 1.40

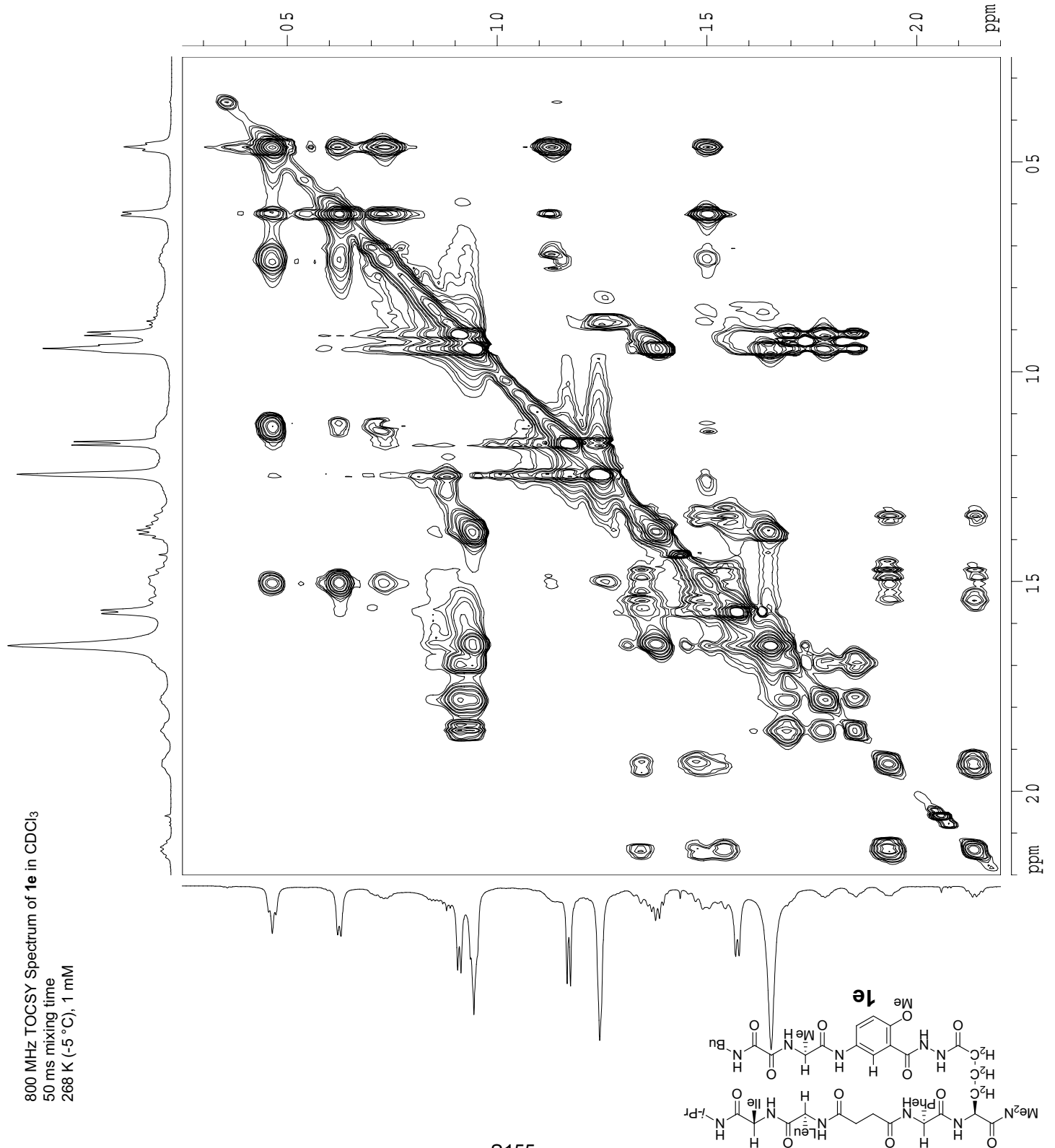
F1 - Processing parameters

SI 2048
 MC2 States
 SF 799.8064116 MHz
 WDW QSTINE
 SSB 2
 LB 0.00 Hz
 GB 0

2D NMR plot parameters

CX2 15.00 cm
 CX1 15.00 cm
 F2PLO 2.200 ppm
 F2LO 1759.57 Hz
 F2PHI 0.250 ppm
 F2HI 199.75 Hz
 F1PLO 2.200 ppm
 F1LO 1759.57 Hz
 F1PHI 0.250 ppm
 F1HI 199.75 Hz
 F2PPMCM 0.13002 ppm/cm
 F2HZCM 103.98820 Hz/cm
 F1PPMCM 0.13002 ppm/cm
 F1HZCM 103.98820 Hz/cm

800 MHz TOCSY Spectrum of **1e** in CDCl₃
 50 ms mixing time
 268 K (-5 °C), 1 mM



Supporting Information

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Current Data Parameters
 USER slevin
 NAME SL-7-137-800-H
 EXNO 5
 PROCNO 1

F2 - Acquisition Parameters

Date_ 20061108
 Time 0.00
 INSTRUM varian
 PROBHD 40:5mm broadband
 PULPROG noesyh2o_pfg_800_pln
 TD 4096
 SOLVENT CDCl3
 NS 16
 DS 64
 SMH 11001.101 Hz
 FIDRES 2.685816 Hz
 AQ 0.1862132 sec
 RG 128
 DW 45.450 usec
 DE 6.00 usec
 TE 268.5 K

F1 - Acquisition parameters

ND0 1
 TD 512
 SF01 799.8107 MHz
 FIDRES 21.486525 Hz
 SW 13.755 ppm
 F1MODE undefined

F2 - Processing parameters

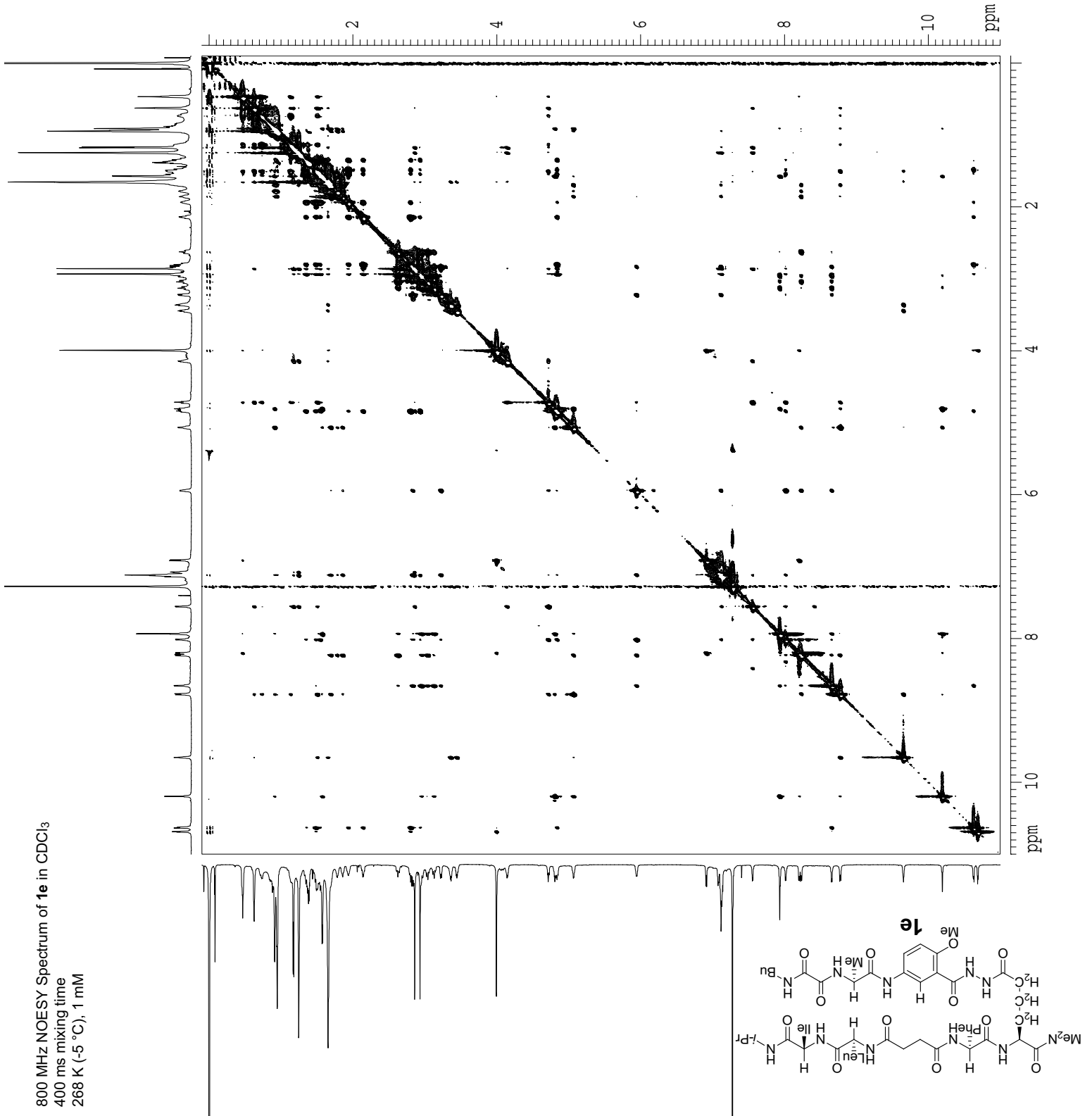
SI 4096
 SF 799.8064116 MHz
 QSI 2
 SSB 2
 LB 0.00 Hz
 GB 0
 PC 1.40

F1 - Processing parameters

SI 1024
 MC2 States
 SF 799.8064116 MHz
 QSI 2
 SSB 2
 LB 0.00 Hz
 GB 0

2D NMR plot parameters

CX2 15.00 cm
 CX1 15.00 cm
 F2PLO 11.000 ppm
 F2LO 8797.87 Hz
 F2PHI -0.100 ppm
 F2HI -79.98 Hz
 F1PLO 11.000 ppm
 F1LO 8797.87 Hz
 F1PHI -0.100 ppm
 F1HI -79.98 Hz
 F2PPMCM 0.74000 ppm/cm
 F2HZCM 591.85669 Hz/cm
 F1PPMCM 0.74000 ppm/cm
 F1HZCM 591.85669 Hz/cm



800 MHz NOESY Spectrum of **1e** in CDCl₃
 400 ms mixing time
 268 K (-5 °C), 1 mM

Supporting Information

S. Levin and J. S. Nowick

Current Data Parameters
 USER slevin
 NAME SL-7-137-800-H
 EXPNO 5
 PROCNO 1

F2 - Acquisition Parameters

Date_ 20061108
 Time 0.00
 INSTRUM varian
 PROBHD 40:5mm broadband
 PULPROG noesyh2o_pfg_800_pln
 TD 4096
 SOLVENT CDCl3
 NS 16
 DS 64
 SWH 11001.101 Hz
 FIDRES 2.685816 Hz
 AQ 0.1862132 sec
 RG 128
 DW 45.450 usec
 DE 6.00 usec
 TE 268.5 K

F1 - Acquisition Parameters

ND0 1
 TD 512
 SF01 799.8107 MHz
 FIDRES 21.486525 Hz
 SW 13.755 ppm
 F1MODE undefined

F2 - Processing parameters

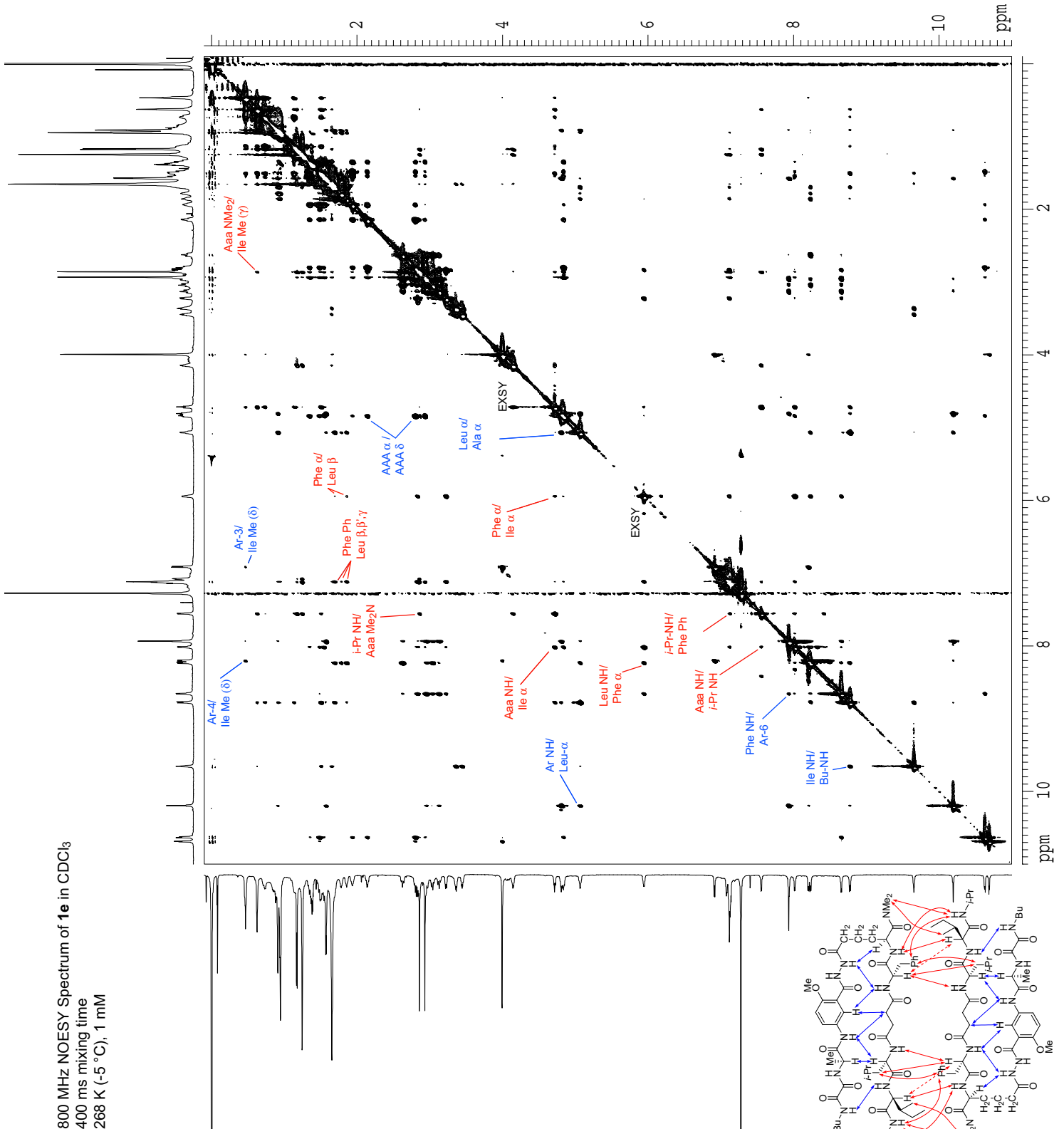
SI 4096
 SF 799.8064116 MHz
 QSIINE QSIINE
 SSB 2
 LB 0.00 Hz
 GB 0
 PC 1.40

F1 - Processing parameters

SI 1024
 MC2 States
 SF 799.8064116 MHz
 QSIINE QSIINE
 SSB 2
 LB 0.00 Hz
 GB 0

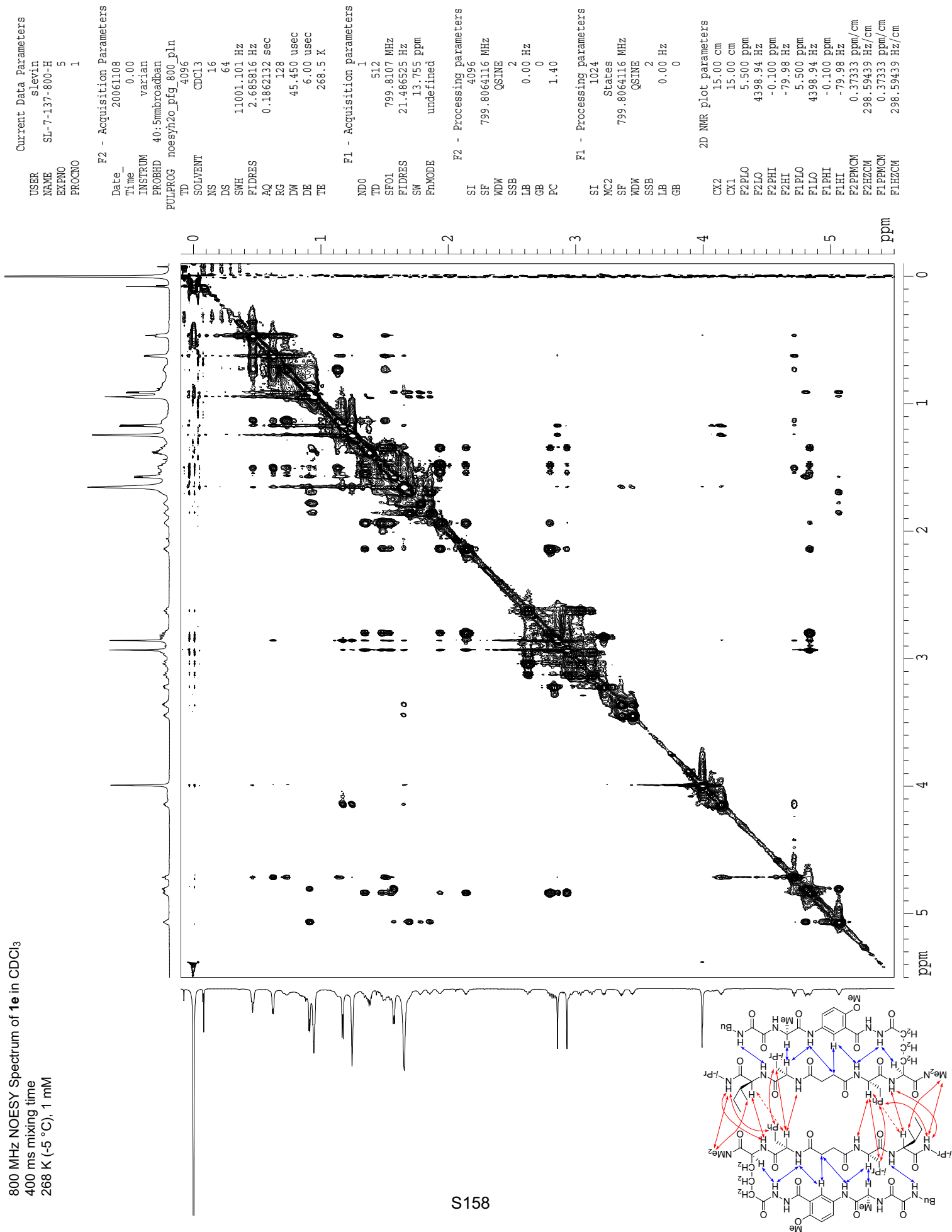
2D NMR plot parameters

CX2 15.00 cm
 CX1 15.00 cm
 F2PLO 11.000 ppm
 F2LO 8797.87 Hz
 F2PHI -0.100 ppm
 F2HI -79.98 Hz
 F1PLO 11.000 ppm
 F1LO 8797.87 Hz
 F1PHI -0.100 ppm
 F1HI -79.98 Hz
 F2PPMCM 0.74000 ppm/cm
 F2HZCM 591.85669 Hz/cm
 F1PPMCM 0.74000 ppm/cm
 F1HZCM 591.85669 Hz/cm



800 MHz NOESY Spectrum of **1e** in CDCl₃
 400 ms mixing time
 268 K (-5 °C), 1 mM

800 MHz NOESY Spectrum of **1e** in CDCl₃
 400 ms mixing time
 268 K (-5 °C), 1 mM



Current Data Parameters
 USER slevin
 NAME SL-7-137-800-H
 EXPNO 5
 PROCNO 1

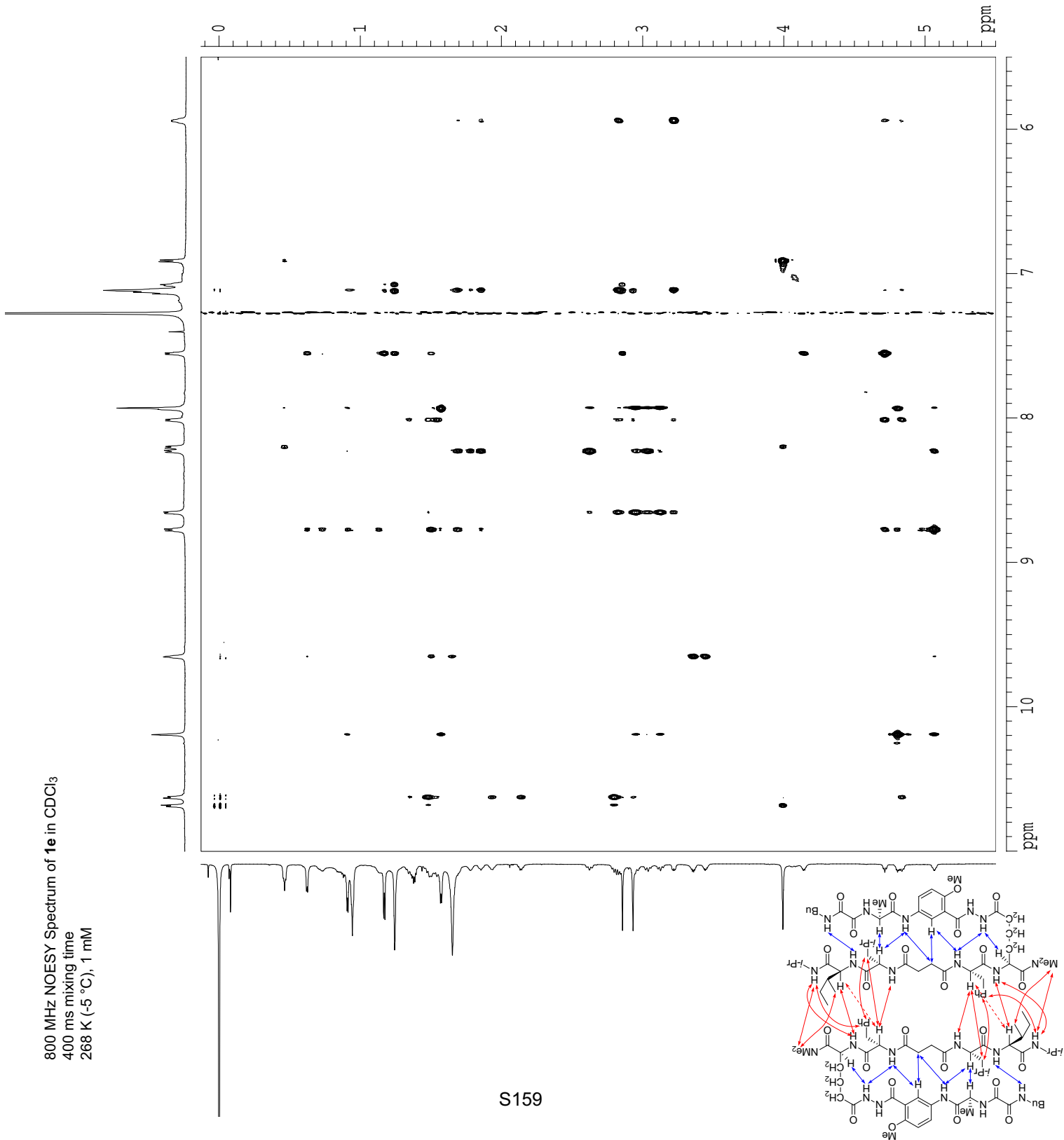
F2 - Acquisition Parameters
 Date_ 20061108
 Time_ 0.00
 INSTRUM varian
 PROBHD 40:5mm broadband
 PULPROG noesyh2o_pfg 800_p1n
 TD 4096
 SOLVENT CDCl3
 NS 16
 DS 64
 SWH 11001.101 Hz
 FIDRES 2.685816 Hz
 AQ 0.1862132 sec
 RG 128
 DW 45.450 usec
 DE 6.00 usec
 TE 268.5 K

F1 - Acquisition Parameters
 ND0 1
 TD 512
 SF01 799.8107 MHz
 FIDRES 21.486525 Hz
 SW 13.755 ppm
 FMODE undefined

F2 - Processing parameters
 SI 4096
 SF 799.8064116 MHz
 WDW QSINE
 SSB 2
 LB 0.00 Hz
 GB 0
 PC 1.40

F1 - Processing parameters
 SI 1024
 MC2 States
 SF 799.8064116 MHz
 WDW QSINE
 SSB 2
 LB 0.00 Hz
 GB 0

2D NMR plot parameters
 CX2 15.00 cm
 CX1 15.00 cm
 F2PLO 11.002 ppm
 F2LO 8799.73 Hz
 F2PHI 5.500 ppm
 F2HI 4398.93 Hz
 F1PLO 5.502 ppm
 F1LO 4400.37 Hz
 F1PHI -0.126 ppm
 F1HI -101.06 Hz
 F2PPMCM 0.36682 ppm/cm
 F2HZCM 293.38644 Hz/cm
 F1PPMCM 0.37521 ppm/cm
 F1HZCM 300.09509 Hz/cm



800 MHz NOESY Spectrum of **1e** in CDCl₃
 400 ms mixing time
 268 K (-5 °C), 1 mM

Supporting Information

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Current Data Parameters
 USER slevin
 NAME SL-7-137-800-H
 EXPNO 5
 PROCNO 1

F2 - Acquisition Parameters

Date_ 20061108
 Time 0.00
 INSTRUM varian
 PROBHD 40:5mm broadband
 PULPROG noesyh2o_pfg_800_pln
 TD 4096
 SOLVENT CDCl3
 NS 16
 DS 64
 SWH 11001.101 Hz
 FIDRES 2.685816 Hz
 AQ 0.1862132 sec
 RG 128
 DW 45.450 usec
 DE 6.00 usec
 TE 268.5 K

F1 - Acquisition Parameters

ND0 1
 TD 512
 SFO1 799.8107 MHz
 FIDRES 21.486525 Hz
 SW 13.755 ppm
 F1MODE undefined

F2 - Processing parameters

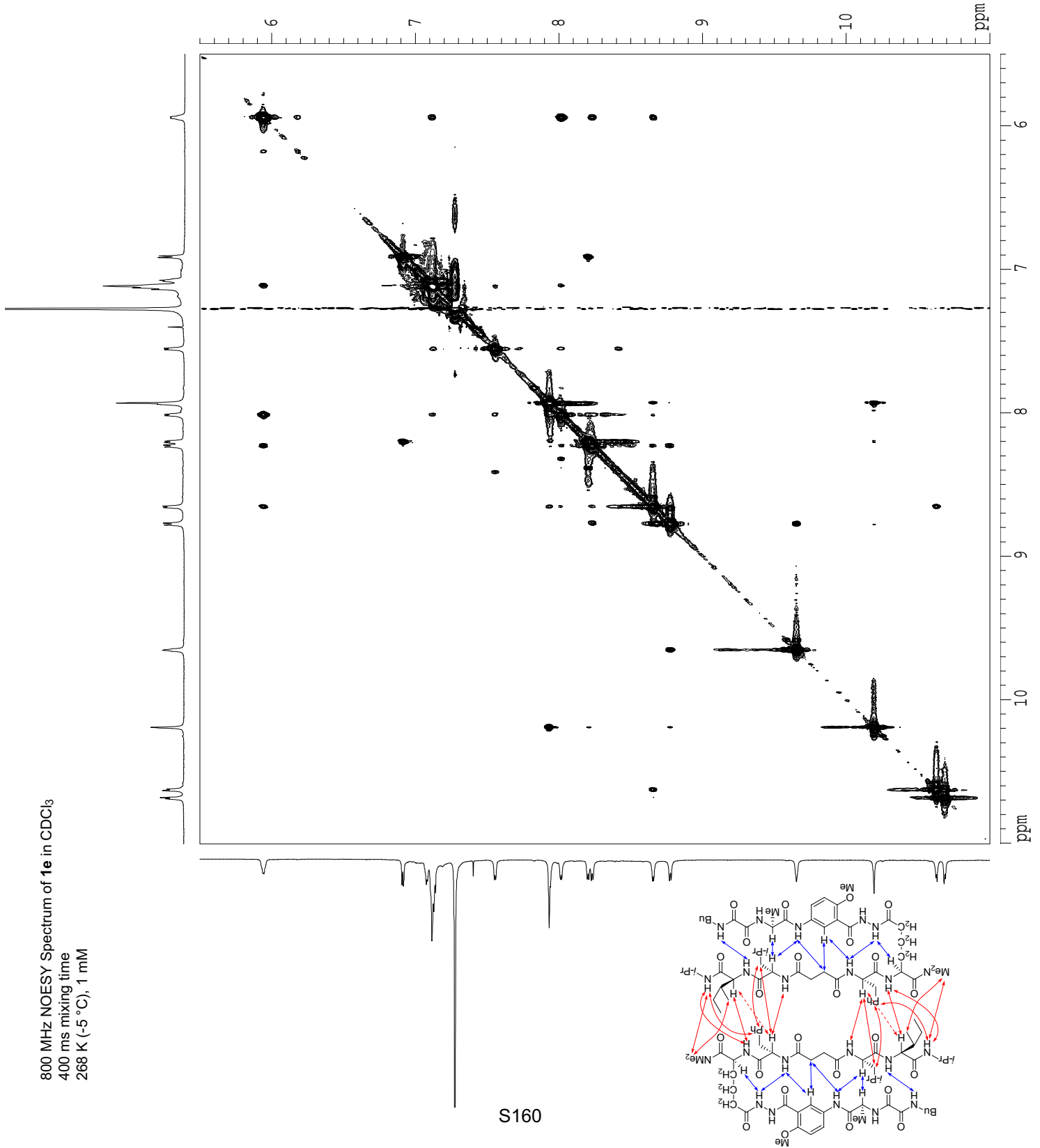
SI 4096
 SF 799.8064116 MHz
 MDW QSINE
 SSB 2
 LB 0.00 Hz
 GB 0
 PC 1.40

F1 - Processing parameters

SI 1024
 MC2 States
 SF 799.8064116 MHz
 MDW QSINE
 SSB 2
 LB 0.00 Hz
 GB 0

2D NMR plot parameters

CX2 15.00 cm
 CX1 15.00 cm
 F2PLO 11.006 ppm
 F2LO 8802.42 Hz
 F2PHI 5.500 ppm
 F2HI 4398.94 Hz
 F1PLO 11.000 ppm
 F1LO 8797.87 Hz
 F1PHI 5.500 ppm
 F1HI 4398.94 Hz
 F2PFCM 0.36705 ppm/cm
 F2H2CM 293.56552 Hz/cm
 F1PFCM 0.36667 ppm/cm
 F1H2CM 293.26236 Hz/cm



800 MHz NOESY Spectrum of **1e** in CDCl₃
 400 ms mixing time
 268 K (-5 °C), 1 mM

Current Data Parameters
 USER sleivin
 NAME SL-7-137-800-H
 EXPNO 5
 PROCNO 1

F2 - Acquisition Parameters

Date_ 20061108
 Time_ 0.00
 INSTRUM varian
 PROBHD 40:5mmbrodban
 PULPROG noesy2o_pfg_800_p1n
 TD 4096
 SOLVENT CDCl3
 NS 16
 DS 64
 SWH 11001.101 Hz
 FIDRES 2.685816 Hz
 AQ 0.1862132 sec
 RG 128
 DW 45.450 usec
 DE 6.00 usec
 TE 268.5 K

F1 - Acquisition parameters

ND0 1
 TD 512
 SF01 799.8107 MHz
 FIDRES 21.486525 Hz
 SW 13.755 ppm
 FMODE undefined

F2 - Processing parameters

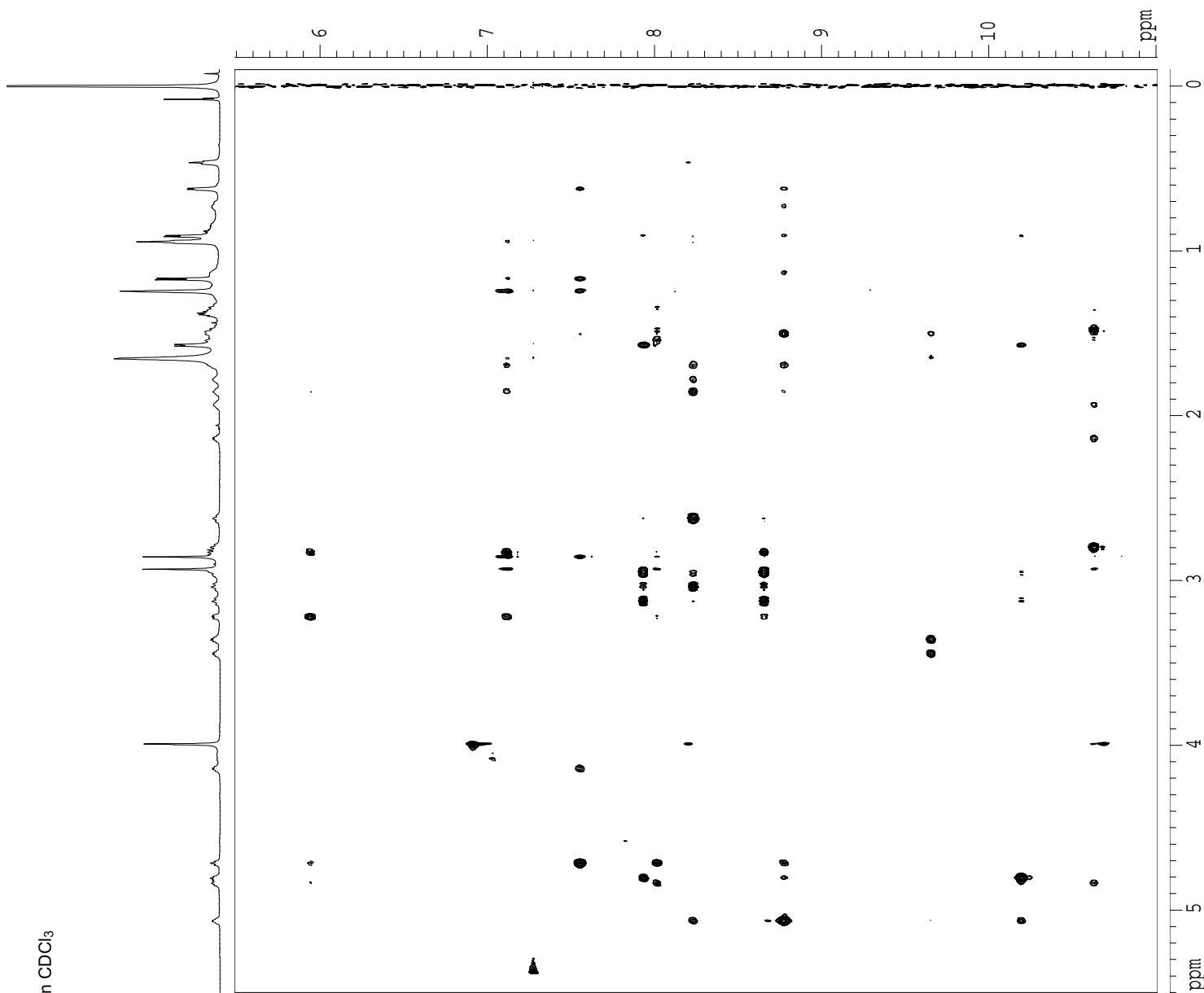
SI 4096
 SF 799.8064116 MHz
 WDM QSINE
 SSB 2
 LB 0.00 Hz
 GB 0
 PC 1.40

F1 - Processing parameters

SI 1024
 MC2 States
 SF 799.8064116 MHz
 WDM QSINE
 SSB 2
 LB 0.00 Hz
 GB 0

2D NMR plot parameters

CX2 15.00 cm
 CX1 15.00 cm
 F2PLO 5.500 ppm
 F2LO 4398.94 Hz
 F2PHI -0.100 ppm
 F2HI -79.98 Hz
 F1PLO 11.009 ppm
 F1LO 8805.10 Hz
 F1PHI 5.488 ppm
 F1HI 4389.62 Hz
 F2PPMCM 0.37333 ppm/cm
 F2HZCM 298.59439 Hz/cm
 F1PPMCM 0.36805 ppm/cm
 F1HZCM 294.36536 Hz/cm



800 MHz NOESY Spectrum of **1e** in CDCl₃
 400 ms mixing time
 268 K (-5 °C), 1 mM

Supporting Information

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Current Data Parameters
 USER slevin
 NAME SL-7-137-800-H
 EXPNO 5
 PROCNO 1

F2 - Acquisition Parameters

Date_ 20061108
 Time 0.00
 INSTRUM varian
 PROBHD 40:5mm broadband
 PULPROG noesyh2o_pfg_800_pln
 TD 4096
 SOLVENT CDCl3
 NS 16
 DS 64
 SWH 11001.101 Hz
 FIDRES 2.685816 Hz
 AQ 0.1862132 sec
 RG 128
 DW 45.450 usec
 DE 6.00 usec
 TE 268.5 K

F1 - Acquisition Parameters

ND0 1
 TD 512
 SF01 799.8107 MHz
 FIDRES 21.486525 Hz
 SW 13.755 ppm
 FMODE undefined

F2 - Processing parameters

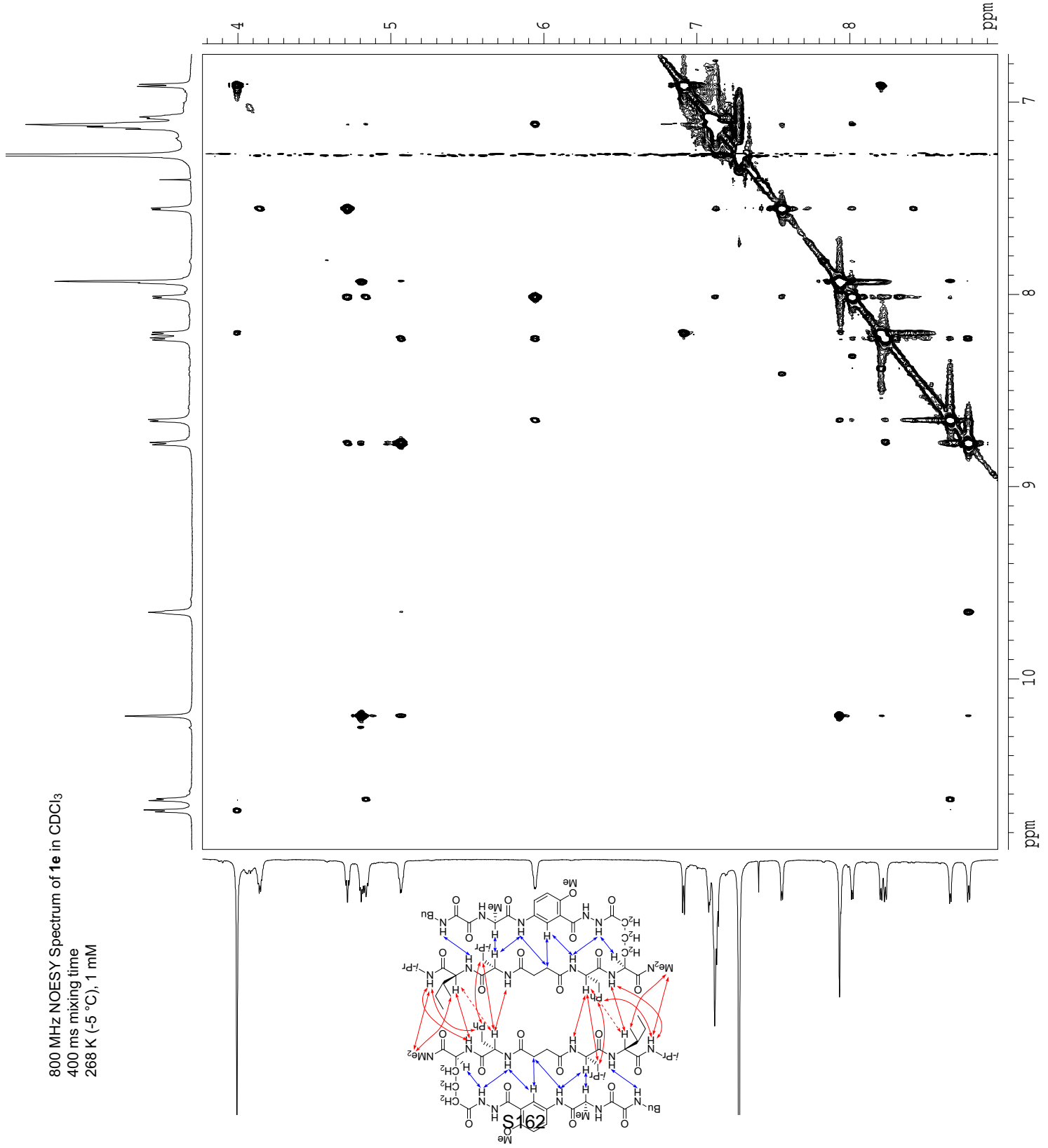
SI 4096
 SF 799.8064116 MHz
 WDW QSINE
 SSB 2
 LB 0.00 Hz
 GB 0
 PC 1.40

F1 - Processing parameters

SI 1024
 MC2 States
 SF 799.8064116 MHz
 WDW QSINE
 SSB 2
 LB 0.00 Hz
 GB 0

2D NMR plot parameters

CX2 15.00 cm
 CX1 15.00 cm
 F2PLO 10.888 ppm
 F2LO 8708.41 Hz
 F2PHI 6.751 ppm
 F2HI 5399.49 Hz
 F1PLO 8.967 ppm
 F1LO 7172.13 Hz
 F1HI 3.769 ppm
 F1HI 3014.49 Hz
 F2PNCM 0.27581 ppm/cm
 F2HZCM 220.59497 Hz/cm
 F1PNCM 0.34655 ppm/cm
 F1HZCM 277.17615 Hz/cm



800 MHz NOESY Spectrum of **1e** in CDCl₃
 400 ms mixing time
 268 K (-5 °C), 1 mM

Supporting Information

S. Levin and J. S. Nowick

Current Data Parameters
 USER slevin
 NAME SL-7-137-800-H
 EXPNO 5
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20061108
 Time 0.00

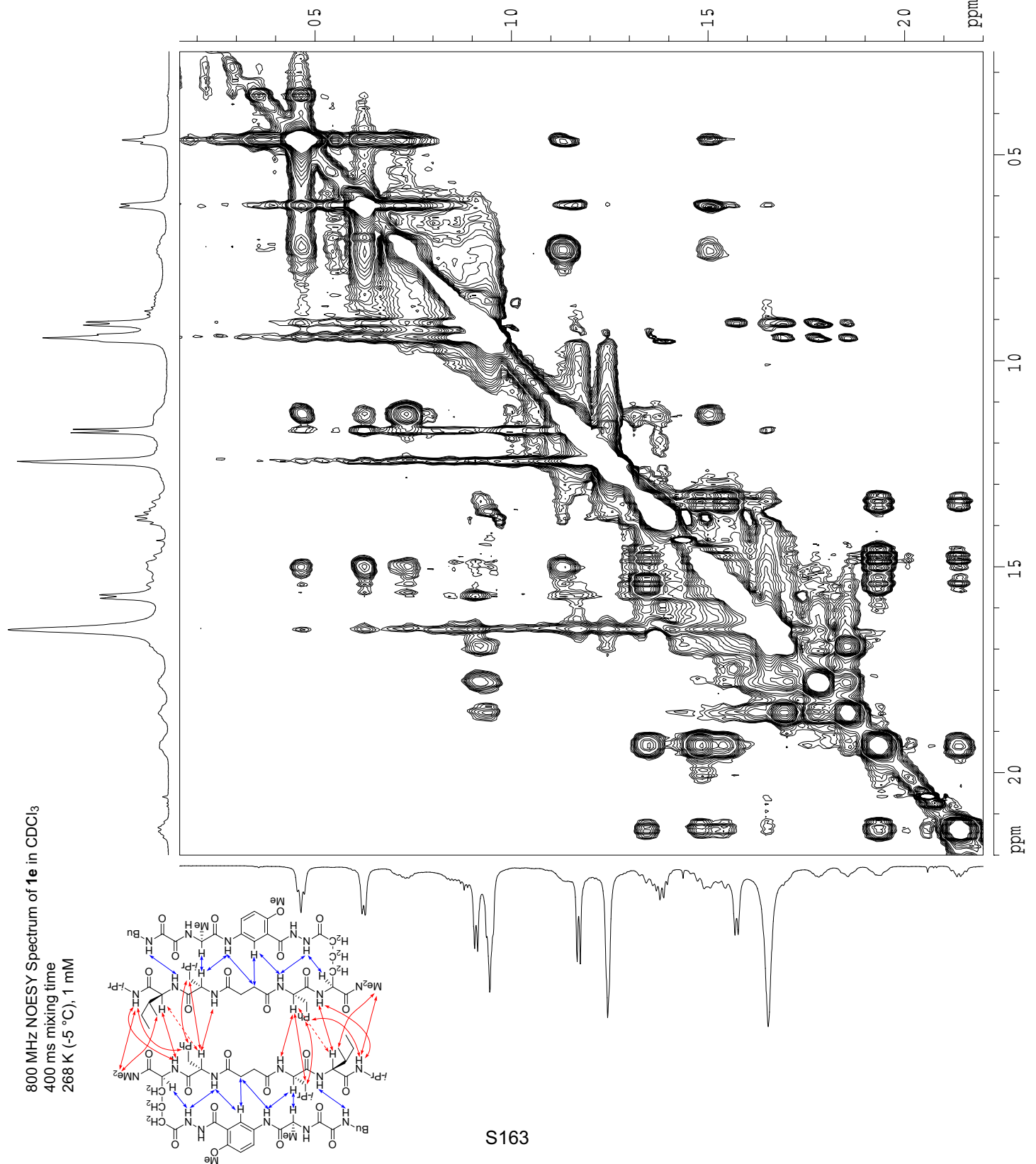
INSTRUM varian
 PROBRD 40:5mmrbroadban
 PULPROG noesyh2o_pfg_800_pln
 TD 4096
 SOLVENT CDCl3
 NS 16
 DS 64
 SWH 11001.101 Hz
 FIDRES 2.683816 Hz
 AQ 0.1862132 sec
 RG 128
 DM 45.450 usec
 DE 6.00 usec
 TE 268.5 K

F1 - Acquisition parameters
 ND0 1
 TD 512
 SF01 799.8107 MHz
 FIDRES 21.486525 Hz
 SW 13.755 ppm
 FreqMODE undefined

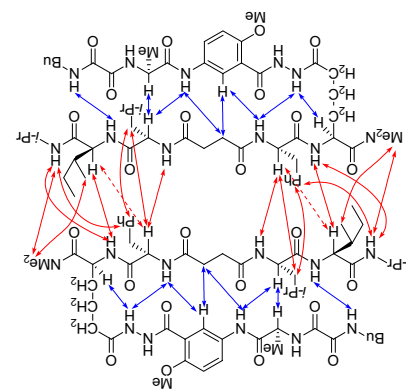
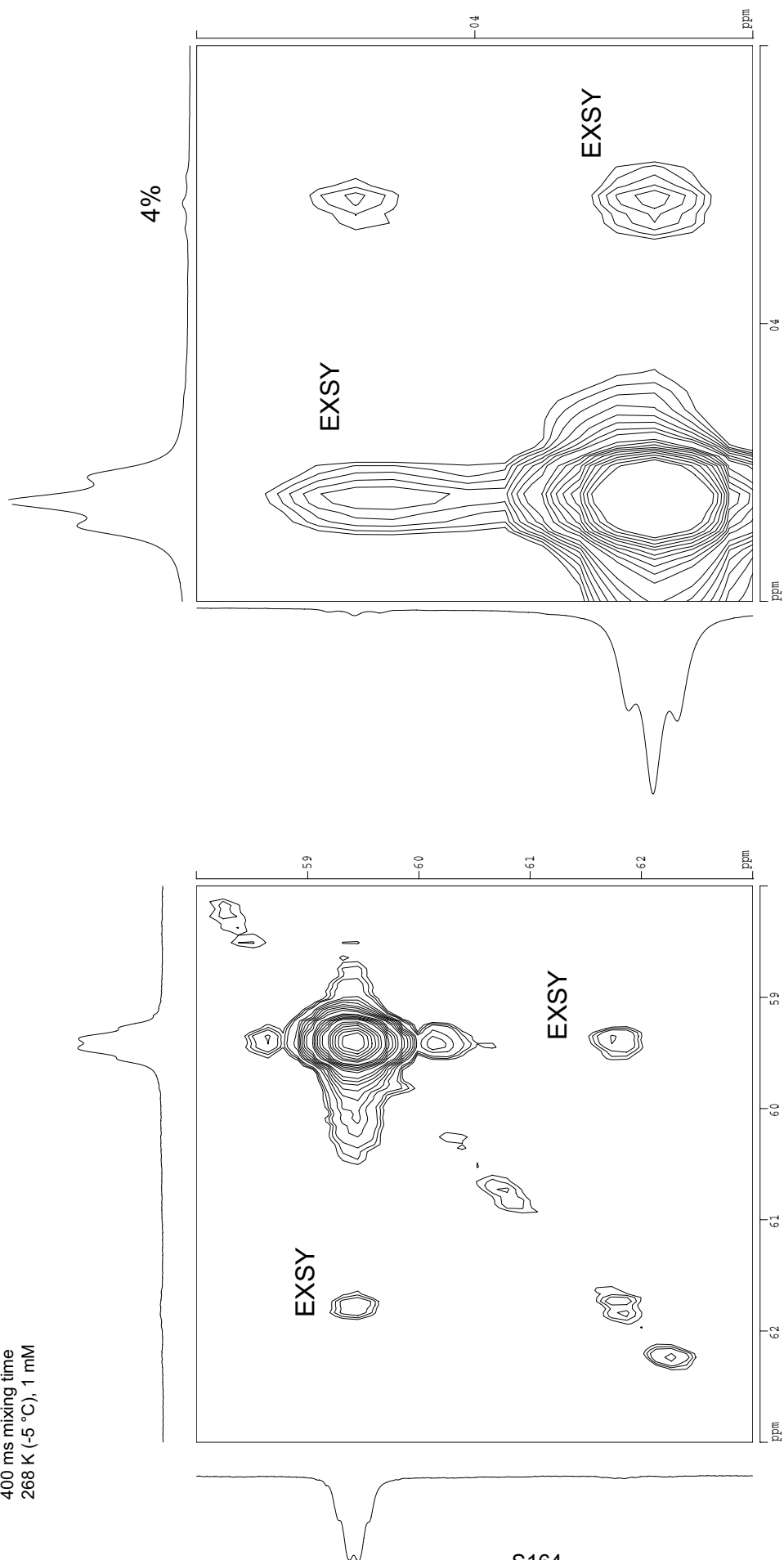
F2 - Processing parameters
 SI 4096
 SF 799.8064116 MHz
 WDM QSINE
 SSB 2
 LB 0.00 Hz
 GB 0
 PC 1.40

F1 - Processing parameters
 SI 1024
 MC2 States
 SF 799.8064116 MHz
 WDM QSINE
 SSB 2
 LB 0.00 Hz
 GB 0

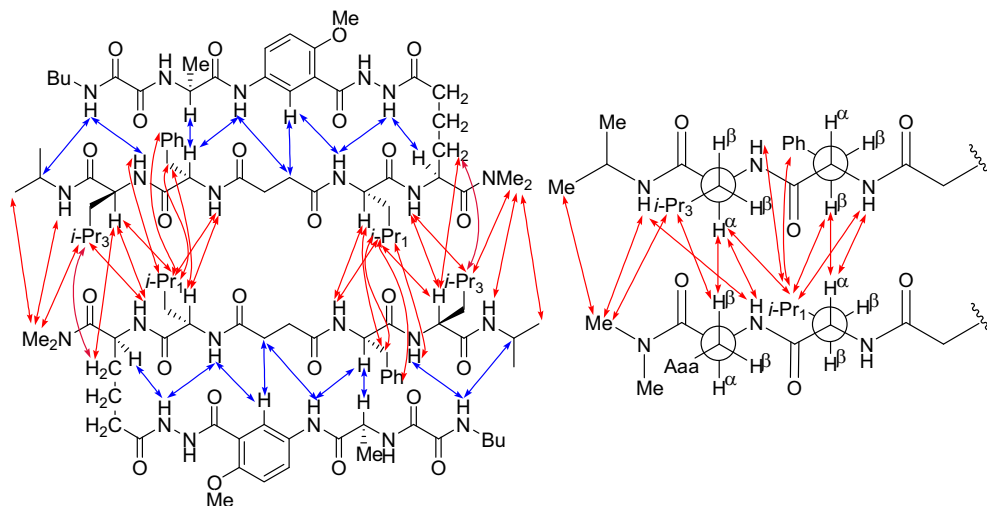
2D NMR plot parameters
 CX2 15.00 cm
 CX1 15.00 cm
 F2PLO 2.200 ppm
 F2LO 1759.57 Hz
 F2PHI 0.250 ppm
 F2HI 199.95 Hz
 F1LO 1759.57 Hz
 F1HI 124.55 Hz
 F2PPMCM 0.13000 ppm/cm
 F2HZCM 103.97483 Hz/cm
 F1PPMCM 0.13629 ppm/cm
 F1HZCM 109.00172 Hz/cm



800 MHz NOESY Spectrum of **1e** in CDCl₃
400 ms mixing time
268 K (-5 °C), 1 mM



Spectroscopic DATA for the compound **1f**
(4 mM, CDCl₃ 268K)



Key NOEs assigned as *intermolecular* are represented with red arrows.
Key NOEs assigned as *intramolecular* are represented with blue arrows.

Key data for amino acids.

Amino acid	H _α Shift ppm	NH Shift ppm	³ J _{NHα} Hz
Aaa	5.18	8.50	8.4
R ₁ = Leu ¹	5.60	8.41	8.0
R ₂ = Phe	5.13	8.55	9.7
R ₃ = Leu ²	5.07	8.80	9.7
R ₄ = Ala	4.60	8.06	overlap

Amino adipic acid (Aaa) δ proton resonances.

pro-R: 2.94 ppm, t, (*overlap*)

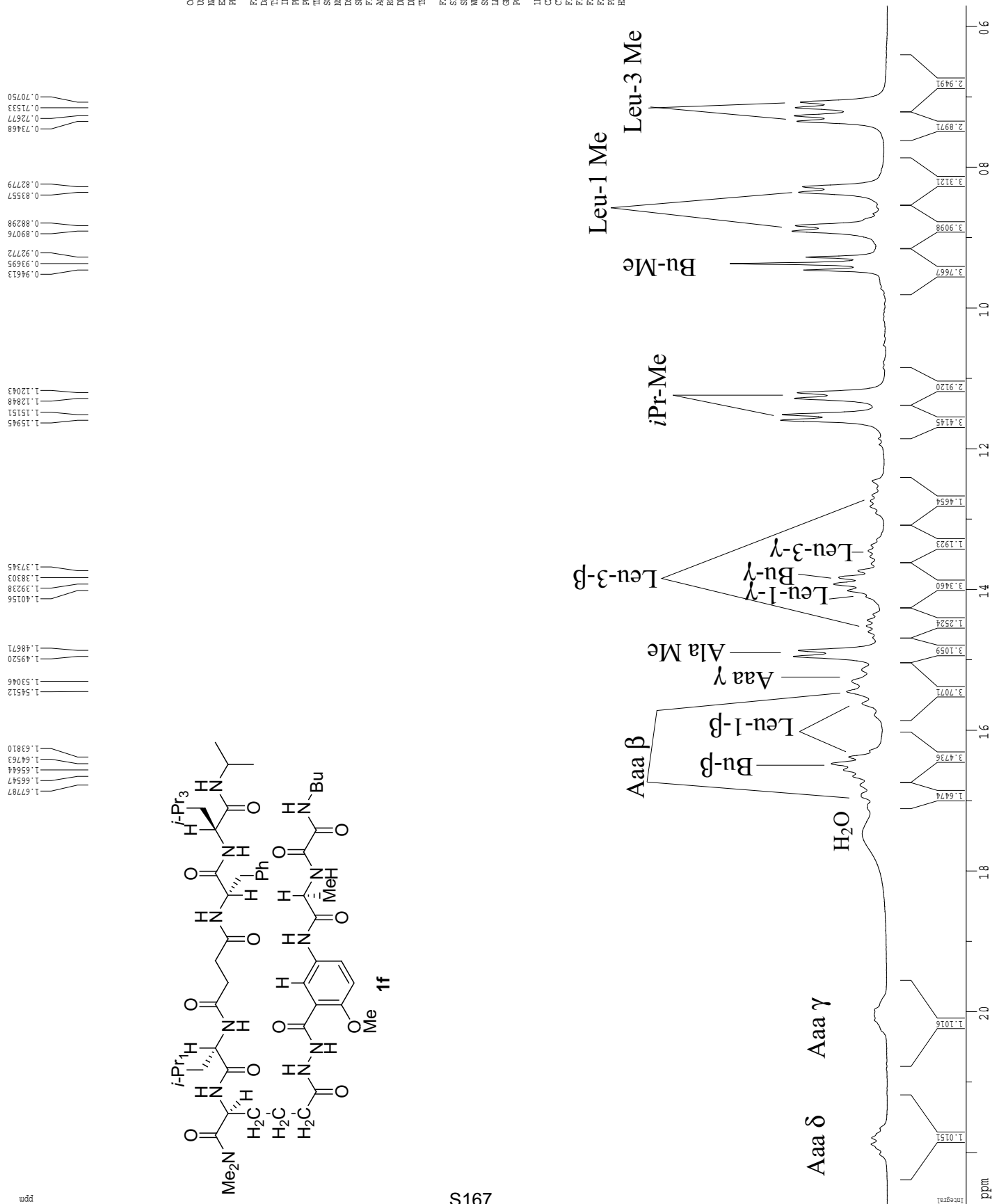
pro-S: 2.18 ppm, td, (*J*₁ = 11.2 Hz; *J*₂ = 7.0 Hz)

anisotropy = 0.76ppm

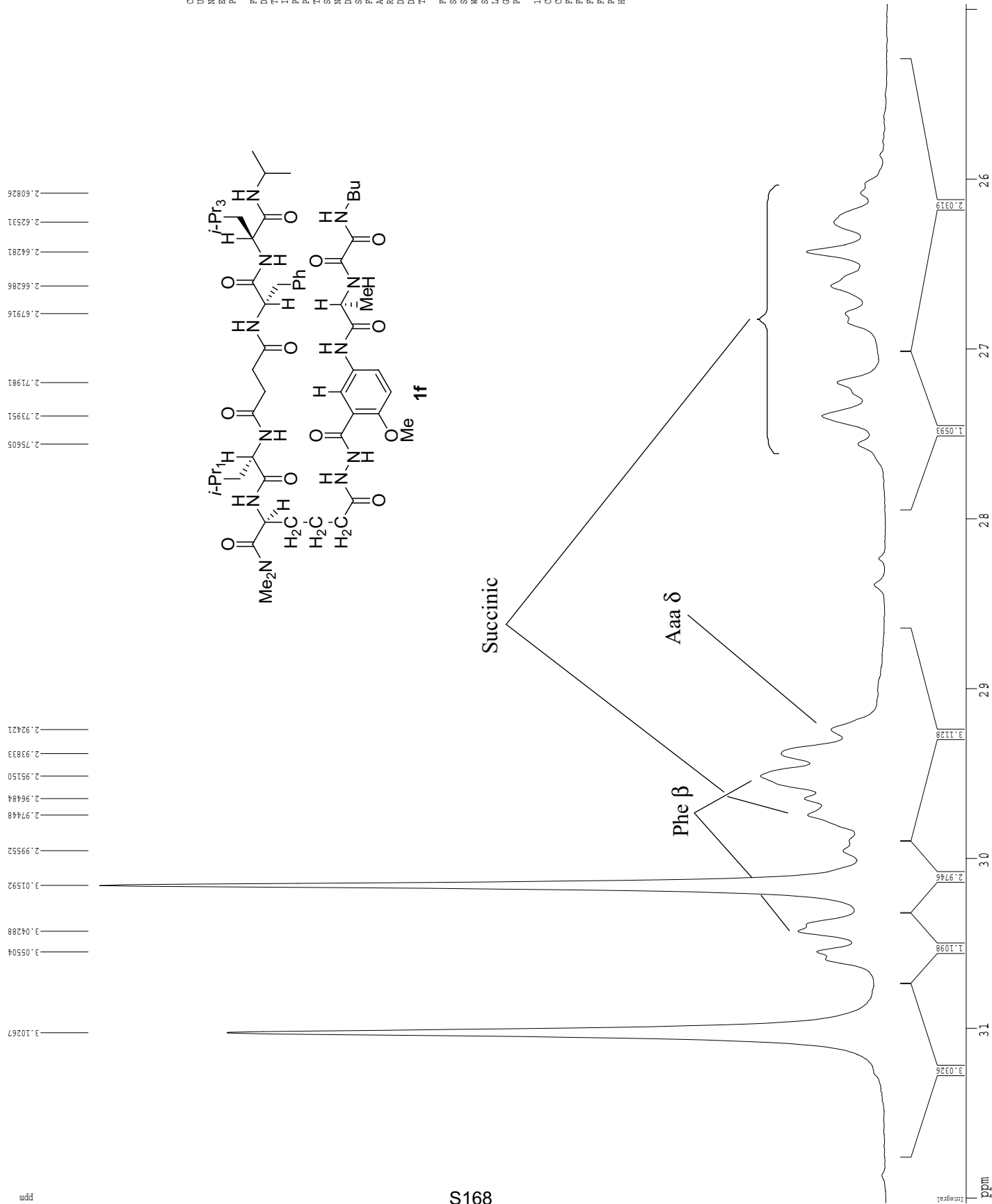
Key data for other NH protons.

Proton	NH Shift ppm	<i>J</i> Hz
Ar-NH	10.09	-
Hydrazide Ar	10.58	7.4
Hydrazide Aaa	10.40	7.4
Bu-NH	9.55	broad
<i>i</i> -Pr-NH	8.06	overlap

ESI MS *m/z* for C₅₃H₈₂N₁₁O₁₂ [M+H]⁺ calcd 1064.61, found 1064.48.

800 MHz ¹H NMR Spectrum of **1f** in CDCl₃
268 K (-5 °C), 4 mM

800 MHz ¹H NMR Spectrum of **1f** in CDCl₃
 268 K (-5 °C), 4 mM



Current Data Parameters
 USER slevin
 NAME SL-7124-800-H
 EXPNO 1
 PROCNO 1
 F2 - Acquisition Parameters
 Date_ 20061030
 Time 0.00
 INSTRUM varian
 PROBRD 40:5mmbroadban
 PULPROG zgpg30
 AD 4392
 SOLVENT cdcl3
 NS 4
 DS 4
 SWH 11001.101 Hz
 FIDRES 0.250070 Hz
 AQ 1.9994864 sec
 RG 81.92
 DW 45.450 usec
 DE 4.50 usec
 TE 268.5 K
 F2 - Processing parameter
 SI 32768
 SF 799.8064096 MHz
 MDW EN
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 2.00
 1D NMR plot parameters
 CX 22.80 cm
 CY 15.00 cm
 F1P 3.203 ppm
 F1 2561.83 Hz
 F2P 2.497 ppm
 F2 1997.21 Hz
 PPMCM 0.03096 ppm/cm
 HZCM 24.76393 Hz/cm

Current Data Parameters
 USER slevin
 NAME SL-7-124-800-H
 EXPNO 2
 PROCNO 1

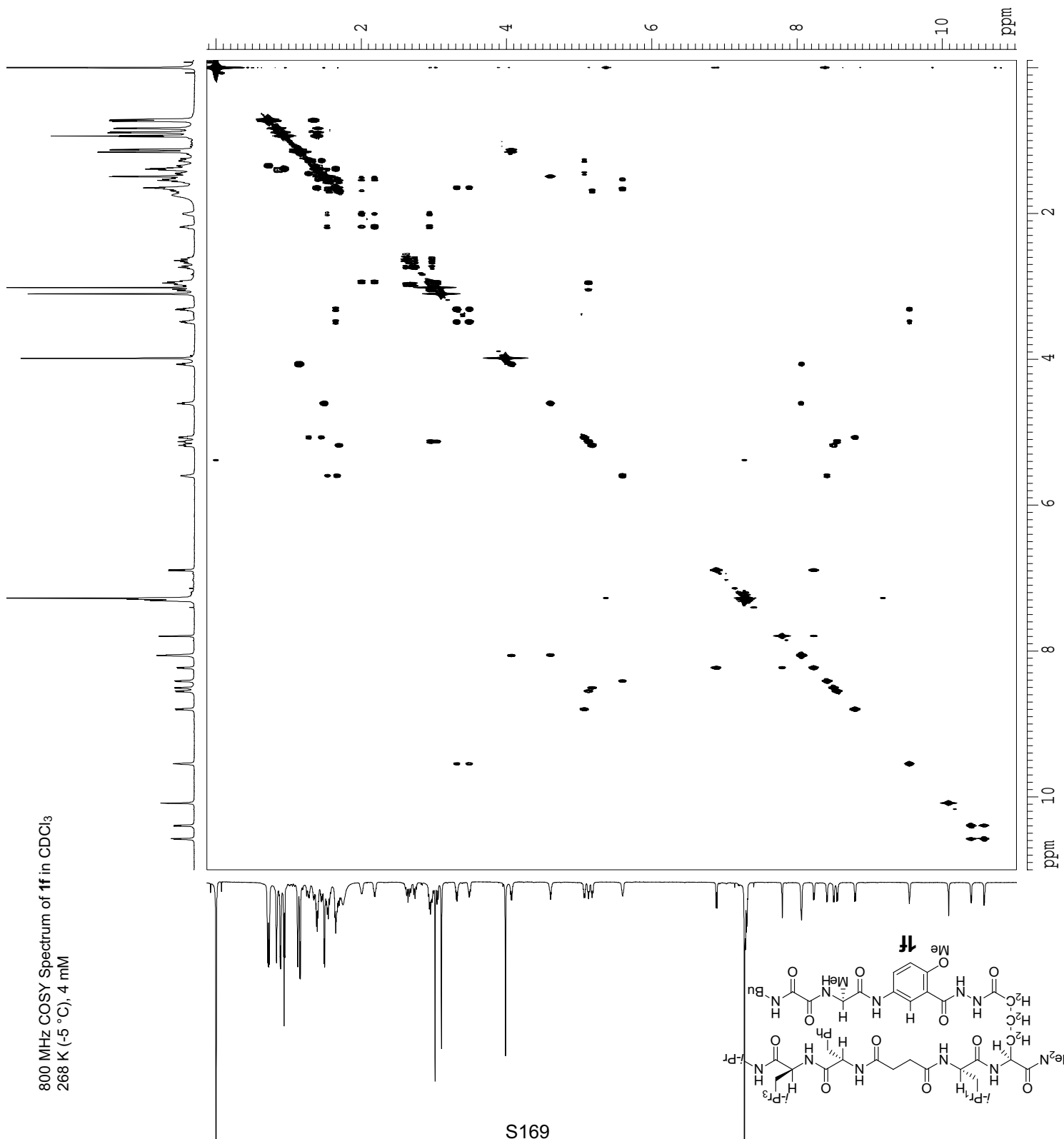
F2 - Acquisition Parameters
 Date_ 20061030
 Time_ 0.00
 INSTRUM varian
 PROBHD 40:5mmrbroadban
 PULPROG gcosy
 TD 4096
 SOLVENT cdcl3
 NS 16
 DS 64
 SWH 11001.101 Hz
 FIDRES 2.685816 Hz
 AQ 0.1843700 sec
 RG 4096
 DW 45.450 usec
 DE 231.43 usec
 TE 268.5 K

F1 - Acquisition parameters
 ND0 1
 TD 512
 SFO1 799.8107 MHz
 FIDRES 21.486525 Hz
 SW 13.755 ppm
 FhMODE undefined

F2 - Processing parameters
 SI 4096
 SF 799.8064116 MHz
 WDW SINE
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.40

F1 - Processing parameters
 SI 512
 MC2 QF
 SF 799.8064116 MHz
 WDW SINE
 SSB 0
 LB 0.00 Hz
 GB 0

2D NMR plot parameters
 CX2 15.00 cm
 CX1 15.00 cm
 F2PLO 11.002 ppm
 F2LO 8799.72 Hz
 F2PHI -0.103 ppm
 F2HI -82.27 Hz
 F1PLO 11.022 ppm
 F1LO 8815.84 Hz
 F1PHI -0.126 ppm
 F1HI -101.07 Hz
 F2PPMCM 0.74035 ppm/cm
 F2ZCM 592.13275 Hz/cm
 F1PPMCM 0.74326 ppm/cm
 F1ZCM 594.46051 Hz/cm



Current Data Parameters
 USER slevin
 NAME SJ-7-124-800-H
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters

Date_ 20061030
 Time 0.00
 INSTRUM varian
 PROBHD 40.5mmroadban
 PULPROG gcosy
 TD 4096
 SOLVENT cdcl3
 NS 16
 DS 64
 SWH 11001.101 Hz
 FIDRES 2.685816 Hz
 AQ 0.1843700 sec
 RG 4096
 DW 45.450 usec
 DE 231.43 usec
 TE 268.5 K

F1 - Acquisition parameters

ND0 1
 TD 512
 SF01 799.8107 MHz
 FIDRES 21.486525 Hz
 SW 13.755 ppm
 F1MODE undefined

F2 - Processing parameters

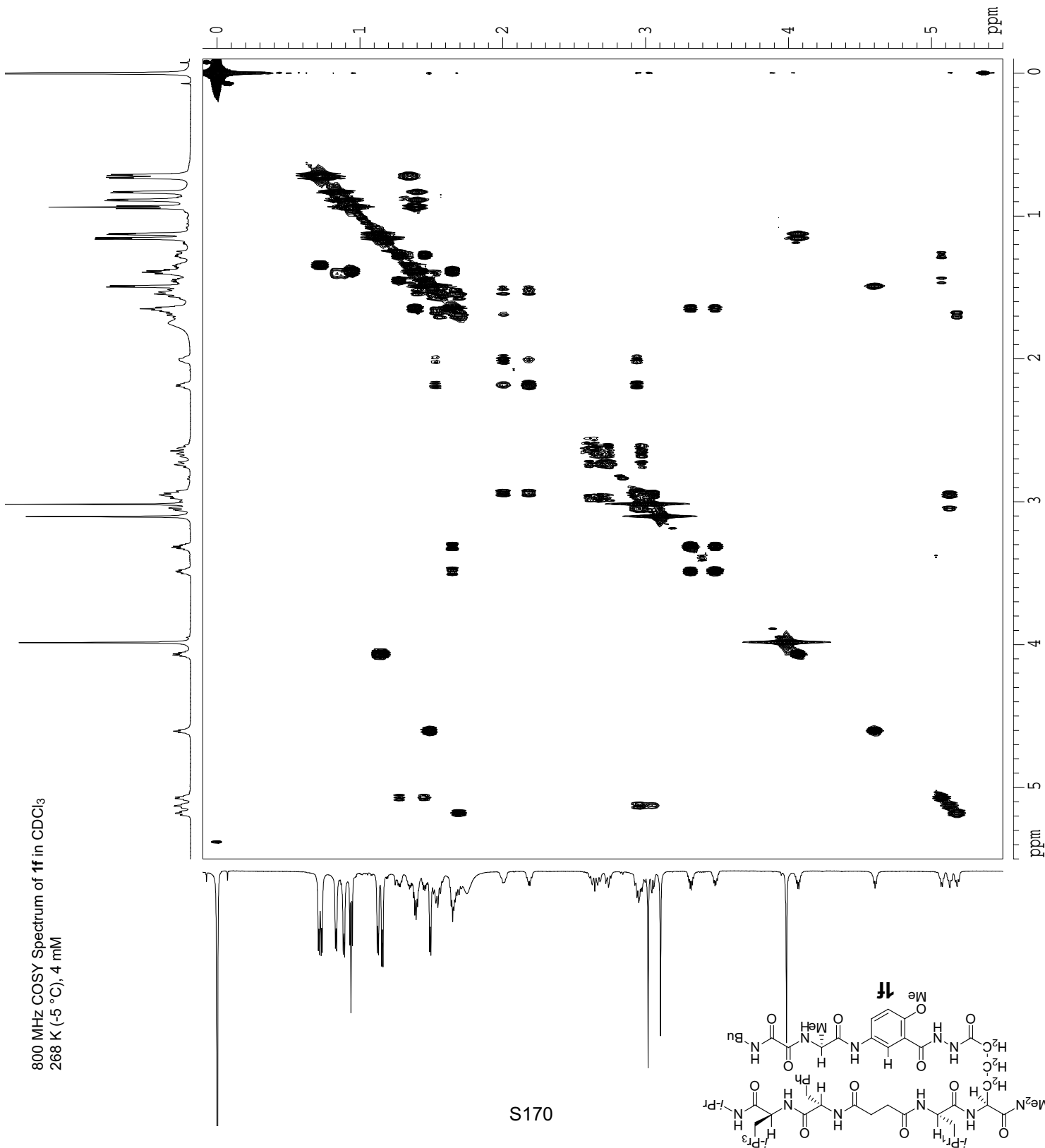
SI 4096
 SF 799.8064116 MHz
 WDW SINE
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.40

F1 - Processing parameters

SI 512
 MC2 QF
 SF 799.8064116 MHz
 WDW SINE
 SSB 0
 LB 0.00 Hz
 GB 0

2D NMR plot parameters

CX2 15.00 cm
 CX1 15.00 cm
 F2PLO 5.500 ppm
 F2LO 4398.94 Hz
 F2PHI -0.100 ppm
 F2HI -79.98 Hz
 F1PLO 5.500 ppm
 F1LO 4398.94 Hz
 F1PHI -0.100 ppm
 F1HI -79.98 Hz
 F2PPMCM 0.37333 ppm/cm
 F2HZCM 298.59439 Hz/cm
 F1PPMCM 0.37333 ppm/cm
 F1HZCM 298.59439 Hz/cm



Supporting Information

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Current Data Parameters
 USER slevin
 NAME SL-7-124-800-H
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters

Date_ 20061030
 Time_ 0.00
 INSTRUM varian
 PROBHD 40:5mmrbroadban
 PULPROG gcosy
 TD 4096
 SOLVENT cdcl3
 NS 16
 DS 64
 SWH 11001.101 Hz
 FIDRES 2.685816 Hz
 AQ 0.1843700 sec
 RG 4096
 DW 45.450 usec
 DE 231.43 usec
 TE 268.5 K

F1 - Acquisition Parameters

ND0 1
 TD 512
 SFO1 799.8107 MHz
 FIDRES 21.486525 Hz
 SW 13.755 ppm
 FTMODE undefined

F2 - Processing parameters

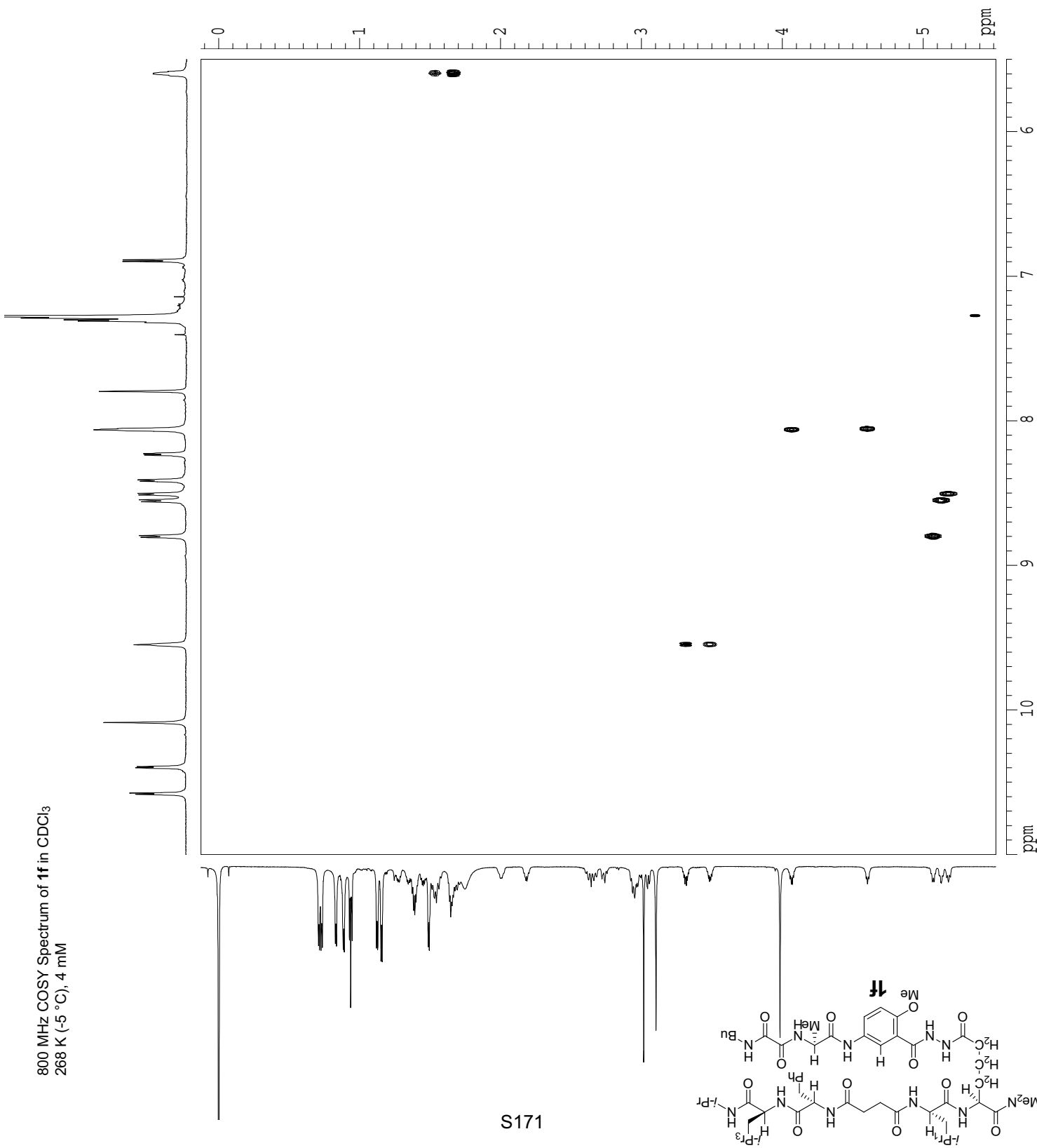
SI 4096
 SF 799.8064116 MHz
 WDW SINE
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.40

F1 - Processing parameters

SI 512
 MC2 QF
 SF 799.8064116 MHz
 WDW SINE
 SSB 0
 LB 0.00 Hz
 GB 0

2D NMR plot parameters

CX2 15.00 cm
 CX1 15.00 cm
 F2PLO 11.000 ppm
 F2LO 8797.87 Hz
 F2PHI 5.500 ppm
 F2HI 4398.94 Hz
 F1PLO 5.515 ppm
 F1LO 4411.10 Hz
 F1PHI -0.126 ppm
 F1HI -101.07 Hz
 F2PFCM 0.36667 ppm/cm
 F2HZCM 293.26236 Hz/cm
 F1PFCM 0.37611 ppm/cm
 F1HZCM 300.81134 Hz/cm



Supporting Information

Current Data Parameters
 USER slevin
 NAME SL-7-124-800-H
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters

Date_ 20061030
 Time 0.00
 INSTRUM varian
 PROBHD 40:5mmroadban
 PULPROG gcosy
 TD 4096
 SOLVENT cdc13
 NS 16
 DS 64
 SWH 11001.101 Hz
 FIDRES 2.685816 Hz
 AQ 0.1843700 sec
 RG 4096
 DW 45.450 usec
 DE 231.43 usec
 TE 268.5 K

F1 - Acquisition Parameters

ND0 1
 TD 512
 SF01 799.8107 MHz
 FIDRES 21.486525 Hz
 SW 13.755 ppm
 F1MODE undefined

F2 - Processing parameters

SI 4096
 SF 799.8064116 MHz
 WDW SINE
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.40

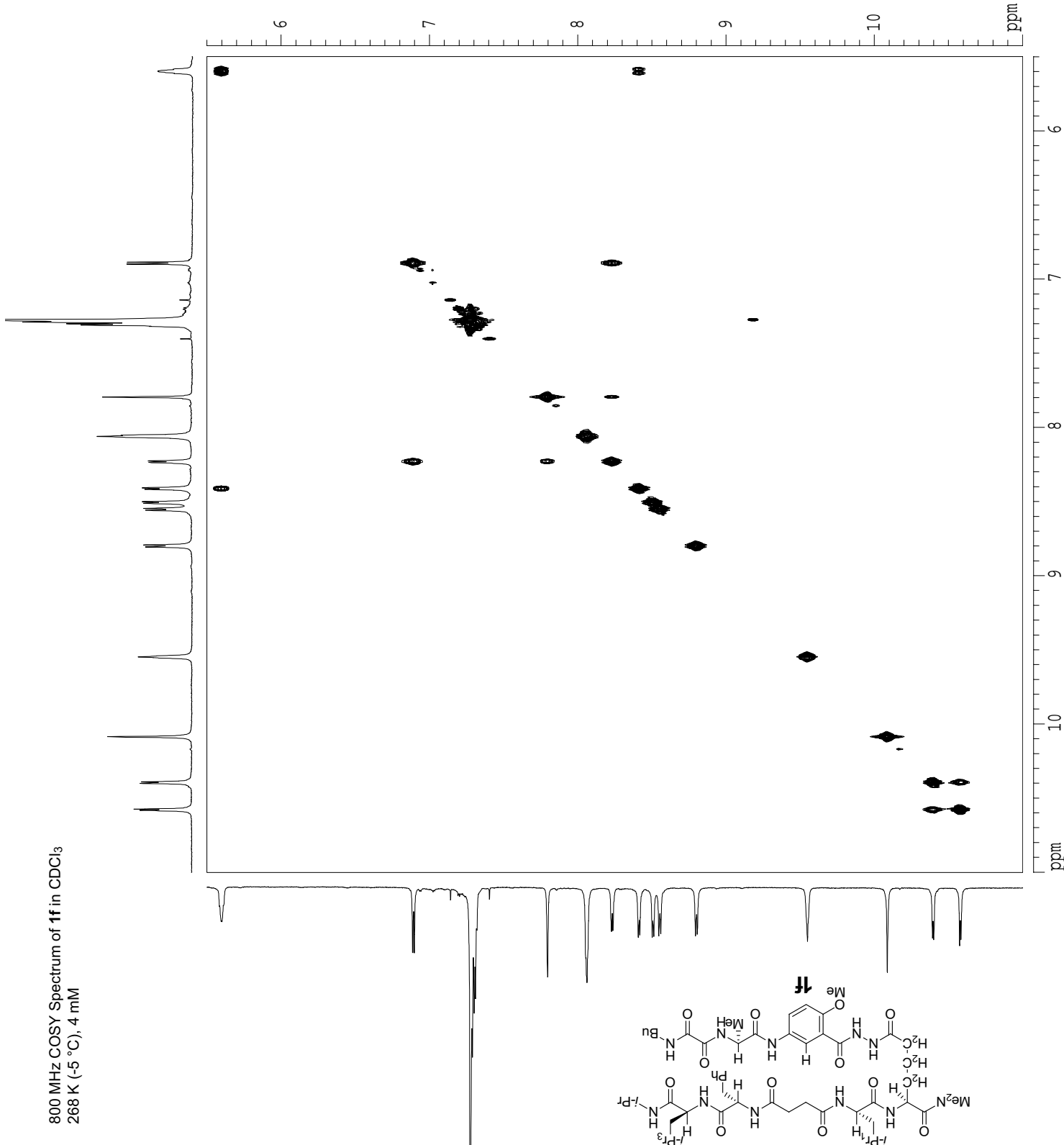
F1 - Processing parameters

SI 512
 MC2 QF
 SF 799.8064116 MHz
 WDW SINE
 SSB 0
 LB 0.00 Hz
 GB 0

S. Levin and J. S. Nowick

2D NMR plot parameters

CX2 15.00 cm
 CX1 15.00 cm
 F2PLO 11.002 ppm
 F2LO 8799.72 Hz
 F2PHI 5.498 ppm
 F2HI 4397.67 Hz
 F1PLO 11.000 ppm
 F1LO 8797.87 Hz
 F1PHI 5.500 ppm
 F1HI 4398.94 Hz
 F2PDMCM 0.36693 ppm/cm
 F2HZCM 293.47009 Hz/cm
 F1PDMCM 0.36667 ppm/cm
 F1HZCM 293.26236 Hz/cm



Supporting Information

Current Data Parameters
 USER slevin
 NAME SL-7-124-800-H
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters

Date 20061030
 Time 0.00
 INSTRUM varian
 PROBHD 40:5mm broadband
 PULPROG gcosy
 TD 4096
 SOLVENT cdcl3
 NS 16
 DS 64
 SWH 11001.101 Hz
 FIDRES 2.685816 Hz
 AQ 0.1843700 sec
 RG 4096
 DW 45.450 usec
 DE 231.43 usec
 TE 268.5 K

F1 - Acquisition parameters

ND0 1
 TD 512
 SFO1 799.8107 MHz
 FIDRES 21.486525 Hz
 SW 13.755 ppm
 FMODE undefined

F2 - Processing parameters

SI 4096
 SF 799.8064116 MHz
 WDW SINE
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.40

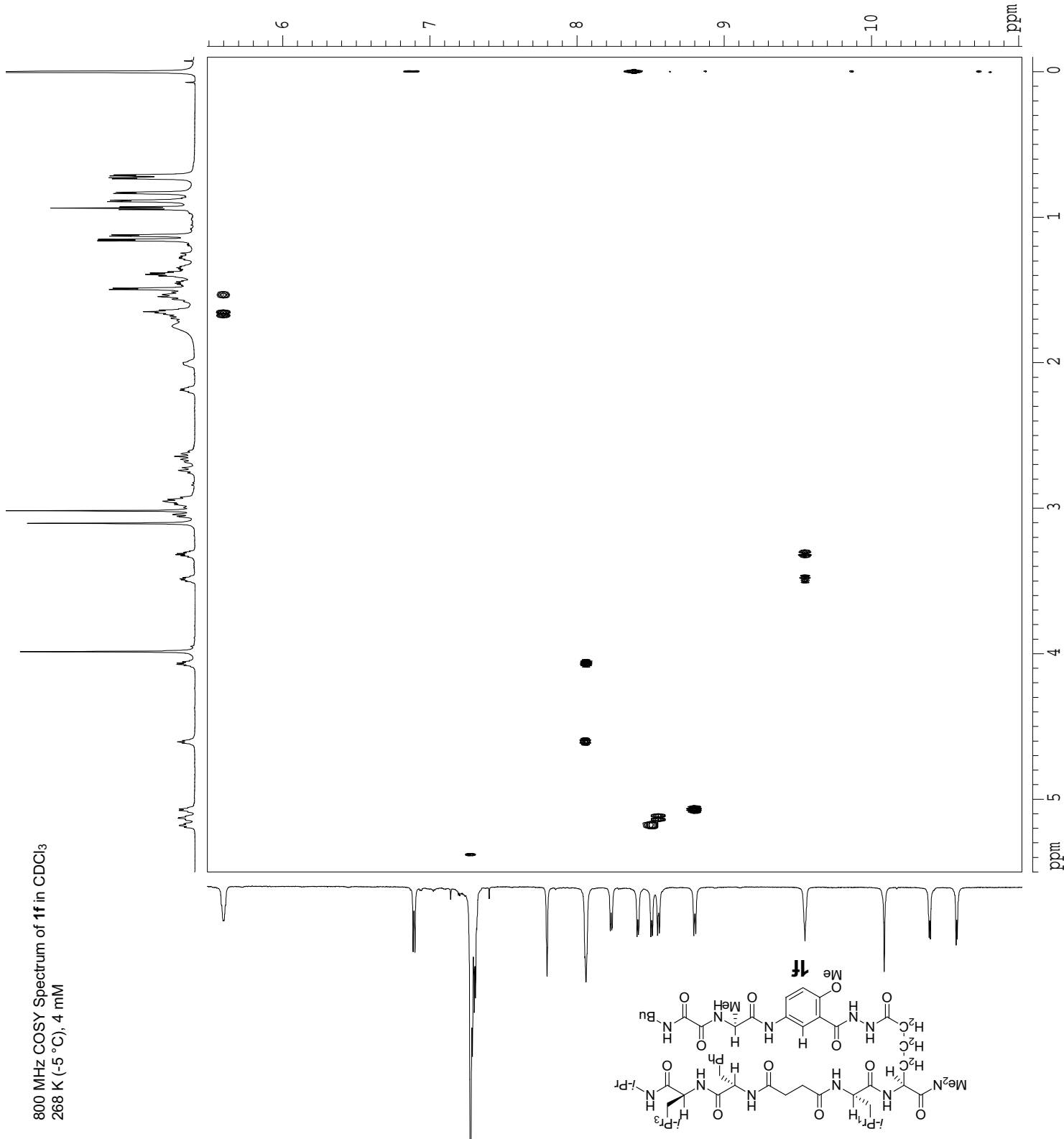
F1 - Processing parameters

SI 512
 MC2 OF
 SF 799.8064116 MHz
 WDW SINE
 SSB 0
 LB 0.00 Hz
 GB 0

S. Levin and J. S. Nowick

2D NMR plot parameters

CX2 15.00 cm
 CX1 15.00 cm
 F2PLO 5.500 ppm
 F2LO 4398.94 Hz
 F2PHI -0.100 ppm
 F2HI -79.98 Hz
 F1PLO 11.022 ppm
 F1LO 8815.84 Hz
 F1PHI 5.488 ppm
 F1HI 4389.61 Hz
 F2PPMCM 0.37333 ppm/cm
 F2HZCM 298.59439 Hz/cm
 F1PPMCM 0.36894 ppm/cm
 F1HZCM 295.08160 Hz/cm



Supporting Information

Current Data Parameters
 USER slevin
 NAME SL-7-124-800-H
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters

Date 20061030
 Time 0.00
 INSTRUM varian
 PROBHD 40:5mm broadband
 PULPROG gcosy
 TD 4096
 SOLVENT cdcl3
 NS 16
 DS 64
 SWH 11001.101 Hz
 FIDRES 2.685816 Hz
 AQ 0.1843700 sec
 RG 4096
 DW 45.450 usec
 DE 231.43 usec
 TE 268.5 K

F1 - Acquisition Parameters

ND0 1
 TD 512
 SF01 799.8107 MHz
 FIDRES 21.486525 Hz
 SW 13.755 ppm
 FmMODE undefined

F2 - Processing Parameters

SI 4096
 SF 799.8064116 MHz
 WDW SINE
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.40

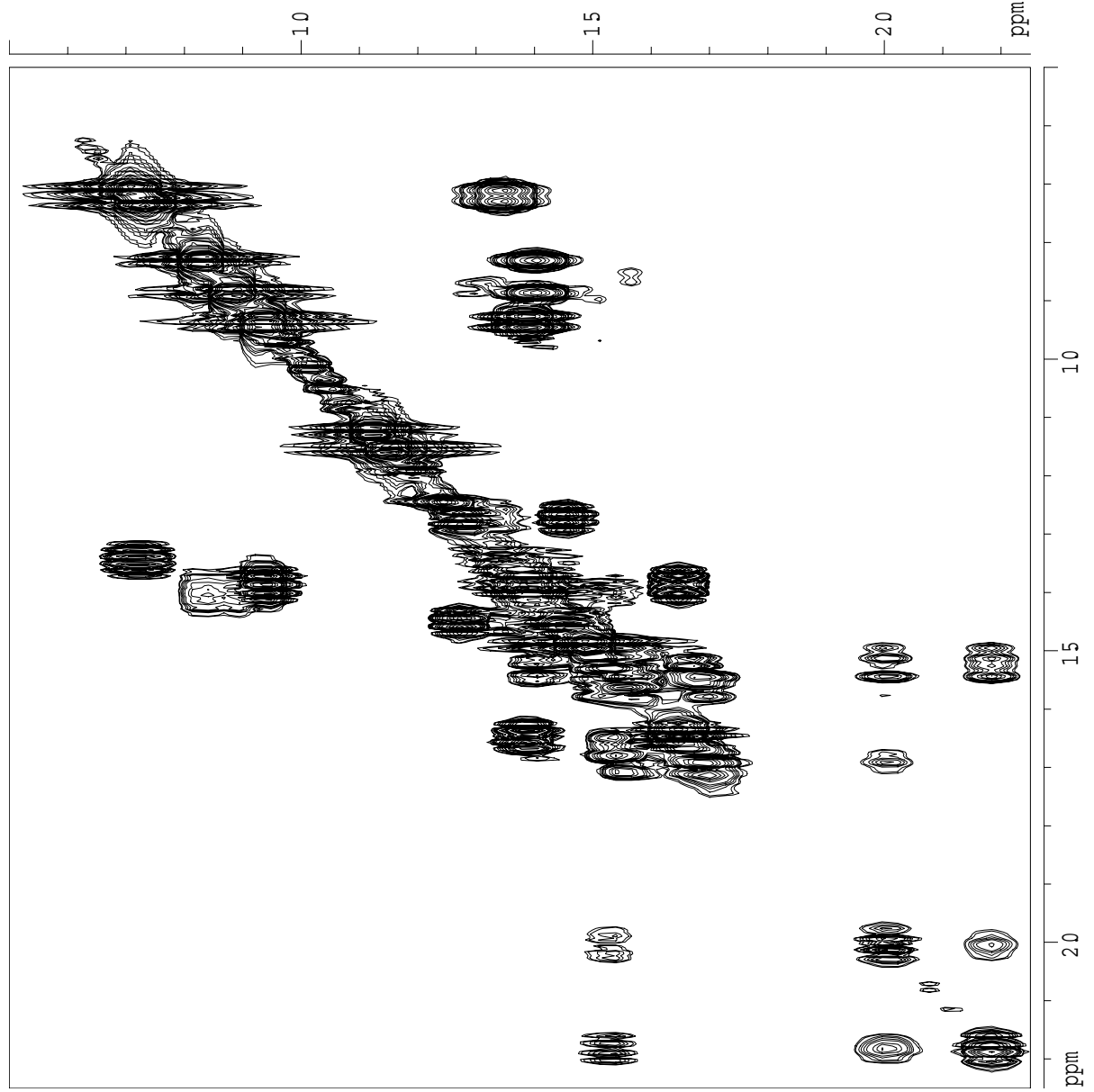
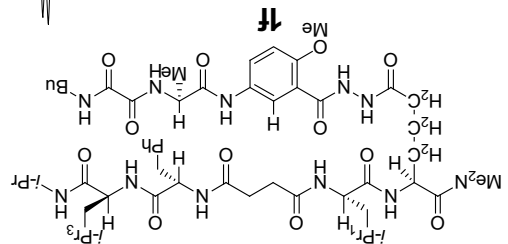
F1 - Processing Parameters

SI 512
 MC2 QF
 SF 799.8064116 MHz
 WDW SINE
 SSB 0
 LB 0.00 Hz
 GB 0

S. Levin and J. S. Nowick

2D NMR plot parameters
 CX2 15.00 cm
 CX1 15.00 cm
 F2PLO 2.250 ppm
 F2LO 1799.56 Hz
 F2PHI 0.500 ppm
 F2HI 399.90 Hz
 F1PLO 2.250 ppm
 F1LO 1799.56 Hz
 F1PHI 0.500 ppm
 F1HI 399.90 Hz
 F2PFCM 0.11667 Hz/cm
 F2HZCM 93.31075 Hz/cm
 F1PFCM 0.11667 Hz/cm
 F1HZCM 93.31075 Hz/cm

800 MHz COSY Spectrum of **1f** in CDCl₃
 268 K (-5 °C), 4 mM



Supporting Information

Current Data Parameters
 USER slewin
 NAME SL-7-124-800-H
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20061030
 Time 0.00
 INSTRUM varian
 PROBHD 40:5mm broadband
 PULPROG gcosy
 TD 4096
 SOLVENT cdcl3
 NS 16
 DS 64
 SWH 11001.101 Hz
 FIDRES 2.685816 Hz
 AQ 0.1843700 sec
 RG 4096
 DW 45.450 usec
 DE 231.43 usec
 TE 268.5 K

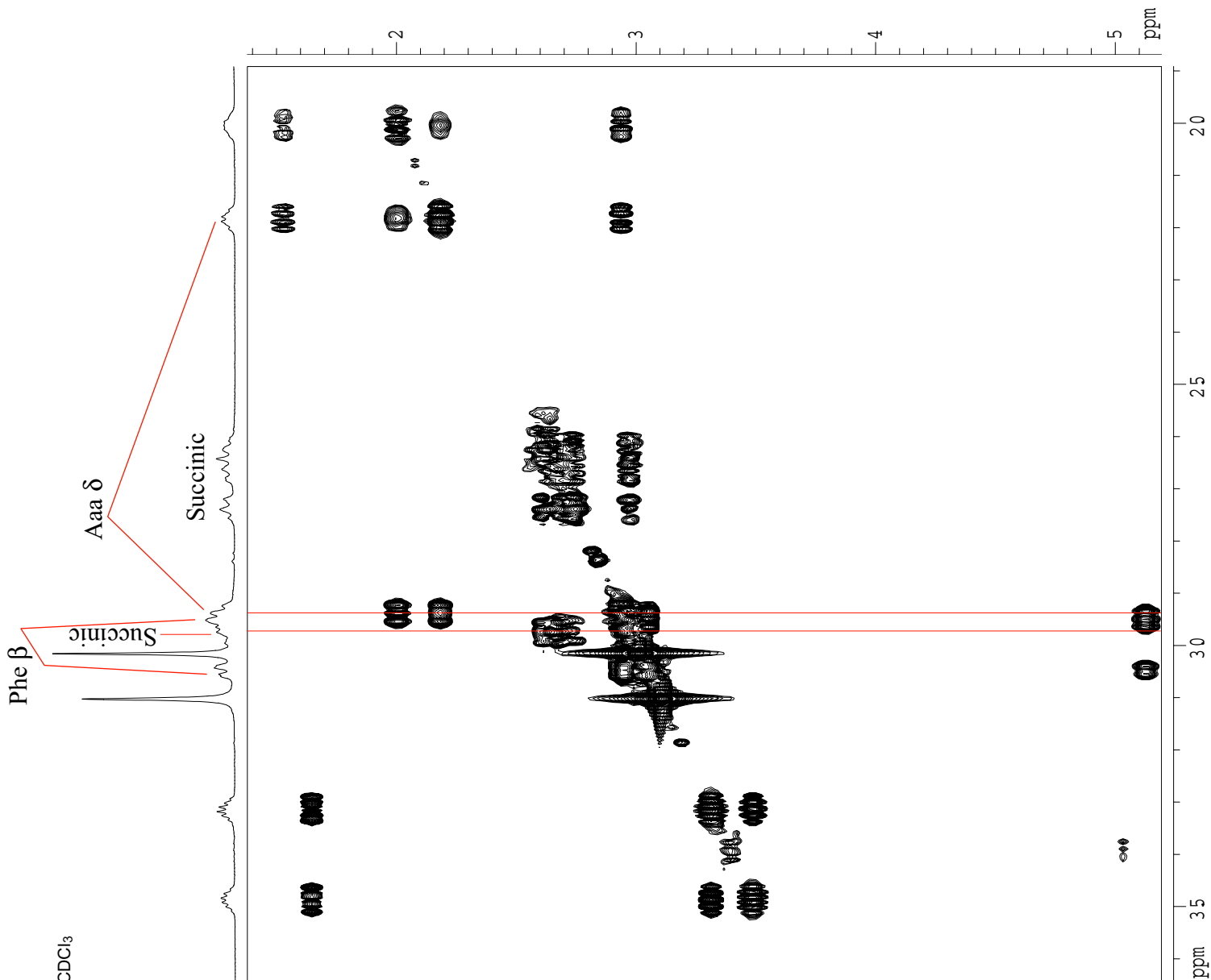
F1 - Acquisition parameters
 NDO 1
 TD 512
 SFO1 799.8107 MHz
 FIDRES 21.486525 Hz
 SW 13.755 ppm
 FwMODE undefined

F2 - Processing parameters
 SI 4096
 SF 799.8064116 MHz
 WDW SINE
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.40

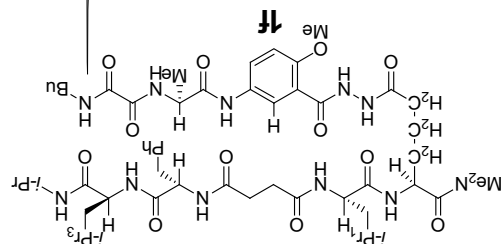
F1 - Processing parameters
 SI 512
 MC2 QF
 SF 799.8064116 MHz
 WDW SINE
 SSB 0
 LB 0.00 Hz
 GB 0

S. Levin and J. S. Nowick

2D NMR plot parameters
 CX2 15.00 cm
 CX1 15.00 cm
 F2PLO 3.641 ppm
 F2LO 2912.42 Hz
 F2PHI 1.892 ppm
 F2HI 1513.11 Hz
 F1PLO 5.193 ppm
 F1LO 4153.26 Hz
 F1PHI 1.378 ppm
 F1HI 1102.18 Hz
 F2PPMCM 0.11664 ppm/cm
 FHZCM 93.28732 Hz/cm
 F1PPMCM 0.25432 ppm/cm
 F1HZCM 203.40576 Hz/cm



800 MHz COSY Spectrum of **1f** in CDCl₃
 268 K (-5 °C), 4 mM



Supporting Information

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Current Data Parameters
 USER slevin
 NAME SL-7-124-800-H
 EXPNO 3
 PROCNO 1

F2 - Acquisition Parameters

Date_ 20061030
 Time 0.00
 INSTRUM varian
 PROBHD 40:5mmroadban
 PULPROG wgtocsy_bt
 TD 4096
 SOLVENT CDCl3
 NS 32
 DS 64
 SWH 11001.101 Hz
 FIDRES 2.685816 Hz
 AQ 0.1862132 sec
 RG 287.4
 DW 45.450 usec
 DE 6.00 usec
 TE 268.5 K

F1 - Acquisition parameters

ND0 1
 TD 256
 SF01 799.8107 MHz
 FIDRES 42.973049 Hz
 SW 13.755 ppm
 F1MODE undefined

F2 - Processing parameters

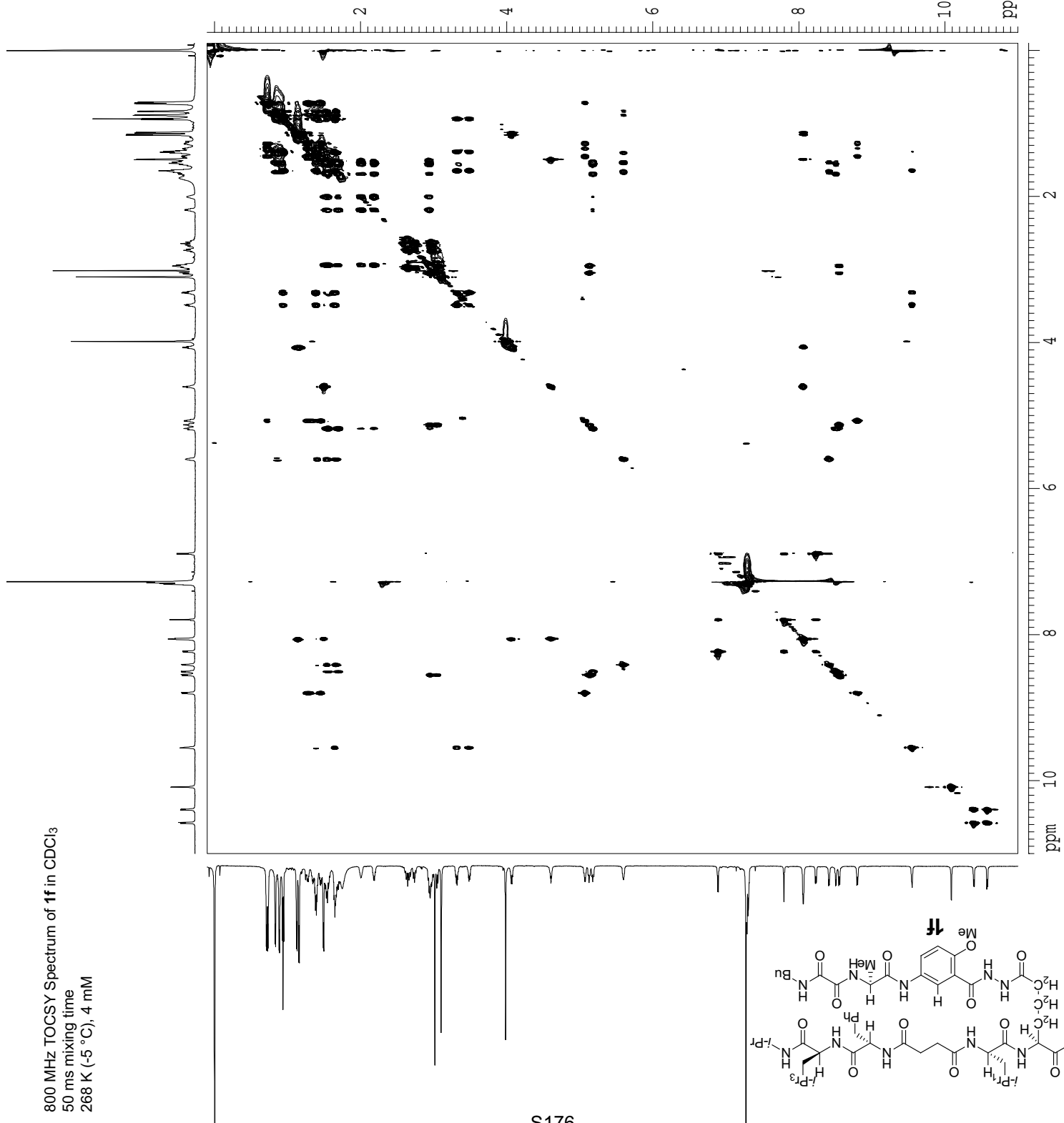
SI 2048
 SF 799.8064116 MHz
 WDW QSI
 SSB 2
 LB 0.00 Hz
 GB 0
 PC 1.40

F1 - Processing parameters

SI 1024
 MC2 States
 SF 799.8064116 MHz
 WDW QSI
 SSB 2
 LB 0.00 Hz
 GB 0

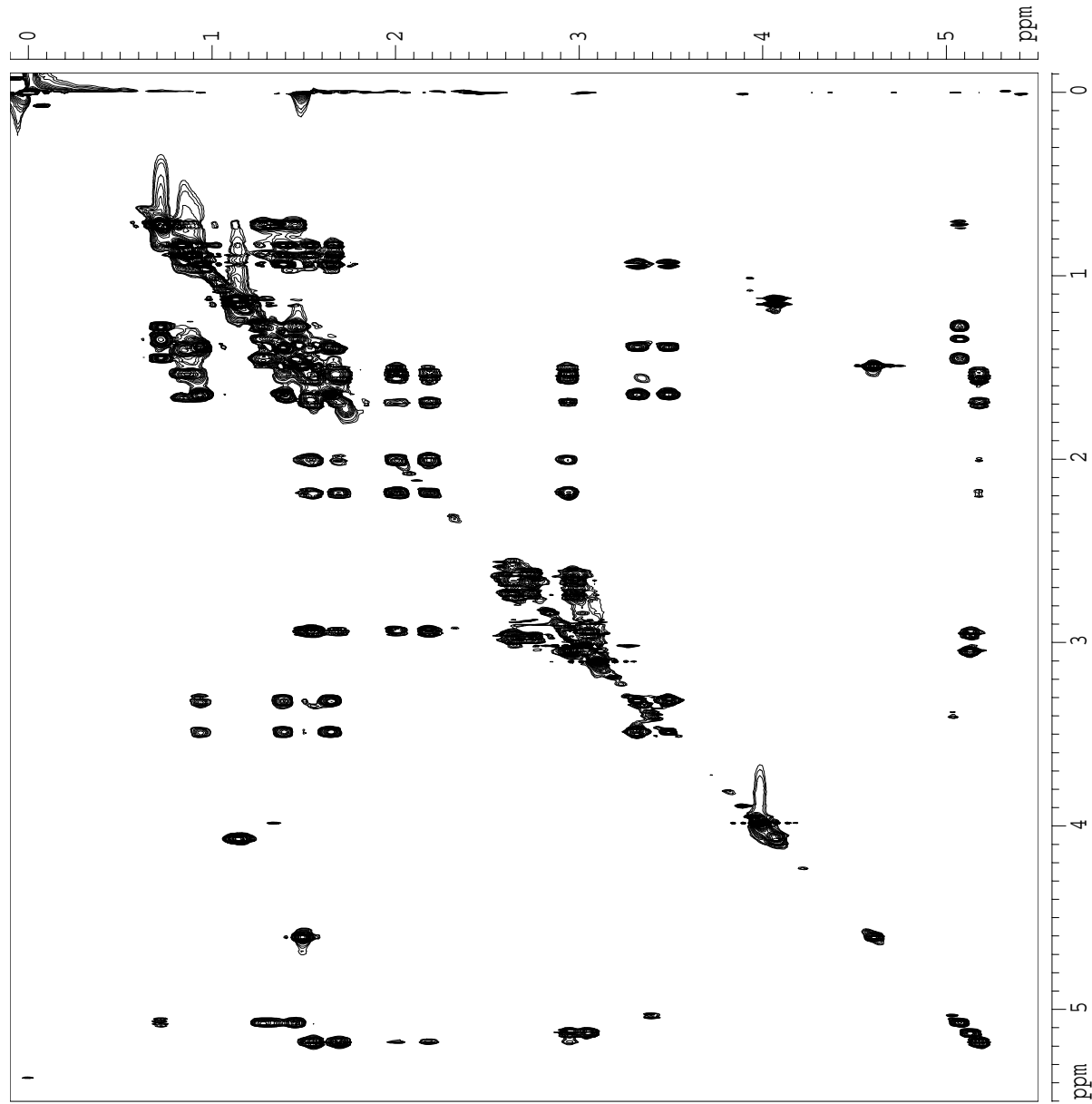
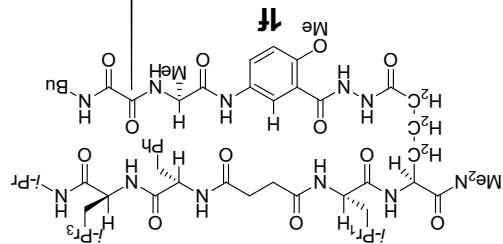
2D NMR plot parameters

CX2 15.00 cm
 CX1 15.00 cm
 F2PLO 11.000 ppm
 F2LO 8797.87 Hz
 F2PHI -0.100 ppm
 F2HI -79.98 Hz
 F1PLO 11.000 ppm
 F1LO 8797.87 Hz
 F1PHI -0.100 ppm
 F1HI -79.98 Hz
 F2PPMCM 0.74000 ppm/cm
 F2HZCM 591.85669 Hz/cm
 F1PPMCM 0.74000 ppm/cm
 F1HZCM 591.85669 Hz/cm



800 MHz TOCSY Spectrum of **1f** in CDCl₃
 50 ms mixing time
 268 K (-5 °C), 4 mM

800 MHz TOCSY Spectrum of **1f** in CDCl₃
 50 ms mixing time
 268 K (-5 °C), 4 mM



S177

Supporting Information

Current Data Parameters
 USER slewin
 NAME SL-7-124-800-H
 EXPNO 3
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20061030
 Time 0.00
 INSTRUM varian
 PROBHD 40-5mm broadband
 PULPROG wgtocsy_bn
 TD 4096
 SOLVENT CDCl₃
 NS 32
 DS 64
 SWH 11001.101 Hz
 FIDRES 2.685816 Hz
 AQ 0.1862132 sec
 RG 287.4
 DW 45.450 usec
 DE 6.00 usec
 TE 268.5 K

F1 - Acquisition parameters
 ND0 1
 TD 256
 SF01 799.8107 MHz
 FIDRES 42.973049 Hz
 SW 13.755 ppm
 FMODE undefined

F2 - Processing parameters
 SI 2048
 SF 799.8064116 MHz
 WDW QSINE
 SSB 2
 LB 0.00 Hz
 GB 0
 PC 1.40

F1 - Processing parameters
 SI 1024
 MC2 States
 SF 799.8064116 MHz
 WDW QSINE
 SSB 2
 LB 0.00 Hz
 GB 0

2D NMR plot parameters
 CX2 15.00 cm
 CX1 15.00 cm
 F2PLO 5.502 ppm
 F2LO 4400.36 Hz
 F2PHI -0.106 ppm
 F2HI -84.95 Hz
 F1PLO 5.502 ppm
 F1LO 4400.36 Hz
 F1PHI -0.100 ppm
 F1HI -79.98 Hz
 F2PPCM 0.37387 ppm/cm
 F2HZCM 299.02078 Hz/cm
 F1PPCM 0.37345 ppm/cm
 F1HZCM 298.68924 Hz/cm

S. Levin and J. S. Nowick

Supporting Information

Current Data Parameters
 USER slevin
 NAME SL-7-124-800-H
 EXPNO 3
 PROCNO 1

F2 - Acquisition Parameters

Date 20061030
 Time 0.00
 INSTRUM varian
 PROBHD 40-5mm broadband
 PULPROG wgtocsy_bn
 TD 4096
 SOLVENT CDCl3
 NS 32
 DS 64
 SWH 11001.101 Hz
 FIDRES 2.685816 Hz
 AQ 0.1862132 sec
 RG 287.4
 DW 45.450 usec
 DE 6.00 usec
 TE 268.5 K

F1 - Acquisition Parameters

ND0 1
 TD 256
 SF01 799.8107 MHz
 FIDRES 42.973049 Hz
 SW 13.755 ppm
 FMODE undefined

F2 - Processing parameters

SI 2048
 SF 799.8064116 MHz
 WDW QSINE
 SSB 2
 LB 0.00 Hz
 GB 0
 PC 1.40

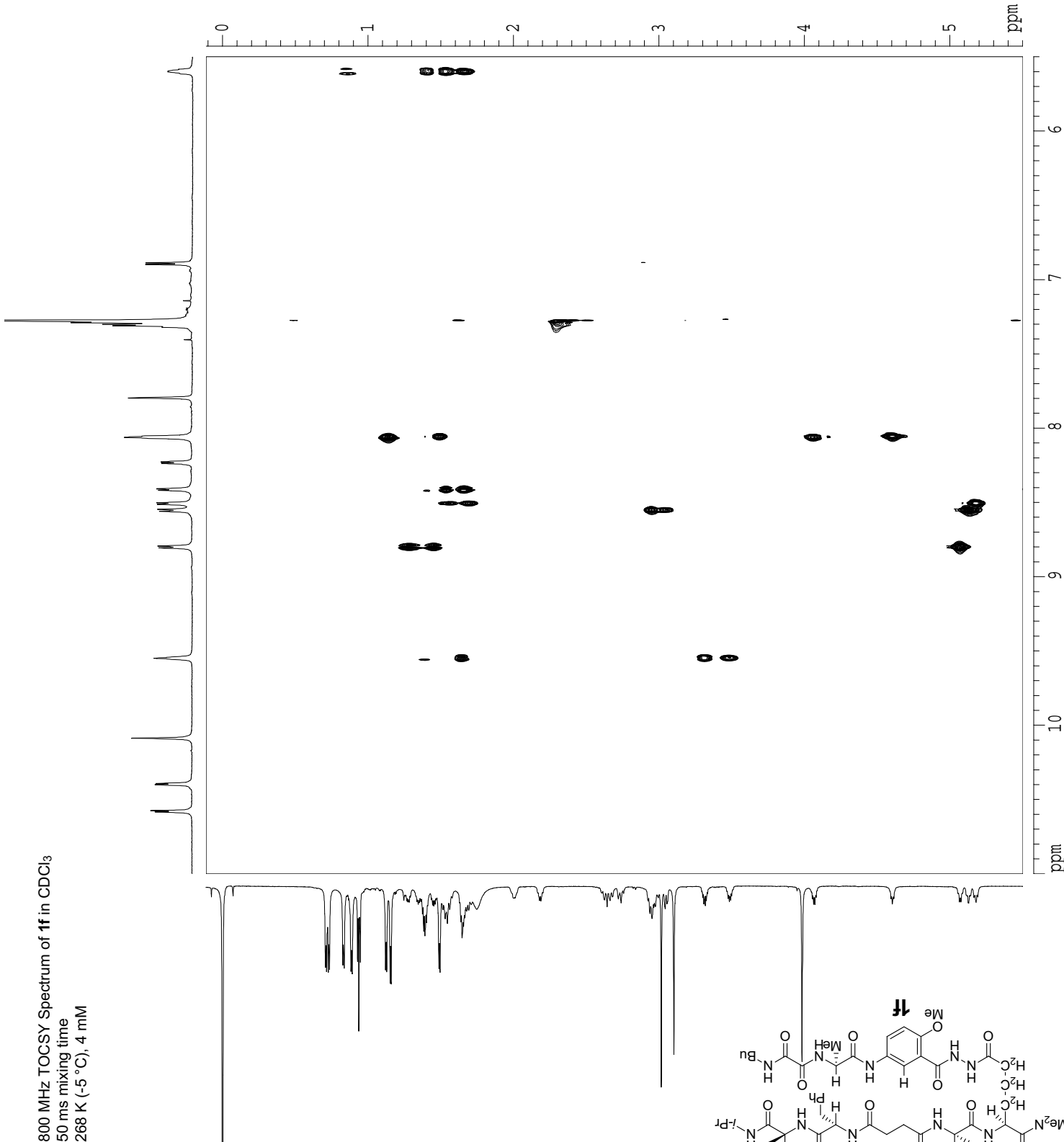
F1 - Processing parameters

SI 1024
 MC2 States
 SF 799.8064116 MHz
 WDW QSINE
 SSB 2
 LB 0.00 Hz
 GB 0

S. Levin and J. S. Nowick

2D NMR plot parameters

CX2 15.00 cm
 CX1 15.00 cm
 F2PLO 11.000 ppm
 FZLO 8797.87 Hz
 F2PHI 5.500 ppm
 F2HI 4398.94 Hz
 F1PLO 5.502 ppm
 F1LO 4400.36 Hz
 F1PHI -0.113 ppm
 F1HI -90.33 Hz
 F2PFCM 0.36667 ppm/cm
 F2HZCM 293.26236 Hz/cm
 F1PFCM 0.37431 ppm/cm
 F1HZCM 299.37891 Hz/cm



800 MHz TOCSY Spectrum of **1f** in CDCl₃
 50 ms mixing time
 268 K (-5 °C), 4 mM

Supporting Information

Current Data Parameters
 USER slewin
 NAME SL-7-124-800-H
 EXPNO 3
 PROCNO 1

F2 - Acquisition Parameters

Date 20061030
 Time 0.00
 INSTRUM varian
 PROBHD 40:5mm broadband
 PULPROG wgtocsy_bn
 TD 4096
 SOLVENT CDCl3
 NS 32
 DS 64
 SWH 11001.101 Hz
 FIDRES 2.685816 Hz
 AQ 0.1862132 sec
 RG 287.4
 DW 45.450 usec
 DE 6.00 usec
 TE 268.5 K

F1 - Acquisition Parameters

ND0 1
 TD 256
 SF01 799.8107 MHz
 FIDRES 42.973049 Hz
 SW 13.755 ppm
 FmMODE undefined

F2 - Processing Parameters

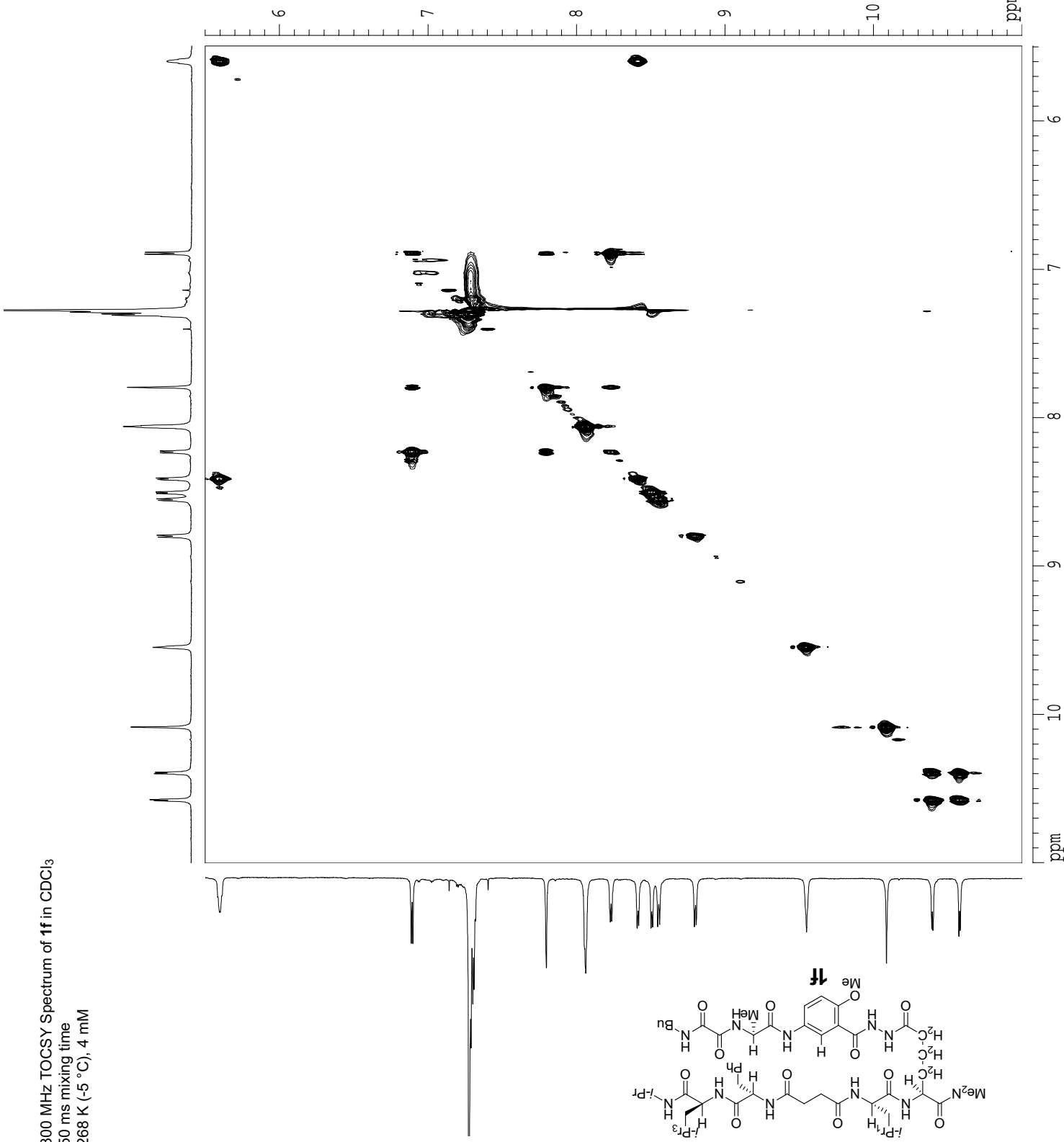
SI 2048
 SF 799.8064116 MHz
 WDW QSI
 SSB 2
 LB 0.00 Hz
 GB 0
 PC 1.40

F1 - Processing Parameters

SI 1024
 MC2 States
 SF 799.8064116 MHz
 WDW QSI
 SSB 2
 LB 0.00 Hz
 GB 0

S. Levin and J. S. Nowick

2D NMR plot parameters
 CX2 15.00 cm
 CX1 15.00 cm
 F2PLO 11.002 ppm
 F2LO 8799.72 Hz
 F2PHI 5.495 ppm
 F2HI 4394.99 Hz
 F1PLO 11.000 ppm
 F1LO 8797.87 Hz
 F1PHI 5.500 ppm
 F1HI 4398.94 Hz
 F2PFCM 0.36715 ppm/cm
 F2HZCM 293.64917 Hz/cm
 F1PFCM 0.36667 ppm/cm
 F1HZCM 293.26236 Hz/cm



800 MHz TOCSY Spectrum of **1f** in CDCl₃
 50 ms mixing time
 268 K (-5 °C), 4 mM

Supporting Information

Current Data Parameters
 USER slevin
 NAME SL-7-124-800-H
 EXPNO 3
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20061030
 Time_ 0.00
 INSTRUM varian
 PROBHD 40:5mmBroadban
 PULPROG wgtocsy_bn
 TD 4096
 SOLVENT CDCl3
 NS 32
 DS 64
 SWH 11001.101 Hz
 FIDRES 2.685816 Hz
 AQ 0.1862132 sec
 RG 287.4
 DW 45.450 usec
 DE 6.00 usec
 TE 268.5 K

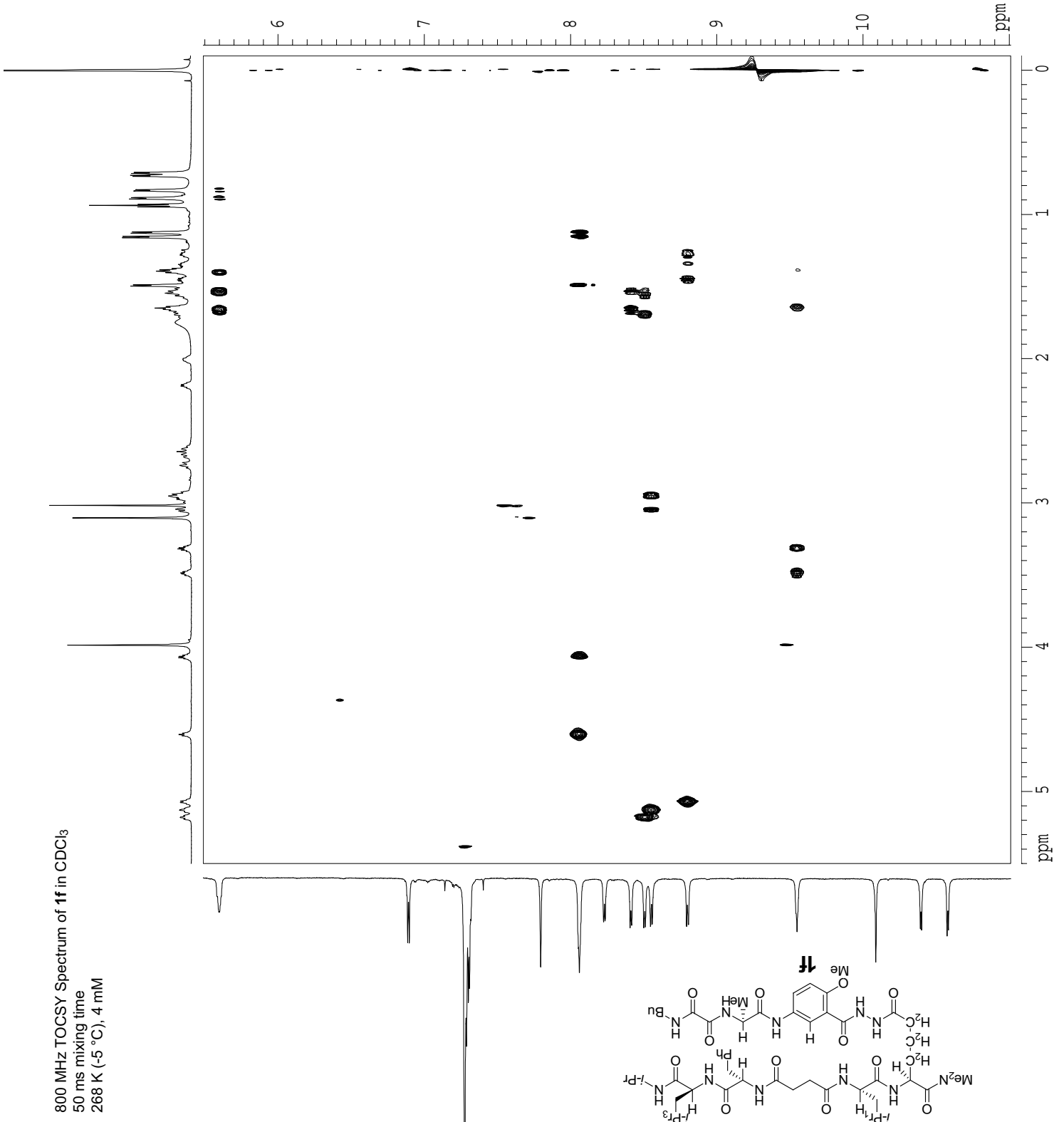
F1 - Acquisition parameters
 ND0 1
 TD 256
 SFO1 799.8107 MHz
 FIDRES 42.973049 Hz
 SW 13.755 ppm
 F1MODE undefined

F2 - Processing parameters
 SI 2048
 SF 799.8064116 MHz
 WDW QSI
 SSB 2
 LB 0.00 Hz
 GB 0
 PC 1.40

F1 - Processing parameters
 SI 1024
 MC2 States
 SF 799.8064116 MHz
 WDW QSI
 SSB 2
 LB 0.00 Hz
 GB 0

S. Levin and J. S. Nowick

2D NMR plot parameters
 CX2 15.00 cm
 CX1 15.00 cm
 F2PLO 5.500 ppm
 F2LO 4398.94 Hz
 F2PHI -0.100 ppm
 F2HI -79.98 Hz
 F1PLO 11.009 ppm
 F1LO 8805.09 Hz
 F1PHI 5.488 ppm
 F1HI 4389.61 Hz
 F2PPMCM 0.37333 ppm/cm
 F2HZCM 298.59439 Hz/cm
 F1PPMCM 0.36805 ppm/cm
 F1HZCM 294.36536 Hz/cm



800 MHz TOCSY Spectrum of **1f** in CDCl₃
 50 ms mixing time
 268 K (-5 °C), 4 mM

Supporting Information

Current Data Parameters
 USER slewin
 NAME SL-7-124-800-H
 EXPNO 3
 PROCNO 1

F2 - Acquisition Parameters

Date_ 20061030
 Time_ 0.00
 INSTRUM varian
 PROBHD 40:5mmBroadban
 PULPROG wgtocsy_bn
 TD 4096
 SOLVENT CDC13
 NS 32
 DS 64
 SWH 11001.101 Hz
 FIDRES 2.685816 Hz
 AQ 0.1862132 sec
 RG 287.4
 DW 45.450 usec
 DE 6.00 usec
 TE 268.5 K

F1 - Acquisition Parameters

ND0 1
 TD 256
 SFO1 799.8107 MHz
 FIDRES 42.973049 Hz
 SW 13.755 ppm
 FreqMODE undefined

F2 - Processing parameters

SI 2048
 SF 799.8064116 MHz
 WDW QSI
 SSB 2
 LB 0.00 Hz
 GB 0
 PC 1.40

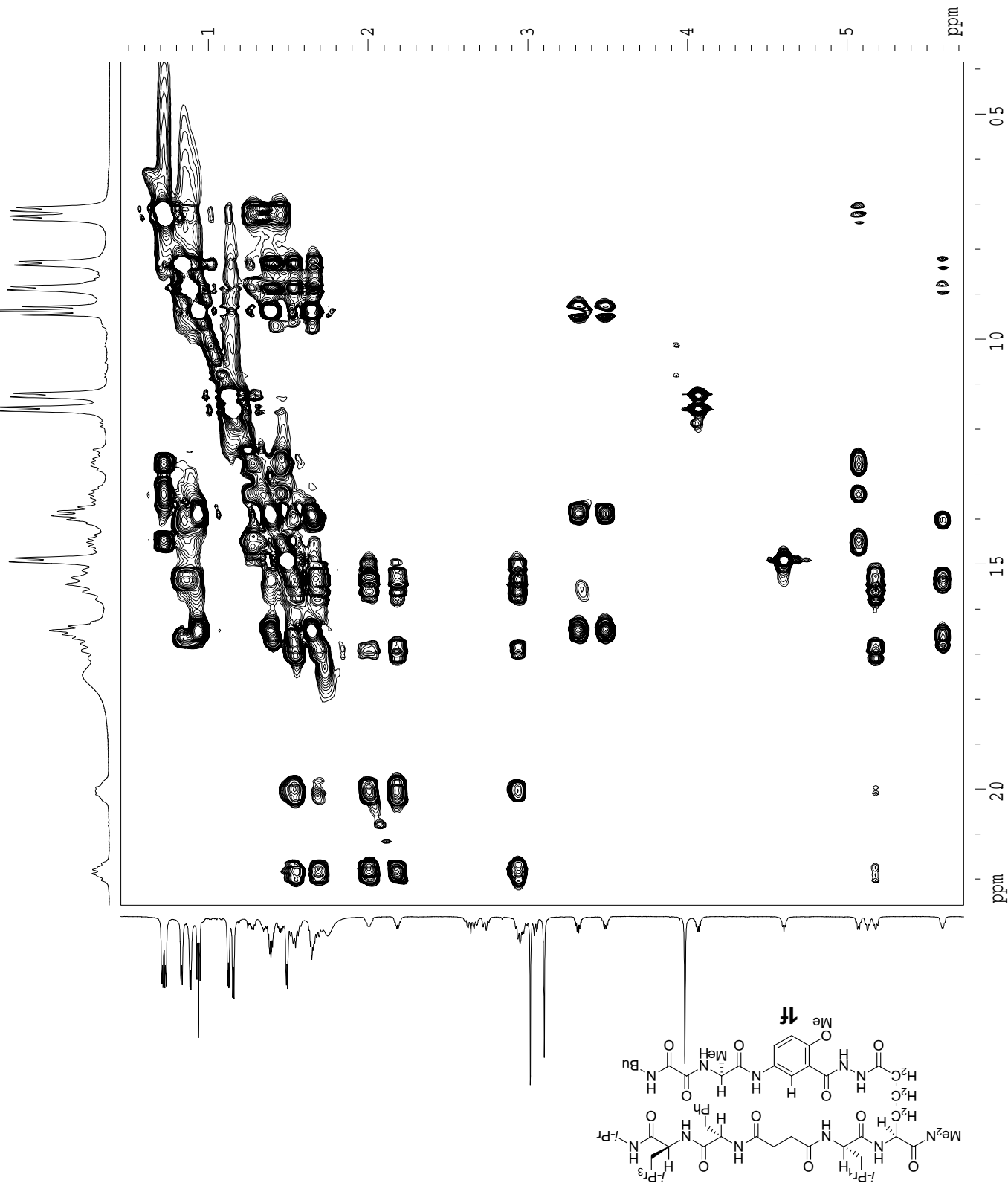
F1 - Processing parameters

SI 1024
 MC2 States
 SF 799.8064116 MHz
 WDW QSI
 SSB 2
 LB 0.00 Hz
 GB 0

2D NMR plot parameters

CX2 15.00 cm
 CX1 15.00 cm
 F2FLO 2.258 ppm
 F2LO 1805.86 Hz
 F2PHI 0.384 ppm
 F2HI 307.18 Hz
 F1FLO 5.730 ppm
 F1LO 4582.99 Hz
 F1PHI 0.451 ppm
 F1HI 360.89 Hz
 F2PPMCM 0.12492 ppm/cm
 F2HZCM 99.91232 Hz/cm
 F1PPMCM 0.35193 ppm/cm
 F1HZCM 281.47345 Hz/cm

800 MHz TOCSY Spectrum of **1f** in CDCl₃
 50 ms mixing time
 268 K (-5 °C), 4 mM



Supporting Information

Current Data Parameters
 USER slevin
 NAME SL-7-124-800-H
 EXPNO 3
 PROCNO 1

F2 - Acquisition Parameters

Date_ 20061030
 Time_ 0.00
 INSTRUM varian
 PROBHD 40:5mmroadban
 PULPROG wgtocsy_bn
 TD 4096
 SOLVENT CDCl3
 NS 32
 DS 64
 SWH 11001.101 Hz
 FIDRES 2.685816 Hz
 AQ 0.1862132 sec
 RG 287.4
 DW 45.450 usec
 DE 6.00 usec
 TE 268.5 K

F1 - Acquisition Parameters

ND0 1
 TD 256
 SF01 799.8107 MHz
 FIDRES 42.973049 Hz
 SW 13.755 ppm
 F1MODE undefined

F2 - Processing parameters

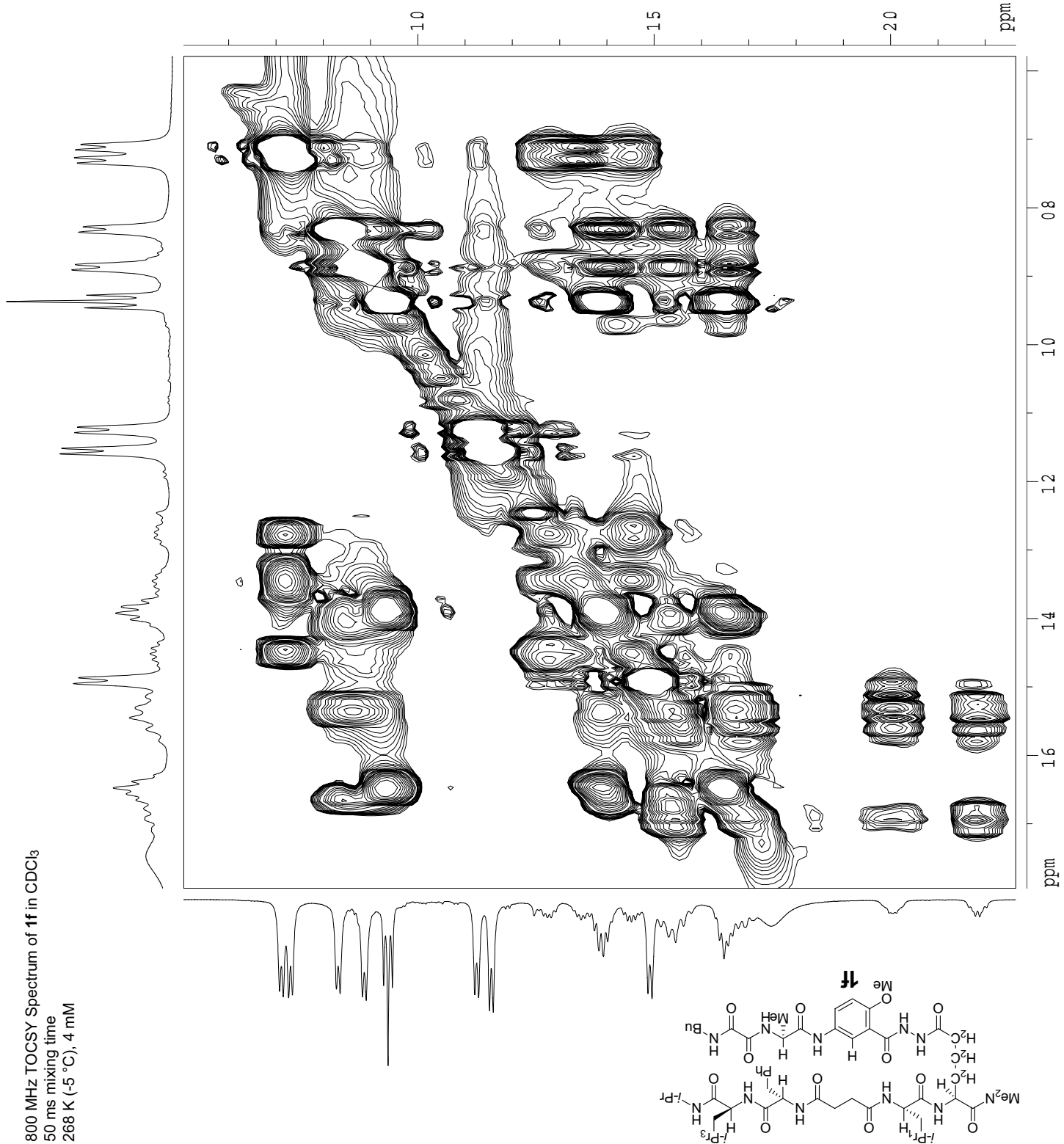
SI 2048
 SF 799.8064116 MHz
 WDW QSIINE
 SSB 2
 LB 0.00 Hz
 GB 0
 PC 1.40

F1 - Processing parameters

SI 1024
 MC2 States
 SF 799.8064116 MHz
 WDW QSIINE
 SSB 2
 LB 0.00 Hz
 GB 0

S. Levin and J. S. Nowick

2D NMR plot parameters
 CX2 15.00 cm
 CX1 15.00 cm
 F2PLO 1.794 ppm
 F2LO 1435.22 Hz
 F2PHI 0.579 ppm
 F2HI 462.95 Hz
 F1PLO 2.265 ppm
 F1LO 1811.23 Hz
 F1PHI 0.505 ppm
 F1HI 403.86 Hz
 F2P1MCM 0.08104 ppm/cm
 F2HZCM 64.81768 Hz/cm
 F1P1MCM 0.11731 ppm/cm
 F1HZCM 93.82449 Hz/cm



800 MHz TOCSY Spectrum of **1f** in CDCl₃
 50 ms mixing time
 268 K (-5 °C), 4 mM

Current Data Parameters
 USER slevin
 NAME SL-7-124-800-H
 EXPNO 4
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20061030
 Time 0.00
 INSTRUM varian
 PROBHD 40:5mmrbroadban
 PULPROG noesy2o_pfg_800_pln

TD 4096
 SOLVENT CDCl3
 NS 32
 DS 64
 SMH 11001.101 Hz
 FIDRES 2.685816 Hz
 AQ 0.1862132 sec
 RG 128
 DW 45.450 usec
 DE 6.00 usec
 TE 268.5 K

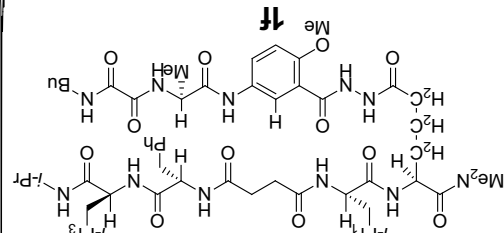
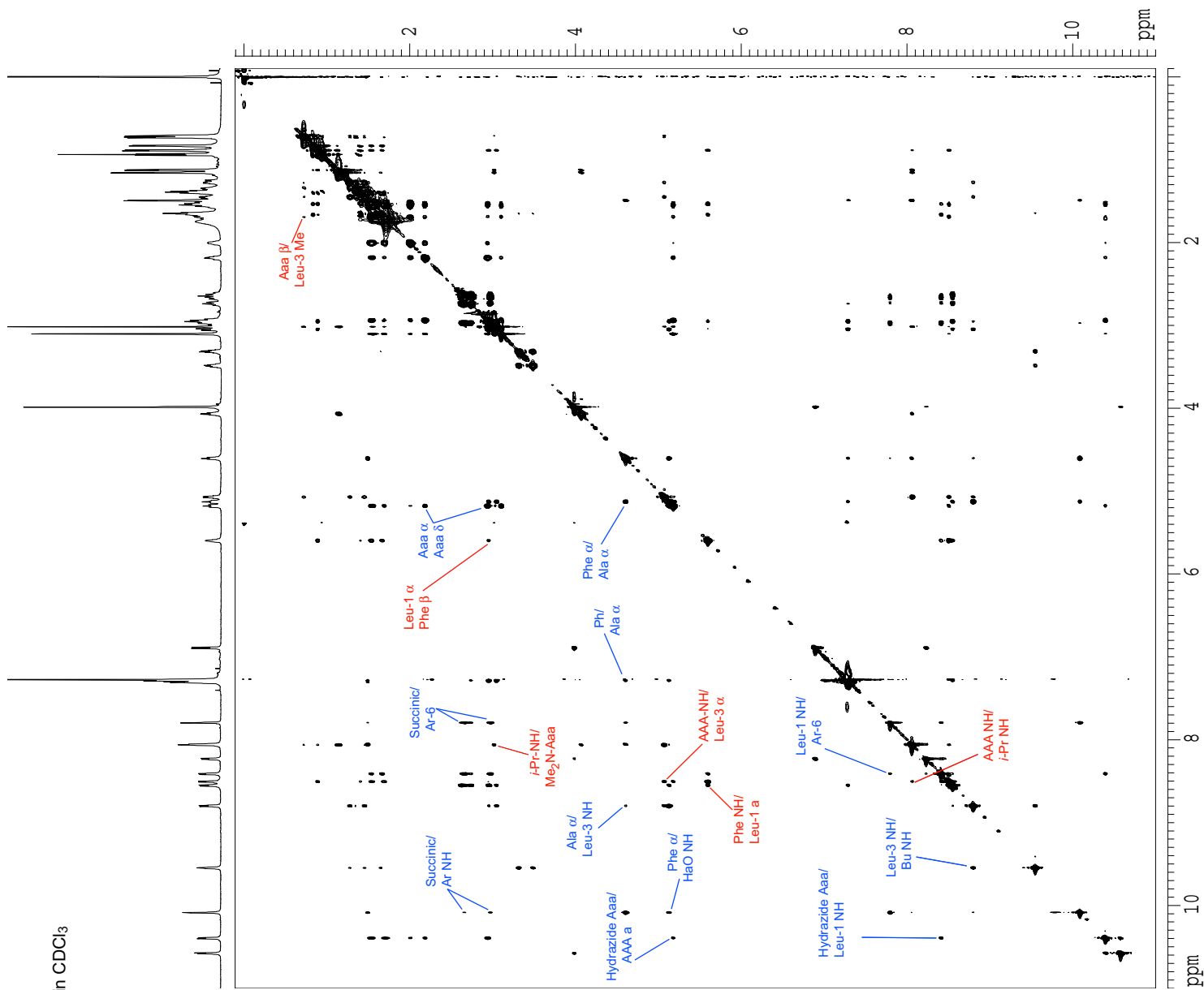
F1 - Acquisition parameters
 NDO 1
 TD 512
 SFO1 799.8107 MHz
 FIDRES 21.486525 Hz
 SW 13.755 ppm
 F1MODE undefined

F2 - Processing parameters
 SI 4096
 SF 799.8064116 MHz
 WDM QSINE
 SSB 2
 LB 0.00 Hz
 GB 0
 PC 1.40

F1 - Processing parameters
 SI 2048
 MC2 States
 SF 799.8064116 MHz
 WDM QSINE
 SSB 2
 LB 0.00 Hz
 GB 0

2D NMR plot parameters
 CX2 15.00 cm
 CX1 15.00 cm
 F2PLO 11.002 ppm
 F2LO 8799.72 Hz
 F2PHI -0.103 ppm
 F2HI -82.27 Hz
 F1PLO 11.002 ppm
 F1LO 8799.72 Hz
 F1PHI -0.106 ppm
 F1HI -84.95 Hz
 F2PFCM 0.74035 ppm/cm
 F2H2CM 592.13275 Hz/cm
 F1PFCM 0.74057 ppm/cm
 F1H2CM 592.31183 Hz/cm

800 MHz NOESY Spectrum of **1f** in CDCl₃
 400 ms mixing time
 268 K (-5 °C), 4 mM



Current Data Parameters
 USER slewin
 NAME SL-7-124-800-H
 EXPNO 4
 PROCNO 1

F2 - Acquisition Parameters

Date_ 20061030
 Time 0.00
 INSTRUM varian
 PROBRD 40:5mm broadband
 PULPROG noesyh2o_pfg_800_pln
 TD 4096
 SOLVENT CDCl3
 NS 32
 DS 64
 SWH 11001.101 Hz
 FIDRES 2.685816 Hz
 AQ 0.1862132 sec
 RG 128
 DW 45.450 usec
 DE 6.00 usec
 TE 268.15 K

F1 - Acquisition parameters

ND0 1
 TD 512
 SFO1 799.8107 MHz
 FIDRES 21.486525 Hz
 SW 13.755 ppm
 F1MODE undefined

F2 - Processing parameters

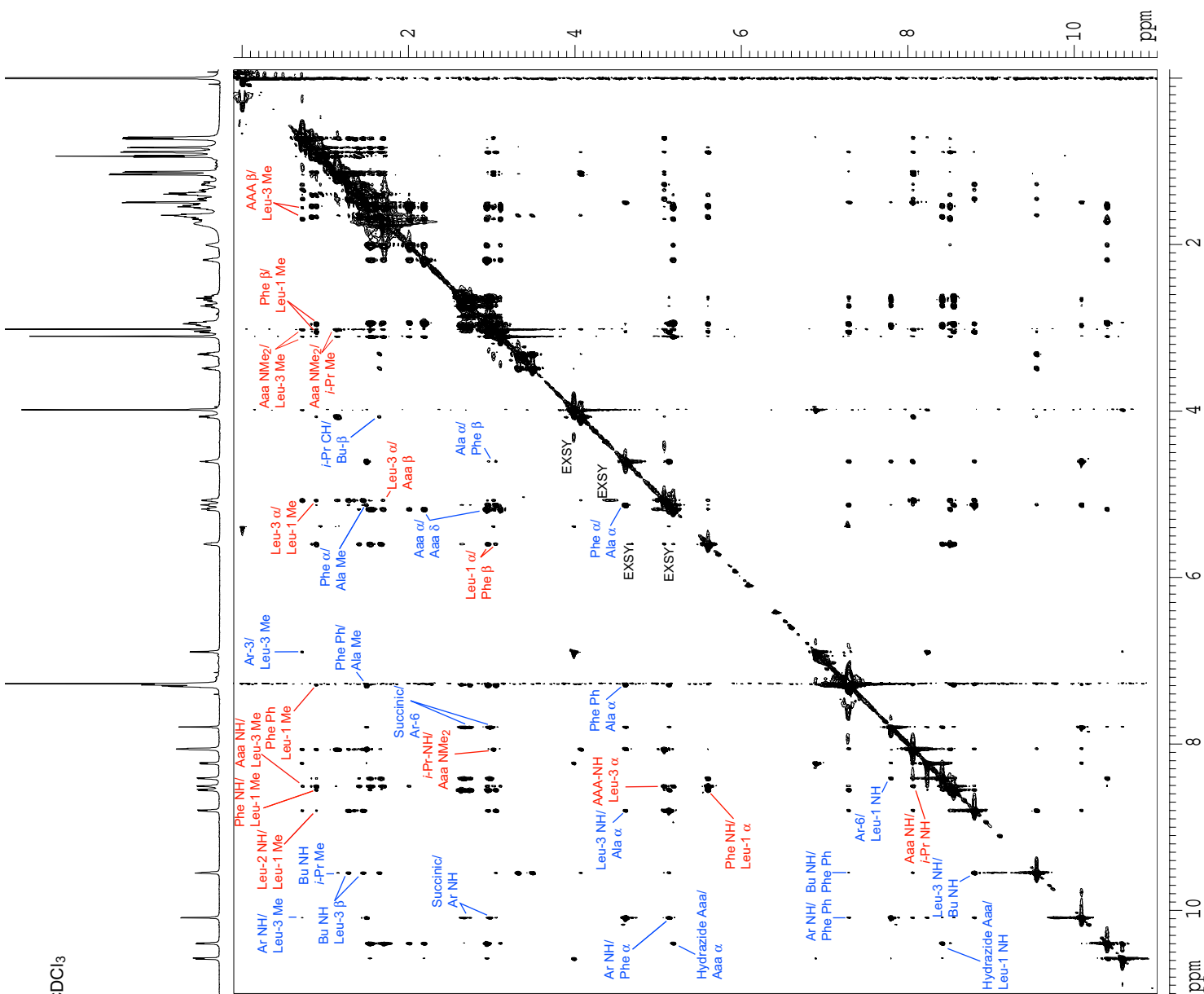
SI 4096
 SF 799.8064116 MHz
 WDW QSI
 SSB 2
 LB 0.00 Hz
 GB 0
 PC 1.40

F1 - Processing parameters

SI 2048
 MC2 States
 SF 799.8064116 MHz
 WDW QSI
 SSB 2
 LB 0.00 Hz
 GB 0

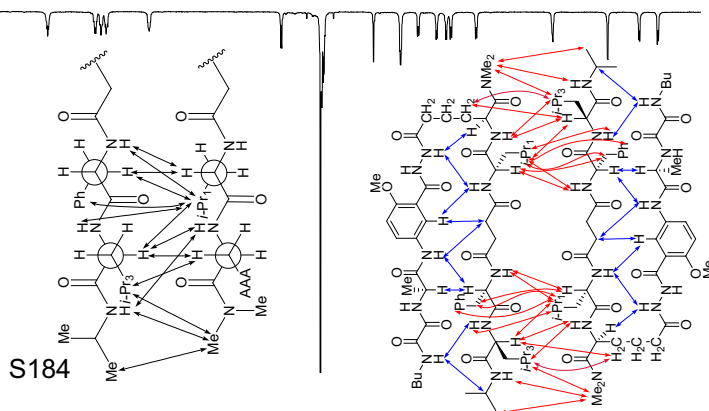
2D NMR plot parameters

CX2 15.00 cm
 CX1 15.00 cm
 F2PLO 11.000 ppm
 F2LO 8797.87 Hz
 F2PHI -0.100 ppm
 F2HI -79.98 Hz
 F1PLO 11.000 ppm
 F1LO 8797.87 Hz
 F1PHI -0.100 ppm
 F1HI -79.98 Hz
 F2PFCM 0.74000 ppm/cm
 F2HZCM 591.85669 Hz/cm
 F1PFCM 0.74000 ppm/cm
 F1HZCM 591.85669 Hz/cm



800 MHz NOESY Spectrum of **1f** in CDCl₃
 400 ms mixing time
 268 K (-5 °C), 4 mM

Deeper slice



Current Data Parameters

USER slevin
 NAME SL-7-124-800-H
 EXNO 4
 PROCNO 1

F2 - Acquisition Parameters

Date_ 20061030
 Time_ 0.00
 INSTRUM varian
 PROBHD 40:5mm broadband
 PULPROG noesyh2o_pfg_800_pln
 TD 4096
 SOLVENT CDCl3

NS 32
 DS 64
 SWH 11001.101 Hz
 FIDRES 2.685816 Hz
 AQ 0.1862132 sec
 RG 128
 DW 45.450 usec
 DE 6.00 usec
 TE 268.5 K

F1 - Acquisition Parameters

ND0 1
 TD 512
 SFO1 799.8107 MHz
 FIDRES 21.486525 Hz
 SW 13.755 ppm
 FRMODE undefined

F2 - Processing parameters

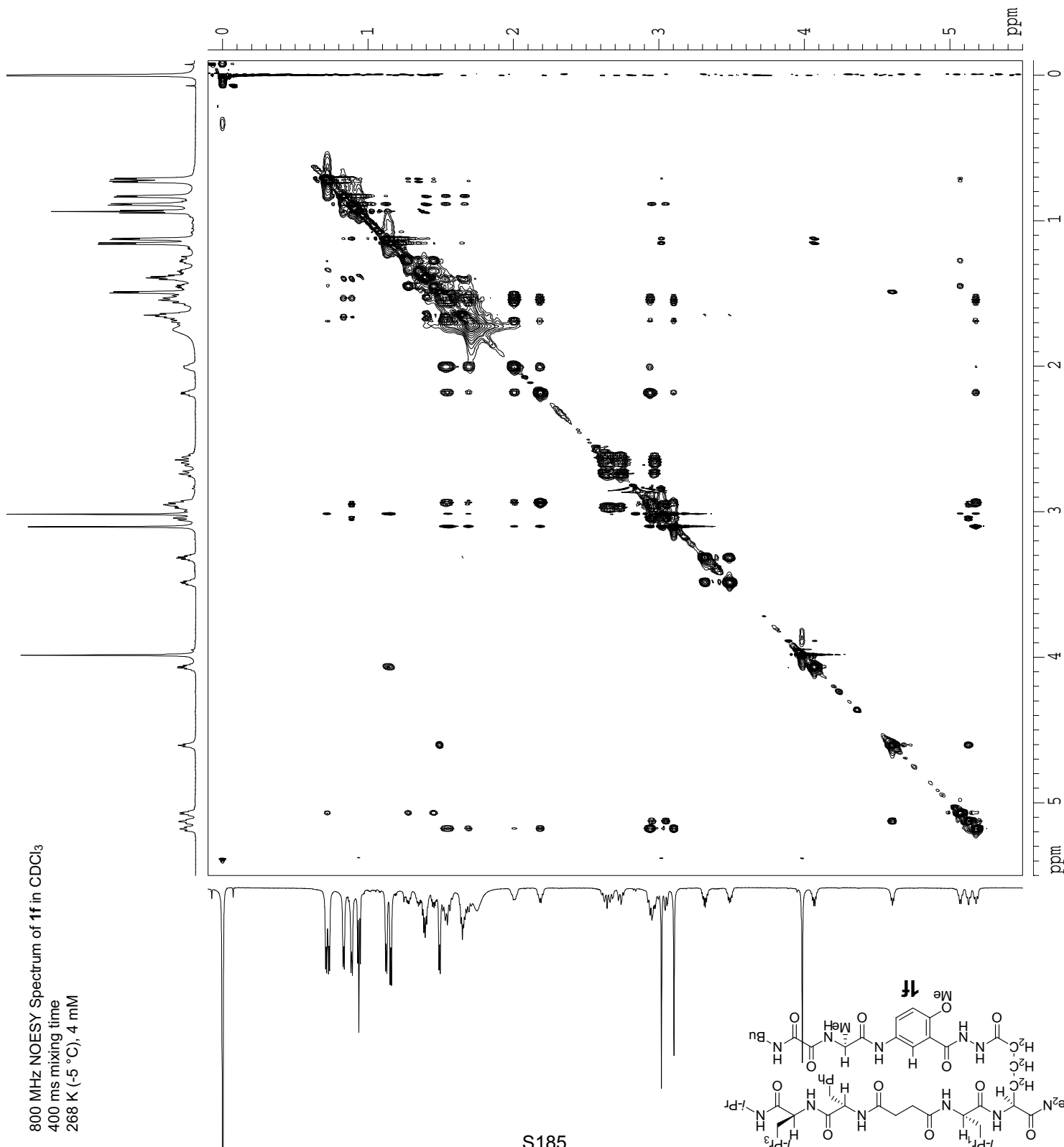
SI 4096
 SF 799.8064116 MHz
 WDM QSINE
 SSB 2
 LB 0.00 Hz
 GB 0
 PC 1.40

F1 - Processing parameters

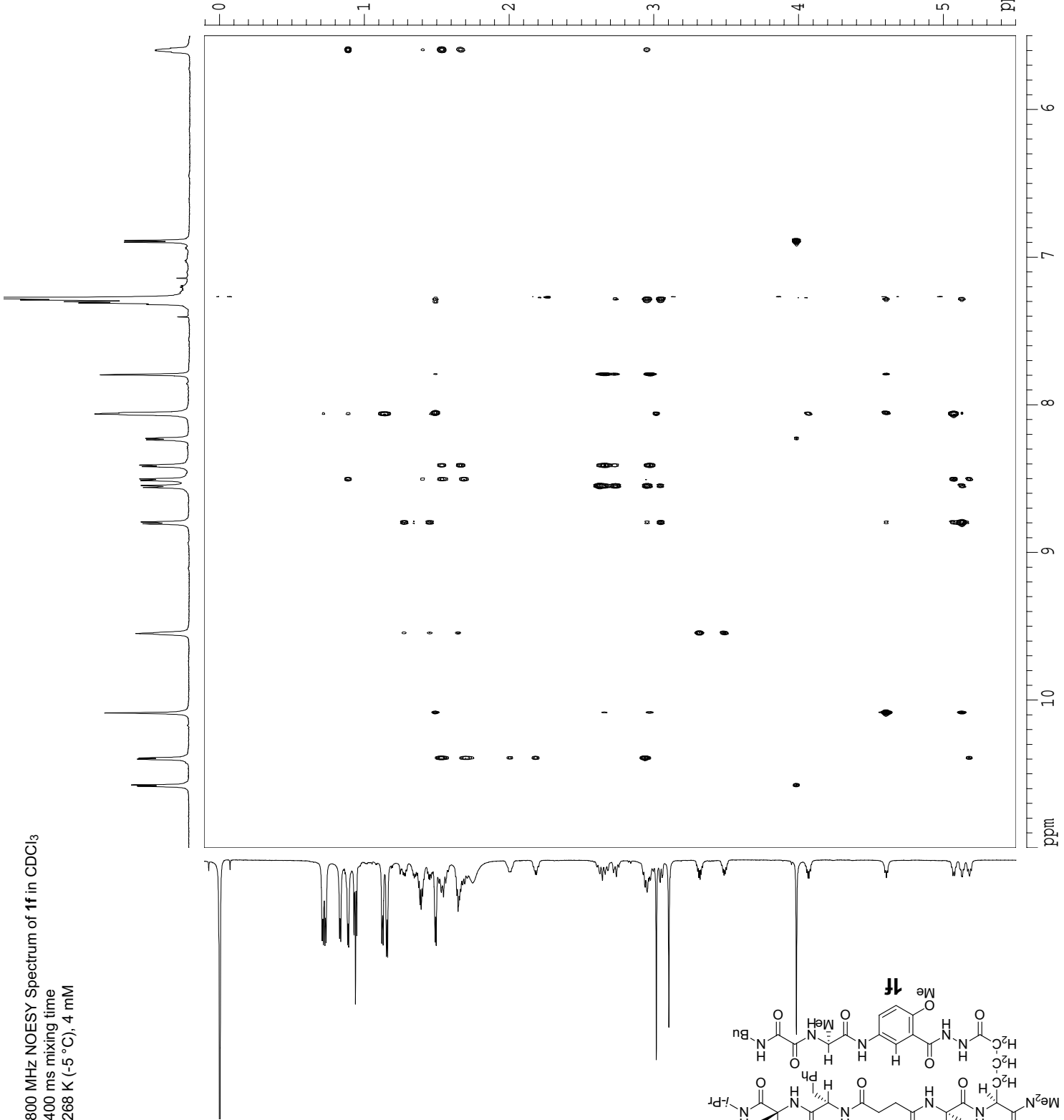
SI 2048
 MC2 States
 SF 799.8064116 MHz
 WDM QSINE
 SSB 2
 LB 0.00 Hz
 GB 0

2D NMR plot parameters

CX2 15.00 cm
 CX1 15.00 cm
 F2PLO 5.500 ppm
 F2LO 4398.94 Hz
 F2PHI -0.100 ppm
 F2HI -79.98 Hz
 F1PLO 5.500 ppm
 F1LO 4398.94 Hz
 F1PHI -0.100 ppm
 F1HI -79.98 Hz
 F2PPMCM 0.37333 ppm/cm
 F2HZCM 298.59439 Hz/cm
 F1PPMCM 0.37333 ppm/cm
 F1HZCM 298.59439 Hz/cm



800 MHz NOESY Spectrum of **1f** in CDCl₃
 400 ms mixing time
 268 K (-5 °C), 4 mM



Supporting Information

Current Data Parameters
 USER slewin
 NAME SL-7-124-800-H
 EXPNO 4
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20061030
 Time_ 0.00
 INSTRUM varian
 PROBHD 40:5mmroadban
 PULPROG noesyh2o_pfg_800_pln
 TD 4096
 SOLVENT CDCl3
 NS 32
 DS 64
 SWH 11001.101 Hz
 FIDRES 2.685816 Hz
 AQ 0.1862132 sec
 RG 128
 DW 45.450 usec
 DE 6.00 usec
 TE 268.5 K

F1 - Acquisition Parameters
 ND0 1
 TD 512
 SFO1 799.8107 MHz
 FIDRES 21.486525 Hz
 SW 13.755 ppm
 FMODE undefined

F2 - Processing parameters
 SI 4096
 SF 799.8064116 MHz
 WDW QSINE
 SSB 2
 LB 0.00 Hz
 GB 0
 PC 1.40

F1 - Processing parameters
 SI 2048
 MC2 States
 SF 799.8064116 MHz
 WDW QSINE
 SSB 2
 LB 0.00 Hz
 GB 0

2D NMR plot parameters
 CX2 15.00 cm
 CX1 15.00 cm
 F2PLO 11.000 ppm
 F2LO 8797.87 Hz
 F2PHI 5.500 ppm
 F2HI 4398.94 Hz
 F1PLO 5.502 ppm
 F1LO 4400.36 Hz
 F1PHI -0.106 ppm
 F1HI -84.95 Hz
 F2PPMCM 0.36667 ppm/cm
 F2HZCM 293.26236 Hz/cm
 F1PPMCM 0.37387 ppm/cm
 F1HZCM 299.02078 Hz/cm

S. Levin and J. S. Nowick

Current Data Parameters
 USER slewin
 NAME SL-7-124-800-H
 EXPNO 4
 PROCNO 1

F2 - Acquisition Parameters

Date_ 20061030
 Time_ 0.00
 INSTRUM varian
 PROBHD 40:5mmrbroadban
 PULPROG noesyh2o_pfg 800_plh
 TD 4096
 SOLVENT CDC13
 NS 32
 DS 64
 SWH 11001.101 Hz
 FIDRES 2.685816 Hz
 AQ 0.1862132 sec
 RG 128
 DW 45.450 usec
 DE 6.00 usec
 TE 268.5 K

F1 - Acquisition Parameters

ND0 1
 TD 512
 SF01 799.8107 MHz
 FIDRES 21.486525 Hz
 SW 13.755 ppm
 FMODE undefined

F2 - Processing parameters

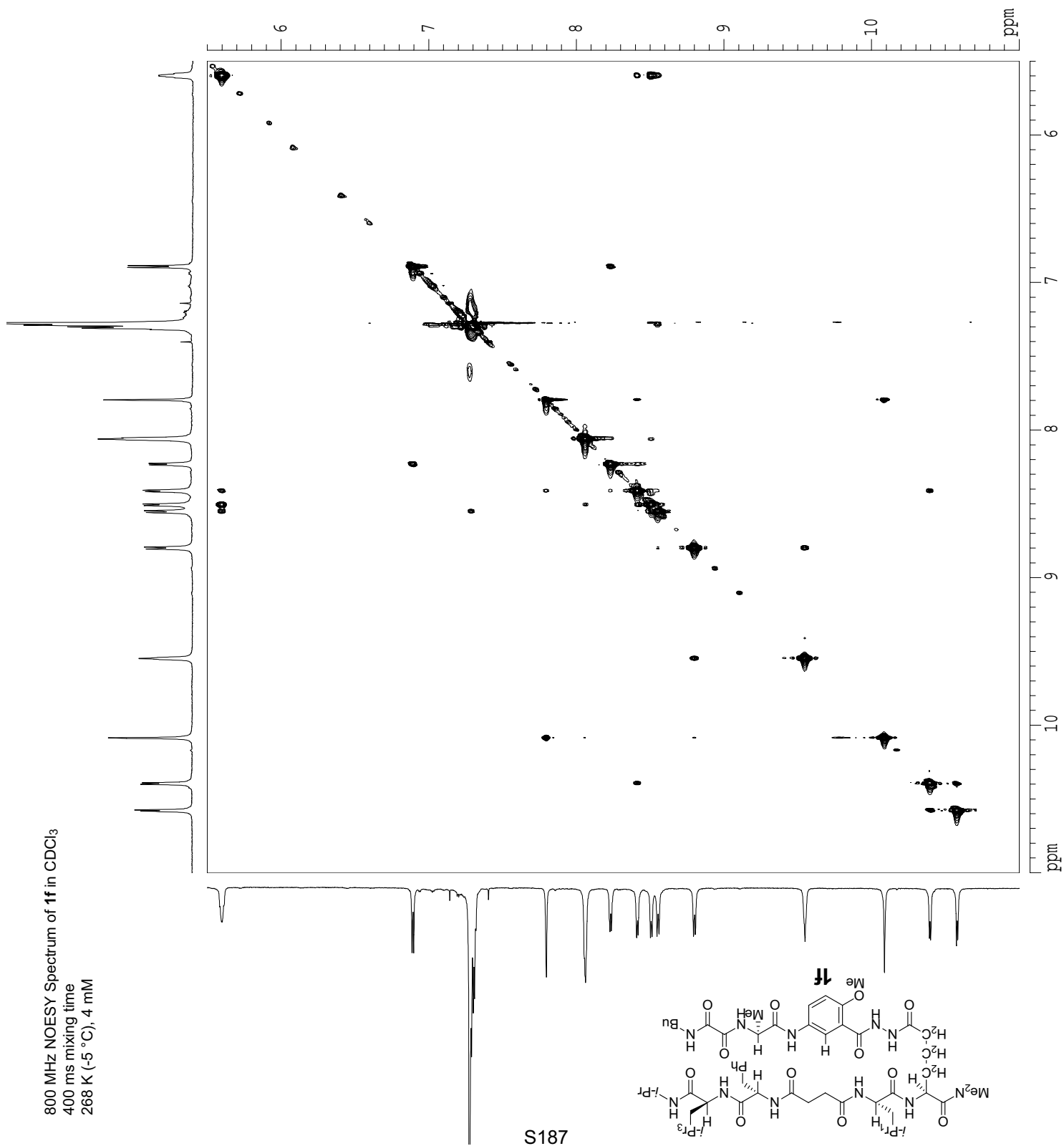
SI 4096
 SF 799.8064116 MHz
 WDW QSI
 SSB 2
 LB 0.00 Hz
 GB 0
 PC 1.40

F1 - Processing parameters

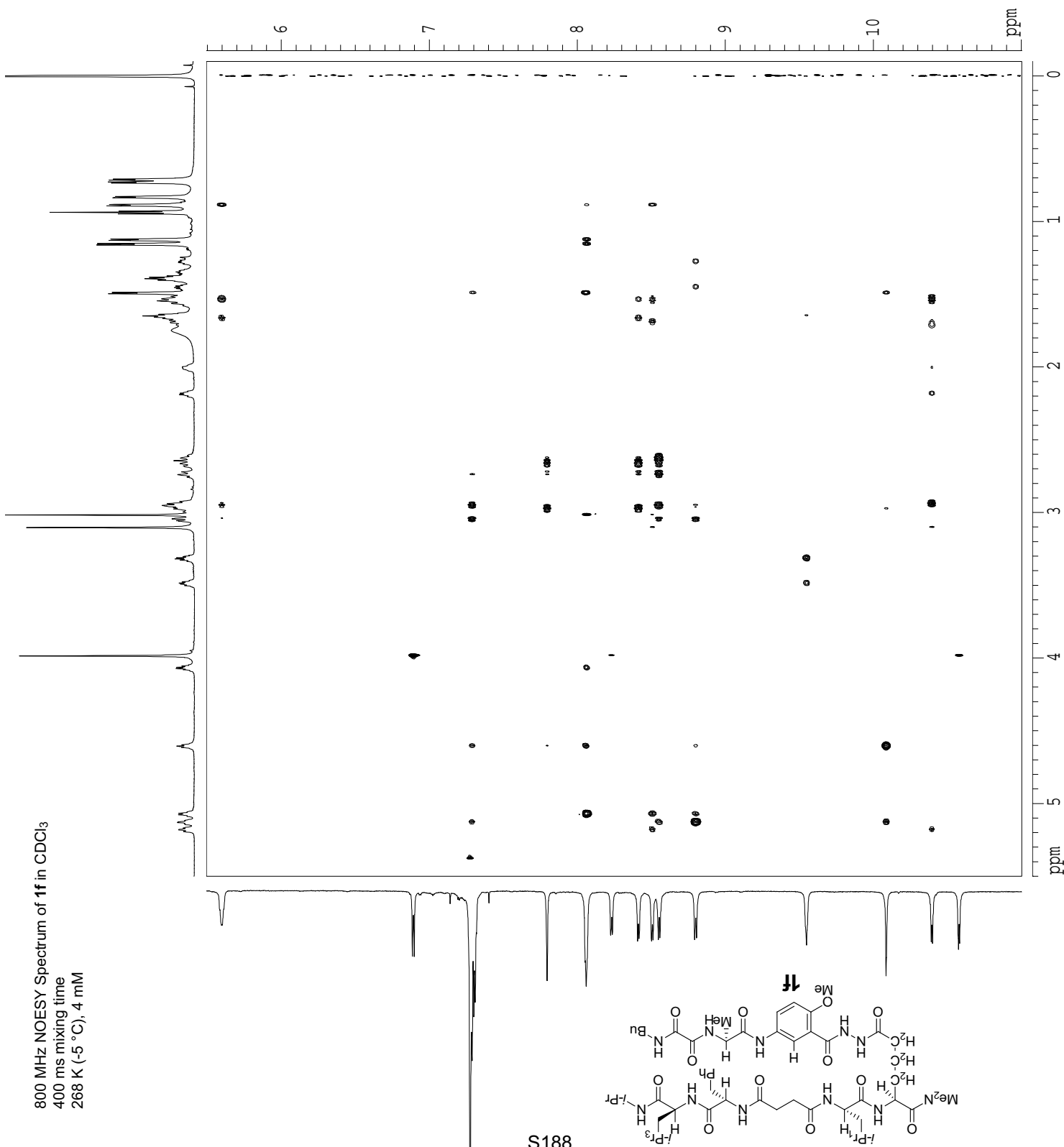
SI 2048
 MC2 States
 SF 799.8064116 MHz
 WDW QSI
 SSB 2
 LB 0.00 Hz
 GB 0

2D NMR plot parameters

CX2 15.00 cm
 CX1 15.00 cm
 F2PLO 11.002 ppm
 F2LO 8799.72 Hz
 F2PHI 5.498 ppm
 F2HI 4397.67 Hz
 F1PLO 11.000 ppm
 F1LO 8797.87 Hz
 F1PHI 5.500 ppm
 F1HI 4398.94 Hz
 F2PQCM 0.36693 ppm/cm
 F2HZCM 293.47009 Hz/cm
 F1PQCM 0.36667 ppm/cm
 F1HZCM 293.26236 Hz/cm



800 MHz NOESY Spectrum of **1f** in CDCl₃
 400 ms mixing time
 268 K (-5 °C), 4 mM



S188

Current Data Parameters
 USER slevin
 NAME SL-7-124-800-H
 EXPNO 4
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20061030
 Time 0.00
 INSTRUM varian
 PROBHD 40:5mm broadband
 PULPROG noesyh2o_pfg_800_pln
 TD 4096
 SOLVENT CDCl3
 NS 32
 DS 64
 SWH 11001.101 Hz
 FIDRES 2.685816 Hz
 AQ 0.1862132 sec
 RG 128
 DW 45.450 usec
 DE 6.00 usec
 TE 268.5 K

F1 - Acquisition parameters
 ND0 1
 TD 512
 SFO1 799.8107 MHz
 FIDRES 21.486525 Hz
 SW 13.755 ppm
 FMODE undefined

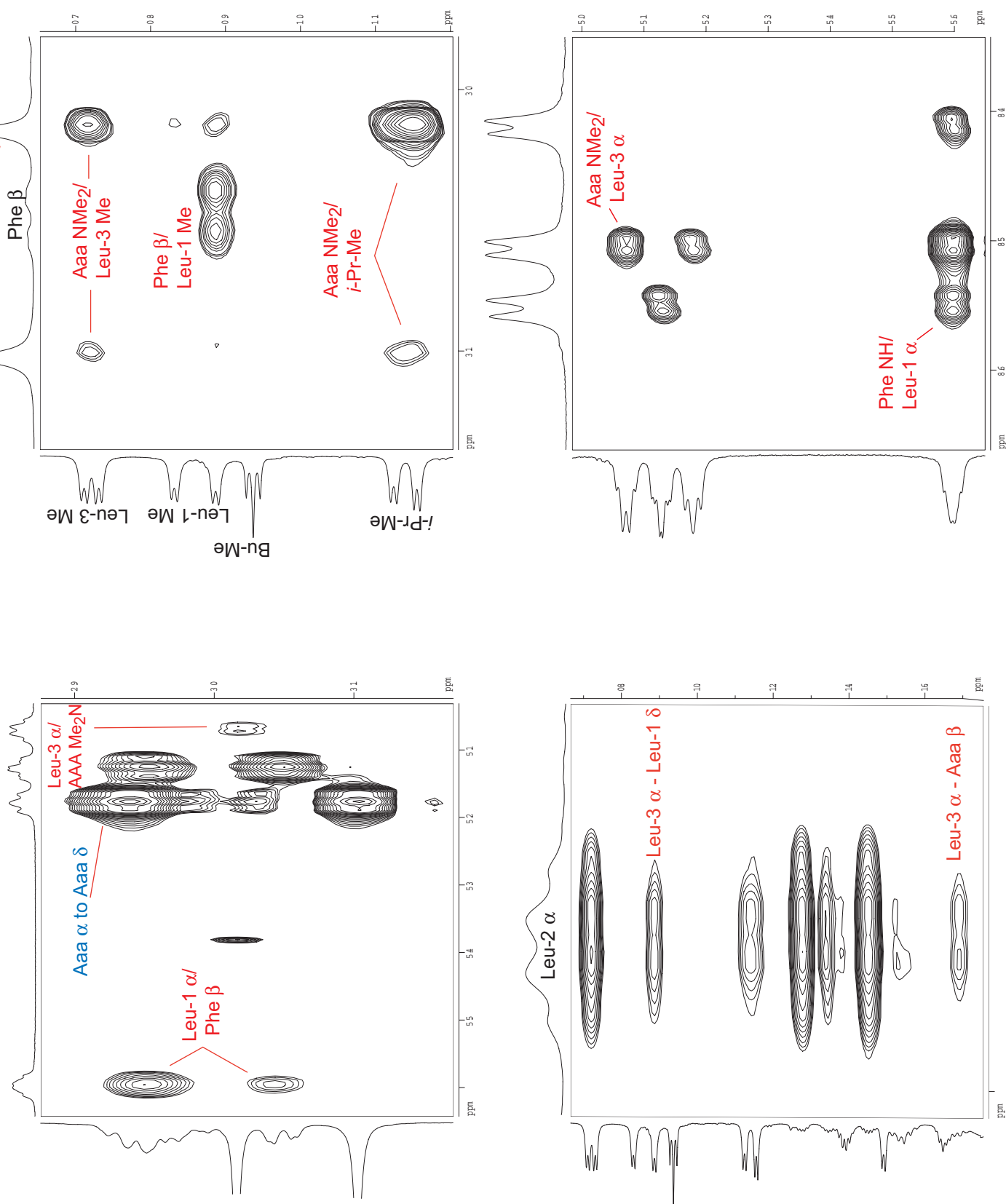
F2 - Processing parameters
 SI 4096
 SF 799.8064116 MHz
 WDW QSI
 SSB 2
 LB 0.00 Hz
 GB 0
 PC 1.40

F1 - Processing parameters
 SI 2048
 MC2 States
 SF 799.8064116 MHz
 WDW QSI
 SSB 2
 LB 0.00 Hz
 GB 0

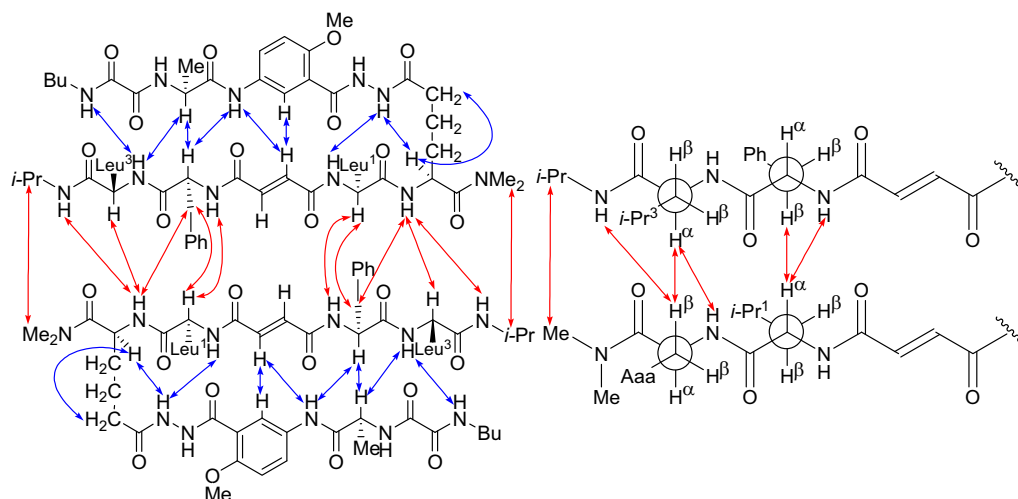
2D NMR plot parameters
 CX2 15.00 cm
 CX1 15.00 cm
 F2PLO 5.500 ppm
 F2LO 4398.94 Hz
 F2PHI -0.100 ppm
 F2HI -79.98 Hz
 F1PLO 11.002 ppm
 F1LO 8799.72 Hz
 F1PHI 5.495 ppm
 F1HI 4394.99 Hz
 F2PNCM 0.37333 ppm/cm
 F2ZCM 298.59439 Hz/cm
 F1PNCM 0.36715 ppm/cm
 F1ZCM 293.64917 Hz/cm

Selected NOEs

800 MHz NOESY Spectrum of **1f** in CDCl₃
 400 ms mixing time
 268 K (-5 °C), 4 mM



Spectroscopic DATA for the compound **2a**
(3 mM, CDCl₃ 268K)



Key NOEs assigned as *intermolecular* are represented with red arrows.
Key NOEs assigned as *intramolecular* are represented with blue arrows.

Key data for amino acids.

Amino acid	H _α Shift ppm	NH Shift ppm	³ J _{NHα} Hz
Aaa	5.20	8.77	8.2
R ₁ = Leu ¹	5.80	8.55	8.2
R ₂ = Phe	5.20	9.20	9.8
R ₃ = Leu ²	5.05	8.74	broad
R ₄ = Ala	4.50	8.05	broad

Aminoacidic acid (Aaa) δ proton resonances.

pro-R: 2.85 ppm, t, (*J* = 12.0 Hz)

pro-S: 2.20 ppm, td, (*J*₁ = 11.5 Hz; *J*₂ = 7.0 Hz)

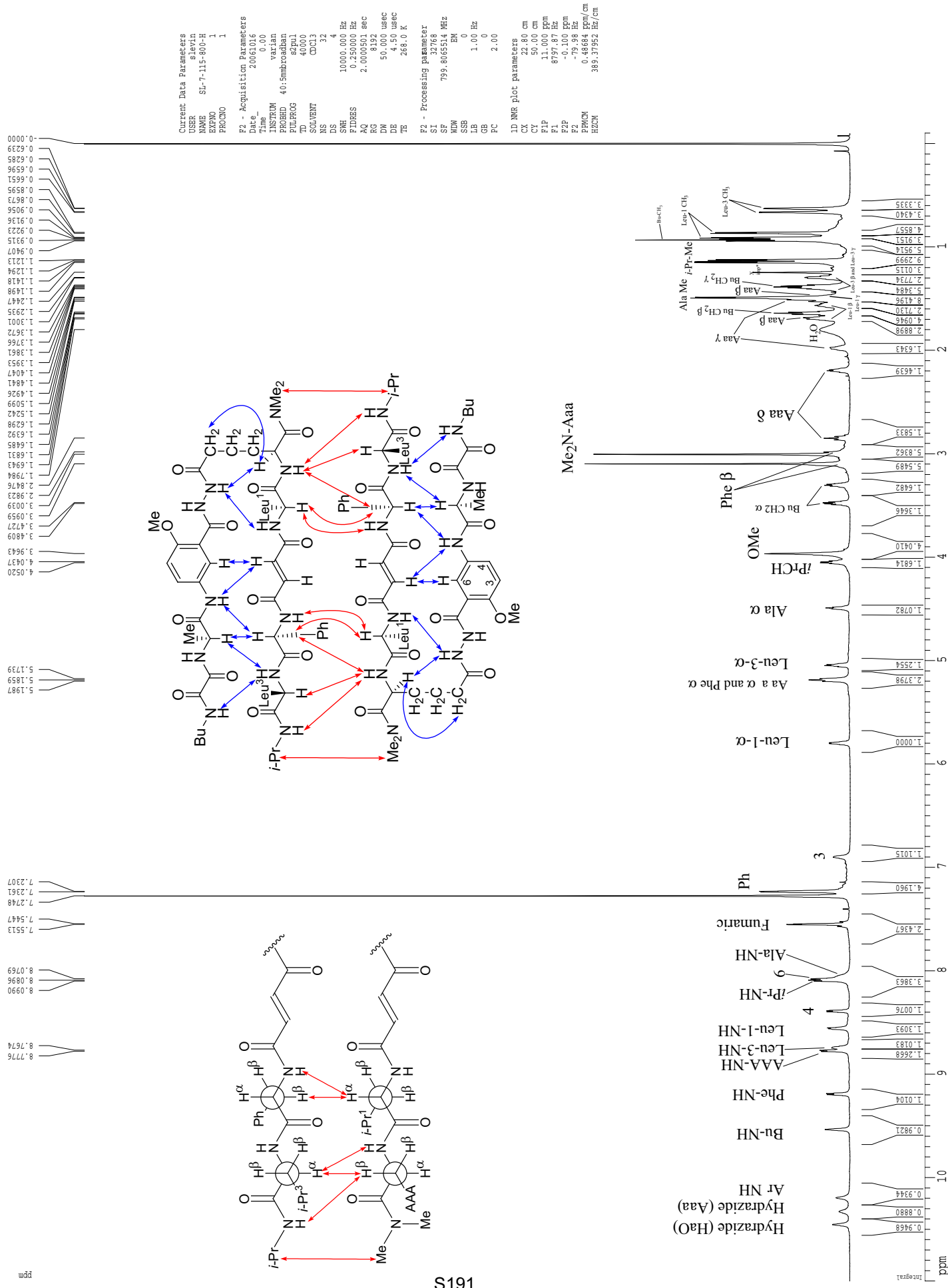
anisotropy = 0.65ppm

Key data for other NH protons.

Proton	NH Shift ppm	<i>J</i> Hz
Ar-NH	10.20	-
Hydrazide Ar	10.45	broad
Hydrazide Aaa	10.33	broad
Bu-NH	9.53	broad
<i>i</i> -Pr-NH	8.10	7.6

ESI MS *m/z* for C₅₃H₈₀N₁₁O₁₂ [M+H]⁺ calcd 1062.60, found 1062.48.

800 MHz ¹H NMR Spectrum of **2a** in CDCl₃
268 K (-5 °C), 3 mM



Supporting Information

Current Data Parameters
 USER sleVIN
 NAME SL-7-115-cr-600-268K-H
 EXPNO 6
 PROCNO 1

F2 - Acquisition Parameters

Date_ 20061011
 Time 19:39
 INSTRUM av600
 PROBHD 5 mm TBI IH/13
 PULPROG cosy90pf
 TD 1912
 SOLVENT CDCl3
 NS 8
 DS 16
 SWH 7211.539 Hz
 FIDRES 3.771725 Hz
 AQ 0.1326151 sec
 RG 362
 DW 69.333 usec
 DE 6.00 usec
 TE 268.0 K
 d0 0.00000300 sec
 d1 1.48689198 sec
 d13 0.00000400 sec
 d16 0.00020000 sec
 INU 0.00013885 sec

==== CHANNEL f1 =====

NUC1 1H
 P0 8.00 usec
 P1 8.00 usec
 PL1 -1.00 dB
 SFO1 600.1334803 MHz

==== GRADIENT CHANNEL =====

GENAM1 SINE.100
 GENAM2 SINE.100
 GPZ1 10.00 %
 GPZ2 10.00 %
 P16 10000.00 usec

F1 - Acquisition Parameters

ND0 1
 TD 256
 SFO1 600.1335 MHz
 FIDRES 28.132877 Hz
 SW 12.001 ppm
 PRMODE QF

F2 - Processing Parameters

SI 1024
 SF 600.1300262 MHz
 SINE
 WDW 0
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.00

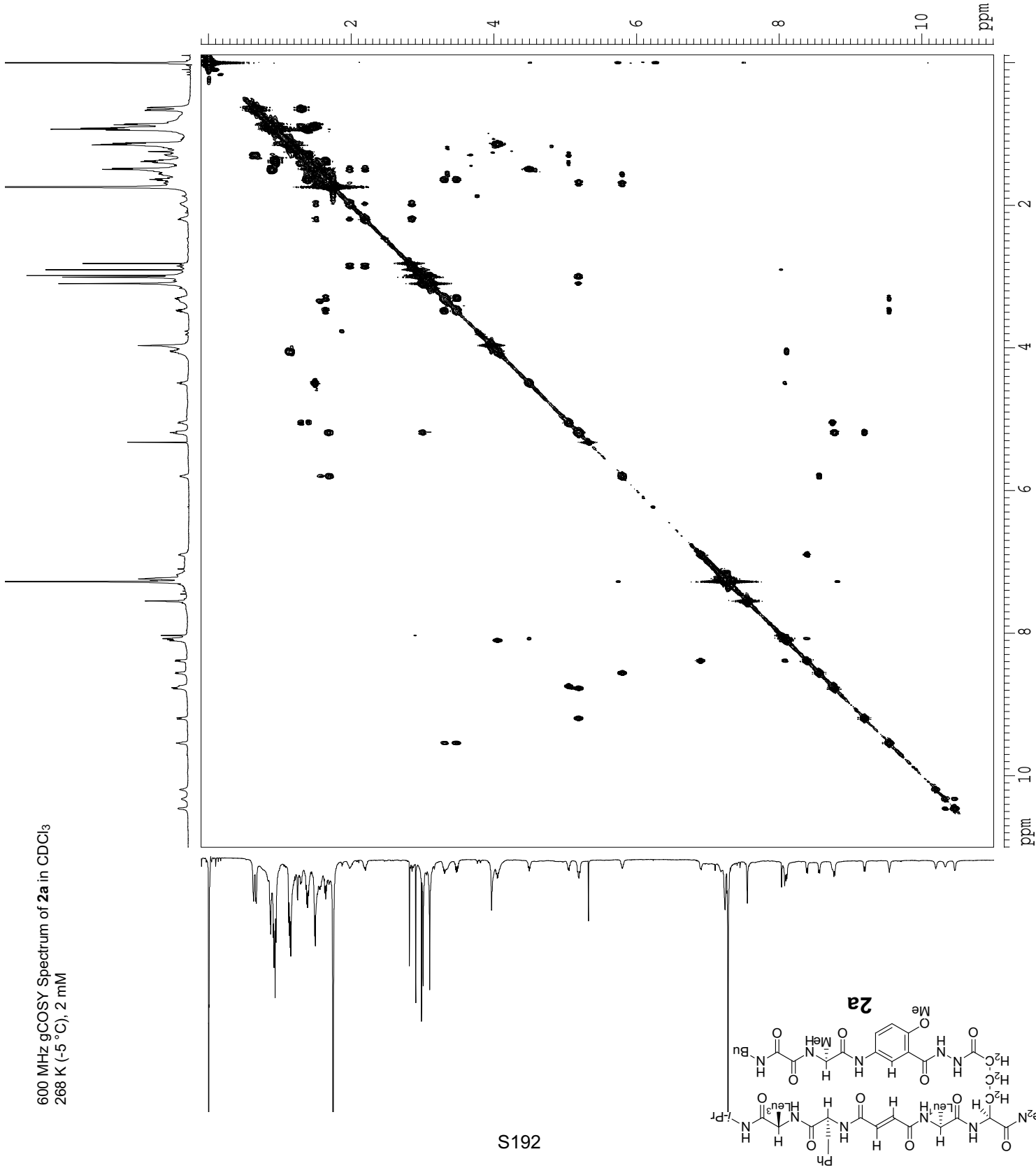
F1 - Processing Parameters

SI 1024
 MC2 QF
 SF 600.1300262 MHz
 SINE
 WDW 0
 SSB 0
 LB 0.00 Hz
 GB 0

2D NMR plot parameters

CY2 15.00 cm
 CX1 15.00 cm
 FZPLO 11.002 Fpm
 FZLO 6602.60 Hz
 FZPHI -0.111 ppm
 FZHI -66.67 Hz
 F1PLO 11.007 ppm
 F1LO 6605.48 Hz
 F1PHI -0.103 ppm
 F1HI -62.02 Hz
 F2PDMCM 0.74087 Fpm/cm
 F2HZCM 444.61761 Hz/cm
 F1PDMCM 0.74067 Fpm/cm
 F1HZCM 444.49945 Hz/cm

600 MHz gCOSY Spectrum of **2a** in CDCl₃
 268 K (-5 °C), 2 mM



Current Data Parameters
 USER slevin
 NAME SL-7-115-cr-600-268K-H
 EXPNO 6
 PROCNO 1

F2 - Acquisition Parameters

Date_ 20061011
 Time 19:39
 INSTRUM av600
 PROBED 5 mm TBI 1H/13
 PULPROG cosygpgf
 TD 1912
 SOLVENT CDCl3
 NS 8
 DS 16
 SWH 7211.539 Hz
 FIDRES 3.771725 Hz
 AQ 0.1326153 sec
 RG 362
 DW 69.333 usec
 DE 6.00 usec
 TE 268.0 K
 d0 0.0000300 sec
 d1 1.48689198 sec
 d13 0.0000400 sec
 d16 0.0002000 sec
 INO 0.00013885 sec

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

NUC1 1H
 P0 8.00 usec
 PL 8.00 usec
 PL1 -1.00 dB
 SF01 600.1334808 MHz

===== GRADIENT CHANNEL =====

GPM1 SINE.100
 GPM2 SINE.100
 GPZ1 10.00 %
 GPZ2 10.00 %
 PL6 1000.00 usec

F1 - Acquisition parameters

ND0 1
 TD 256
 SF01 600.1335 MHz
 FIDRES 28.132877 Hz
 SW 12.001 ppm
 PHMODE QF

F2 - Processing parameters

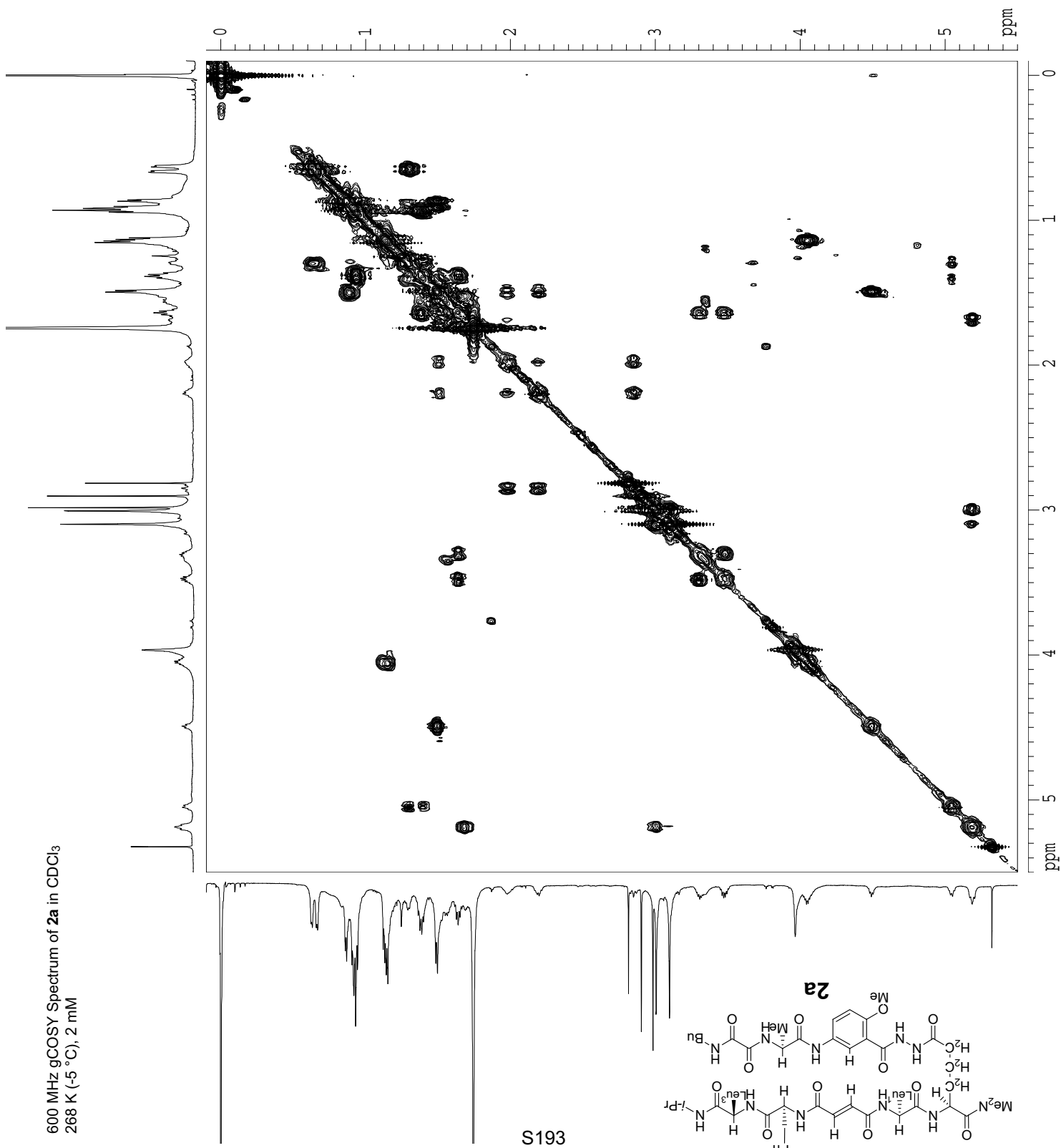
SI 1.024
 SF 600.1300262 MHz
 SINE SINE
 WDW 0
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.00

F1 - Processing parameters

SI 1.024
 MC2 QF
 SF 600.1300262 MHz
 SINE SINE
 WDW 0
 SSB 0
 LB 0.00 Hz
 GB 0

2D NMR plot parameters

CV2 15.00 cm
 CX1 15.00 cm
 F2PLO 5.500 ppm
 F2LO 3300.72 Hz
 F2PHI -0.100 ppm
 F2HT -60.01 Hz
 F1PLO 5.500 ppm
 F1LO 3300.72 Hz
 F1PHI -0.100 ppm
 F1HT -60.01 Hz
 F2PPMCM 0.37333 ppm/cm
 F2HZCM 224.04854 Hz/cm
 F1PPMCM 0.37333 ppm/cm
 F1HZCM 224.04854 Hz/cm



Supporting Information

S. Levin and J. S. Nowick

Current Data Parameters
 USER slevin
 NAME SL-7-115-cr-600-268K-H
 EXPNO 6
 PROCNO 1

F2 - Acquisition Parameters

Date_ 20061011
 Time_ 19:39
 INSTRUM av600
 PROHD 5 mm TBI IH/13
 PULPROG cosyppf
 TD 1912
 SOLVENT CDCl3
 NS 8
 DS 16
 SWH 7211.539 Hz
 FIDRES 3.771725 Hz
 AQ 0.1326153 sec
 RG 362
 DW 69.333 usec
 DE 6.00 usec
 TE 268.0 K
 d0 0.0000300 sec
 d1 1.48689198 sec
 d13 0.0000400 sec
 d16 0.0002000 sec
 INO 0.0001385 sec

==== CHANNEL f1 =====

NUC1 1H
 P0 8.00 usec
 PL 8.00 usec
 PL1 -1.00 dB
 SFO1 600.1334808 MHz

==== GRADIENT CHANNEL =====

GENAM1 SINE.100
 GENAM2 SINE.100
 GFZ1 10.00 %
 GFZ2 10.00 %
 PL6 1000.00 usec

F1 - Acquisition parameters

ND0 1
 TD 256
 SFO1 600.1335 MHz
 FIDRES 28.132877 Hz
 SW 12.001 ppm
 PRMODE QF

F2 - Processing parameters

SI 1024
 SF 600.1300262 MHz
 NDW SINE
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.00

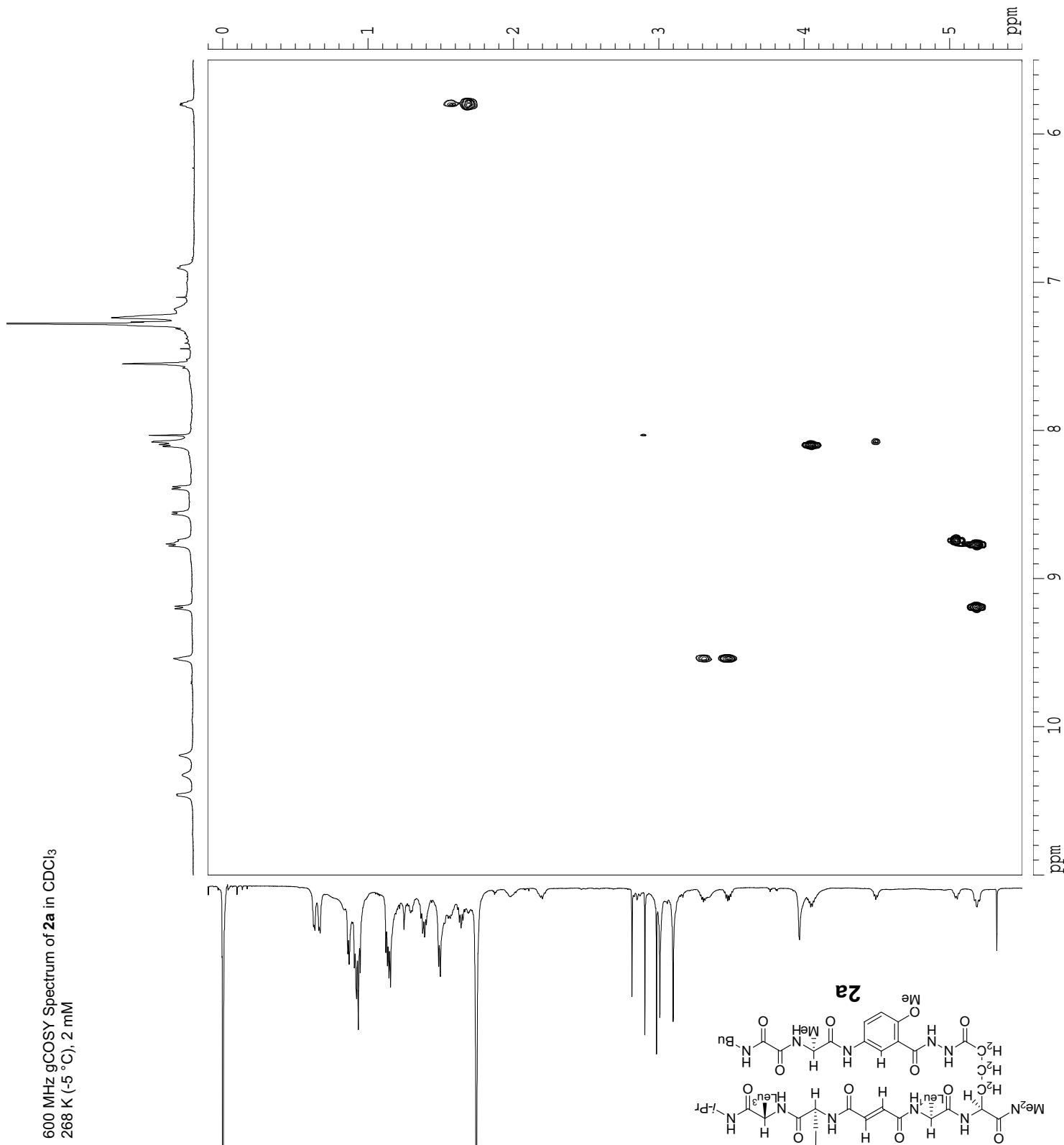
F1 - Processing parameters

SI 1024
 MC2 QF
 SF 600.1300262 MHz
 NDW SINE
 SSB 0
 LB 0.00 Hz
 GB 0

2D NMR plot parameters

CX2 15.00 cm
 CX1 15.00 cm
 F2PLO 11.000 ppm
 FZLO 6601.43 Hz
 FZPHI 5.500 ppm
 F3PHI 3300.72 Hz
 F1PLO 5.500 ppm
 F1LO 3300.72 Hz
 F1PHI -0.103 ppm
 FIHI -62.01 Hz
 F2PDMCM 0.36667 ppm/cm
 F2HZCM 220.04767 Hz/cm
 F1PDMCM 0.37356 ppm/cm
 F1HZCM 224.18199 Hz/cm

600 MHz gCOSY Spectrum of **2a** in CDCl₃
 268 K (-5 °C), 2 mM



Current Data Parameters
 USER slevin
 NAME SJ-7-115-cr-600-268K-H
 EXPNO 6
 PROCNO 1

F2 - Acquisition Parameters

Date 20061011
 Time 19.39
 INSTRUM av600
 PROBHD 5 mm TBI 1H/13
 PULPROG cosygpcf
 TD 1312
 SOLVENT CDCl3
 NS 8
 DS 16
 SWH 7211.539 Hz
 FIDRES 3.771725 Hz
 AQ 0.1326153 sec
 RG 362
 DW 69.333 usec
 DE 6.00 usec
 TE 288.0 K
 d0 0.0000300 sec
 d1 1.48689139 sec
 d13 0.0000400 sec
 d16 0.0002000 sec
 INO 0.00013885 sec

***** CHANNEL f1 *****

NUC1 ¹H
 P0 8.00 usec
 P1 8.00 usec
 PL1 -1.00 dB
 SFO1 600.1334808 MHz

***** GRADIENT CHANNEL *****

GENAM1 SINE.100
 GENAM2 SINE.100
 GPZ1 10.00 %
 GPZ2 10.00 %
 PL6 1000.00 usec

F1 - Acquisition parameters

ND0 1
 TD 256
 SFO1 600.1335 MHz
 FIDRES 28.132877 Hz
 SW 12.001 Epm
 FMODE QF

F2 - Processing parameters

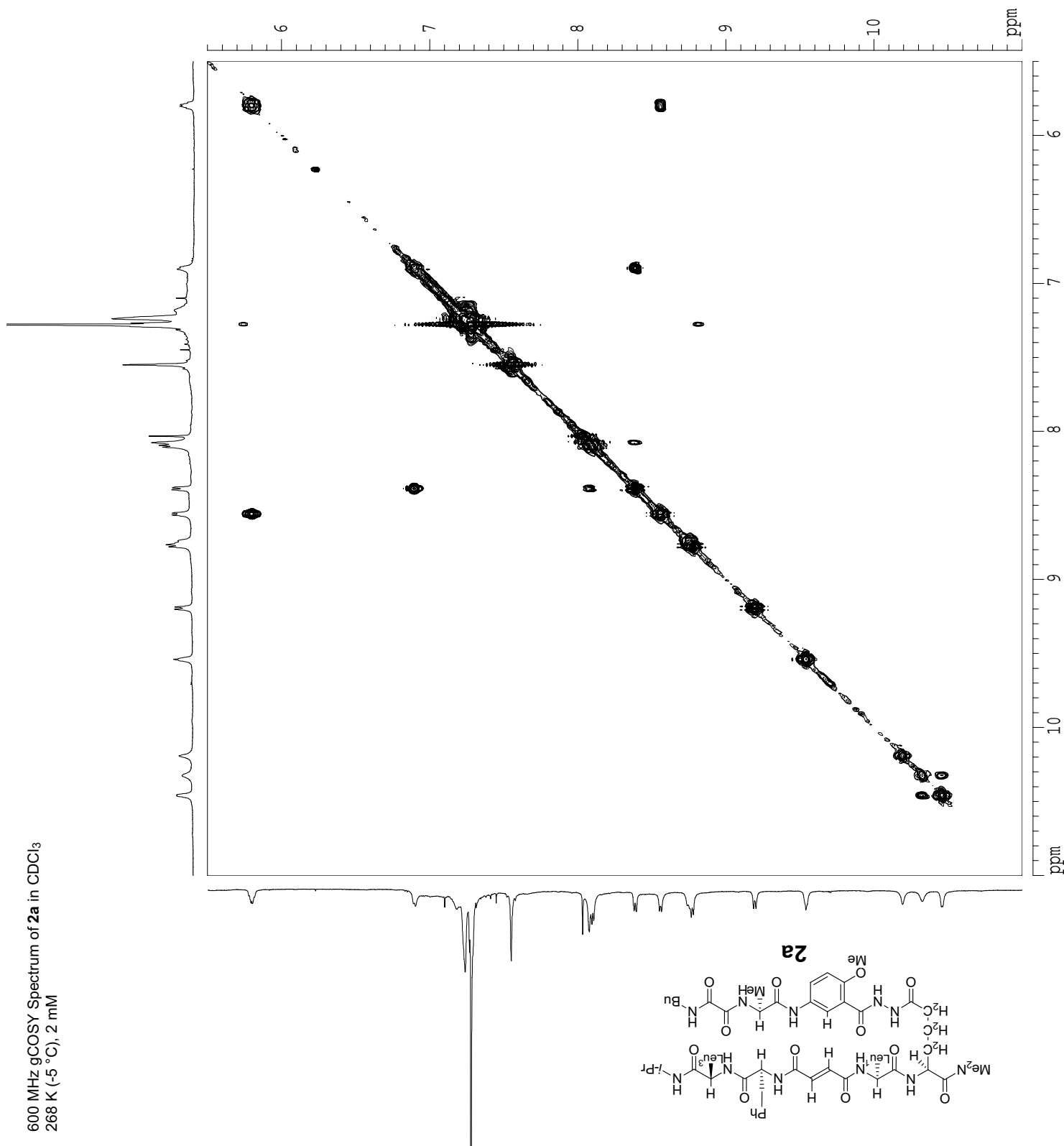
SI 1024
 SF 600.1300262 MHz
 NQW SINE
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.00

F1 - Processing parameters

SI 1024
 MC2 QF
 SF 600.1300262 MHz
 NQW SINE
 SSB 0
 LB 0.00 Hz
 GB 0

2D NMR plot parameters

CX2 15.00 cm
 CX1 15.00 cm
 F2PLO 11.002 ppm
 F2LO 6602.60 Hz
 F2PHI 5.488 ppm
 F2HL 3299.66 Hz
 F1PLO 11.000 ppm
 F1LO 6601.43 Hz
 F1PHI 5.500 ppm
 F1HI 3300.72 Hz
 F2PPMCM 0.36691 ppm/cm
 F2HZCM 220.19606 Hz/cm
 F1PPMCM 0.36667 ppm/cm
 F1HZCM 220.04767 Hz/cm



Supporting Information

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Current Data Parameters
 USER sievin
 NAME SL-7-115-cr-600-268K-H
 EXPNO 6
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20061011
 Time 19.39

INSTRUM av600
 PROBHD 5 mm TBI IH/13
 PULPROG cosy90pf
 TD 1912
 SOLVENT CDCl3
 NS 8
 DS 16
 SWH 7211.538 Hz
 FIDRES 3.771725 Hz
 AQ 0.1326151 sec
 RG 362
 DW 69.333 usec
 DE 6.00 usec
 TE 268.0 K
 d0 0.0000300 sec
 d1 1.48689198 sec
 d13 0.0000300 sec
 d16 0.0002000 sec
 IN0 0.00013885 sec

===== CHANNEL f1 =====
 NUC1 1H
 P0 8.00 usec
 PL 8.00 usec
 PL1 -1.00 dB
 SFO1 600.1334808 MHz

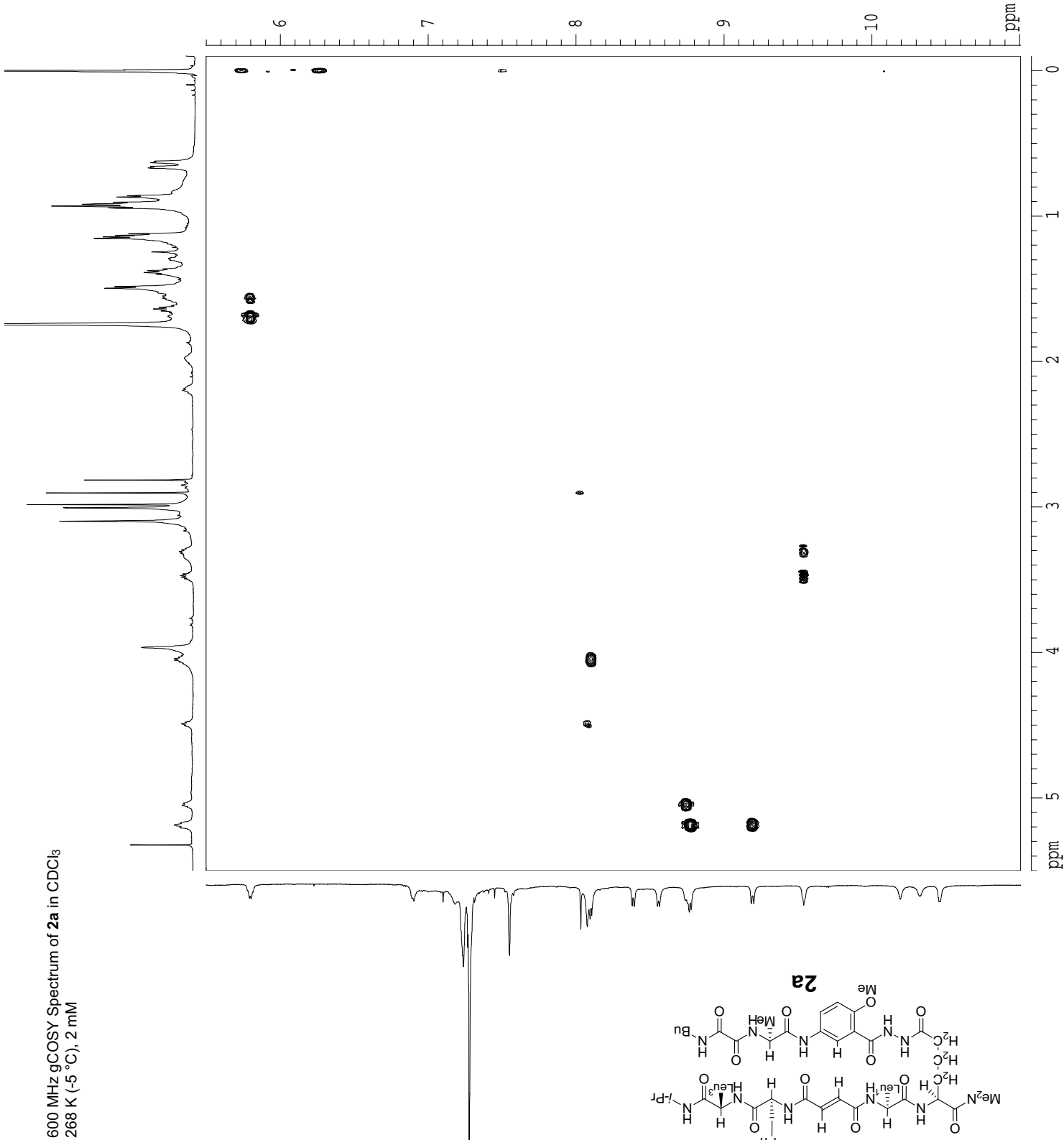
===== GRADIENT CHANNEL =====
 GENAM1 SINE.100
 GENAM2 SINE.100
 GFZ1 10.00 %
 GFZ2 10.00 %
 P16 10000.00 usec

F1 - Acquisition Parameters
 ND0 1
 TD 256
 SFO1 600.1335 MHz
 FIDRES 28.132877 Hz
 SW 12.001 ppm
 PRMODE QF

F2 - Processing Parameters
 SI 1024
 SF 600.1300262 MHz
 SINE
 NDUW 0
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.00

F1 - Processing Parameters
 SI 1024
 MC2 QF
 SF 600.1300262 MHz
 SINE
 NDUW 0
 SSB 0
 LB 0.00 Hz
 GB 0

2D NMR plot parameters
 CV2 15.00 cm
 CX1 15.00 cm
 F2PLO 5.500 ppm
 F2ALO 3300.72 Hz
 F2PHI -0.100 ppm
 F2HI -60.01 Hz
 F1PLO 11.007 ppm
 F1LO 6605.48 Hz
 F1PHI 5.493 ppm
 F1HI 3299.86 Hz
 F2PPMCM 0.37333 ppm/cm
 F2HZCM 224.04854 Hz/cm
 F1PPMCM 0.36721 ppm/cm
 F1HZCM 220.37421 Hz/cm



600 MHz gCOSY Spectrum of **2a** in CDCl₃
 268 K (-5 °C), 2 mM

Supporting Information

Current Data Parameters

USER slevin
 NAME SL-7-115-800-H
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters

Date_ 20061016
 Time_ 0.00
 INSTRUM varian
 PROBHD 40:5mmBroadban
 PULPROG wgtocsy_bn
 TD 4096
 SOLVENT CDCl3
 NS 32
 DS 64
 SWH 10000.000 Hz
 FIDRES 2.441406 Hz
 AQ 0.2048500 sec
 RG 287.4
 DW 50.000 usec
 DE 6.00 usec
 TE 268.5 K

F1 - Acquisition parameters

ND0 1
 TD 256
 SFO1 799.811 MHz
 FIDRES 39.062500 Hz
 SW 12.503 ppm
 F1MODE undefined

F2 - Processing parameters

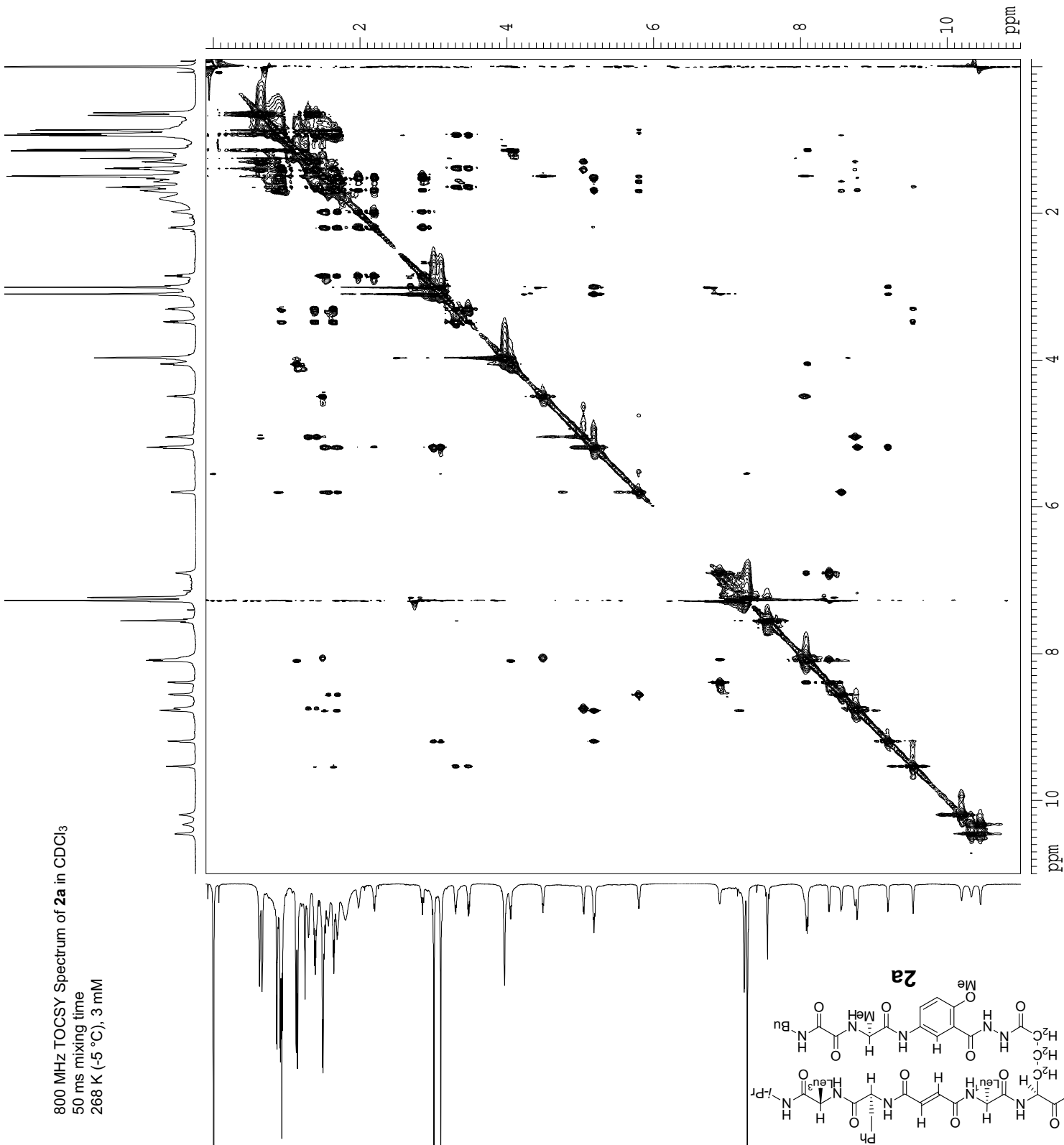
SI 2048
 SF 799.8065514 MHz
 WDW QSIINE
 SSB 2
 LB 0.00 Hz
 GB 0
 PC 1.40

F1 - Processing parameters

SI 2048
 MC2 States
 SF 799.8065514 MHz
 WDW QSIINE
 SSB 2
 LB 0.00 Hz
 GB 0

2D NMR plot parameters

CX2 15.00 cm
 CX1 15.00 cm
 F2PLO 11.000 ppm
 F2LO 8797.87 Hz
 F2PHI -0.100 ppm
 F2HI -79.98 Hz
 F1PLO 11.000 ppm
 F1LO 8797.87 Hz
 F1PHI -0.100 ppm
 F1HI -79.98 Hz
 F2FPMCM 0.74000 ppm/cm
 F2HZCM 591.85681 Hz/cm
 F1FPMCM 0.74000 ppm/cm
 F1HZCM 591.85681 Hz/cm



800 MHz TOCSY Spectrum of **2a** in CDCl₃
 50 ms mixing time
 268 K (-5 °C), 3 mM

Current Data Parameters

USER slevin
 NAME SL-7-115-800-H
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters

Date_ 20061016
 Time_ 0.00
 INSTRUM varian
 PROBDH 40.5mmrbroadban
 PULPROG wgtocpsy_bn
 TD 4096
 SOLVENT CDCl3
 NS 32
 DS 64
 SWH 10000.000 Hz
 FIDRES 2.441406 Hz
 AQ 0.2048500 sec
 RG 287.4
 DW 50.000 usec
 DE 6.00 usec
 TE 268.5 K

F1 - Acquisition Parameters

ND0 1
 TD 256
 SF01 799.811 MHz
 FIDRES 39.062500 Hz
 SW 12.503 ppm
 FMODE undefined

F2 - Processing parameters

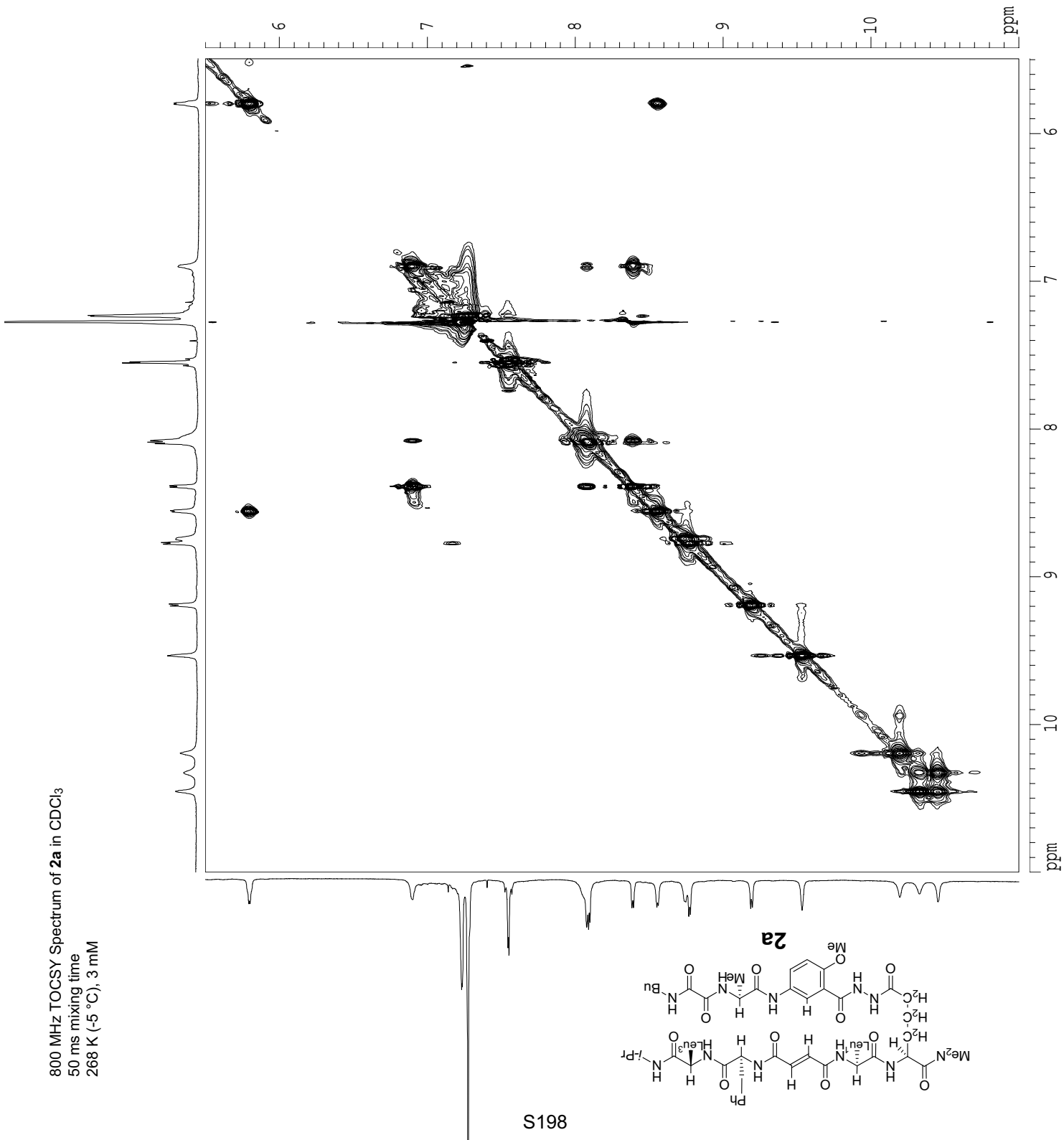
SI 2048
 SF 799.8065514 MHz
 WDW QSI
 SSB 2
 LB 0.00 Hz
 GB 0
 PC 1.40

F1 - Processing parameters

SI 2048
 MC2 States
 SF 799.8065514 MHz
 WDW QSI
 SSB 2
 LB 0.00 Hz
 GB 0

2D NMR plot parameters

CX2 15.00 cm
 CX1 15.00 cm
 F2PLO 11.000 ppm
 F2LO 8798.22 Hz
 F2PHI 5.494 ppm
 F2HI 4393.32 Hz
 F1PLO 11.000 ppm
 F1LO 8797.87 Hz
 F1PHI 5.500 ppm
 F1HI 4398.81 Hz
 F2PMCM 0.36711 ppm/cm
 F2HCM 293.161978 Hz/cm
 F1PMCM 0.36668 ppm/cm
 F1HCM 293.271103 Hz/cm



Current Data Parameters
 USER slevin
 NAME SL-7-115-800-H
 EXPNO 2
 PROCNO 1

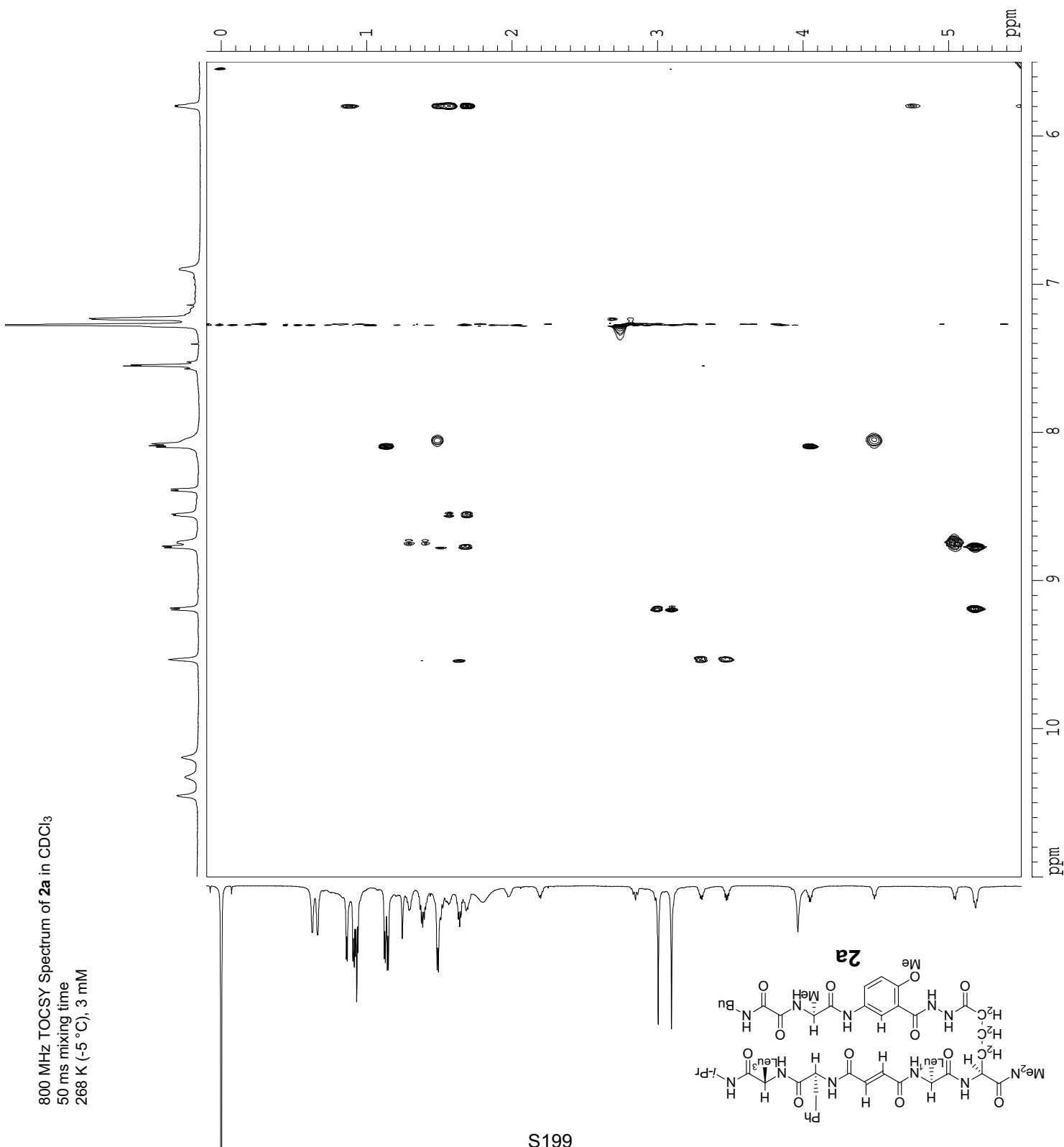
F2 - Acquisition Parameters
 Date_ 20061016
 Time_ 0.00
 INSTRUM varian
 PROBHD 40:5mm broadband
 PULPROG wgtocsy_bn
 TD 4096
 SOLVENT CDCl3
 NS 32
 DS 64
 SWH 10000.000 Hz
 FIDRES 2.441406 Hz
 AQ 0.2048500 sec
 RG 287.4
 DW 50.000 usec
 DE 6.00 usec
 TE 288.5 K

F1 - Acquisition parameters
 ND0 1
 TD 256
 SFO1 799.811 MHz
 FIDRES 39.062500 Hz
 SW 12.503 ppm
 F1MODE undefined

F2 - Processing parameters
 SI 2048
 SF 799.8065514 MHz
 WDW QSI
 SSB 2
 LB 0.00 Hz
 GB 0
 PC 1.40

F1 - Processing parameters
 SI 2048
 MC2 States
 SF 799.8065514 MHz
 WDW QSI
 SSB 2
 LB 0.00 Hz
 GB 0

2D NMR plot parameters
 CX2 15.00 cm
 CX1 15.00 cm
 F2PLO 11.000 ppm
 F2LO 8797.87 Hz
 F2PHI 5.500 ppm
 F2HI 4398.94 Hz
 F1PLO 5.500 ppm
 F1LO 4398.94 Hz
 F1PHI -0.100 ppm
 F1HI -79.98 Hz
 F2PMCM 0.36667 ppm/cm
 F2HZCM 293.26242 Hz/cm
 F1PMCM 0.37333 ppm/cm
 F1HZCM 298.59445 Hz/cm



Current Data Parameters
 USER slevin
 NAME SL-7-115-800-H
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters

Date 20061016
 Time 0.00
 INSTRUM varian
 PROBHD 40:5mmbroadban
 PULPROG wgtocsy_bn
 TD 4096
 SOLVENT CDCl₃
 NS 32
 DS 64
 SWH 10000.000 Hz
 FIDRES 2.441406 Hz
 AQ 0.2048500 sec
 RG 287.4
 DW 50.000 usec
 DE 6.00 usec
 TE 268.5 K

F1 - Acquisition Parameters

ND0 1
 TD 256
 SF01 799.811 MHz
 FIDRES 39.062500 Hz
 SW 12.503 ppm
 FMODE undefined

F2 - Processing parameters

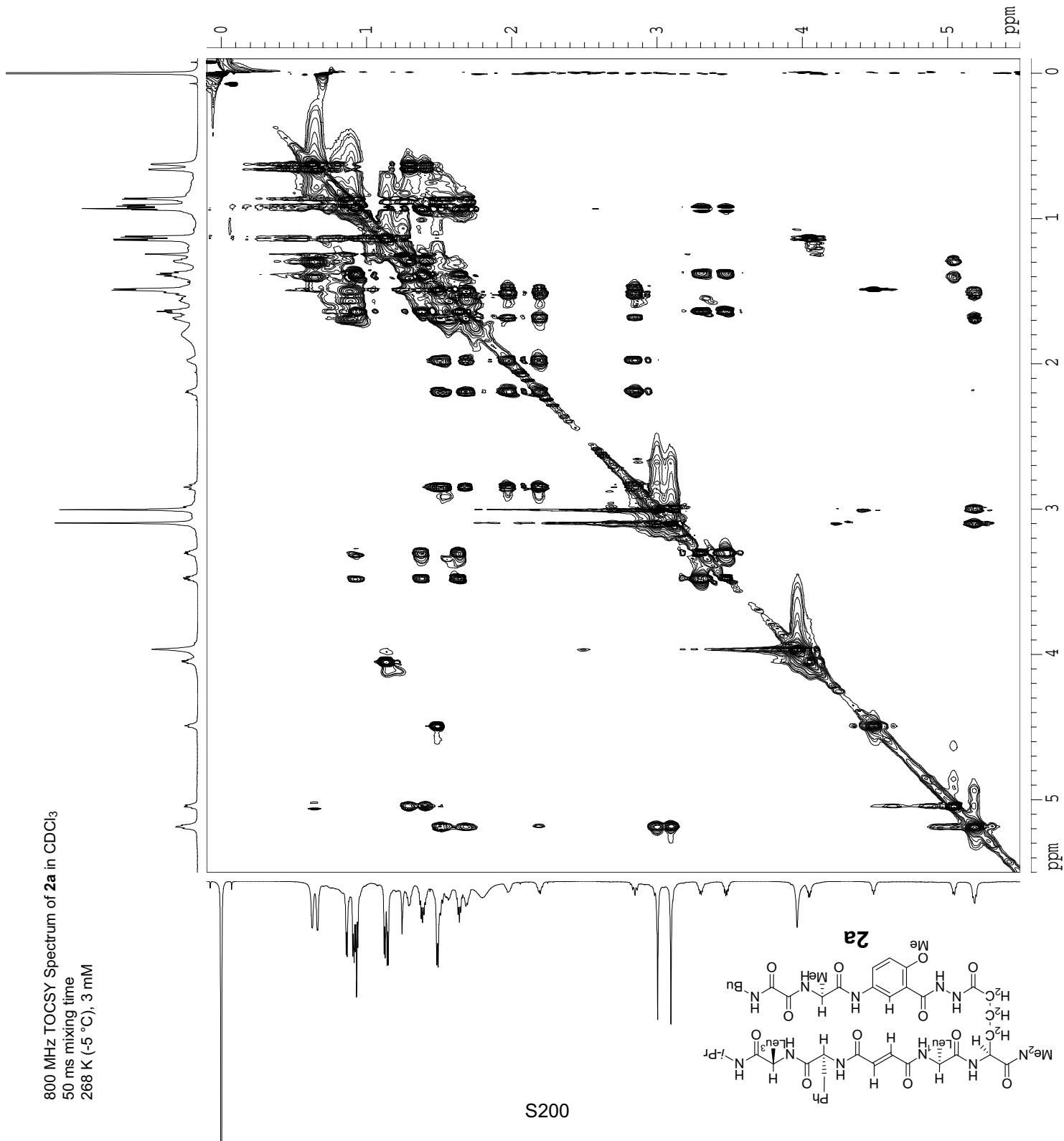
SI 2048
 SF 799.8065514 MHz
 WDW QSI
 SSB 2
 LB 0.00 Hz
 GB 0
 PC 1.40

F1 - Processing parameters

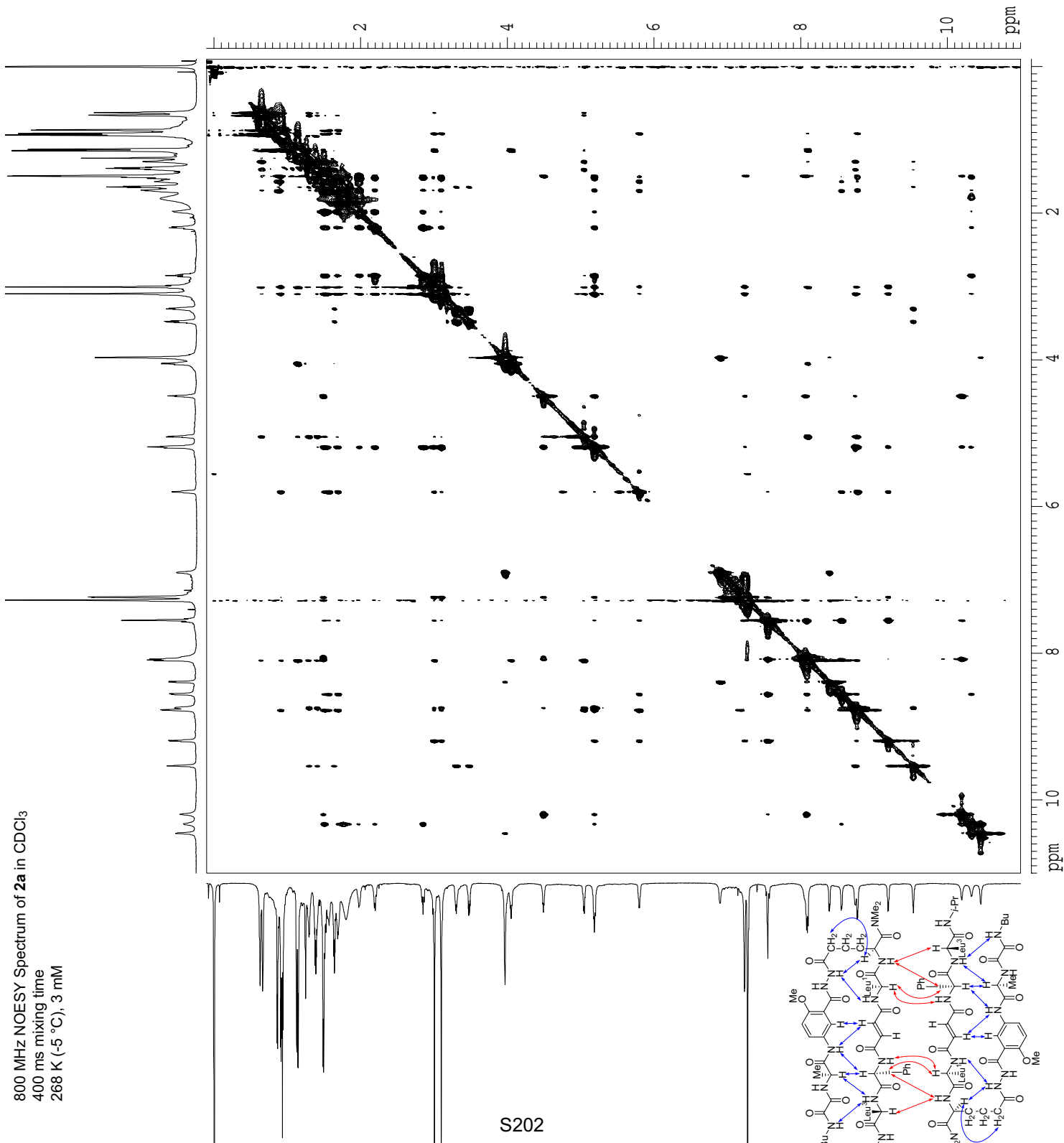
SI 2048
 MC2 States
 SF 799.8065514 MHz
 WDW QSI
 SSB 2
 LB 0.00 Hz
 GB 0

2D NMR plot parameters

CX2 15.00 cm
 CX1 15.00 cm
 F2PLO 5.500 ppm
 F2LO 4398.94 Hz
 F2PHI -0.100 ppm
 F2HI -79.98 Hz
 F1LO 5.500 ppm
 F1LO 4398.94 Hz
 F1PHI -0.100 ppm
 F1HI -79.98 Hz
 F2PNCM 0.37333 ppm/cm
 F2H2CM 298.59445 Hz/cm
 F1PNCM 0.37333 ppm/cm
 F1H2CM 298.59445 Hz/cm



800 MHz NOESY Spectrum of **2a** in CDCl₃
 400 ms mixing time
 268 K (-5 °C), 3 mM



S202

Current Data Parameters
 USER slevin
 NAME SL-7-115-800-H
 EXPNO 3
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20061016
 Time 0.00
 INSTRUM varian
 PROBHD 40:5mm broadband
 PULPROG noesyh2o_pfg_800_pln
 TD 4096
 SOLVENT CDCl3
 NS 32
 DS 64
 SMH 10000.000 Hz
 FIDRES 2.441406 Hz
 AQ 0.2048500 sec
 RG 128
 DW 50.000 usec
 DE 6.00 usec
 TE 268.5 K

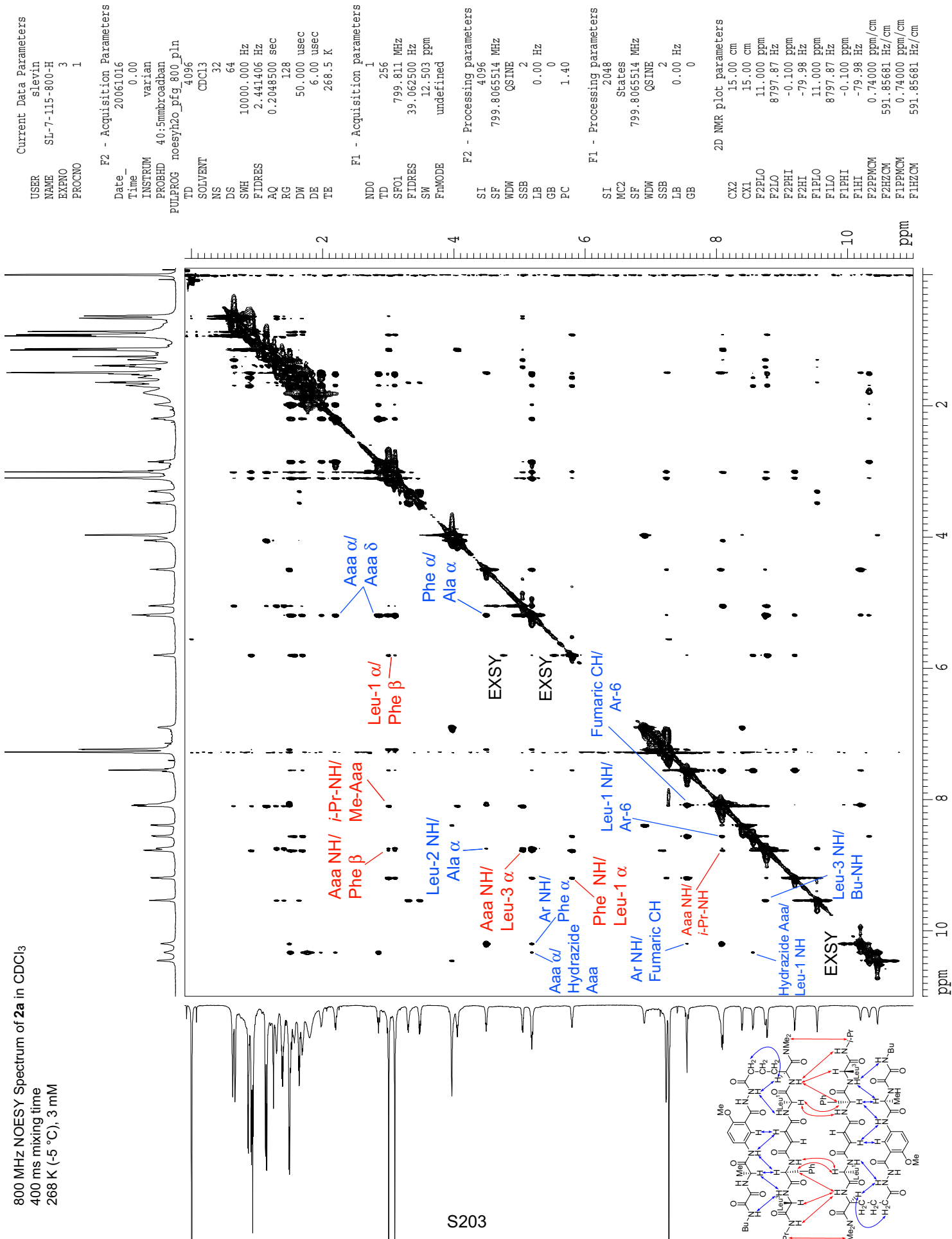
F1 - Acquisition parameters
 ND0 1
 TD 256
 SF01 799.811 MHz
 FIDRES 39.062500 Hz
 SW 12.503 ppm
 FnmODE undefined

F2 - Processing parameters
 SI 4096
 SF 799.8065514 MHz
 WDW QSIGNE
 SSB 2
 LB 0.00 Hz
 GB 0
 PC 1.40

F1 - Processing parameters
 SI 2048
 MC2 States
 SF 799.8065514 MHz
 WDW QSIGNE
 SSB 2
 LB 0.00 Hz
 GB 0

2D NMR plot parameters
 CX2 15.00 cm
 CX1 15.00 cm
 F2PLO 11.000 ppm
 F2LO 8797.87 Hz
 F2PHI -0.100 ppm
 F2HI -79.98 Hz
 F1PLO 11.000 ppm
 F1LO 8797.87 Hz
 F1PHI -0.100 ppm
 F1HI -79.98 Hz
 F2PPMCM 0.74000 ppm/cm
 F2HZCM 591.85681 Hz/cm
 F1PPMCM 0.74000 ppm/cm
 F1HZCM 591.85681 Hz/cm

800 MHz NOESY Spectrum of **2a** in CDCl₃
 400 ms mixing time
 268 K (-5 °C), 3 mM



Current Data Parameters

USER sleVII
 NAME SL-7-1115-800-H
 EXPNO 3
 PROCNO 1

F2 - Acquisition Parameters

Date 20061016
 Time 0.00
 INSTRUM varian
 PROBHD 40:5mmbroadban
 PULPROG noesyh2o_pfg_800_pln
 TD 4096
 SOLVENT CDCl3
 NS 32
 DS 64
 SWH 10000.000 Hz
 FIDRES 2.441406 Hz
 AQ 0.2048500 sec
 RG 128
 DW 50.000 usec
 DE 6.00 usec
 TE 268.5 K

F1 - Acquisition Parameters

ND0 1
 TD 256
 SFO1 799.811 MHz
 FIDRES 39.062500 Hz
 SW 12.503 ppm
 FMODE undefined

F2 - Processing parameters

SI 4096
 SF 799.8065514 MHz
 WDW QSINE
 SSB 2
 LB 0.00 Hz
 GB 0
 PC 1.40

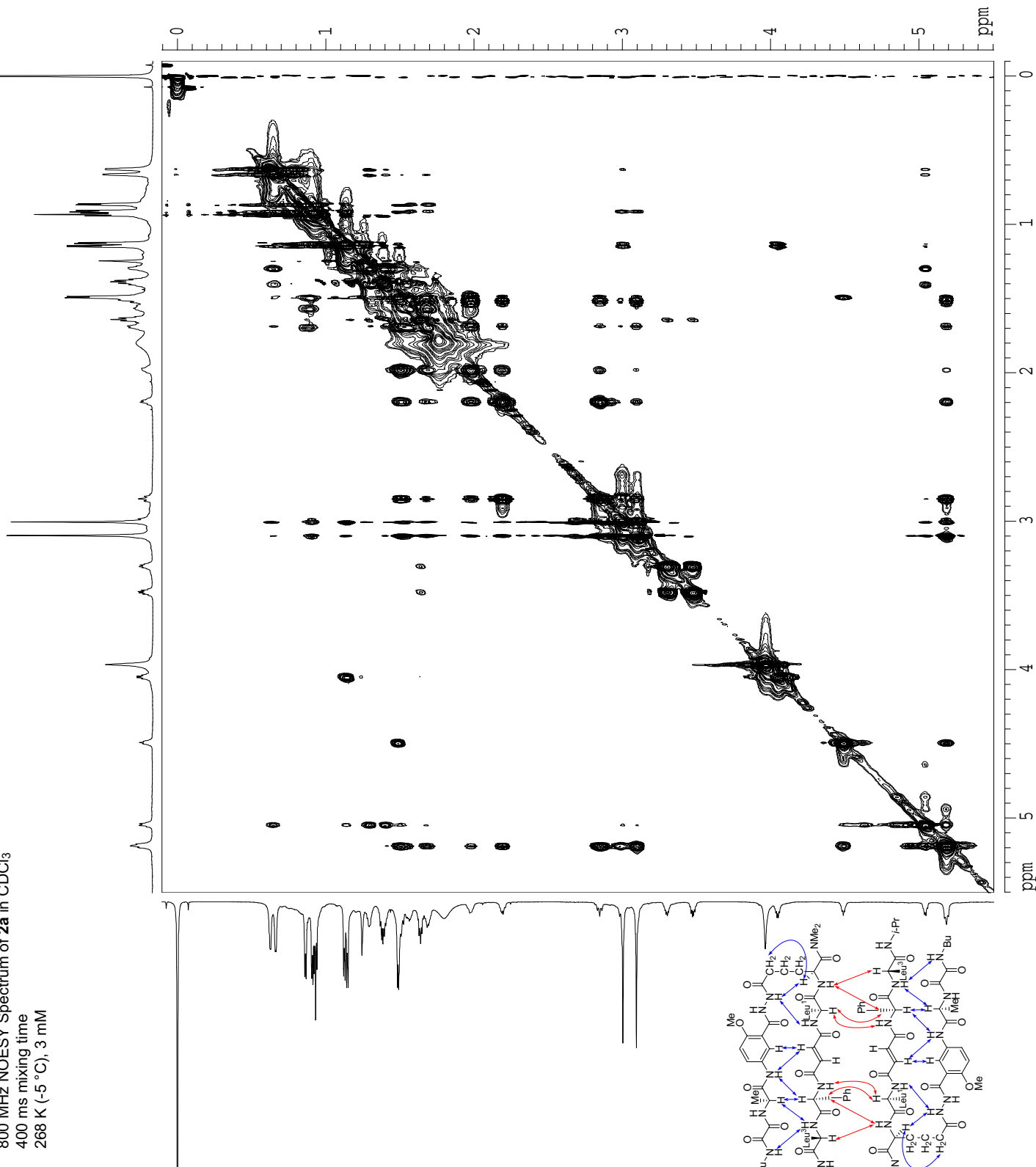
F1 - Processing parameters

SI 2048
 MC2 States
 SF 799.8065514 MHz
 WDW QSINE
 SSB 2
 LB 0.00 Hz
 GB 0

2D NMR plot parameters

CX2 15.00 cm
 CX1 15.00 cm
 F2PLO 5.503 ppm
 F2LO 4401.25 Hz
 F2PHI -0.101 ppm
 F2HI -81.17 Hz
 F1PLO 5.506 ppm
 F1LO 4403.69 Hz
 F1PHI -0.105 ppm
 F1HI -83.62 Hz
 F2PPMCM 0.37363 ppm/cm
 F2HZCM 298.82816 Hz/cm
 F1PPMCM 0.37403 ppm/cm
 F1HZCM 299.15366 Hz/cm

800 MHz NOESY Spectrum of **2a** in CDCl₃
 400 ms mixing time
 268 K (-5 °C), 3 mM



Supporting Information

Current Data Parameters
 USER slevin
 NAME SL-7-115-800-H
 EXPNO 3
 PROCNO 1

F2 - Acquisition Parameters

Date_ 20061016
 Time_ 0.00
 INSTRUM varian
 PROBHD 40:5mmbracdban
 PULPROG noesyh2o_pfg_800_pln
 TD 4096
 SOLVENT CDCl3
 NS 32
 DS 64
 SWH 10000.000 Hz
 FIDRES 2.441406 Hz
 AQ 0.2048500 sec
 RG 128
 DM 50.000 usec
 DE 6.00 usec
 TE 268.5 K

F1 - Acquisition Parameters

ND0 1
 TD 256
 SF01 799.811 MHz
 FIDRES 39.062500 Hz
 SW 12.503 ppm
 FhMODE undefined

F2 - Processing parameters

SI 4096
 SF 799.8065514 MHz
 WDW QSI
 SSB 2
 LB 0.00 Hz
 GB 0
 PC 1.40

F1 - Processing parameters

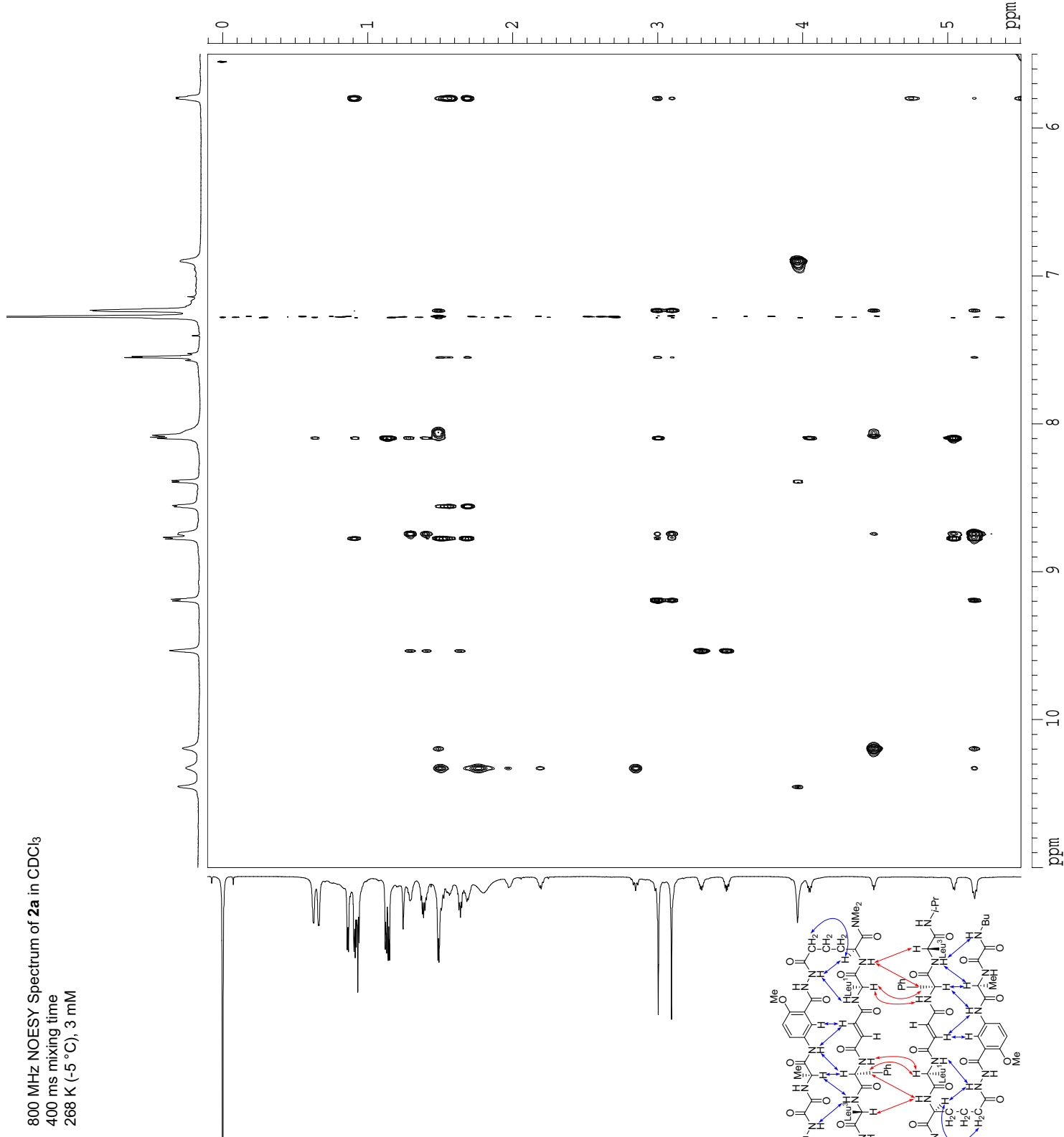
SI 2048
 MC2 States
 SF 799.8065514 MHz
 WDW QSI
 SSB 2
 LB 0.00 Hz
 GB 0

2D NMR plot parameters

CX2 15.00 cm
 CX1 15.00 cm
 F2PLO 11.000 ppm
 F2LO 8797.87 Hz
 F2PHI 5.500 ppm
 F2HI 4398.94 Hz
 F1PLO 5.506 ppm
 F1LO 4403.69 Hz
 F1PHI -0.105 ppm
 F1HI -83.62 Hz
 F2PPMCM 0.36667 ppm/cm
 F2HZCM 293.26242 Hz/cm
 F1PPMCM 0.37403 ppm/cm
 F1HZCM 299.15366 Hz/cm

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800 MHz NOESY Spectrum of **2a** in CDCl₃
 400 ms mixing time
 268 K (-5 °C), 3 mM



800 MHz NOESY Spectrum of **2a** in CDCl₃
 400 ms mixing time
 268 K (-5 °C), 3 mM

Supporting Information

Current Data Parameters
 USER slevin
 NAME SL-7-115-800-H
 EXPNO 3
 PROCNO 1

F2 - Acquisition Parameters

Date 20061016
 Time 0.00
 INSTRUM varian
 PROBHD 40:5mmrbroadban
 PULPROG noesyh2o_pfg_800_pln
 TD 4096
 SOLVENT CDCl₃
 NS 32
 DS 64
 SWH 10000.000 Hz
 FIDRES 2.441406 Hz
 AQ 0.2048500 sec
 RG 128
 DW 50.000 usec
 DE 6.00 usec
 TE 268.5 K

F1 - Acquisition parameters

ND0 1
 TD 256
 SFO1 799.811 MHz
 FIDRES 39.062500 Hz
 SW 12.503 ppm
 FMODE undefined

F2 - Processing parameters

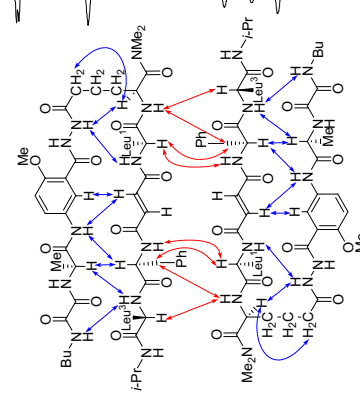
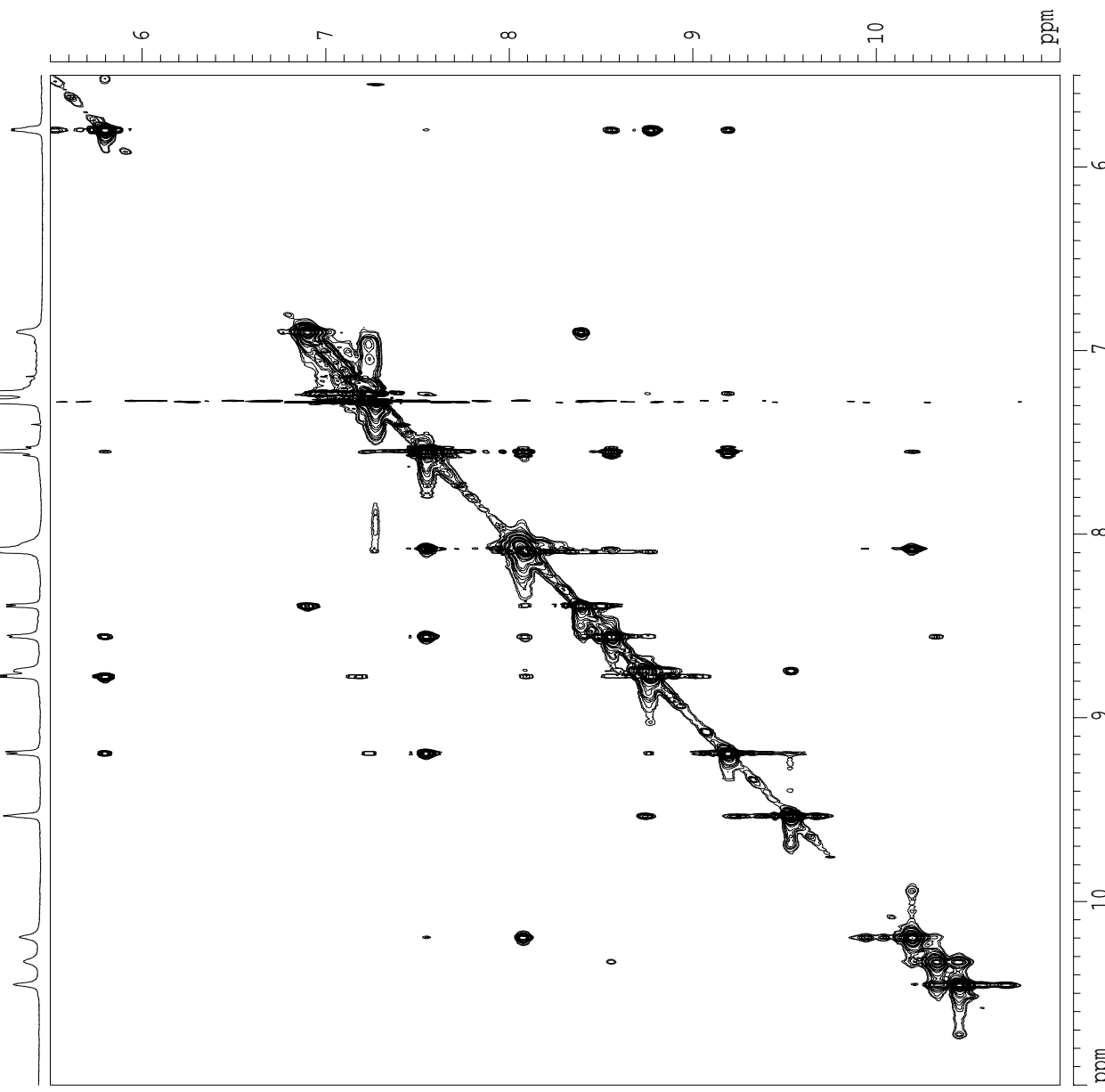
SI 4096
 SF 799.8065514 MHz
 WDW QSINE
 SSB 2
 LB 0.00 Hz
 GB 0
 PC 1.40

F1 - Processing parameters

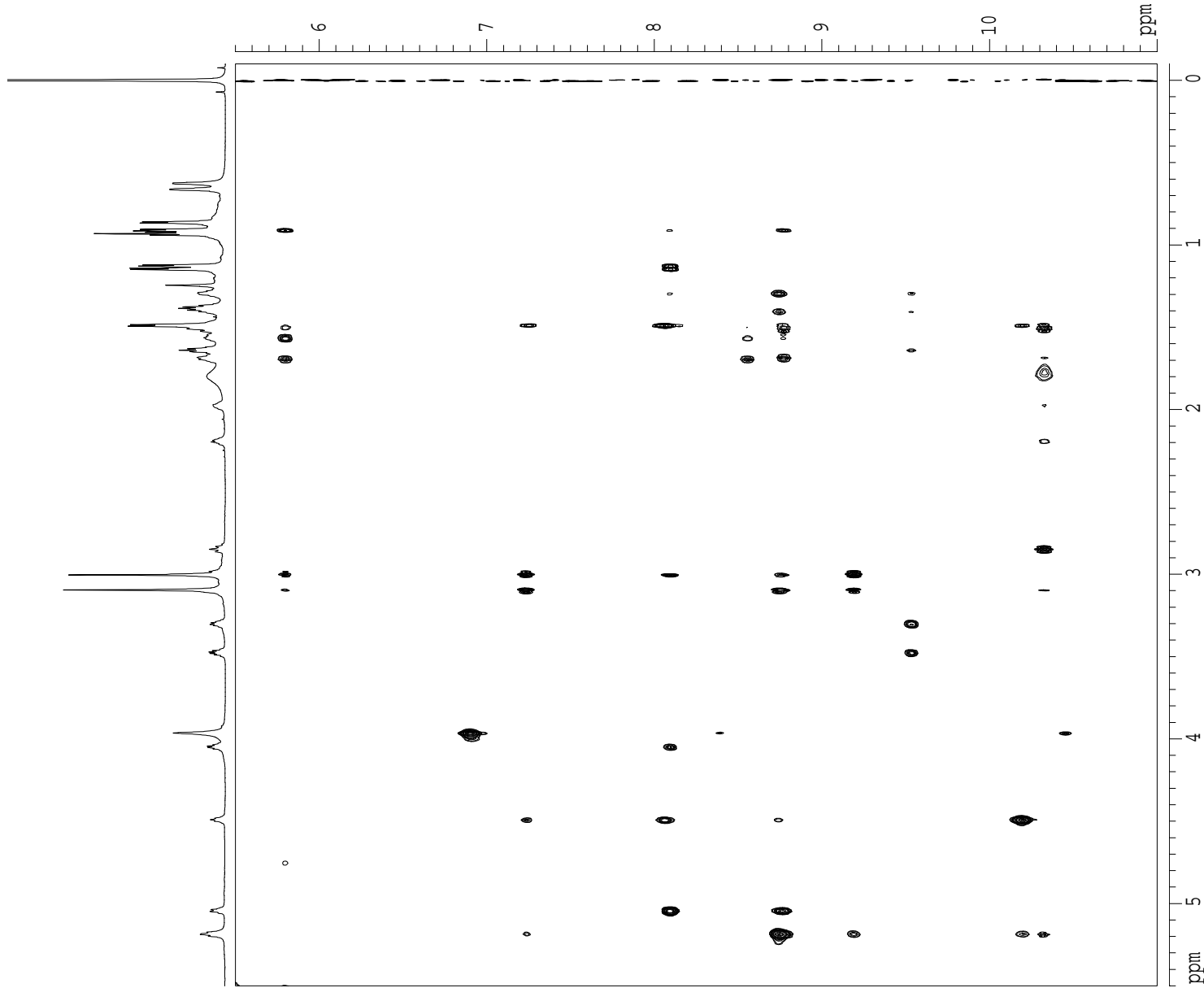
SI 2048
 MC2 States
 SF 799.8065514 MHz
 WDW QSINE
 SSB 2
 LB 0.00 Hz
 GB 0

2D NMR plot parameters

CX2 15.00 cm
 CX1 15.00 cm
 F2PLO 11.000 ppm
 FZLO 8798.22 Hz
 F2PHI 5.500 ppm
 F2HI 4398.81 Hz
 F1PLO 11.000 ppm
 F1LO 8797.87 Hz
 F1PHI 5.500 ppm
 F1HI 4398.94 Hz
 F2PPMCM 0.36671 ppm/cm
 F2HZCM 293.29428 Hz/cm
 F1PPMCM 0.36667 ppm/cm
 F1HZCM 293.26242 Hz/cm



800 MHz NOESY Spectrum of **2a** in CDCl₃
 400 ms mixing time
 268 K (-5 °C), 3 mM



S207

Supporting Information

Current Data Parameters
 USER slevin
 NAME SL-7-115-800-H
 EXPNO 3
 PROCNO 1

F2 - Acquisition Parameters

Date 20061016
 Time 0.00
 INSTRUM varian
 PROBHD 40:5mmroadban
 PULPROG noesyh2o_pfg_800_p1n
 TD 4096
 SOLVENT CDCl₃

NS 32
 DS 64
 SMH 10000.000 Hz
 FIDRES 2.441406 Hz
 AQ 0.2048500 sec
 RG 128
 DW 50.000 usec
 DE 6.00 usec
 TE 268.5 K

F1 - Acquisition Parameters

ND0 1
 TD 256
 SF01 799.811 MHz
 FIDRES 39.062500 Hz
 SW 12.503 ppm
 FwMODE undefined

F2 - Processing parameters

SI 4096
 SF 799.8065514 MHz
 WDW QSI
 SSB 2
 LB 0.00 Hz
 GB 0
 PC 1.40

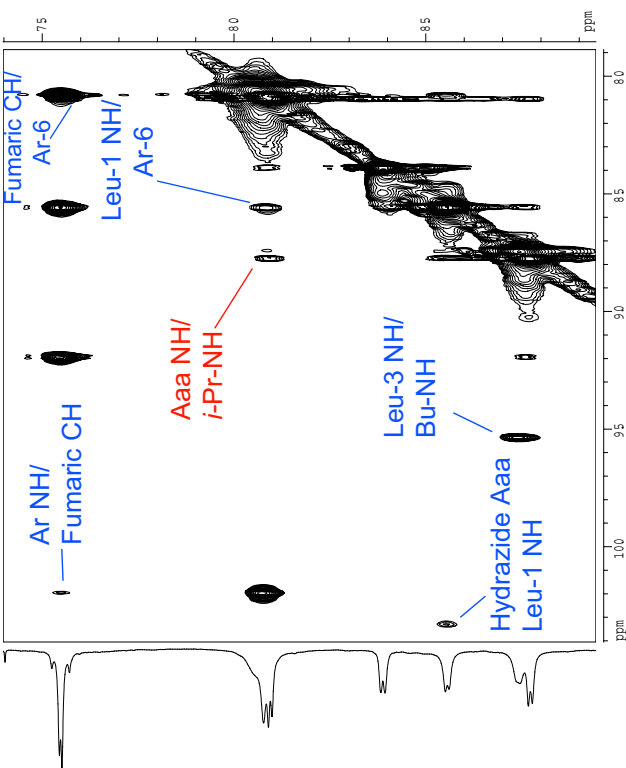
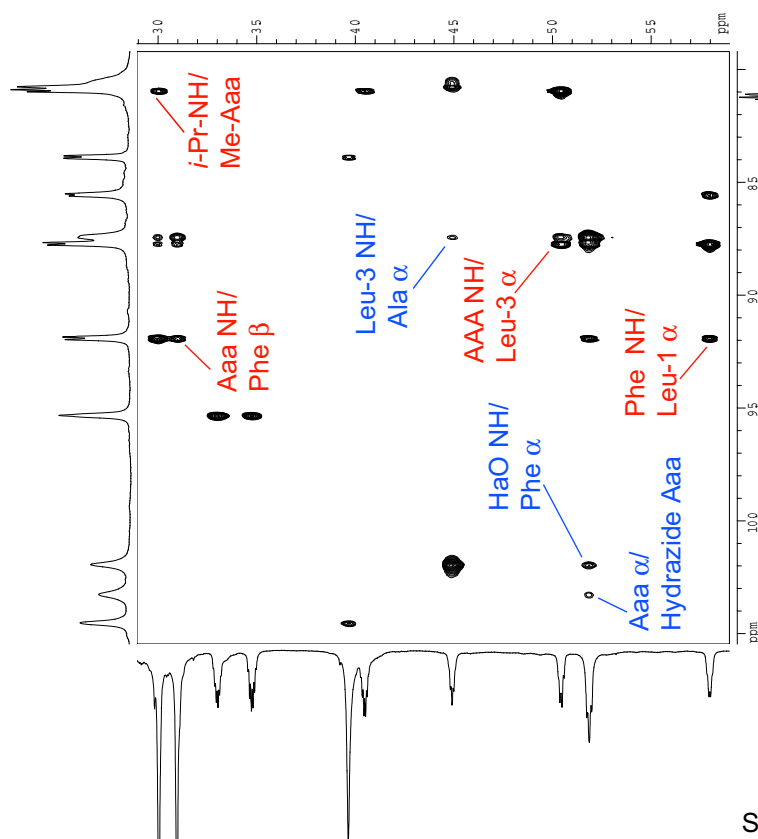
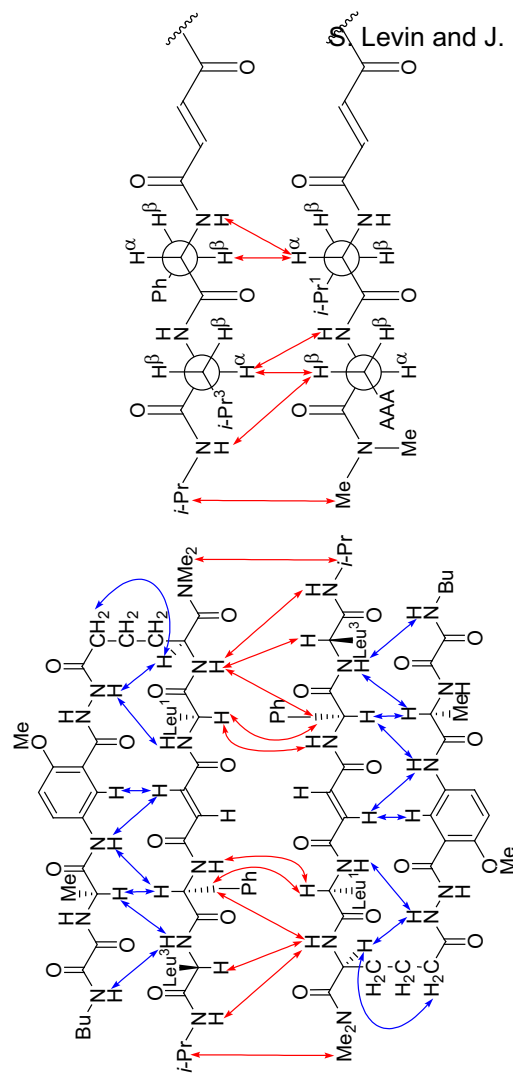
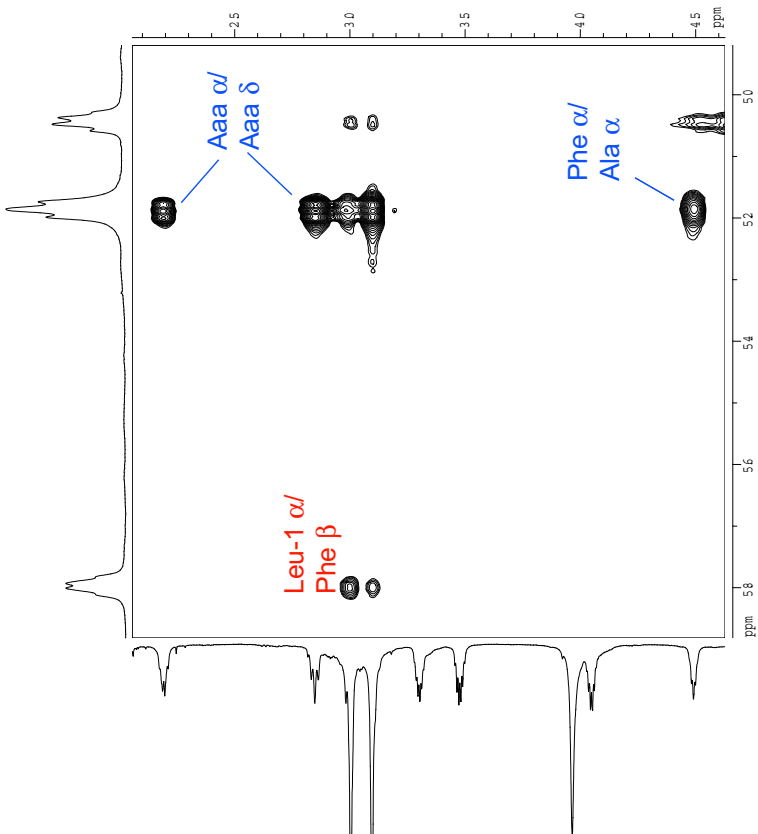
F1 - Processing parameters

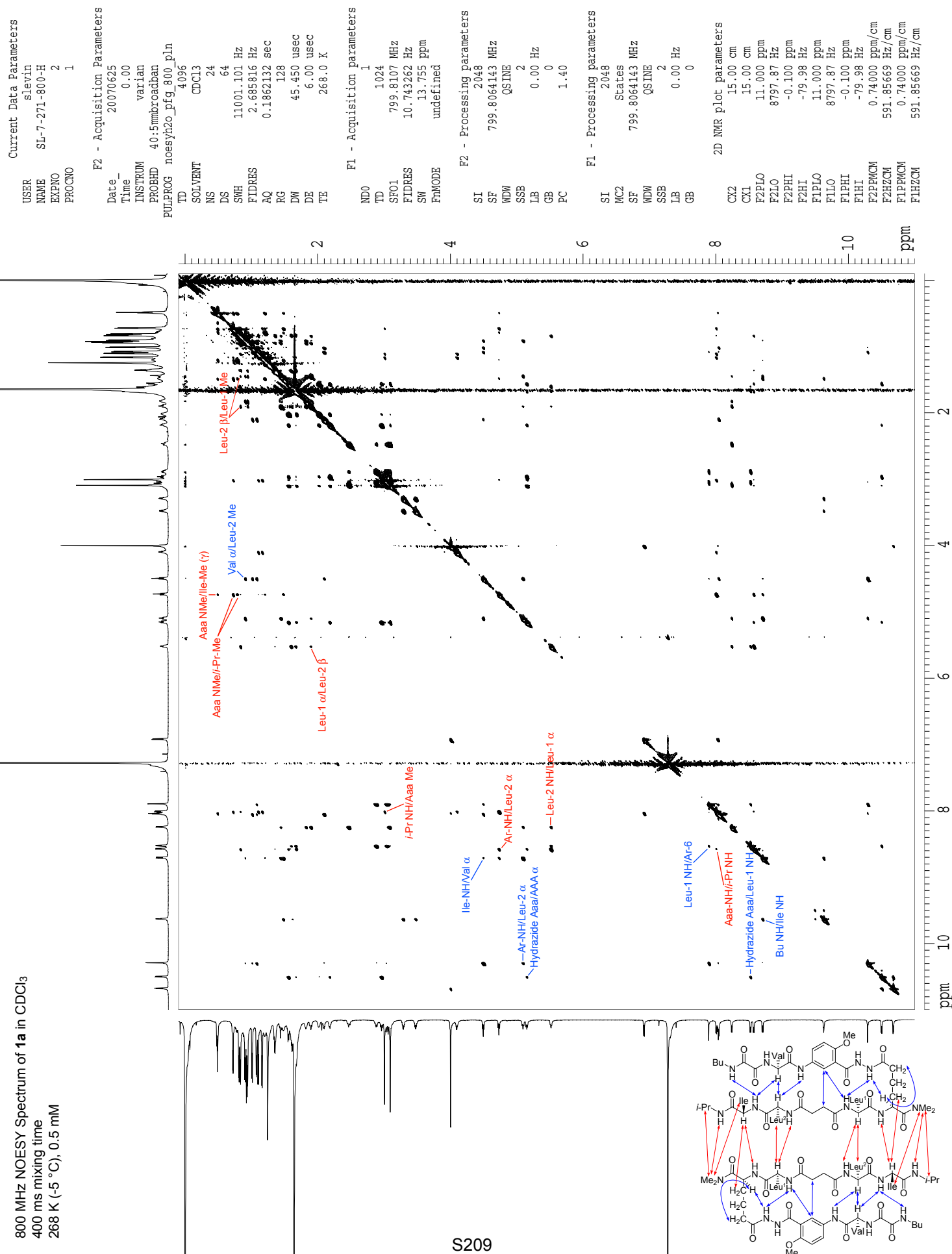
SI 2048
 MC2 States
 SF 799.8065514 MHz
 WDW QSI
 SSB 2
 LB 0.00 Hz
 GB 0

2D NMR plot parameters

CX2 15.00 cm
 CX1 15.00 cm
 F2PLO 5.500 ppm
 F2LO 4398.94 Hz
 F2PHI -0.100 ppm
 F2HI -79.98 Hz
 F1PLO 11.000 ppm
 F1LO 8798.22 Hz
 F1PHI 5.500 ppm
 F1HI 4398.81 Hz
 F2PPMCM 0.37333 ppm/cm
 F2HZCM 298.59445 Hz/cm
 F1PPMCM 0.36671 ppm/cm
 F1HZCM 293.29428 Hz/cm

S. Levin and J. S. Nowick





Supporting Information

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Current Data Parameters
 USER slevin
 NAME SL-7-271-800-H
 EXPNO 2
 PROCNO 1

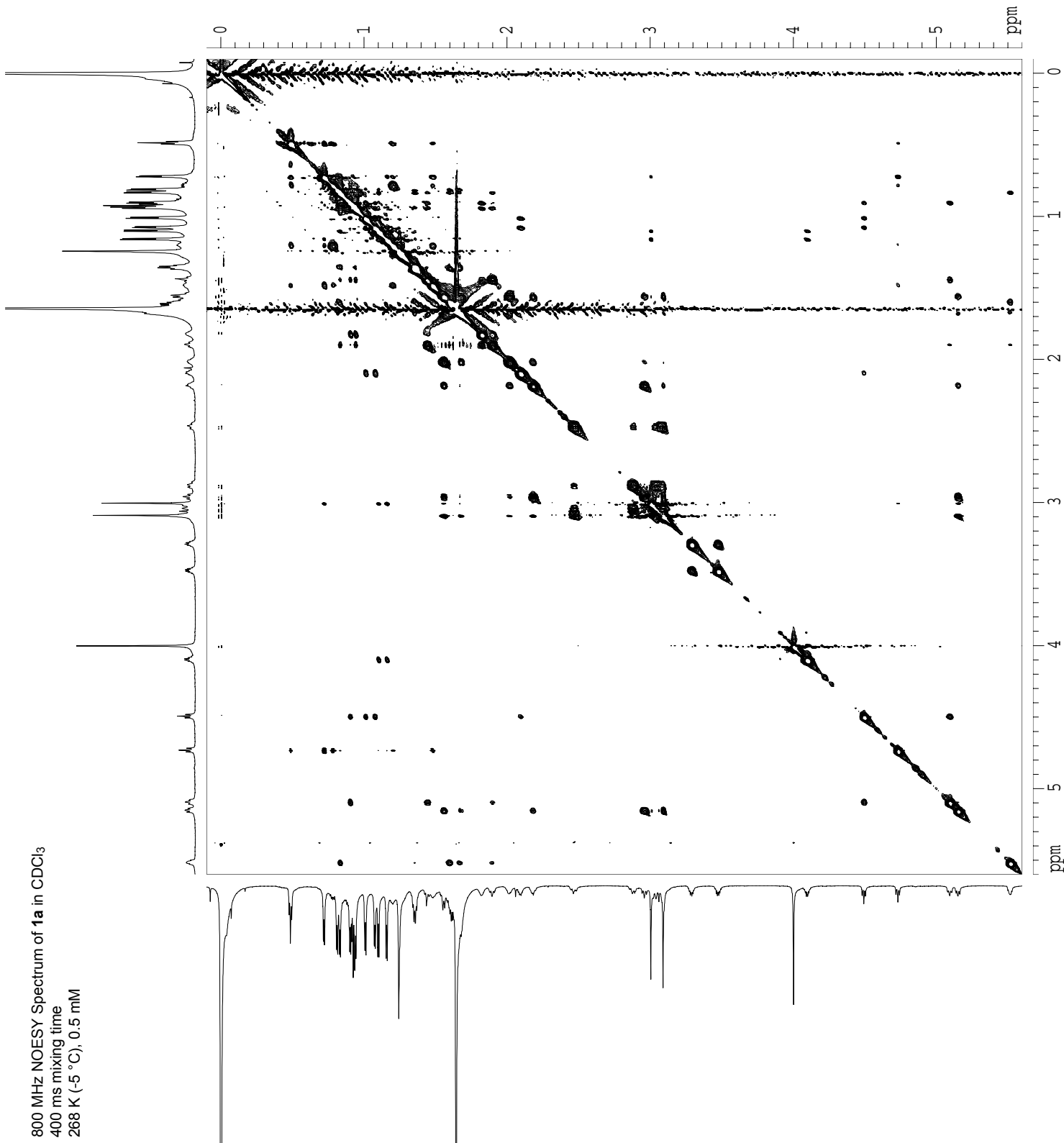
F2 - Acquisition Parameters
 Date_ 20070625
 Time_ 0.00
 INSTRUM varian
 PROBHD 40:5mm broadband
 PULPROG noesyh2o_pfg_800_pln
 TD 4096
 SOLVENT CDCl3
 NS 24
 DS 64
 SWH 11001.101 Hz
 FIDRES 2.683816 Hz
 AQ 0.1862132 sec
 RG 128
 DM 45.450 usec
 DE 6.00 usec
 TE 268.0 K

F1 - Acquisition parameters
 ND0 1
 TD 1024
 SF01 799.8107 MHz
 FIDRES 10.743262 Hz
 SW 13.755 ppm
 FreqMODE undefined

F2 - Processing parameters
 SI 2048
 SF 799.8064143 MHz
 WDM QSIINE
 SSB 2
 LB 0.00 Hz
 GB 0
 PC 1.40

F1 - Processing parameters
 SI 2048
 MC2 States
 SF 799.8064143 MHz
 WDM QSIINE
 SSB 2
 LB 0.00 Hz
 GB 0

2D NMR plot parameters
 CX2 15.00 cm
 CX1 15.00 cm
 F2PLO 5.600 ppm
 F2LO 4478.92 Hz
 F2PHI -0.100 ppm
 F2HI -79.98 Hz
 F1PLO 5.600 ppm
 F1LO 4478.92 Hz
 F1PHI -0.100 ppm
 F1HI -79.98 Hz
 F2PPMCM 0.38000 ppm/cm
 F2HZCM 303.92645 Hz/cm
 F1PPMCM 0.38000 ppm/cm
 F1HZCM 303.92645 Hz/cm



800 MHz NOESY Spectrum of **1a** in CDCl₃
 400 ms mixing time
 268 K (-5 °C), 0.5 mM

Supporting Information

Current Data Parameters
 USER sievin
 NAME SL-7-271-800-H
 EXNO 2
 PROCNO 1

F2 - Acquisition Parameters

Date_ 20070625
 Time_ 0.00
 INSTRUM varian
 PROBHD 40:5mmbroadban
 PULPROG noesyh2o_pfg_800_pin
 TD 4096
 SOLVENT CDCl3
 NS 24
 DS 64
 SWH 11001.101 Hz
 FIDRES 2.685816 Hz
 AQ 0.1862132 sec
 RG 128
 DW 45.450 usec
 DE 6.00 usec
 TE 268.0 K

F1 - Acquisition parameters

ND0 1
 TD 1024
 SFO1 799.8107 MHz
 FIDRES 10.743262 Hz
 SW 13.755 ppm
 FwMODE undefined

F2 - Processing parameters

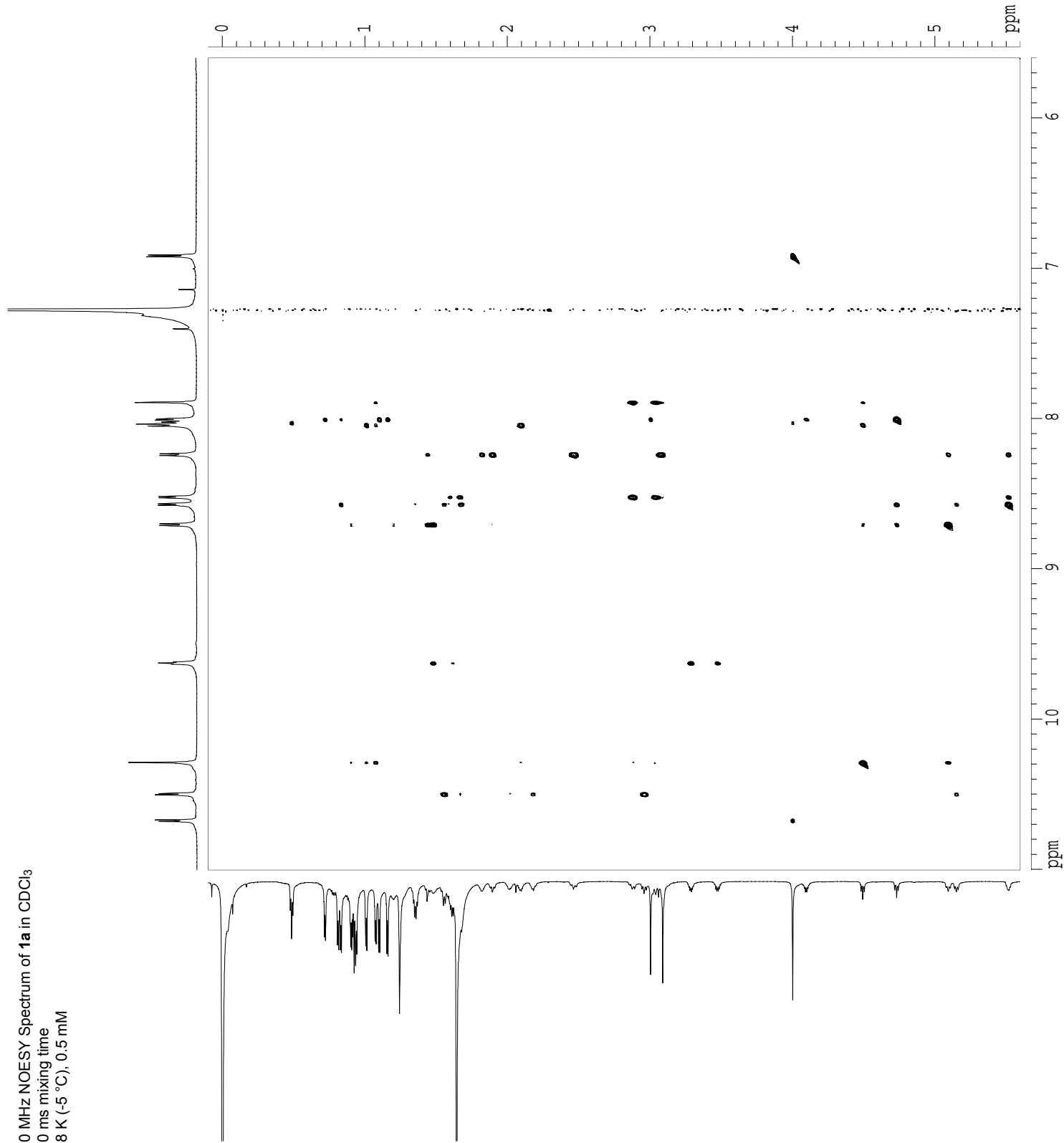
SI 2048
 SF 799.8064143 MHz
 WDW QSINE
 SSB 2
 LB 0.00 Hz
 GB 0
 PC 1.40

F1 - Processing parameters

SI 2048
 MC2 States
 SF 799.8064143 MHz
 WDW QSINE
 SSB 2
 LB 0.00 Hz
 GB 0

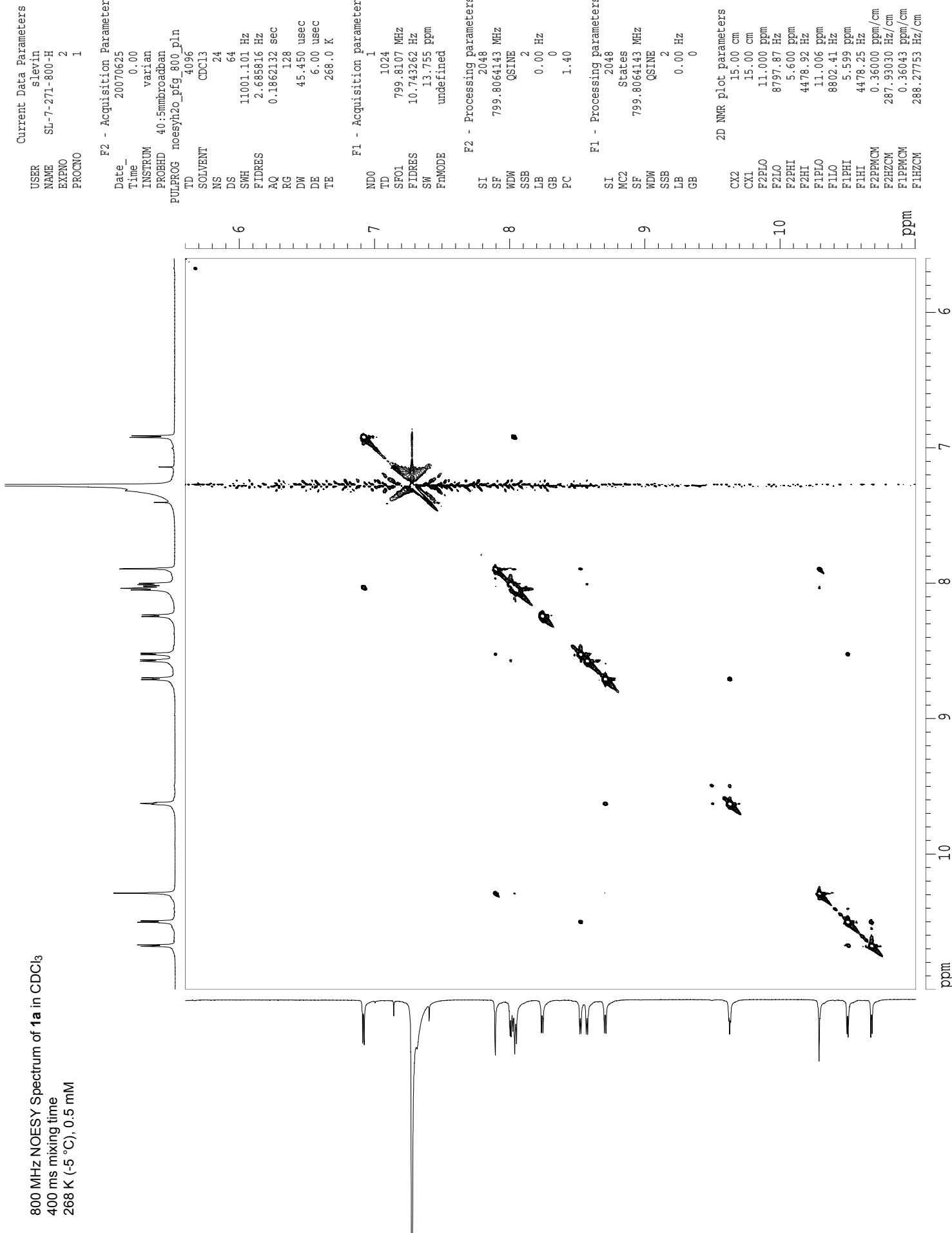
2D NMR plot parameters

CX2 15.00 cm
 CX1 15.00 cm
 F2PLO 11.006 ppm
 F2LO 8802.41 Hz
 F2PHI 5.599 ppm
 F2HI 4478.25 Hz
 F1PLO 5.600 ppm
 F1LO 4478.92 Hz
 F1PHI -0.100 ppm
 F1HI -79.98 Hz
 F2PPMCM 0.36043 ppm/cm
 F2HZCM 288.27753 Hz/cm
 F1PPMCM 0.38000 ppm/cm
 F1HZCM 303.92645 Hz/cm



Supporting Information

S. Levin and J. S. Nowick



Supporting Information

S. Levin and J. S. Nowick

Current Data Parameters
 USER slevin
 NAME SL-7-271-800-H
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters

Date_ 20070625
 Time 0.00
 INSTRUM varian
 PROBHD 40:5mmbrdabban
 PULPROG noesyh2o_pfg_800_pln
 TD 4096

SOLVENT CDCl3
 NS 24
 DS 64
 SWH 11001.101 Hz
 FIDRES 2.685816 Hz
 AQ 0.1862132 sec
 RG 128
 DW 45.450 usec
 DE 6.00 usec
 TE 268.0 K

F1 - Acquisition Parameters

ND0 1
 TD 1024
 SFO1 799.8107 MHz
 FIDRES 10.743262 Hz
 SW 13.755 ppm
 F1MODE undefined

F2 - Processing parameters

SI 2048
 SF 799.8064143 MHz
 WDW QSI
 SSB 2
 LB 0.00 Hz
 GB 0
 PC 1.40

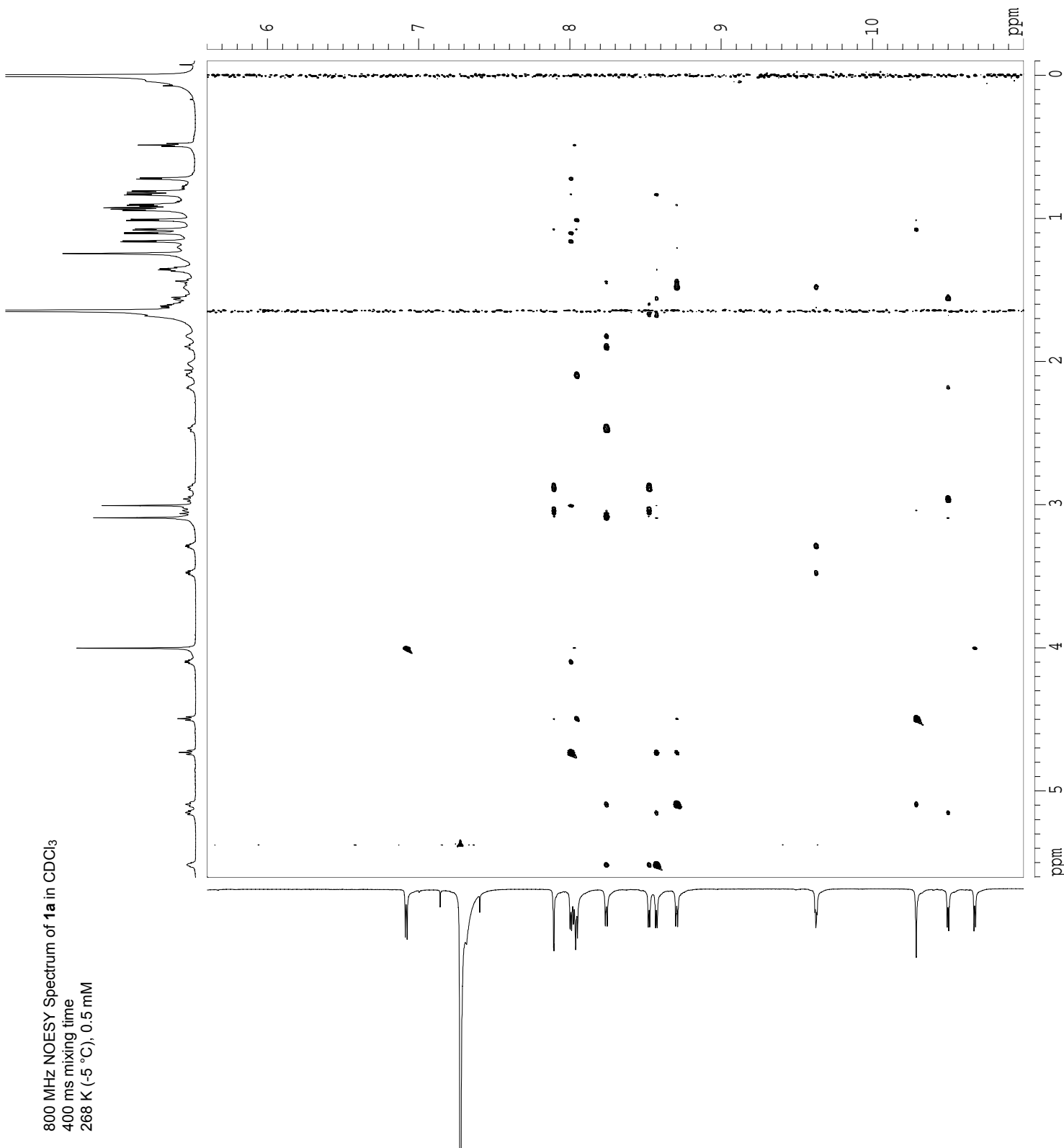
F1 - Processing parameters

SI 2048
 MC2 States
 SF 799.8064143 MHz
 WDW QSI
 SSB 2
 LB 0.00 Hz
 GB 0

2D NMR plot parameters

CX2 15.00 cm
 CX1 15.00 cm
 F2PLO 5.606 ppm
 F2LO 4483.62 Hz
 F2PHI -0.103 ppm
 F2HI -82.27 Hz
 F1PLO 11.000 ppm
 F1LO 8797.87 Hz
 F1PHI 5.600 ppm
 F1HI 4478.92 Hz
 F2P1MCM 0.38058 ppm/cm
 F2H1MCM 304.39243 Hz/cm
 F1P1MCM 0.36000 ppm/cm
 F1H1MCM 287.93030 Hz/cm

800 MHz NOESY Spectrum of **1a** in CDCl₃
 400 ms mixing time
 268 K (-5 °C), 0.5 mM



```

Current Data Parameter
USER      slevin
NAME     SL-7-23-HMQC-N-H
PROCNO   4
PROBHD   5 mm TBI 1H/13
PULPROG  hmqcspcf
TD       888
SOLVENT  CDCl3
NS       16
DS       16
SWH      7211.539 Hz
FIDRES   8.121102 Hz
AQ       0.0616180 sec
RG       2050
DM       69.333 usec
DE       6.00 usec
TE       268.0 K
CNS2     145.0000000
D0       0.0000300 sec
D1       1.1600000 sec
d2       0.0344838 sec
d12      0.0002000 sec
d13      0.0000400 sec
D16      0.0022000 sec
DELTA1   0.0222438 sec
IN0      0.0001655 sec

***** CHANNEL f1 *****
NUC1     1H
P1       8.00 usec
PL1      0.00 dB
PC1      1.00
SFO1     600.1335488 MHz

***** CHANNEL f2 *****
CPDPRG2  gsp
NUC2     13C
P2       15.00 usec
PL2      -1.00 dB
PC2      1.00
SFO2     150.9179793 MHz

***** GRADIENT CHANNEL *****
GPM1     SINE.100
GPM2     SINE.100
GPM3     SINE.100
GPZ1     50.00 %
GPZ2     30.00 %
GPZ3     40.10 %
P16      1000.00 usec

F1 - Acquisition parameter
NU0      2
TD       512
SFO1     150.9179 MHz
FIDRES   59.006798 Hz
SW       200.185 ppm
PwMODE   QF

F2 - Processing parameter
SI       2048
SF       600.1300263 MHz
AQ       0.0616180 sec
SFO      150.9179793 MHz
SSB      0
LB       5.00 Hz
GB       0
PC       1.00

F1 - Processing parameter
SI       2048
MC2     QF
SF       150.9028353 MHz
AQ       0.0616180 sec
SFO      150.9179793 MHz
SSB      0
LB       5.00 Hz
GB       0

2D NMR plot parameter
CX2     18.00 cm
CX1     15.00 cm
F2P2LO  3.161 ppm
F2P2HI  1908.776 Hz
F2P1HI  2.36 ppm
F2P1LO  140.10 ppm
F1P2LO  4796.79 Hz
F1P2HI  23.050 ppm
F1P1HI  4383.75 Hz
F2P2MCM 0.04694 ppm/cm
F2P1MCM 28.17007 Hz/cm
F1P2MCM 0.18248 ppm/cm
F1P1MCM 27.53650 Hz/cm
    
```

