

Supporting information for

A Tetramer Derived from Islet Amyloid Polypeptide

Yilin Wang, Adam G. Kreutzer, Nicholas L. Truex, and James S. Nowick*

Department of Chemistry, University of California, Irvine, Irvine, CA 92697-2025

*To whom correspondence should be addressed: jsnowick@uci.edu

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I. SUPPLEMENTAL FIGURES

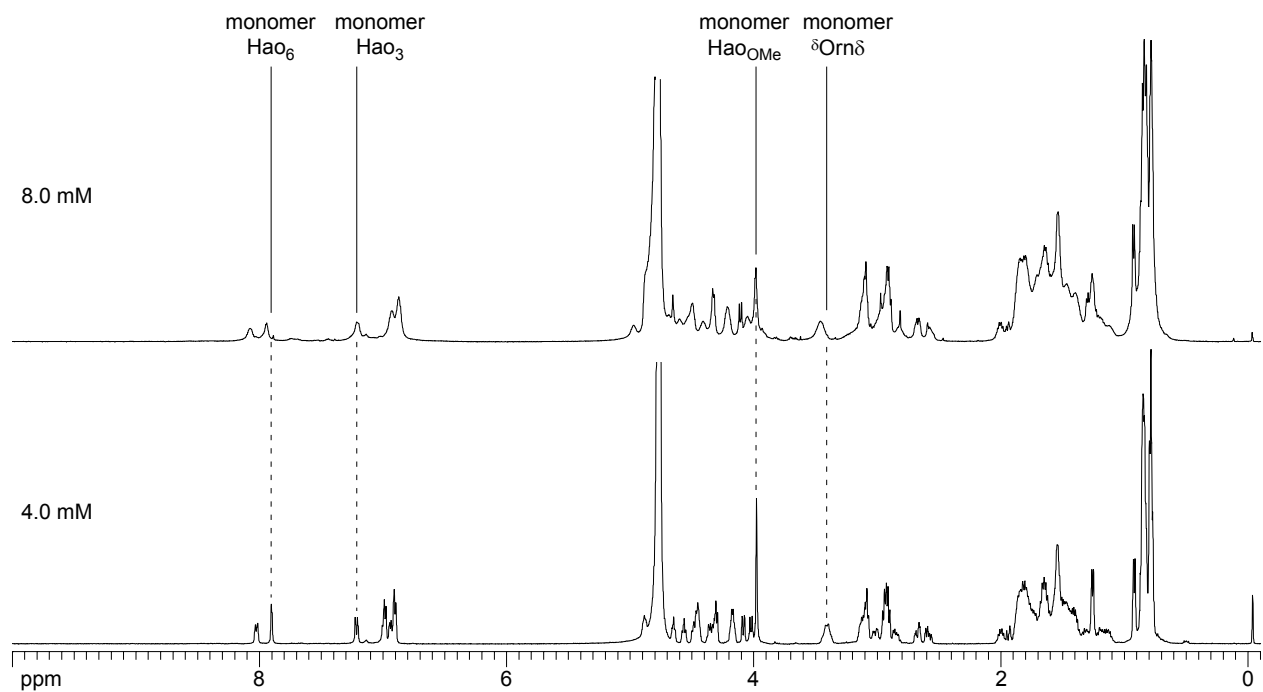


Fig S1. ^1H NMR spectra of peptide $\mathbf{1}_{\text{Arg}}$ at 4 mM and 8 mM in 50 mM CD_3COOD and 50 mM CD_3COONa buffer in D_2O at 500 MHz and 298 K.

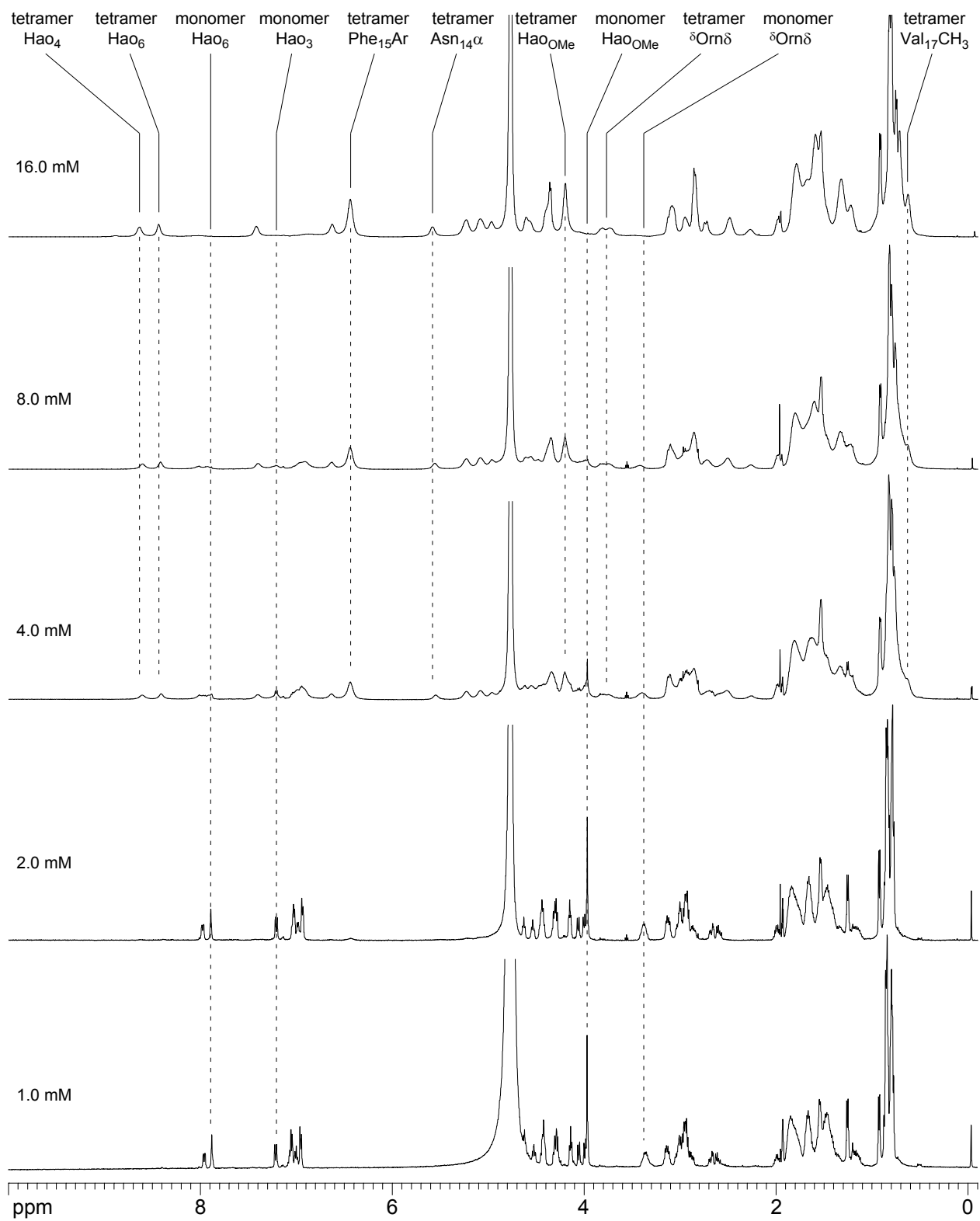


Fig S2. ^1H NMR spectra of peptide **1_{Cit}** at various concentrations in 50 mM CD_3COOD and 50 mM CD_3COONa in D_2O at 500 MHz and 298 K.

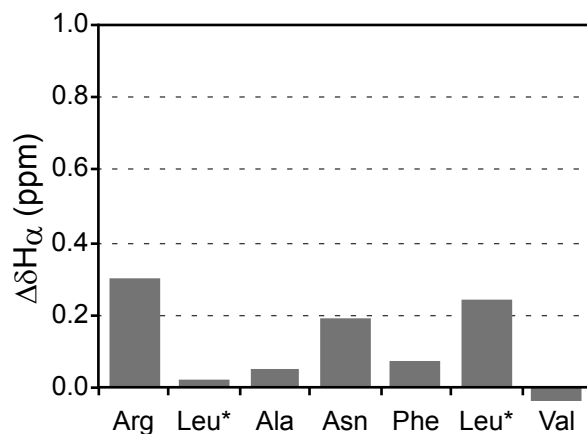


Fig. S3. Downfield shifting of the α -protons of peptide $\mathbf{1}_{\text{Arg}}$ at 4 mM relative to those of random coil chemical shifts. *Leucine residues are not assigned in a sequence-specific fashion.

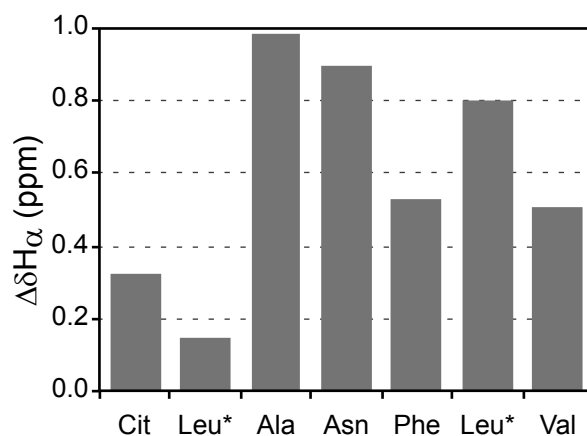


Fig. S4. Downfield shifting of the α -protons of peptide $\mathbf{1}_{\text{Cit}}$ at 16 mM relative to those of random coil chemical shifts. The random coil chemical shift of arginine was used for citrulline. *Leucine residues are not assigned in a sequence-specific fashion.

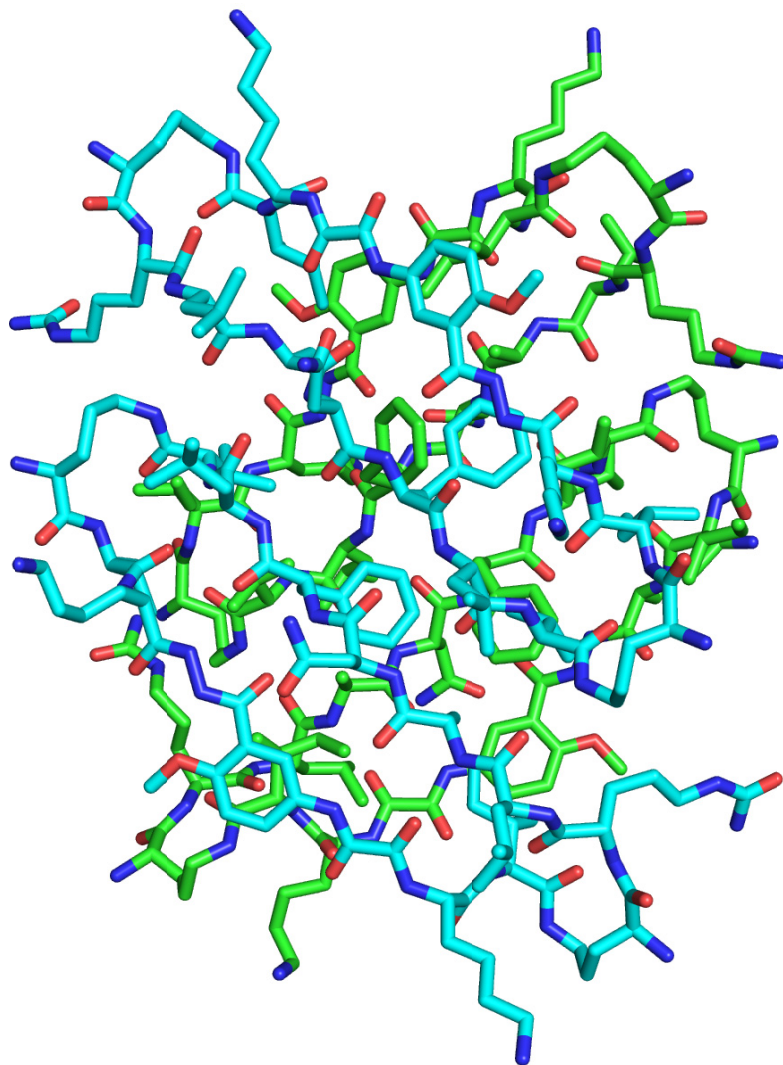


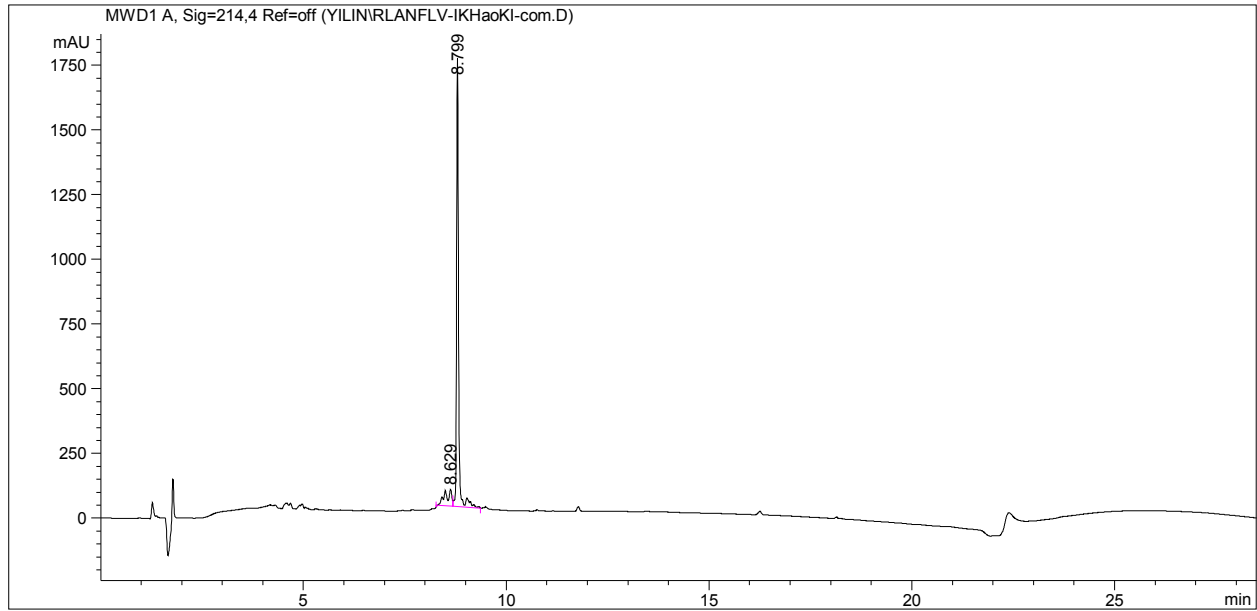
Fig. S5. Crystallographically based molecular model of the tetramer formed by peptide **1_{Cit}**. The model was generated in MacroModel with the MMFFs force field with GB/SA water solvation.

Table S1. Crystallographic properties, crystallization conditions, data collection, and model refinement statistics for peptide **2_{Cit}**.

peptide	peptide 2_{Cit}
PDB ID	5UHR
space group	<i>P4₁2₁2</i>
<i>a, b, c</i> (Å)	33.88, 33.88, 99.05
α, β, λ (°)	90, 90, 90
peptides per asymmetric unit	4
crystallization conditions	0.1 M sodium citrate at pH 4.9, 20% (v/v) isopropanol, 18% PEG 4000
wavelength (Å)	0.92
resolution (Å)	27.96–1.798 (1.862–1.798)
total reflections	11672 (1079)
unique reflections	5838 (541)
multiplicity	2.0 (2.0)
completeness (%)	99.51 (95.41)
mean I/σ	41.22 (9.47)
Wilson B factor	24.70
R_{merge}	0.01553 (0.06924)
R_{measure}	0.02196 (0.09792)
$CC_{1/2}$	1.000 (0.988)
CC^*	1.000 (0.997)
R_{work}	0.2257 (0.2928)
R_{free}	0.2687 (0.3045)
number of non-hydrogen atoms	540
$\text{RMS}_{\text{bonds}}$	0.020
$\text{RMS}_{\text{angles}}$	2.04
Ramachandran favored (%)	100
outliers (%)	0
clashscore	3.30
average B-factor	32.91
number of TLS groups	4
ligands/ions	Cl (1)
water molecules	39

IV. CHARACTERIZATION DATA

RP-HPLC of Macrocytic β -Sheet 1Arg



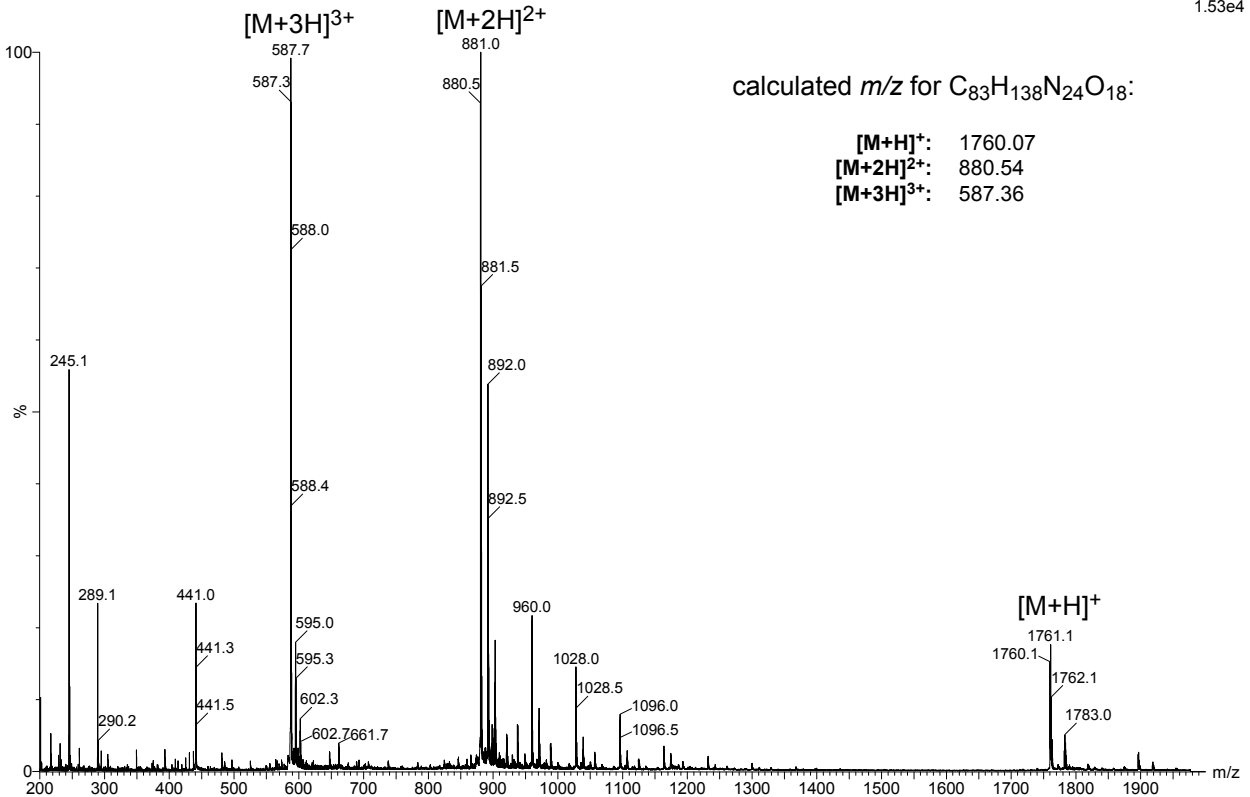
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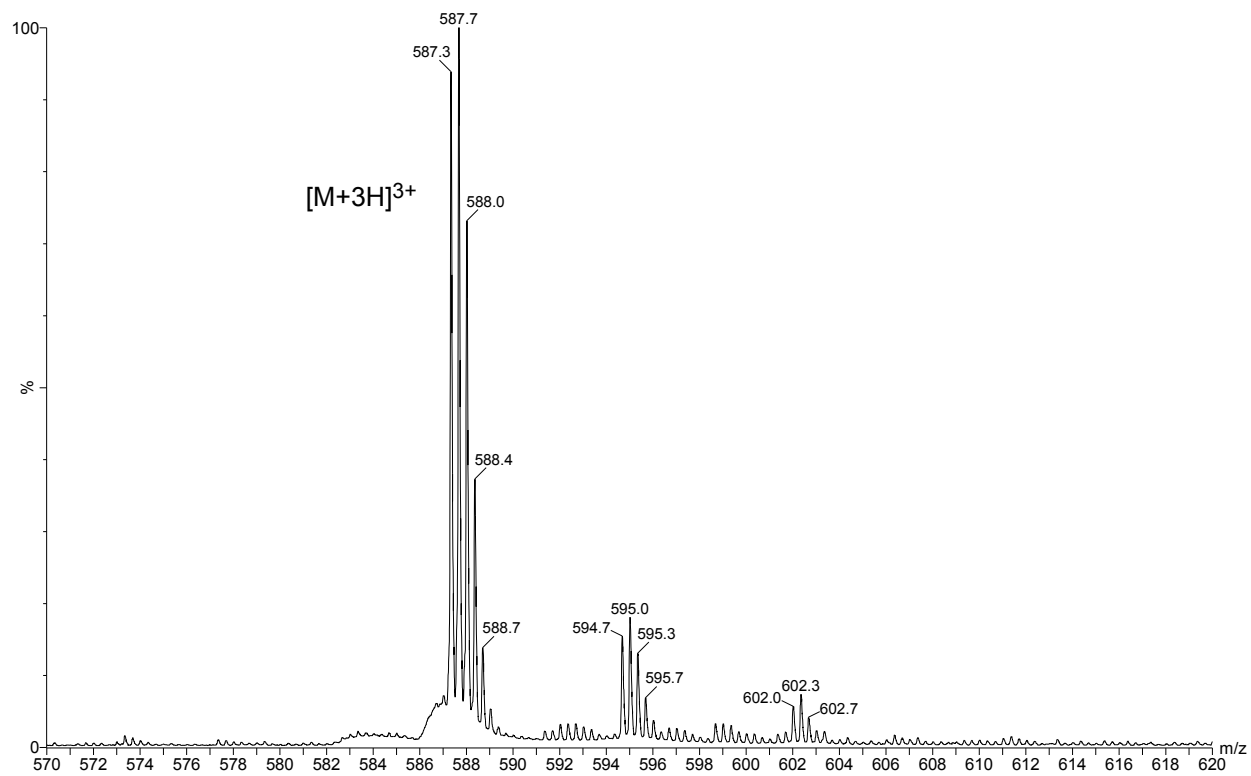
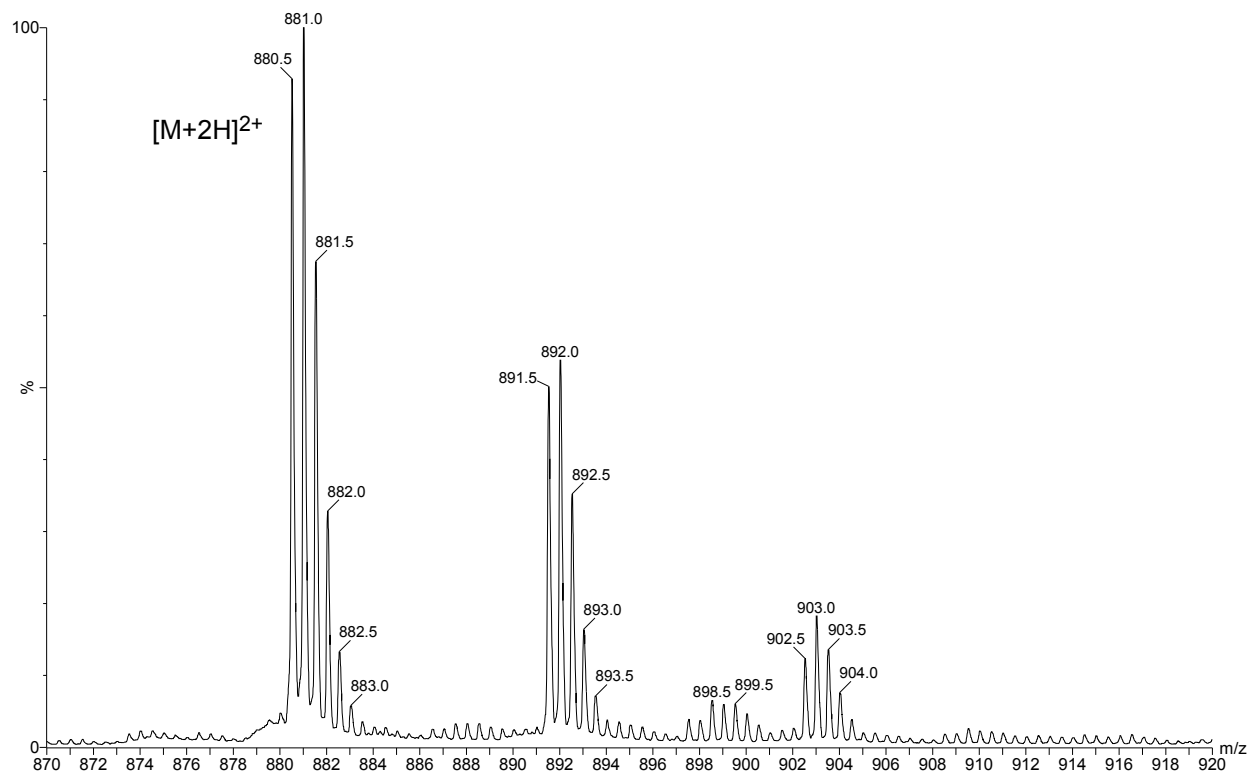
column: Aeris XB-C18 2.6 μ
dimensions: 150 mm x 4.6 mm
mobile phase: A: H₂O, 0.1% TFA
 B: CH₃CN, 0.1% TFA
gradient: A/B (95:5) to (0:100) in 20 min
flow rate: 1.0 mL/min
detection: VWD, wavelength = 214 nm
temperature: 298 K

MS (ESI) of Macrocytic β -Sheet 1Arg

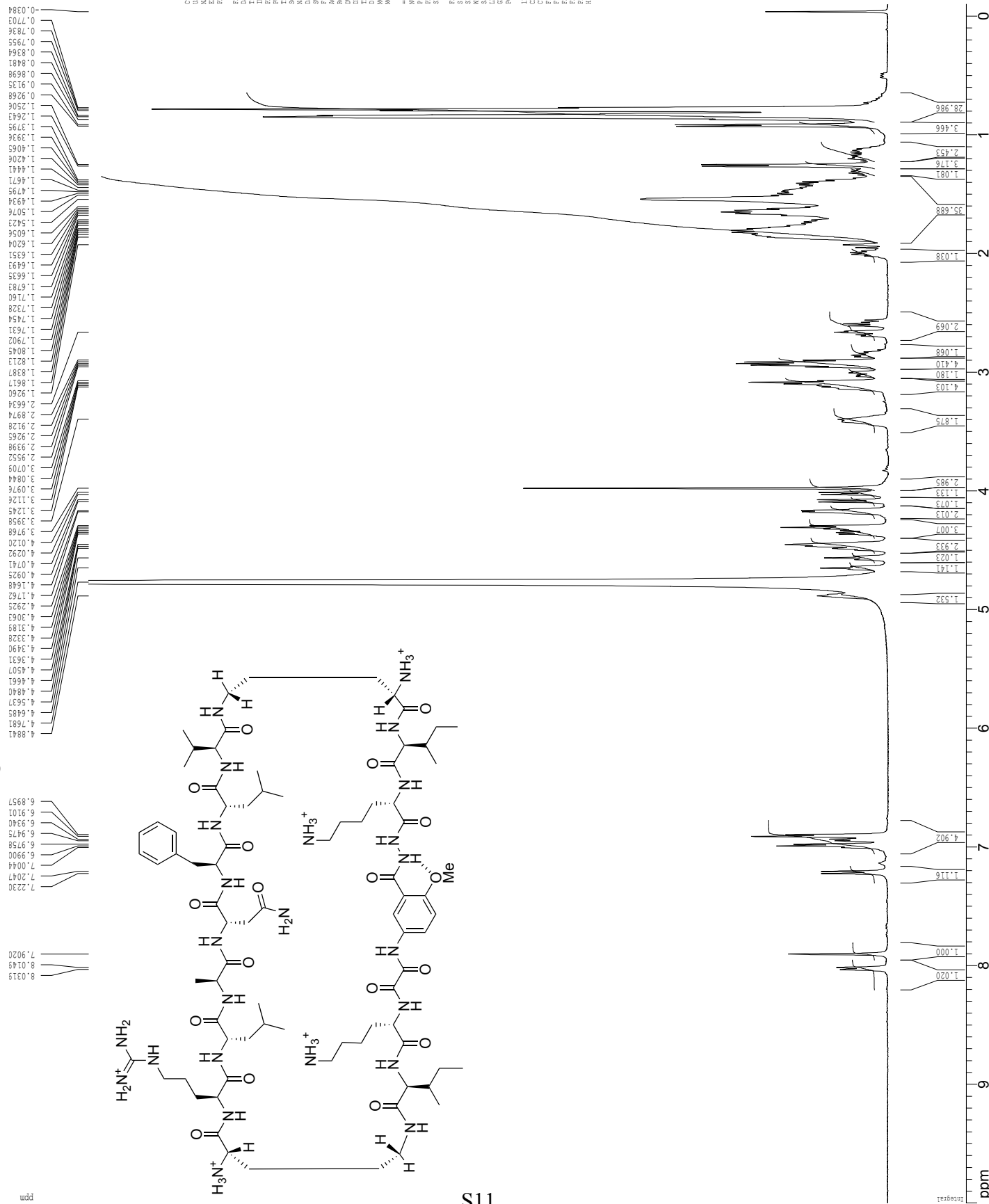
yilinw8-rianflv-ikhaoki-1 26 (0.477) Sm (Md, 3.00); Cm (2:55)

TOF MS ES+
1.53e4

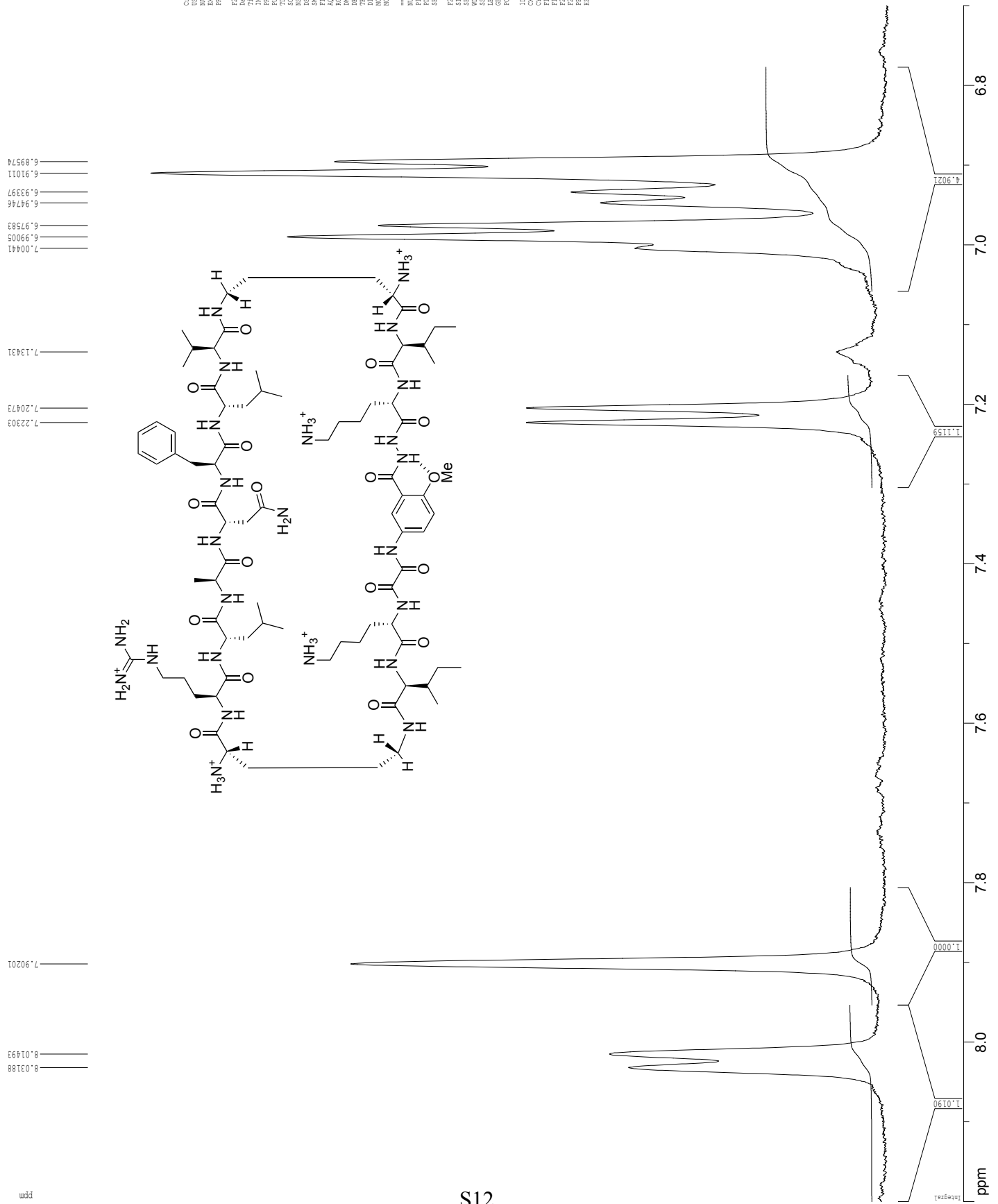




¹H NMR of macrocyclic β-sheet peptide 1Arg, 4 mM in 100 mM deuterioacetate buffer in D₂O at 500 MHz and 298 K



¹H NMR of macrocyclic β-sheet peptide 1Arg, 4 mM in 100 mM deuterioacetate buffer in D₂O at 500 MHz and 298 K

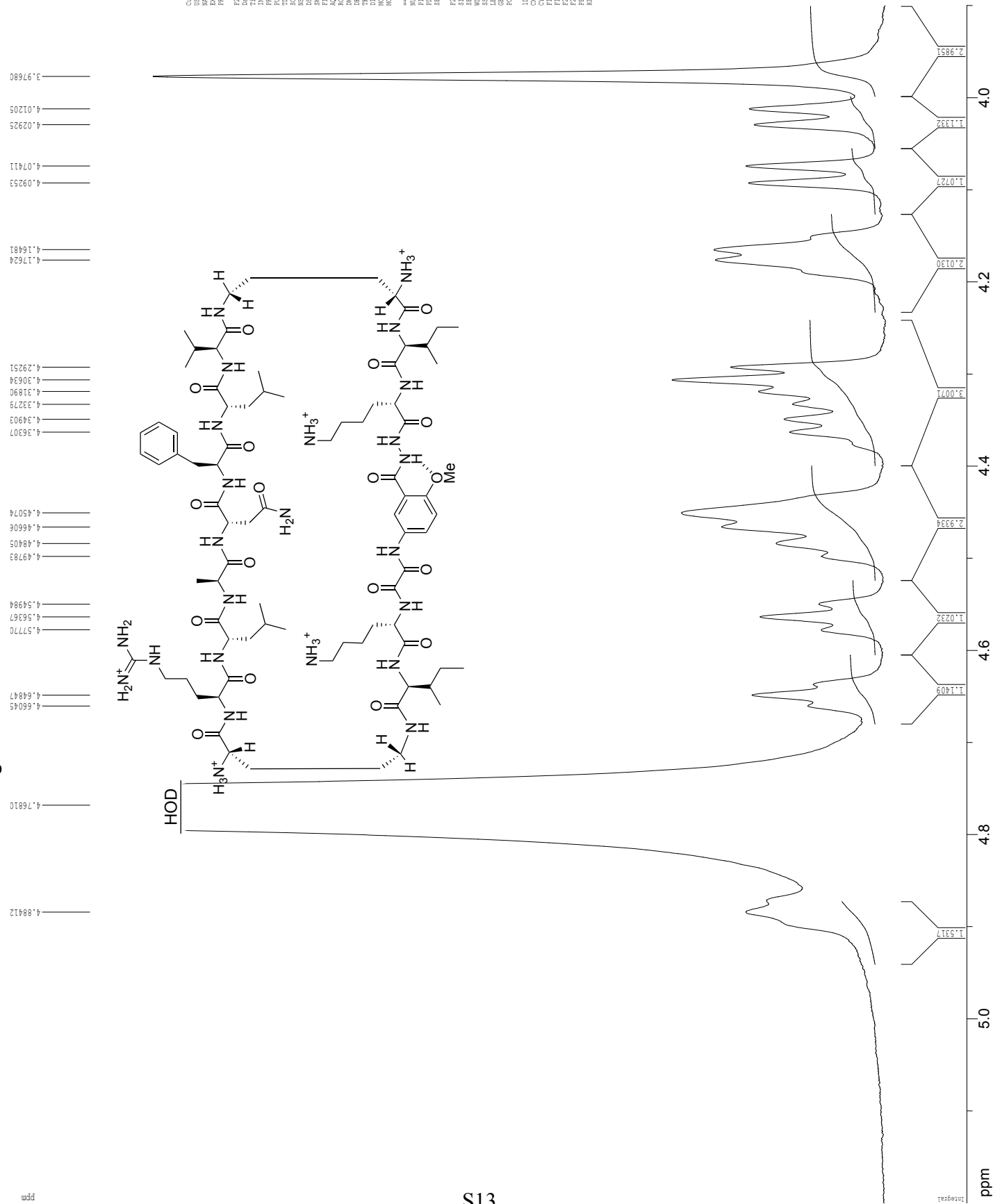


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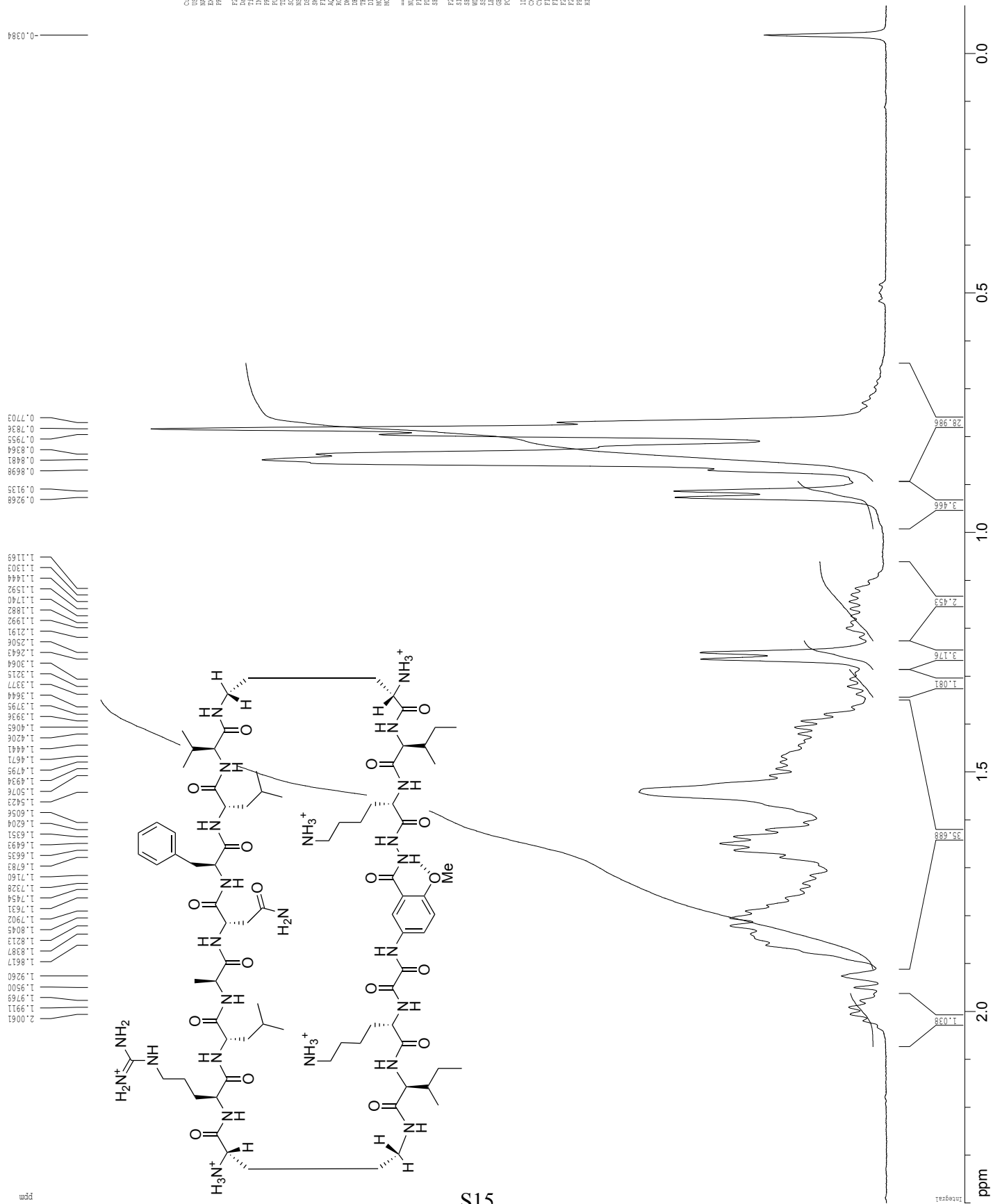
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 T99 0.1000000 sec
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¹H NMR of macrocyclic β-sheet peptide 1Arg, 4 mM in 100 mM deuterioacetate buffer in D₂O at 500 MHz and 298 K



¹H NMR of macrocyclic β-sheet peptide 1Arg, 4 mM in 100 mM deuterioacetate buffer in D₂O at 500 MHz and 298 K

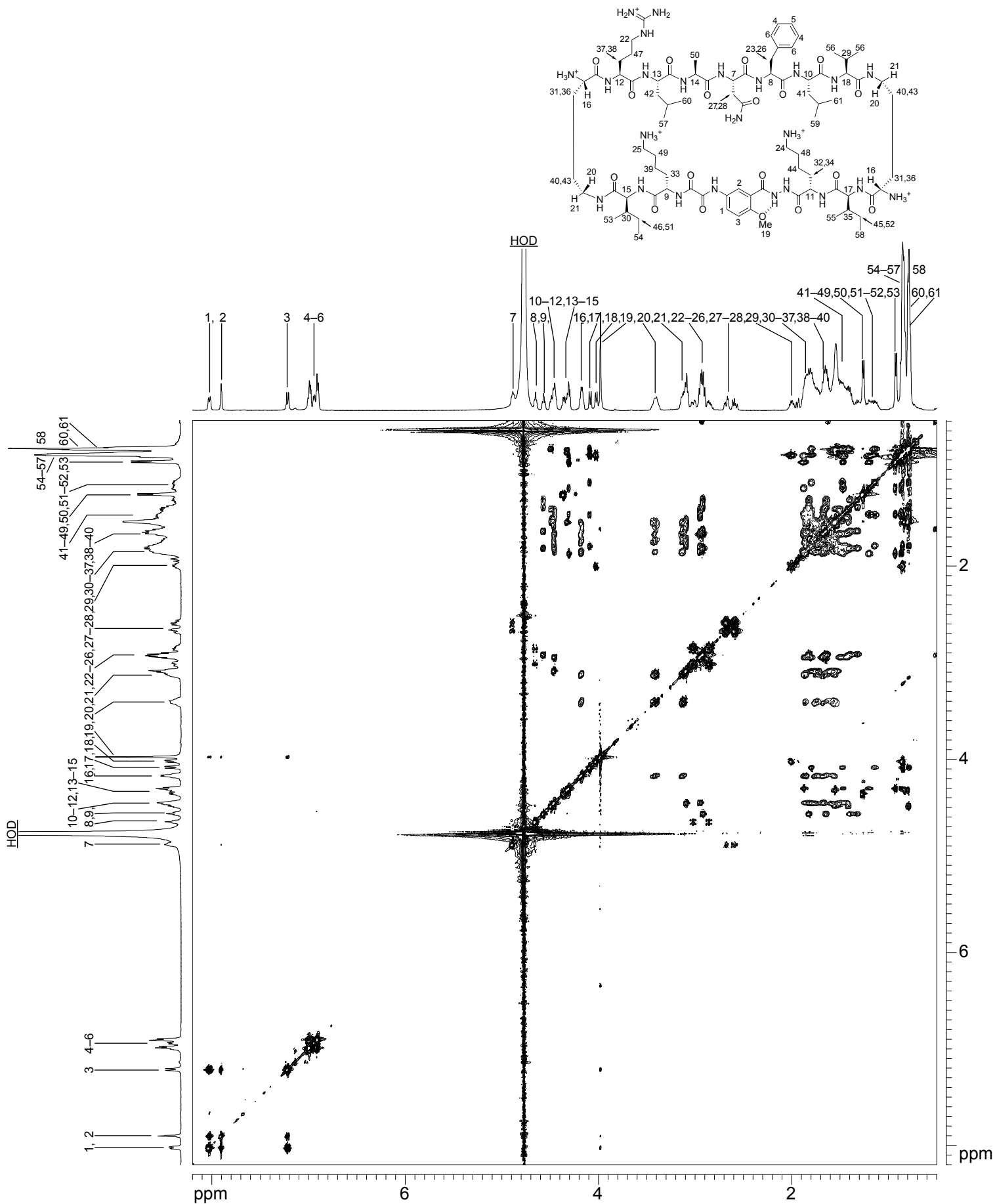


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 WDW EM
 SSB 0
 GB 0
 PC 4.100

1D NMR plot parameters
 CX 22.80 cm
 CY 14.00 cm
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 F2P -0.110 ppm
 F3P -30.02 Hz
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 HZCX 54.94865 ppm/cm

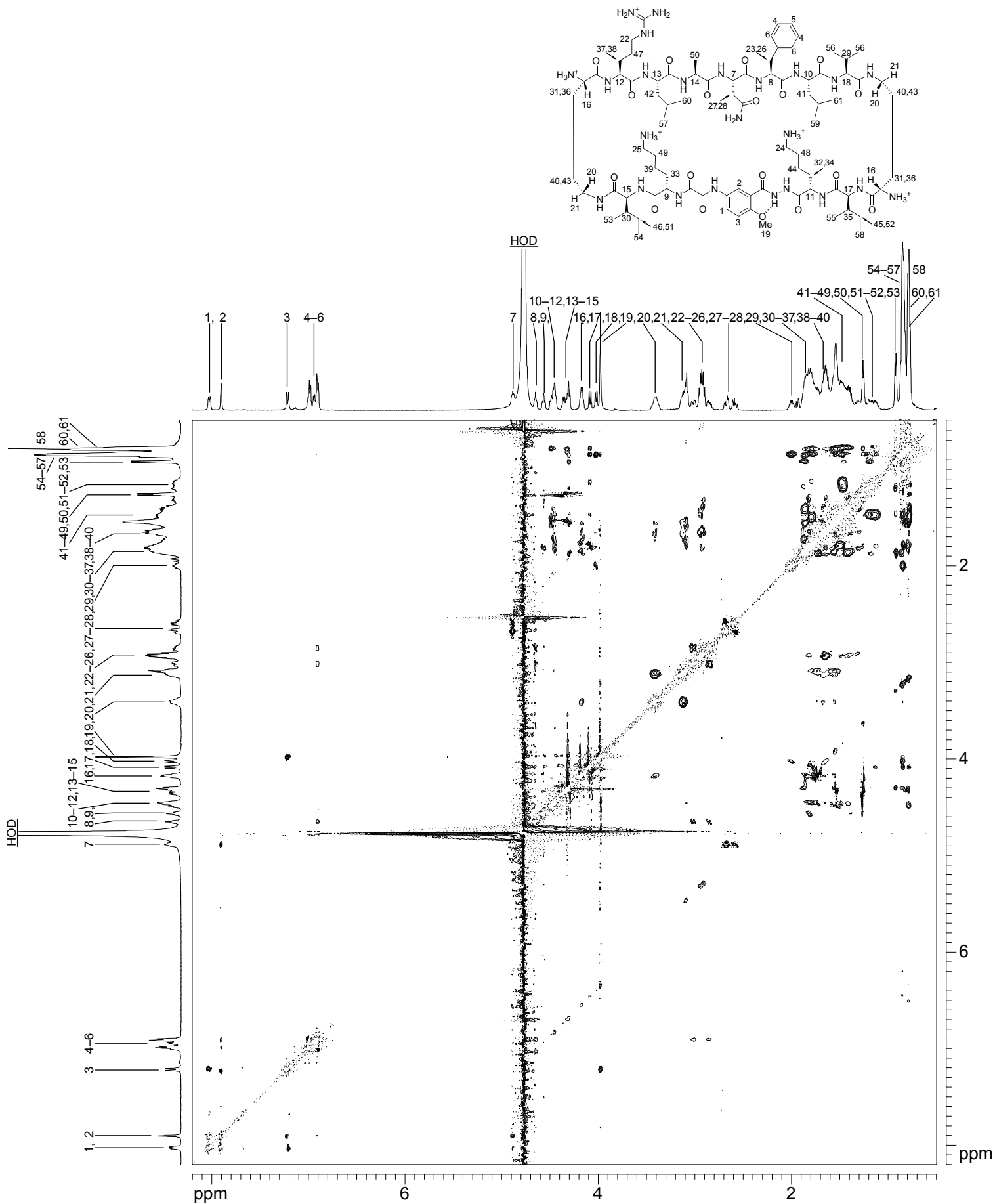
^1H NMR 2D TOCSY of macrocyclic β -sheet peptide **1Arg** with 150-ms spin-lock mixing time
4 mM in 100 mM deuterioacetate buffer in D_2O at 500 MHz and 298 K



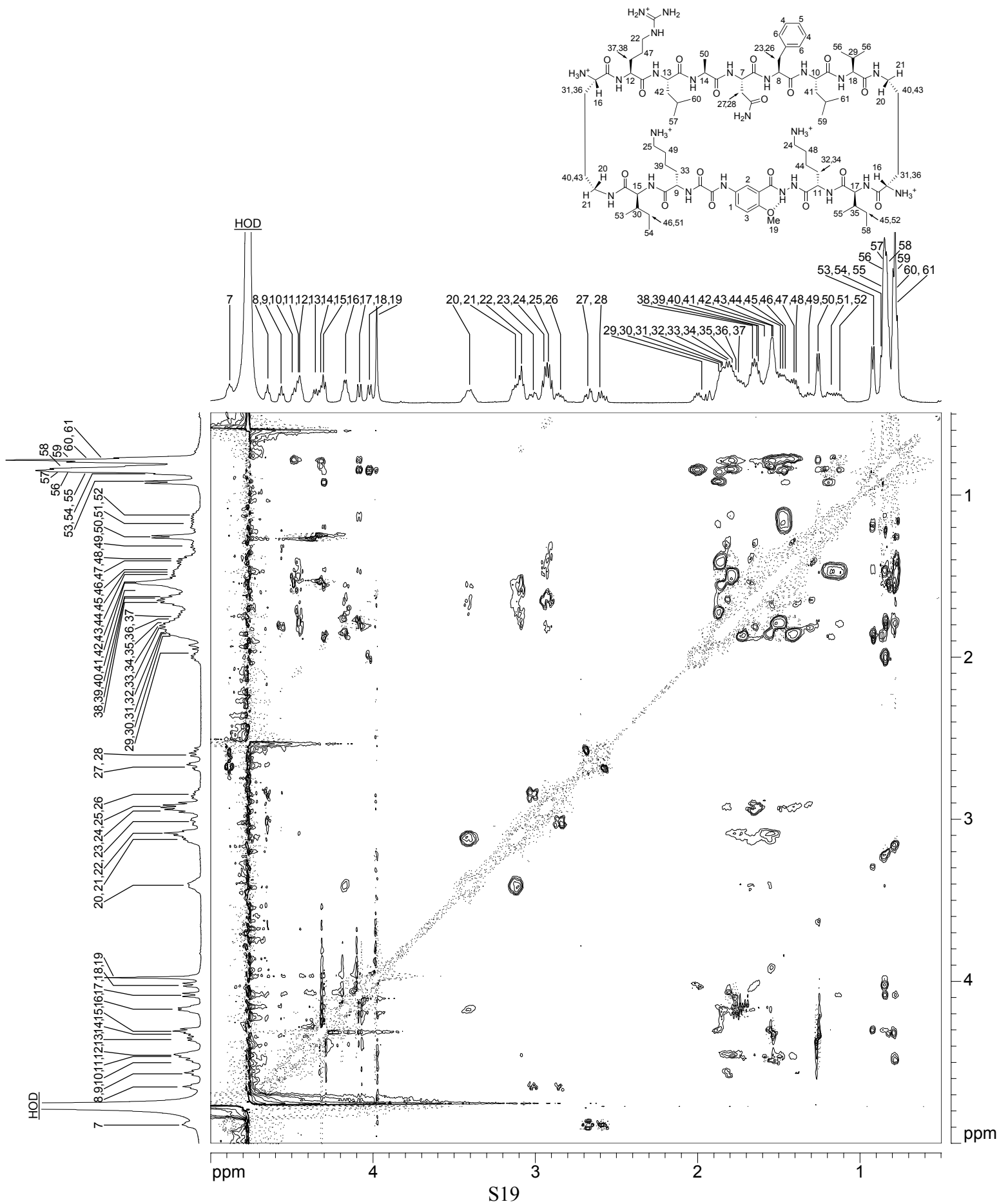
^1H NMR 2D TOCSY of macrocyclic β -sheet peptide **1Arg** with 150-ms spin-lock mixing time
4 mM in 100 mM deuterioacetate buffer in D_2O at 500 MHz and 298 K



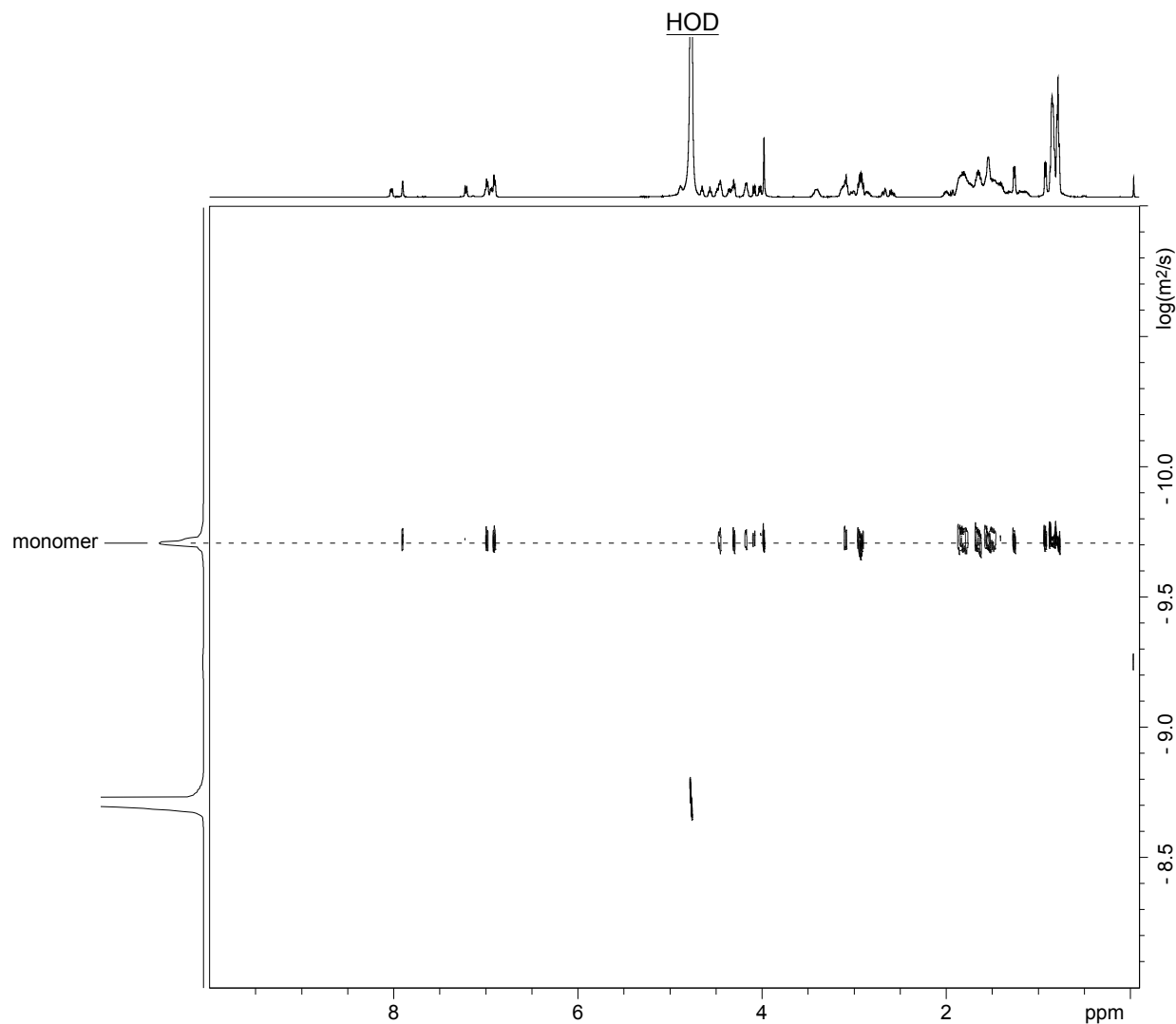
^1H NMR 2D ROESY of macrocyclic β -sheet peptide **1Arg** with 150-ms spin-lock mixing time
4 mM in 100 mM deuterioacetate buffer in D_2O at 500 MHz and 298 K



^1H NMR 2D ROESY of macrocyclic β -sheet peptide **1Arg** with 150-ms spin-lock mixing time
4 mM in 100 mM deuterioacetate buffer in D_2O at 500 MHz and 298 K



^1H NMR DOSY of macrocyclic β -sheet peptide **1Arg** at 500 MHz and 298 K
4 mM in 100 mM deuterioacetate buffer in D_2O



Calculations for macrocyclic β -sheet peptide **1Arg** at 4 mM

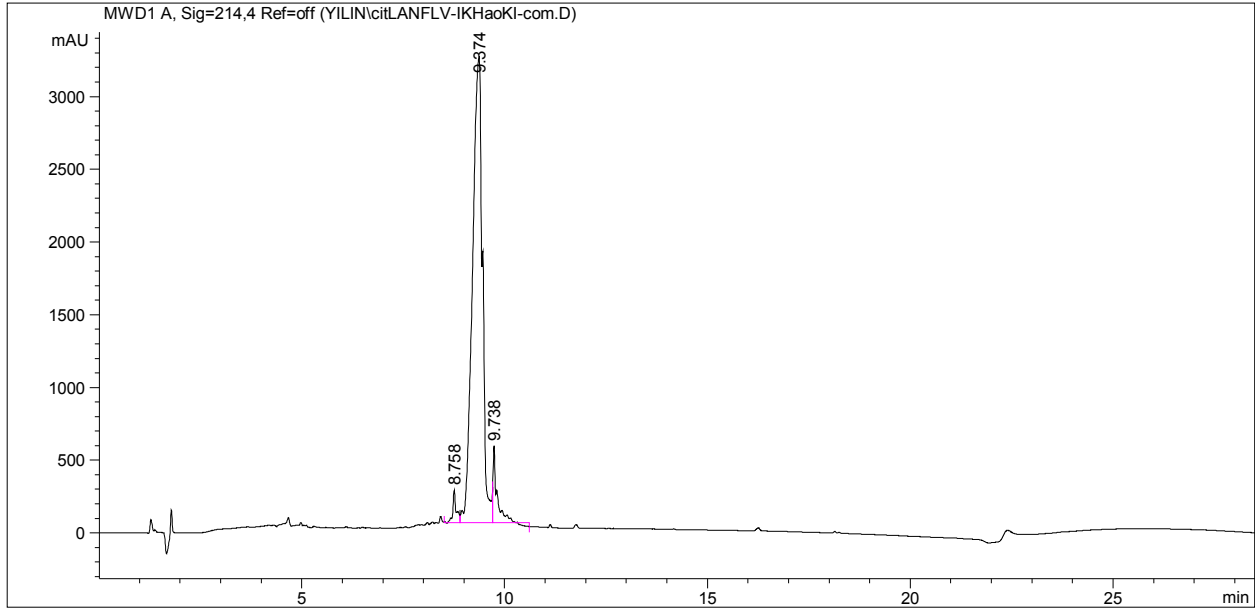
$$D_{\text{HOD}} = 19.0 \times 10^{-10} \text{ m}^2/\text{s} \text{ }^a$$

$$\log(D_{\text{HOD}}) = -8.721$$

$$D_{\text{monomer}} : \log(D) = -9.708; D = 10^{-9.708} = 19.6 \pm 0.6 \times 10^{-11} \text{ m}^2/\text{s}$$

^aLongworth, L. G. *J. Phys. Chem.* **1960**, *64*, 1914–1917.

RP-HPLC of Macrocytic β -Sheet 1_{cit}



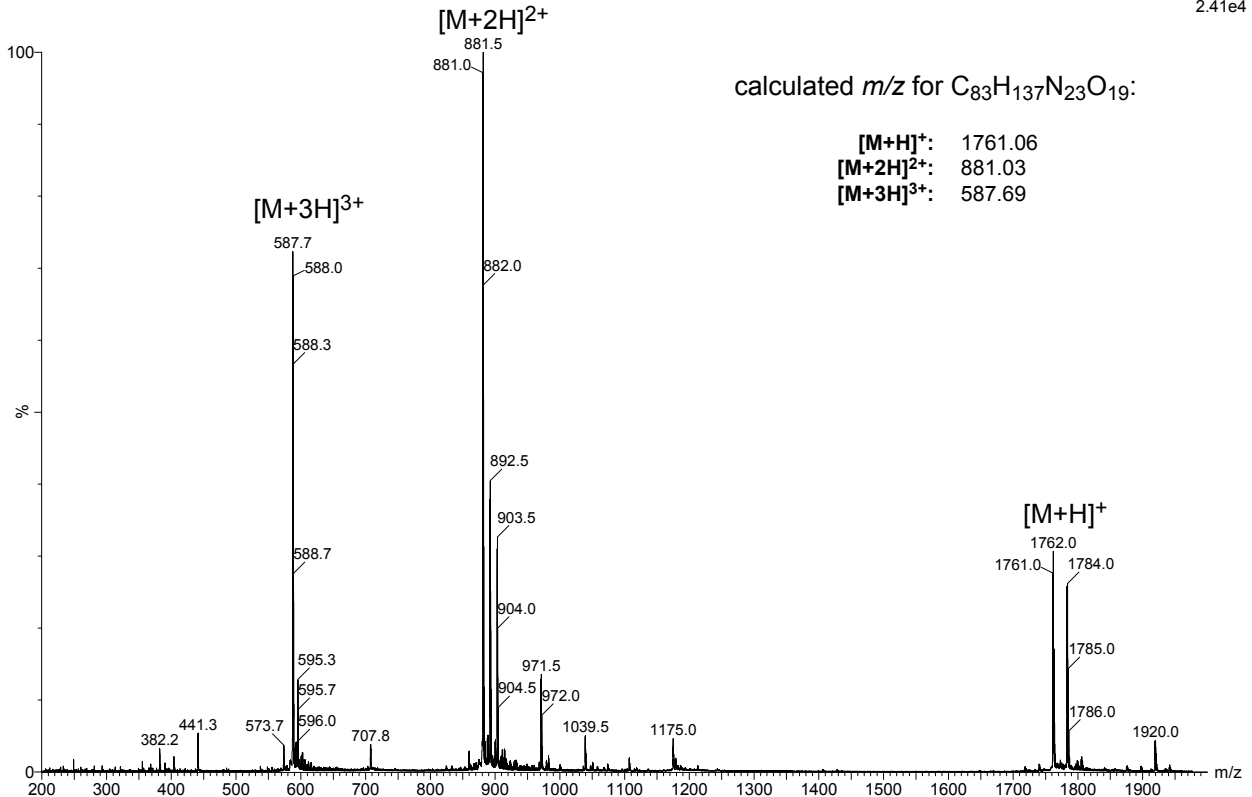
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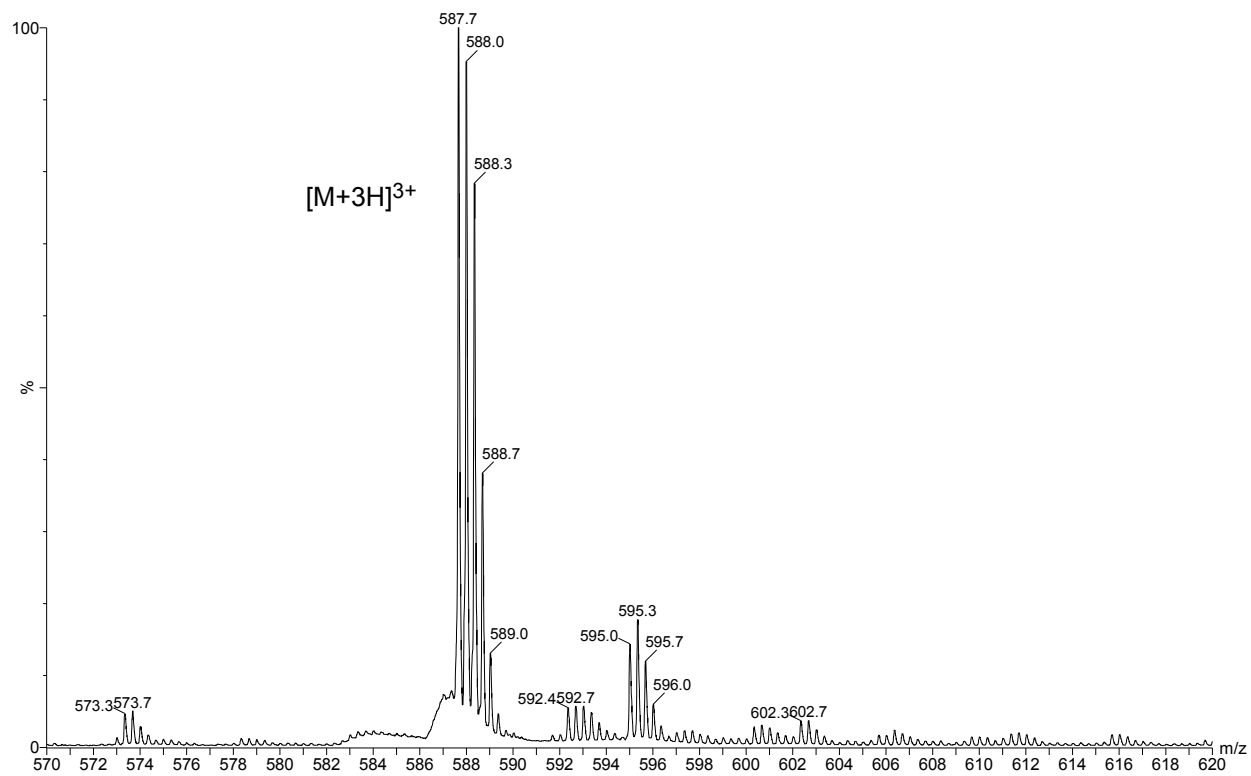
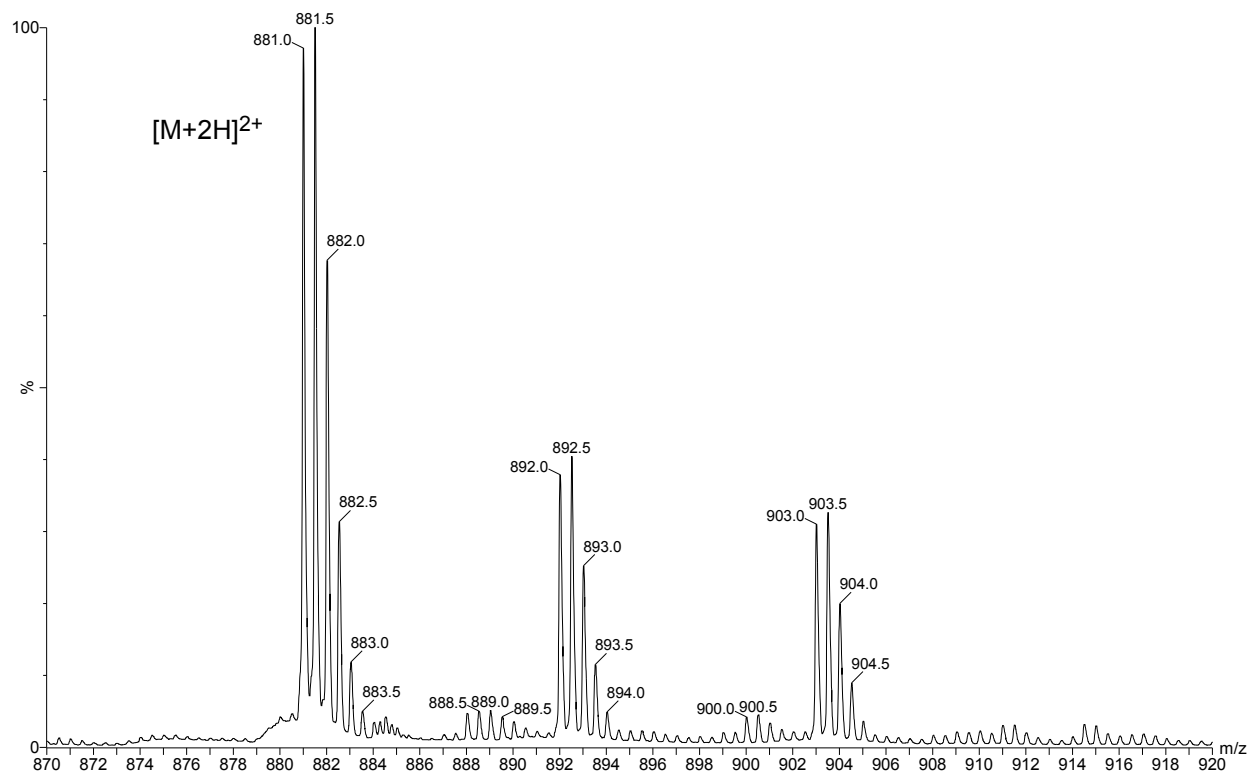
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 B: CH₃CN, 0.1% TFA
gradient: A/B (95:5) to (0:100) in 20 min
flow rate: 1.0 mL/min
detection: VWD, wavelength = 214 nm
temperature: 298 K

MS (ESI) of Macrocytic β -Sheet 1_{cit}

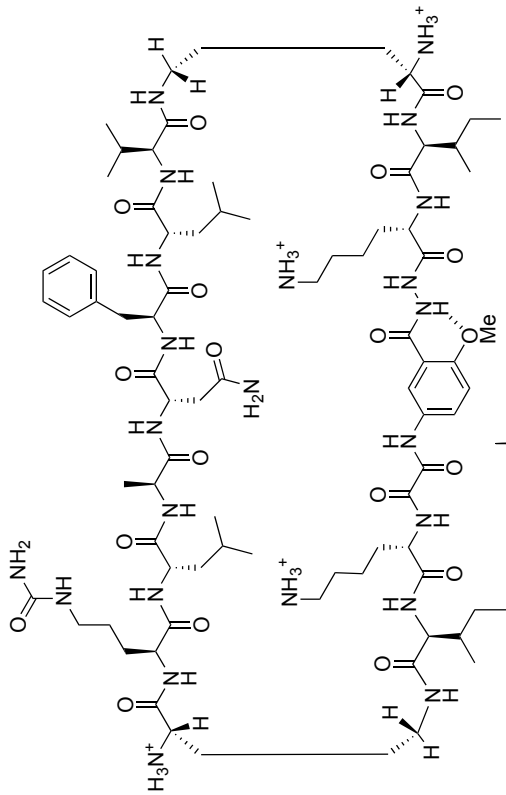
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2.41e4



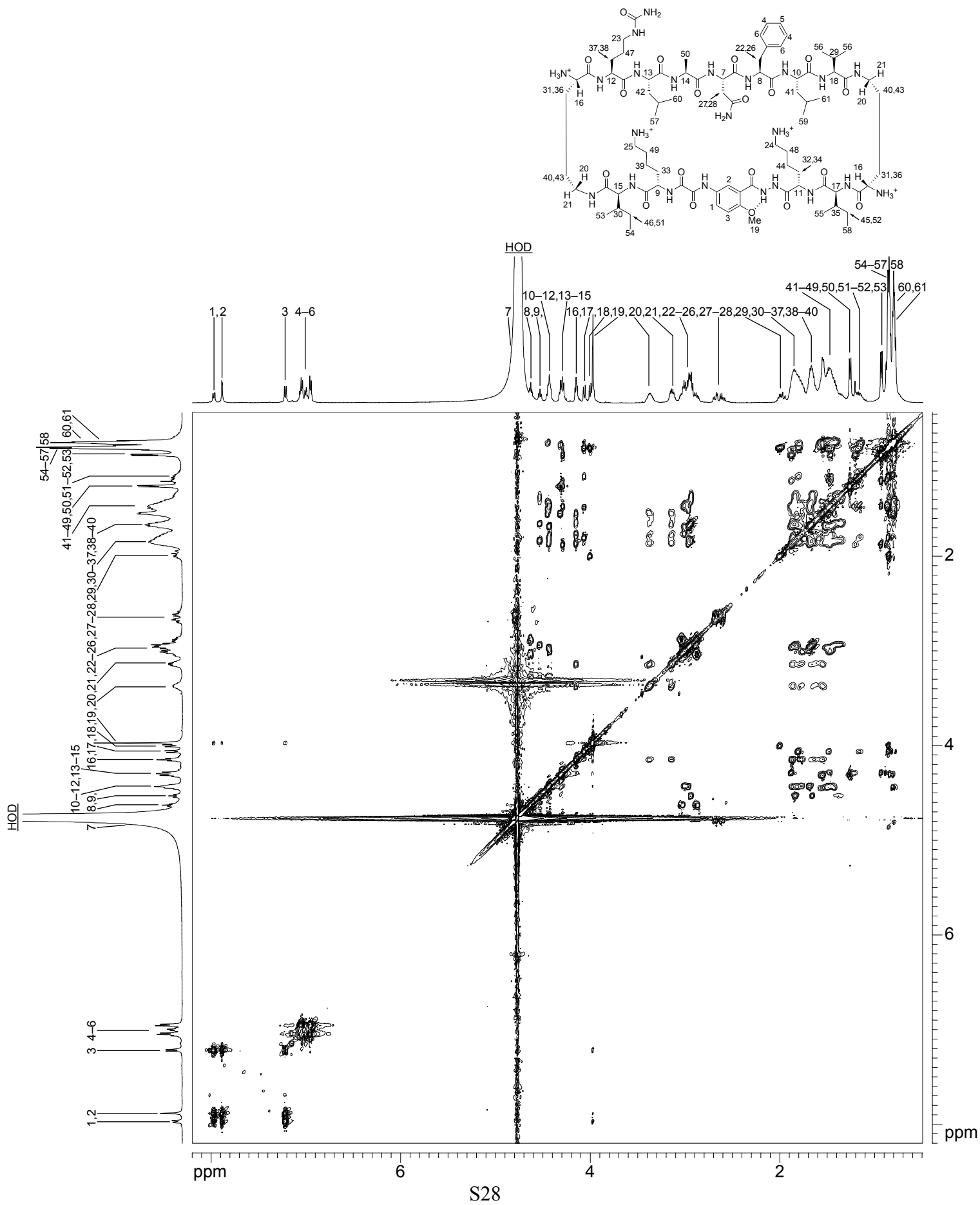


¹H NMR of macrocyclic β-sheet peptide 1cit, 2 mM in 100 mM deuterioacetate buffer in D₂O at 500 MHz and 298 K

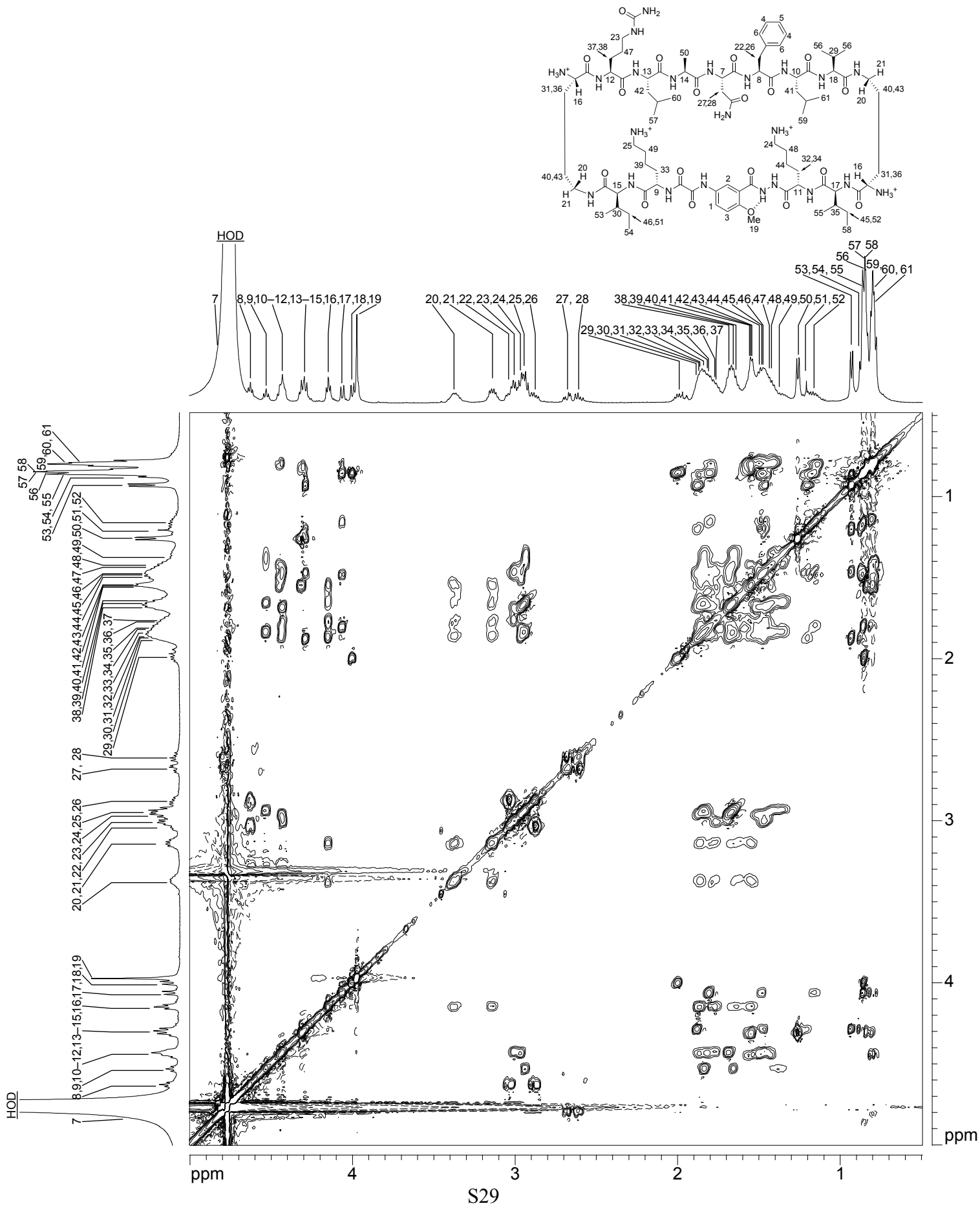


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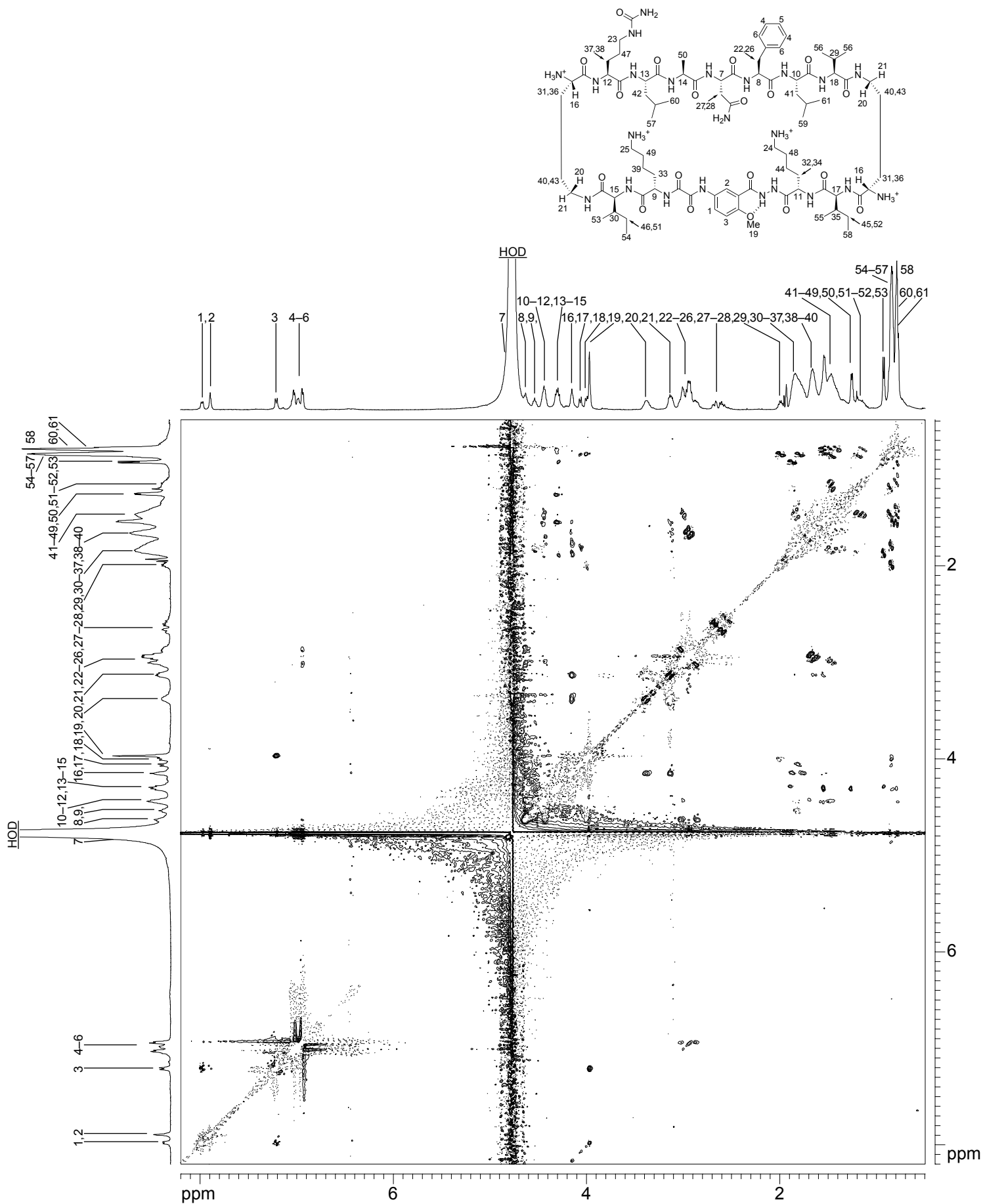
¹H NMR 2D TOCSY of macrocyclic β-sheet peptide **1**_{Cit} with 150-ms spin-lock mixing time
2 mM in 100 mM deuterioacetate buffer in D₂O at 500 MHz and 298 K



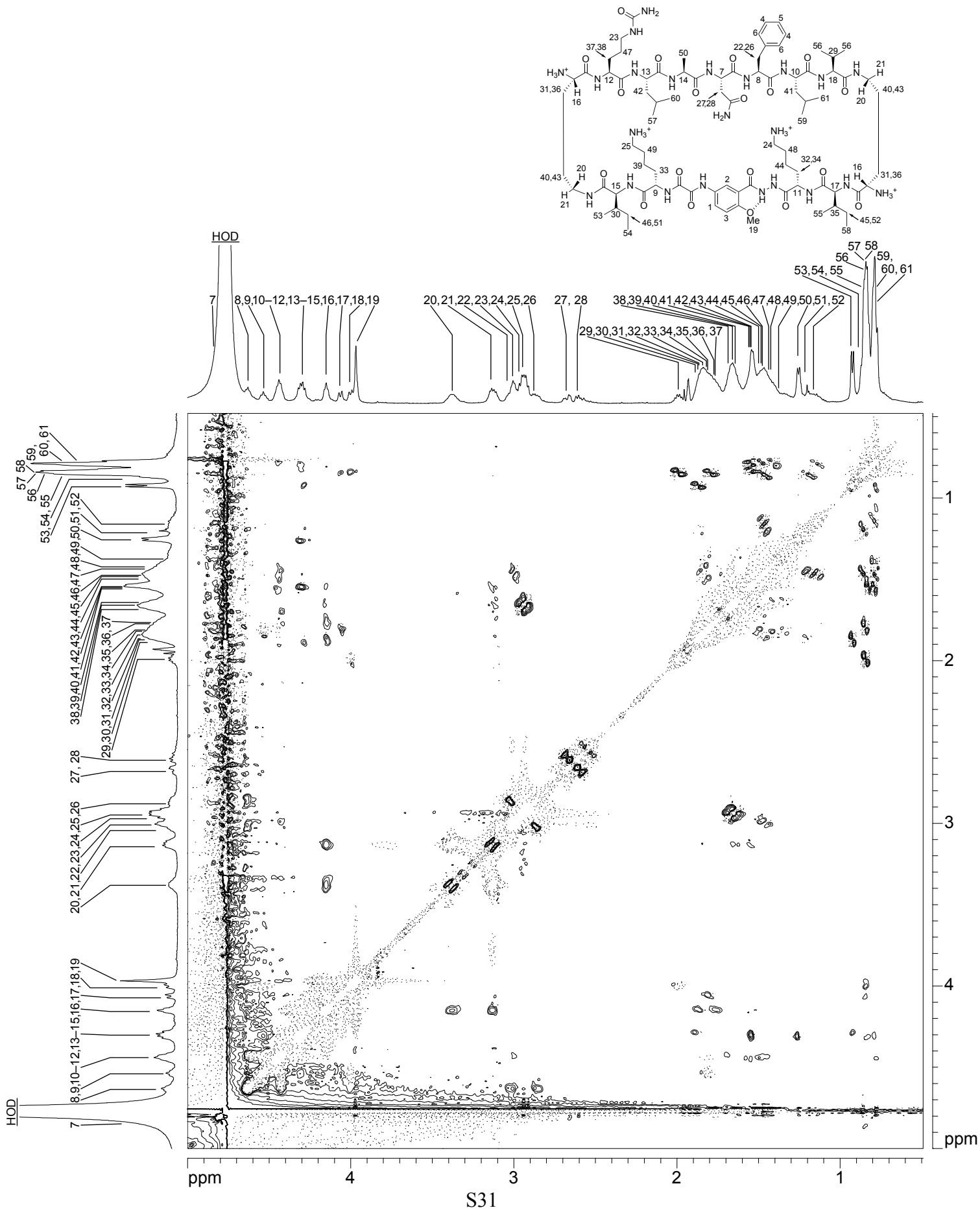
¹H NMR 2D TOCSY of macrocyclic β-sheet peptide **1C_{it}** with 150-ms spin-lock mixing time
2 mM in 100 mM deuterioacetate buffer in D₂O at 500 MHz and 298 K



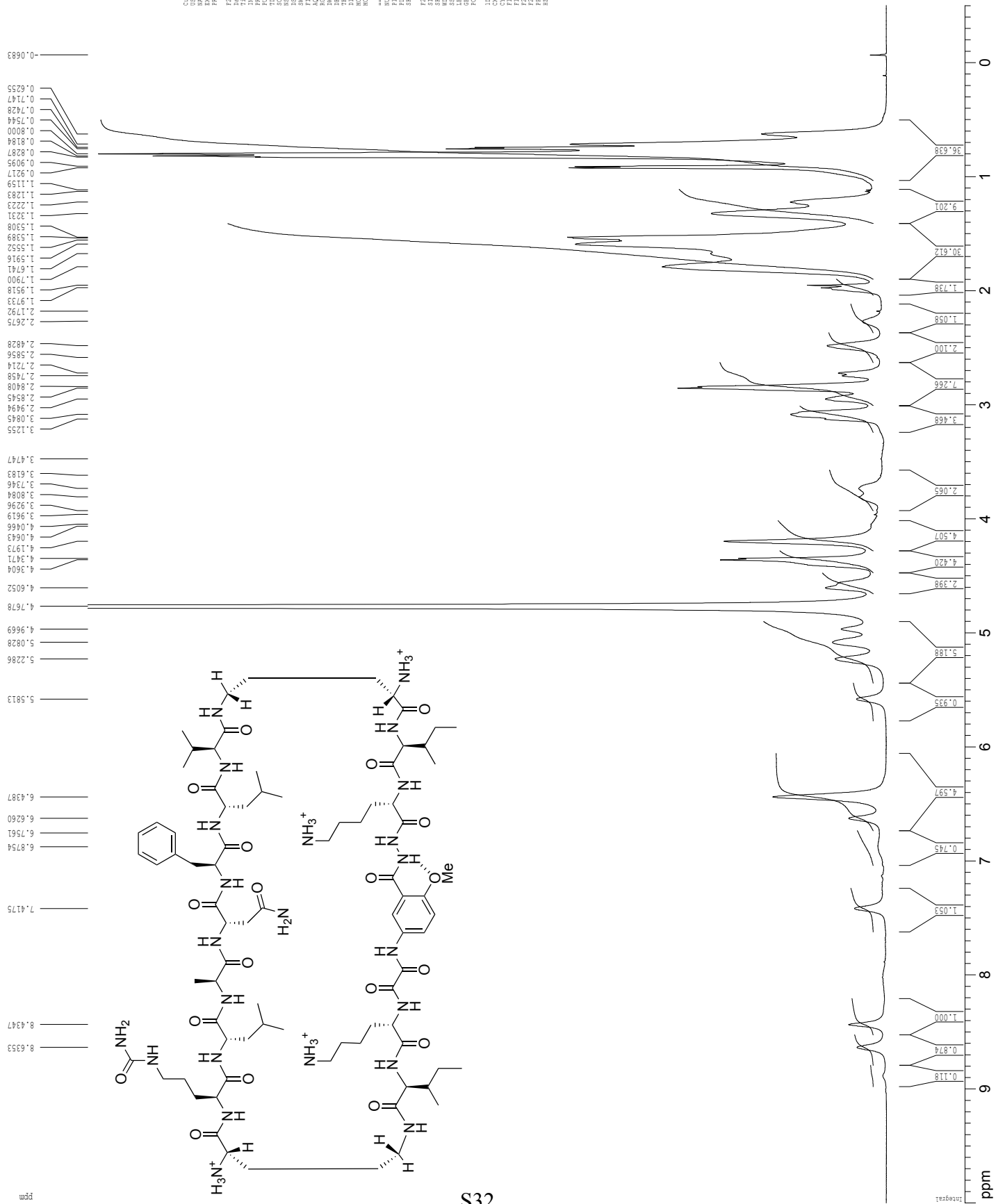
¹H NMR 2D ROESY of macrocyclic β-sheet peptide **1**_{Cit} with 100-ms spin-lock mixing time
2 mM in 100 mM deuterioacetate buffer in D₂O at 500 MHz and 298 K



^1H NMR 2D ROESY of macrocyclic β -sheet peptide **1**_{Cit} with 100-ms spin-lock mixing time
2 mM in 100 mM deuterioacetate buffer in D₂O at 500 MHz and 298 K

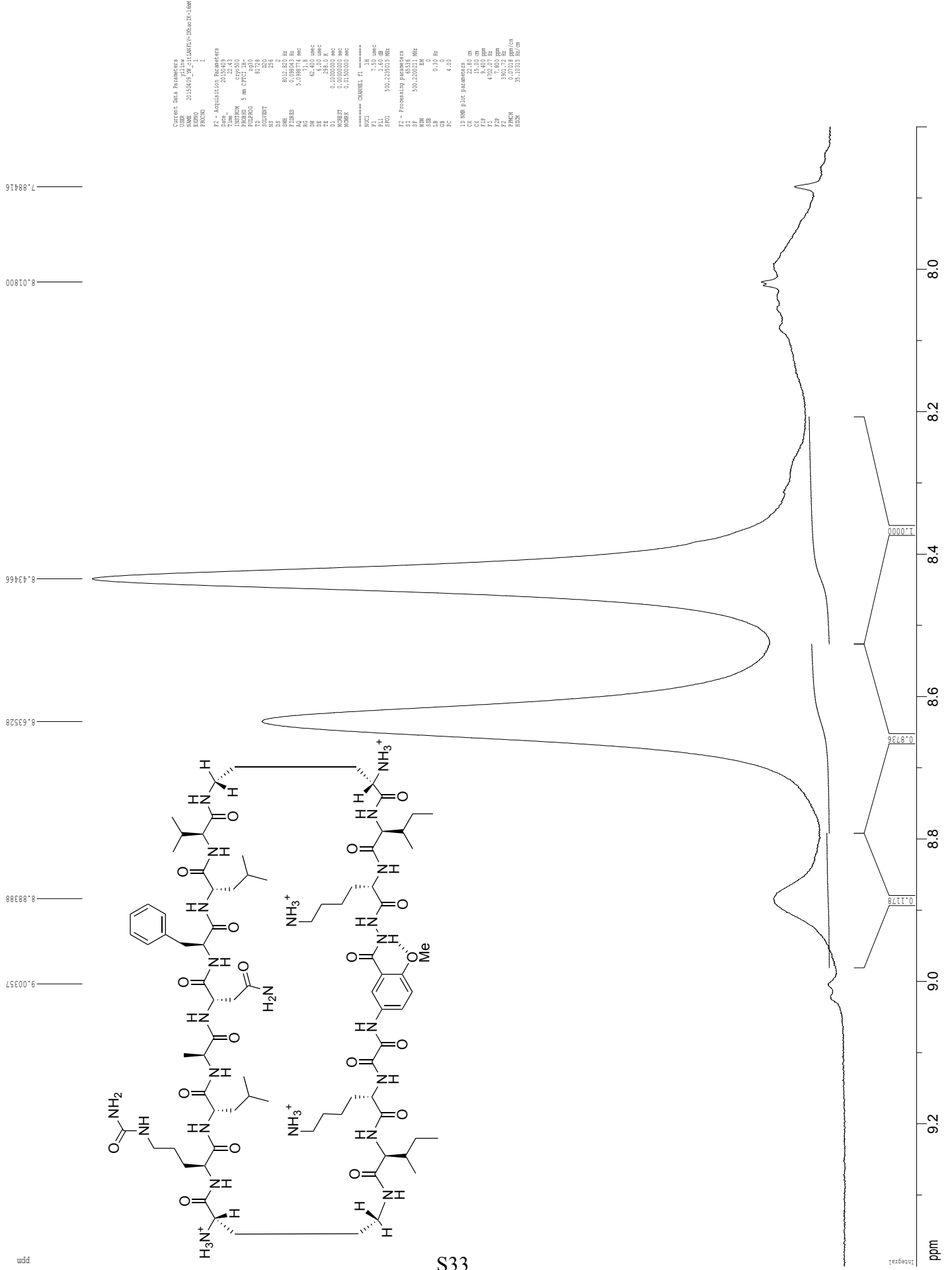


¹H NMR of macrocyclic β-sheet peptide 1cit, 16 mM in 100 mM deuterioacetate buffer in D₂O at 500 MHz and 298 K

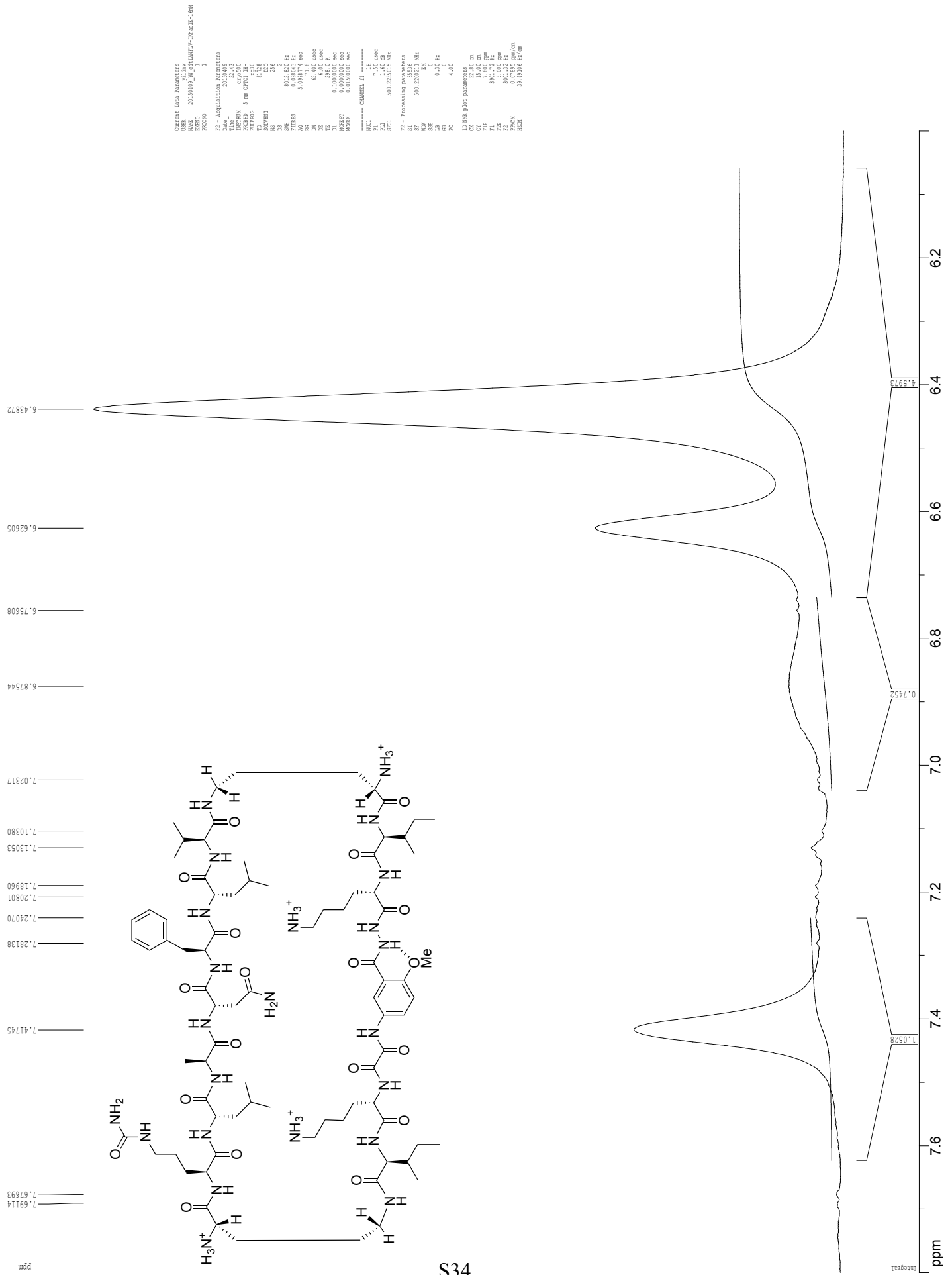


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 FWHZ 0.198863 Hz
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 RG 62.400 usec
 DE 6.00 usec
 D1 0.1000000 sec
 NOISE 0.0000000 sec
 PARRG 0.0100000 sec
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 P1 7.50 usec
 PL 0.00 dB
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 LB 0.30 Hz
 SB 0
 PC 4.00
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¹H NMR of macrocyclic β-sheet peptide 1cit, 16 mM in 100 mM deuterioacetate buffer in D₂O at 500 MHz and 298 K

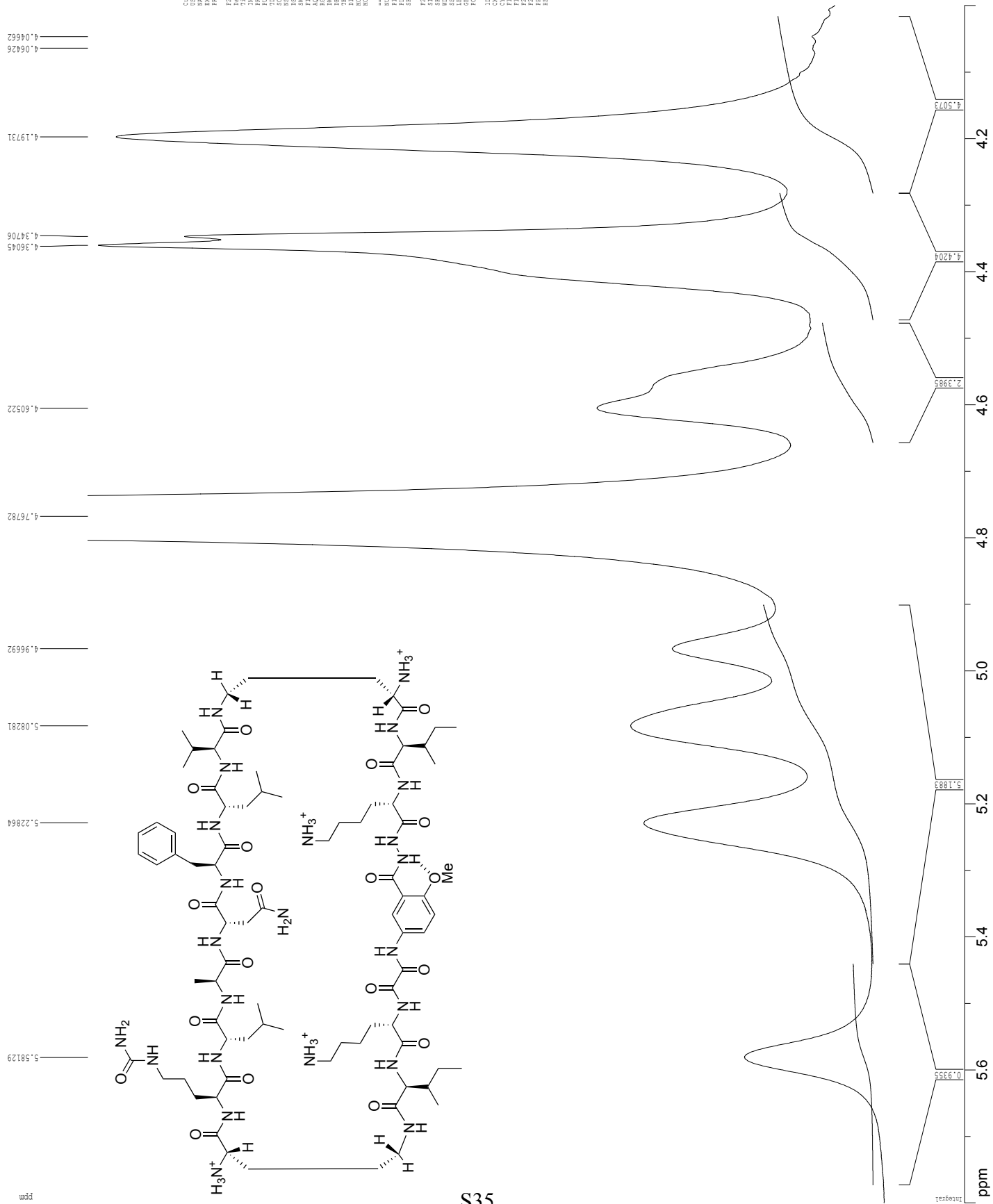


¹H NMR of macrocyclic β-sheet peptide 1cit, 16 mM in 100 mM deuterioacetate buffer in D₂O at 500 MHz and 298 K



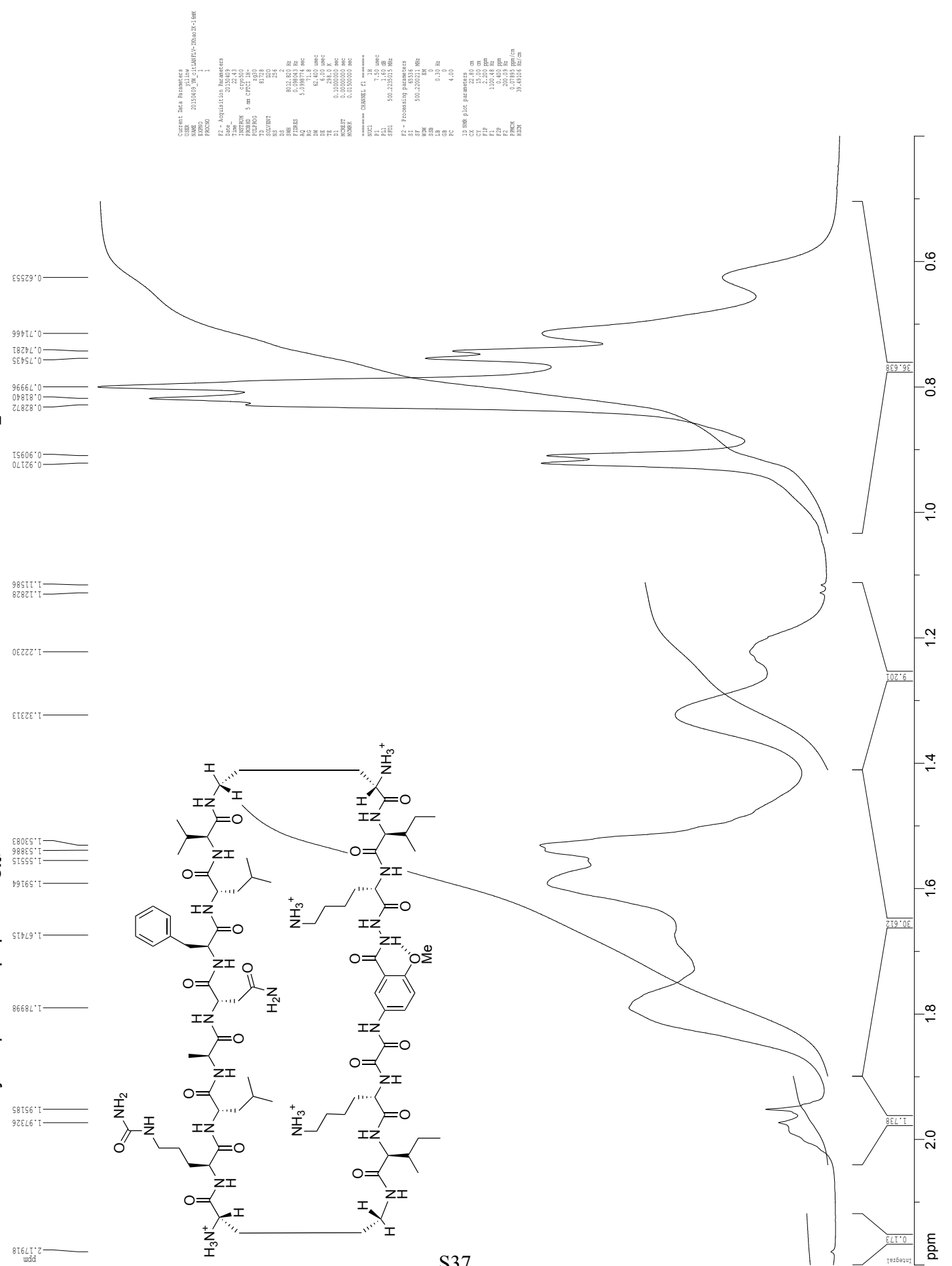
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 CZ 3.00 cm
 F1 3901.72 Hz
 F2 3901.72 Hz
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¹H NMR of macrocyclic β-sheet peptide 1cit, 16 mM in 100 mM deuterioacetate buffer in D₂O at 500 MHz and 298 K



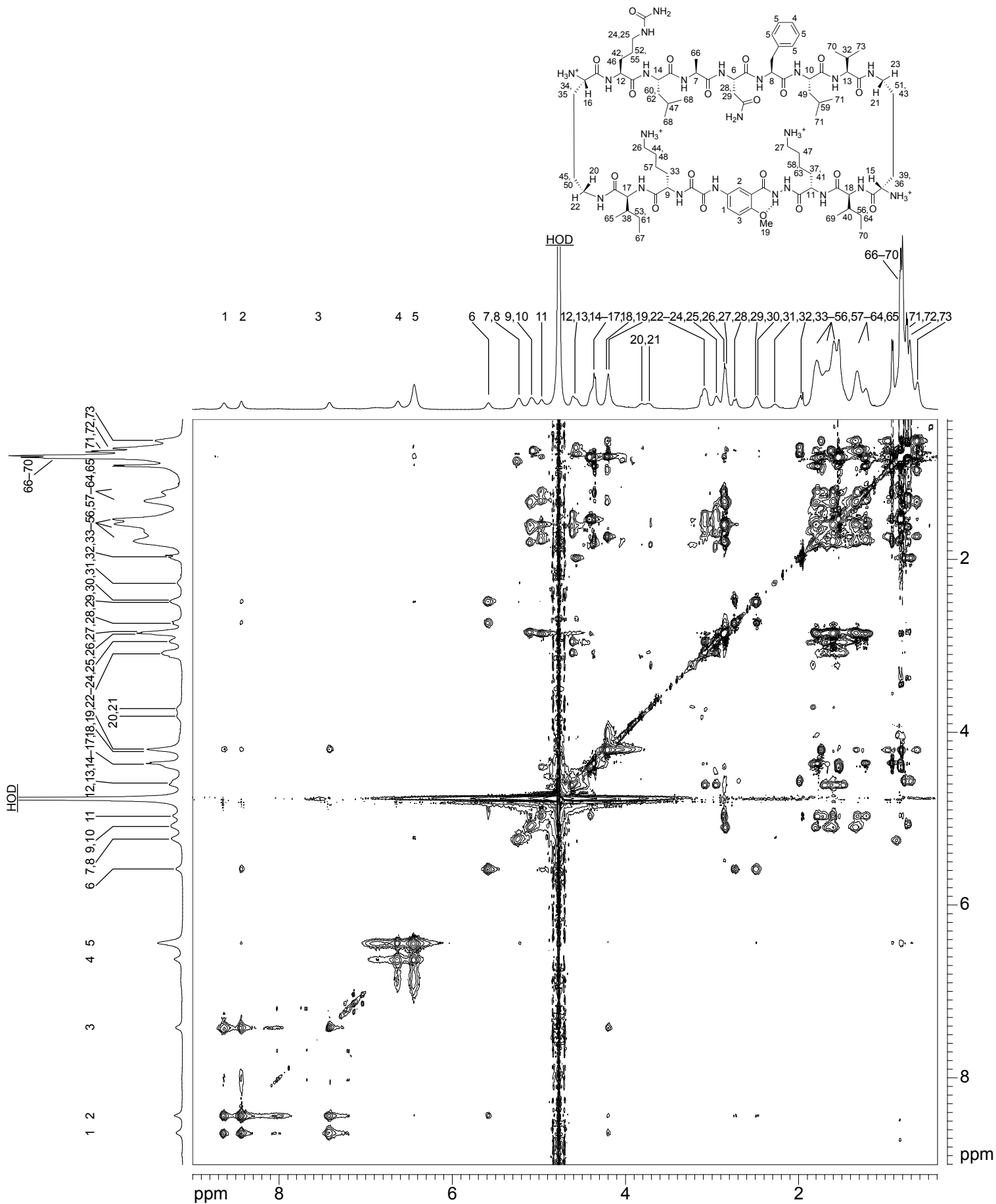
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 RG 62.400 usec
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 DI 0.1000000 sec
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 P1 7.50 usec
 PL 0.00 dB
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 F2 - Processing parameters
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 GB 0
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 CY 3.00 cm
 CZ 3.00 cm
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 F3 2901.48 Hz
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¹H NMR of macrocyclic β-sheet peptide 1cit, 16 mM in 100 mM deuterioacetate buffer in D₂O at 500 MHz and 298 K

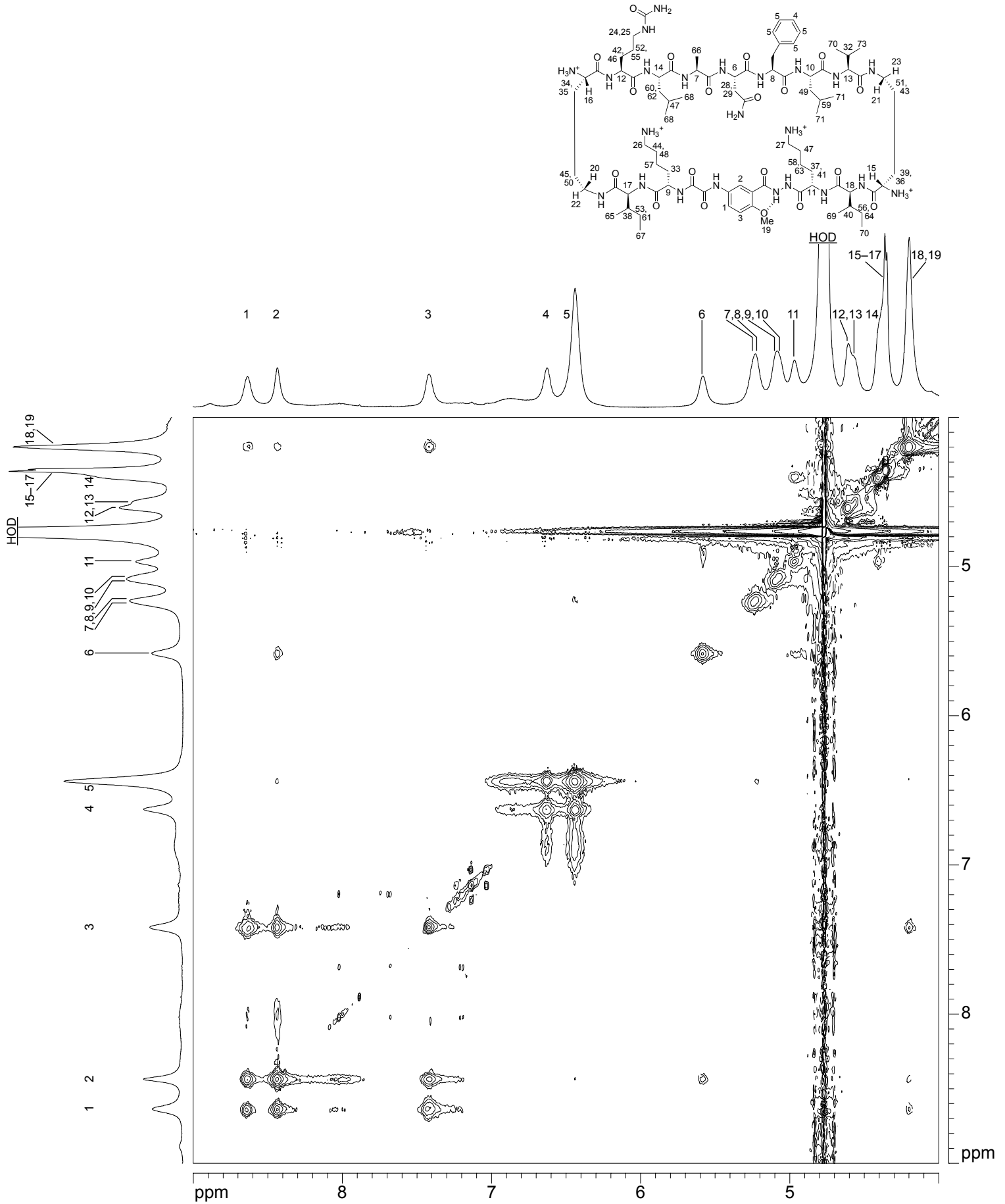


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 PL1 0.00 dB
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 SB 0
 GB 0
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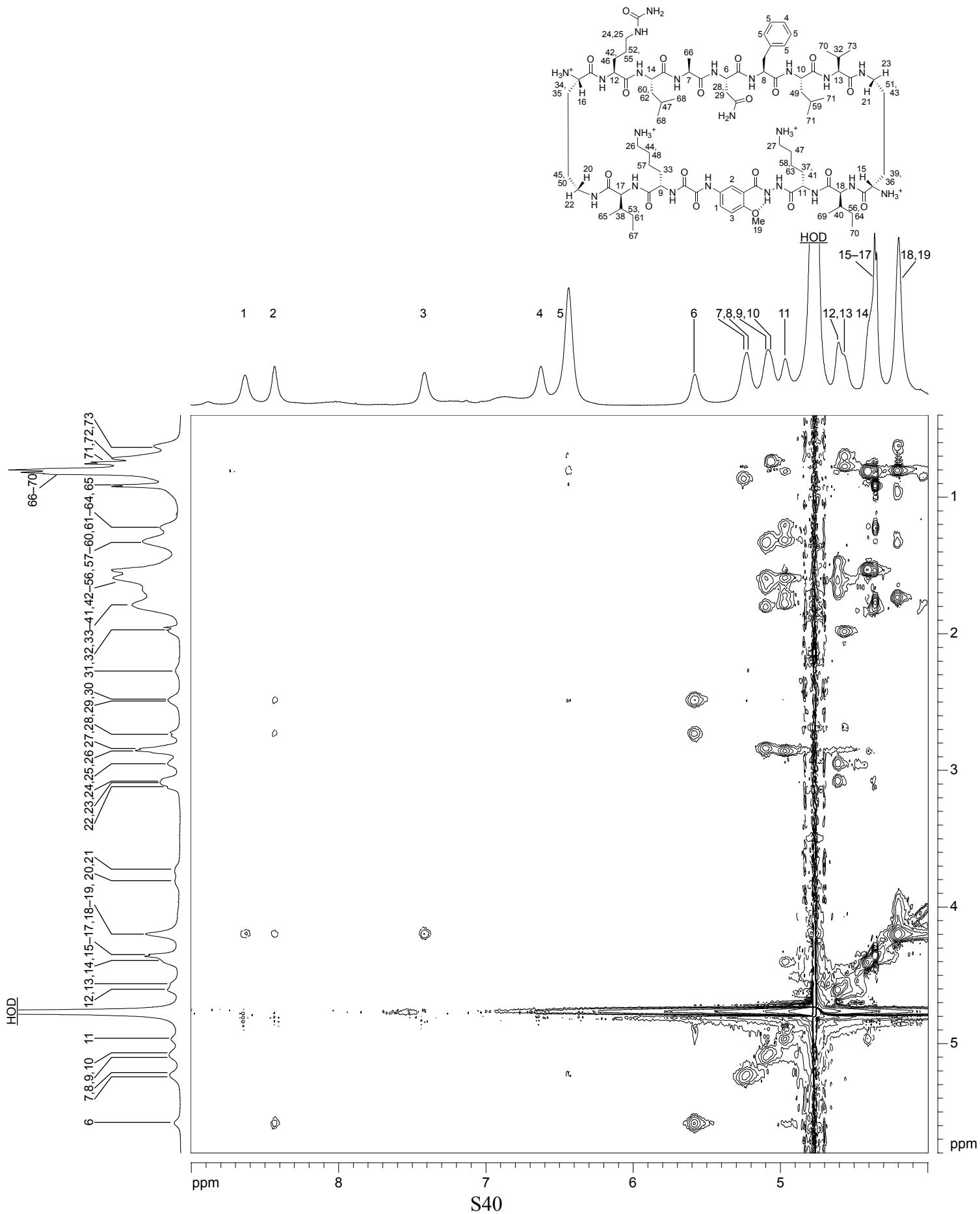
¹H NMR 2D TOCSY of macrocyclic β-sheet peptide **1**_{Cit} with 150-ms spin-lock mixing time
16 mM in 100 mM deuterioacetate buffer in D₂O at 500 MHz and 298 K



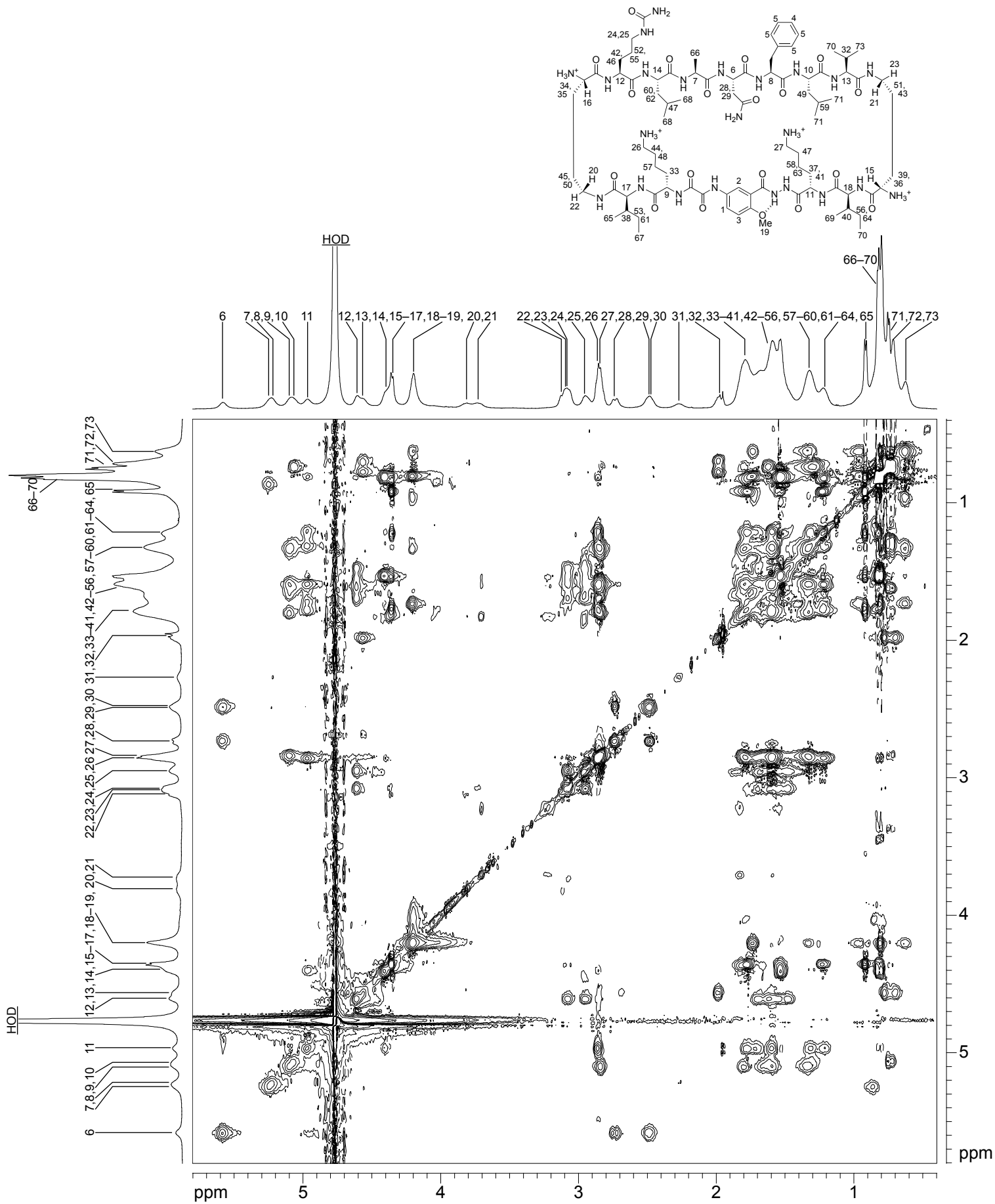
¹H NMR 2D TOCSY of macrocyclic β-sheet peptide **1C_{it}** with 150-ms spin-lock mixing time
16 mM in 100 mM deuterioacetate buffer in D₂O at 500 MHz and 298 K



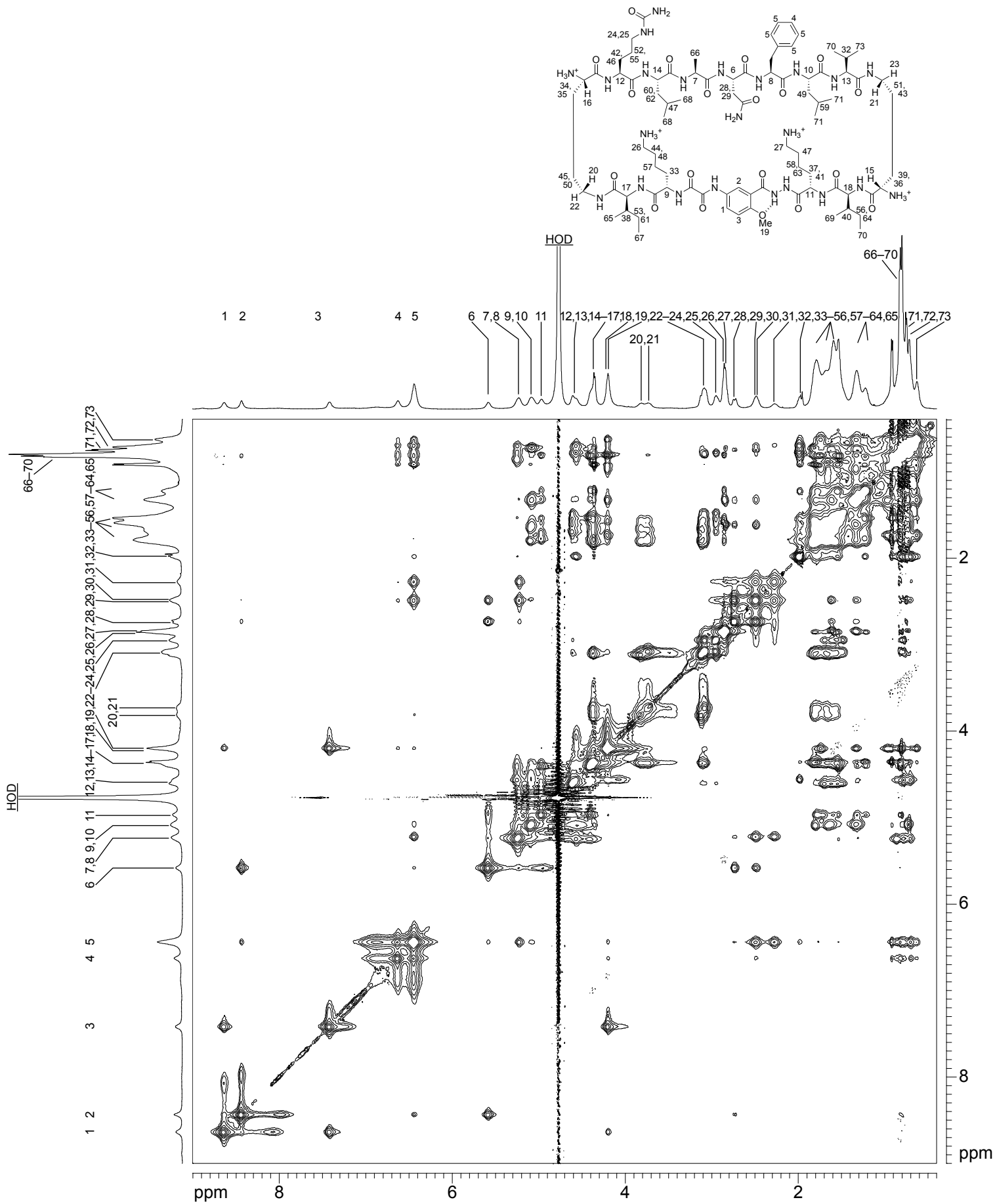
¹H NMR 2D TOCSY of macrocyclic β-sheet peptide **1C_{it}** with 150-ms spin-lock mixing time
16 mM in 100 mM deuterioacetate buffer in D₂O at 500 MHz and 298 K



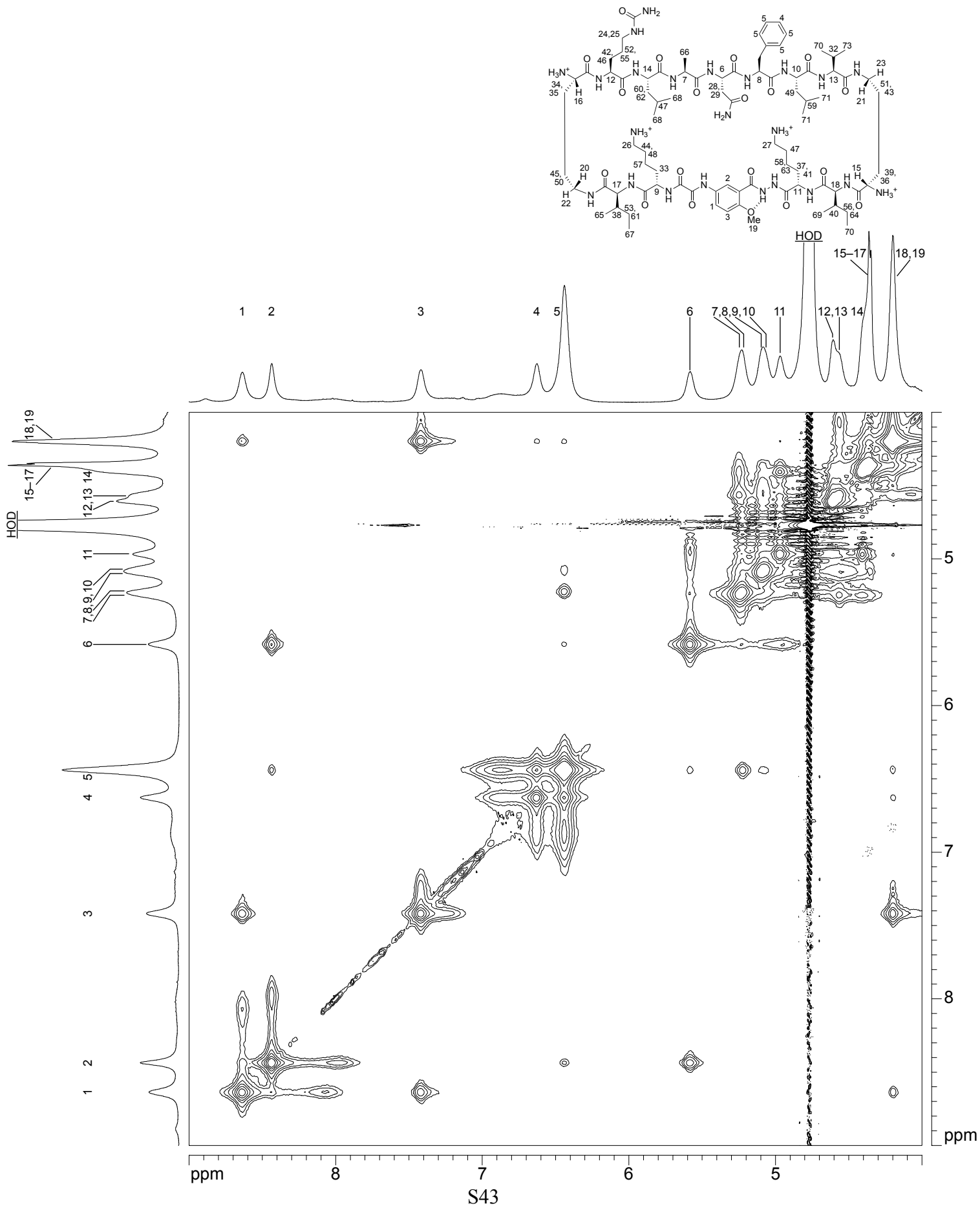
¹H NMR 2D TOCSY of macrocyclic β-sheet peptide **1cit**
16 mM in D₂O at 500 MHz and 298 K with 150-ms spin-lock mixing time



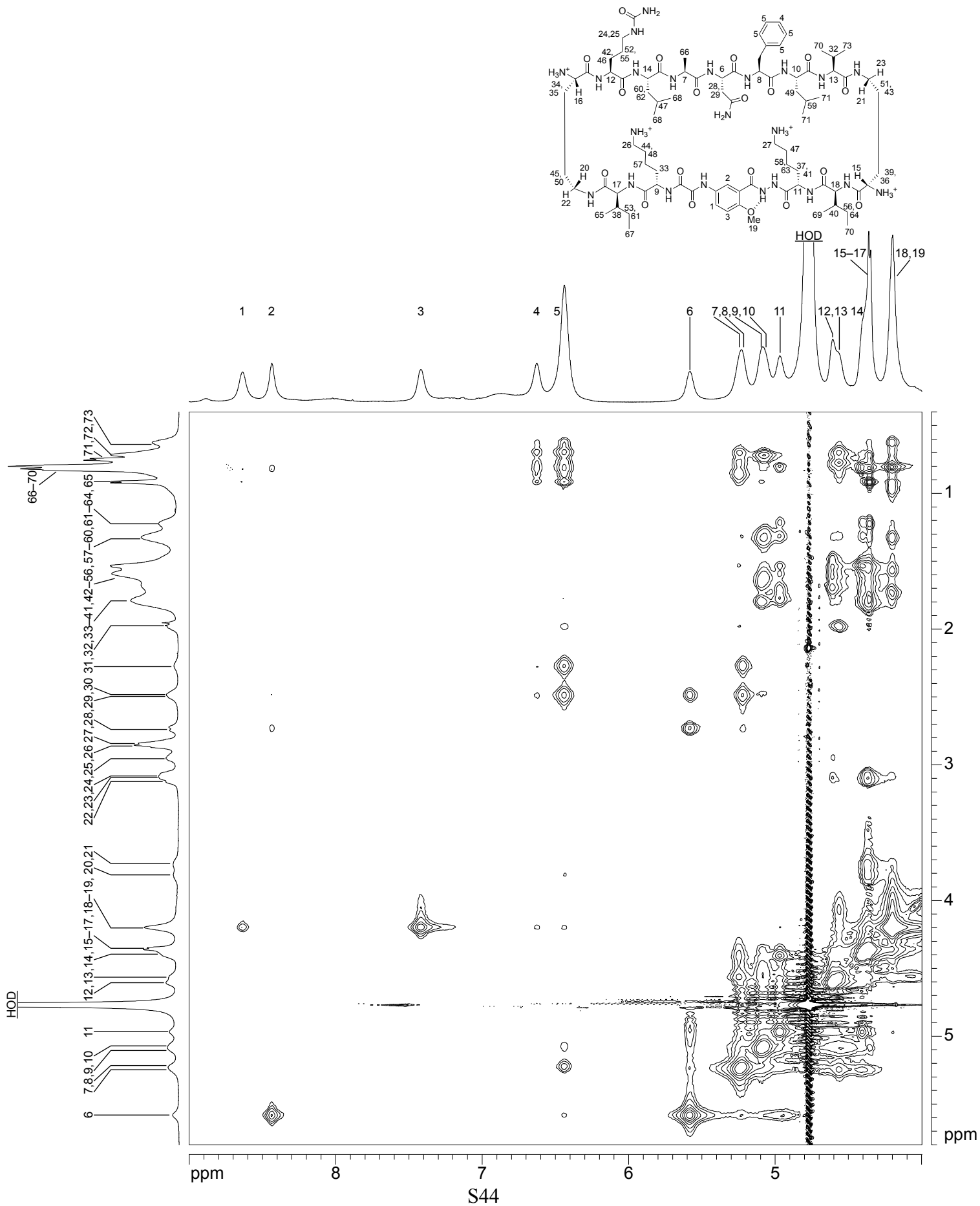
¹H NMR 2D NOESY of macrocyclic β-sheet peptide **1**_{Cit} with 150-ms mixing time
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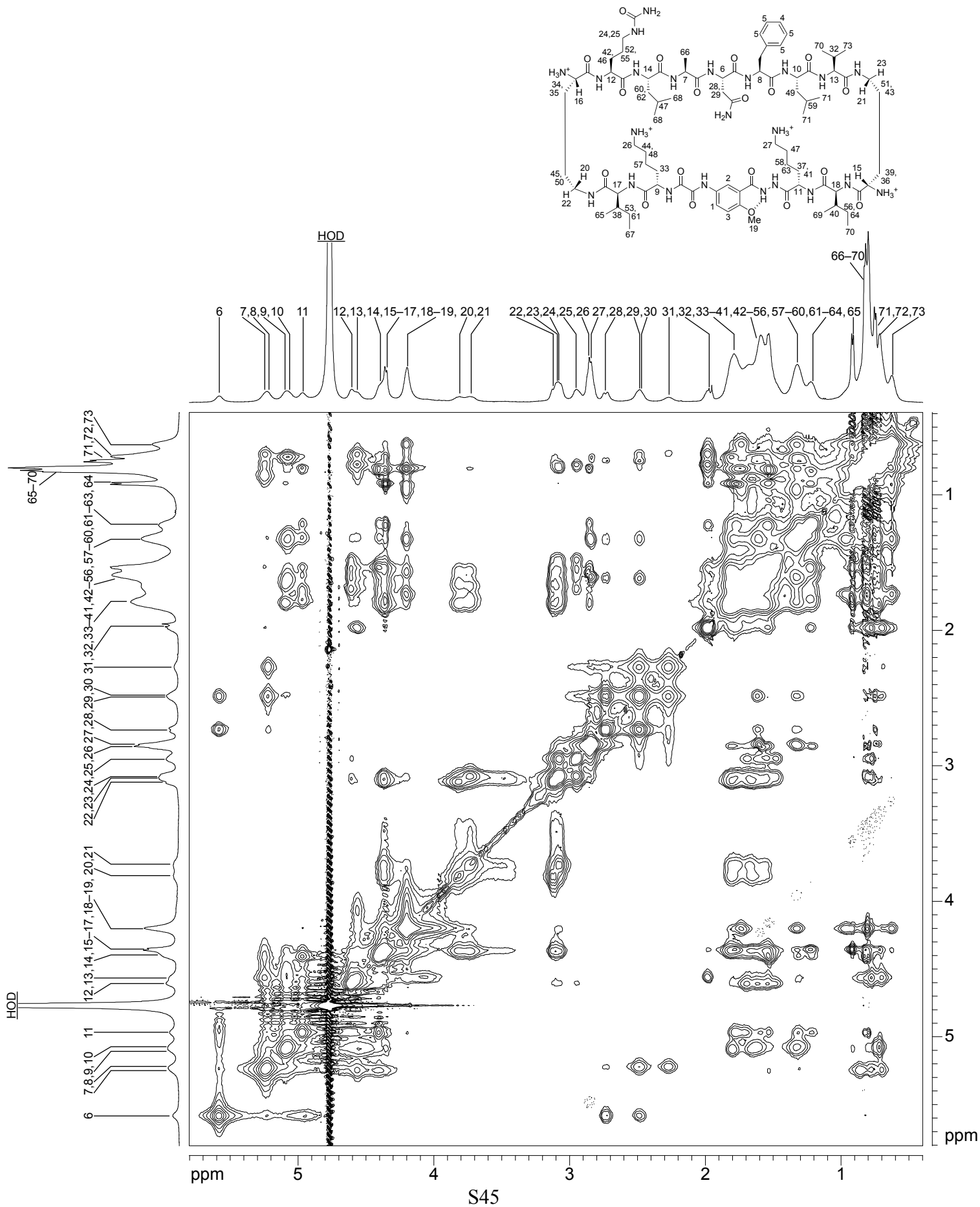
¹H NMR 2D NOESY of macrocyclic β-sheet peptide **1**_{Cit} with 150-ms mixing time
16 mM in 100 mM deuterioacetate buffer in D₂O at 500 MHz and 298 K



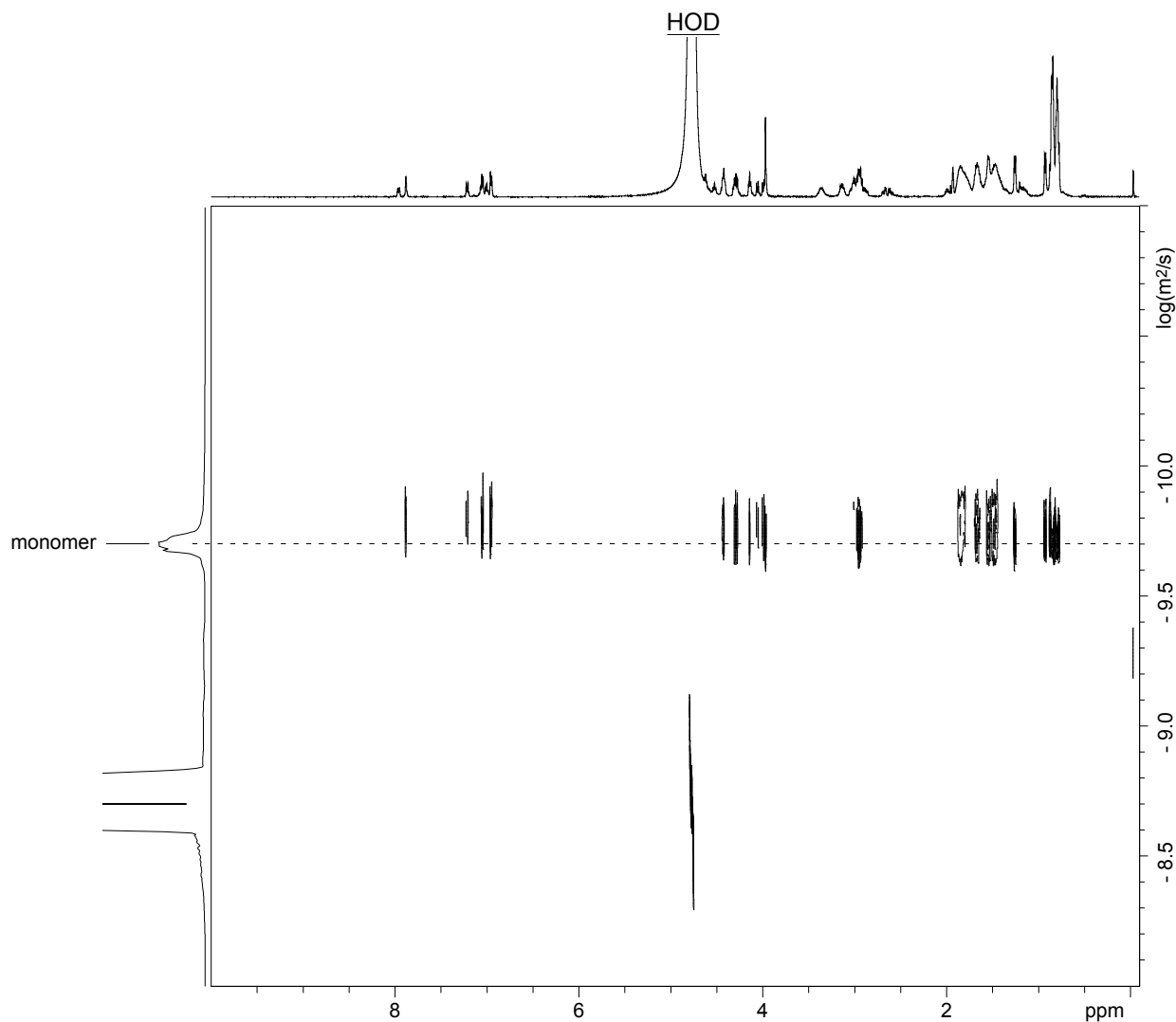
¹H NMR 2D NOESY of macrocyclic β-sheet peptide **1**_{Cit} with 150-ms mixing time
16 mM in 100 mM deuterioacetate buffer in D₂O at 500 MHz and 298 K



¹H NMR 2D NOESY of macrocyclic β-sheet peptide **1C_{it}** with 150-ms mixing time
16 mM in 100 mM deuterioacetate buffer in D₂O at 500 MHz and 298 K



^1H NMR DOSY of macrocyclic β -sheet peptide **1Cit** at 500 MHz and 298 K
1 mM in 100 mM deuterioacetate buffer in D_2O



Calculations for macrocyclic β -sheet peptide **1Cit** at 1 mM

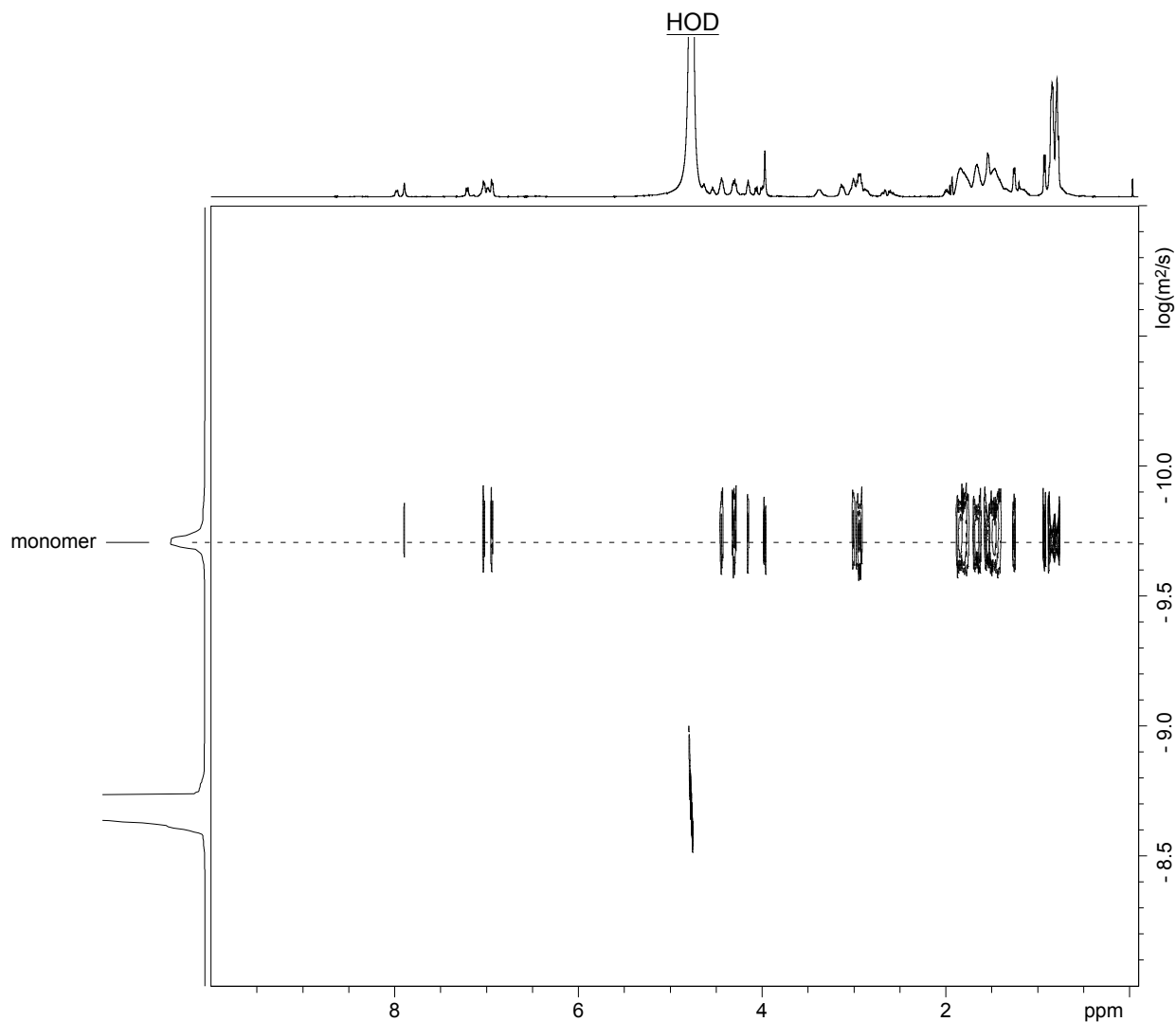
$$D_{\text{HOD}} = 19.0 \times 10^{-10} \text{ m}^2/\text{s} \text{ }^a$$

$$\log(D_{\text{HOD}}) = -8.721$$

$$D_{\text{monomer}} : \log(D) = -9.700; D = 10^{-9.700} = 20.0 \pm 2.0 \times 10^{-11} \text{ m}^2/\text{s}$$

^aLongworth, L. G. *J. Phys. Chem.* **1960**, *64*, 1914–1917.

^1H NMR DOSY of macrocyclic β -sheet peptide **1Cit** at 500 MHz and 298 K
2 mM in 100 mM deuterioacetate buffer in D_2O



Calculations for macrocyclic β -sheet peptide **1Cit** at 2 mM

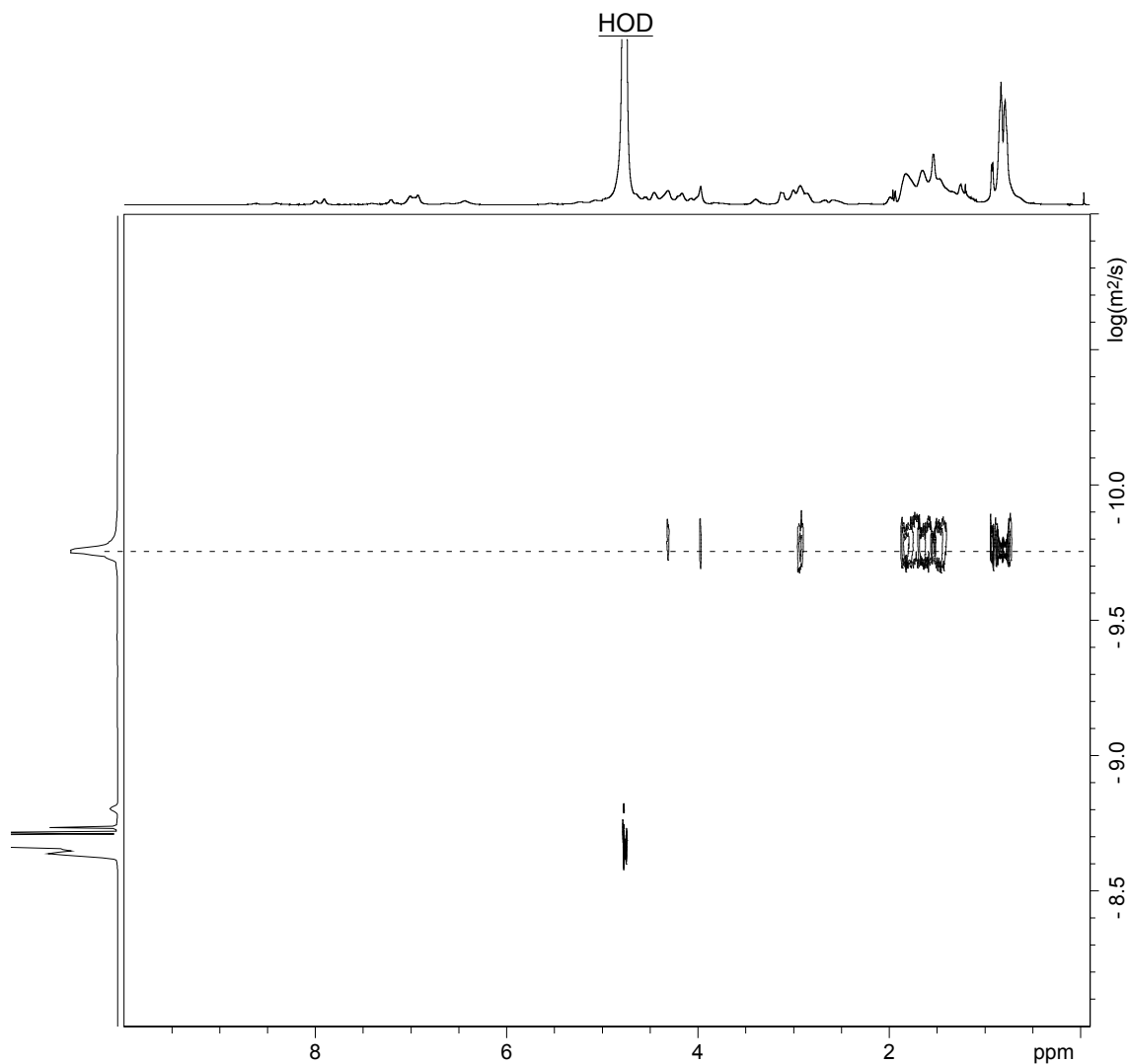
$$D_{\text{HOD}} = 19.0 \times 10^{-10} \text{ m}^2/\text{s} \text{ }^a$$

$$\log(D_{\text{HOD}}) = -8.721$$

$$D_{\text{monomer}} : \log(D) = -9.723; D = 10^{-9.723} = 18.9 \pm 1.2 \times 10^{-11} \text{ m}^2/\text{s}$$

^aLongworth, L. G. *J. Phys. Chem.* **1960**, *64*, 1914–1917.

^1H NMR DOSY of macrocyclic β -sheet peptide **1Cit** at 500 MHz and 298 K
4 mM in 100 mM deuterioacetate buffer in D_2O



Calculations for macrocyclic β -sheet peptide **1Cit** at 4 mM

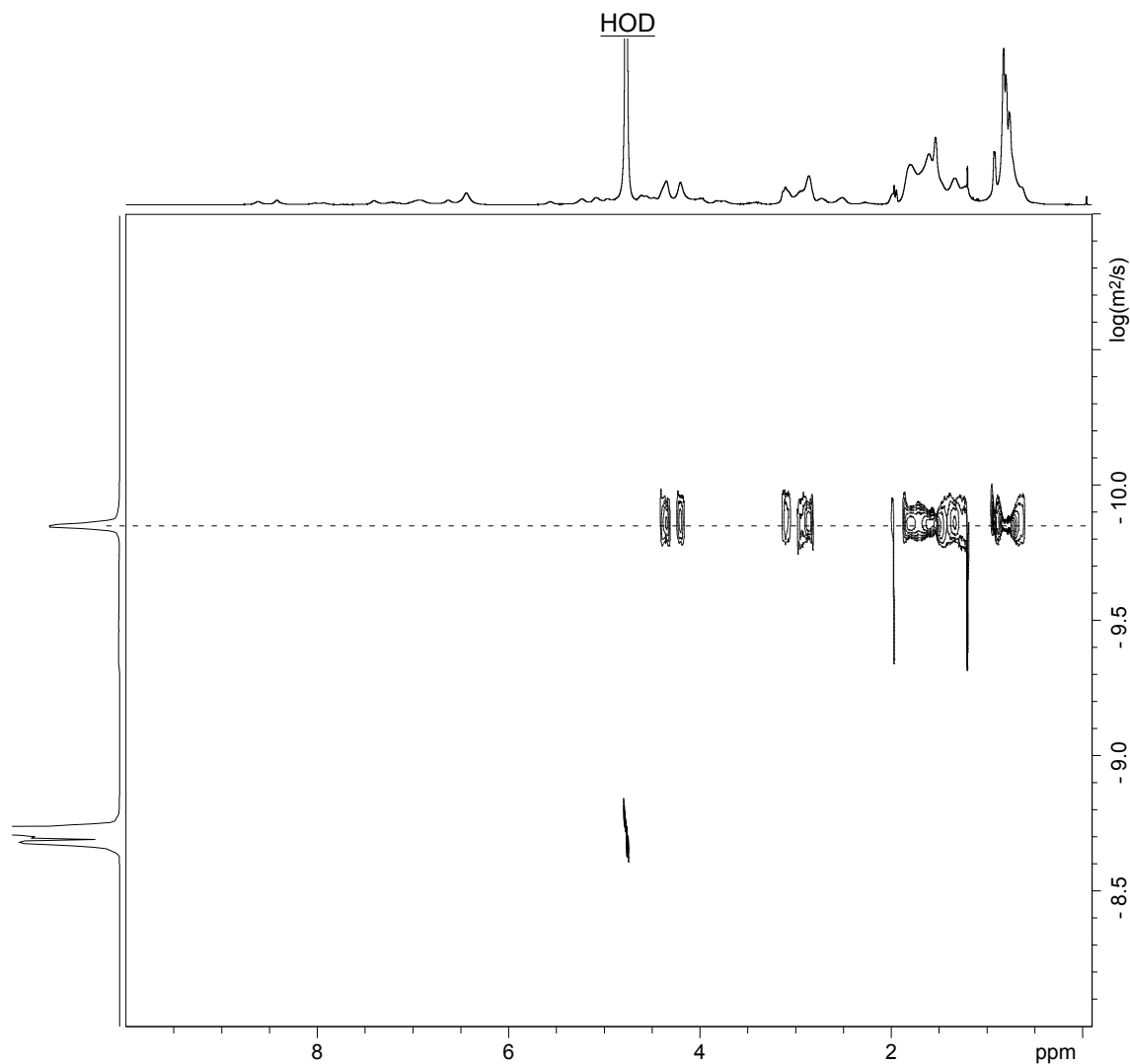
$$D_{\text{HOD}} = 19.0 \times 10^{-10} \text{ m}^2/\text{s} \text{ }^a$$

$$\log(D_{\text{HOD}}) = -8.721$$

$$D_{\text{monomer}} : \log(D) = -9.759; D = 10^{-9.759} = 17.4 \pm 1.2 \times 10^{-11} \text{ m}^2/\text{s}$$

^aLongworth, L. G. *J. Phys. Chem.* **1960**, *64*, 1914–1917.

^1H NMR DOSY of macrocyclic β -sheet peptide **1Cit** at 500 MHz and 298 K
8 mM in 100 mM deuterioacetate buffer in D_2O



Calculations for macrocyclic β -sheet peptide **1Cit** at 8 mM

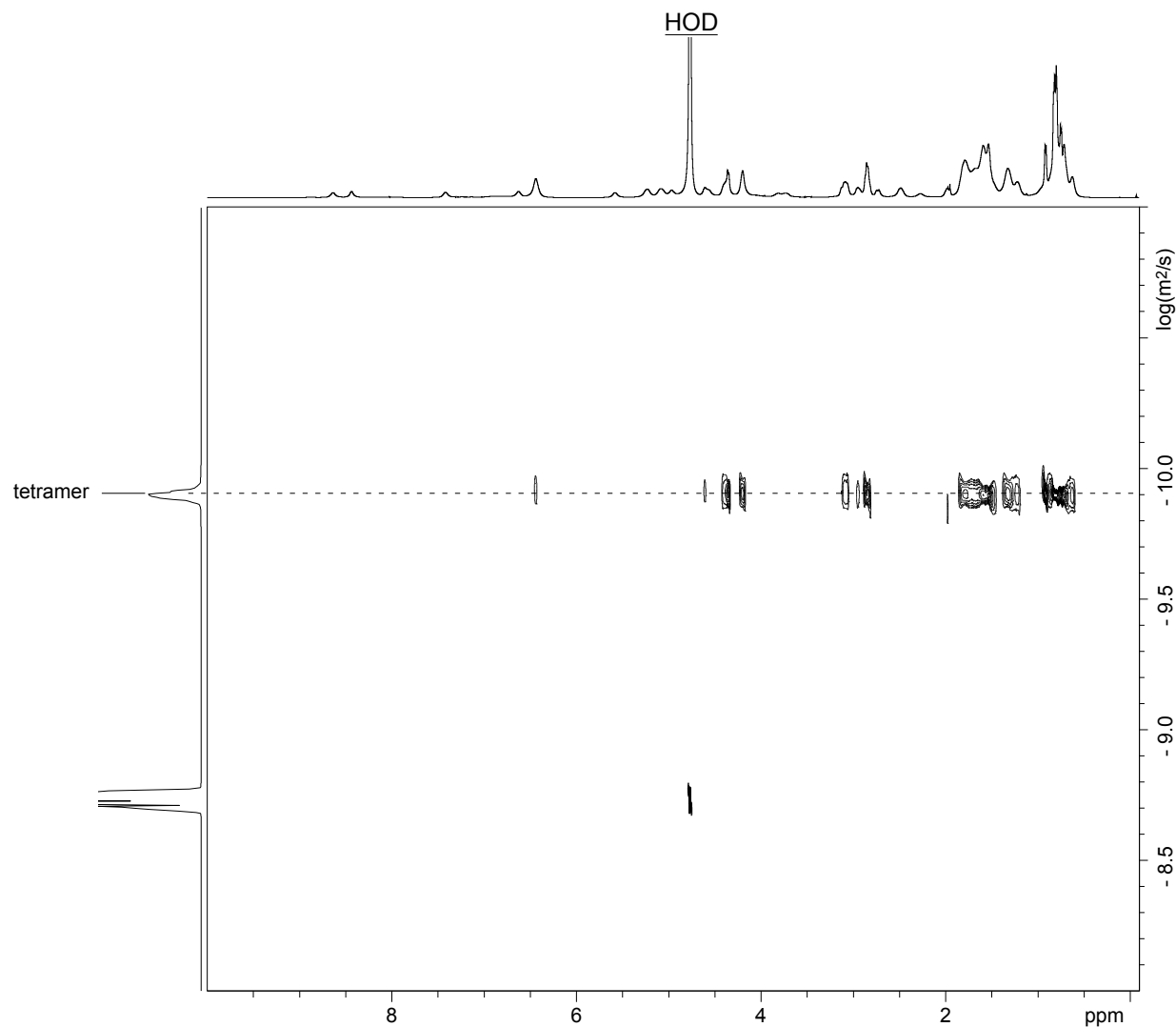
$$D_{\text{HOD}} = 19.0 \times 10^{-10} \text{ m}^2/\text{s} \text{ }^a$$

$$\log(D_{\text{HOD}}) = -8.721$$

$$D_{\text{monomer}} : \log(D) = -9.849; D = 10^{-9.849} = 14.2 \pm 0.3 \times 10^{-11} \text{ m}^2/\text{s}$$

^aLongworth, L. G. *J. Phys. Chem.* **1960**, *64*, 1914–1917.

^1H NMR DOSY of macrocyclic β -sheet peptide **1Cit** at 500 MHz and 298 K
16 mM in 100 mM deuterioacetate buffer in D_2O



Calculations for macrocyclic β -sheet peptide **1Cit** at 16 mM

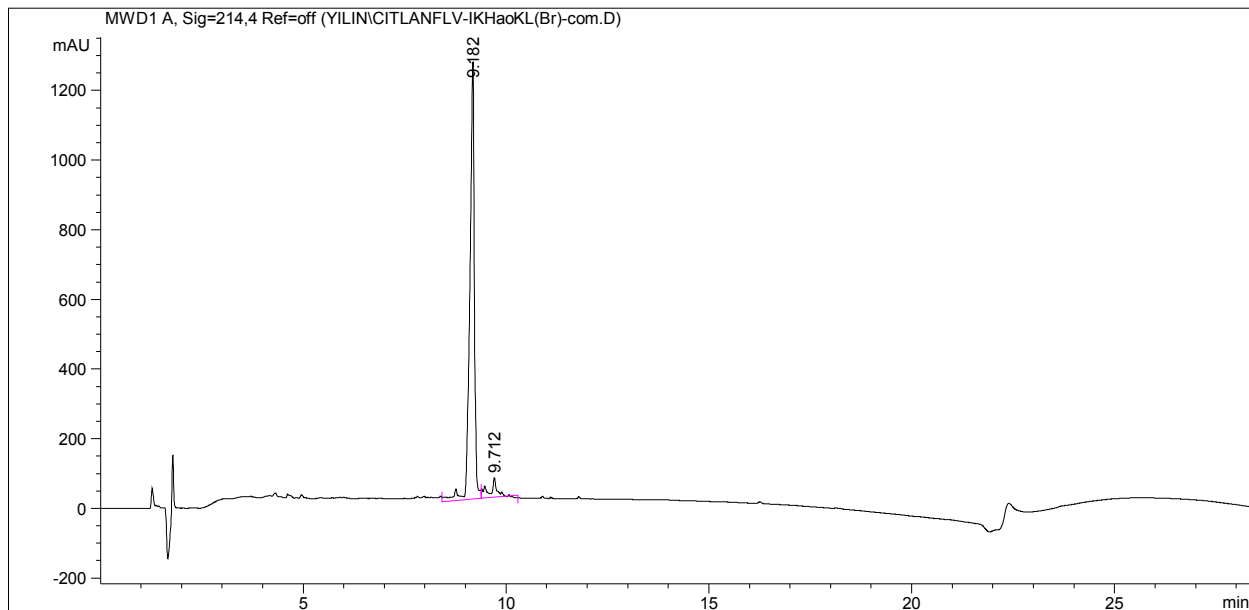
$$D_{\text{HOD}} = 19.0 \times 10^{-10} \text{ m}^2/\text{s} \text{ }^a$$

$$\log(D_{\text{HOD}}) = -8.721$$

$$D_{\text{monomer}} : \log(D) = -9.905; D = 10^{-9.905} = 12.4 \pm 0.3 \times 10^{-11} \text{ m}^2/\text{s}$$

^aLongworth, L. G. *J. Phys. Chem.* **1960**, *64*, 1914–1917.

RP-HPLC of Macrocytic β -Sheet **2**_{Cit}



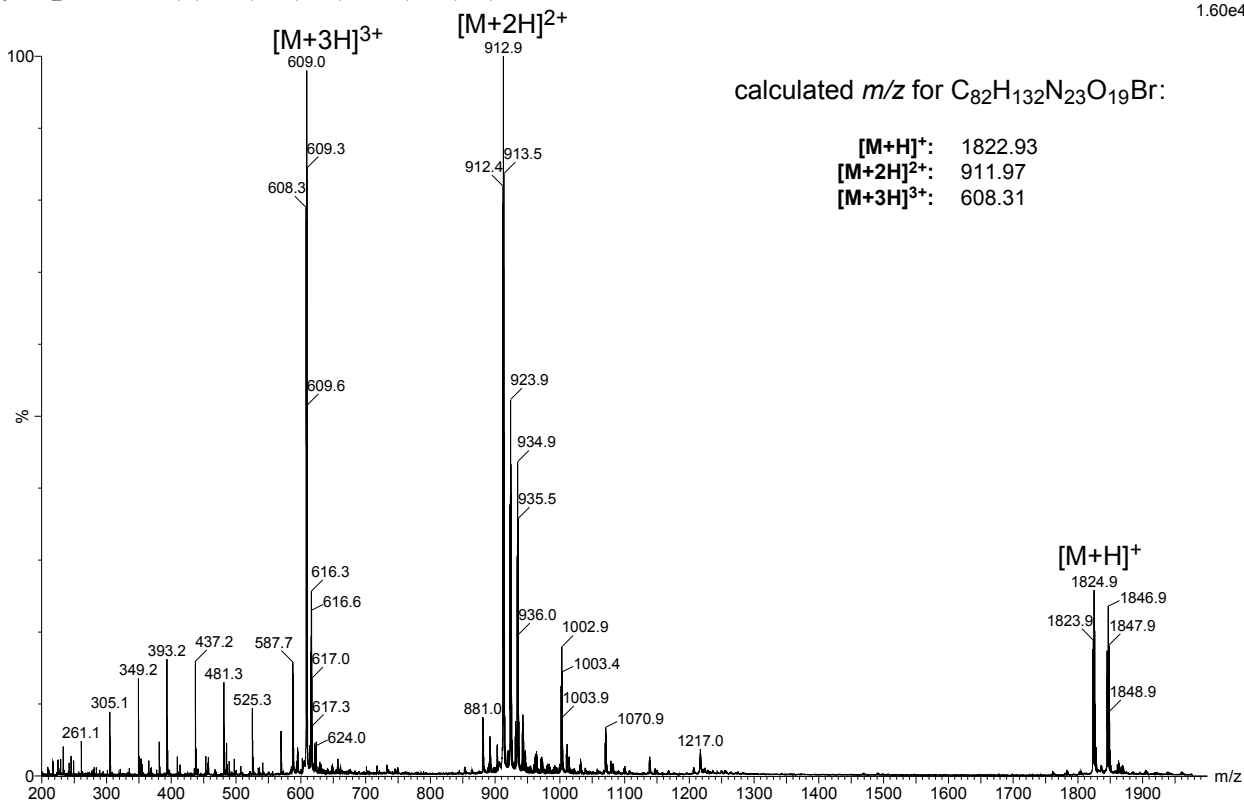
Peak #	RetTime [min]	Type	Width [min]	Area mAU*s	Height [mAU]	Area %
1	9.182	MF	0.1294	9766.9707	1258.4011	93.6334
2	9.712	FM	0.1955	664.1050	56.6224	6.3666

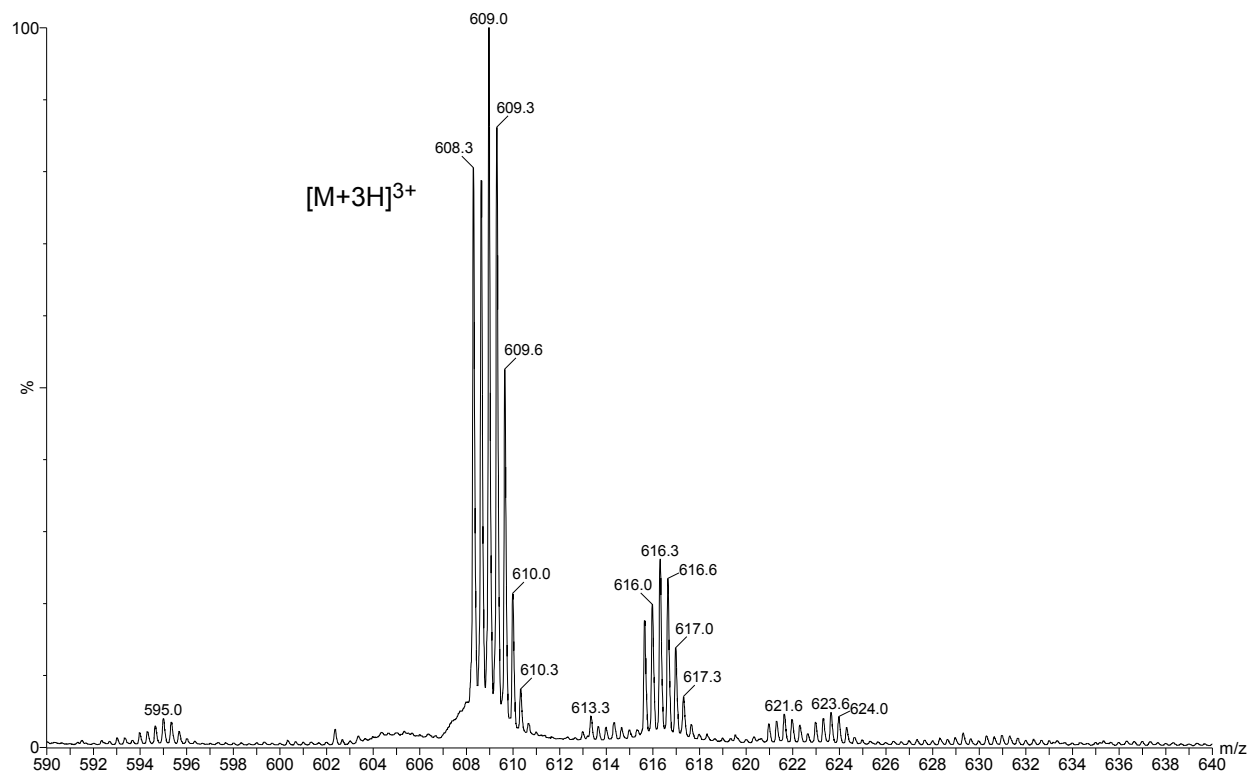
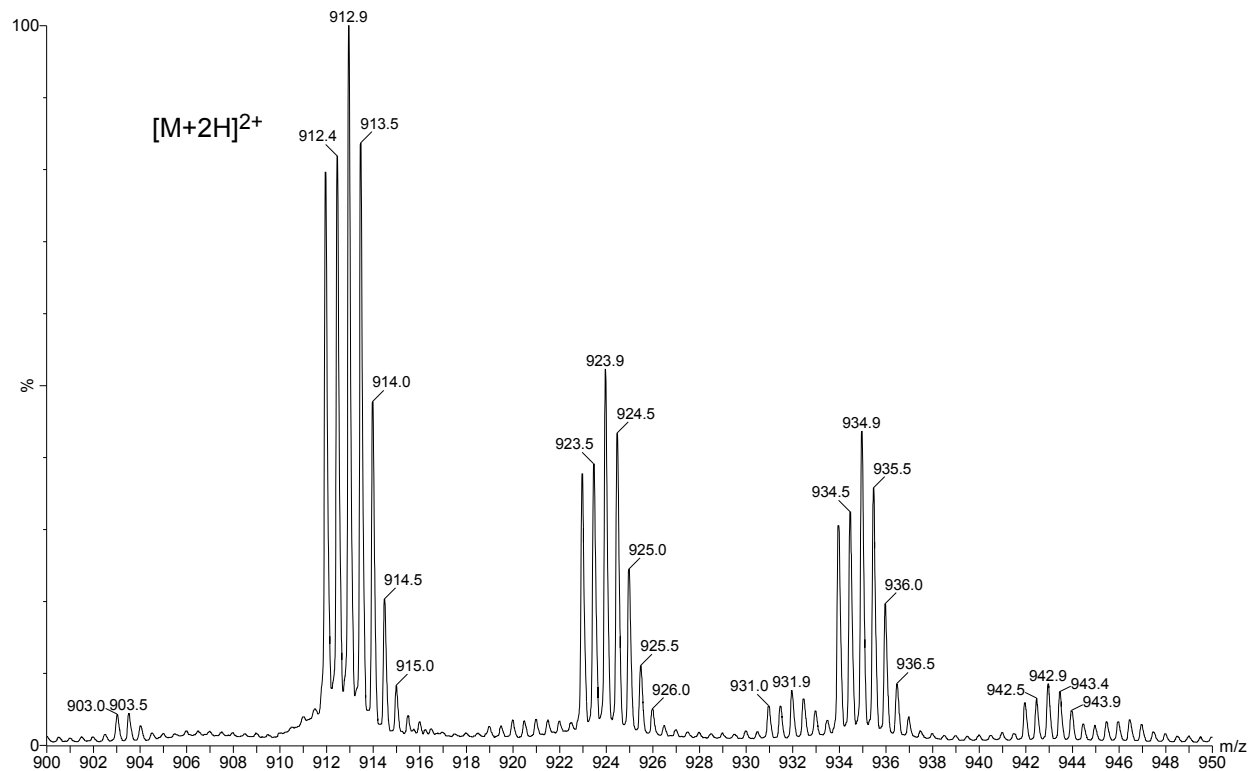
column: Aeris XB-C18 2.6 μ
dimensions: 150 mm x 4.6 mm
mobile phase: A: H₂O, 0.1% TFA
 B: CH₃CN, 0.1% TFA
gradient: A/B (95:5) to (0:100) in 20 min
flow rate: 1.0 mL/min
detection: VWD, wavelength = 214 nm
temperature: 298 K

MS (ESI) of Macrocytic β -Sheet **2**_{Cit}

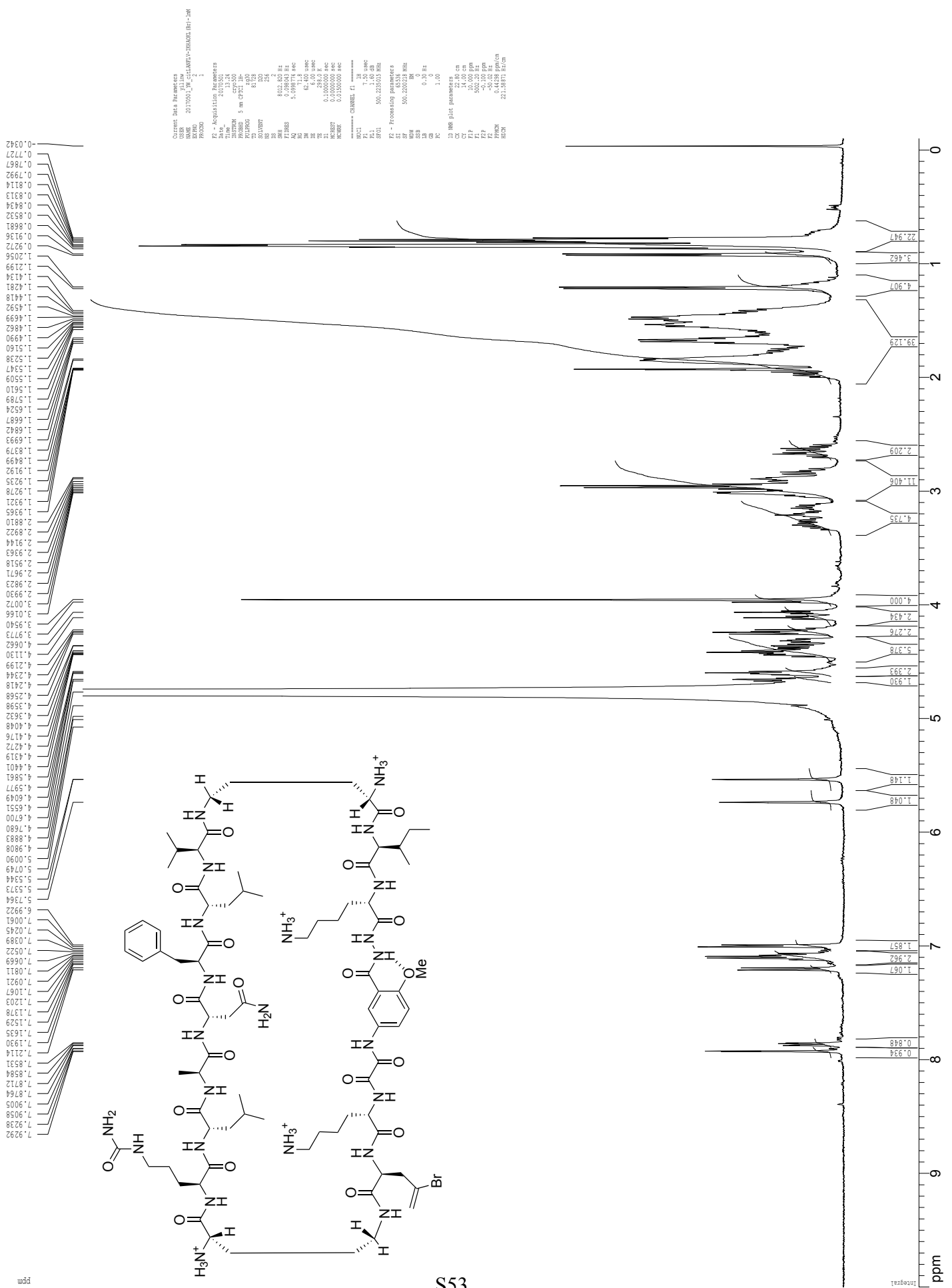
yilinw9_cittanflv-ikhaokl(br)-1 20 (0.367) Sm (Md, 3.00); Cm (2:55)

TOF MS ES+
1.60e4

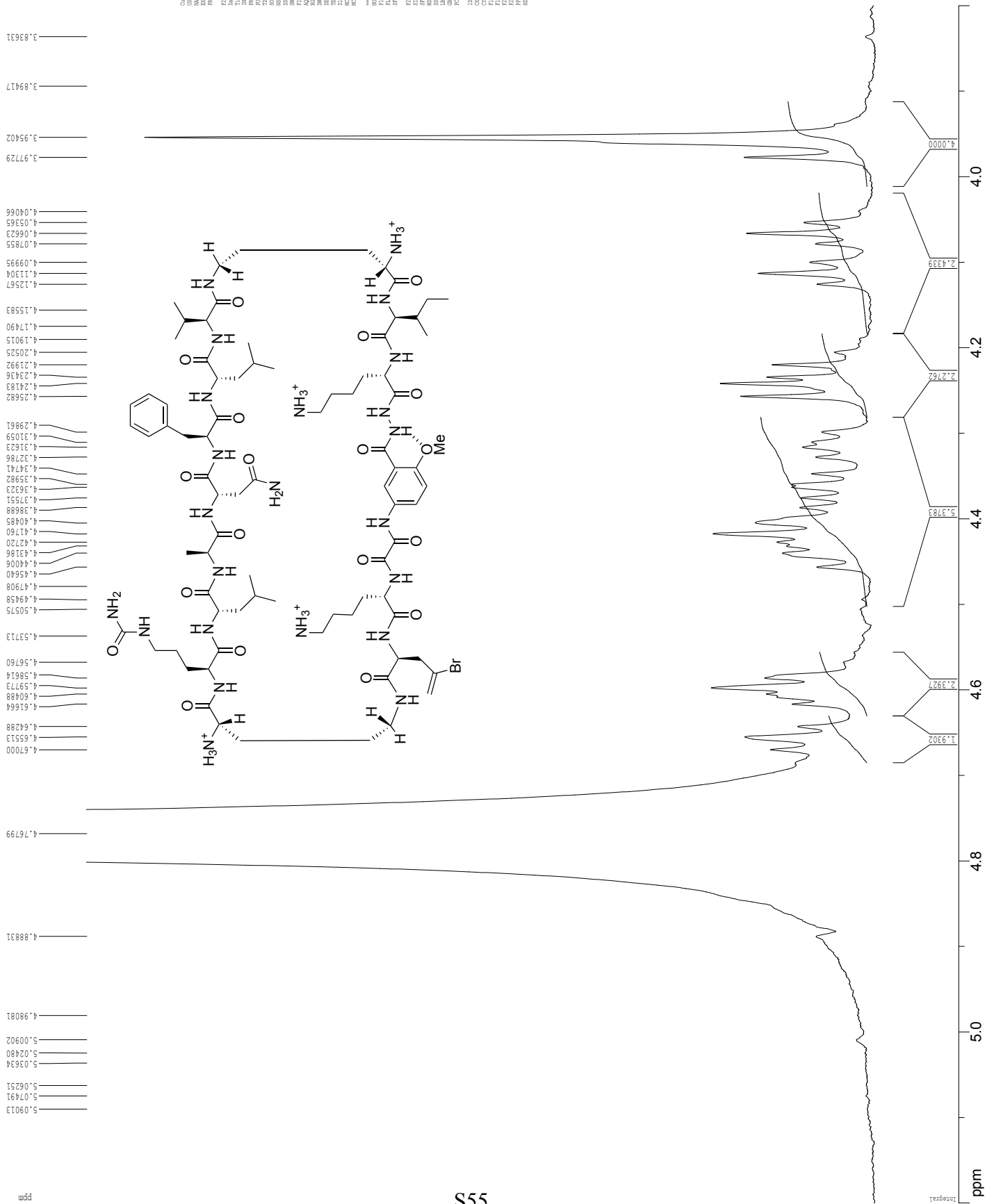




¹H NMR of macrocyclic β-sheet peptide 2cit, 1 mM in 100 mM deuterioacetate buffer in D₂O at 500 MHz and 298 K

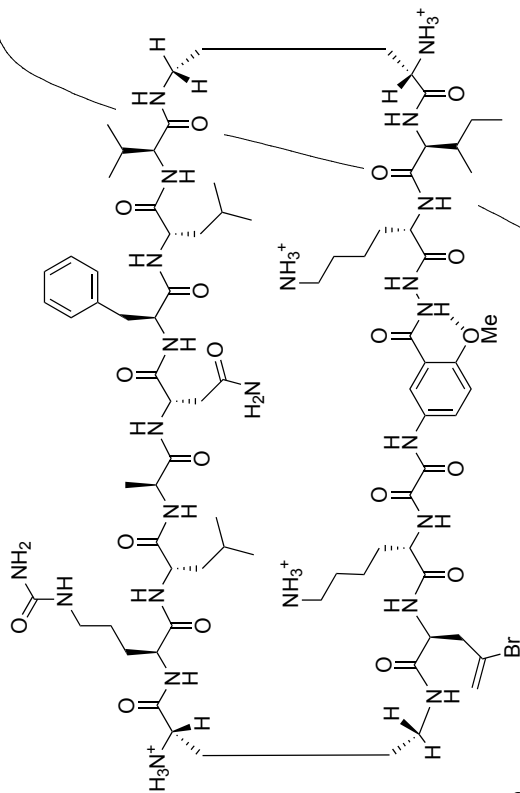
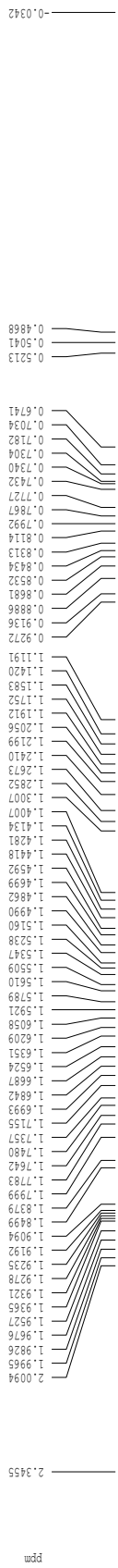


¹H NMR of macrocyclic β-sheet peptide 2cit, 1 mM in 100 mM deuterioacetate buffer in D₂O at 500 MHz and 298 K



Current Date Parameters
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 F2 - Acquisition Parameters
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 Time_ 10:00:00
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 PROCNO 1
 F2PRG1 2D
 AQ 300
 F2 300 MHz
 P1 12.00
 PL1 0.00
 SFO1 500.1362610 MHz
 F2 - Processing parameters
 SI 32768
 SF 500.1362610 MHz
 W 65536
 LB 3.00
 GB 0
 PC 1.00
 TO 088 plot parameters
 CX 22.80 cm
 CY 1.00 cm
 F1 5.2000 ppm
 F2 2601.14 Hz
 F3 1000.54 Hz
 F4 1000.54 Hz
 F5 1000.54 Hz
 F6 1000.54 Hz
 F7 1000.54 Hz

¹H NMR of macrocyclic β-sheet peptide 2cit, 1 mM in 100 mM deuterioacetate buffer in D₂O at 500 MHz and 298 K



Current Data Parameters
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 NAME 2017001_W_CITLMBL100MMADEUHEI-2M
 PROBN 1
 F2 - Acquisition Parameters
 Date_ 20171001
 Time 08:57:00
 INSTRUM cpd500
 PROCESSOR 2.0.10
 PULPROG zgpg30
 ACQPROG 300
 F2 - Processing parameters
 SI 32768
 SF 500.1362618 MHz
 DS 4
 AS 32
 SC 0.30 Hz
 RC 1.00
 10 NMR pit parameters
 CR 22.80 cm
 PI 1.500 ppm
 F1 120.15 Hz
 F2 -50.02 Hz
 SFO 0.714364 ppm/cm
 SFO2 0.714364 ppm/cm

