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Supporting Information

Streamlined Construction of Peptide Macrocycles via Palladium-catalyzed Intramolecular S-Arylation in Solution and on DNA

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1. Reagents & Instruments

Unless otherwise noted, chemicals were purchased from Sigma Aldrich, *J&K* Chemical, or Energy Chemical and were used without further purification. Protected Fmoc-amino acids and coupling reagents were purchased from Bidepharm and Shanghai Haohong Scientific Co. TLC were performed on silica gel Huanghai HSGF254 plates and visualization of the developed chromatogram was performed by fluorescence quenching of UV fluorescence (λ_{max} = 254 nm). Flash chromatography was performed using Silica gel (200-300 mesh) purchased from Qingdao Haiyang Chemical. Rink-AM amide resin (0.667 mmol/g) and 2-Cl-Trt resin (0.99 mmol/g) were purchased from Tianjin Nankai HECHENG. Pd-G_3-XantPhos (98%, Ark Pharm.) was used in the Pd-catalyzed intramolecular S-arylation.

NMR spectra were recorded on Bruker AVANCE AV 400 instruments. UPLC-MS analyses were performed with a Dionex UltiMate 3000 connected to a thermo scientific MSQ PLUS mass spectrometer using Thermo Scientific Hypersil GOLD C18 (1.9 μm, 2.1 × 100 mm) or Acclaim RSLC 120 C18 (2.2 μm, 2.1 × 100 mm) UPLC analytical column. Linear gradients using A: H_2O (0.1% HCOOH) and B: MeCN (0.1% HCOOH) were run over varying periods of time. High-resolution mass spectra (HRMS) were recorded on a Thermo Q Exactive Focus using ESI. Heating reactions were performed by heating blocks which purchased from Boost Tech. Co., Ltd., Ltd. Semi preparative HPLC was carried out on a Dionex UltiMate 3000 using a Thermo Scientific Hypersil GOLD C18 (5 μm, 21.2 × 150 mm) preparative column. Linear gradients using A: H_2O (0.1% HCOOH or TFA) and B: MeCN (0.1% HCOOH or TFA) were run over varying periods of time. Peptide centrifugation was performed by DM0412 low speed centrifuge purchased from DLAB Scientific Co., Ltd. Peptide freeze drying was achieved by means of VirTis/SP SCIENTIFIC BenchTop Pro.

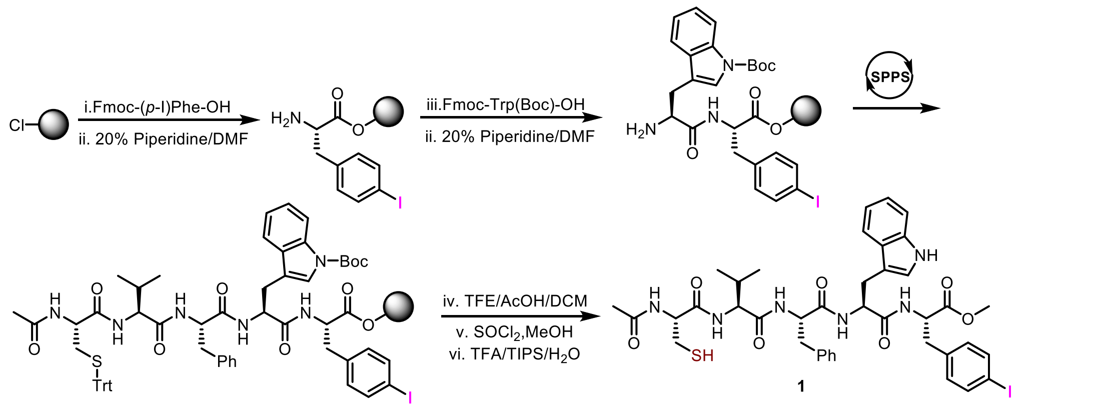
Analysis on DNA was performed by HPLC/ESI-MS. After reaction, an aliquot of the reaction mixture solution was diluted (typically a 1 μL aliquot diluted with 40 μL of water) for LC/MS. Reverse-phase chromatography column (Optimize Opti-Lynx Trap 20 μL, C18AQ-40u) was applied. The sample was eluted [Inject at 4%B, step 90%B at

0.1 min., 1 mL/min flow rate; Solvent A: 0.75%v/v hexafluoroisopropanol (HFIP)/0.038% v/v triethylamine /5 μM EDTA in deionized water; Solvent B: 0.75% v/v HFIP/ 0.038% triethylamine /5 μM EDTA in 90/ 10 methanol/ deionized water] with detection at UV 260 nm.

2. Preparation of linear peptide

All the linear peptides obtained in this work were synthesized following the reported SPPS procedures[1].

Peptide **1** is taken as an example to give the detailed operation:



i) 2-Cl-Trt resin loading; ii) Fmoc group deprotection; iii) Amino acids coupling; iv) 2-Cl-Trt resin cleavage; v) Methyl esterification; vi) removal of PGs.

Scheme S1. Synthesis of linear peptide 1

Preparation of linear peptides 1 from 2-Cl-Trt resin:

2-Chlorotrityl chloride resin (1 g, 0.99 mmol, 1.0 equiv) was swelled in 1% DI-PEA/DCM for 10 min before added into a 25 mL peptide synthesis tube. After sucking the solvent under vacum, a solution of the Fmoc-(*p*-I)Phe-OH (620 mg, 1.2 mmol, 1.2 equiv) and DIPEA (1.1 mL, 6.0 mmol, 6.0 equiv) in DCM (20 mL) was added. The tube was capped and shaken for 1 h at room temperature, then DIPEA (0.53 mL, 3.0 mmol, 3.0 equiv) and MeOH (1 mL) were added. The mixture shaken for another 20 minutes. The tube was then drained, rinsed with CH_2Cl_2 (15 mL). The resin was treated with 20% piperidine/DMF (15 mL) for 10 minutes followed by thorough washing with DMF (10 mL) and DCM (10 mL), which was performed twice. A solution of Fmoc-Trp (Boc)-OH (1.58 g, 3.0 mmol, 3.0 equiv) and Oxyma (0.43 g, 1.8 mmol, 3 equiv) in NMP (15 mL) followed by DIC (0.51 mL, 3.3 mmol, 3.3 equiv) were added to the resin and the mixture was shaken for 1 h at room temperature. The resin was then drained and rinsed with DMF (2 x 10 mL) and DCM (2 x 10mL). Repeating the coupling and deprotection steps, peptide chain can be elongated with Phe, Val and Cys successively. After the completion of peptide elongation, the resin was treated with a solution of TFE/AcOH/DCM (20 mL, 1/1/3, v/v/v) twice for 1 h each time. The combined solvent was concentrated *in vacuo* to give the peptide with a free carboxylic acid group which was treated with the $SOCl_2$ (0.37 mL, 5.0 mmol, 5.0 equiv) in MeOH (25 mL) at 0 ^oC. The solution was gradually warmed to room temperature and stirred for 3 hours. After removing the solvent under vacuum, and the mixture was added the cocktails of TFA/ H_2O/TIPS (95:2.5:2.5) for 1 hours. Then the solvents were evaporated at 30 ^oC and the crude peptide was precipitated by the addition of cold diethyl ether. After centrifugation the supernatant was taken out to give the crude peptide which was dried under vacuum. Finally got 786 mg white solid in 90% yield. All of the products were pure enough for next cyclization step. For peptides that are not methylated at the C-terminus, Mmt protected Cys can be used. Mmt can be removed using DCM/TES/TFA (95:3:2).

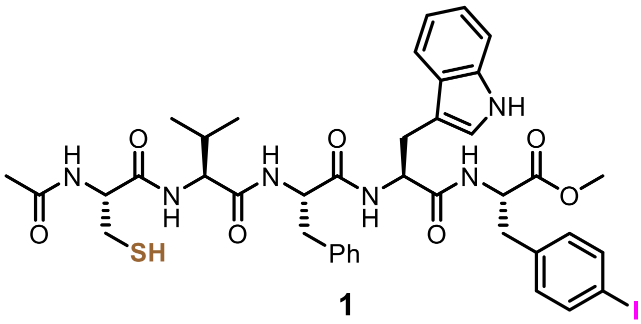
Preparation of linear peptides from Rink-amide AM resin:

Rink-amide AM resin (1.0 equiv) was swelled in DCM for 10 min and then was added into a peptide synthesis tube. After sucking the solvent under vacuum, a solution of 20% piperidine in DMF was added and the tube was capped and shaken for 25 min (15 min + 10min). The tube was then drained, rinsed with DCM (2 x 10 mL) and DMF (2 x 10 mL). DIC (3.3 equiv) was added to a freshly prepared solution of the first loading Fmoc amino acid (3.0 equiv) and Oxyma (3.0 equiv) in NMP (15 mL) and the solution was stirred under ice-water bath for 5 minutes. Then the clear solution was added to the tube and shaken for 2 h at room temperature. The tube was then drained, the resin was rinsed with DMF (2 x 10 mL), DCM (2 x 10 mL). The amount of amino acid loaded on the resin was then measured by Fmoc determination.

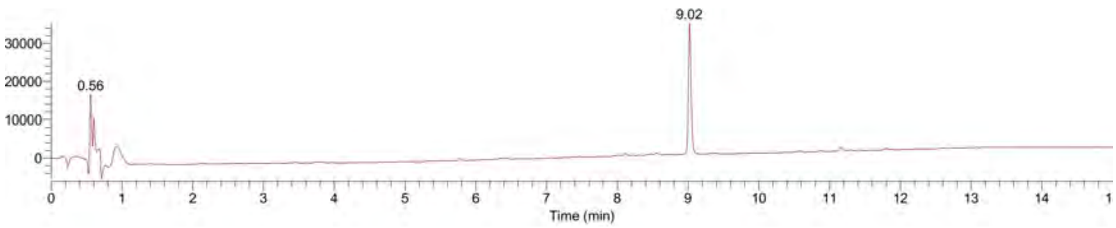
The dry Rink-AM amide resin was treated with a solution of TFA/H_2O/TIPS (95:2.5:2.5) for 2 hours. The solvents were concentrated in vacuo at 30 ^oC and the crude peptide was precipitated by the addition of cold diethyl ether. After centrifugation (5 min, 4000 r/min, 25°C) the supernatant was removed to give the crude peptide which was dried under vacuum. All of the products were used for next step without any purification.

Coupling amino acids in solution:

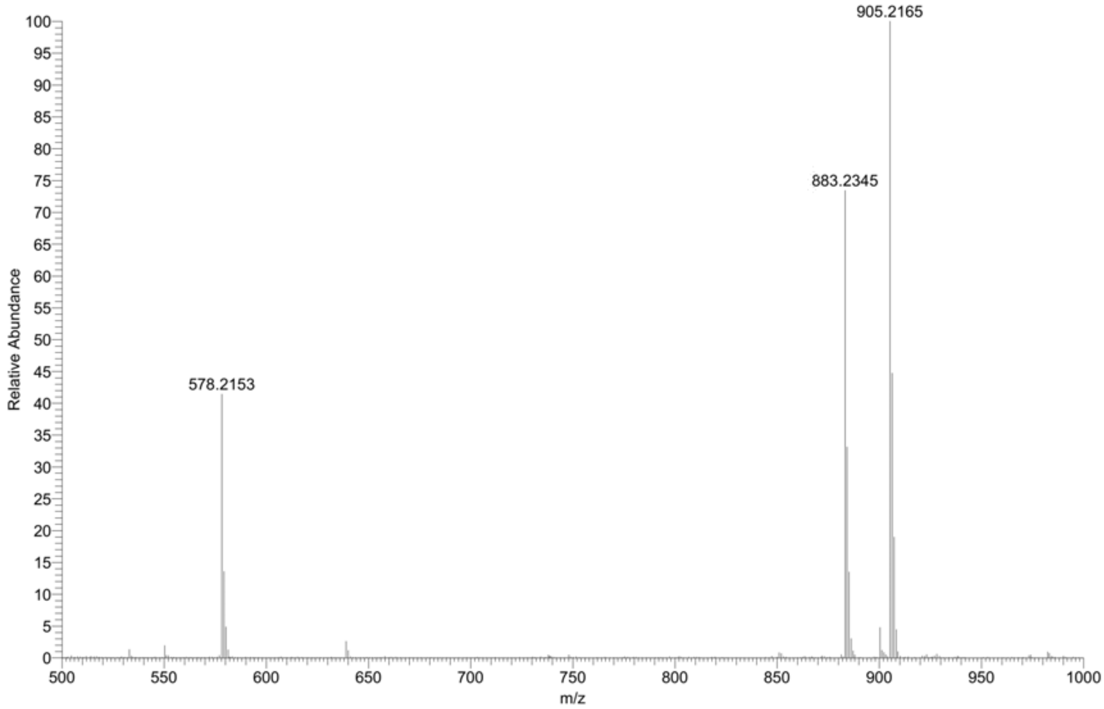
To a solution of the crude peptide (1.0 equiv) prepared from 2-Cl-Trt resin, HOAt (1.0 equiv) and HATU (1.0 equiv) in DMF, the corresponding amino acid derivative (1.1 equiv) and DIPEA (1.1 equiv) were added at 0 °C. Then the reaction mixture was gradually warmed to room temperature and stirred for 6 h. The reaction was quenched with 1 N HCl and extracted with EtOAc. The combined organic phase was sequentially washed with saturated $NaHCO_3$ and brine, dried over anhydrous Na_2SO_4 . The organic phase was concentrated in vacuo, the resulting residue was purified by silica gel flash chromatography to give the desired product.



1



t_R = 9.02 min, 5% to 95% B for 10 min, then 95% B 10-15 min, λ = 254 nm



HRMS: Calcd for $C_{40}H_{47}IN_6O_7S$ [M+H$^+$]:883.2344; found: 883.2345

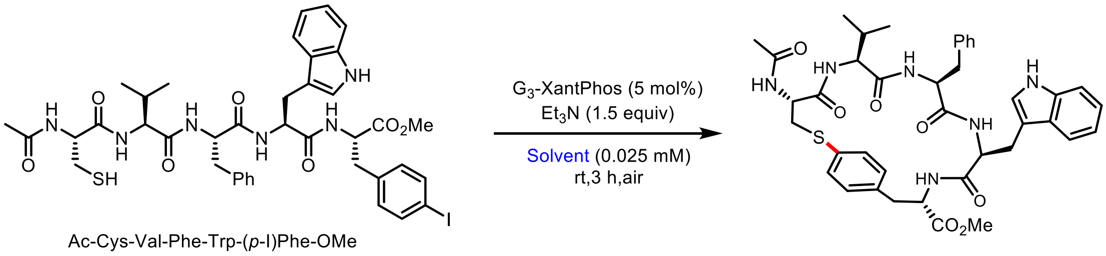
^{1}H NMR (400 MHz, 5%MeOD in DMSO) δ 8.42 (d, *J* = 7.6 Hz, 1H), 8.12 (dd, *J* = 8.0, 3.5 Hz, 1H), 7.96 (d, *J* = 8.0 Hz, 1H), 7.78 (d, *J* = 8.8 Hz, 1H), 7.57 (dd, *J* = 14.0, 8.0 Hz, 3H), 7.32 (t, *J* = 8.0 Hz, 2H), 7.25-7.03 (m, 9H), 7.00-6.95 (m, 2H), 4.57 (dd, *J* = 9.4, 5.4 Hz, 2H), 4.49-4.34 (m, 2H), 4.09 (dd, *J* = 8.8, 6.4 Hz, 1H), 3.57 (s, 3H), 3.06 (dd, *J* = 14.8, 6.0 Hz, 1H), 2.99-2.82 (m, 4H), 2.77-2.65 (m, 2H), 2.64-2.56 (m, 1H), 2.20 (t, *J* = 8.4 Hz, 1H), 1.87 (s, 3H), 0.70 (dd, *J* = 6.9, 2.0 Hz, 6H).

3. Optimization of intramolecular C-S arylation reaction

General procedure for optimization of reaction conditions

The linear peptide **1** (88.2 mg, 0.1 mmol, 1.0 equiv), G_3-XantPhos catalyst **(4.8 mg, 5 mol%)**, base and solvent were added into a 8 mL glass vial according the specific conditions listed below. The vial was sealed with PTFE cap (air and moisture were not vigorously excluded). The reaction mixture was stirred at room temperature. 50 µL of the mixture was taken out. Then 1 mL MeOH was added to dissolve the residue and the insoluble was removed by filtration with filter membrane (0.2 µm), the filtrate was used for LCMS analysis.

Evaluation of different solvents

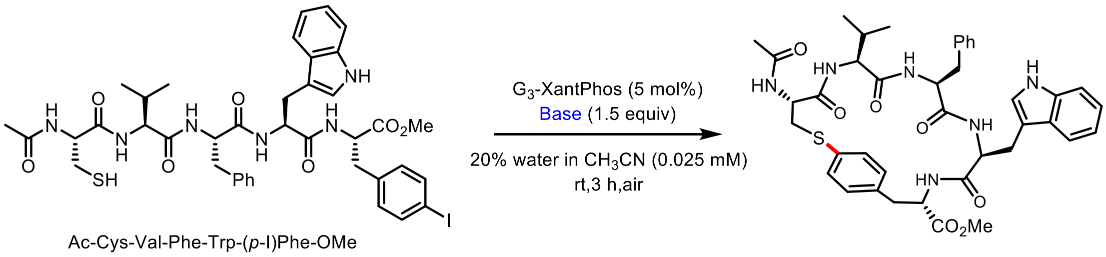


Entry	Solvent	Yield (%)[a]
1	20% water in THF	74
2	40% water in THF	81
3	60% water in THF	66
4	80% water in THF	40
5	water	<10
6	20% water in Acetone	64
7	20% water in CH_3CN	82
8	20% water in dioxane	30
9	20% water in MeOH	<10
10	20% water in EtOH	<10
11	20% water in HFIP	<10

a: LCMS Yield

Scheme S2

Evaluation of different bases



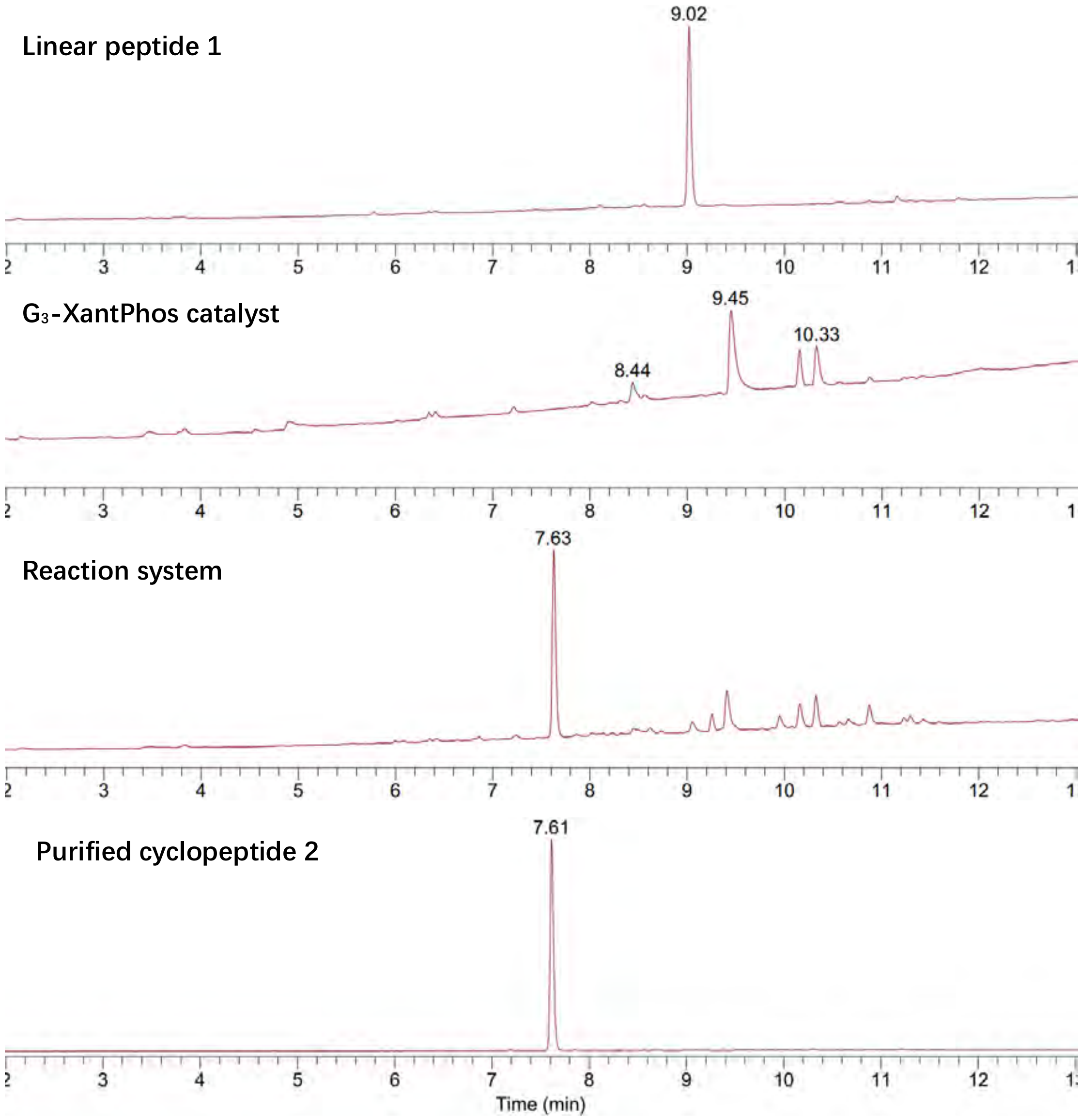
Entry	Base	Yield (%)[a]
1	Et_3N	82
2	4-Methylmorpholine	62
3	TMEDA	57
4	DIPEA	84

5	DMAP	62
6	TEDA	50
7	K_2CO_3	37
8	PhCOOK	42
9	Cs_2CO_3	47

a: LCMS Yield

Scheme S3

The Optimized condition for Pd-catalyzed intramolecular C-S arylation of peptide 1 is: peptide **1** (44.1 mg, 0.05 mmol, 1.0 equiv), G_3-XantPhos catalyst **(2.4 mg, 5 mol%), DIPEA (26.0 μL, 0.15 mmol, 1.5 equiv), in 20% water in Acetonitrile (2 mL), rt, 3 h.**



Scheme S4. HPLC spectrum of the intramolecular C-S arylation reaction of compound **1** under optimal condition.

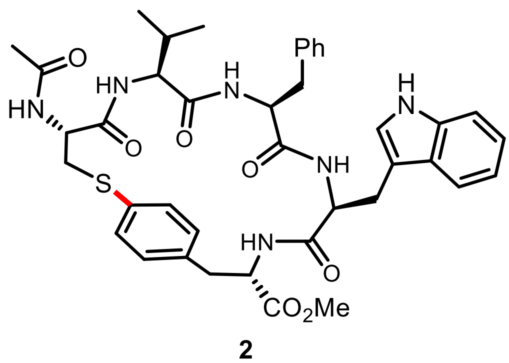
4. General procedure for Pd-catalyzed peptide macrocyclization

General condition A:

A mixture of linear peptide substrate (0.1 mmol, 1.0 equiv), G_3-XantPhos catalyst **(4.7 mg, 5 mol%), and DIPEA (52.0 μL, 0.1 mmol, 1.5 equiv) in 2 mL of 20% water in Acetonitrile was stirred in a 8 mL glass vial (sealed with PTFE cap under air atmosphere) at rt for 3 hours. The reaction mixture was diluted with MeOH (5 mL) and filtered through a pad of celite. The filtrate was concentrated *in vacuo* and the resulting residue was purified by silica gel flash chromatography to give the cyclized product.**

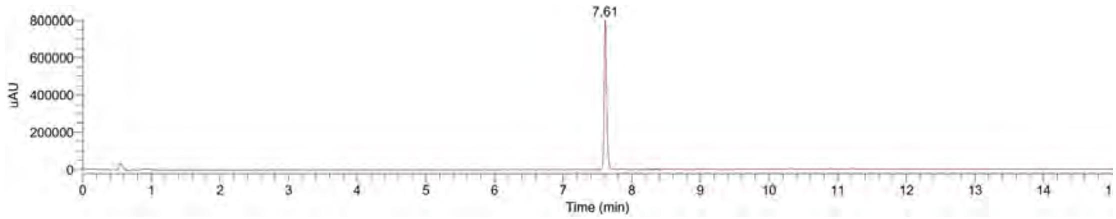
General conditions B (heated at 45 °C):

A mixture of linear peptide substrate (0.1 mmol, 1.0 equiv), G_3-XantPhos catalyst **(4.7 mg, 5 mol%), and DIPEA (52.0 μL, 0.1 mmol, 1.5 equiv) in 2 mL of 20% water in Acetonitrile was heated in a 8 mL glass vial (sealed with PTFE cap under air atmosphere) at 45 °C for 2 hours. After been cooled to room temperature, the reaction mixture was diluted with MeOH (5 mL) and filtered through a pad of celite. The filtrate was concentrated in vacuo and the resulting residue was purified by silica gel flash chromatography to give the cyclized product.**

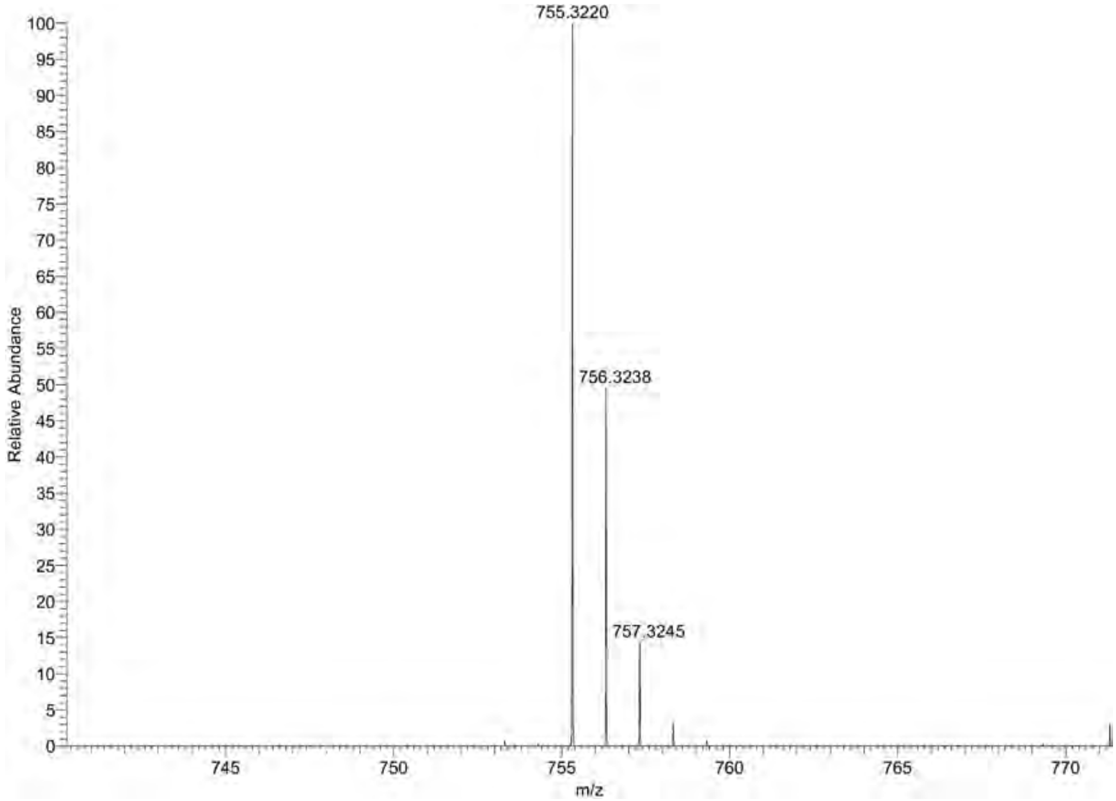


2

Compound **2** was isolated in 72% yield (54 mg) as a white powder under the general condition A.



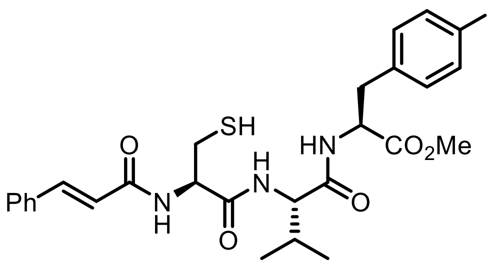
t_R = 7.61 min, 5% to 95% B for 10 min, then 95% B 10-15 min, λ = 254 nm



HRMS: Calcd for $C_{40}H_{46}N_6O_7S$ [M+H$^+$]:755.3221; found: 755.3220

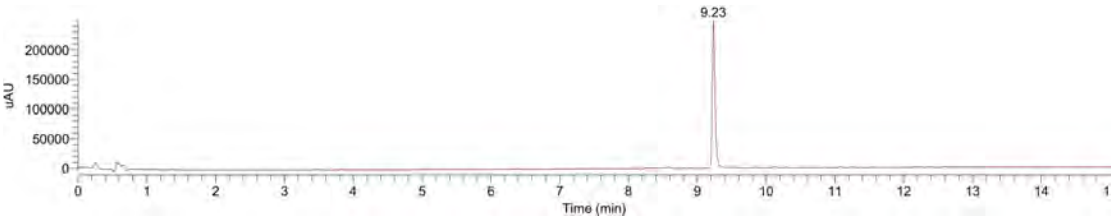
^{1}H NMR (400 MHz, CD_3Cl) δ 7.42 (d, *J* = 7.8 Hz, 1H), 7.32 (dd, *J* = 10.8, 8.2 Hz, 3H), 7.23-7.14 (m, 4H), 7.08 (dd, *J* = 23.6, 7.8 Hz, 3H), 7.00-6.89 (m, 3H), 6.78 (d, *J* = 6.8 Hz, 1H), 6.61-6.54 (m, 2H), 6.15 (d, *J* = 7.6 Hz, 1H), 4.78 (t, *J* = 10.8 Hz, 1H), 4.64-4.48 (m, 2H), 4.23-4.16 (m, 1H), 3.98 (t, *J* = 6.4 Hz, 1H), 3.77 (s, 3H), 3.46 (dd, *J* = 13.8, 4.7 Hz, 1H), 3.38-3.20 (m, 2H), 3.12 (dd, *J* = 14.0, 7.8 Hz, 1H), 2.92 (m, 1H), 2.83 (dd, *J* = 14.2, 10.0 Hz, 1H), 2.56 (dd, *J* = 13.8, 7.2 Hz, 1H), 2.38-2.27 (m, 1H), 2.24-2.13 (m, 1H), 2.09 (s, 3H), 0.84 (d, *J* = 6.8 Hz, 3H), 0.72 (d, *J* = 6.8 Hz, 3H).

^{13}C NMR (101 MHz, DMSO) δ 174.27, 172.15, 171.50, 170.33, 170.15, 169.49, 137.62, 136.04, 135.23, 133.68, 130.12, 129.89, 129.61, 129.17, 127.87, 127.14, 126.11, 123.45, 120.92, 118.39, 118.18, 111.30, 109.84, 58.77, 53.53, 53.06, 52.37, 52.17, 52.07, 35.08, 31.24, 29.65, 26.52, 25.07, 22.29, 22.05, 18.94, 17.50, 13.90.

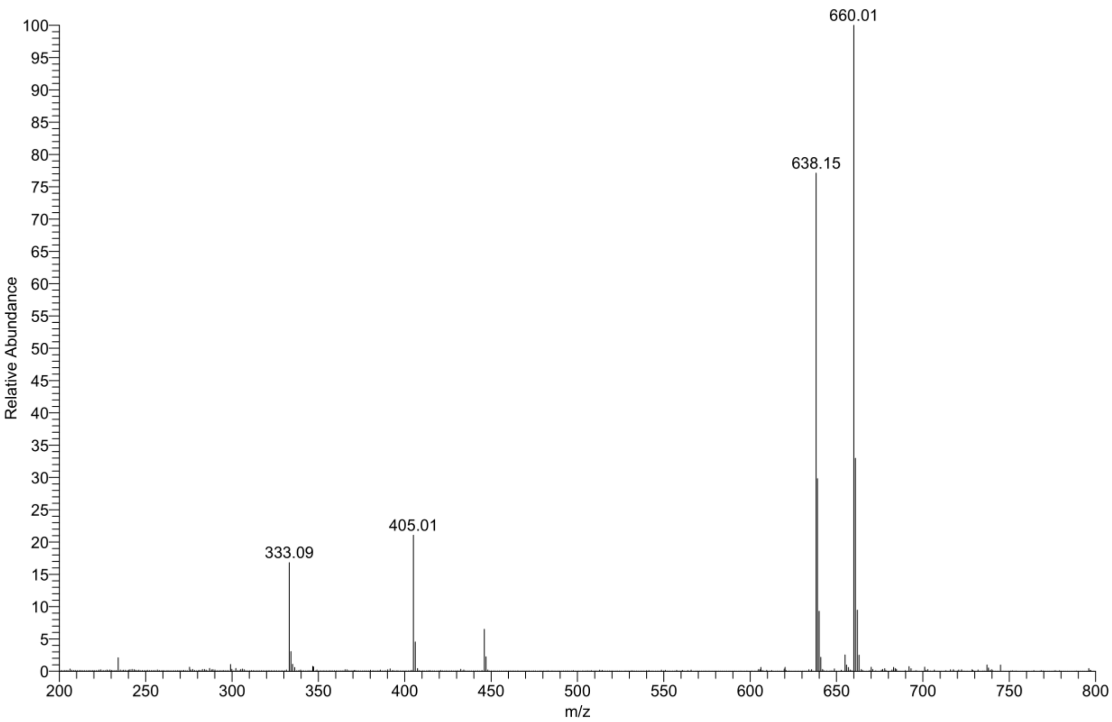


S3

Compound **S3** was prepared as a white solid in 92% yield from 2-Cl-Trt resin following the SPPS procedure.

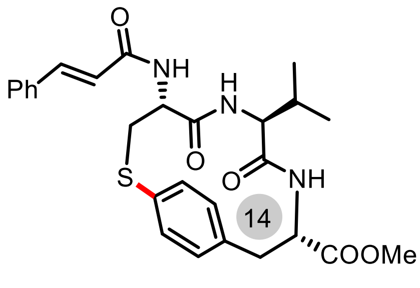


t_R = 9.23 min, 5% to 95% B for 10 min, then 95% B 10-15 min, λ = 254 nm



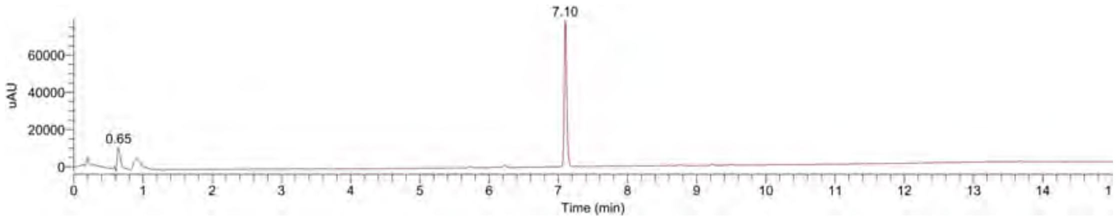
LRMS: $[M+H]^+$ 638.15; $[M+Na]^+$ 660.01.

^{1}H NMR (400 MHz, AcOD) δ 7.77-7.56 (m, 5H), 7.43-7.38 (m, 3H), 7.04-6.96 (m, 2H), 6.76 (d, J = 15.8 Hz, 1H), 4.94 (dd, J = 7.4, 5.2 Hz, 2H), 4.43 (d, J = 8.0 Hz, 1H), 3.77 (s, 3H), 3.23-3.16 (m, 1H), 3.14-2.98 (m, 2H), 2.98-2.84 (m, 2H), 0.97-0.90 (m, 6H).

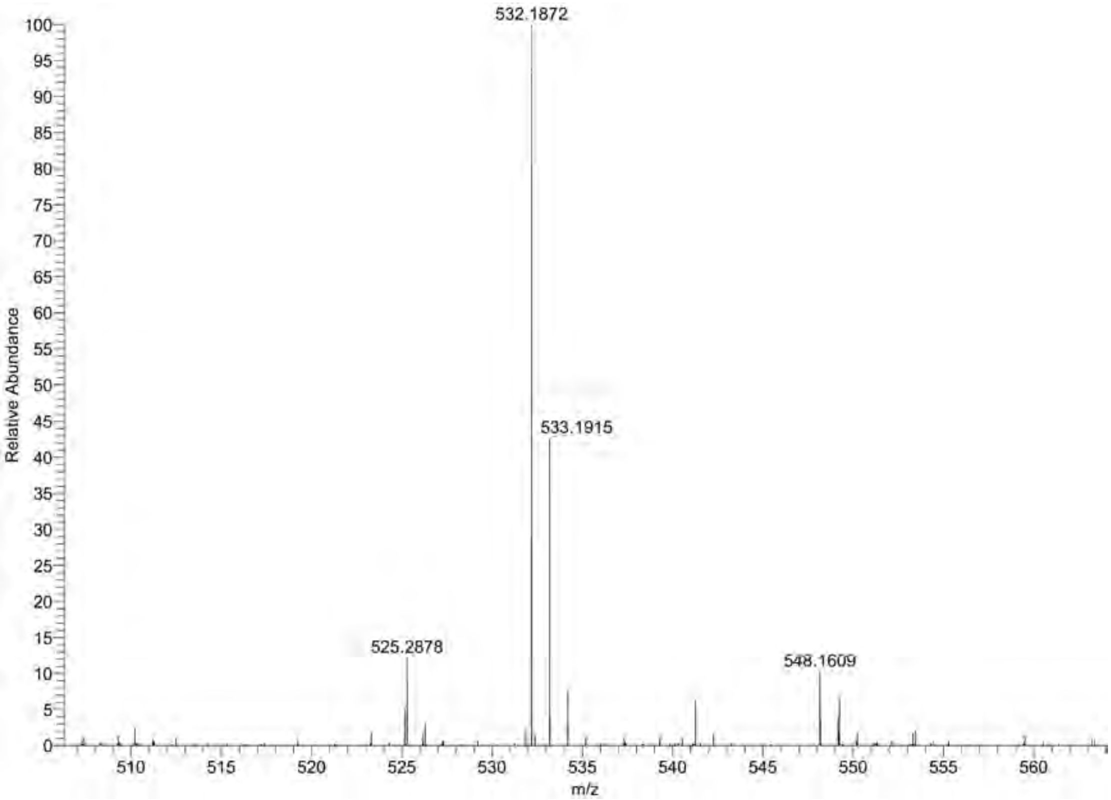


3 (25%)

Compound **3** was isolated in 25% yield (13 mg) as a white powder under the general condition A.



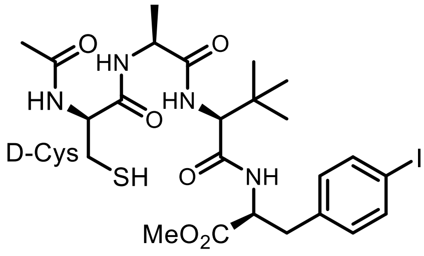
t_R = 7.10 min, 5% to 95% B for 10 min, then 95% B 10-15 min, λ = 254 nm



HRMS: Calcd for $C_{27}H_{31}N_3O_5S$ [M+Na$^+$]: 532.1877; found: 532.1872

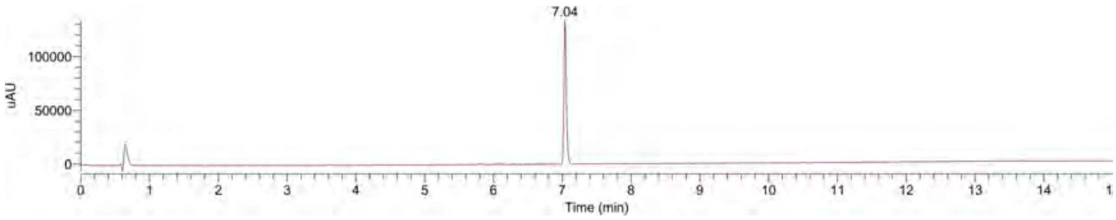
^{1}H NMR (600 MHz, AcOD) δ 7.40 (t, *J* = 11.4 Hz, 4H), 7.27-7.20 (m, 3H), 7.18-7.11 (m, 3H), 6.96 (d, *J* = 8.0 Hz, 1H), 5.44 (d, *J* = 4.4 Hz, 1H), 5.38 (d, *J* = 5.0 Hz, 2H), 3.82 (s, 3H), 3.67 (d, J = 4.4 Hz, 1H), 3.61 (d, J = 16.4 Hz, 1H), 3.49 (d, J = 21.0 Hz, 3H), 1.47 (d, J = 12.8 Hz, 1H), 0.81 (dd, J = 30.2, 6.4 Hz, 6H).

^{13}C NMR (101 MHz, DMSO) δ 174.63, 171.28, 169.60, 167.45, 139.08, 136.82, 134.85, 129.47, 128.68, 127.51, 122.01, 57.20, 53.59, 52.04, 51.92, 35.13, 31.26, 26.55, 25.10.

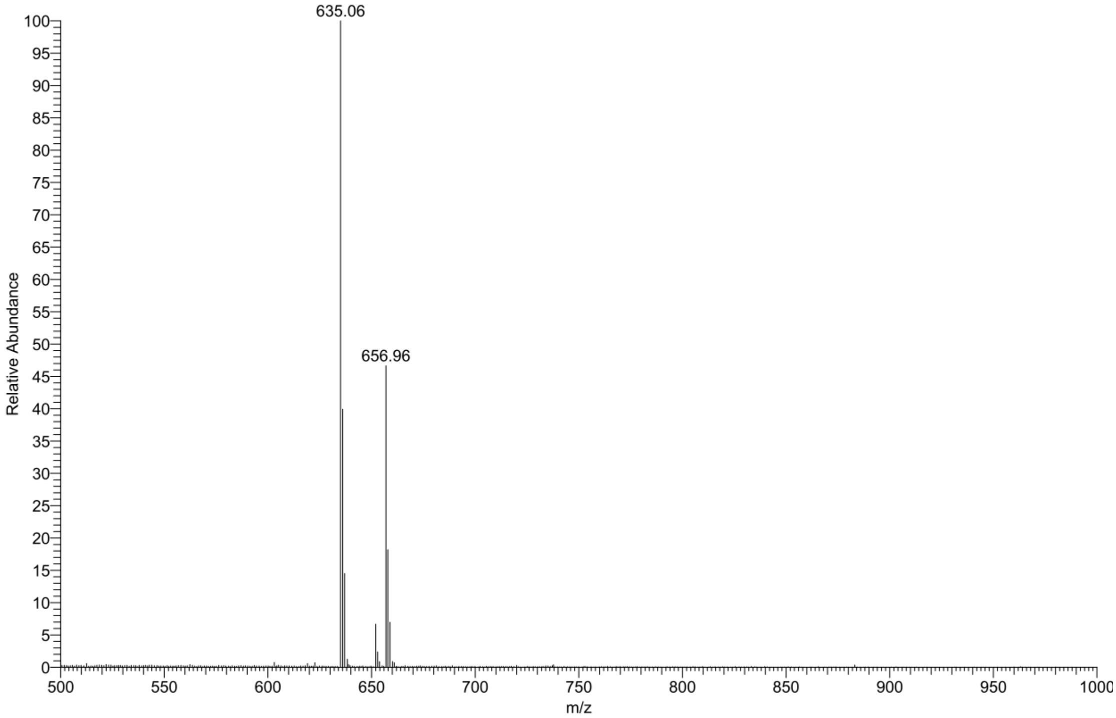


S4

Compound **S4** was prepared as a white solid in 93% yield from 2-Cl-Trt resin following the SPPS procedure.

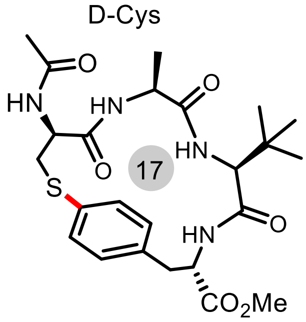


t_R = 7.04 min, 5% to 95% B for 10 min, then 95% B 10-15 min, λ = 254 nm



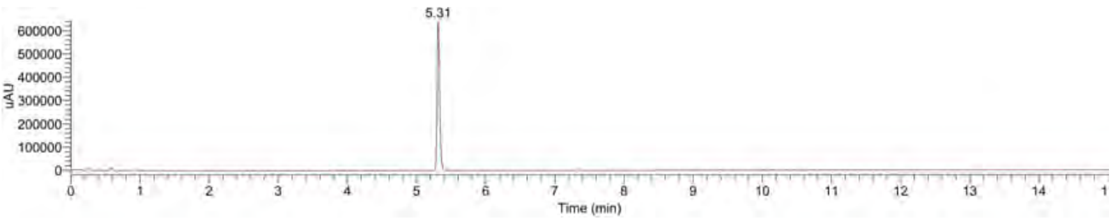
LRMS: [M+H] $^+$ 635.06; [M+Na] $^+$ 656.96.

^{1}H NMR (400 MHz, MeOD) δ 7.62 (d, *J* = 8.0 Hz, 2H), 7.01 (d, *J* = 8.0 Hz, 2H), 4.71 (dd, *J* = 8.8, 5.6 Hz, 1H), 4.53 (t, *J* = 6.4 Hz, 1H), 4.42 (q, *J* = 7.0 Hz, 1H), 4.26 (s, 1H), 3.71 (s, 3H), 3.15 (dd, *J* = 13.8, 5.4 Hz, 1H), 2.94 (dd, *J* = 13.8, 9.0 Hz, 1H), 2.89-2.75 (m, 2H), 2.03 (s, 3H), 1.34 (d, *J* = 7.0 Hz, 3H), 0.98 (s, 9H).

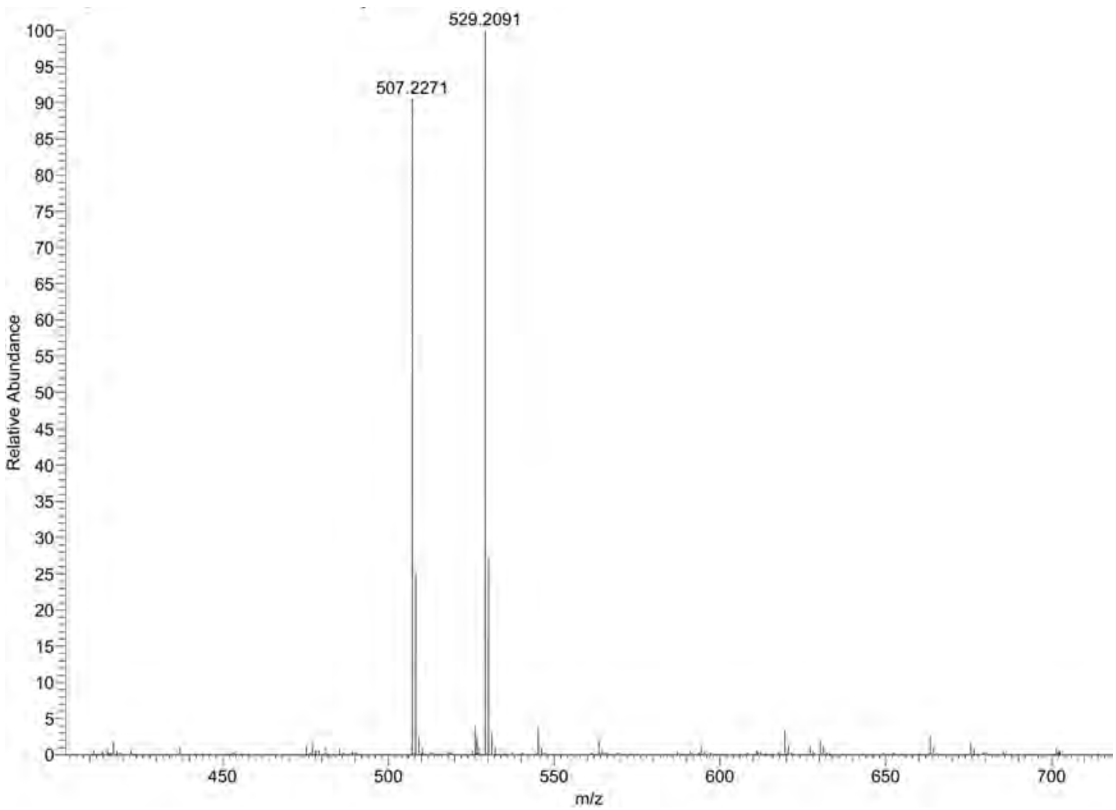


4 (63%)

Compound **4** was isolated in 31% yield (17 mg) as a white powder under the general condition A.



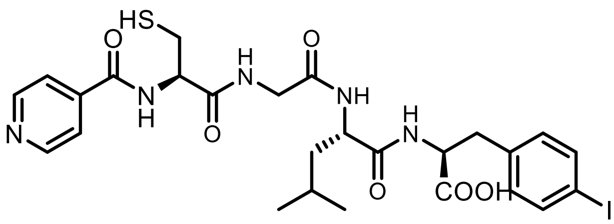
t_R = 5.31 min, 5% to 95% B for 10 min, then 95% B 10-15 min, λ = 254 nm



HRMS: Calcd for $C_{24}H_{34}N_4O_6S$ [M+H$^+$]: 507.2272; found: 507.2271

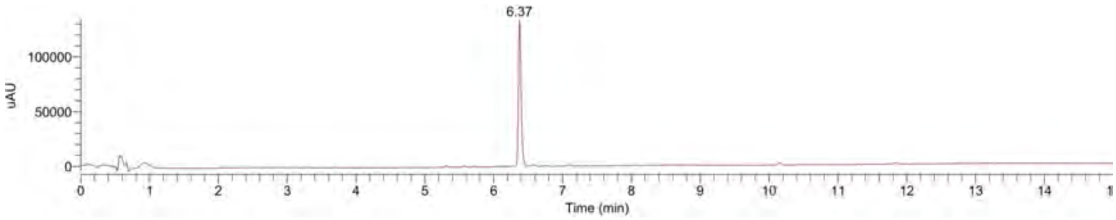
^{1}H NMR (400 MHz, MeOD) δ 7.23 (d, *J* = 8.0 Hz, 2H), 7.06 (d, *J* = 8.0 Hz, 2H), 4.74 (s, 1H), 4.60 (d, *J* = 7.4 Hz, 1H), 4.27 (dd, *J* = 14.8, 7.6 Hz, 1H), 4.23 (d, *J* = 6.4 Hz, 1H), 3.82 (s, 3H), 3.28 (d, *J* = 13.0 Hz, 1H), 3.20 (dd, *J* = 15.0, 7.5 Hz, 1H), 2.99 (dd, *J* = 14.8, 10.2 Hz, 1H), 2.57 (t, *J* = 12.8 Hz, 1H), 2.07 (s, 3H), 1.43-1.39 (m, 3H), 0.92 (s, 9H).

^{13}C NMR (101 MHz, DMSO) δ 171.81, 171.74, 170.18, 169.68, 169.21, 136.89, 133.95, 131.07, 130.50, 130.10, 59.62, 55.22, 52.63, 52.54, 52.18, 35.41, 31.73, 29.46, 29.13, 27.00, 26.86, 22.97, 19.16, 19.08.

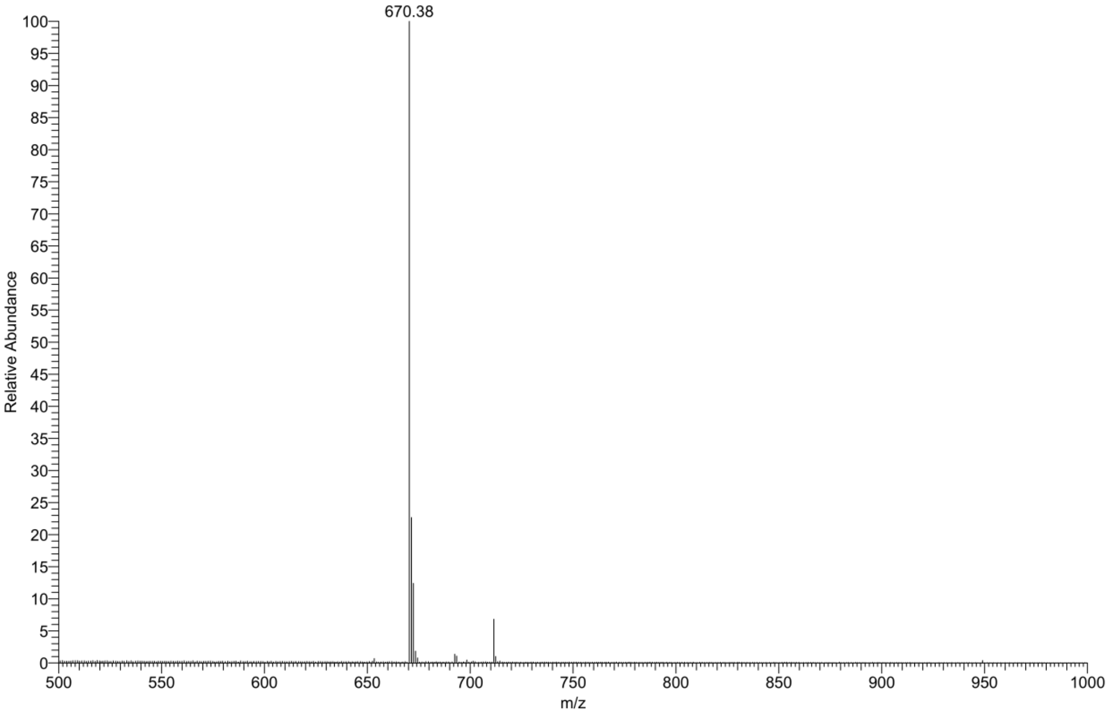


S5

Compound **S5** was prepared as a white solid in 90% yield from 2-Cl-Trt resin following the SPPS procedure.

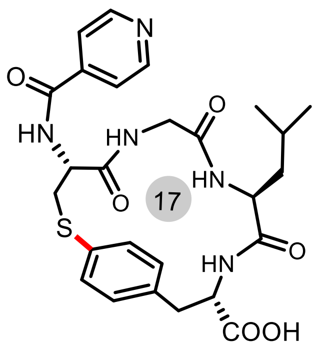


t_R = 6.37 min, 5% to 95% B for 10 min, then 95% B 10-15 min, λ = 254 nm



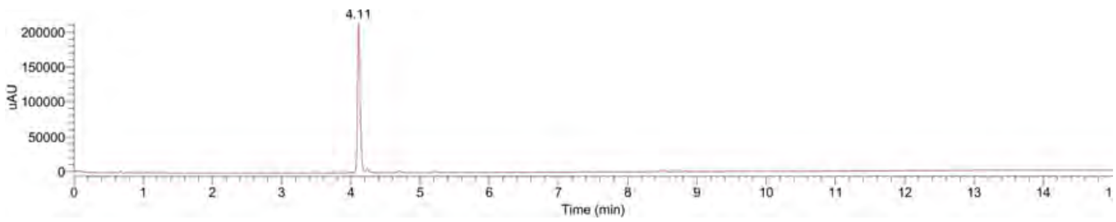
LRMS: $[M+H]^+$ 670.38.

^{1}H NMR (400 MHz, MeOD) δ 8.81 (d, *J* = 5.2 Hz, 2H), 8.04 (d, *J* = 4.5 Hz, 2H), 7.60 (d, *J* = 7.8 Hz, 2H), 7.02 (d, *J* = 7.9 Hz, 2H), 4.70-4.53 (m, 2H), 4.43 (d, *J* = 7.6 Hz, 1H), 4.01-3.76 (m, 2H), 3.22-3.04 (m, 2H), 2.97 (t, *J* = 11.6 Hz, 2H), 1.58 (s, 1H), 1.51 (t, *J* = 7.3 Hz, 2H), 0.85 (d, *J* = 5.1 Hz, 6H).

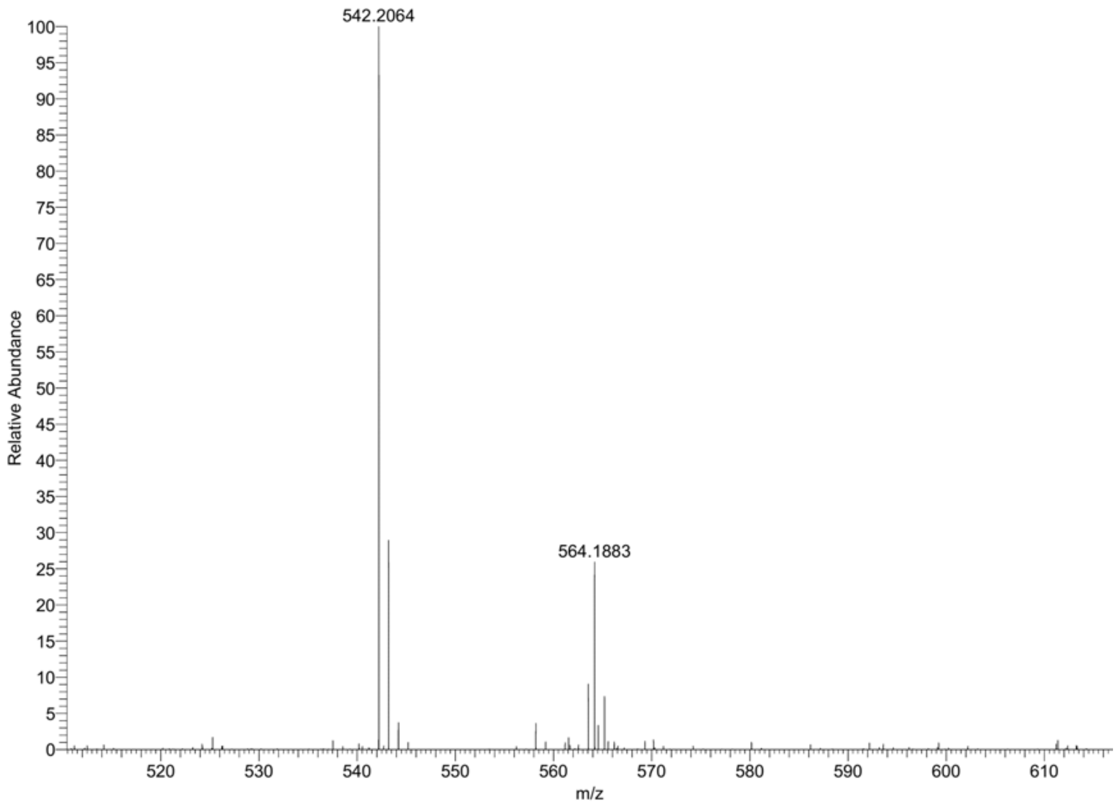


5 (69%)

Compound **5** was isolated in 69% yield (37 mg) as a white powder (TFA salt) under the general condition A.



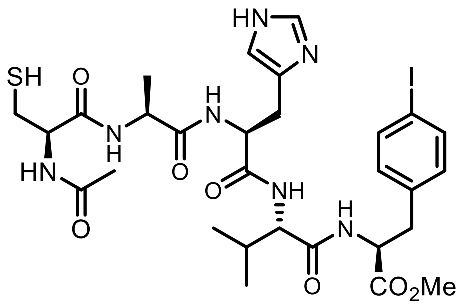
t_R = 4.11 min, 5% to 95% B for 10 min, then 95% B 10-15 min, λ = 254 nm



HRMS: Calcd for $C_{26}H_{31}N_5O_6S$ [M+H$^+$]: 542.2068; found: 542.2064

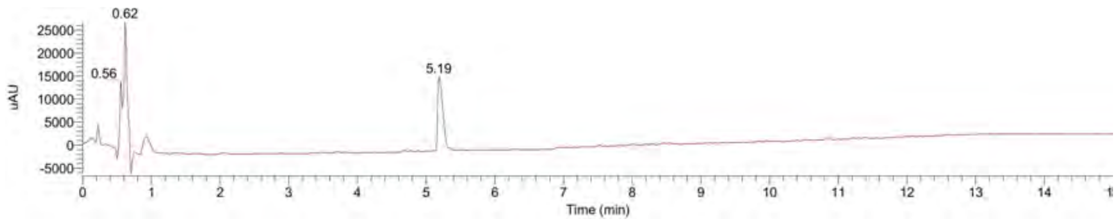
^{1}H NMR (400 MHz, 5%D_2O in DMSO) δ 8.67 (d, *J* = 5.2 Hz, 2H), 7.81-7.73 (m, 2H), 7.22 (d, *J* = 8.2 Hz, 2H), 7.05 (d, *J* = 8.2 Hz, 2H), 4.57-4.46 (m, 1H), 4.39 (d, *J* = 4.0 Hz, 1H), 3.79-3.70 (d, *J* = 15.2 Hz, 1H), 3.46 (t, *J* = 3.8 Hz, 2H), 3.25 (s, 1H), 3.17-3.03 (m, 2H), 2.89-2.75 (m, 1H), 1.60-1.46 (m, 1H), 1.45-1.35 (m, 2H), 0.79 (d, *J* = 6.4 Hz, 6H).

^{13}C NMR (101 MHz, DMSO) δ 171.11, 169.39, 168.03, 164.66, 150.75, 141.16, 136.42, 133.11, 130.45, 130.11, 121.86, 55.80, 53.37, 51.13, 42.66, 35.58, 31.73, 27.01, 24.51, 23.13, 22.59, 22.54.

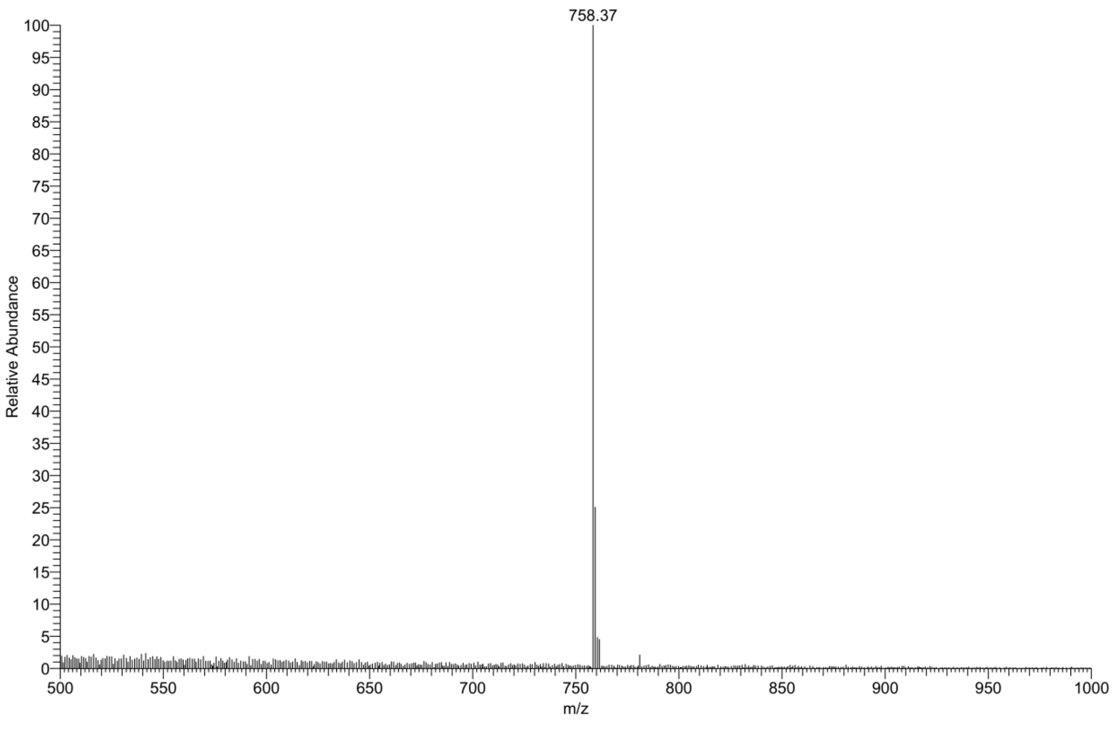


S6

Compound **S6** was prepared as a white solid in 85% yield from 2-Cl-Trt resin following the SPPS procedure.

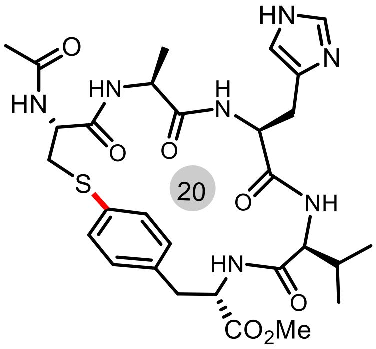


t_R = 5.19 min, 5% to 95% B for 10 min, then 95% B 10-15 min, λ = 254 nm



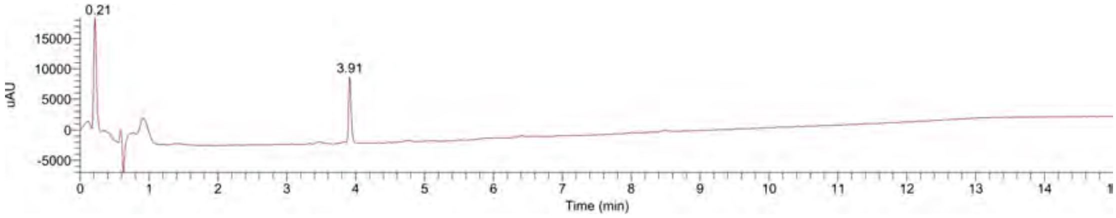
LRMS: [M+H] $^+$ 758.37.

^{1}H NMR (400 MHz, AcOD) δ 8.68 (s, 1H), 7.60 (d, *J* = 7.8 Hz, 2H), 7.15 (s, 1H), 7.02 (d, *J* = 7.8 Hz, 2H), 4.69 (s, 2H), 4.47 (t, *J* = 5.8 Hz, 1H), 4.29 (d, *J* = 7.0 Hz, 1H), 4.15 (d, *J* = 6.8 Hz, 1H), 3.68 (s, 3H), 3.33 (s, 1H), 3.25-3.02 (m, 3H), 3.00-2.74 (m, 3H), 1.34 (d, J = 6.8 Hz, 3H), 0.91 (t, J = 6.0 Hz, 6H).

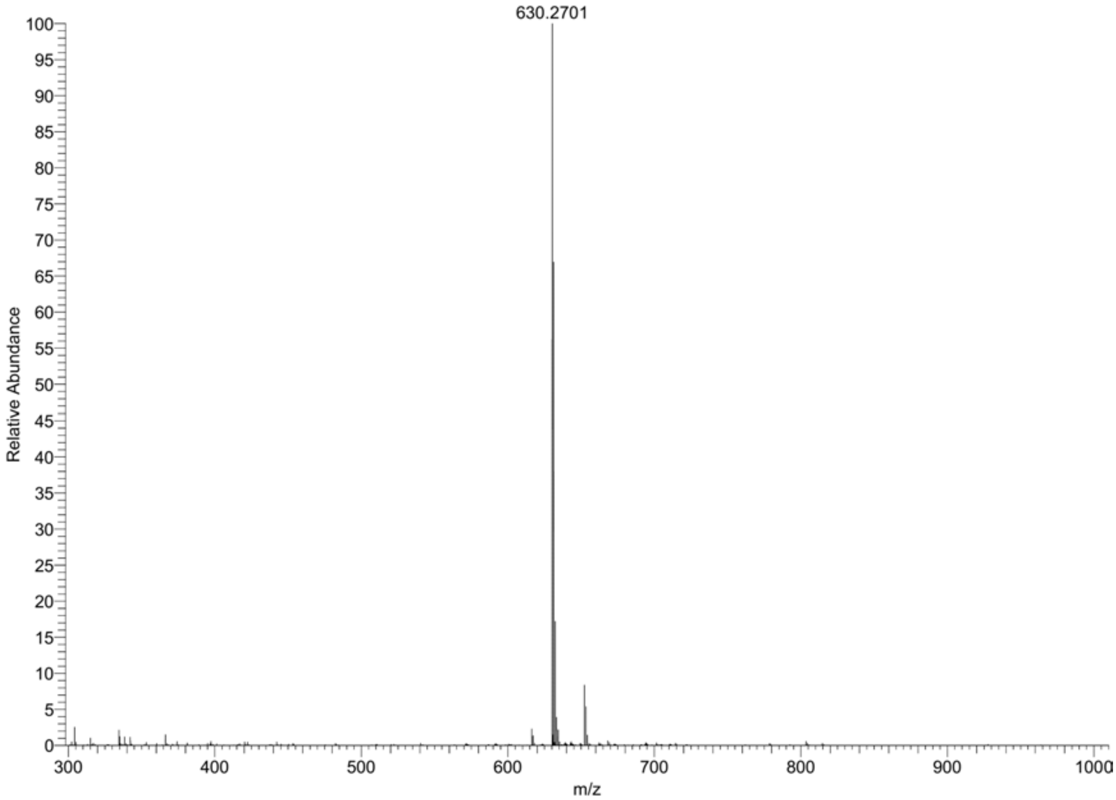


6 (80%)

Compound **6** was isolated in 80% yield (50 mg) as a white powder (TFA salt) under the general condition A.



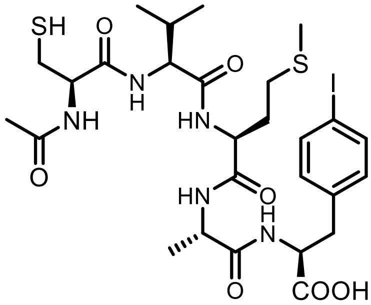
t_R = 3.91 min, 5% to 95% B for 10 min, then 95% B 10-15 min, λ = 254 nm



HRMS: Calcd for $C_{29}H_{39}N_7O_7S$ [M+H$^+$]: 630.2704; found: 630.2701

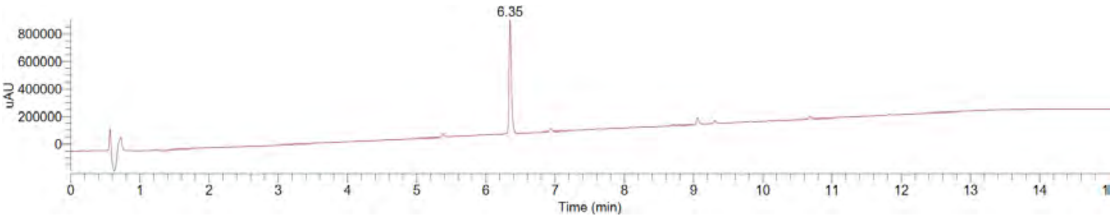
^{1}H NMR (400 MHz, MeOD) δ 8.29 (s, 1H), 7.34 (d, *J* = 8.2 Hz, 2H), 7.21 (d, *J* = 8.0 Hz, 2H), 7.10-7.04 (m, 1H), 4.85 (d, *J* = 12.4 Hz, 1H), 4.56 (d, *J* = 4.6 Hz, 1H), 4.50 (t, *J* = 7.4 Hz, 1H), 4.39 (q, *J* = 7.2 Hz, 1H), 3.89 (d, *J* = 6.6 Hz, 1H), 3.78 (s, 3H), 3.34 (d, *J* = 3.4 Hz, 1H), 3.21 (d, *J* = 7.4 Hz, 2H), 3.08 (d, *J* = 15.2 Hz, 1H), 2.95 (d, *J* = 10.0 Hz, 1H), 2.80 (t, *J* = 13.2 Hz, 1H), 2.13-2.05 (m, 1H), 1.34 (d, *J* = 7.2 Hz, 3H), 1.00 (dd, *J* = 15.6, 6.8 Hz, 6H).

^{13}C NMR (101 MHz, MeOD) δ 172.92, 172.35, 172.03, 171.72, 171.36, 169.62, 135.90, 134.42, 133.39, 130.88, 129.81, 129.62, 118.41, 59.41, 53.25, 53.14, 51.52, 51.39, 48.94, 37.94, 36.13, 29.83, 28.24, 20.97, 18.14, 17.14, 15.55.

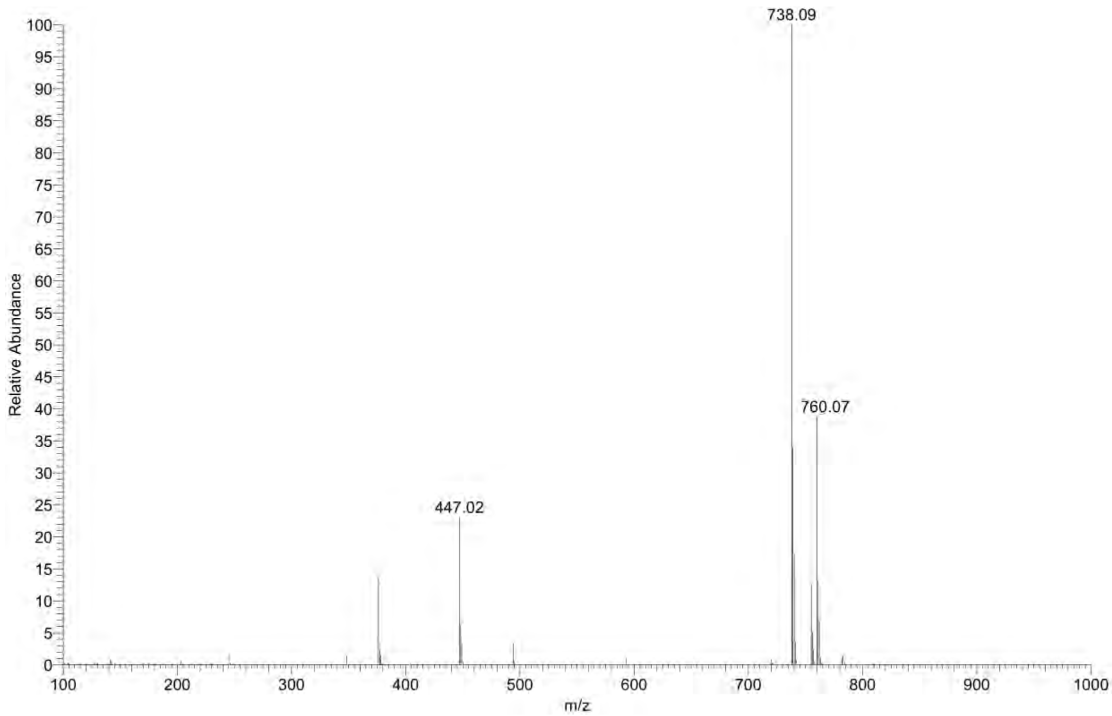


S7

Compound **S7** was prepared as a white solid in 87% yield from 2-Cl-Trt resin following the SPPS procedure.

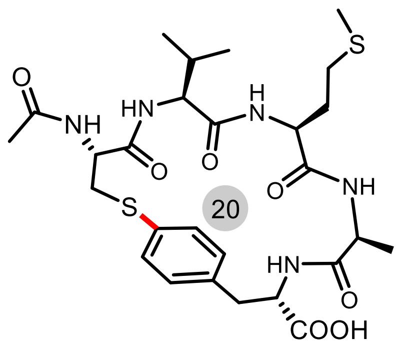


t_R = 7.79 min, 5% to 95% B for 10 min, then 95% B 10-15 min, λ = 254 nm



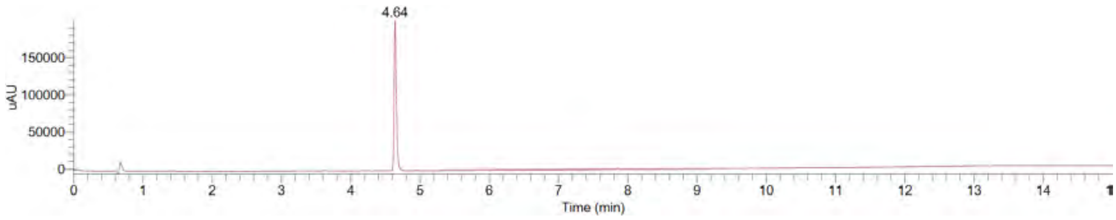
LRMS: [M+H] $^{+}$ 738.09; [M+Na] $^{+}$ 760.07.

^{1}H NMR (400 MHz, MeOD) δ 8.38 (d, *J* = 4.9 Hz, 2H), 7.80 (d, *J* = 5.1 Hz, 2H), 5.25 (dd, *J* = 7.7, 5.5 Hz, 1H), 5.15 (dd, *J* = 9.0, 4.8 Hz, 1H), 5.11-5.00 (m, 3H), 3.94 (s, 2H), 3.82 (dd, *J* = 13.6, 5.0 Hz, 1H), 3.68 (dd, *J* = 13.6, 6.7 Hz, 1H), 3.57 (dd, *J* = 13.5, 5.6 Hz, 1H), 3.46 (dd, *J* = 13.7, 7.9 Hz, 1H), 3.28-3.18 (m, 2H), 2.69 (s, 3H), 2.63-2.53 (m, 1H), 2.04 (s, 3H), 1.98 (d, *J* = 7.1 Hz, 3H), 1.64 (dd, *J* = 8.1, 5.4 Hz, 6H).

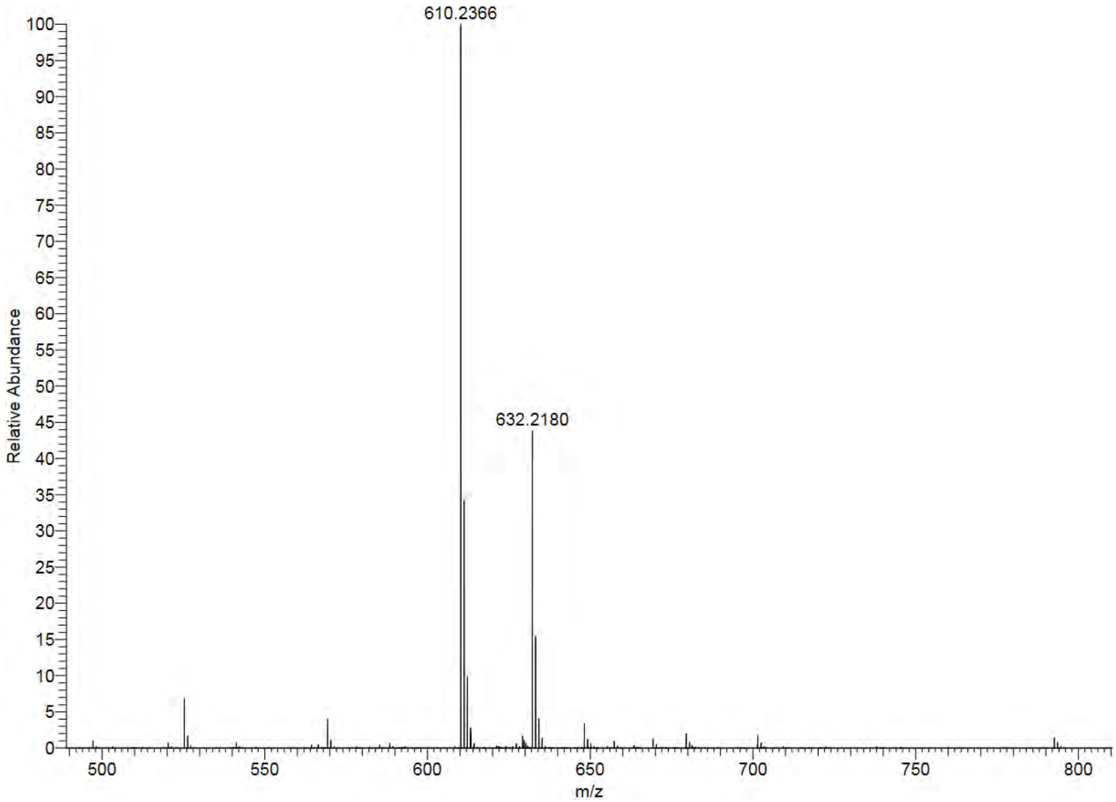


7 (70%)

Compound **7** was isolated in 70% yield (42 mg) as a white powder under the general condition A.



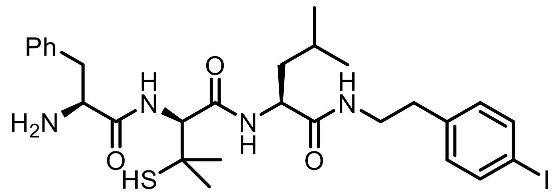
t_R = 4.64 min, 5% to 95% B for 10 min, then 95% B 10-15 min, λ = 254 nm



HRMS: Calcd for $C_{27}H_{39}N_5O_7S_2$ [M+H$^+$]: 610.2366; found: 610.2364.

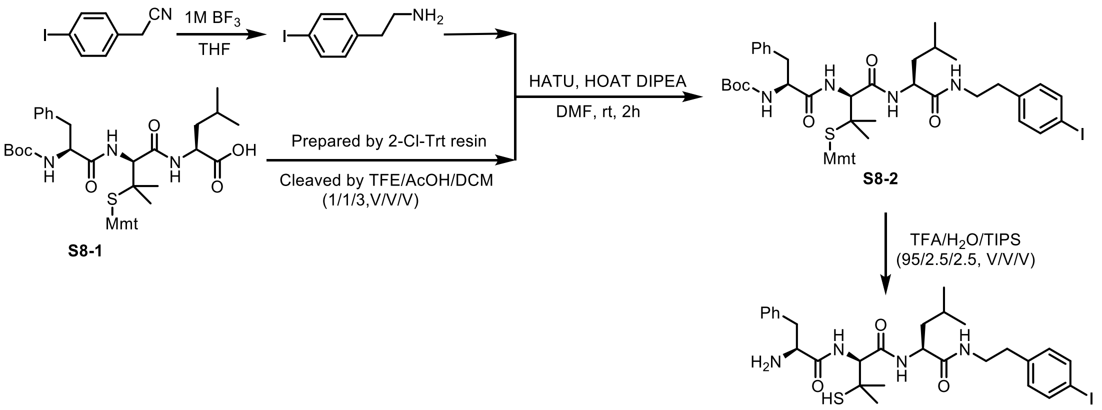
^{1}H NMR (400 MHz, MeOD) δ 7.39 (d, *J* = 8.2 Hz, 2H), 7.20 (d, *J* = 8.2 Hz, 2H), 4.70-4.54 (m, 2H), 4.41-4.28 (m, 2H), 4.10-3.98 (m, 1H), 3.33 (d, *J* = 8.8 Hz, 2H), 3.31 (q, *J* = 1.8 Hz, 2H), 2.83-2.68 (m, 1H), 2.50-2.37 (m, 2H), 2.36-2.25 (m, 1H), 2.06 (d, *J* = 1.6 Hz, 3H), 2.01 (s, 3H), 1.83-1.68 (m, 1H), 1.30 (dd, *J* = 7.4, 2.6 Hz, 3H), 0.93 (dd, *J* = 15.8, 6.8 Hz, 6H).

^{13}C NMR (101 MHz, MeOD) δ 174.85, 173.51, 172.80, 171.60, 137.81, 134.82, 132.92, 131.18, 60.20, 55.04, 54.71, 52.99, 39.53, 37.89, 33.73, 30.74, 30.46, 22.33, 19.84, 17.67, 17.27, 15.33.



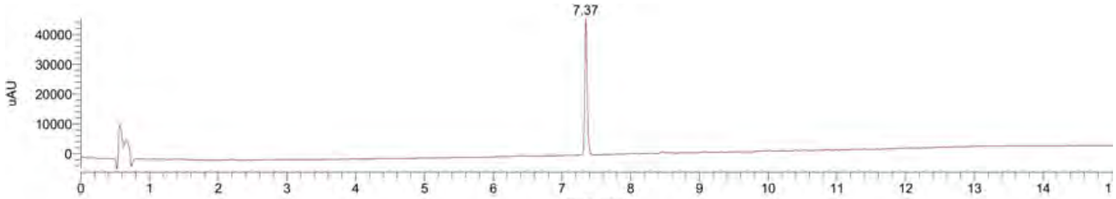
S8

Compound **S8** was prepared in 70% yield as follows:

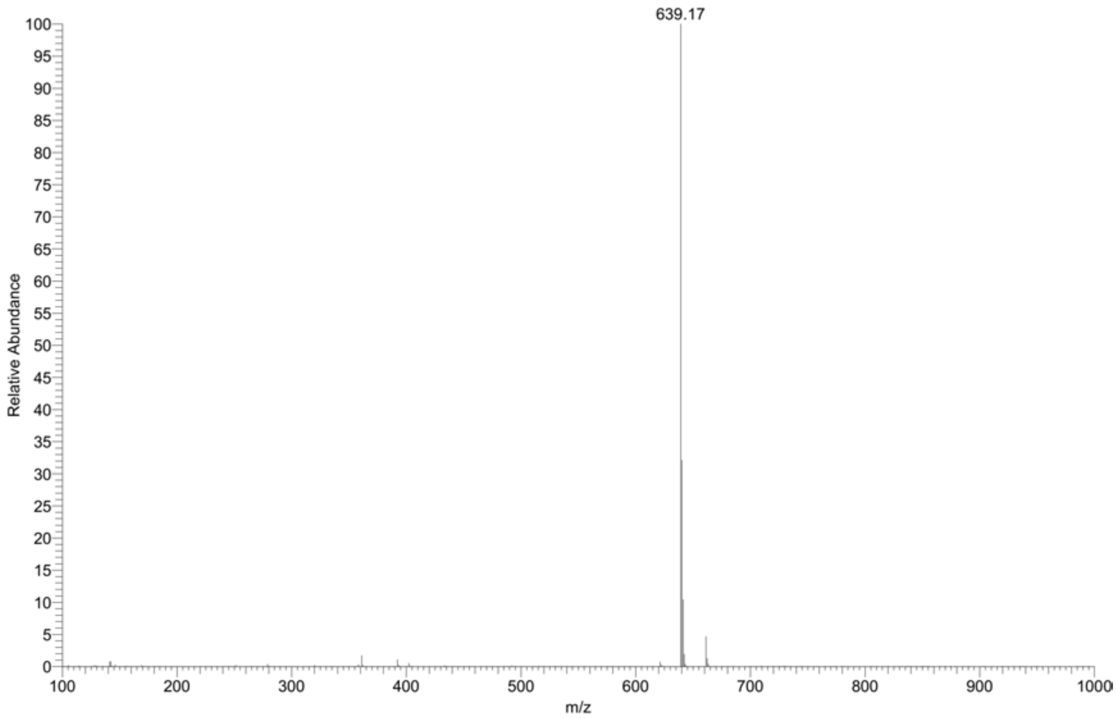


Scheme S5

To a solution of 3-iodophenylacetonitrile (1 g, 4.12 mmol) in dry THF (6 mL) at 0 °C was added dropwise a solution of BH_3 (10 mL of 1M solution in THF, 10 mmol) and was refluxed for 2h. EtOH (4 mL) was added to the mixture under ice-cooling and 1N HCl-CH_3OH (6 mL) was added. The mixture was evaporated to give 3-iodophenylethylamine (1.2 g, quantitative), which was used in the next step without purification. S8-1 was prepared by 2-Cl-Trt resin and cleaved by TFE/AcOH/DCM (1/1/3, V/V/V). 3-iodophenylethylamine was couple with S8-1, following the general amide coupling procedure to give compound **S8** as yellow solid in 70% yield.

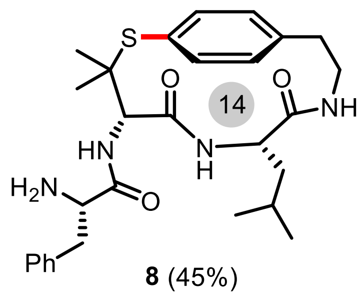


t_R = 7.37 min, 5% to 95% B for 10 min, then 95% B 10-15 min, λ = 254 nm



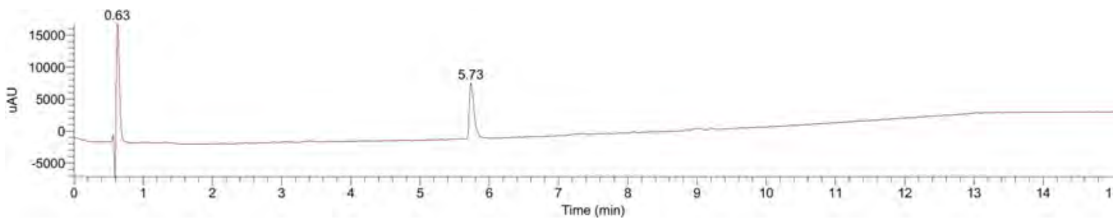
LRMS: $[M+H]^+$ 639.17.

^{1}H NMR (400 MHz, DMSO) δ 7.60 (d, *J* = 8.17 Hz, 2H), 7.30-7.10 (m, 5H), 7.00 (d, *J* = 8.17 Hz, 2H), 4.45 (s, 1H), 4.27-4.13 (m, 1H), 3.65-3.53 (m, 1H), 3.39-3.18 (m, 4H), 2.99 (dd, *J* = 13.4, 5.0 Hz, 1H), 2.67 (t, *J* = 7.2 Hz, 2H), 2.59 (dd, *J* = 13.4, 8.6 Hz, 1H), 1.57-1.45 (m, 1H), 1.35 (s, 3H), 1.24 (s, 3H), 0.81 (dd, *J* = 17.8, 6.4 Hz, 6H).

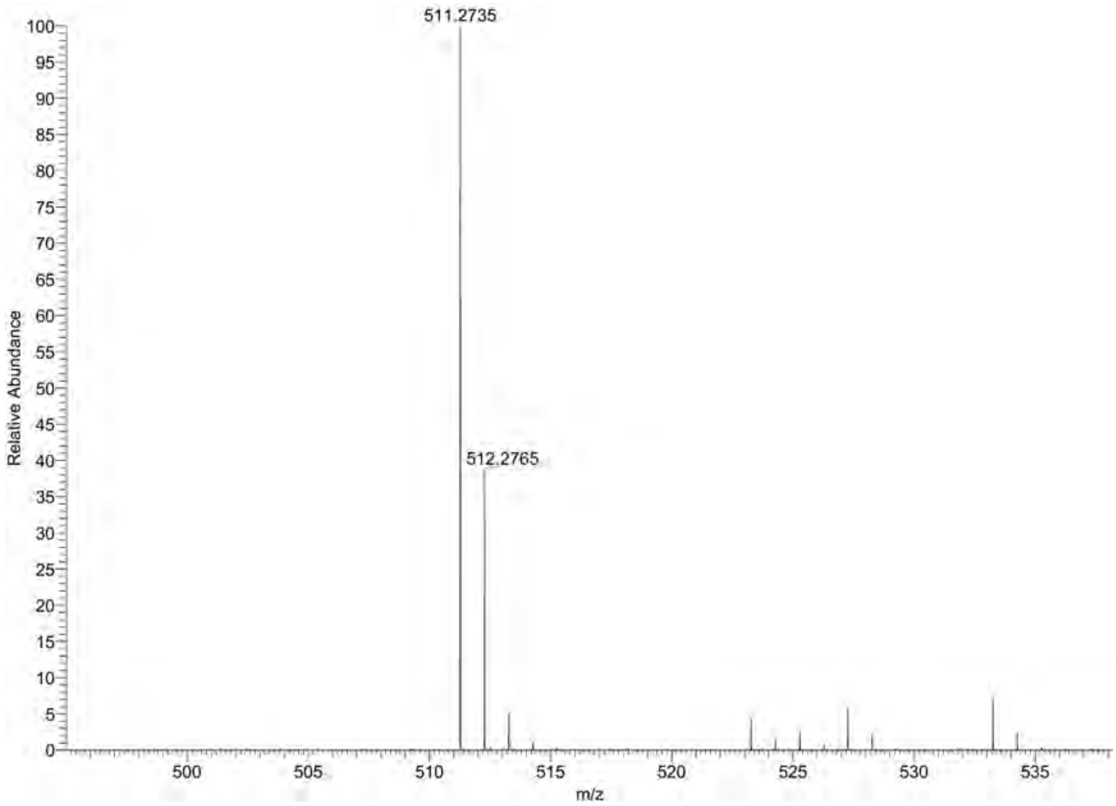


8 (45%)

Compound **8** was isolated in 45% yield (22 mg) as a white powder (TFA salt) under the general condition A (16 h).

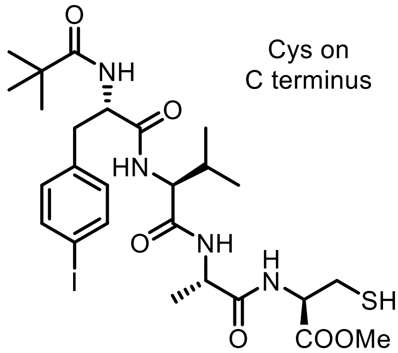


t_R = 5.73 min, 5% to 95% B for 10 min, then 95% B 10-15 min, λ = 254 nm



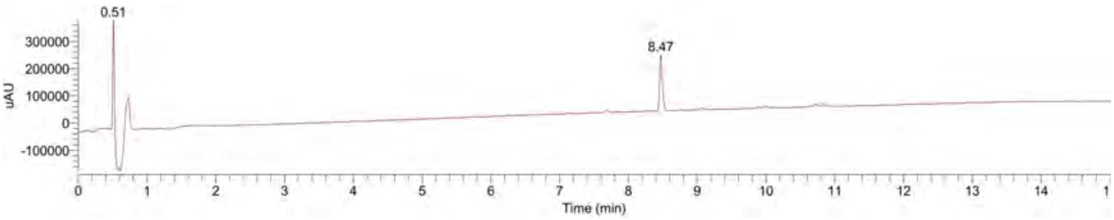
HRMS: Calcd for $C_{28}H_{38}N_4O_3S$ [M+H$^+$]: 511.2737; found: 511.2735

^{1}H NMR (400 MHz, MeOD) δ 7.48-7.41 (m, 2H), 7.38 (s, 1H), 7.36 (d, *J* = 2.4 Hz, 2H), 7.34 (s, 1H), 7.30 (d, *J* = 6.6 Hz, 1H), 7.21-7.17 (m, 1H), 7.05 (dd, *J* = 7.8, 2.0 Hz, 1H), 4.25-4.19 (m, 1H), 3.95 (t, *J* = 7.4 Hz, 2H), 3.25-3.14 (m, 2H), 3.12-3.03 (m, 2H), 2.92 (dd, *J* = 13.6, 8.4 Hz, 2H), 2.75-2.62 (m, 2H), 1.24-1.21 (m, 1H), 1.09 (s, 3H), 0.92 (s, 3H), 0.85 (dd, *J* = 9.8, 6.6 Hz, 6H).

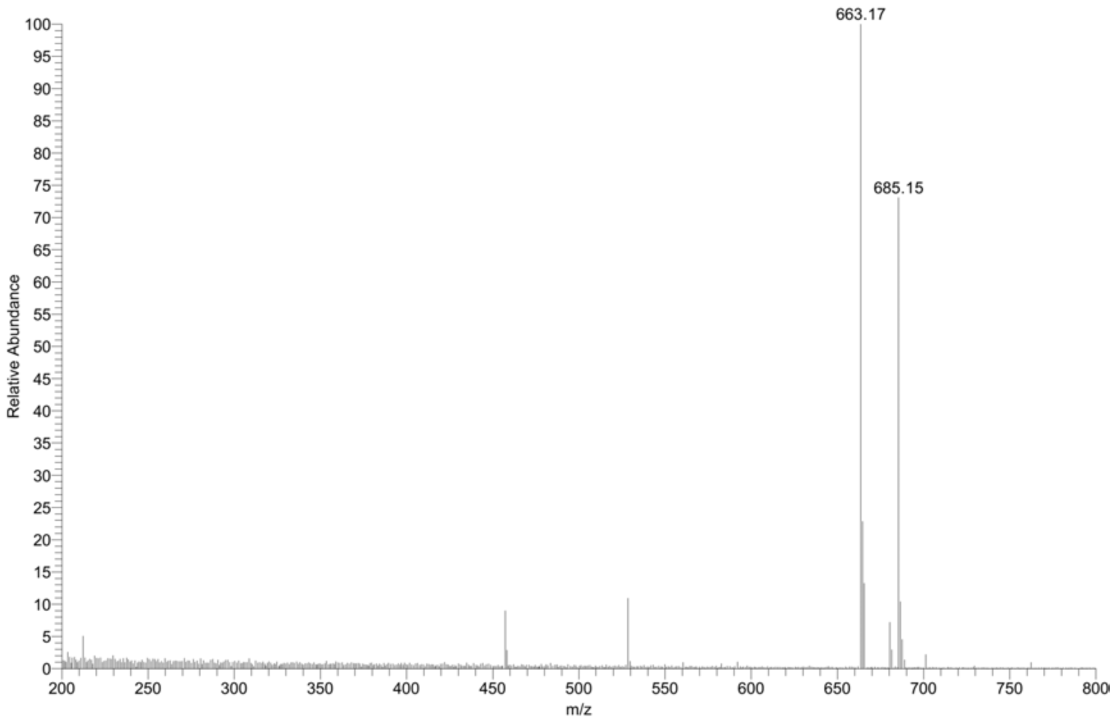


S9

Compound **S9** was prepared as a white solid in 89% yield from 2-Cl-Trt resin following the SPPS procedure.

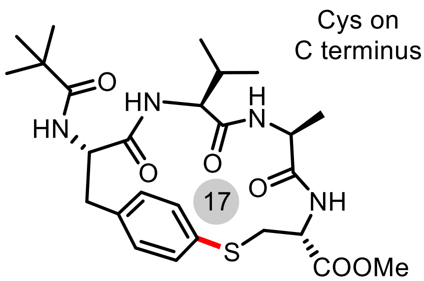


t_R = 8.47 min, 5% to 95% B for 10 min, then 95% B 10-15 min, λ = 254 nm



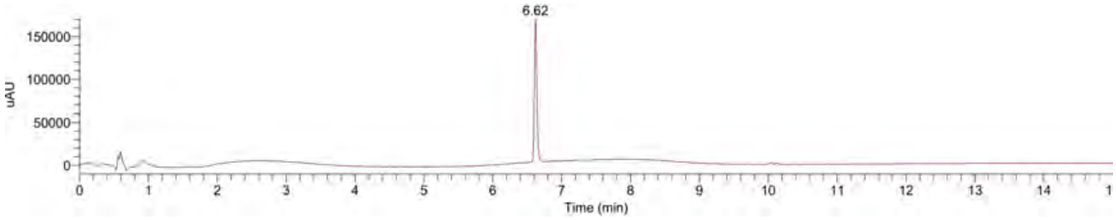
LRMS: [M+H] $^+$ 663.17; [M+Na] $^+$ 685.15.

^{1}H NMR (400 MHz, MeOD) δ 7.60 (d, J = 8.3 Hz, 2H), 7.00 (d, J = 8.2 Hz, 2H), 4.68 (dd, J = 9.2, 5.0 Hz, 1H), 4.65 (dd, J = 6.2, 4.6 Hz, 1H), 4.41 (q, J = 7.0 Hz, 1H), 4.19 (d, J = 7.0 Hz, 1H), 3.74 (s, 3H), 3.17-3.09 (m, 1H), 2.97-2.84 (m, 3H), 2.14-2.01 (m, 1H), 1.39 (d, J = 7.0 Hz, 3H), 1.08 (s, 9H), 0.95 (dd, J = 10.8, 6.6 Hz, 6H).

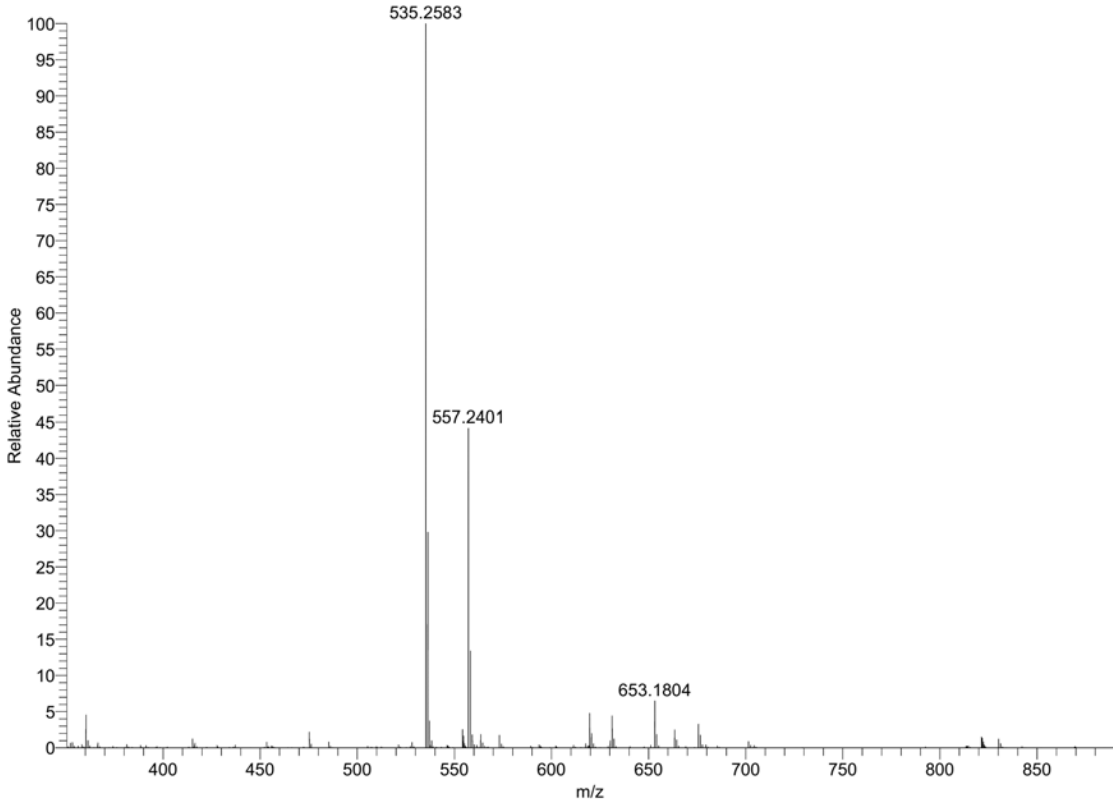


9 (45%)

Compound **9** was isolated in 45% yield (24 mg) as a white powder under the general condition A.



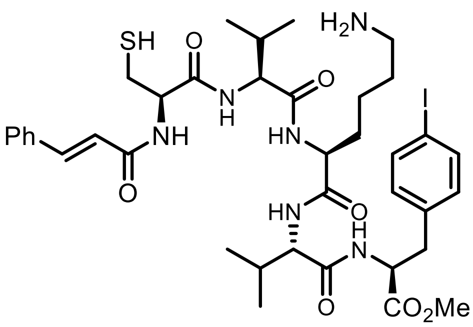
t_R = 6.62 min, 5% to 95% B for 10 min, then 95% B 10-15 min, λ = 254 nm



HRMS: Calcd for $C_{26}H_{38}N_4O_6S$ [M+H$^+$]: 535.2585; found: 535.2583

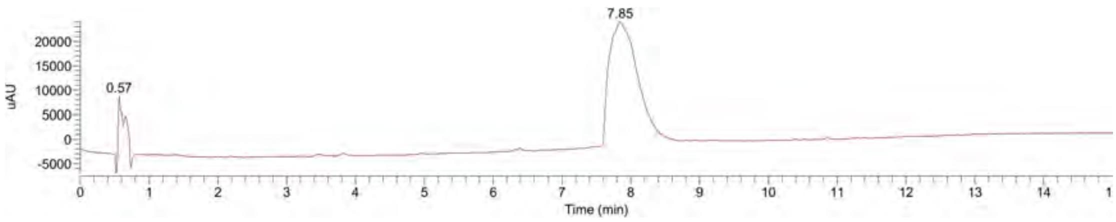
^{1}H NMR (400 MHz, CD_3Cl) δ 7.33 (d, *J* = 8.2 Hz, 2H), 7.17 (d, *J* = 8.2 Hz, 2H), 6.63 (d, *J* = 7.8 Hz, 1H), 6.57 (s, 1H), 6.23 (d, *J* = 8.0 Hz, 1H), 5.97 (d, *J* = 6.0 Hz, 1H), 4.78-4.72 (m, 1H), 4.59-4.51 (m, 1H), 4.22 (q, *J* = 6.2 Hz, 1H), 4.16-4.10 (m, 1H), 3.84 (s, 3H), 3.76 (dd, *J* = 15.0, 4.4 Hz, 1H), 3.52-3.48 (m, 1H), 3.16 (t, *J* = 12.2 Hz, 1H), 2.83 (dd, *J* = 12.2, 3.6 Hz, 1H), 2.16-1.94 (m, 2H), 1.34 (d, *J* = 6.6 Hz, 3H), 1.22 (s, 9H), 0.88 (s, 6H).

^{13}C NMR (101 MHz, DMSO) δ 177.54, 171.85, 171.01, 170.87, 170.55, 136.77, 133.97, 131.81, 130.35, 130.12, 59.95, 55.15, 54.11, 52.90, 48.79, 38.47, 31.74, 30.58, 27.70, 27.02, 22.54, 19.43, 18.76.

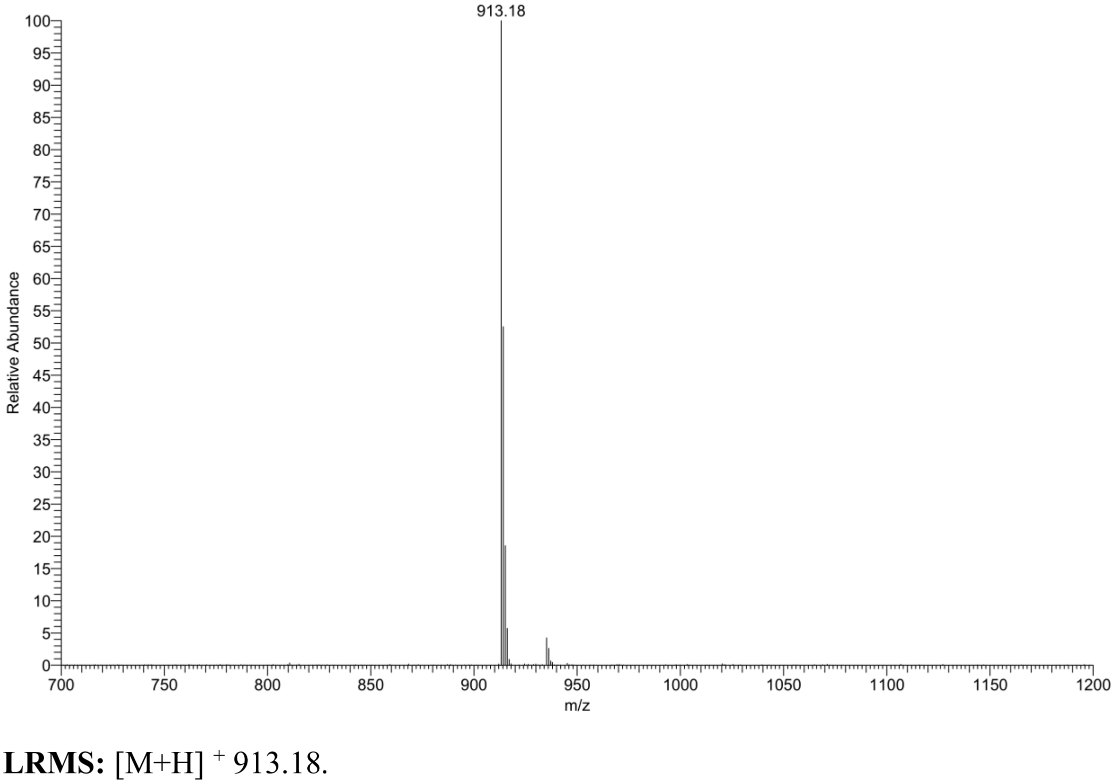


S10

Compound **S10** was prepared as a white solid in 92% yield from 2-Cl-Trt resin following the SPPS procedure.

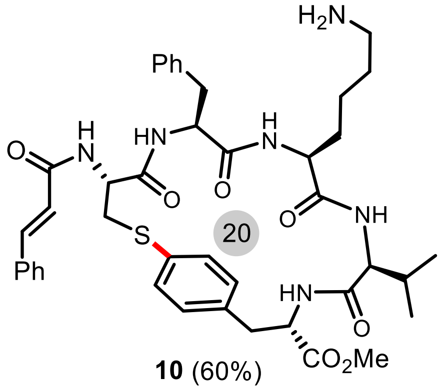


t_R = 7.85 min, 5% to 95% B for 10 min, then 95% B 10-15 min, λ = 254 nm



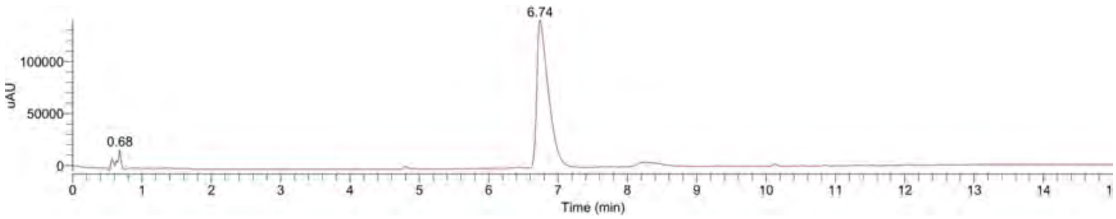
LRMS: [M+H] $^+$ 913.18.

^{1}H NMR (400 MHz, DMSO) δ 8.48 (dd, *J* = 20.2, 7.8 Hz, 2H), 8.26 (d, *J* = 7.8 Hz, 1H), 8.13 (d, *J* = 7.8 Hz, 1H), 7.85 (d, *J* = 5.2 Hz, 2H), 7.60 (d, *J* = 7.8 Hz, 3H), 7.55 (d, *J* = 7.0 Hz, 2H), 7.47 (d, *J* = 15.6 Hz, 1H), 7.39 (d, *J* = 6.4 Hz, 3H), 7.24-7.09 (m, 5H), 7.03 (d, J = 7.8 Hz, 2H), 6.71 (d, J = 15.6 Hz, 1H), 4.80-4.67 (m, 1H), 4.65-4.54 (m, 1H), 4.51-4.43 (m, 1H), 4.33 (q, J = 7.6 Hz, 1H), 4.21 (t, J = 7.8 Hz, 1H), 3.58 (s, 3H), 3.10-3.02 (m, 2H), 3.02-2.96 (m, 1H), 2.92-2.82 (m, 3H), 2.76 (q, J = 8.2, 7.2 Hz, 2H), 1.93 (q, J = 6.6 Hz, 1H), 1.69-1.60 (m, 1H), 1.55 (t, J = 7.6 Hz, 3H), 1.38-1.23 (m, 2H), 0.82 (dd, J = 6.6, 4.2 Hz, 6H).

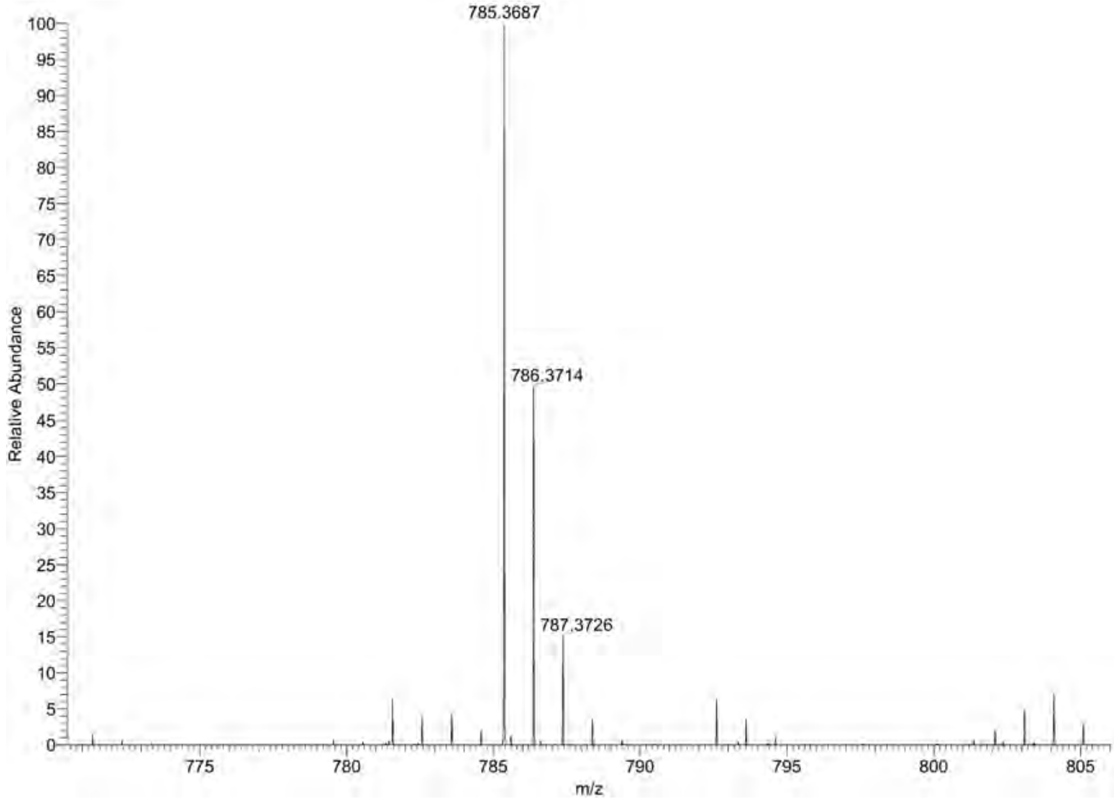


10 (60%)

Compound **10** was isolated in 60% yield (47 mg) as a white powder (TFA salt) under the general condition A.



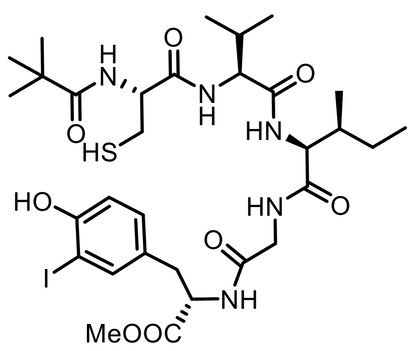
t_R = 6.74 min, 5% to 95% B for 10 min, then 95% B 10-15 min, λ = 254 nm



HRMS: Calcd for $C_{42}H_{52}N_6O_7S$ [M+H$^+$]: 785.3691; found: 785.3687

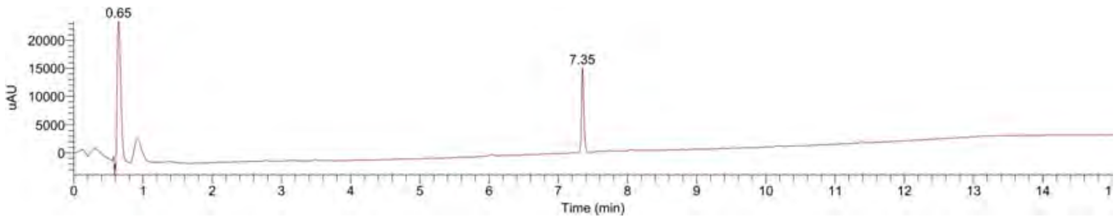
^{1}H NMR (400 MHz, MeOD) δ 7.53-7.48 (m, 2H), 7.44 (s, 1H), 7.32 (m, 5H), 7.15-7.10 (m, 4H), 7.07 (t, *J* = 7.4 Hz, 2H), 6.95 (t, *J* = 7.2 Hz, 1H), 6.47 (dd, *J* = 15.8, 3.2 Hz, 1H), 4.64 (dd, *J* = 10.0, 4.4 Hz, 1H), 4.59 (dd, *J* = 6.4, 2.8 Hz, 1H), 4.50 (dd, *J* = 12.4, 3.0 Hz, 1H), 4.22 (dd, *J* = 7.4, 4.2 Hz, 1H), 3.82 (d, *J* = 8.8 Hz, 1H), 3.66 (s, 3H), 3.30 (dd, *J* = 13.2, 9.0 Hz, 1H), 3.19-3.16 (m, 1H), 3.16-3.08 (m, 2H), 2.84-2.75 (m, 1H), 2.73-2.62 (m, 3H), 1.90-1.80 (m, 1H), 1.58-1.49 (m, 1H), 1.45-1.34 (m, 2H), 1.12-1.04 (m, 1H), 0.89 (t, *J* = 6.6 Hz, 6H), 0.82-0.75 (m, 3H).

^{13}C NMR (101 MHz, MeOD) δ 171.69, 171.18, 166.70, 141.38, 137.30, 135.79, 134.76, 133.61, 130.02, 129.71, 128.90, 128.67, 128.14, 127.55, 126.16, 59.68, 54.45, 53.81, 51.46, 38.95, 36.26, 35.45, 31.28, 29.61, 26.62, 18.16.

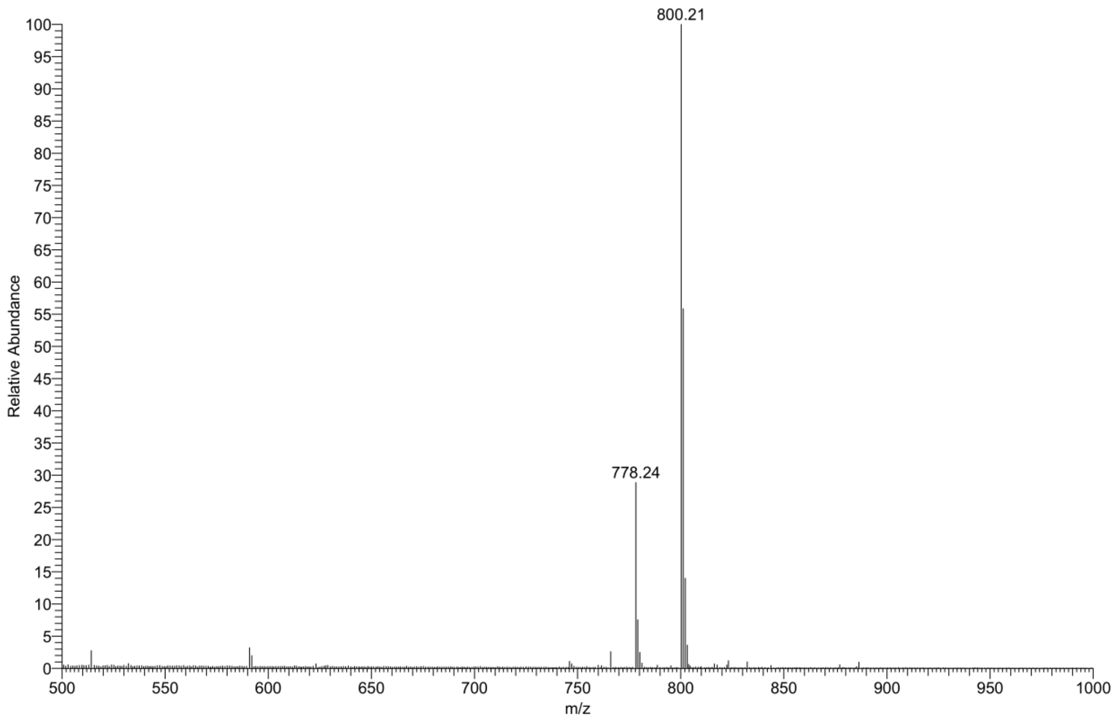


S11

Compound **S11** was prepared as a white solid in 94% yield from 2-Cl-Trt resin following the SPPS procedure.

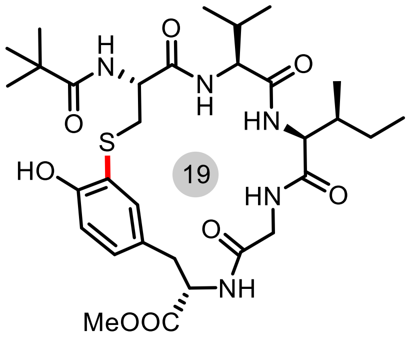


t_R = 7.35 min, 5% to 95% B for 10 min, then 95% B 10-15 min, λ = 254 nm



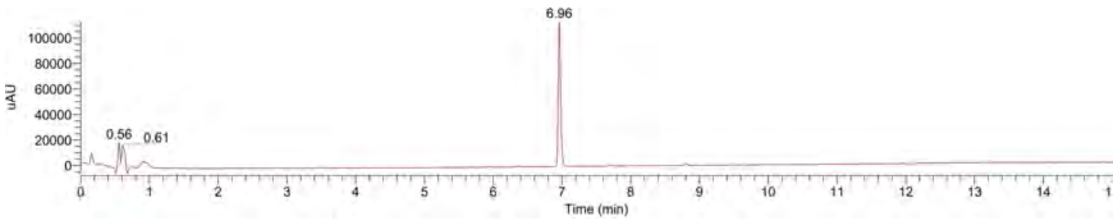
LRMS: $[M+H]^+$ 778.24; $[M+Na]^+$ 800.21.

^{1}H NMR (400 MHz, MeOD) δ 7.54 (d, *J* = 3.2 Hz, 1H), 7.05 (dd, *J* = 8.2, 2.2 Hz, 1H), 6.77 (d, *J* = 8.2 Hz, 1H), 4.67-4.52 (m, 2H), 4.29-4.16 (m, 2H), 3.97-3.80 (m, 2H), 3.70 (s, 3H), 3.05 (dd, *J* = 14.4, 6.4 Hz, 1H), 2.98-2.88 (m, 2 H), 2.85 (dd, *J* = 13.8, 7.0 Hz, 1H), 2.17-1.98 (m, 1H), 1.87 (d, J = 11.0 Hz, 1H), 1.69-1.51 (m, 1H), 1.24 (s, 9H), 0.99-0.83 (m, 12H).

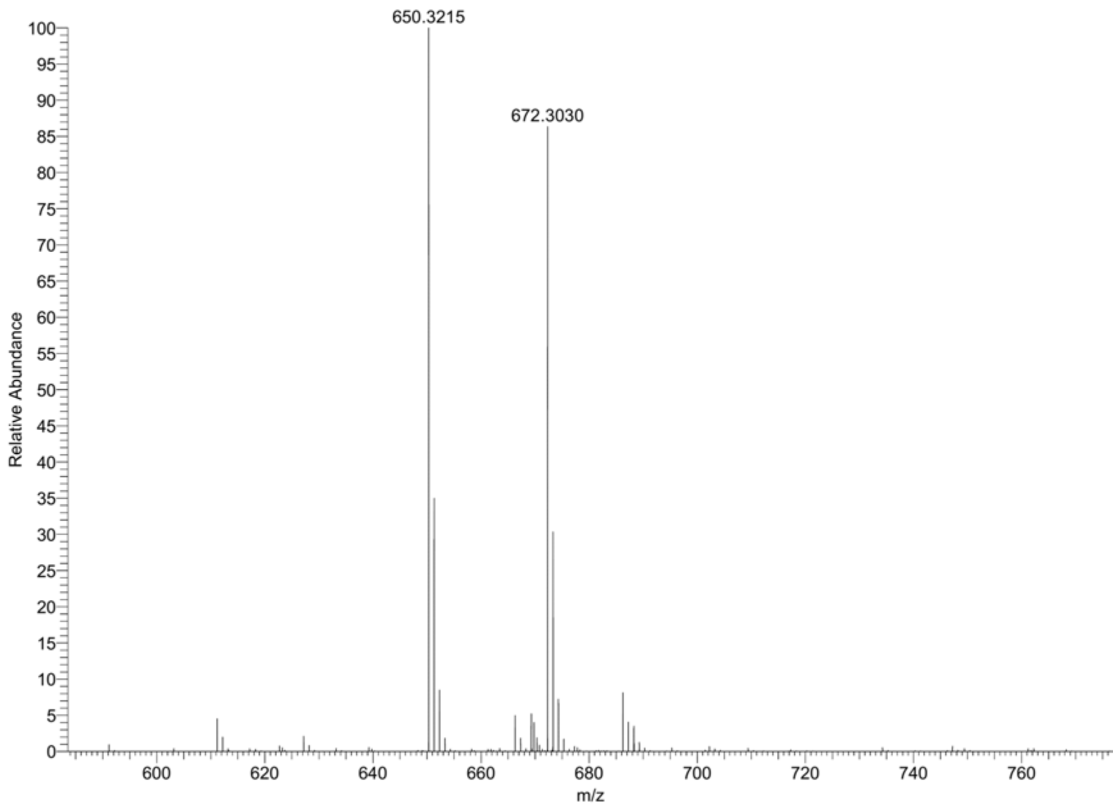


11 (40%)

Compound **11** was isolated in 40% yield (26 mg) as a white powder under the general condition A.



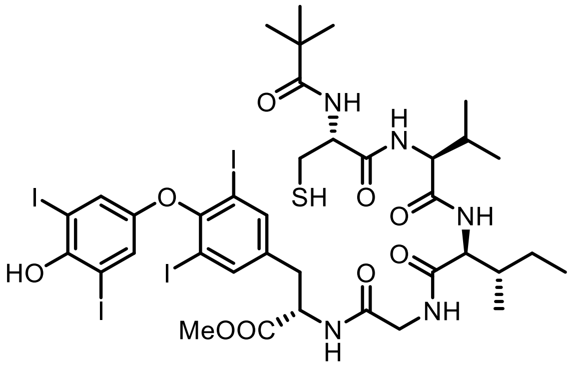
t_R = 6.96 min, 5% to 95% B for 10 min, then 95% B 10-15 min, λ = 254 nm



HRMS: Calcd for $C_{31}H_{47}N_5O_8S$ [M+H$^+$]: 650.3218; found: 650.3215

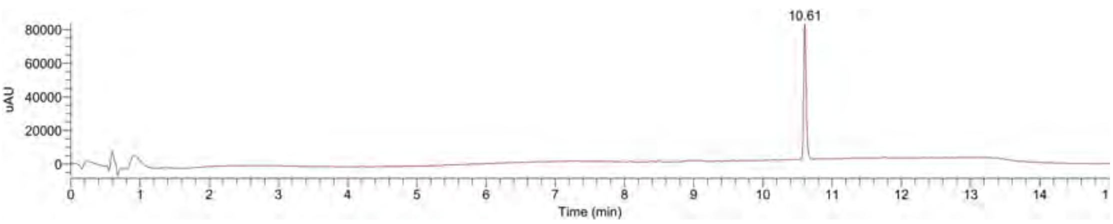
^{1}H NMR (400 MHz, MeOD) δ 7.28 (s, 1H), 6.84 (d, *J* = 7.0 Hz, 1H), 6.64 (d, *J* = 8.2 Hz, 1H), 4.60 (dd, *J* = 9.0, 3.0 Hz, 1H), 4.40 (dd, *J* = 9.0, 6.0 Hz, 1H), 4.20 (d, *J* = 6.2 Hz, 1H), 3.92 (d, *J* = 6.2 Hz, 1H), 3.76 (d, *J* = 16.2 Hz, 1H), 3.62 (s, 3H), 3.52 (d, *J* = 16.4 Hz, 1H), 3.14 (dd, *J* = 14.8, 7.6 Hz, 2H), 3.02 (dd, *J* = 14.0, 3.4 Hz, 1H), 2.82 (dd, *J* = 14.0, 9.2 Hz, 1H), 2.10-2.00 (m, 1H), 1.80 (d, *J* = 7.8 Hz, 1H), 1.45-1.36 (m, 1H), 1.10 (s, 9 H), 1.04-0.98 (m, 1H), 0.91 (dd, *J* = 6.8, 3.0 Hz, 6H), 0.85-0.77 (m, 6H).

^{13}C NMR (101 MHz, DMSO) δ 178.03, 171.61, 171.50, 171.45, 171.01, 169.14, 153.23, 129.52, 128.70, 127.12, 123.68, 114.59, 60.68, 56.64, 54.10, 52.20, 52.03, 43.07, 38.55, 38.19, 36.20, 33.54, 29.88, 27.70, 24.63, 19.65, 18.83, 15.79, 11.69.

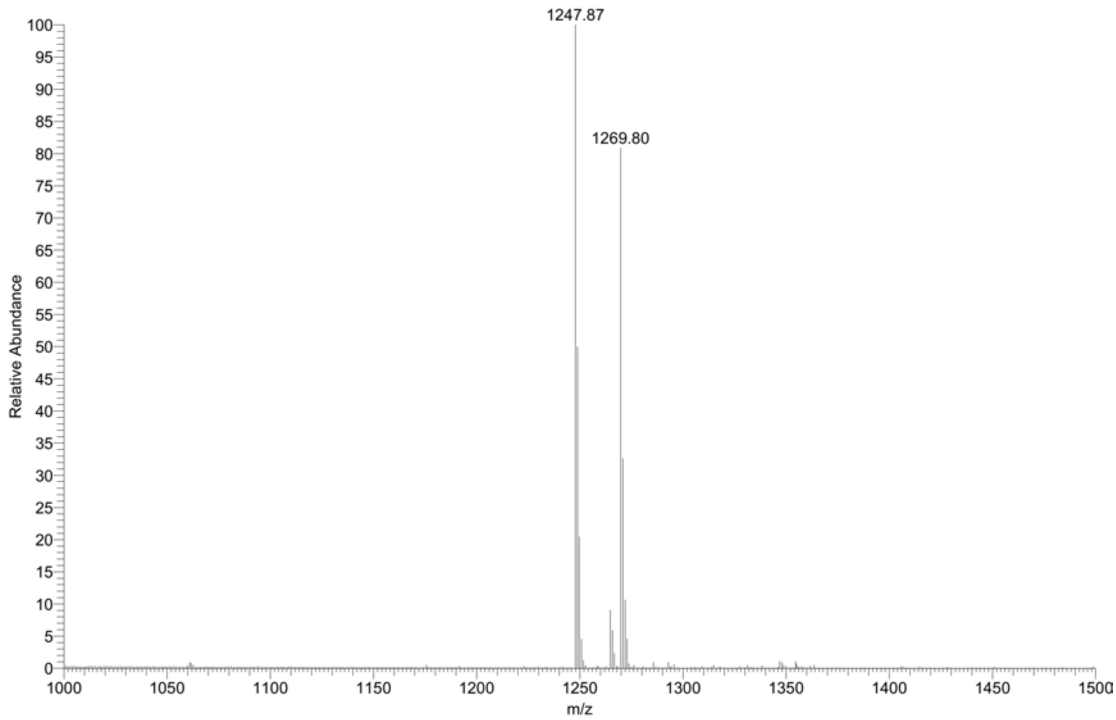


S12

Compound **S12** was prepared as a yellow solid in 94% yield from 2-Cl-Trt resin following the SPPS procedure.

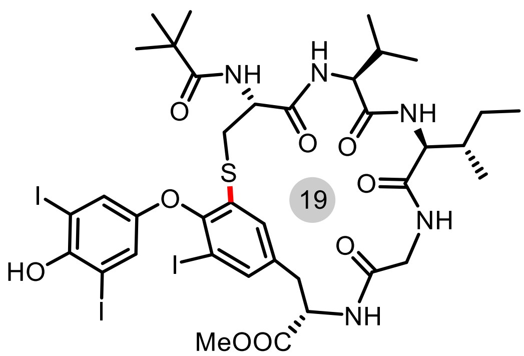


t_R = 10.61 min, 5% to 95% B for 10 min, then 95% B 10-15 min, λ = 254 nm



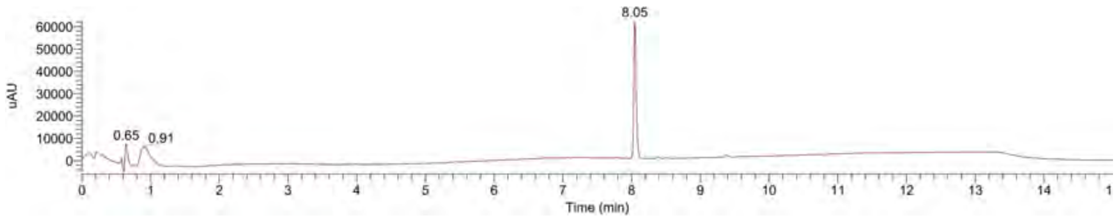
LRMS: [M+H] $^+$ 1247.87; [M+Na] $^+$ 1269.80.

^{1}H NMR (400 MHz, MeOD) δ 7.82 (s, 2H), 7.09 (s, 2H), 4.61 (t, *J* = 7.0 Hz, 1H), 4.55-4.45 (m, 1H), 4.22 (d, *J* = 6.6 Hz, 1H), 4.18-4.11 (m, 1H), 3.81 (dd, *J* = 70.8, 16.8 Hz, 2H), 3.65 (s, 3H), 3.16-2.94 (m, 2H), 2.94-2.75 (m, 2H), 2.11-1,98 (m, 1H), 1.86-1.74 (m, 1H), 1.66-1.43 (m, 2H), 1.17 (s, 9H), 0.94-0.84 (m, 12H).

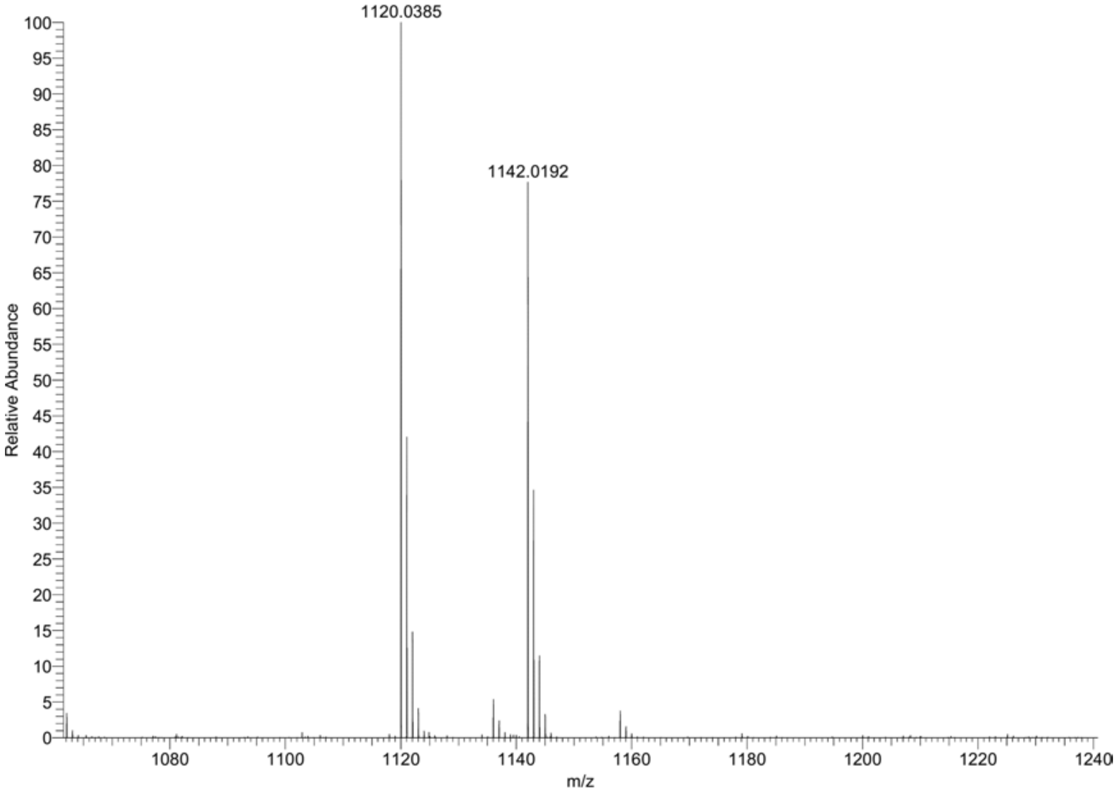


12 (44%)

Compound **12** was isolated in 44% yield (49 mg) as a white powder under the general condition A. The reaction site of thyroxine can be judged by ^{1}H NMR spectrum of **S12** and **12**.



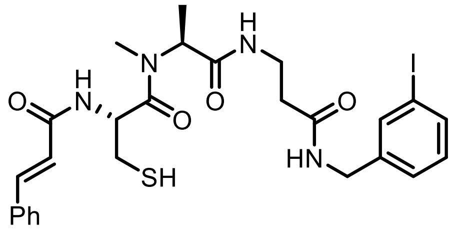
t_R = 8.05 min, 5% to 95% B for 10 min, then 95% B 10-15 min, λ = 254 nm



HRMS: Calcd for $C_{37}H_{48}I_3N_5O_9S$ [M+H$^+$]: 1120.0380; found: 1120.0385

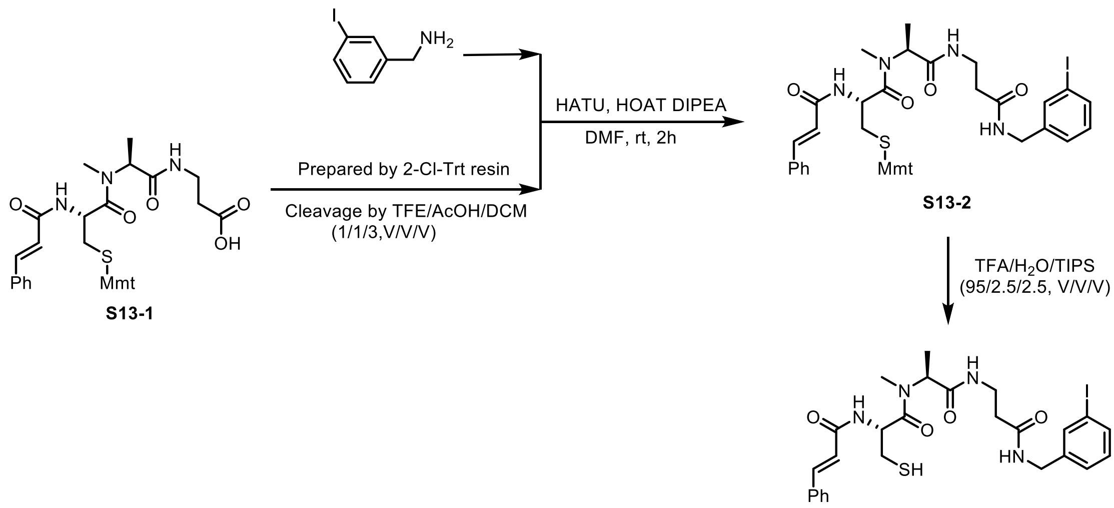
^{1}H NMR (400 MHz, MeOD) δ 7.57 (d, J = 1.8 Hz, 1H), 7.50 (d, J = 1.8 Hz, 1H), 7.04 (s, 2H), 4.70 (dd, J = 11.0, 4.2 Hz, 1H), 4.29 (d, J = 6.4 Hz, 1H), 3.89 (d, J = 6.6 Hz, 1H), 3.80 (d, J = 15.6 Hz, 1H), 3.74 (s, 3H), 3.64 (d, J = 15.6 Hz, 1H), 3.53 (dd, J = 12.0, 4.2 Hz, 1H), 3.32 (d, J = 8.6 Hz, 1H), 3.26 (d, J = 11.8 Hz, 1H), 3.14 (dd, J = 13.8, 3.6 Hz, 1H), 3.06 (dd, J = 13.8, 6.8 Hz, 1H), 2.15-2.04 (m, 1H), 1.86-1.76 (m, 1H), 1.54-1.41 (m, 1H), 1.13 (dd, J = 6.6, 2.6 Hz, 1H), 1.08 (s, 9H), 1.01 (dd, J = 6.9, 4.4 Hz, 6H), 0.97 (d, J = 6.8 Hz, 3H), 0.90 (t, J = 7.4 Hz, 3H).

^{13}C NMR (101 MHz, DMSO) δ 177.46, 171.11, 170.80, 170.68, 170.44, 168.88, 147.50, 137.51, 136.75, 135.76, 133.67, 129.62, 128.60, 128.19, 128.00, 127.88, 126.37, 124.92, 92.01, 87.47, 77.70, 62.83, 55.84, 53.23, 51.80, 50.61, 42.45, 29.32, 28.98, 28.78, 28.65, 28.53, 27.19, 26.51, 24.02, 19.20, 18.48, 15.38, 13.92, 11.33.



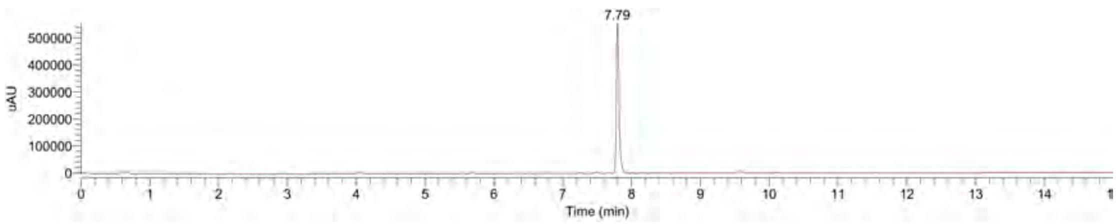
S13

Compound **S13** was prepared in 88% yield as follows:

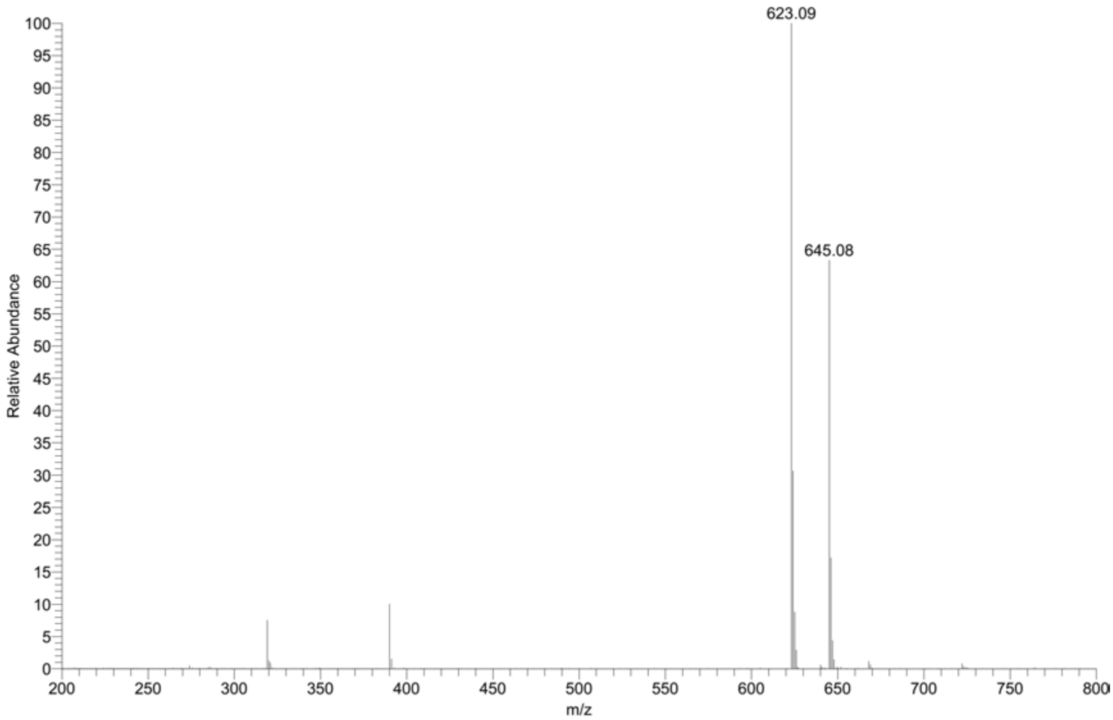


Scheme S6

S13-1 was prepared by 2-Cl-Trt resin and cleaved by TFE/AcOH/DCM (1/1/3, V/V/V). 3-iodobenzylamine was couple with S13-1, following the general amide coupling procedure to give compound **S13** as white solid in 88% yield.

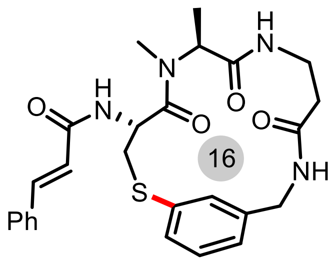


t_R = 7.79 min, 5% to 95% B for 10 min, then 95% B 10-15 min, λ = 254 nm



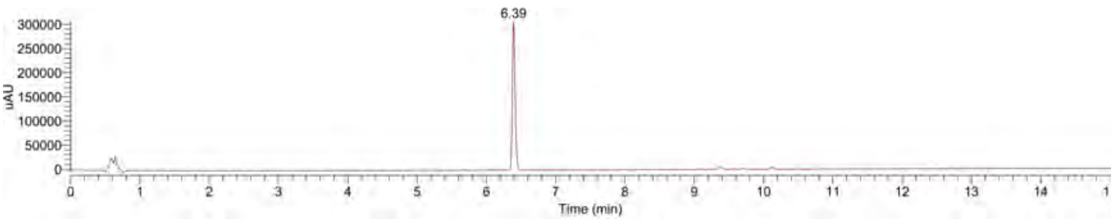
LRMS: [M+H] $^{+}$ 623.09; [M+Na] $^{+}$ 645.08.

^{1}H NMR (400 MHz, MeOD) δ 7.67 (s, 1H), 7.64-7.68 (m, 4H), 7.39 (s, 3H), 7.32-7.18 (m, 1H), 7.15-7.00 (m, 1H), 6.65 (dd, J = 26.4, 15.8 Hz, 1H), 5.09-4.99 (m, 1H), 4.98-4.89 (m, 1H), 4.29 (dd, J = 18.8, 3.0 Hz, 2H), 3.57-3.38 (m, 2H), 3.11 (s, 2H), 3.02-2.88 (m, 1H), 2.87-2.73 (m, 2H), 2.54-2.38 (m, 2H), 1.51-1.31 (m, 3H).

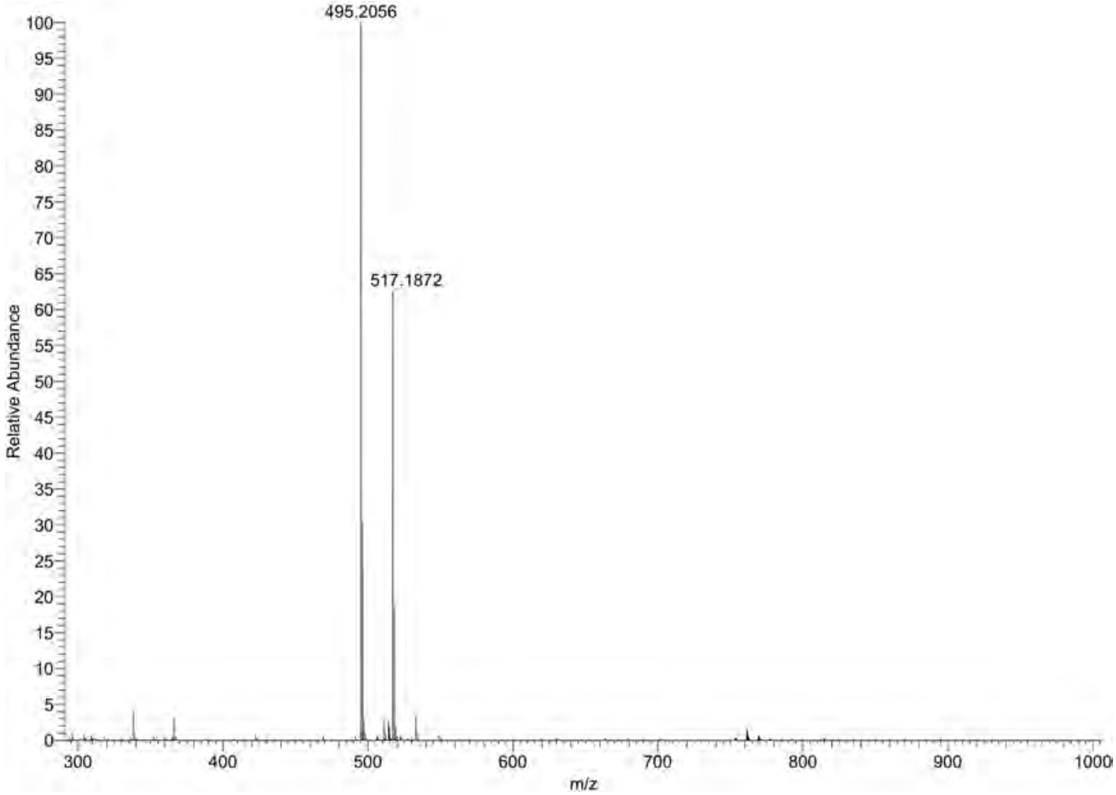


13 (41%)

Compound **13** was isolated in 41% yield (20 mg) as a white powder under the general condition A.



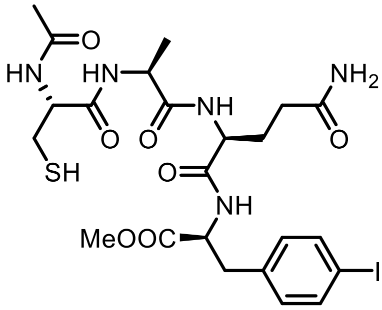
t_R = 6.39 min, 5% to 95% B for 10 min, then 95% B 10-15 min, λ = 254 nm



HRMS: Calcd for $C_{26}H_{30}N_4O_4S$ [M+H$^+$]: 495.2061; found: 495.2056

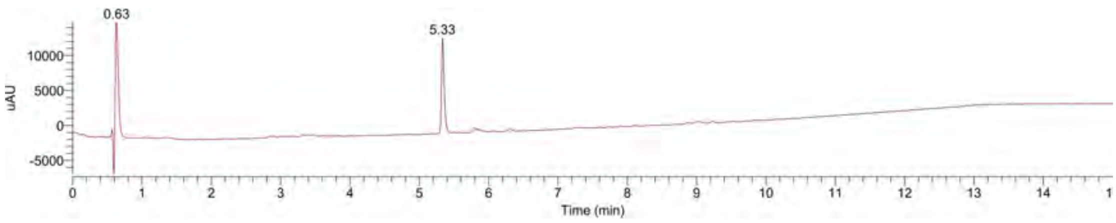
^{1}H NMR (400 MHz, MeOD) δ 7.72-7.49 (m, 4H), 7.47-7.36 (m, 4H), 7.32 (t, *J* = 7.6 Hz, 1H), 7.21 (d, *J* = 7.4 Hz, 1H), 6.73 (d, *J* = 15.6 Hz, 1H), 5.03 (q, *J* = 6.8 Hz, 1H), 4.80 (d, *J* = 14.6 Hz, 1H), 4.72 (dd, *J* = 8.4, 5.0 Hz, 1H), 4.01 (d, *J* = 14.2 Hz, 1H), 3.81-3.72 (m, 1H), 3.37 (d, *J* = 5.2 Hz, 1H), 3.28-3.19 (m, 1H), 3.15 (dd, *J* = 14.6, 8.4 Hz, 1H), 3.09-2.84 (m, 1H), 2.59-2.46 (m, 1H), 2.41 (s, 3H), 1.13 (d, *J* = 6.8 Hz, 3H).

^{13}C NMR (101 MHz, DMSO) δ 170.63, 170.30, 169.61, 164.81, 141.16, 139.65, 134.67, 129.60, 129.51, 128.94, 128.86, 128.17, 127.69, 127.56, 126.38, 121.21, 52.15, 48.26, 41.84, 35.49, 35.08, 34.70, 29.65, 12.99.

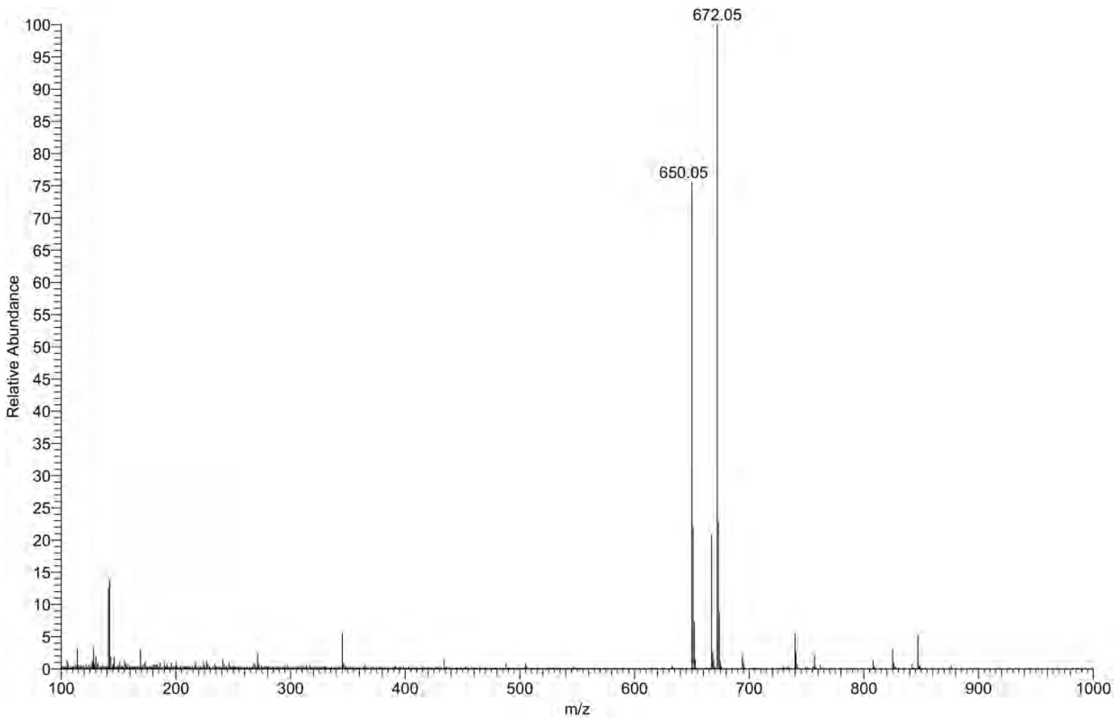


S14

Compound **S14** was prepared as a white solid in 86% yield from 2-Cl-Trt resin following the SPPS procedure.

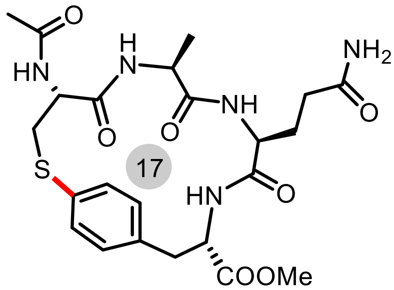


t_R = 5.33 min, 5% to 95% B for 10 min, then 95% B 10-15 min, λ = 254 nm



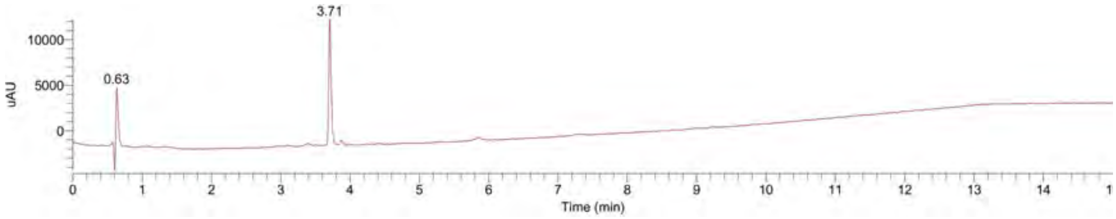
LRMS: $[M+H]^+$ 650.05; $[M+Na]^+$ 672.05.

^{1}H NMR (400 MHz, DMSO) δ 8.34-8.27 (m, 1H), 8.14 (d, *J* = 7.0 Hz, 1H), 8.08 (d, *J* = 7.8 Hz, 1H), 7.89 (d, *J* = 8.4 Hz, 1H), 7.61 (d, *J* = 7.8 Hz, 2H), 7.20 (s, 1H), 7.02 (d, *J* = 8.0 Hz, 2H), 6.75 (s, 1H), 4.50-4.41 (m, 1H), 4.41-4.32 (m, 1H), 4.31-4.17 (m, 2H), 3.59 (s, 3H), 3.01-2.86 (m, 2H), 2.79-2.61 (m, 2H), 2.11-2.03 (m, 2H), 1.87 (s, 3H), 1.85-1.78 (m, 1H), 1.75-1.63 (m, 1H), 1.20-1.11 (m, 3H).

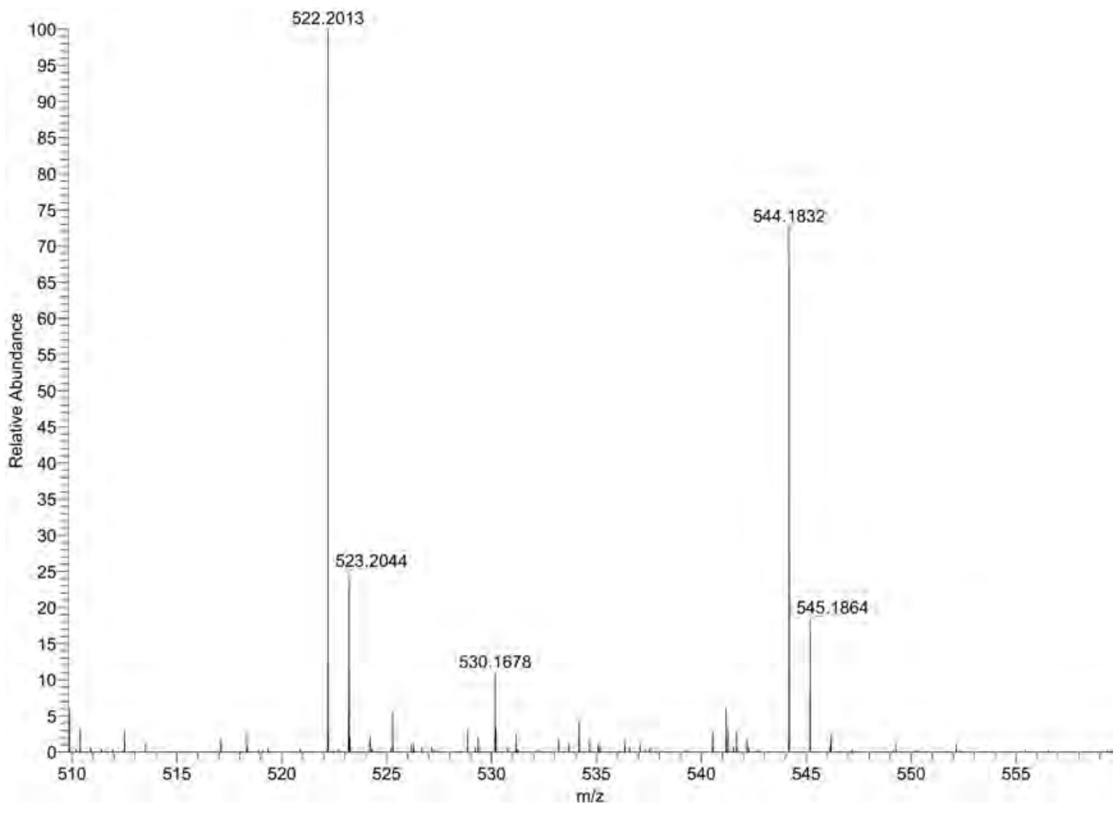


14 (67%)

Compound **14** was isolated in 67% yield (34 mg) as a white powder under the general condition A.



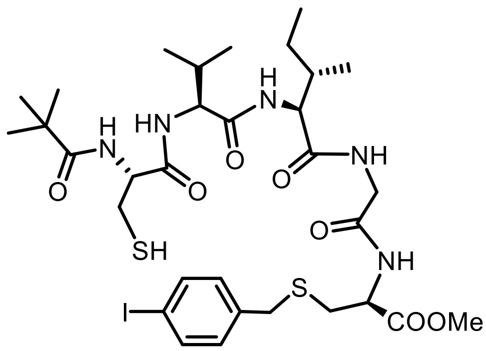
t_R = 3.71 min, 5% to 95% B for 10 min, then 95% B 10-15 min, λ = 254 nm



HRMS: Calcd for $C_{23}H_{31}N_5O_7S$ [M+H$^+$]: 522.2017; found: 522.2013

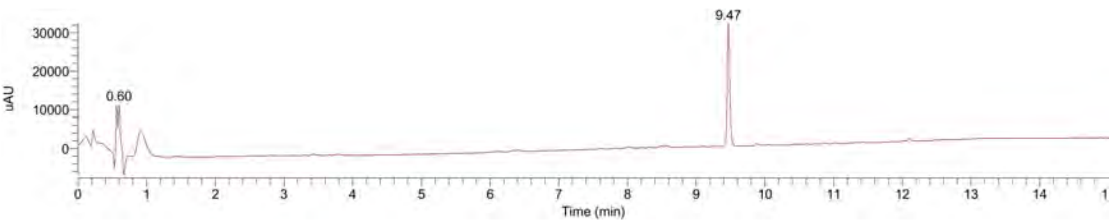
^{1}H NMR (400 MHz, DMSO) δ 8.21 (dd, *J* = 8.2, 4.8 Hz, 2H), 7.95 (d, *J* = 8.6 Hz, 1H), 7.43 (d, *J* = 7.4 Hz, 1H), 7.25 (s, 1H), 7.19 (d, *J* = 7.8 Hz, 2H), 7.09 (d, *J* = 7.8 Hz, 2H), 6.72 (s, 1H), 4.53 (t, J = 10.0 Hz, 1H), 4.35-4.23 (m, 1H), 4.14 (t, J = 7.8 Hz, 1H), 4.00 (q, J = 7.2, 6.8 Hz, 1H), 3.70 (s, 3H), 3.48 (dd, J = 15.2, 4.6 Hz, 1H), 3.17-3.10 (m, 1H), 2.87 (dd, J = 15.0, 4.4 Hz, 1H), 2.68 (t, J = 13.0 Hz, 1H), 1.97 (t, J = 7.4 Hz, 2H), 1.88 (s, 3H), 1.80-1.67 (m, 2H), 1.16 (d, J = 7.2 Hz, 3H).

^{13}C NMR (101 MHz, DMSO) δ 174.14, 172.07, 171.63, 170.66, 169.52, 169.46, 136.42, 133.33, 131.33, 130.32, 54.04, 53.10, 53.00, 52.61, 50.02, 37.43, 36.56, 31.53, 27.50, 22.93, 19.31.

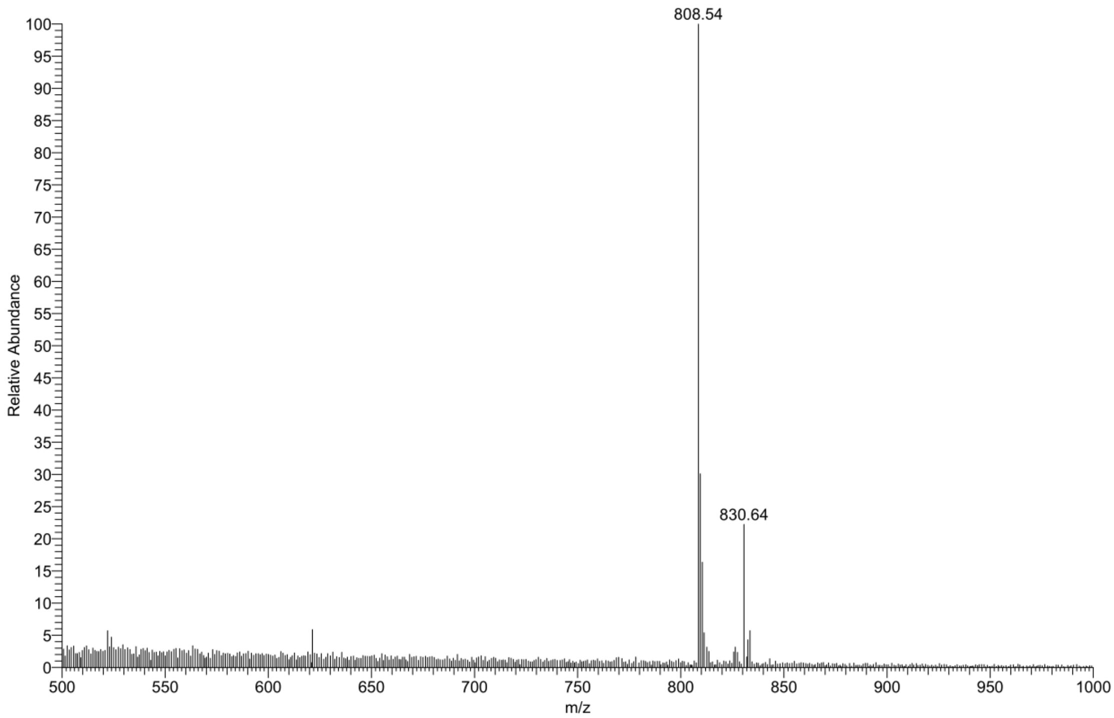


S15

Compound **S15** was prepared as a white solid in 87% yield from 2-Cl-Trt resin following the SPPS procedure.

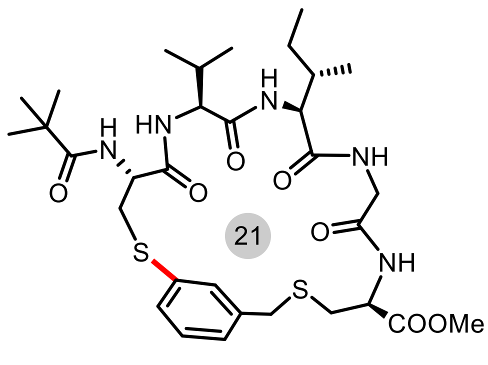


t_R = 9.47 min, 5% to 95% B for 10 min, then 95% B 10-15 min, λ = 254 nm



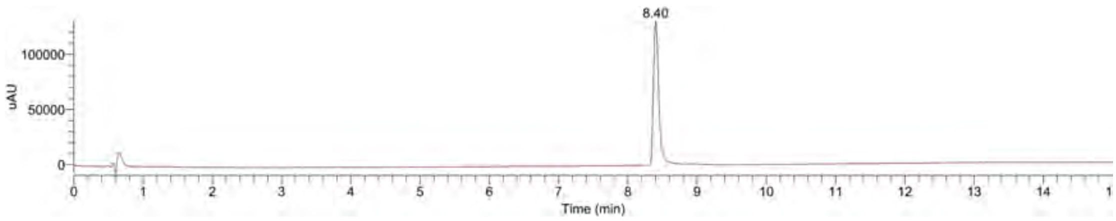
LRMS: [M+H] $^{+}$ 808.54; [M+Na] $^{+}$ 830.64.

^{1}H NMR (400 MHz, AcOD) δ 7.74 (s, 1H), 7.64 (d, *J* = 7.8 Hz, 1H), 7.36 (d, *J* = 7.6 Hz, 1H), 7.11 (t, *J* = 7.8 Hz, 1H), 4.86 (dd, *J* = 7.0, 5.2 Hz, 1H), 4.78 (t, *J* = 6.6 Hz, 1H), 4.54 (d, *J* = 8.2 Hz, 1H), 4.43 (d, *J* = 7.4 Hz, 1H), 4.16 (s, 2H), 3.78 (s, 3H), 3.72 (s, 2H), 3.01-2.89 (m, 2H), 2.88-2.78 (m, 2H), 2.12 (dd, *J* = 13.8, 7.0 Hz, 2H), 1.94-1.83 (m, 1H), 1.66-1.50 (m, 1H), 1.24 (s, 9H), 0.99-0.87 (m, 12H).

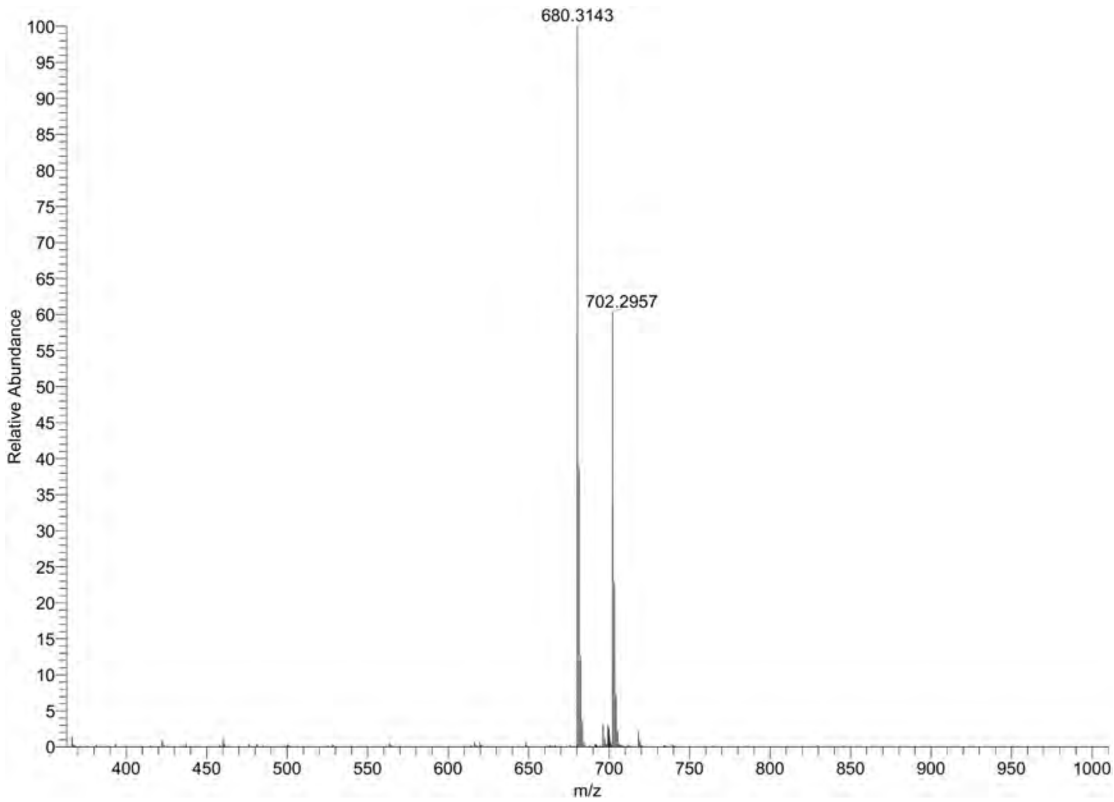


15 (78%)

Compound **15** was isolated in 78% yield (53 mg) as a white powder under the general condition A.



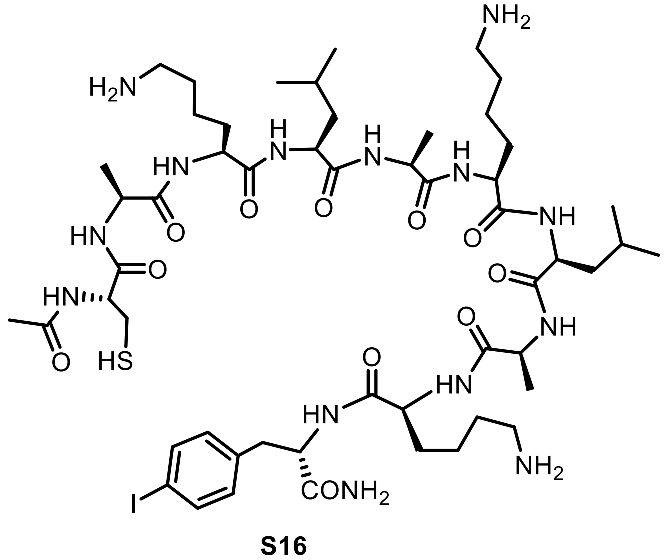
t_R = 8.40 min, 5% to 95% B for 10 min, then 95% B 10-15 min, λ = 254 nm



HRMS: Calcd for $C_{32}H_{49}N_5O_7S_2$ [M+H$^+$]: 680.3146; found: 680.3143

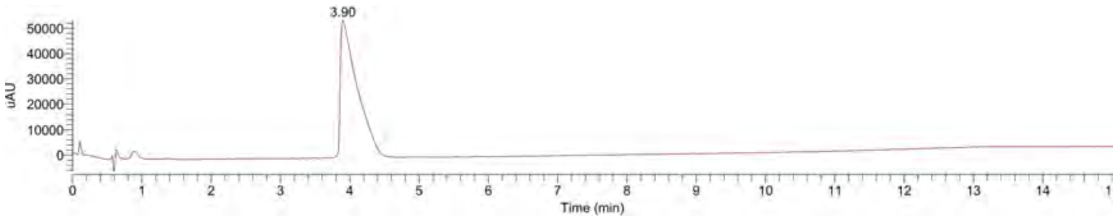
^{1}H NMR (400 MHz, AcOD) δ 7.60 (s, 1H), 7.29-7.19 (m, 3H), 4.85-4.80 (m, 1H), 4.80-4.74 (m, 1H), 4.48 (d, *J* = 7.2 Hz, 1H), 4.40 (d, *J* = 5.6 Hz, 1H), 4.21-4.07 (m, 2H), 3.94 (d, *J* = 12.0 Hz, 1H), 3.81 (s, 1H), 3.77 (s, 3H), 3.47 (dd, *J* = 13.8, 5.4 Hz, 1H), 3.33 (dd, *J* = 13.4, 9.2 Hz, 1H), 3.08 (d, *J* = 5.4 Hz, 2H), 2.36-2.20 (m, 1H), 1.92 (dd, *J* = 12.8, 5.0 Hz, 1H), 1.63-1.53 (m, 1H), 1.23 (d, *J* = 1.4 Hz, 9H), 1.01-0.89 (m, 12H).

^{13}C NMR (101 MHz, DMSO) δ 178.13, 171.71, 171.26, 171.17, 171.10, 169.29, 139.61, 136.94, 129.17, 128.34, 126.99, 126.23, 59.41, 57.16, 53.25, 52.57, 52.19, 42.26, 38.55, 37.26, 36.67, 34.41, 33.27, 30.10, 27.71, 24.70, 19.62, 18.32, 15.66, 11.41.

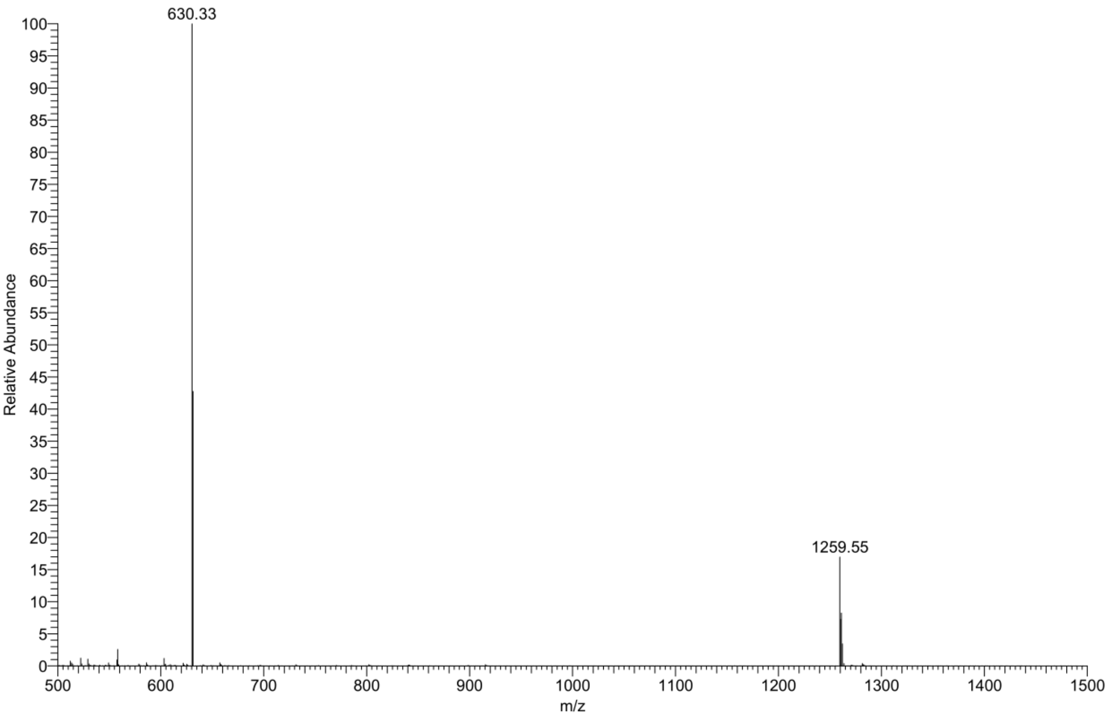


S16

Compound **S16** was prepared as a white solid in 85% yield from **Rink-amide AM resin** following the SPPS procedure.

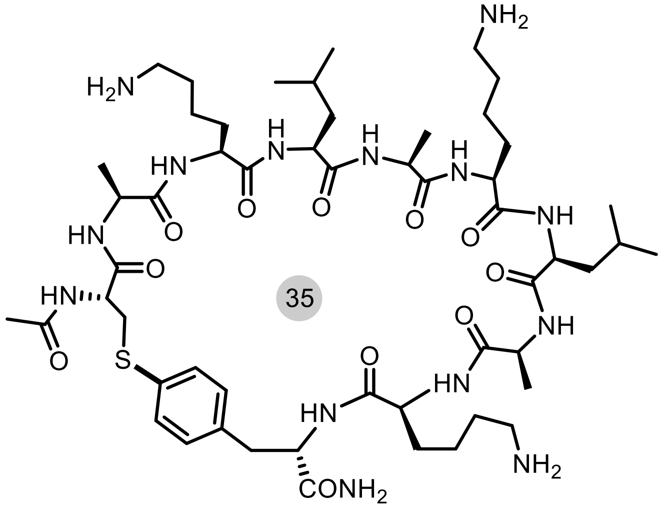


t_R = 3.90 min, 5% to 95% B for 10 min, then 95% B 10-15 min, λ = 254 nm



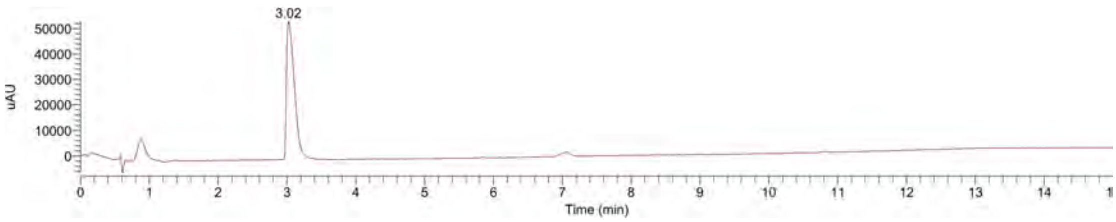
LRMS: $[M+H]^+$ 1259.55.

^{1}H NMR (400 MHz, 5%MeOD in DMSO) δ 7.56 (d, *J* = 7.8 Hz, 2H), 7.05 (d, *J* = 7.8 Hz, 2H), 4.47 (t, *J* = 7.0 Hz, 1H), 4.37-4.27 (m, 2H), 4.19-4.14 (m, 3H), 4.09 (t, *J* = 7.0 Hz, 3H), 2.81-2.64 (m, 9H), 1.89 (s, 3H), 1.69-1.58 (m, 5H), 1.54-1.43 (m, 12H), 1.35-1.28 (m, 3H), 1.23 (dd, *J* = 10.4, 6.8 Hz, 12H), 0.84 (d, *J* = 6.2 Hz, 6H), 0.79 (d, *J* = 6.2 Hz, 6H).

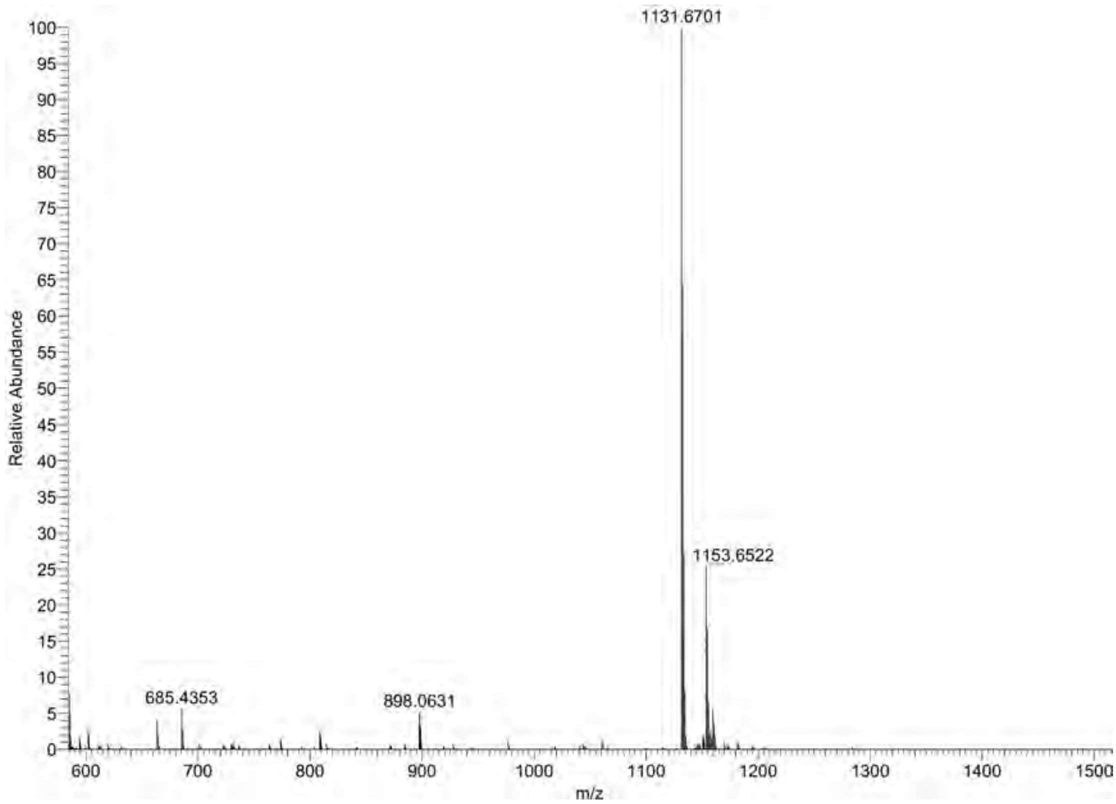


16 (41%)

Compound **16** was isolated in 41% yield (46 mg) as a white powder (TFA salt) under the general condition A.



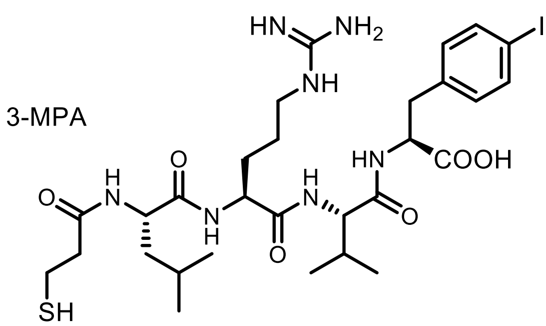
t_R = 3.02 min, 5% to 95% B for 10 min, then 95% B 10-15 min, λ = 254 nm



HRMS: Calcd for $C_{53}H_{90}N_{14}O_{11}S$ [M+H$^+$]: 1131.6707; found: 1131.6701

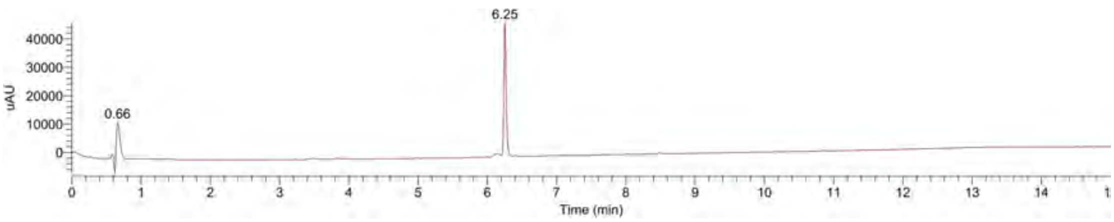
^{1}H NMR (400 MHz, MeOD) δ 7.34 (d, *J* = 7.8 Hz, 2H), 7.21 (d, *J* = 7.8 Hz, 2H), 4.52-4.43 (m, 1H), 4.36-4.28 (m, 2H), 4.27-4.18 (m, 3H), 4.17-4.07 (m, 3H), 3.23 (dd, *J* = 14.0, 7.8 Hz, 1H), 3.15 (dd, *J* = 14.2, 4.4 Hz, 1H), 3.05 (d, *J* = 9.0 Hz, 1H), 3.00-2.84 (m, 6H), 2.05 (s, 3H), 1.93-1.79 (m, 5H), 1.79-1.59 (m, 12H), 1.57-1.44 (m, 6H), 1.40 (d, *J* = 8.0 Hz, 9H), 0.92 (dd, *J* = 10.2, 5.8 Hz, 6H), 0.85 (dd, *J* = 15.0, 6.4 Hz, 6H).

^{13}C NMR (101 MHz, DMSO) δ 173.37, 172.98, 172.81, 172.70, 172.59, 172.31, 171.81, 170.65, 170.39, 136.23, 134.03, 130.33, 128.68, 79.75, 79.63, 79.42, 79.09, 54.39, 53.68, 53.37, 53.09, 52.18, 49.28, 49.05, 37.05, 35.68, 31.26, 30.81, 29.53, 27.21, 24.61, 23.42, 22.95, 22.60, 21.87, 21.78, 18.05, 17.71.

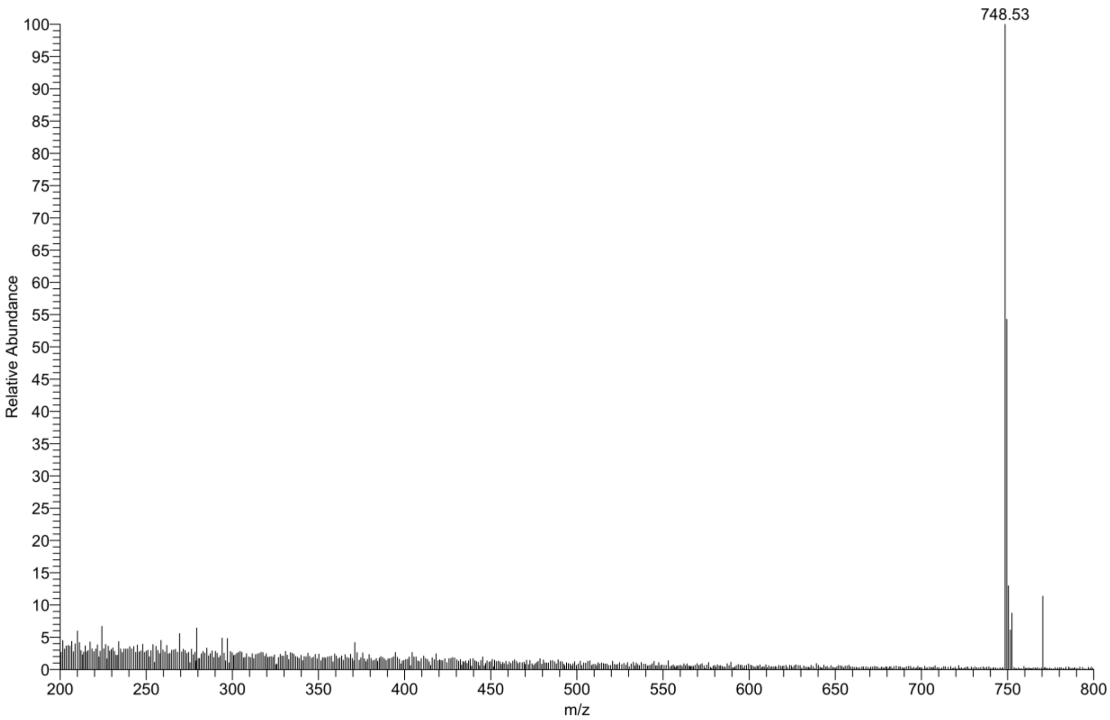


S17

Compound **S17** was prepared as a white solid in 90% yield from 2-Cl-Trt resin following the SPPS procedure.

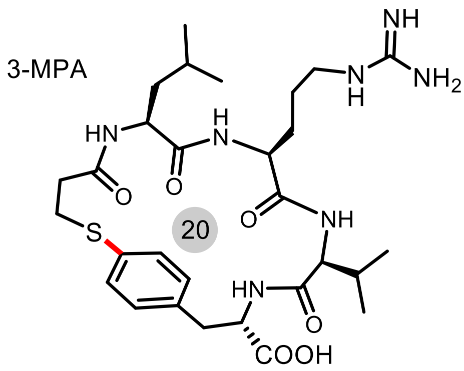


t_R = 6.25 min, 5% to 95% B for 10 min, then 95% B 10-15 min, λ = 254 nm



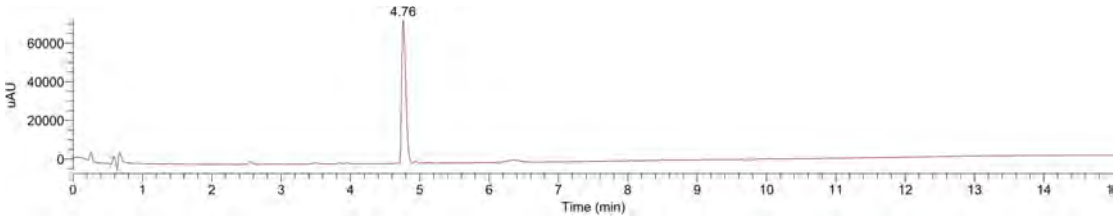
LRMS: $[M+H]^+$ 748.53.

^{1}H NMR (400 MHz, MeOD) δ 7.63 (d, *J* = 8.0 Hz, 2H), 7.06 (d, *J* = 8.0 Hz, 2H), 4.66 (dd, *J* = 8.6, 4.8 Hz, 1H), 4.46-4.34 (m, 2H), 4.18 (d, *J* = 7.2 Hz, 1H), 3.28-3.07 (m, 4H), 3.03-2.86 (m, 2H), 2.79-2.73 (m, 1H), 2.58 (t, *J* = 6.6 Hz, 1H), 2.09-1.99 (m, 1H), 1.80 (dd, *J* = 14.4, 6.6 Hz, 1H), 1.77-1.68 (m, 2H), 1.67-1.54 (m, 4H), 1.01-0.88 (m, 12H).

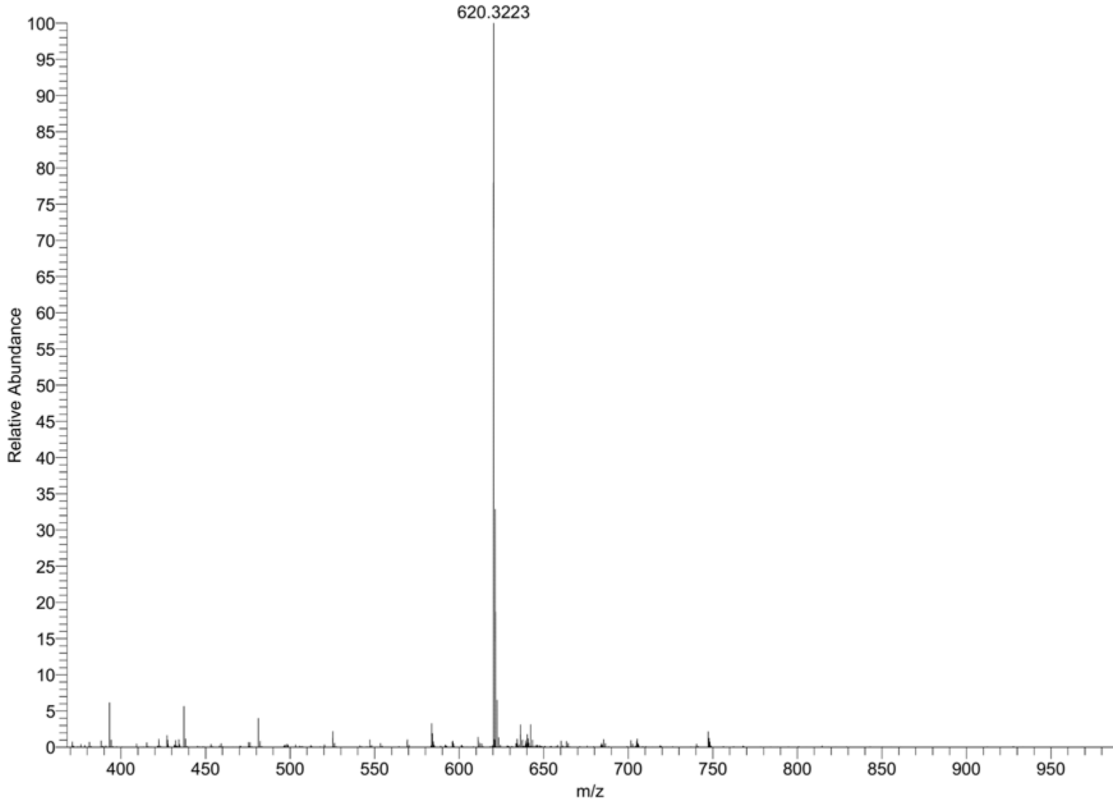


17 (45%)

Compound **17** was isolated in 45% yield (27 mg) as a white powder (TFA salt) under the general condition A.



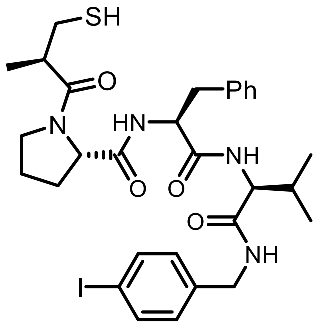
t_R = 4.76 min, 5% to 95% B for 10 min, then 95% B 10-15 min, λ = 254 nm



HRMS: Calcd for $C_{29}H_{45}N_7O_6S$ [M+H$^+$]: 620.3225; found: 620.3223

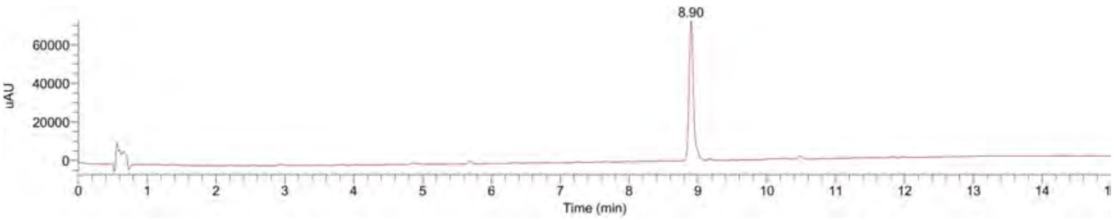
^{1}H NMR (400 MHz, MeOD) δ 7.32 (d, *J* = 7.8 Hz, 2H), 7.18 (d, *J* = 7.8 Hz, 2H), 4.57

(dd, J = 10.0, 4.8 Hz, 1H), 4.38 (d, J = 11.6 Hz, 1H), 4.24 (d, J = 5.4 Hz, 1H), 4.19 (d, J = 8.4 Hz, 1H), 3.39 (d, J = 2.4 Hz, 2H), 3.22 (d, J = 13.4 Hz, 1H), 2.94-2.84 (m, 2H), 2.76-2.65 (m, 2H), 2.64-2.53 (m, 1H), 2.02 (d, J = 6.4 Hz, 2H), 1.94-1.82 (m, 1H), 1.81-1.67 (m, 2H), 1.67-1.58 (m, 2H), 1.42 (dd, J = 15.4, 8.6 Hz, 1H), 1.02-0.86 (m, 12H). **^{13}C NMR (101 MHz, DMSO)** δ 173.92, 171.95, 171.74, 171.70, 170.41, 157.18, 136.22, 133.80, 130.61, 129.33, 59.61, 51.42, 50.90, 40.94, 35.84, 30.15, 24.64, 23.45, 21.64, 19.56, 19.37.

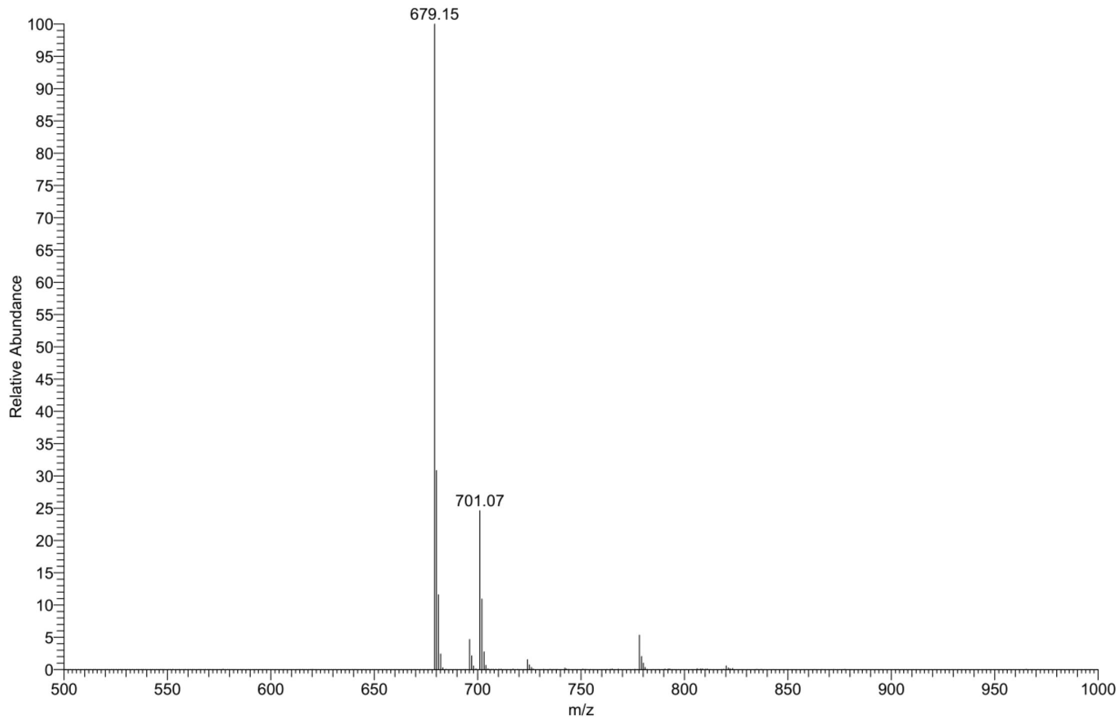


S18

Compound **S18** was prepared as from 2-Cl-Trt resin following the SPPS procedure. 4-iodobenzylamine was coupled, following the general amide coupling procedure to give compound **S18** as white solid in 87% yield.

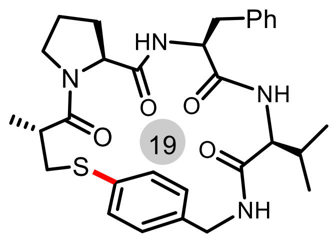


t_R = 8.90 min, 5% to 95% B for 10 min, then 95% B 10-15 min, λ = 254 nm



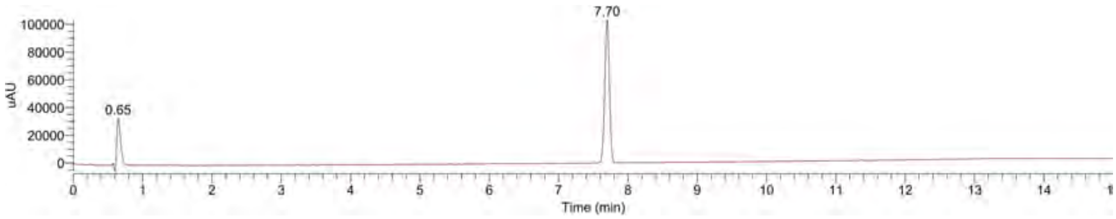
LRMS: [M+H] $^+$ 679.15; [M+Na] $^+$ 701.07.

^{1}**H NMR (400 MHz, MeOD)** δ 7.67 (s, 1H), 7.59 (d, *J* = 7.8 Hz, 1H), 7.30-7.25 (m, 2H), 7.22-7.17 (m, 4H), 7.08 (t, *J* = 7.8 Hz, 1H), 4.58 (t, *J* = 7.0 Hz, 1H), 4.40 (dd, *J* = 8.6, 3.8 Hz, 1H), 4.33-4.27 (m, 2H), 4.17 (dd, *J* = 13.4, 7.2 Hz, 1H), 3.78-3.57 (m, 2H), 3.33-3.27 (m, 1H), 3.18-3.02 (m, 2H), 2.90-2.62 (m, 2H), 2.45 (dd, *J* = 13.2, 5.4 Hz, 1H), 2.13-2.00 (m, 2H), 1.95-1.85 (m, 2H), 1.13 (d, *J* = 6.8 Hz, 3H), 0.91 (d, *J* = 6.8 Hz, 6H).

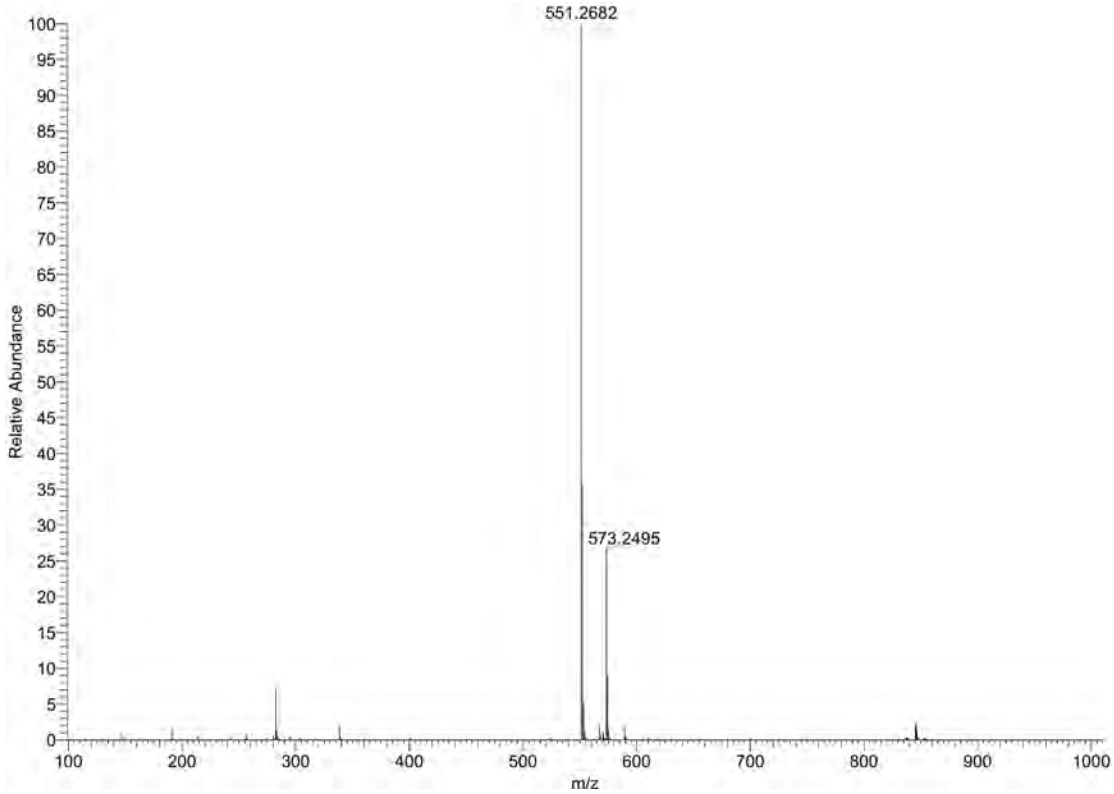


18 (52%)

Compound **18** was isolated in 52% yield (28 mg) as a white powder under the general condition A.



t_R = 7.70 min, 5% to 95% B for 10 min, then 95% B 10-15 min, λ = 254 nm

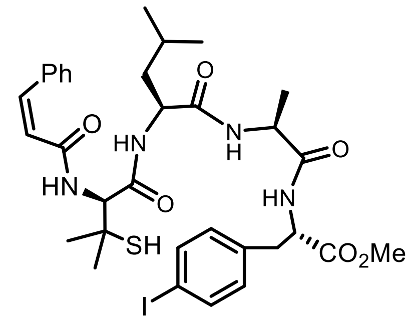


HRMS: Calcd for $C_{30}H_{38}N_4O_4S$ [M+H$^+$]: 551.2687; found: 551.2682

18 should be a mixture of conformational isomers determined by ^{1}H NMR in different deuterated solvents (see ^{1}H NMR spectrum).

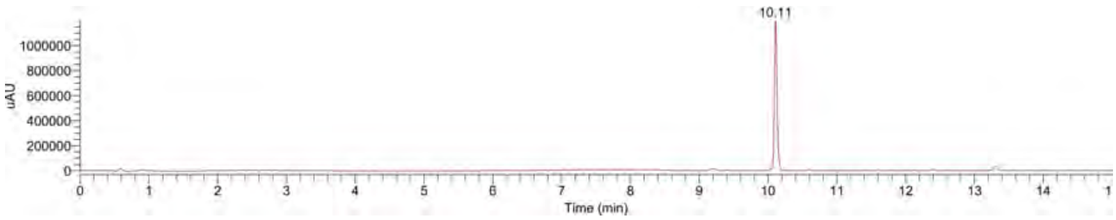
^{1}H NMR (400 MHz, MeOD) δ 7.66 (s, 1H), 7.30-7.19 (m, 6H), 7.18 (d, *J* = 6.0 Hz, 1H), 7.06 (d, *J* = 5.6 Hz, 1H), 4.94 (d, *J* = 14.8 Hz, 1H), 4.67 (d, *J* = 3.8 Hz, 1H), 4.26 (dd, *J* = 9.6, 4.6 Hz, 1H), 3.87 (d, *J* = 14.6 Hz, 2H), 3.62 (q, *J* = 8.6, 8.0 Hz, 1H), 3.49-3.37 (m, 2H), 3.20 (dd, *J* = 14.4, 4.8 Hz, 1H), 3.08 (s, 1H), 2.93 (d, *J* = 14.2 Hz, 1H), 2.84-2.75 (m, 1H), 2.63-2.47 (m, 1H), 1.93 (dd, *J* = 18.0, 6.6 Hz, 2H), 1.84 (d, *J* = 6.6 Hz, 1H), 1.74-1.61 (m, 1H), 1.19 (d, *J* = 6.8 Hz, 3H), 0.97 (dd, *J* = 27.0, 6.8 Hz, 6H).

^{13}C NMR (101 MHz, Acetone) δ 175.50, 173.00, 172.92, 172.31, 172.23, 170.95, 170.88, 140.02, 138.90, 135.73, 135.68, 131.04, 129.62, 129.32, 129.28, 129.18, 128.81, 127.38, 127.18, 127.14, 63.10, 63.07, 58.22, 58.16, 58.07, 57.99, 48.48, 43.54, 43.43, 40.72, 36.69, 36.64, 36.58, 25.39, 20.24, 18.37, 17.55.

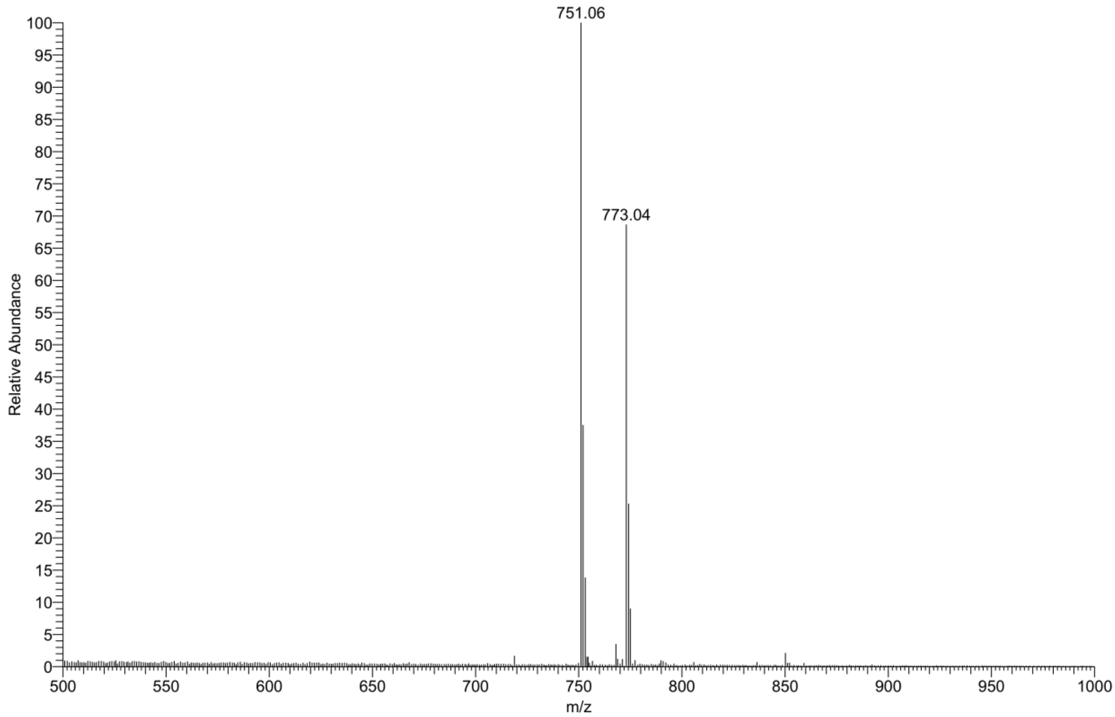


S19

Compound **S19** was prepared as a white solid in 91% yield from 2-Cl-Trt resin following the SPPS procedure.

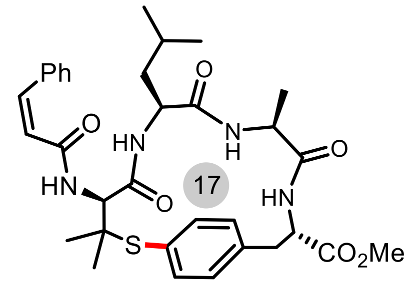


t_R = 10.11 min, 5% to 95% B for 10 min, then 95% B 10-15 min, λ = 254 nm



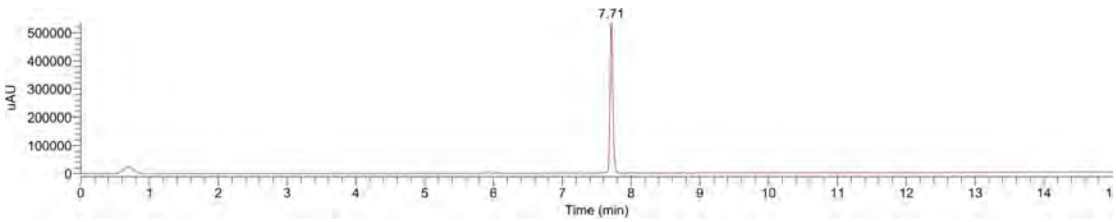
LRMS: [M+H] $^+$ 751.06; [M+Na] $^+$ 773.04.

^{1}H NMR (400 MHz, AcOD) δ 7.73 (d, *J* = 15.8 Hz, 1H), 7.66-7.55 (m, 4H), 7.46-7.36 (m, 3H), 6.94 (d, *J* = 8.2 Hz, 2H), 6.84 (d, *J* = 15.8 Hz, 1H), 4.98 (s, 1H), 4.82 (dd, *J* = 7.2, 5.4 Hz, 1H), 4.65 (q, *J* = 7.0 Hz, 1H), 4.59 (dd, *J* = 10.4, 4.6 Hz, 1H), 3.73 (s, 3H), 3.18-3.09 (m, 1H), 2.99 (dd, *J* = 14.0, 7.4 Hz, 1H), 1.80 (dd, *J* = 12.8, 7.8 Hz, 1H), 1.76-1.67 (m, 1H), 1.58 (dd, *J* = 9.4, 4.4 Hz, 1H), 1.54 (s, 3H), 1.44 (s, 3H), 1.36 (d, *J* = 7.0 Hz, 3H), 0.98 (dd, *J* = 14.8, 6.4 Hz, 6H).

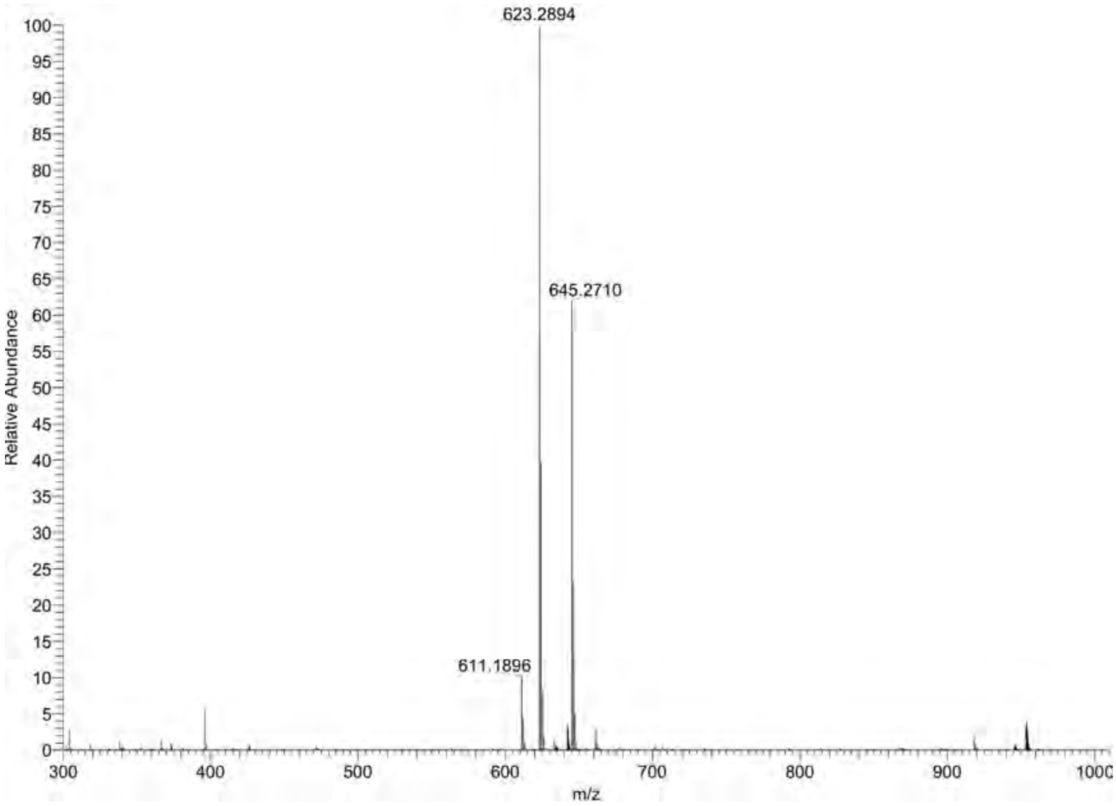


19 (81%)

Compound **19** was isolated in 81% yield (50 mg) as a white powder under the general condition B.



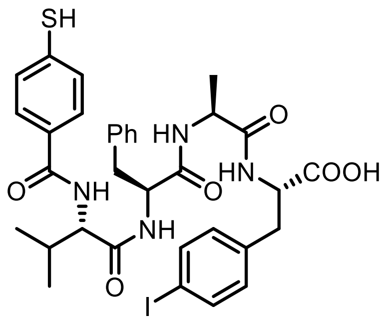
t_R = 7.71 min, 5% to 95% B for 10 min, then 95% B 10-15 min, λ = 254 nm



HRMS: Calcd for $C_{33}H_{42}N_4O_6S$ [M+H$^+$]: 623.2898; found: 623.2894

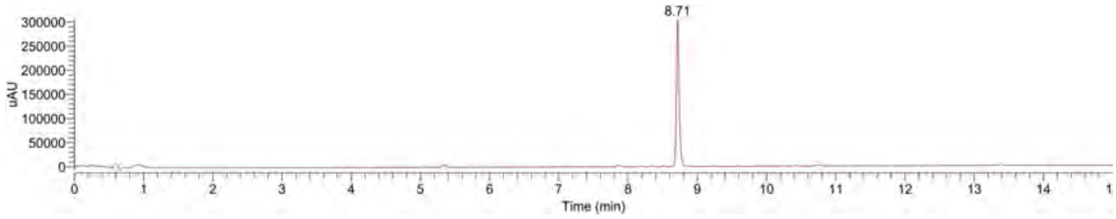
^{1}H NMR (400 MHz, MeOD) δ 7.61-7.54 (m, 3H), 7.47-7.36 (m, 5H), 7.10 (d, *J* = 7.6 Hz, 2H), 6.83 (d, *J* = 15.6 Hz, 1H), 4.70-4.59 (m, 2H), 4.35 (dd, *J* = 9.2, 4.4 Hz, 2H), 3.80 (s, 3H), 3.26 (d, *J* = 3.0 Hz, 1H), 2.71 (t, *J* = 12.6 Hz, 1H), 1.62 (d, *J* = 10.0 Hz, 1H), 1.58 (s, 3H), 1.54-1.43 (m, 2H), 1.22 (t, *J* = 3.5 Hz, 6H), 0.86 (dd, *J* = 25.0, 6.0 Hz, 6H).

^{13}C NMR (101 MHz, DMSO) δ 171.96, 171.46, 171.23, 169.45, 165.21, 139.85, 138.75, 137.91, 135.30, 130.05, 129.75, 129.44, 127.98, 122.13, 64.07, 53.37, 52.68, 49.53, 48.72, 41.67, 37.63, 30.45, 24.41, 24.28, 23.60, 22.02, 17.89.

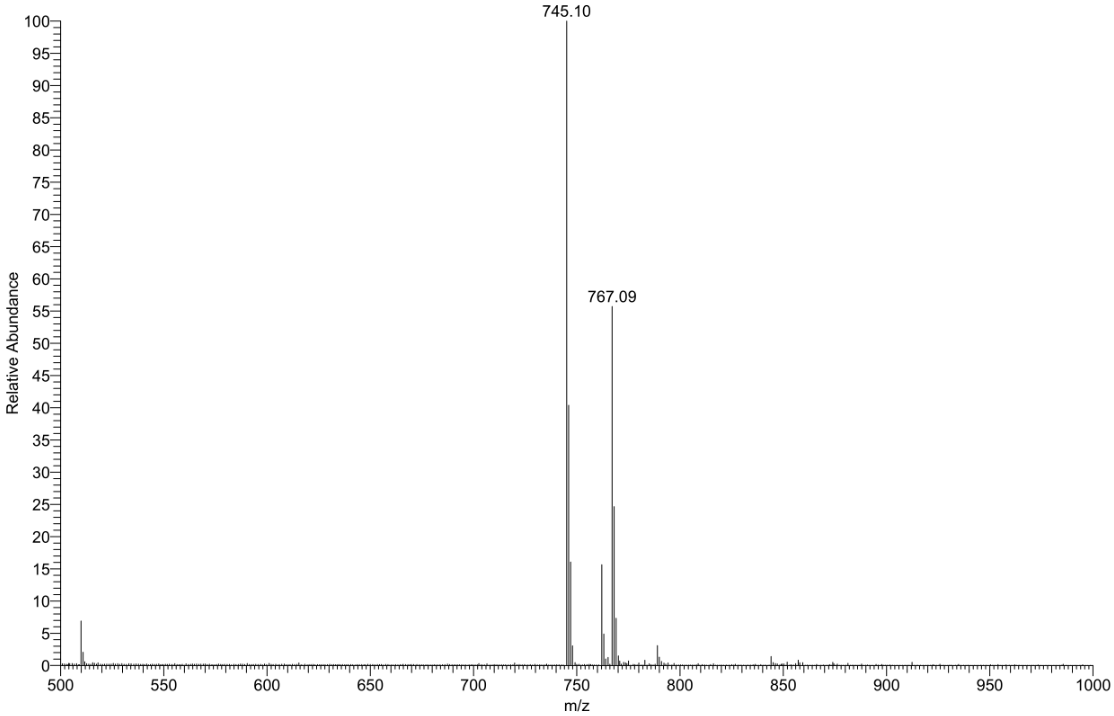


S20

Compound **S20** was prepared as a white solid in 89% yield from 2-Cl-Trt resin following the SPPS procedure.

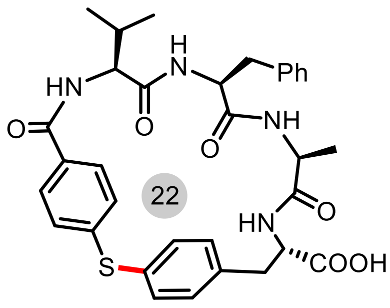


t_R = 8.71 min, 5% to 95% B for 10 min, then 95% B 10-15 min, λ = 254 nm



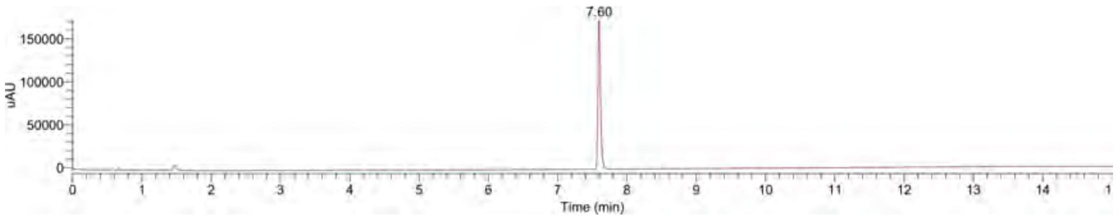
LRMS: [M+H] $^+$ 745.10; [M+Na] $^+$ 767.09.

^{1}H NMR (400 MHz, MeOD) δ 8.84 (d, *J* = 10.0 Hz, 2H), 8.76 (t, *J* = 9.0 Hz, 2H), 8.48 (d, *J* = 8.1 Hz, 1H), 8.33 (d, *J* = 8.1 Hz, 2H), 8.09 (d, *J* = 8.4 Hz, 2H), 7.98-7.14 (m, 2H), 7.90-7.81 (m, 2H), 7.75 (d, *J* = 8.2 Hz, 1H), 5.42-5.33 (m, 1H), 5.32-5.15 (m, 1H), 5.15-5.04 (m, 1H), 4.97 (t, *J* = 8.2 Hz, 1H), 3.84-3.73 (m, 2H), 3.67 (dd, *J* = 13.8, 8.2 Hz, 1H), 3.58 (dd, *J* = 14.0, 9.4 Hz, 1H), 2.80 (q, *J* = 7.0 Hz, 1H), 1.97 (d, *J* = 7.0 Hz, 3H), 1.57 (dd, *J* = 27.8, 6.6 Hz, 6H).

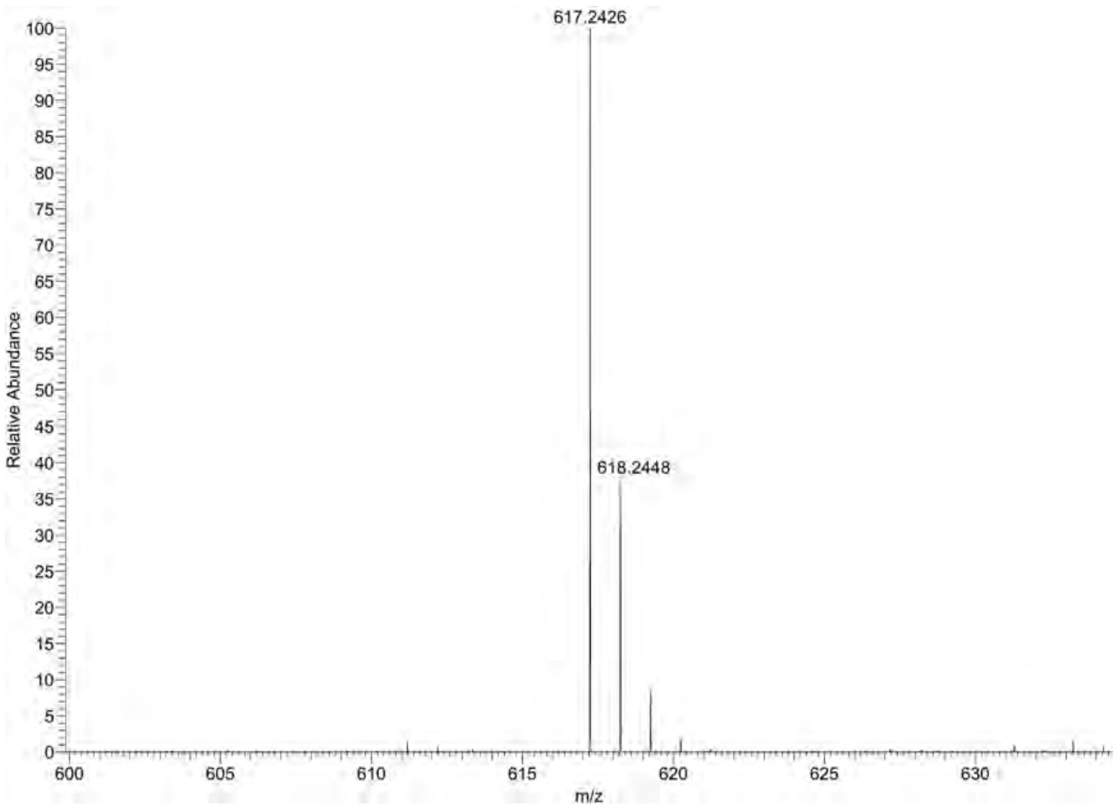


20 (30%)

Compound **20** was isolated in 30% yield (18 mg) as a white powder under the general condition A.

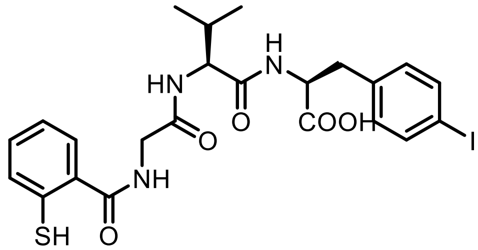


t_R = 7.60 min, 5% to 95% B for 10 min, then 95% B 10-15 min, λ = 254 nm



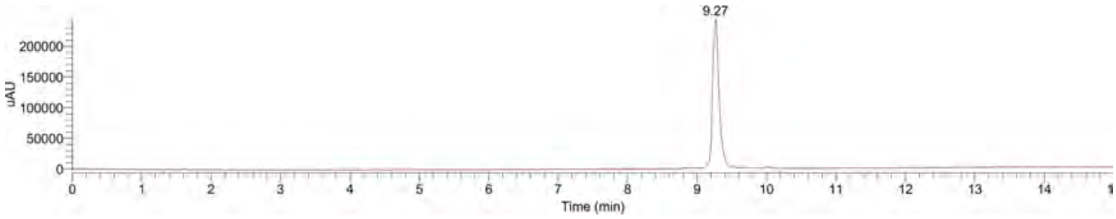
HRMS: Calcd for $C_{33}H_{36}N_4O_6S$ [M+H$^+$]: 617.2428; found: 617.2426

^{1}H NMR (400 MHz, MeOD) δ 7.66 (d, *J* = 8.2 Hz, 2H), 7.34 (s, 4H), 7.18 (d, *J* = 6.8 Hz, 4H), 7.11 (d, *J* = 6.6 Hz, 1H), 6.90 (d, *J* = 8.0 Hz, 2H), 4.64 (dd, *J* = 10.8, 4.4 Hz, 1H), 4.37 (d, J = 11.6 Hz, 1H), 3.95 (d, J = 9.6 Hz, 2H), 3.35-3.25 (m, 2H), 2.86-2.71 (m, 1H), 2.66 (dd, J = 14.0, 10.8 Hz, 1H), 1.71-1.57 (m, 1H), 1.35 (d, J = 7.2 Hz, 3H), 0.82 (d, J = 6.4 Hz, 3H), 0.45 (d, J = 6.6 Hz, 3H).

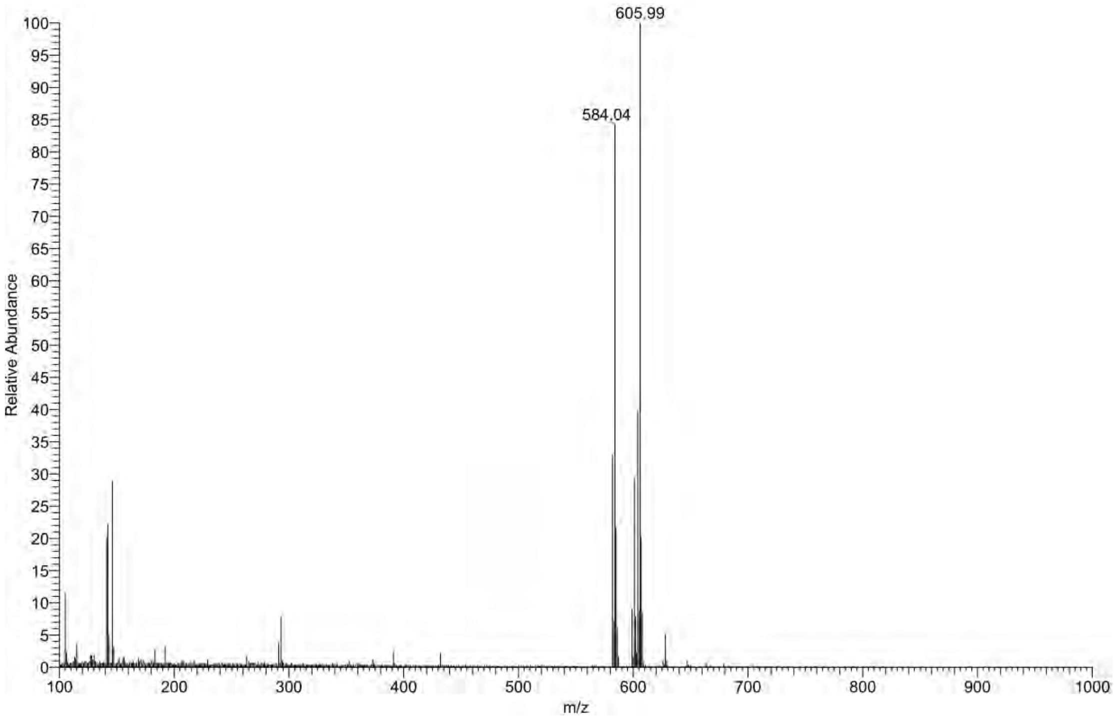


S21

Compound **S21** was prepared as a white solid in 93% yield from 2-Cl-Trt resin following the SPPS procedure.



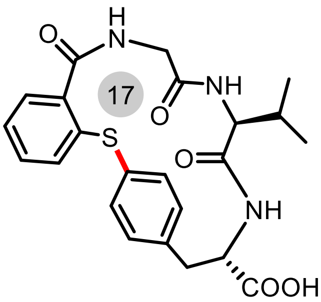
t_R = 9.27 min, 5% to 95% B for 10 min, then 95% B 10-15 min, λ = 254 nm



LRMS: $[M+H]^+$ 584.04; $[M+Na]^+$ 605.99.

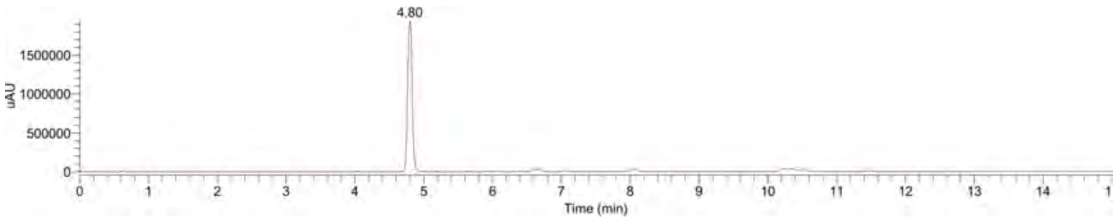
^{1}H NMR (400 MHz, MeOD) δ 7.77 (d, J = 7.6 Hz, 1H), 7.69 (dd, J = 7.6, 1.2 Hz, 1H), 7.58 (d, J = 8.2 Hz, 2H), 7.43-7.36 (m, 1H), 7.35-7.22 (m, 1H), 7.01 (d, J = 8.2

Hz, 2H), 4.65 (dd, J = 8.4, 5.0 Hz, 1H), 4.33-4.22 (m, 1H), 4.07 (s, 2H), 3.14 (dd, J = 13.4, 4.6 Hz, 1H), 2.95 (dd, J = 13.8, 8.6 Hz, 1H), 2.06 (dd, J = 14.4, 7.6 Hz, 1H), 0.91 (dd, J = 15.4, 6.8 Hz, 6H).

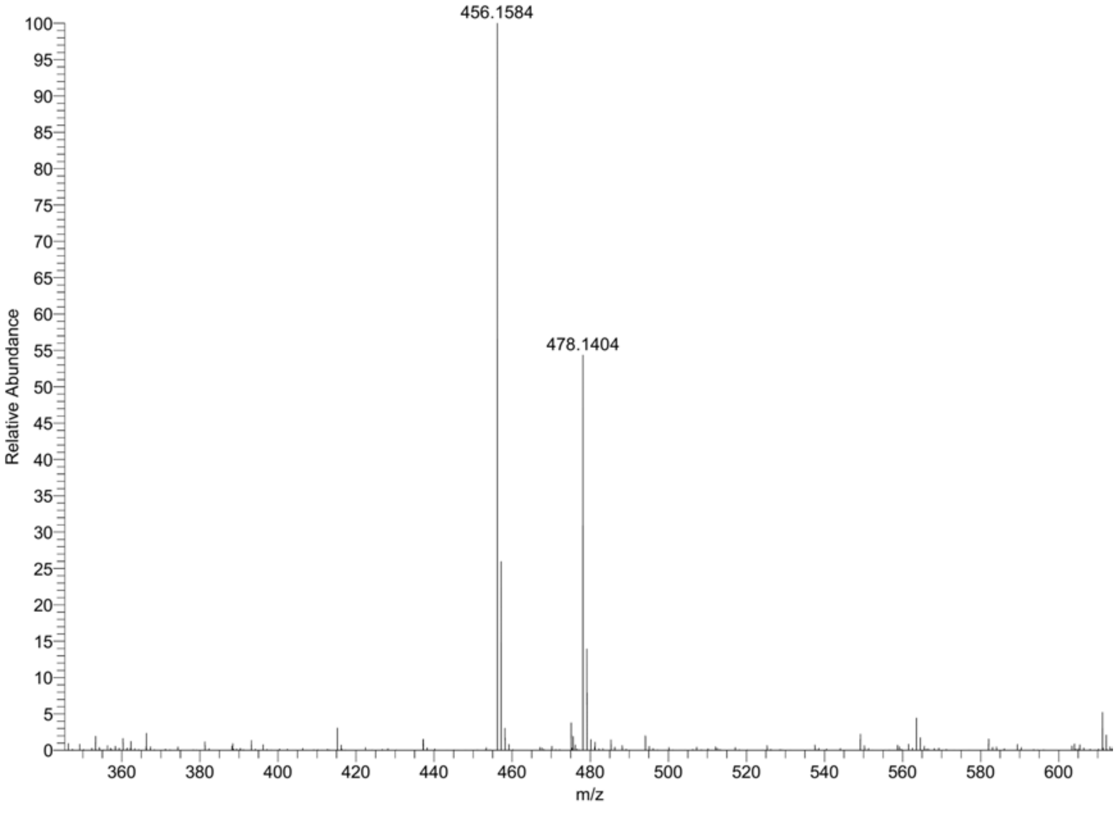


21 (71%)

Compound **21** was isolated in 71% yield (32 mg) as a white powder under the general condition A (6 h).



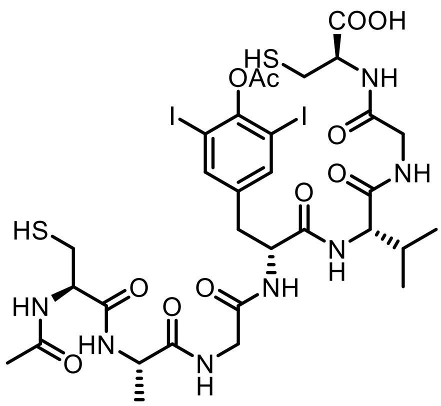
t_R = 4.80 min, 5% to 95% B for 10 min, then 95% B 10-15 min, λ = 254 nm



HRMS: Calcd for $C_{23}H_{25}N_3O_5S$ [M+H$^+$]: 456.1588; found: 456.1584

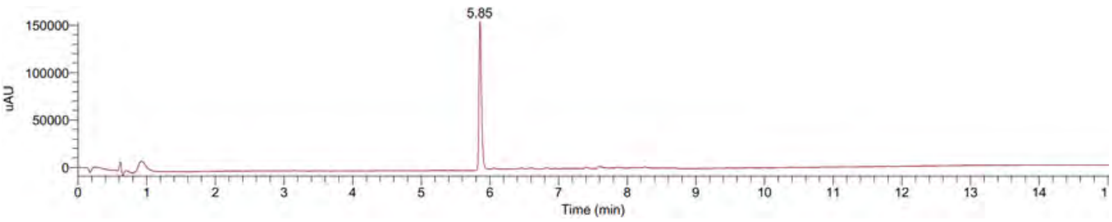
^{1}H NMR (400 MHz, DMSO) δ 8.14 (d, *J* = 8.9 Hz, 1H), 7.88 (d, *J* = 8.8 Hz, 1H), 7.80 (s, 1H), 7.74 (d, *J* = 5.9 Hz, 1H), 7.61-7.50 (m, 3H), 7.03 (d, *J* = 8.1 Hz, 2H), 6.85 (d, *J* = 8.1 Hz, 2H), 4.53 (t, *J* = 9.0 Hz, 1H), 3.98-3.86 (m, 2H), 3.65 (dd, *J* = 15.8, 4.7 Hz, 1H), 3.10 (d, *J* = 10.6 Hz, 1H), 2.63 (t, *J* = 12.8 Hz, 1H), 1.88-1.73 (m, 1H), 0.81 (t, *J* = 6.0 Hz, 6H).

^{13}C NMR (101 MHz, DMSO) δ 173.58, 167.84, 166.79, 141.39, 137.57, 136.59, 133.97, 131.06, 130.51, 130.09, 129.85, 129.57, 127.62, 58.54, 42.84, 29.82, 19.54, 19.18, 18.50.

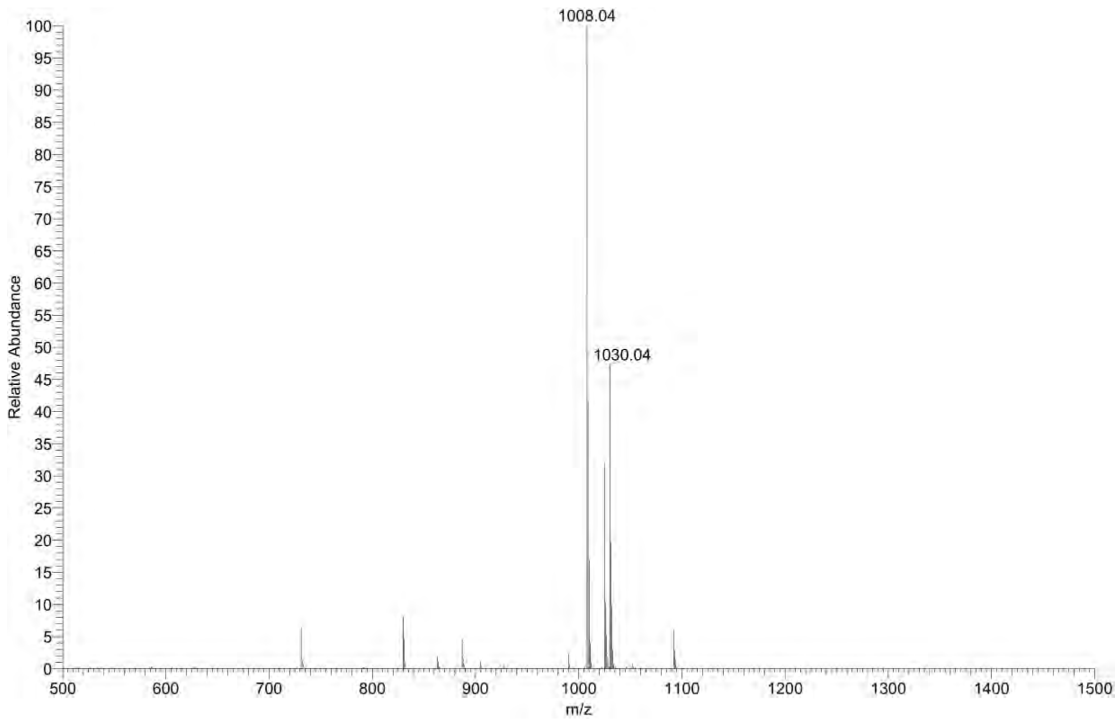


22

Compound **22** was prepared as a white solid in 88% yield from 2-Cl-Trt resin following the SPPS procedure.

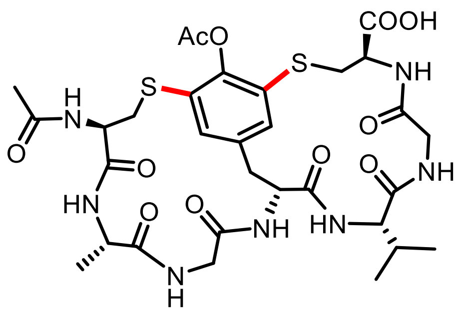


t_R = 5.85 min, 5% to 95% B for 10 min, then 95% B 10-15 min, λ = 254 nm



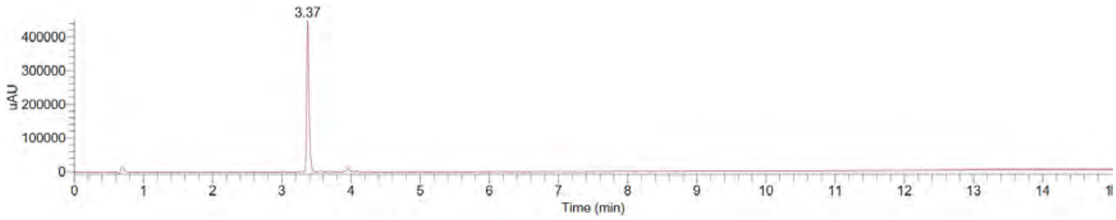
LRMS: [M+H] $^+$ 1008.04; [M+Na] $^+$ 1030.04.

^{1}H NMR (400 MHz, DMSO) δ 7.78 (s, 2H), 4.66-4.56 (m, 1H), 4.48-4.40 (m, 1H), 4.40-4.34 (m, 1H), 4.23 (t, *J* = 7.0 Hz, 1H), 4.17 (dd, *J* = 8.6, 6.6 Hz, 1H), 3.86 (dd, *J* = 16.6, 5.8 Hz, 1H), 3.79-3.68 (m, 2H), 3.60 (dd, *J* = 16.8, 5.4 Hz, 1H), 2.99-2.91 (m, 1H), 2.89-2.83 (m, 1H), 2.81-2.71 (m, 2H), 2.68-2.60 (m, 1H), 2.42 (t, *J* = 8.4 Hz, 1H), 2.35 (s, 3H), 2.04-1.94 (m, 1H), 1.86 (s, 3H), 1.09 (t, *J* = 7.0 Hz, 3H), 0.88 (dd, *J* = 6.8, 2.0 Hz, 6H).

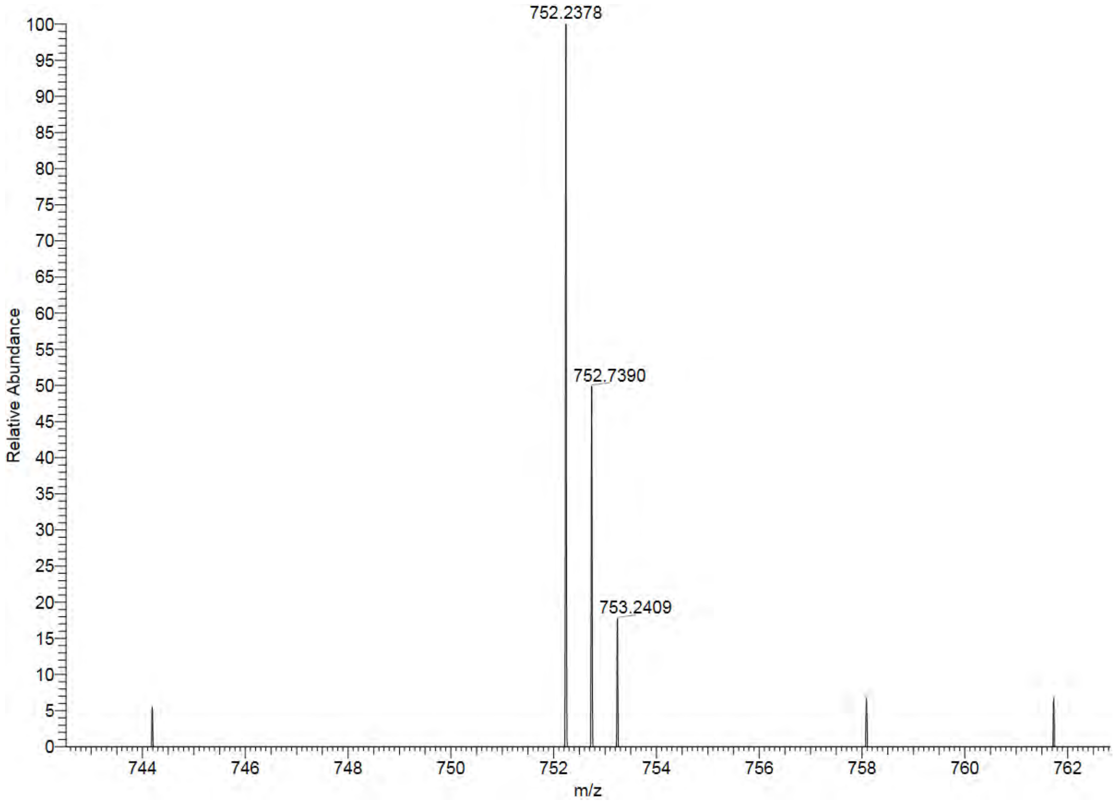


23 (56%)

Compound **23** was isolated in 56% yield (42 mg) as a white powder under the general condition A (10 mol% catalyst, 3 equiv DIPEA, 16h).



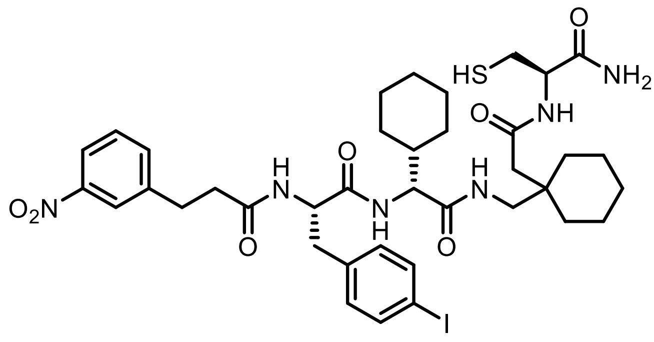
t_R = 3.37 min, 5% to 95% B for 10 min, then 95% B 10-15 min, λ = 254 nm



HRMS: Calcd for $C_{31}H_{41}N_7O_{11}S_2$ [M+H$^+$]: 752.2378; found: 752.2378.

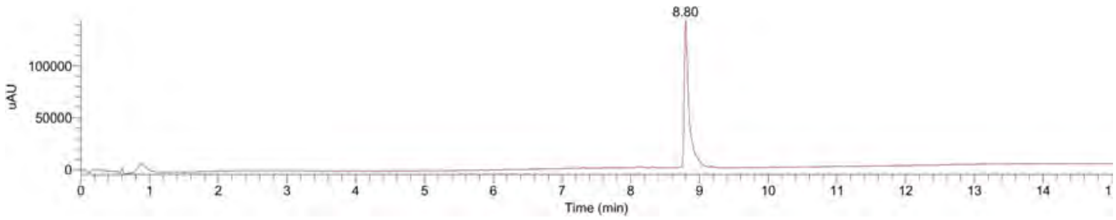
^{1}H NMR (400 MHz, DMSO) δ 7.21 (s, 1H), 7.01 (s, 1H), 5.28-5.09 (m, 1H), 4.98-4.80 (m, 1H), 4.50 (d, *J* = 7.2 Hz, 1H), 4.34 (q, *J* = 7.4 Hz, 2H), 4.23 (s, 1H), 3.93 (dd, *J* = 15.8, 7.2 Hz, 2H), 3.54 (d, *J* = 4.6 Hz, 2H), 3.12 (d, *J* = 13.4 Hz, 3H), 3.03 (d, *J* = 18.6 Hz, 2H), 2.32 (s, 3H), 2.07-1.98 (m, 1H), 1.84 (s, 3H), 1.21 (s, 3H), 0.84 (dd, *J* = 6.8, 3.6 Hz, 6H).

^{13}C NMR (101 MHz, DMSO) δ 171.81, 170.41, 169.73, 169.13, 168.50, 136.12, 134.46, 130.82, 129.86, 128.74, 124.13, 121.73, 57.91, 53.76, 52.34, 48.65, 44.60, 43.09, 37.37, 36.02, 31.79, 31.19, 27.01, 25.57, 22.83, 22.56, 19.82, 18.10.

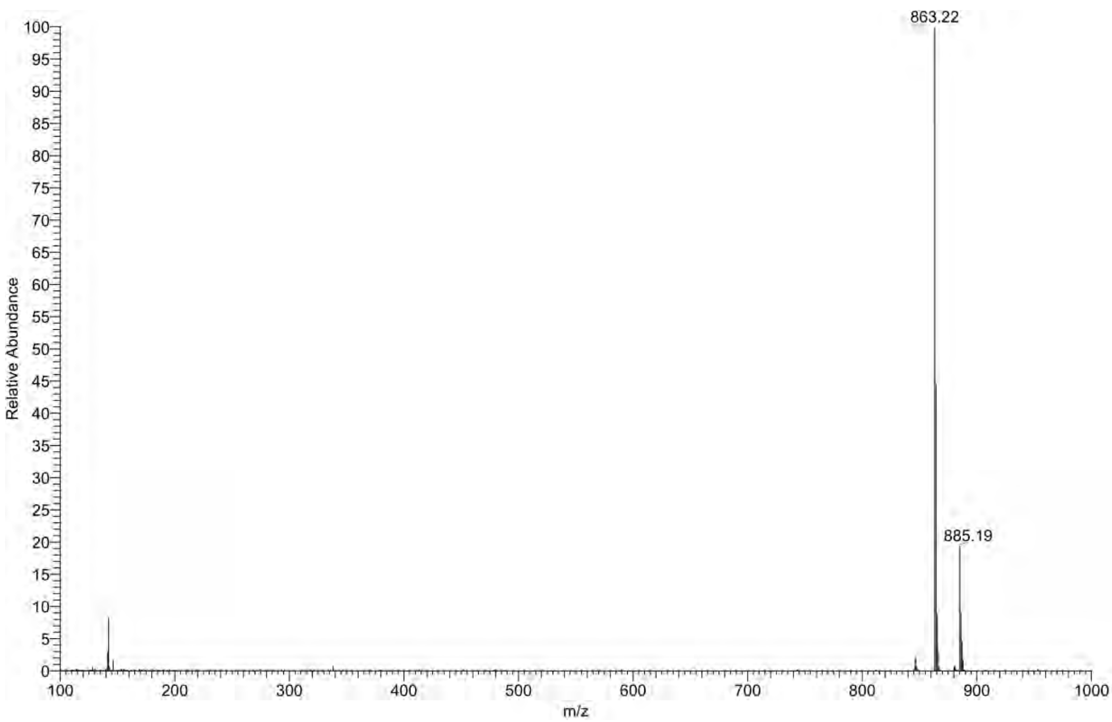


32-L

Compound **32-L** was prepared as a white solid in 90% yield from **Rink-amide AM resin** following the SPPS procedure.



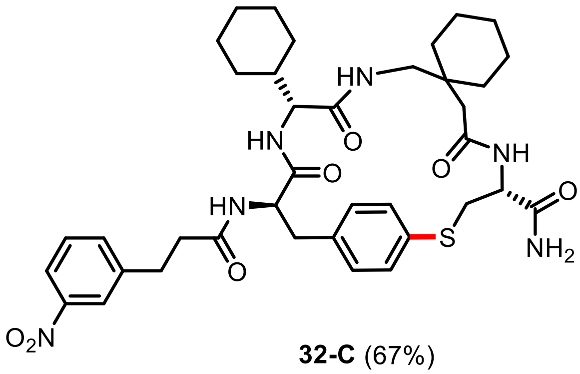
t_R = 8.80 min, 5% to 95% B for 10 min, then 95% B 10-15 min, λ = 254 nm



LRMS: [M+H] $^+$ 863.22; [M+Na] $^+$ 885.19.

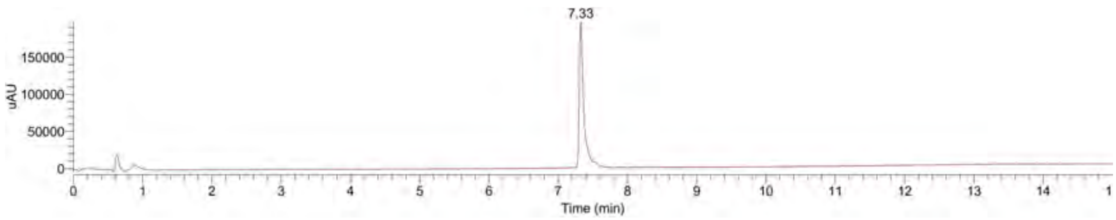
^{1}H NMR (400 MHz, MeOD) δ 8.07 (d, *J* = 5.8 Hz, 2H), 7.61 (d, *J* = 7.6 Hz, 2H), 7.54 (d, *J* = 7.2 Hz, 1H), 7.48 (dd, *J* = 10.2, 6.0 Hz, 1H), 6.98 (d, *J* = 7.6 Hz, 2H), 4.86-4.79

(m, 1H), 4.64 (d, J = 7.6 Hz, 1H), 4.59 (t, J = 8.4 Hz, 1H), 4.08 (d, J = 5.6 Hz, 1H), 3.36-3.21 (m, 2H), 3.06-2.98 (m, 2H), 2.96-2.81 (m, 4H), 2.57 (t, J = 7.4 Hz, 2H), 2.22 (d, J = 4.2 Hz, 2H), 1.71 (d, J = 12.0 Hz, 3H), 1.64 (d, J = 12.4 Hz, 1H), 1.50 (q, J = 10.6, 9.0 Hz, 5H), 1.45-1.39 (m, 3H), 1.36 (t, J = 9.6 Hz, 4H), 1.23-1.13 (m, 2H), 0.85-0.72 (m, 1H), 0.70-0.58 (m, 1H).

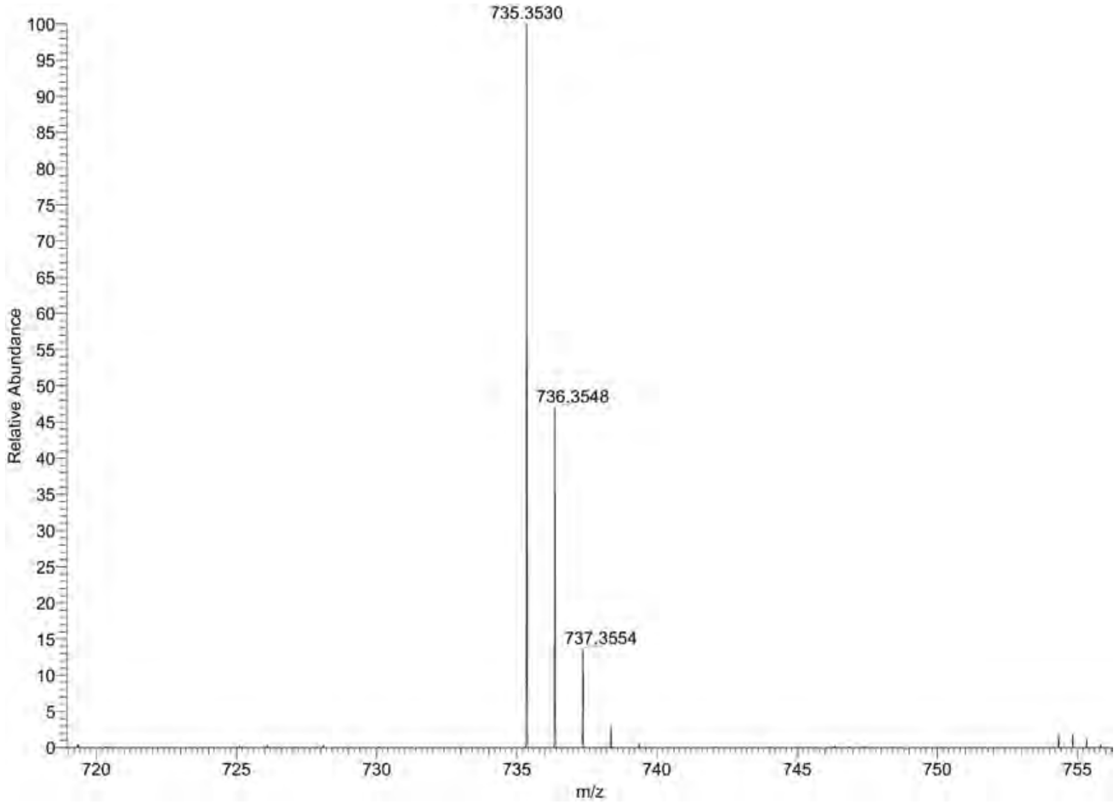


32-C (67%)

Compound **32-C** was isolated in 67% yield (49 mg) as a white powder under the general condition A.



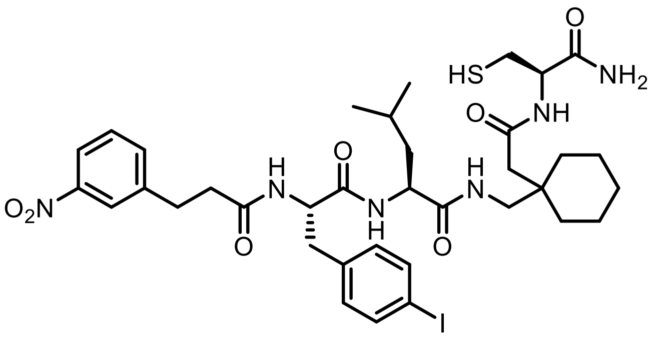
t_R = 7.33 min, 5% to 95% B for 10 min, then 95% B 10-15 min, λ = 254 nm



HRMS: Calcd for $C_{38}H_{50}N_6O_7S$ [M+H$^+$]: 735.3534; found: 735.3530

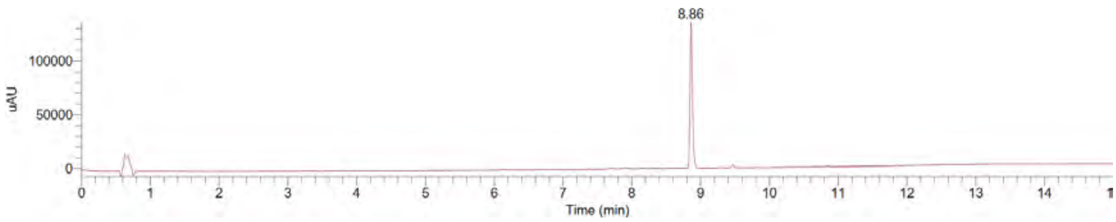
^{1}H NMR (400 MHz, MeOD) δ 8.30 (t, *J* = 6.6 Hz, 1H), 8.13-8.07 (m, 1H), 7.72-7.65 (m, 1H), 7.57 (t, *J* = 7.8 Hz, 1H), 7.31-7.23 (m, 2H), 7.02 (d, *J* = 8.2 Hz, 2H), 4.59 (t, *J* = 5.0 Hz, 1H), 4.47 (dd, *J* = 11.6, 3.2 Hz, 1H), 4.06 (d, *J* = 8.8 Hz, 1H), 3.69 (dd, *J* = 14.2, 3.2 Hz, 1H), 3.48 (dd, *J* = 14.2, 6.0 Hz, 1H), 3.21-3.06 (m, 4H), 2.97 (dd, *J* = 14.2, 11.8 Hz, 1H), 2.82-2.68 (m, 3H), 2.22-2.00 (m, 3H), 1.66 (d, *J* = 9.4 Hz, 2H), 1.64-1.56 (m, 3H), 1.55-1.35 (m, 9H), 1.32 (s, 2H), 1.16 (d, *J* = 15.4 Hz, 3H), 1.06-0.94 (m, 1H), 0.93-0.85 (m, 1H), 0.81 (t, *J* = 11.6 Hz, 1H).

^{13}C NMR (101 MHz, MeOD) δ 175.42, 174.71, 174.19, 174.02, 171.85, 149.86, 144.52, 137.43, 136.12, 135.87, 132.75, 130.97, 130.91, 130.87, 124.13, 122.50, 59.01, 56.62, 55.88, 41.11, 39.43, 38.41, 37.78, 37.64, 35.42, 35.20, 31.97, 30.84, 30.82, 30.01, 27.20, 27.10, 26.79, 22.66, 22.62.

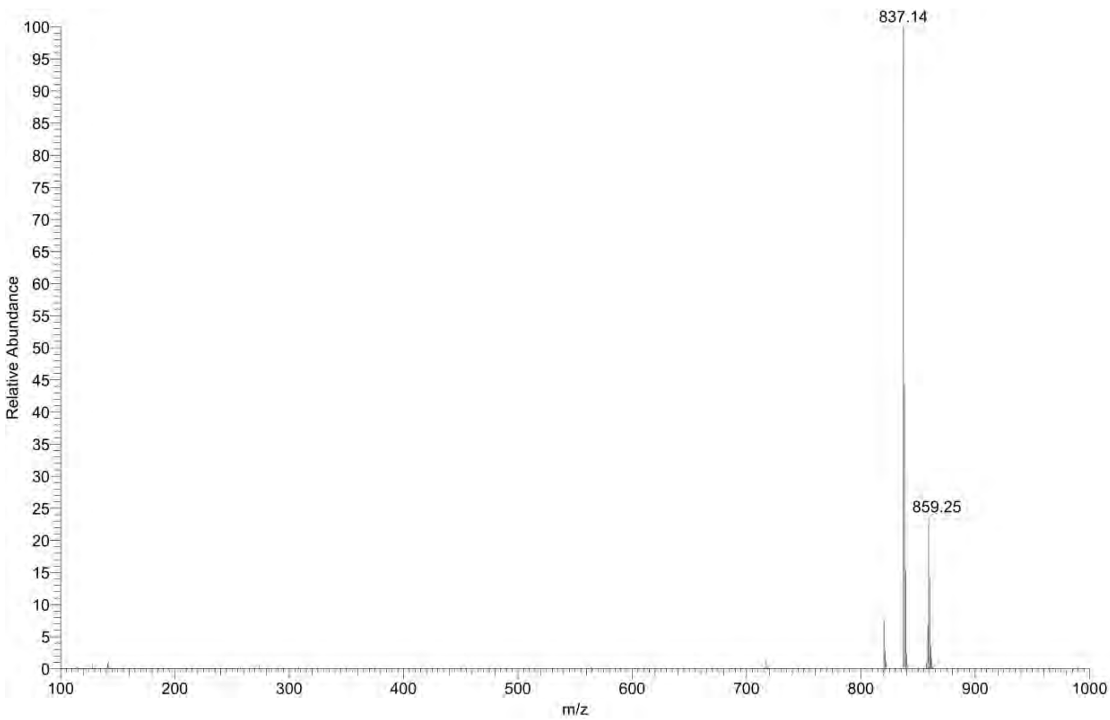


33-L

Compound **33-L** was prepared as a white solid in 85% yield from **Rink-amide AM resin** following the SPPS procedure.

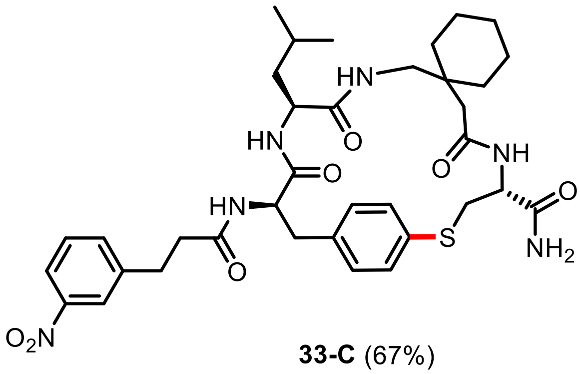


t_R = 8.86 min, 5% to 95% B for 10 min, then 95% B 10-15 min, λ = 254 nm



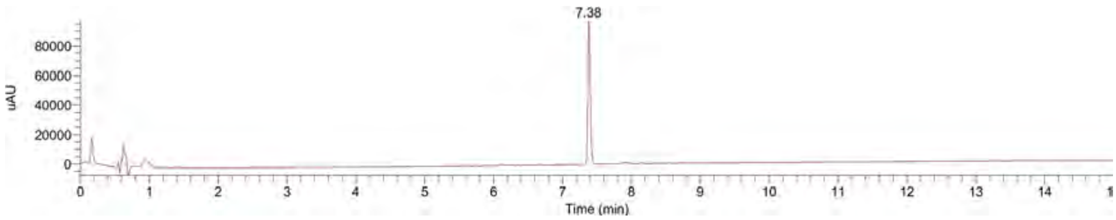
LRMS: $[M+H]^+$ 837.14; $[M+Na]^+$ 859.25.

^{1}H NMR (400 MHz, MeOD) δ 8.17-8.03 (m, 2H), 7.65-7.59 (m, 3H), 7.53 (t, *J* = 7.8 Hz, 1H), 7.02-7.97 (m, 2H), 4.61-4.42 (m, 2H), 4.17 (dd, *J* = 11.2, 4.0 Hz, 1H), 3.38-3.31 (m, 2H), 3.27 (d, *J* = 4.2 Hz, 2H), 3.13-2.99 (m, 2H), 2.97-2.87 (m, 3H), 2.82 (dd, *J* = 13.8, 7.8 Hz, 1H), 2.60 (t, *J* = 7.4 Hz, 2H), 2.22 (s, 2H), 1.60-1.45 (m, 6H), 1.44-1.34 (m, 5H), 0.86 (d, *J* = 6.0 Hz, 3H), 0.75 (d, *J* = 6.0 Hz, 3H).

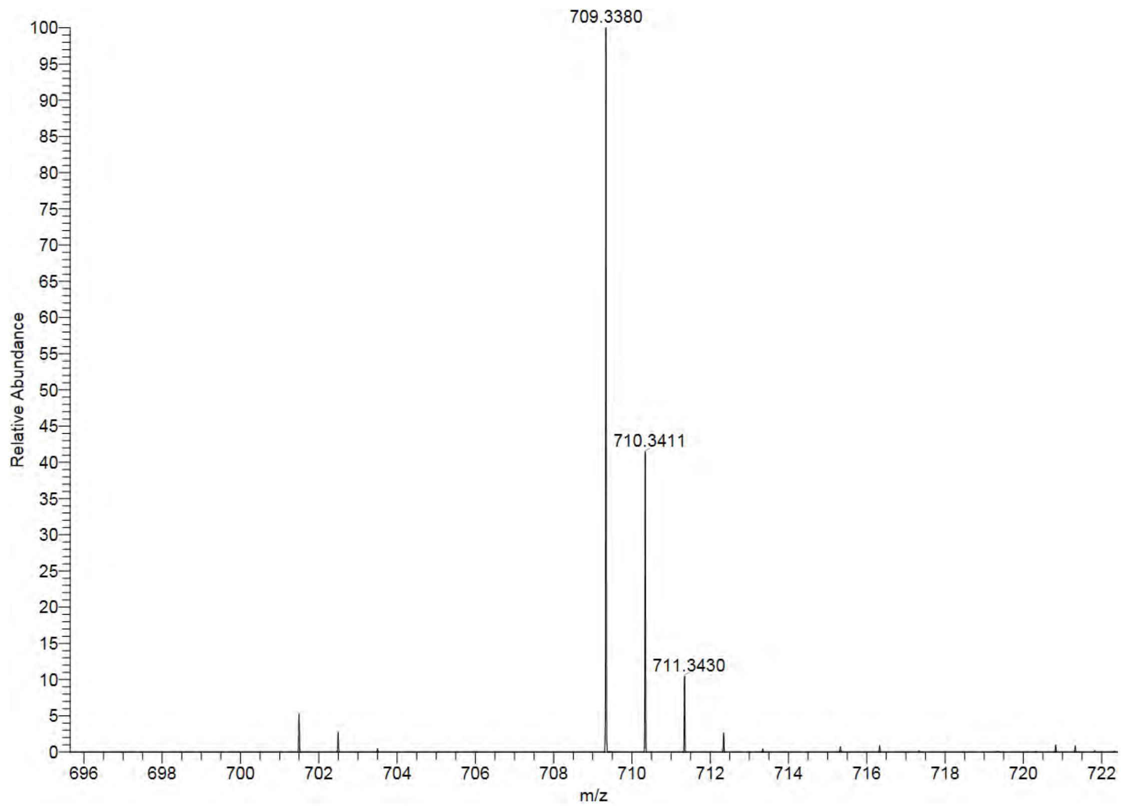


33-C (67%)

Compound **33-C** was isolated in 67% yield (47 mg) as a white powder under the general condition A.



t_R = 7.38 min, 5% to 95% B for 10 min, then 95% B 10-15 min, λ = 254 nm

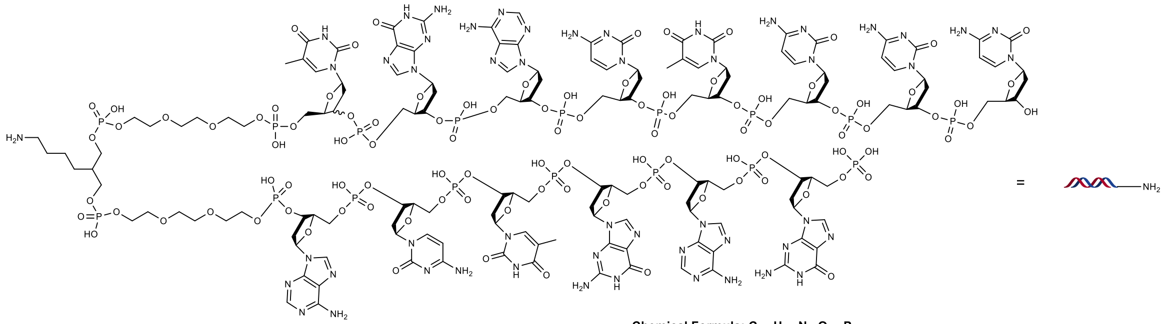


HRMS: Calcd for $C_{38}H_{50}N_6O_7S$ [M+H$^+$]: 709.3378; found: 709.3380.

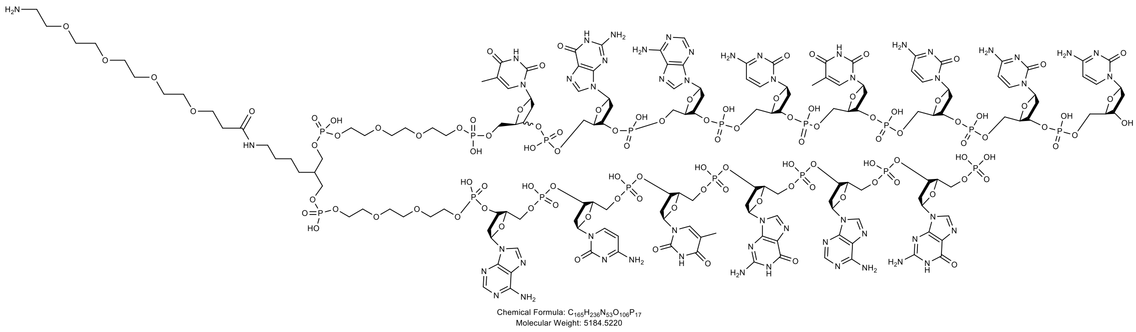
^{1}H NMR (400 MHz, MeOD) δ 8.20-8.12 (m, 1H), 8.11-8.02 (m, 1H), 7.68 (dd, *J* = 8.2, 4.4 Hz, 1H), 7.61-7.49 (m, 1H), 7.31-7.23 (m, 2H), 7.00 (d, *J* = 7.6 Hz, 2H), 4.65 (q, *J* = 5.2 Hz, 1H), 4.61-4.50 (m, 1H), 4.38-4.28 (m, 1H), 3.61 (dd, *J* = 14.4, 3.4 Hz, 1H), 3.35 (s, 1H), 3.32-3.26 (m, 1H), 3.24-3.16 (m, 1H), 3.13-3.05 (m, 2H), 3.03-2.92 (m, 1H), 2.81-2.69 (m, 3H), 2.11-1.97 (m, 2H), 1.58-1.38 (m, 8H), 1.38-1.22 (m, 5H), 0.92-0.78 (m, 6H).

^{13}C NMR (101 MHz, MeOD) δ 173.89, 173.70, 173.02, 172.78, 170.25, 148.41, 143.16, 135.49, 134.78, 131.70, 129.71, 129.46, 122.81, 121.09, 54.82, 54.45, 51.35, 40.94, 37.90, 37.03, 36.50, 33.86, 30.55, 25.71, 24.40, 21.83, 21.02.

5. The structure of Headpiece and AOP-headpiece



Scheme S7. The structure of Headpiece



Scheme S8. The structure of AOP-headpiece

6. DNA-compatible reaction general protocols

On-DNA amidation reaction

Materials

oligonucleotide: 2 mM in water

pH 9.4 borate buffer: 500 mM in water

Amino Acid : 200 mM in DMA

HATU: 200 mM in DMA

DIPEA: 200 mM in DMA

Procedure

1) Premix solution: Amino Acids (67 equiv, 670 nmol, 3.4 μL), HATU (67 equiv, 670 nmol, 3.4 μL) and DIPEA (67 equiv, 670 nmol, 3.4 μL).
2) To the headpiece solution (10 nmol, 5 μL), was added 5 μL pH 9.4 buffer solution and 6 μL premix solution. The mixture was vortexed and react at room temperature for 10 min, then was added 4 μL premix solution. The mixture was vortexed and react at room temperature for 1 h.
3) Add 5 M NaCl solution (10 % by volume) and cold ethanol (2.5 times by volume,

ethanol stored at -20 °C). The mixture was stored at a -80 °C freezer for more than 30 minutes.

4) Centrifuge the sample for around 30 minutes at 4 °C in a microcentrifuge at 10000 rpm. The above supernatant was removed and the pellet (precipitate) was cooled in liquid nitrogen and then placed on a lyophilizer. After lyophilization, the dry pellet was recovered.

On-DNA de-Fmoc reaction

Materials

oligonucleotide: 1 mM in water

piperidine

Procedure

1) To the peptide-linked DNA (5 nmol, 5 μL), was added 0.5 μL piperidine. The mixture was vortexed and react at room temperature for 1 h.
2) Add 5 M NaCl solution (10 % by volume) and cold ethanol (2.5 times by volume, ethanol stored at -20 °C). The mixture was stored at a -80 °C freezer for more than 30 minutes.
3) Centrifuge the sample for around 30 minutes at 4 °C in a microcentrifuge at 10000 rpm. The above supernatant was removed and the pellet (precipitate) was cooled in liquid nitrogen and then placed on a lyophilizer. After lyophilization, the dry pellet was recovered.

On-DNA de-Mmt protection reaction

Materials

oligonucleotide: 1 mM in water

$MgCl_2$: 400 mM in water

pH 5.5 phosphate buffer: 500 mM in water

Procedure

1) To the peptide-linked DNA (5 nmol, 5 μL), was added the solution of $MgCl_2$ (400 equiv, 5 μL) and pH 5.5 phosphate buffer (500 equiv, 5 μL). The mixture was vortexed.
2) The solution was reacted at 80 °C for 10 h.
3) Add 5 M NaCl solution (10 % by volume) and cold ethanol (2.5 times by volume, ethanol stored at -20 °C). The mixture was stored at a -80 °C freezer for more than 30 minutes.

4) Centrifuge the sample for around 30 minutes at 4 °C in a microcentrifuge at 10000 rpm. The above supernatant was removed and the pellet (precipitate) was cooled in liquid nitrogen and then placed on a lyophilizer. After lyophilization, the dry pellet was recovered.

On-DNA S-arylation reaction

Materials

oligonucleotide: 1 mM in water

xantphosPdG3: 5 mM in ACN

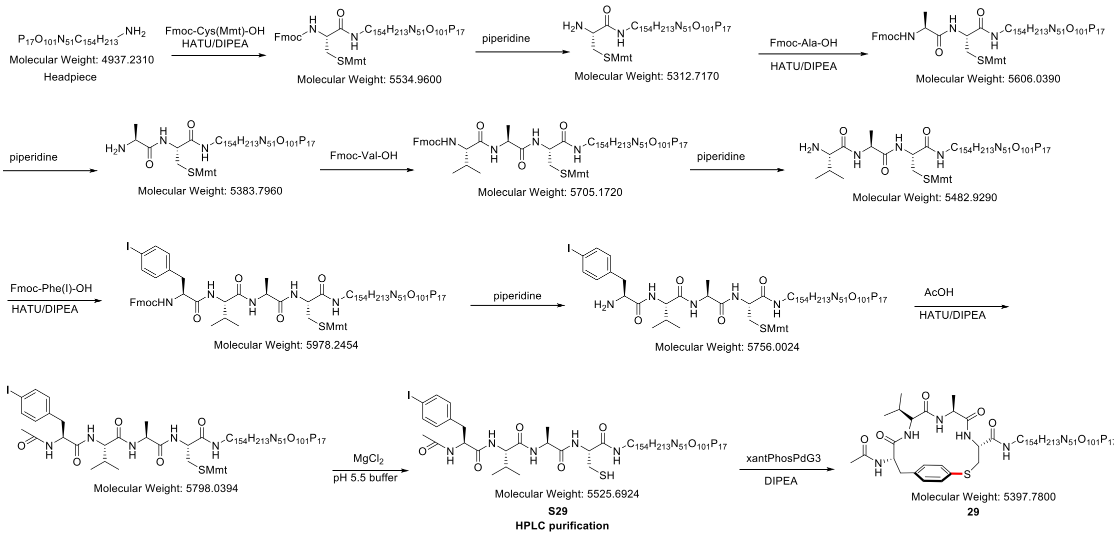
DIPEA: 200 mM in ACN

Procedure

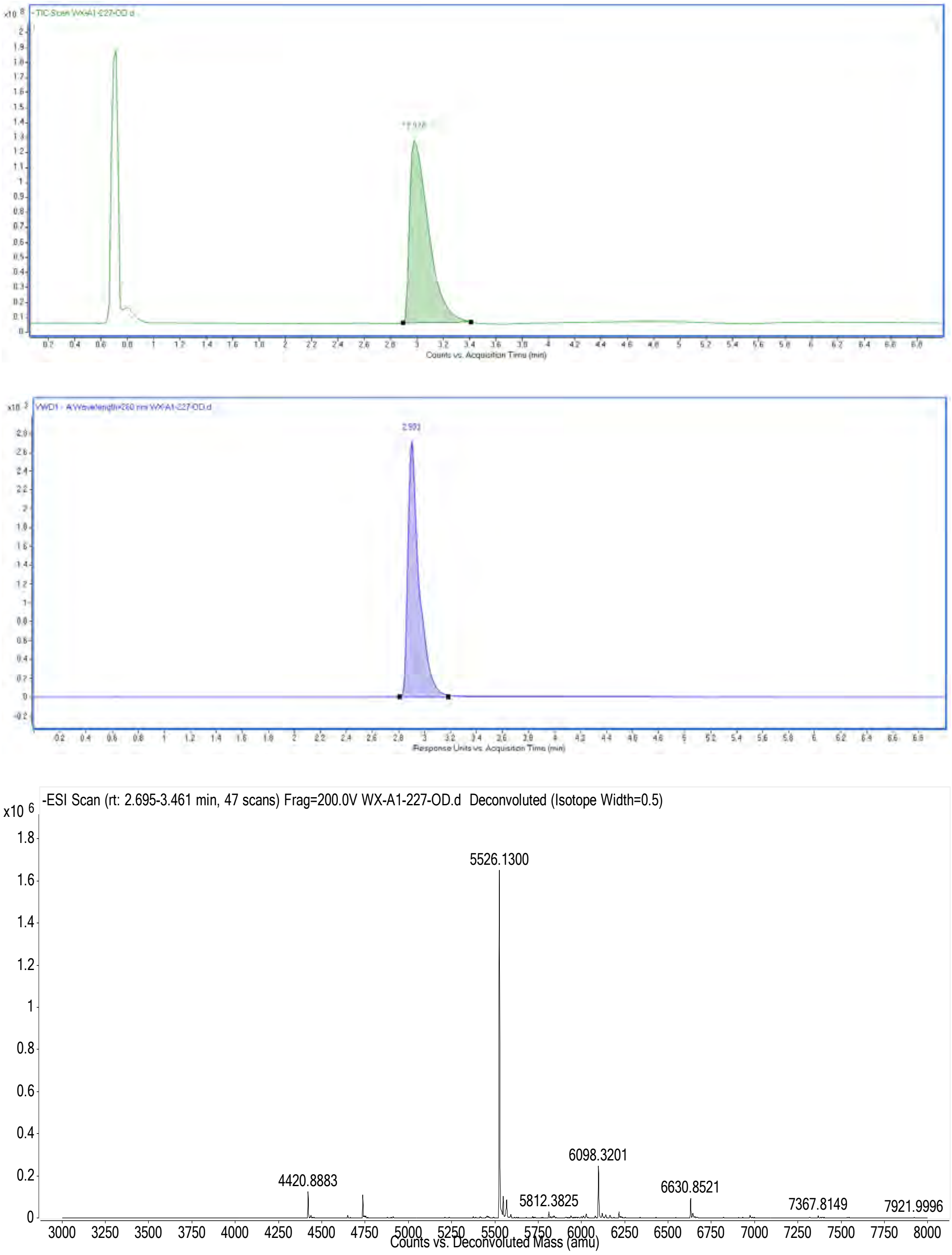
1) To the peptide-linked DNA (5 nmol, 5 µL), was added the solution of Pd catalysis (1 equiv, 1 µL) and DIPEA (100 equiv, 2.5 µL). The mixture was vortexed.
2) The mixture was reacted at room temperature for 1 h.
3) Add 5 M NaCl solution (10 % by volume) and cold ethanol (2.5 times by volume, ethanol stored at -20 °C). The mixture was stored at a -80 °C freezer for more than 30 minutes.
4) Centrifuge the sample for around 30 minutes at 4 °C in a microcentrifuge at 10000 rpm. The above supernatant was removed and the pellet (precipitate) was cooled in liquid nitrogen and then placed on a lyophilizer. After lyophilization, the dry pellet was recovered.

7. Synthetic routes and mass spectrums

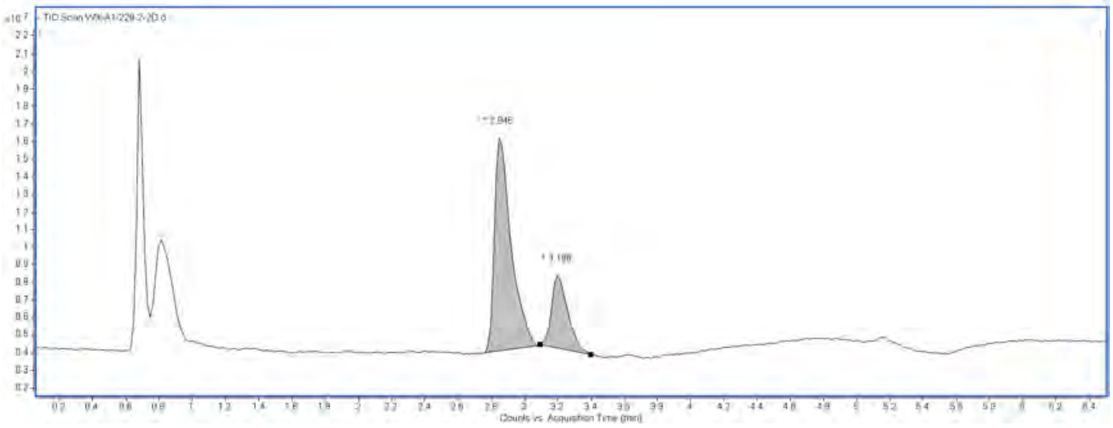
DNA-linked compound 29

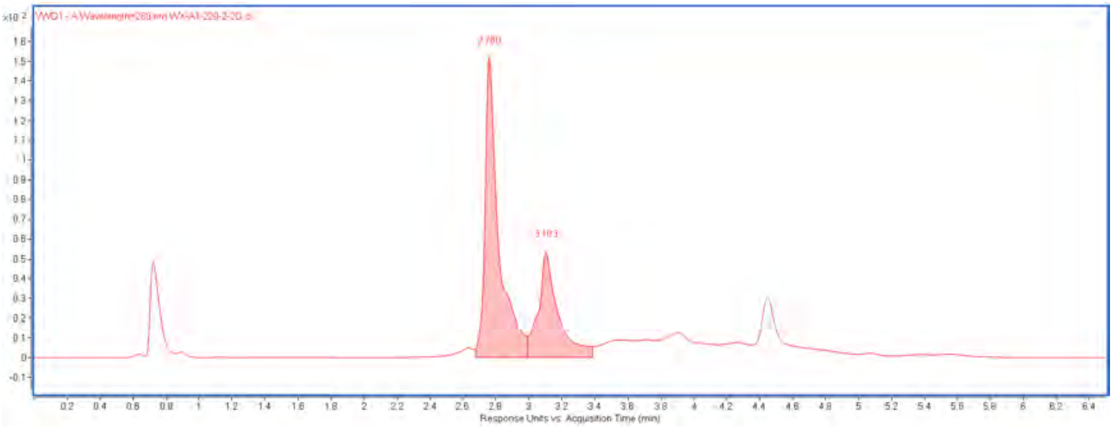


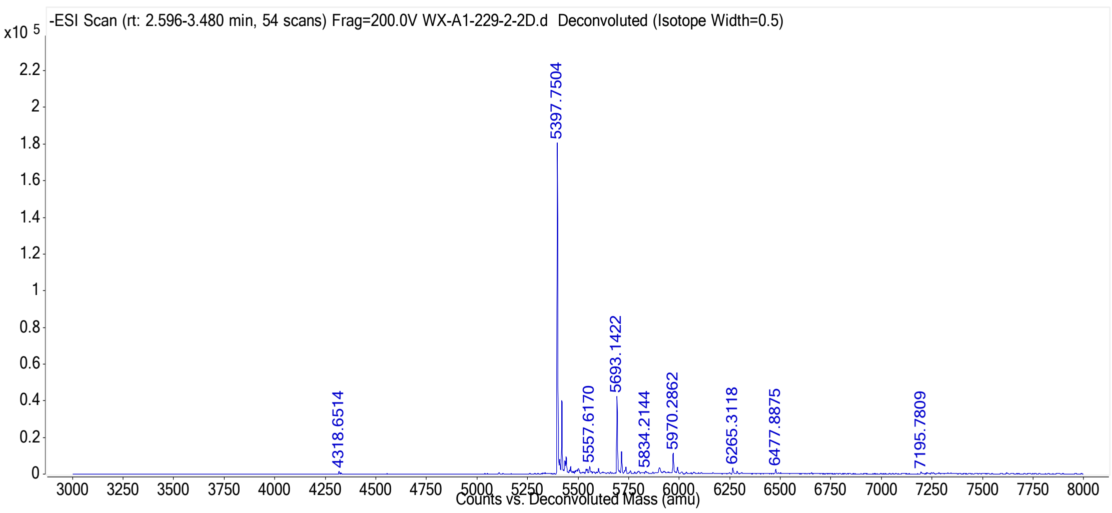
Mass spectrum of S29



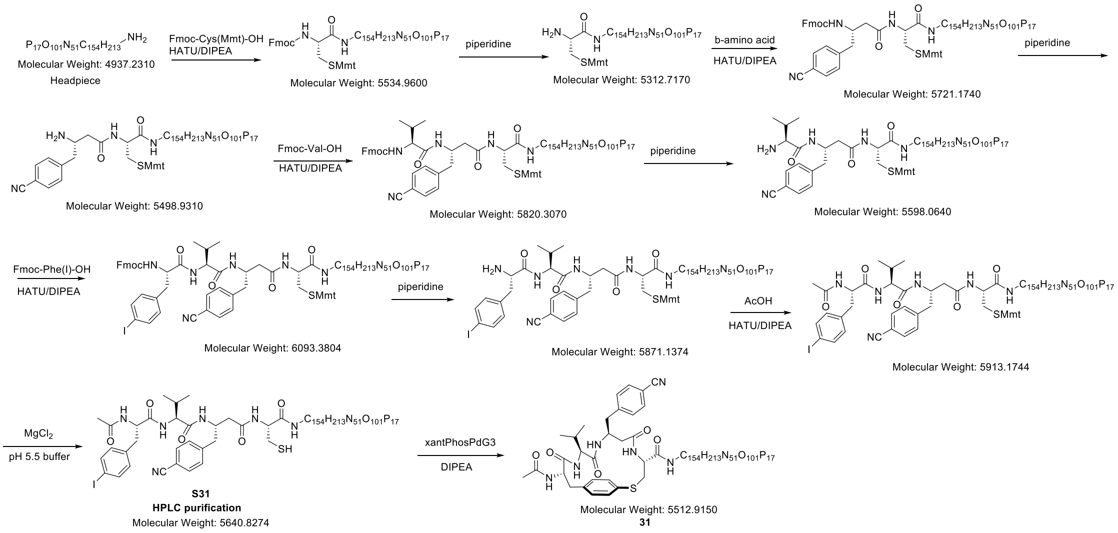
Mass spectrum of 29 and 30



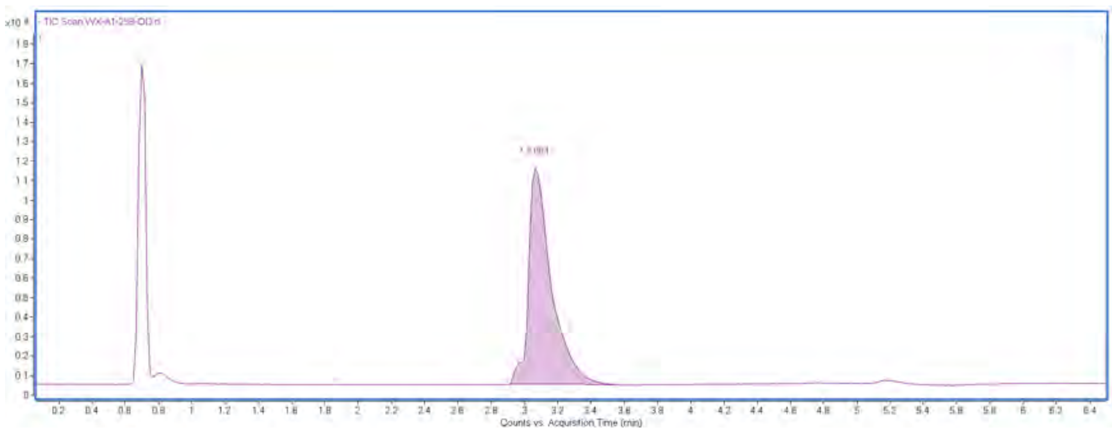


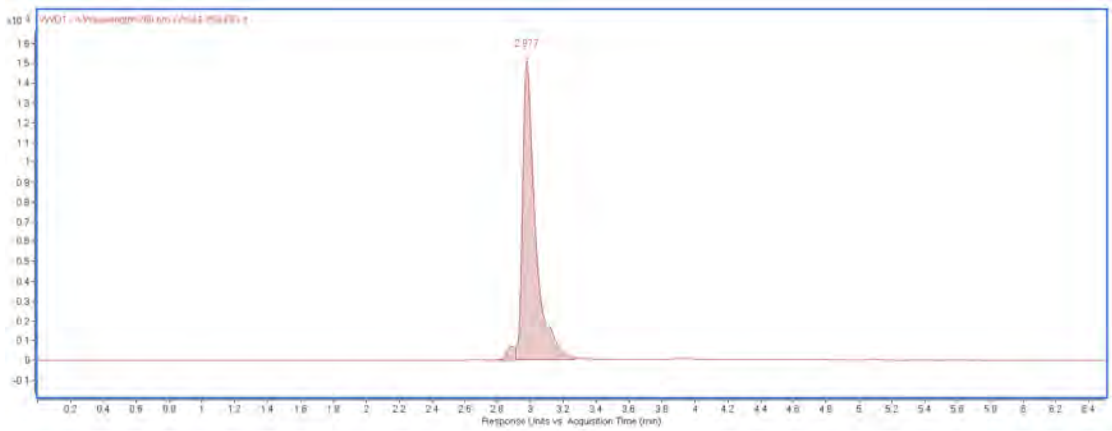


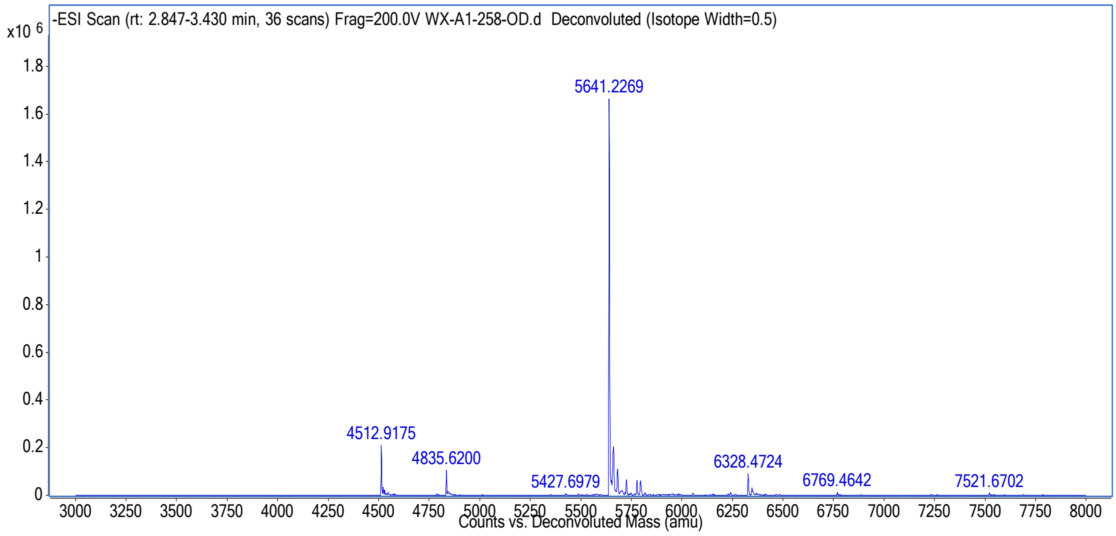
DNA-linked compound 31



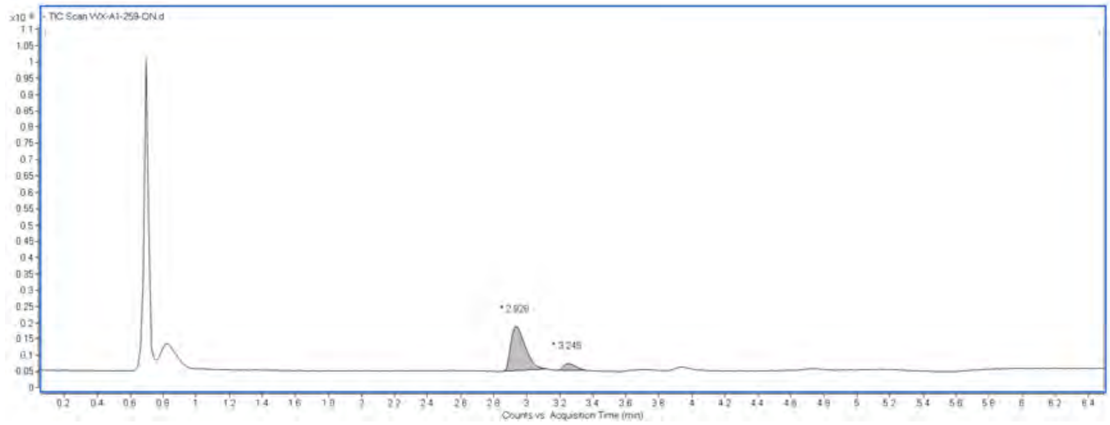
Mass spectrum of S31

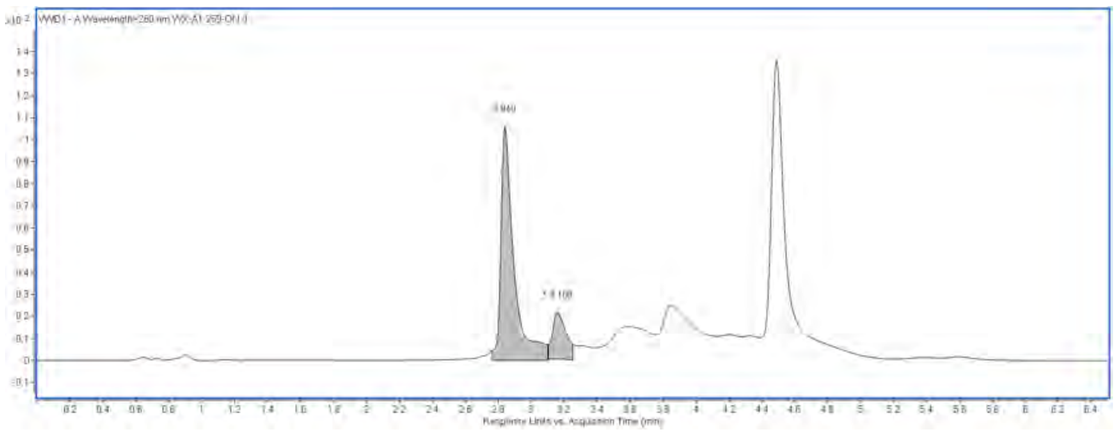


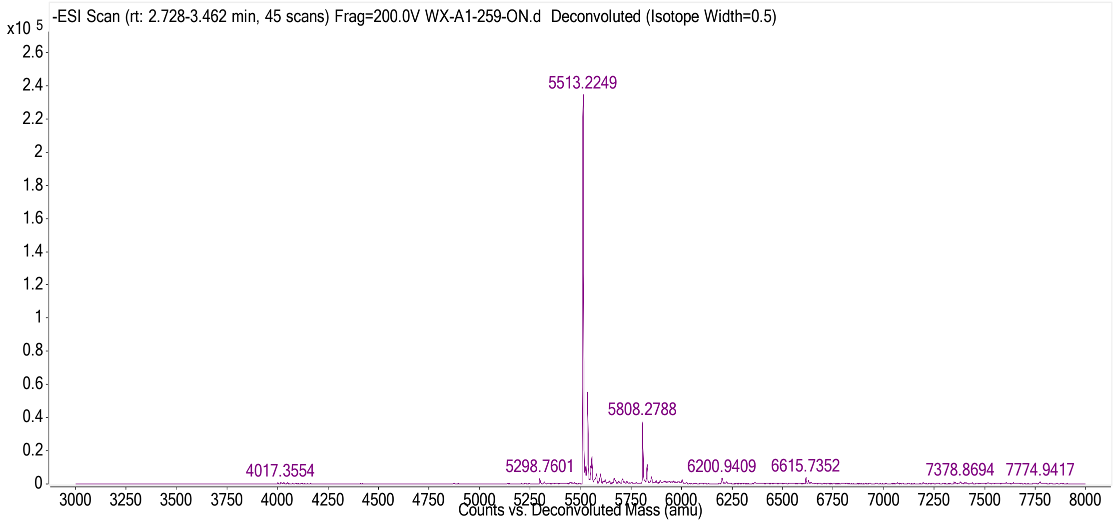




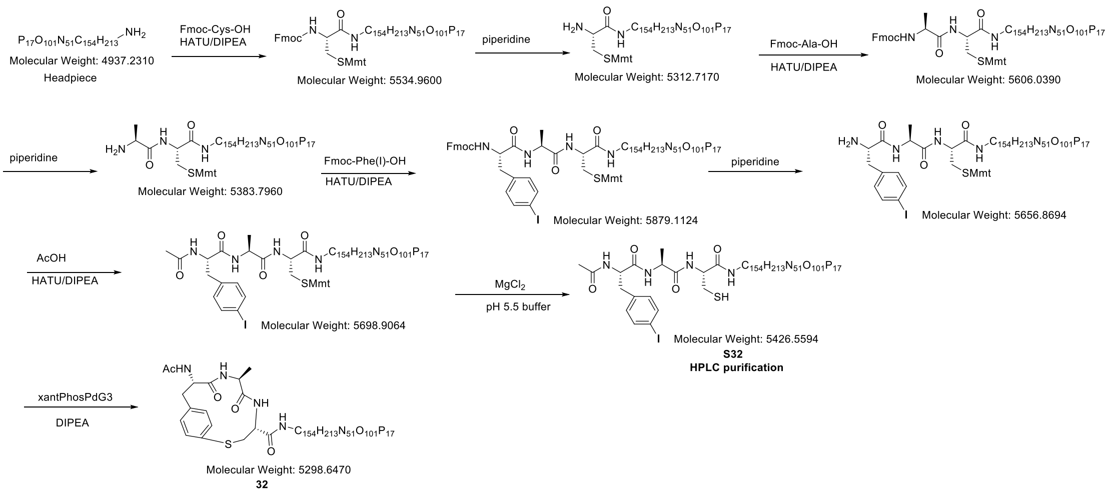
Mass spectrum of 31



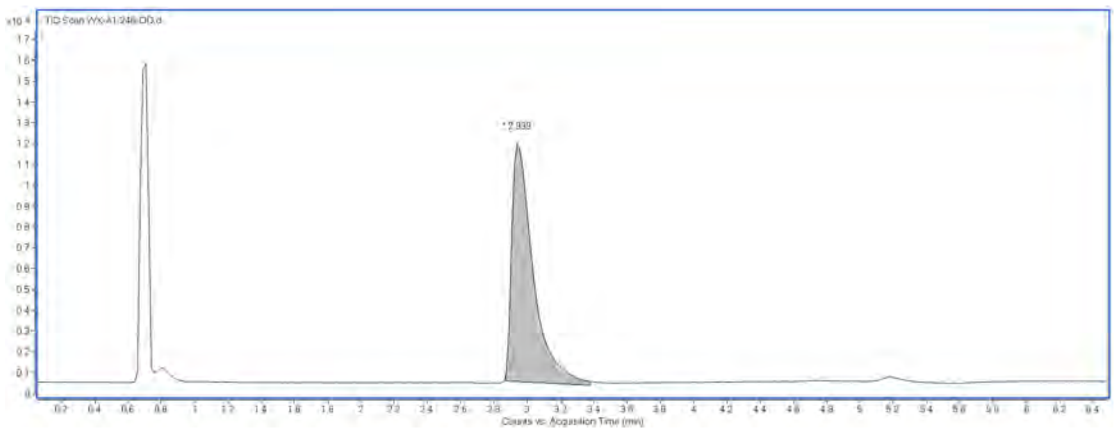


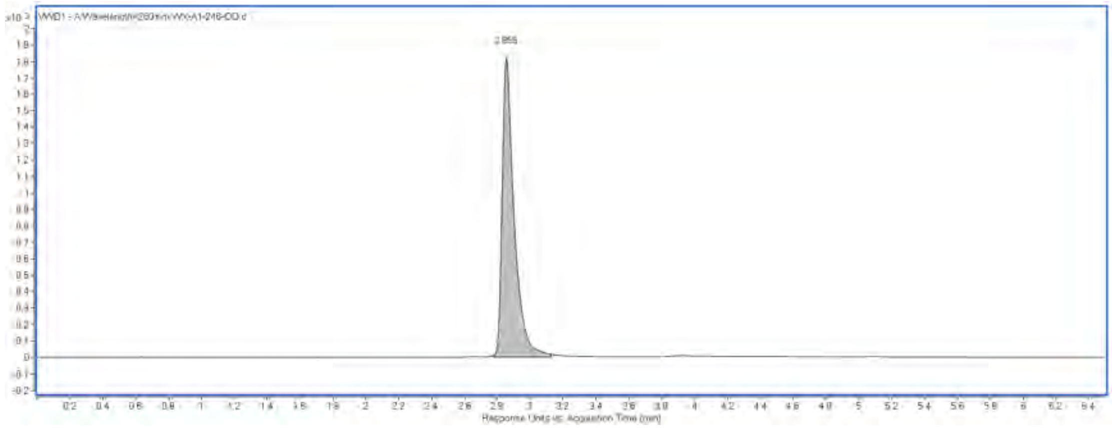


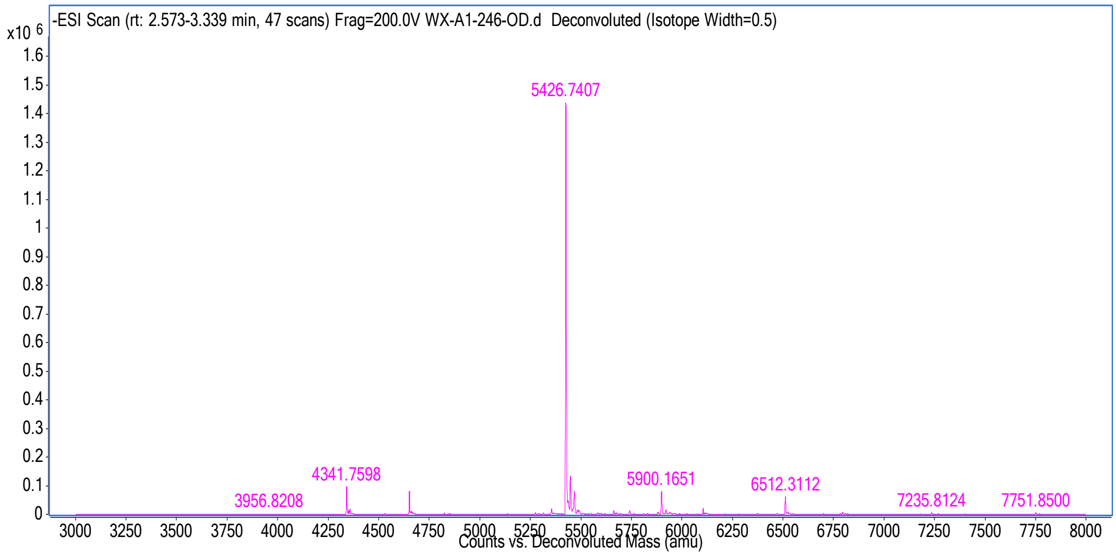
DNA-linked compound 32



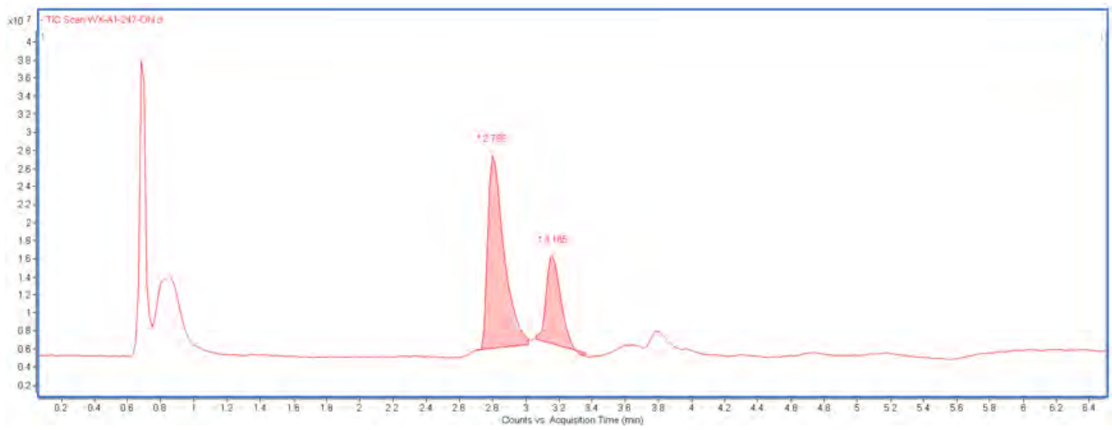
Mass spectrum of S32

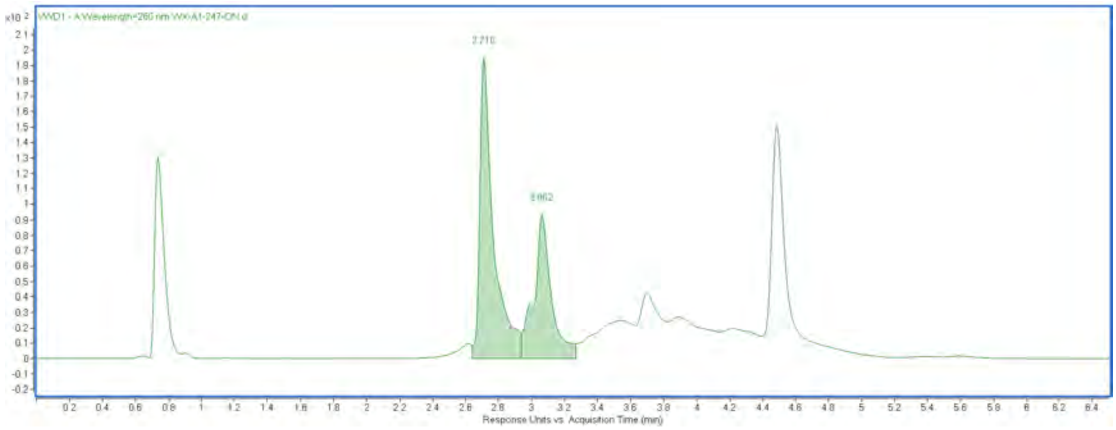


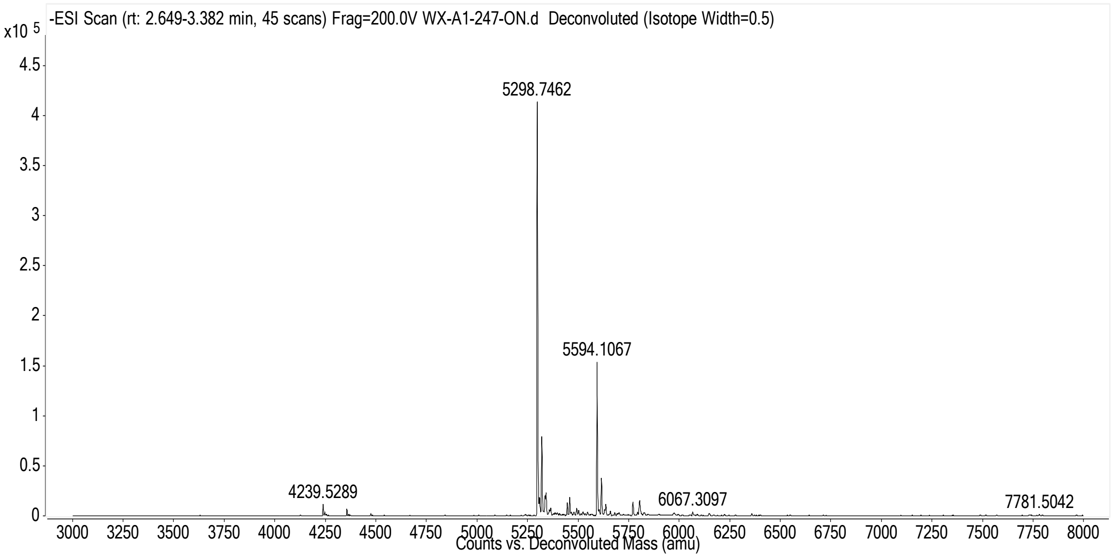




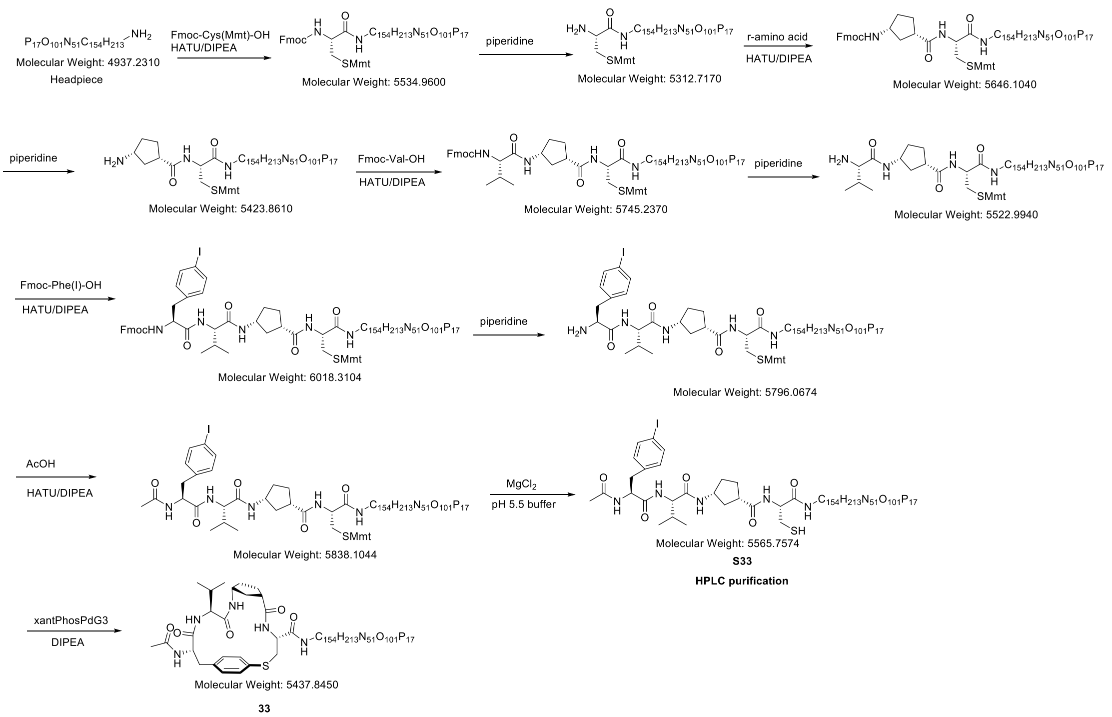
Mass spectrum of 32



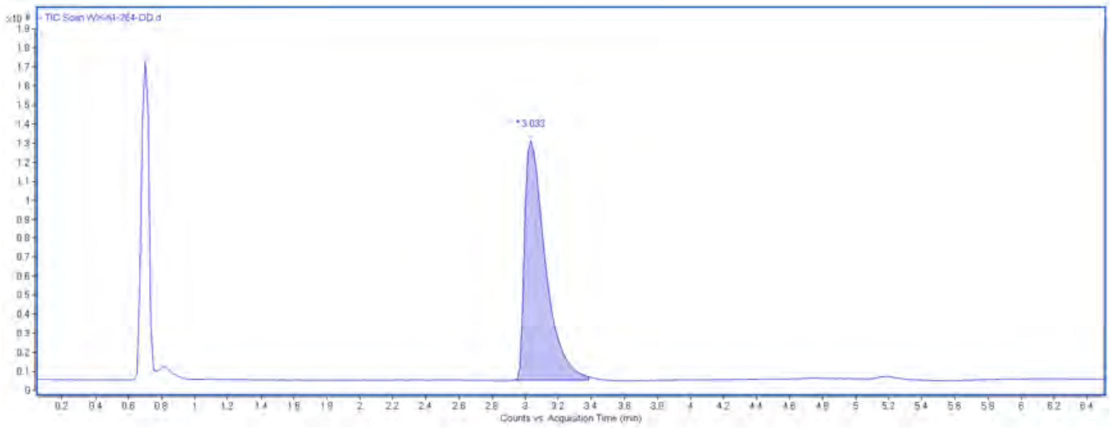


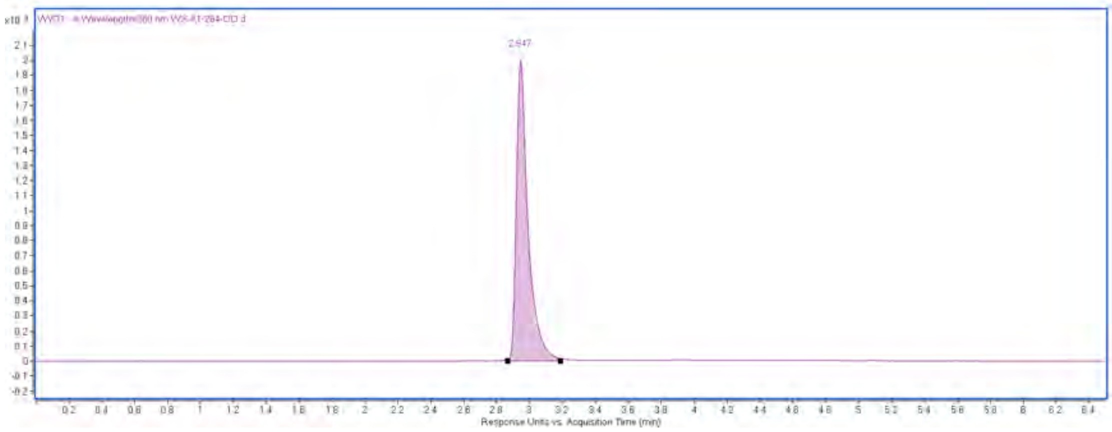


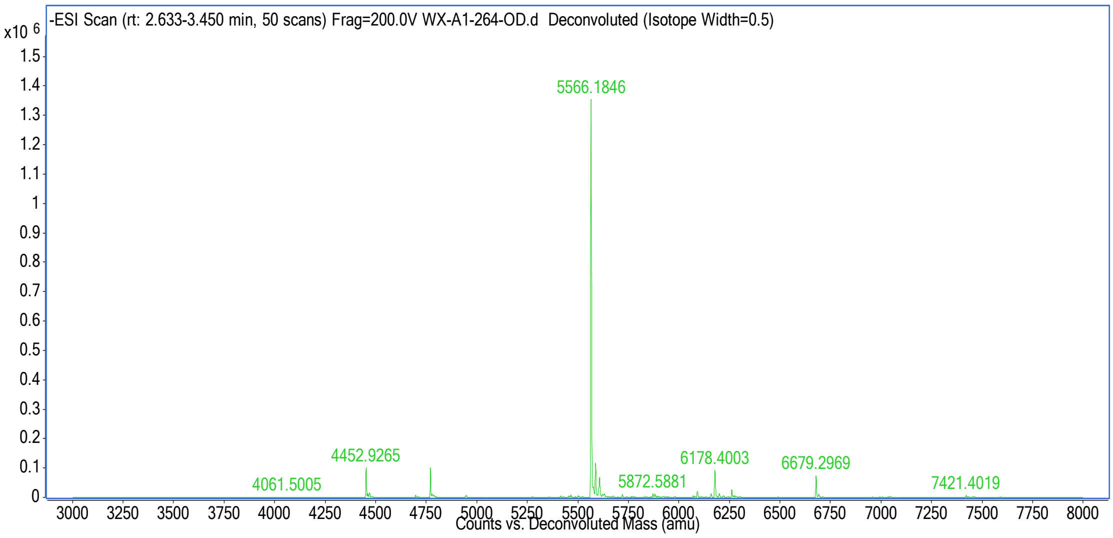
DNA-linked compound 33



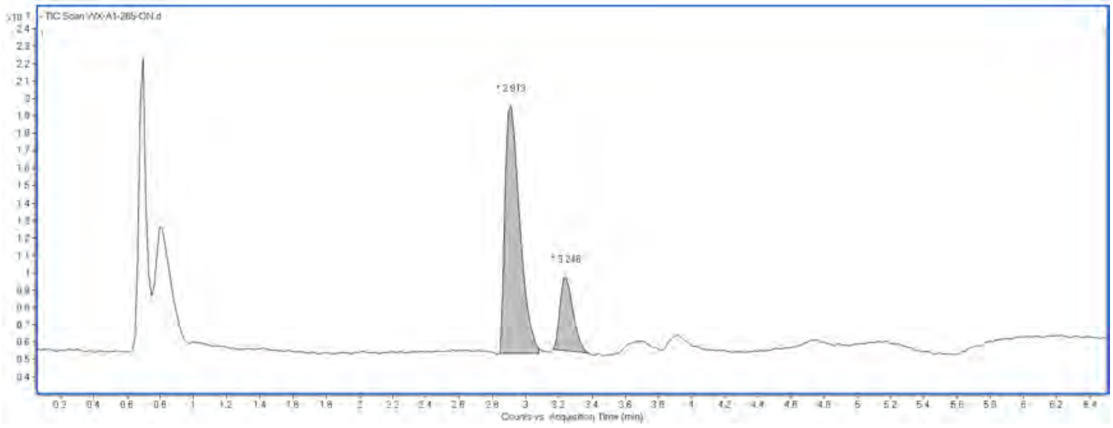
Mass spectrum of S33

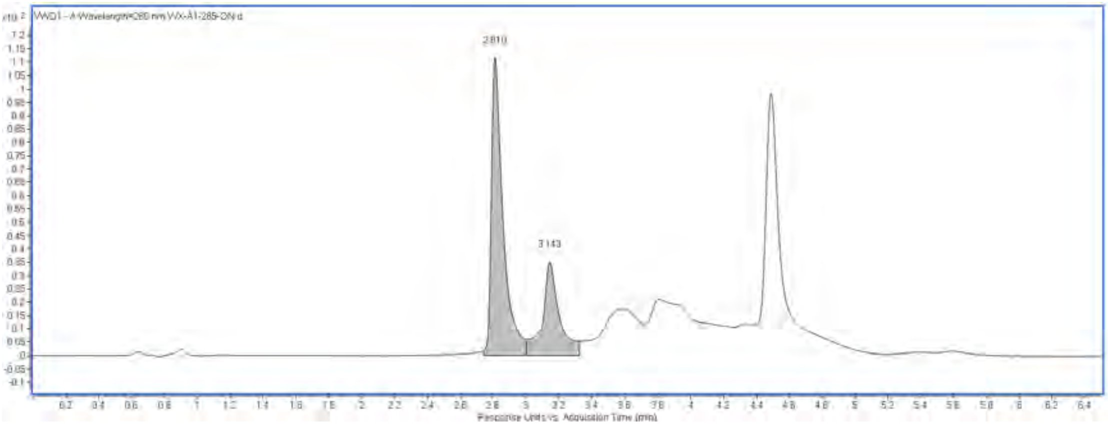


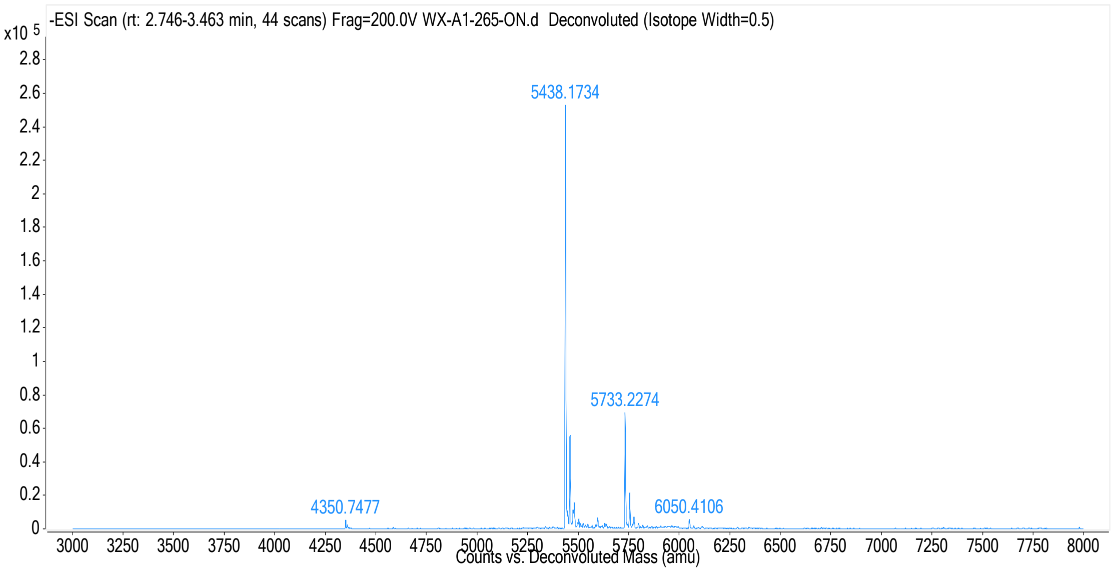




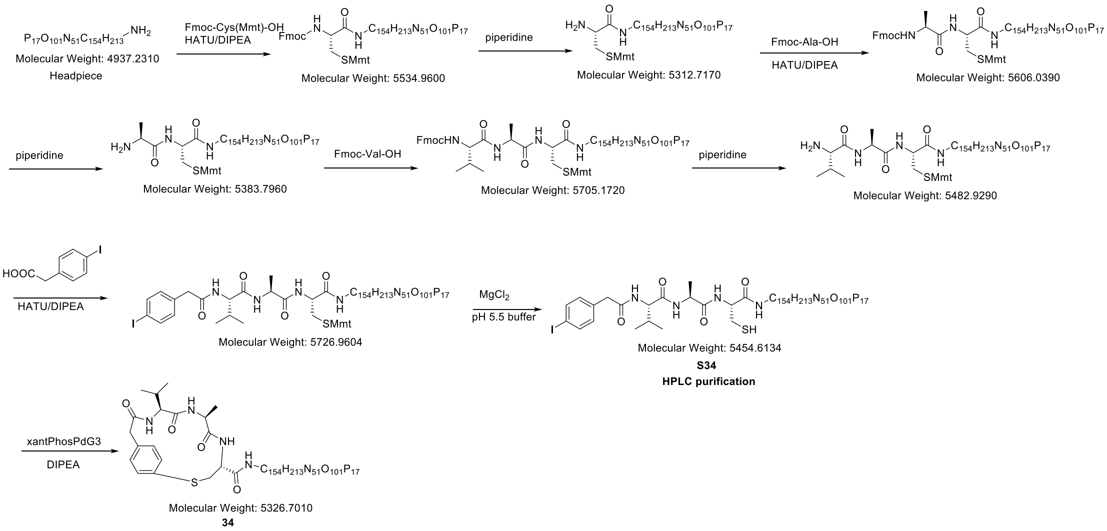
Mass spectrum of 33



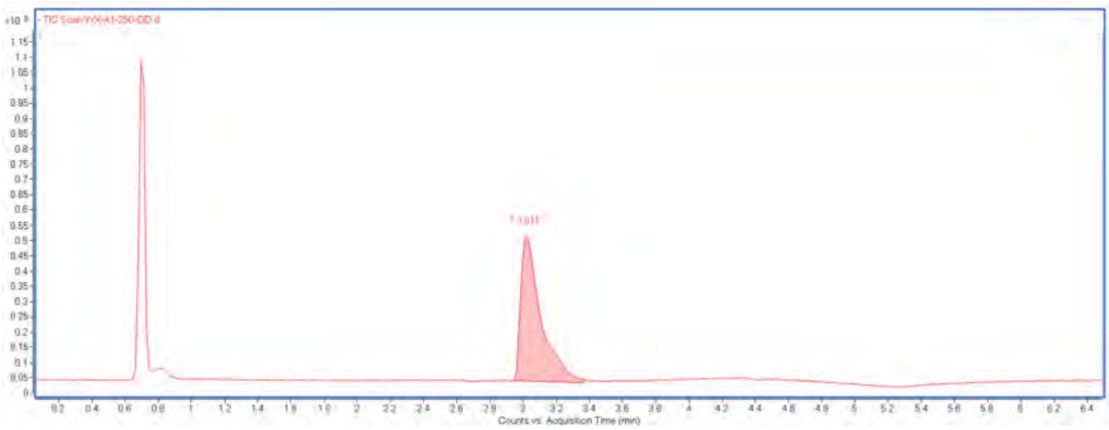


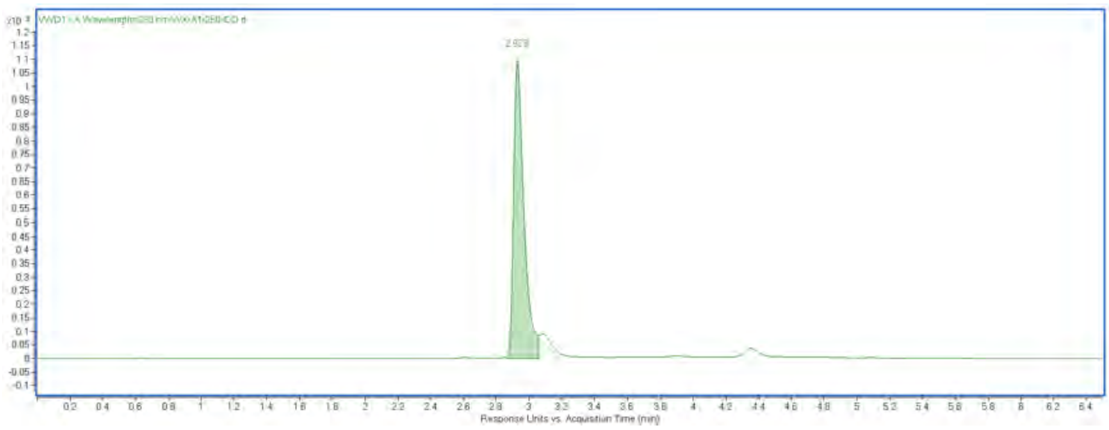


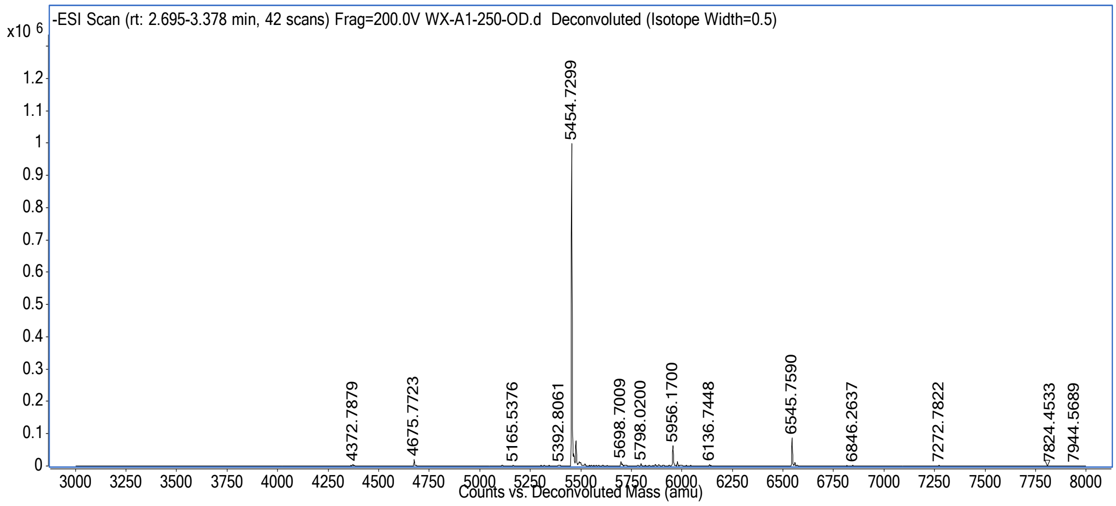
DNA-linked compound 34



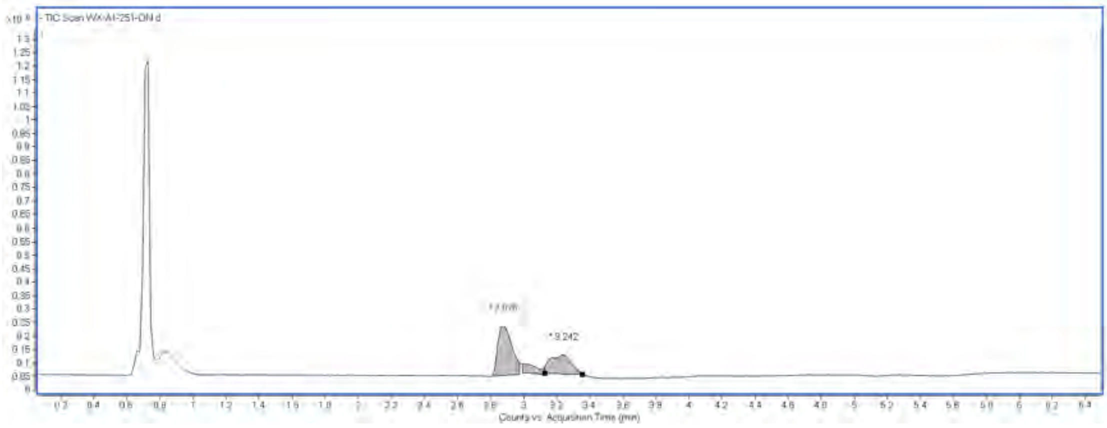
Mass spectrum of S34

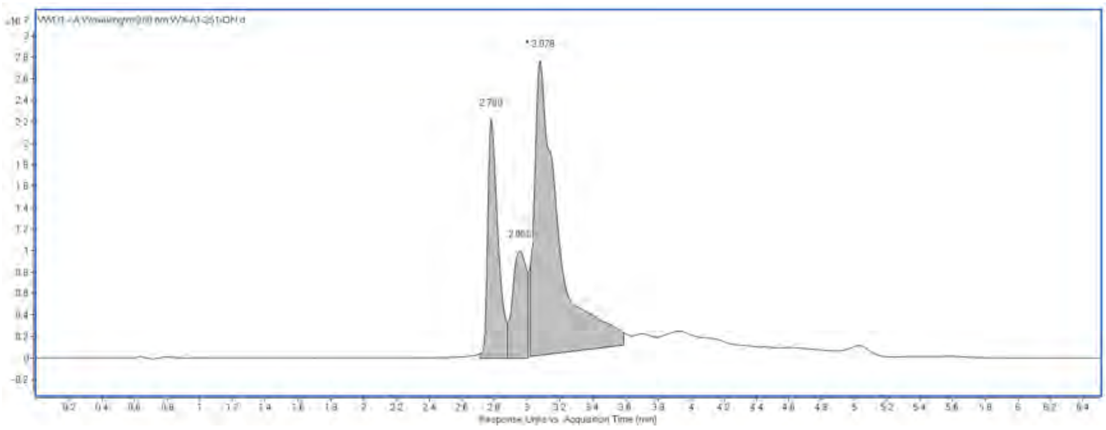


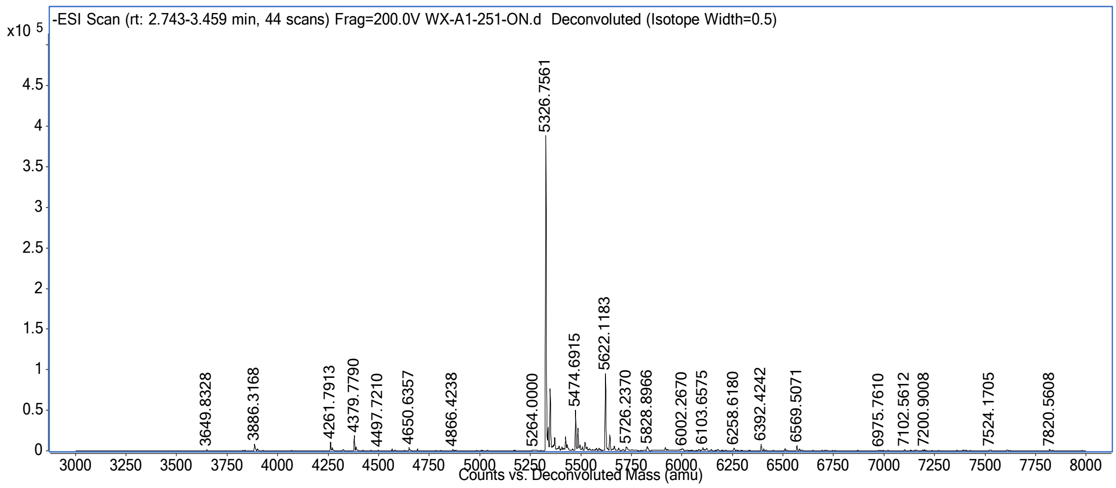




Mass spectrum of 34







8. The construction of DNA-encoded library

Sequence of primer

5’ AAATCGATGTG 3’
3’ GGTTTAGCTAC 5’

Sequence of the extended headpiece

TGACTCCCAAATCGATGTG 3’
ACTGAGGGTTTAGCTAC 5’

Tags: The DNA tags contained a 11bp coding region, flanked by two 2-base 3’ overhangs, all 5’-ends were phosphorylated.

5’ XXXXXXXXXAG XXXXXXXXXGT XXXXXXXXXGA
3’ ACXXXXXXXXX TCXXXXXXXXX CAXXXXXXXXX

Primer/tag ligation

Materials

AOP-Headpiece: 1 mM in water

Primer/tag: 1.8 mM in water

T4 DNA ligase

T4 ligation buffer

Procedure

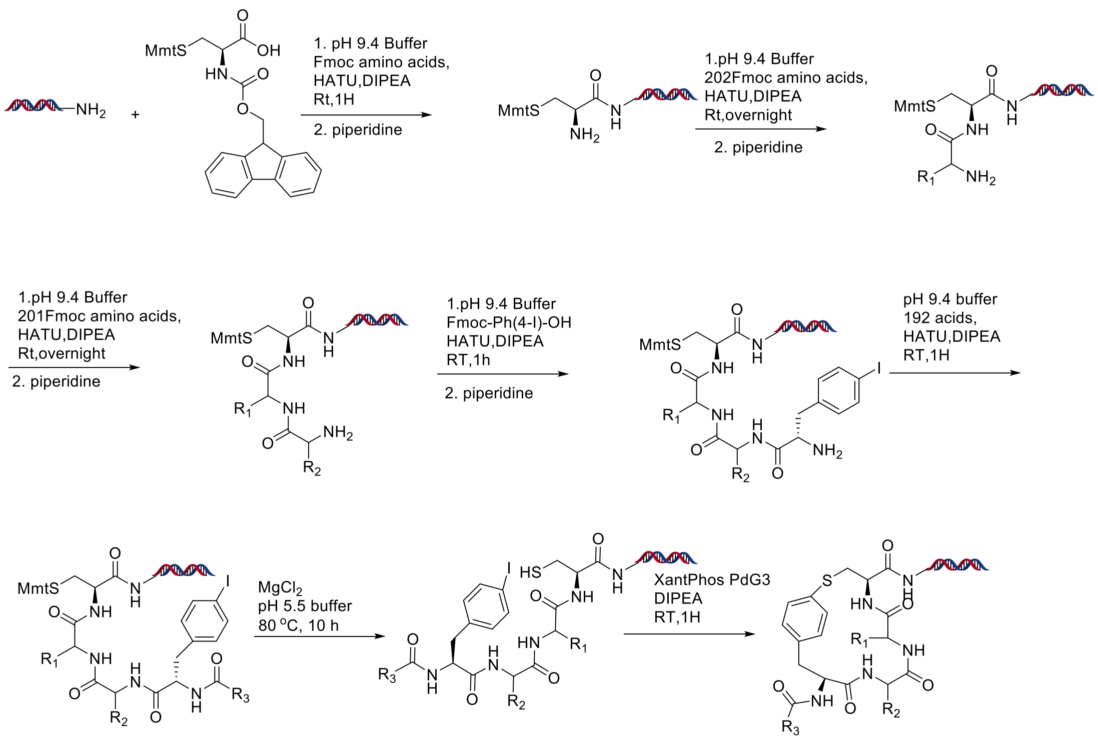
1) To the AOP-Headpiece solution (5 nmol, 5 μL), was added 9.5 μL ddH_2O, 3 μL

primer/tag (1.1 equiv, 5.5 nmol), 2 μL T4 buffer and 0.5 μL T4 ligase. The mixture was vortexed and incubated at 16 °C for 16 h.

2) Add 5 M NaCl solution (10 % by volume) and cold ethanol (2.5 times by volume, ethanol stored at -20 °C). The mixture was stored at a -80 °C freezer for more than 30 minutes.

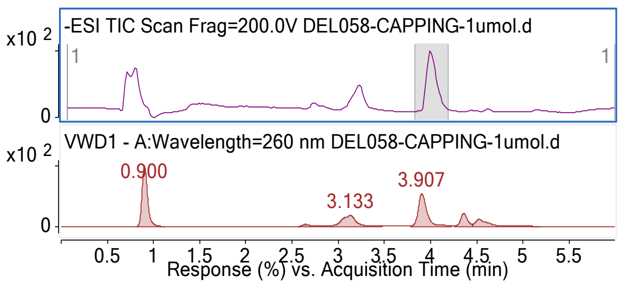
3) Centrifuge the sample for around 30 minutes at 4 °C in a microcentrifuge at 10000 rpm. The above supernatant was removed and the pellet (precipitate) was cooled in liquid nitrogen and then placed on a lyophilizer. After lyophilization, the dry pellet was recovered.

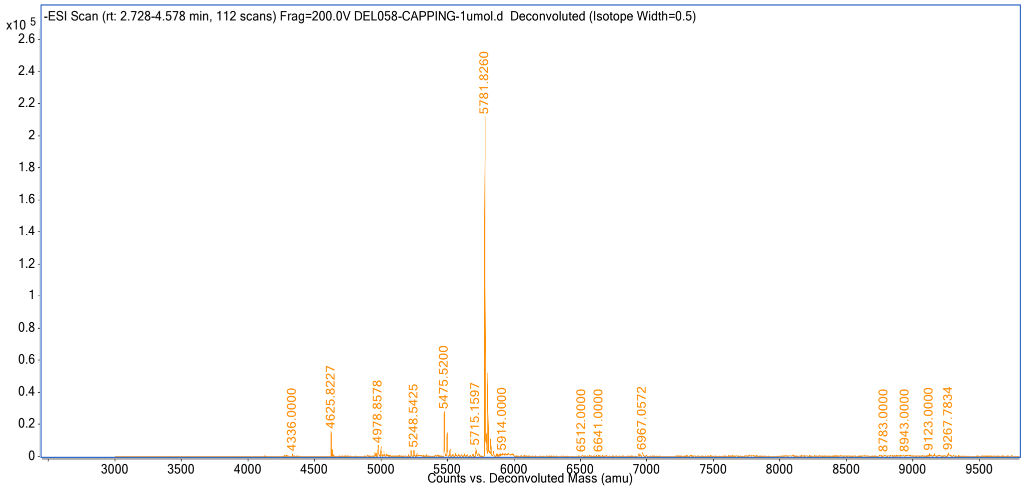
9. Library synthetic route



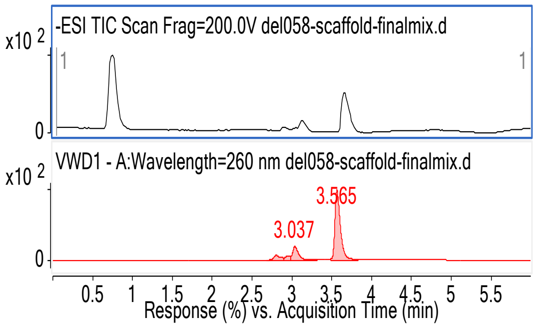
10. The synthesis of DNA-encoded library

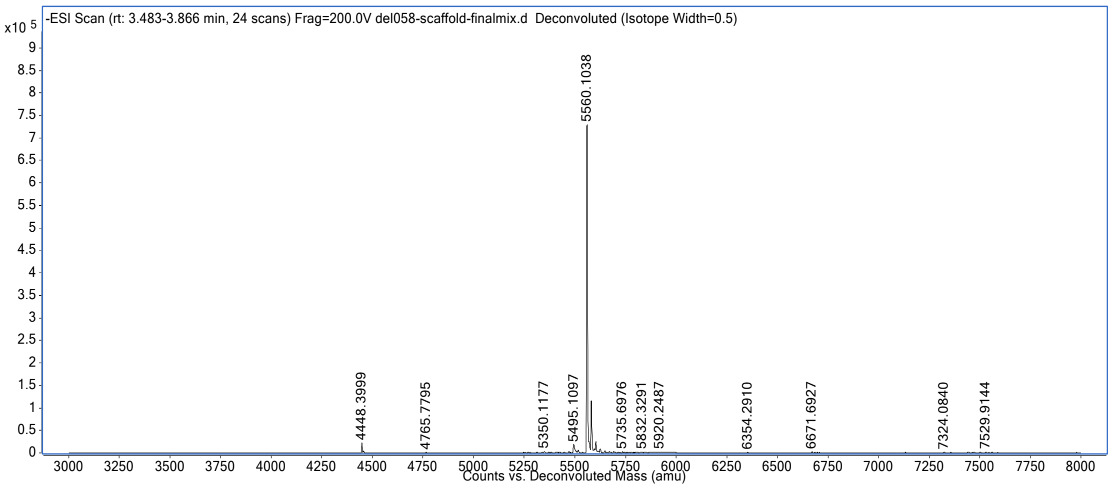
Amidation with Fmoc-Cys(Mmt)-OH



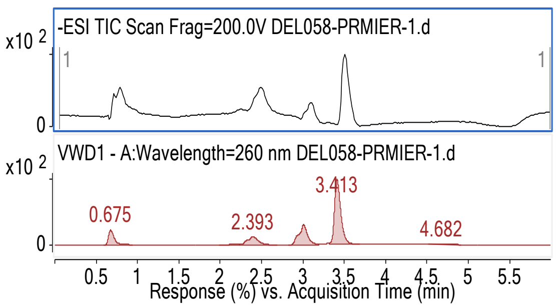


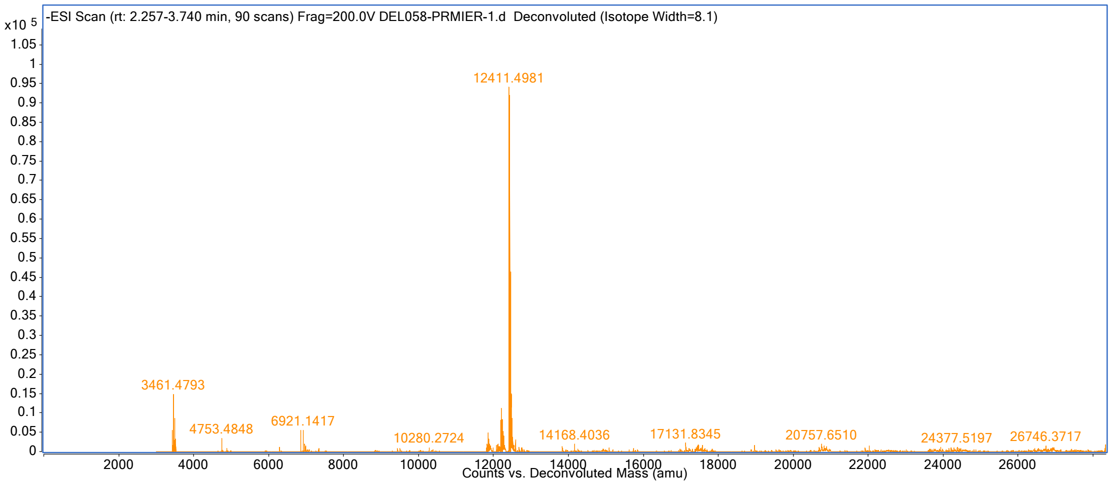
De-Fmoc



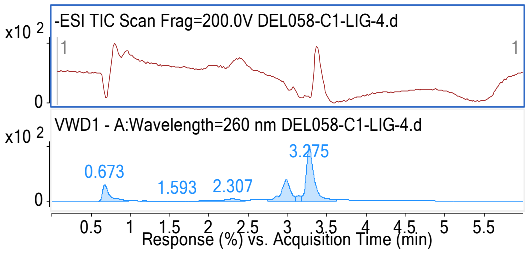


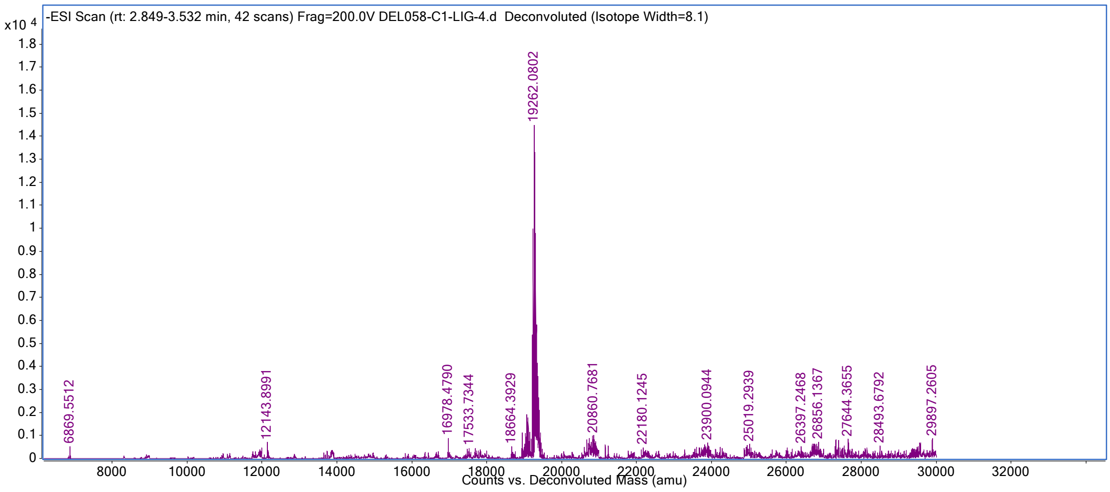
Primer ligation



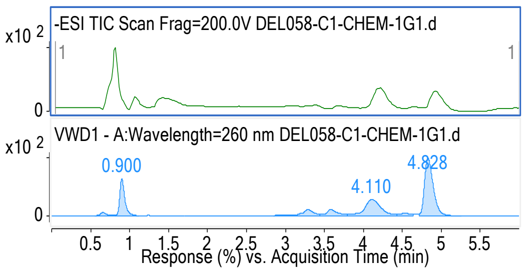


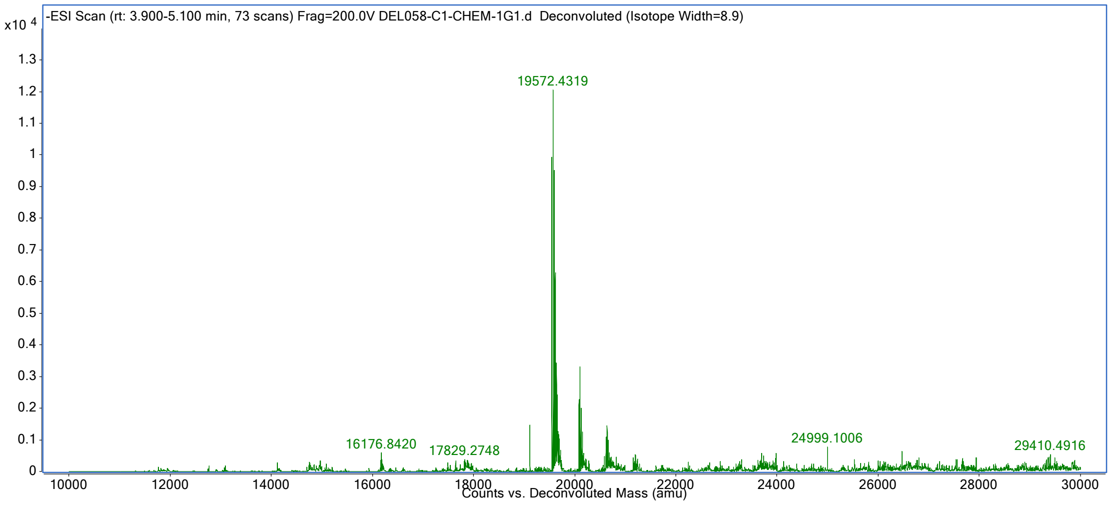
C1-tag ligation



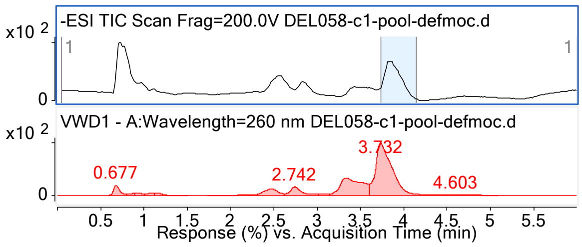


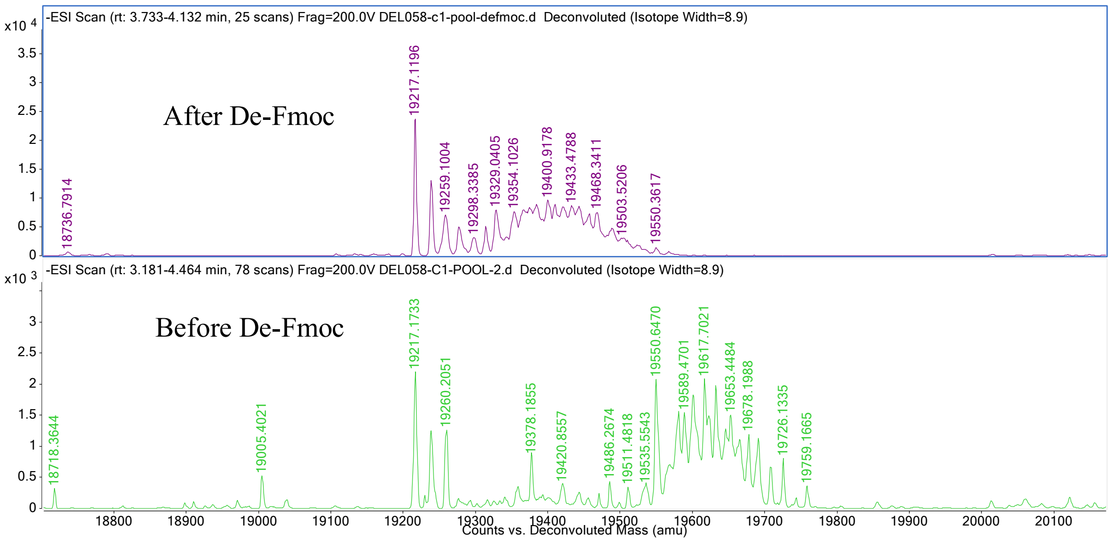
C1-amidation reaction



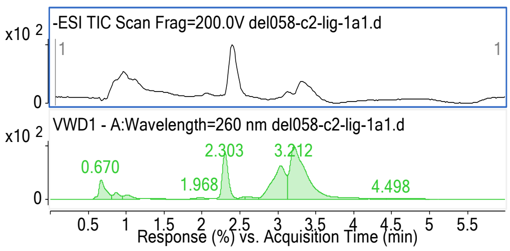


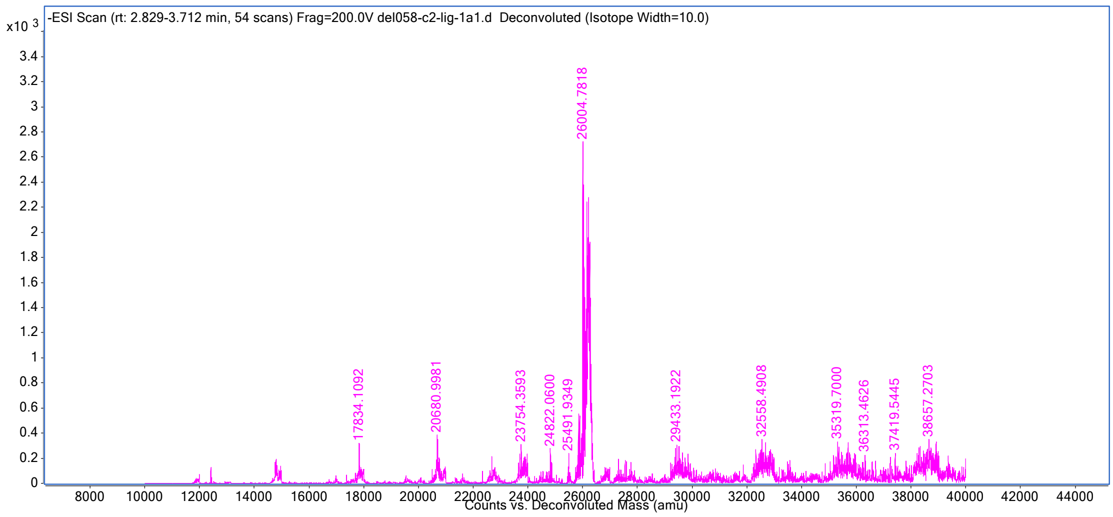
De-Fmoc



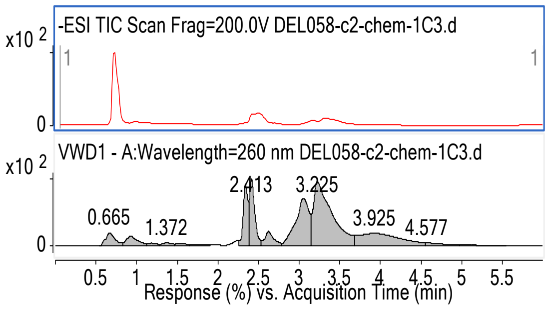


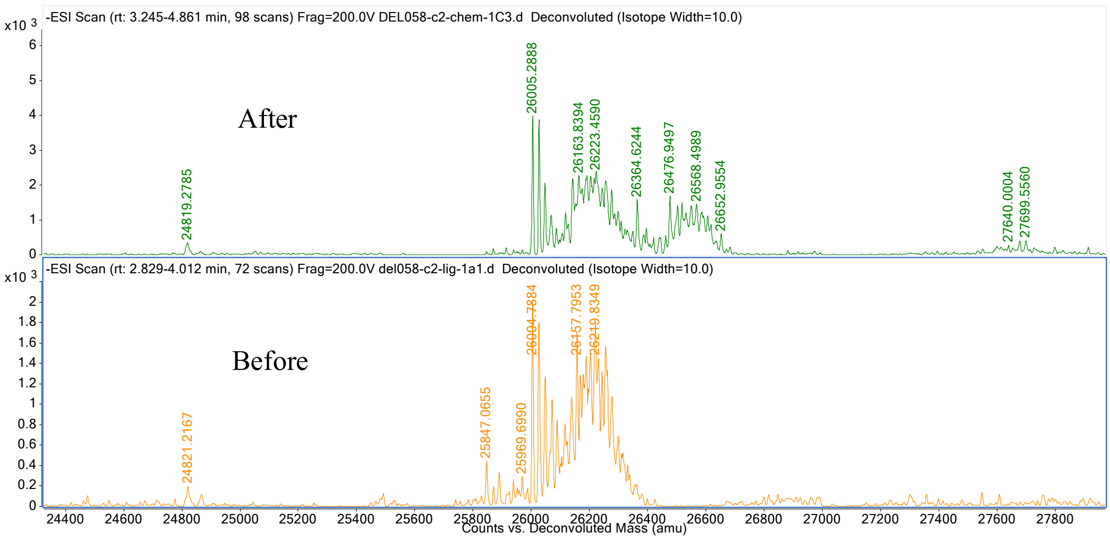
C2-tag ligation



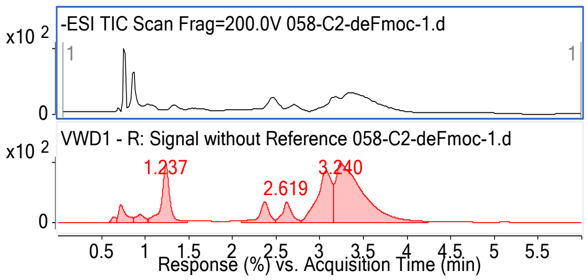


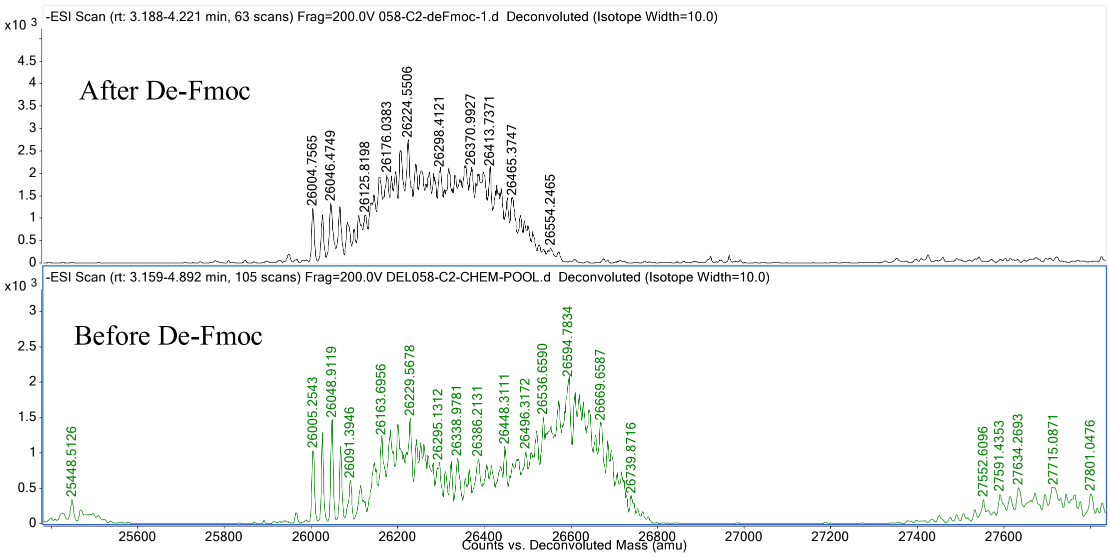
C2-amidation reaction



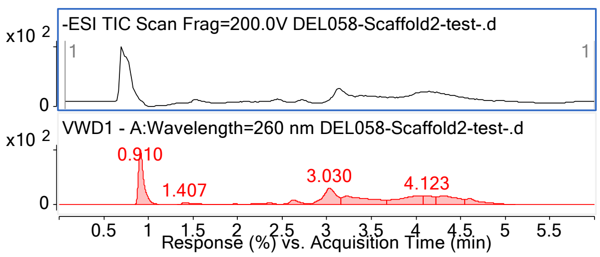


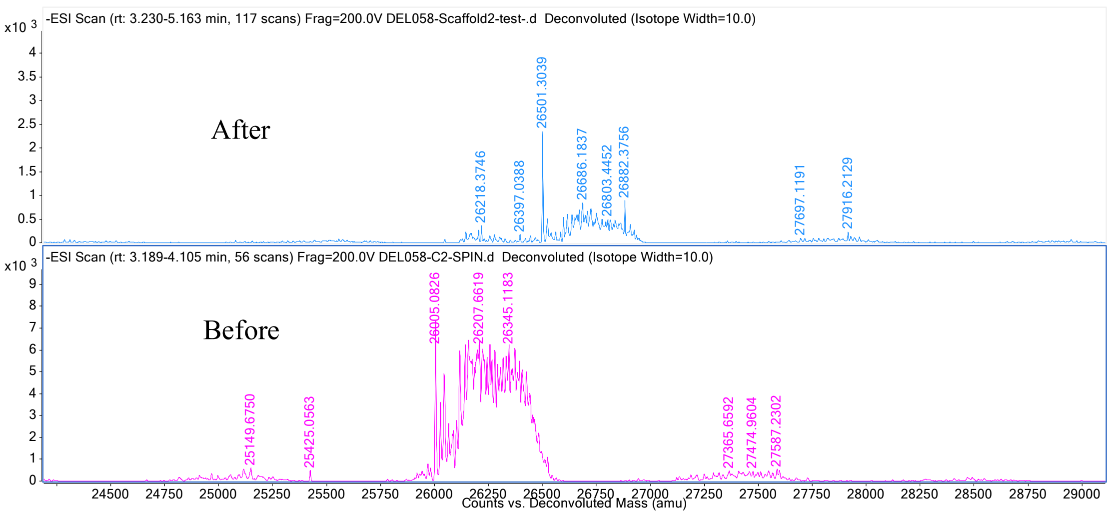
De-Fmoc



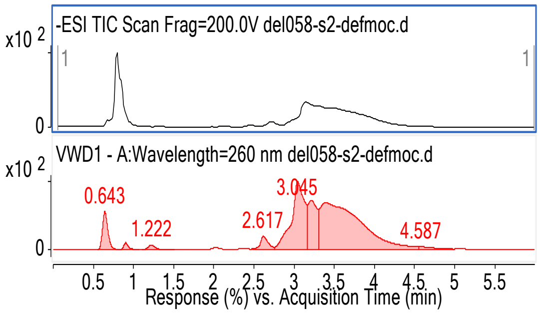


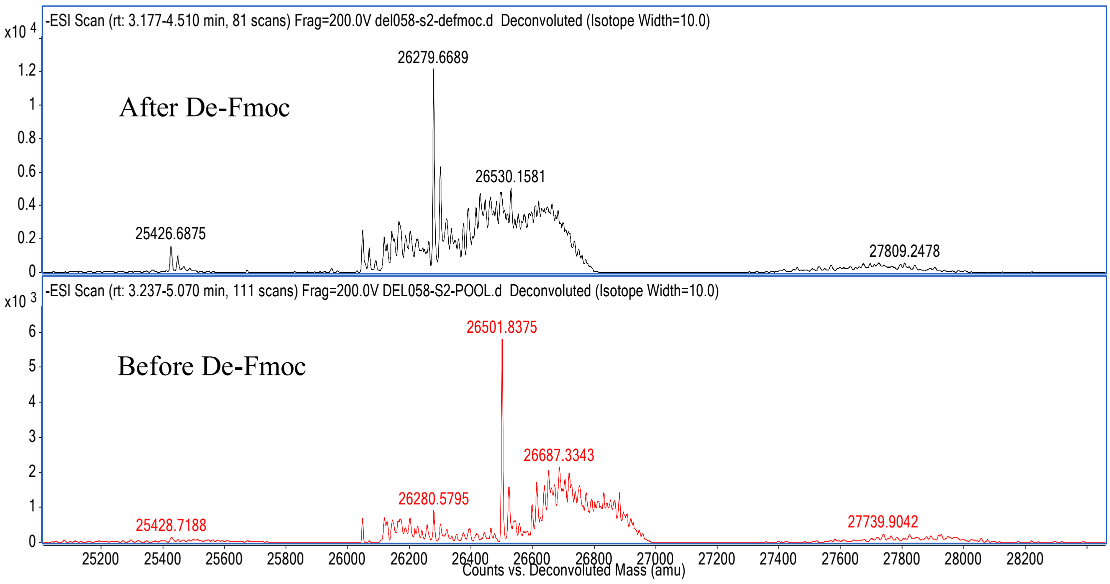
Amidation with Fmoc-Phe(4-I)-OH



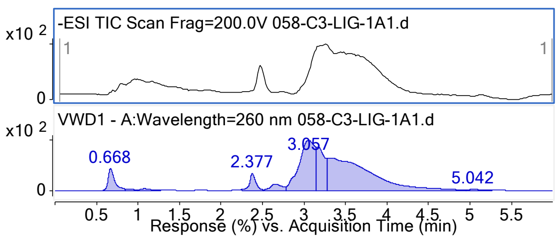


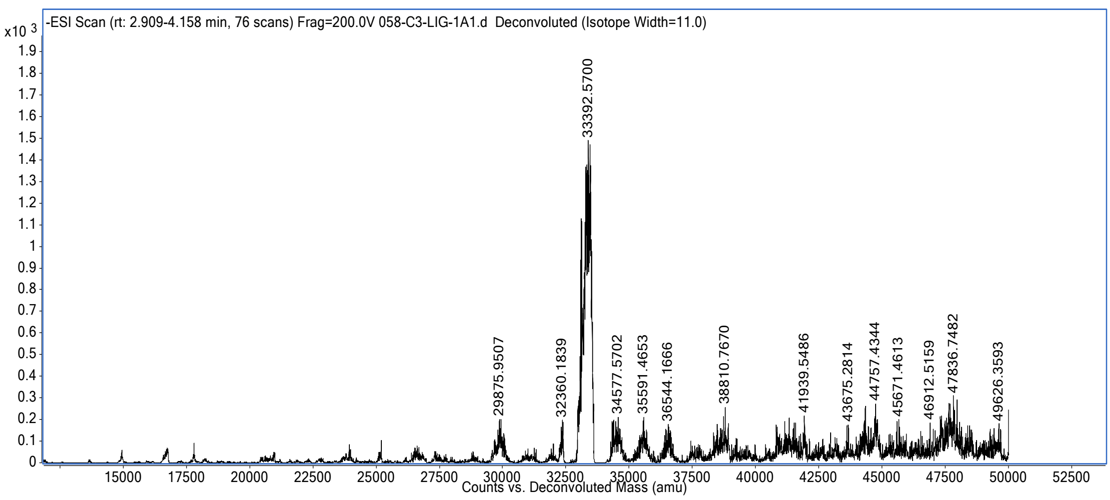
De-Fmoc



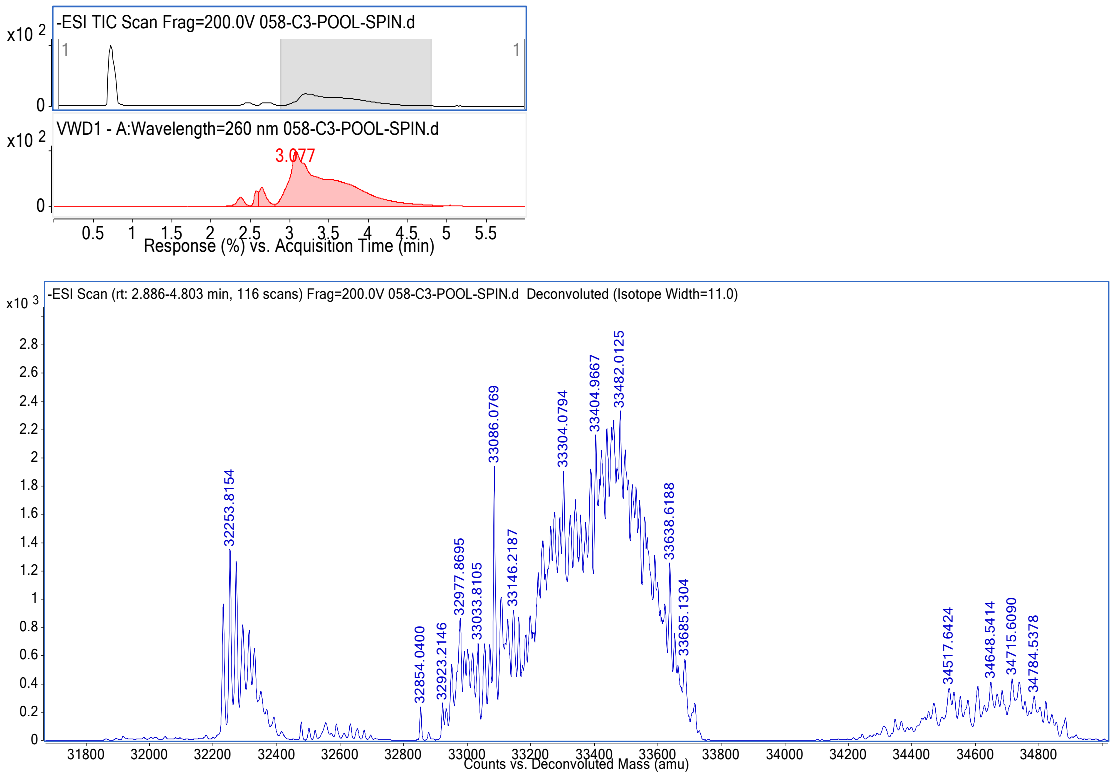


C3-tag ligation

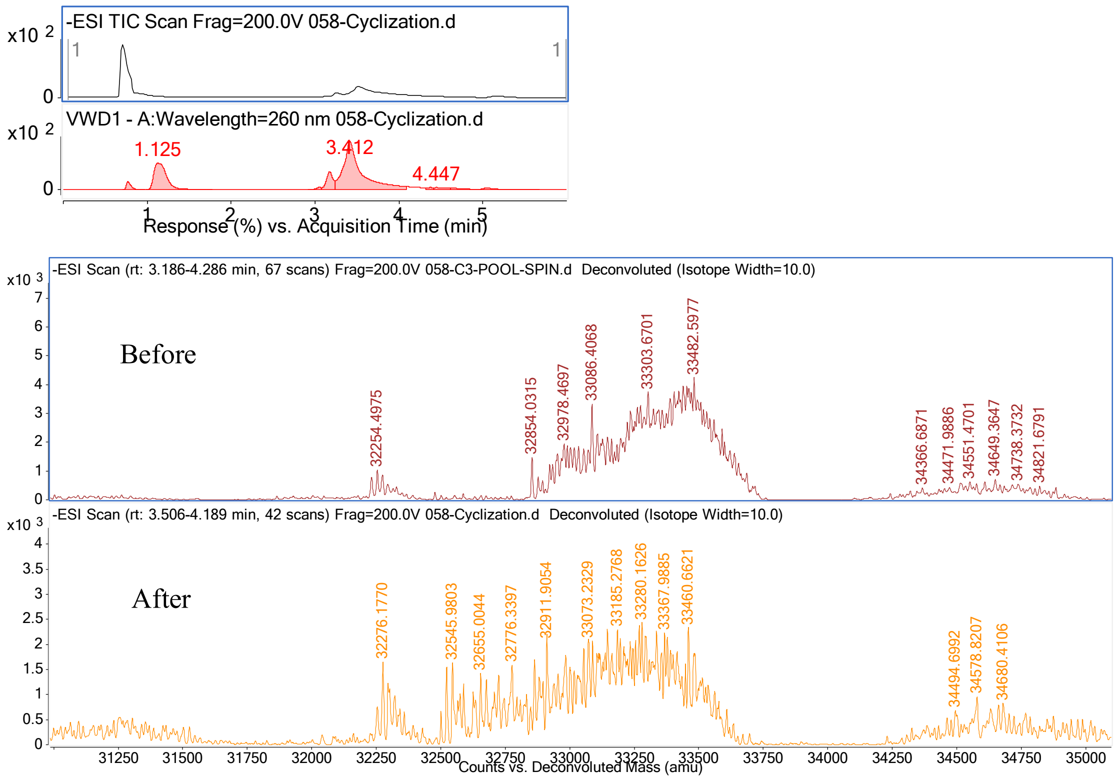




C3-amidation reaction



De-Mmt and S-arylation reaction



Library composition

1		tag	tag	smiles	cas
2	Cycle 1	GAATCCCTGAG	CAGGGATTCCA	C#CC[C@@H](NC(OCC1C2=CC=CC=C2C3=(	332064-94-5
3	Cycle 1	GAGTTCCTCAG	GAGGAACTCCA	FC=1C=CC(=CC1)C[C@H](CC(O)=O)NC(OC(	331763-70-3
4	Cycle 1	CTTCATTGGAG	CCAATGAAGCA	N#CC=1C=CC(=CC1)C[C@@H](CC(O)=O)NC	270065-90-2
5	Cycle 1	TTACGTCCTAG	AGGACGTAACA	FC1=C(F)C(F)=C(F)C(F)=C1C[C@@H](CC(O)	270063-43-9
6	Cycle 1	AAGGAAGACAG	GTCTTCCTTCA	C#CC[C@H](NC(OCC1C2=CC=CC=C2C3=C(	1217669-02-7
7	Cycle 1	ACACCTGCTAG	AGCAGGTGTCA	FC1=C(F)C(F)=C(F)C(F)=C1C[C@H](CC(O)=(	269398-94-9
8	Cycle 1	CCATGTAGCAG	GCTACATGGCA	O=C(O)[C@H]1C[C@H](C=C1)NC(OCC2C3=(	220497-64-3
9	Cycle 1	ATACGTCCGAG	CGGACGTATCA	ClC1=CC2=C(C=C1)C(C[C@H](C(O)=O)NC(O	925916-73-0
10	Cycle 1	CCACCTACTAG	AGTAGGTGGCA	N#CC=1C=CC(=CC1)C[C@H](CC(O)=O)NC(C	269726-87-6
11	Cycle 1	AGTGGGATGAG	CATCCCACTCA	O=C(O)[C@@H](NC(OCC1C2=CC=CC=C2C3	269078-73-1
12	Cycle 1	GACCGGATTAG	AATCCGGTCCA	C1=CC=C2CN([C@@H](CC2=C1)C(=O)O)C(=	136030-33-6
13	Cycle 1	GAACGCCTTAG	AAGGCGTTCCA	ClC=1C=CC(=CC1)C[C@H](C(O)=O)NC(OCC	142994-19-2
14	Cycle 1	ATCGCGTACAG	GTACGCGATCA	N#CC=1C=CC(=CC1)C[C@H](C(O)=O)NC(OC	205526-34-7
15	Cycle 1	GTTCGGTACAG	GTACCGAACCA	C1=CC=C2C(=C1)C3=CC=CC=C3C2COC(=O	101555-63-9
16	Cycle 1	ATGTCGGAAAG	TTCCGACATCA	O=C(O)[C@H](NC(OCC1C2=CC=CC=C2C3=(	198543-96-3
17	Cycle 1	GAAGAGCGTAG	ACGCTCTTCCA	O=C(O)[C@H](NC(OCC1C2=CC=CC=C2C3=(	269078-72-0
18	Cycle 1	CAAAGCCGTAG	ACGGCTTTGCA	O=C([C@@H]1C[C@H](NC(OCC2C3=C(C4=C	220497-66-5
19	Cycle 1	AGGATGTTGAG	CAACATCCTCA	C1=CC=C2C(=C1)C3=CC=CC=C3C2COC(=O	193693-64-0
20	Cycle 1	CGATTGAGAAG	TCTCAATCGCA	C1=CC=C2C(=C1)C3=CC=CC=C3C2COC(=O	129223-22-9
21	Cycle 1	AGGCTGTTGAG	CAACAGCCTCA	O=C(O)[C@H](CC1=CSC=C1)NC(OCC2C3=C	186320-06-9
22	Cycle 1	GTGTTCTCTAG	AGAGAACACCA	ClC1=CC2=C(C=C1)C(C[C@@H](C(O)=O)NC	908847-42-7
23	Cycle 1	CTCATTACGAG	CGTAATGAGCA	O=C(O)[C@H](CC1=CSC=N1)NC(OCC2C3=C	205528-32-1
24	Cycle 1	TTAGAACGGAG	CCGTTCTAACA	CN([C@@H](CC1CCCCC1)C(=O)O)C(=O)OC(	148983-03-3
25	Cycle 1	TCTATCCCTAG	AGGGATAGACA	O=C(O)[C@H](CC1=CC=CO1)NC(OCC2C3=C	159611-02-6
26	Cycle 1	ACGTTCAGAAG	TCTGAACGTCA	O=C(O)[C@H](NC(OCC1C2=CC=CC=C2C3=(	205526-38-1
27	Cycle 1	AAGTCACACAG	GTGTGACTTCA	O=C(O)C1CCC(CC1)CNC(OCC2C3=CC=CC=	188715-40-4
28	Cycle 1	CAGCTAAAGAG	CTTTAGCTGCA	C=CCC(C(O)=O)(NC(OCC1C2=CC=CC=C2C	1311992-97-8
29	Cycle 1	TGGAAACCGAG	CGGTTTCCACA	O=C(O)C[C@H](C1=CC([N+]([O-])=O)=CC=C	374791-04-5
30	Cycle 1	TTCCGAGAGAG	CTCTCGGAACA	NC(NCCC[C@H](C(O)=O)NC(OCC1C2=CC=C	200344-33-8
31	Cycle 1	CCTTATGCTAG	AGCATAAGGCA	O=C(O)C[C@H](C1=CC=C(Br)C=C1)NC(OCC	220498-04-4
32	Cycle 1	CCACAATCGAG	CGATTGTGGCA	CC1=CC=CC=C1[C@H](NC(OCC2C3=CC=C(	507472-27-7
33	Cycle 1	TGGTGTGAGAG	CTCACACCACA	O=C(O)C[C@H](C1=CC=C(C(F)(F)F)C=C1)N(	517905-88-3
34	Cycle 1	TGACGTAGCAG	GCTACGTCACA	O=C(O)CC(C1=CC=C(Br)C=C1)NC(OCC2C3=	269078-76-4
35	Cycle 1	GTAGGTTTGAG	CAAACCTACCA	CC1=CC=C(C(NC(OCC2C3=CC=CC=C3C4=(	284492-08-6
36	Cycle 1	CACTTGTTCAG	GAACAAGTGCA	C1=CC=C(C=C1)C[C@@H](C(=O)N2CCC[C@	138372-76-6
37	Cycle 1	ATGAGCTGCAG	GCAGCTCATCA	C=CCC(NC(OCC1C2=CC=CC=C2C3=CC=C(	221884-63-5
38	Cycle 1	GAATAGGCCAG	GGCCTATTCCA	C1CCC2C(C1)C[C@H](C(=O)O)N2C(=O)OCC	1217512-55-4
39	Cycle 1	GTACATCAGAG	CTGATGTACCA	O=C(O)C[C@@H](CC1=CC=CS1)NC(OCC2C	270262-98-1
40	Cycle 1	AGGCGTTCAAG	TGAACGCCTCA	C=CC[C@@H](NC(OCC1C2=CC=CC=C2C3=	170642-28-1
41	Cycle 1	GAGAATGCTAG	AGCATTCTCCA	C#CCCC[C@@H](C(=O)O)NC(=O)OCC1C2=C	1097192-05-6
42	Cycle 1	TCACGATCCAG	GGATCGTGACA	FC1=C(F)C(F)=C(F)C(F)=C1C[C@@H](C(O)=(	205526-32-5
43	Cycle 1	ACGGGAACAAG	TGTTCCCGTCA	CC1=CC=C(C[C@H](NC(OCC2C3=CC=CC=(	199006-54-7
44	Cycle 1	CAACGACACAG	GTGTCGTTGCA	CC1=C(C(C)=CC(O)=C1)C[C@H](NC(OCC2C	206060-54-0
45	Cycle 1	GTAAGGGTCAG	GACCCTTACCA	O=C(O)[C@H](CC1=CSC2=CC=CC=C12)NC(	177966-60-8
46	Cycle 1	CACATGACTAG	AGTCATGTGCA	O=C([C@H]1N(C(OCC2C3=C(C4=C2C=CC=C	130309-37-4
47	Cycle 1	ATAGCAGTGAG	CACTGCTATCA	O=C(O)C1=CC=CC(CNC(OCC2C3=CC=CC=(	155369-11-2
48	Cycle 1	TCCAGACATAG	ATGTCTGGACA	FC1=CC(C[C@H](C(O)=O)NC(OCC2C3=CC=(	205526-31-4
49	Cycle 1	TCAATCAGGAG	CCTGATTGACA	ClC=1C=CC(=CC1Cl)C[C@@H](C(O)=O)NC(	177966-59-5
50	Cycle 1	TCCCGAACTAG	AGTTCGGGACA	C1=CC=C2C(=C1)C3=CC=CC=C3C2COC(=O	885951-89-3
51	Cycle 1	GTAAGAGAGAG	CTCTCTTACCA	IC=1C=CC(=CC1)C[C@@H](C(O)=O)NC(OCC	82565-68-2
52	Cycle 1	CTCGCAACTAG	AGTTGCGAGCA	IC=1C=CC(=CC1)C[C@H](C(O)=O)NC(OCC2(	205526-29-0
53	Cycle 1	GTTGGCTTGAG	CAAGCCAACCA	C1=CC=C2C(=C1)C[C@@H](C(=O)O)N2C(=O	198560-38-2
54	Cycle 1	TCTTCAGGGAG	CCCTGAAGACA	O=[N+]([O-])C=1C=CC(=C(C1)[N+]([O-])=O)N(	140430-54-2
55	Cycle 1	GAAGTATGCAG	GCATACTTCCA	O=C(O)[C@@H](CC1=CSC2=CC=CC=C12)N(	177966-61-9
56	Cycle 1	CTAAGTCACAG	GTGACTTAGCA	O=C(O)[C@H](CC1CC1)NC(OCC2C3=CC=CC	214750-76-2
57	Cycle 1	AGAGTAAGGAG	CCTTACTCTCA	O=C(O)C[C@H](CC1=CC=CO1)NC(OCC2C3=	270263-07-5
58	Cycle 1	GTTTACCCCAG	GGGGTAAACCA	O=C(O)C1(NC(OCC2C3=CC=CC=C3C4=CC=	162648-54-6
59	Cycle 1	CTTTCGGGAAG	TCCCGAAAGCA	FC1=CC2=C(C=C1)C(CC(C(O)=O)NC(OCC3C	1219392-55-8
60	Cycle 1	CTAGGGAGTAG	ACTCCCTAGCA	ClC=1C=CC(=CC1Cl)C[C@H](C(O)=O)NC(OC	177966-58-4

61	Cycle 1	GTAAAGCTCAG	GAGCTTTACCA	BrC=1C=CC(=CC1)C[C@@H](C(O)=O)NC(OC	198561-04-5
62	Cycle 1	CCTACTTGCAG	GCAAGTAGGCA	O=[N+]([O-])C=1C=CC(=CC1)C[C@H](C(O)=	177966-63-1
63	Cycle 1	AAGCTCGTAAG	TACGAGCTTCA	O=C(O)C[C@@H](NC(OCC1C2=CC=CC=C2C	1217460-65-5
64	Cycle 1	ACGATTAGCAG	GCTAATCGTCA	O=C(O)[C@@H](CC1=CN=CC=C1)NC(OCC2	142994-45-4
65	Cycle 1	AACGGAGTAAG	TACTCCGTTCA	O=C(O)[C@@H](NC(OCC1C2=CC=CC=C2C3	220497-61-0
66	Cycle 1	CAACTGAAGAG	CTTCAGTTGCA	O=C(O)C=1C=CC(=CC1)CNC(OCC2C3=CC=	164470-64-8
67	Cycle 1	AAGAATGGCAG	GCCATTCTTCA	O=C(O)C1(CCCC1)NC(OCC2C3=CC=CC=C3	117322-30-2
68	Cycle 1	AGGGGAACAAG	TGTTCCCCTCA	O=C(O)C1(CCC1)NC(OCC2C3=CC=CC=C3C	885951-77-9
69	Cycle 1	CGCGAATATAG	ATATTCGCGCA	FC(F)(F)C=1C=CC(=CC1)C[C@@H](C(O)=O)	247113-86-6
70	Cycle 1	AAGTCGGATAG	ATCCGACTTCA	C1=CC=C2C(=C1)C3=CC=CC=C3C2COC(=O	178432-49-0
71	Cycle 1	GTTCTGCTTAG	AAGCAGAACCA	COC1=C(OC)C=C(C[C@H](NC(OCC2C3=CC=	184962-88-7
72	Cycle 1	CACCACTTAAG	TAAGTGGTGCA	O=C(O)[C@H](CC1=CC=CS1)NC(OCC2C3=C	130309-35-2
73	Cycle 1	CATGATGAGAG	CTCATCATGCA	OC=1C=CC2=C(C1)C(=CN2)C[C@@H](C(O)=	178119-94-3
74	Cycle 1	CACGATCATAG	ATGATCGTGCA	O=C(O)[C@H]1CCC[C@@H]1NC(OCC2C3=C	359586-64-4
75	Cycle 1	GCCCTATTAAG	TAATAGGGCCA	O=C(O)C[C@H](CC1=CSC=C1)NC(OCC2C3=	270263-01-9
76	Cycle 1	GACCTTTGGAG	CCAAAGGTCCA	O=C(O)C1(CCOCC1)NC(OCC2C3=CC=CC=C	285996-72-7
77	Cycle 1	ATGCCTCCTAG	AGGAGGCATCA	O=C(O)[C@H](C1=CSC=C1)NC(OCC2C3=CC	1217706-09-6
78	Cycle 1	TGTTCAGGCAG	GCCTGAACACA	O=C(O)C1(CC1)NC(OCC2C3=CC=CC=C3C4=	126705-22-4
79	Cycle 1	TTCCCAGTAAG	TACTGGGAACA	C1=CC=C2C(=C1)C3=CC=CC=C3C2COC(=O	185116-43-2
80	Cycle 1	GGACTTCGAAG	TCGAAGTCCCA	C#CC[C@@H](NC(OCC1C2=CC=CC=C2C3=	220497-98-3
81	Cycle 1	TAAGAAGCGAG	CGCTTCTTACA	C#CC[C@H](NC(OCC1C2=CC=CC=C2C3=C	198561-07-8
82	Cycle 1	CTAGCGGTTAG	AACCGCTAGCA	ClC=1C=CC(=C(C1)Cl)C[C@@H](C(O)=O)NC	352351-62-3
83	Cycle 1	TGCGATCAGAG	CTGATCGCACA	FC1=CC(C[C@@H](C(O)=O)NC(OCC2C3=CC	205526-30-3
84	Cycle 1	CGCAAAGACAG	GTCTTTGCGCA	O=C(O)[C@H](CC1=CN=CC=C1)NC(OCC2C3	175453-07-3
85	Cycle 1	CCCGGTTATAG	ATAACCGGGCA	O=C(O)[C@H](NC(OCC1C2=CC=CC=C2C3=	136555-16-3
86	Cycle 1	CCGAATAGGAG	CCTATTCGGCA	O=C(O)[C@@H](NC(OCC1C2=CC=CC=C2C3	138775-07-2
87	Cycle 1	GGCCAGTTTAG	AAACTGGCCCA	FC(F)(F)C(NCCCC[C@@H](C(O)=O)NC(OCC	76265-69-5
88	Cycle 1	ACTAGTACCAG	GGTACTAGTCA	O=C(CC[C@H](NC(OCC1C2=CC=CC=C2C3=	150047-85-1
89	Cycle 1	ACCTATCTCAG	GAGATAGGTCA	[N-]=[N+]=NCCC[C@@H](C(O)=O)NC(OCC1	1097192-04-5
90	Cycle 1	AGGAGCAGTAG	ACTGCTCCTCA	C#CC[C@](C(O)=O)(NC(OCC1C2=CC=CC=C	1198791-65-9
91	Cycle 1	GCTCGAAGAAG	TCTTCGAGCCA	C[C@@H](OCC1=CC=CC=C1)[C@H](NC(OC	117872-75-0
92	Cycle 1	CAGAATCCCAG	GGGATTCTGCA	O=C(O)C[C@H](C1=CC=C([N+]([O-])=O)C=C	507472-26-6
93	Cycle 1	ACGCTCCAAAG	TTGGAGCGTCA	COC1=CC(OC)=CC([C@H](NC(OCC2C3=CC=	511272-41-6
94	Cycle 1	TCTCCGATCAG	GATCGGAGACA	O=C(O)C[C@H](C1=CN=CC=C1)NC(OCC2C3	511272-43-8
95	Cycle 1	GTCAAAGAGAG	CTCTTTGACCA	O=C(O)C[C@H](C1=CC=CS1)NC(OCC2C3=C	511272-45-0
96	Cycle 1	CGTTCGTATAG	ATACGAACGCA	O=C(O)C[C@H](C1=CC=CO1)NC(OCC2C3=C	1217662-55-9
97	Cycle 1	TAGTAGGAGAG	CTCCTACTACA	CC(C1=CC=C(C[C@H](NC(OCC2C3=CC=CC	204716-07-4
98	Cycle 1	CCGTTACACAG	GTGTAACGGCA	O=C(O)C1=CC(NC(OCC2C3=CC=CC=C3C4=	1071446-05-3
99	Cycle 1	AGAGATTCGAG	CGAATCTCTCA	C1(C2=C(C=CC=C2)C3=C1C=CC=C3)COC(N	1260596-73-3
100	Cycle 1	GAGTGGACTAG	AGTCCACTCCA	O=C(O)[C@H](CC1=CNC2=C1C=CC=N2)NC(	737007-45-3
101	Cycle 1	TTATGGCCGAG	CGGCCATAACA	N1([C@H](C(=O)O)C[C@H](C1)F)C(=O)OCC1	1228307-81-0
102	Cycle 1	GTAGCCTGTAG	ACAGGCTACCA	FC1=CC(C[C@H](C(O)=O)NC(OCC2C3=CC=	205526-25-6
103	Cycle 1	TGGCGTTTTAG	AAAACGCCACA	FC=1C=CC(=C(C1)F)C[C@@H](C(O)=O)NC(	1032337-49-7
104	Cycle 1	TACTCGGGAAG	TCCCGAGTACA	C1=CC=C2C(=C1)C3=CC=CC=C3C2COC(=O	133054-21-4
105	Cycle 1	TGAGTTCAGAG	CTGAACTCACA	C1(C2=C(C=CC=C2)C3=C1C=CC=C3)COC(N	1217716-50-1
106	Cycle 1	TATGTGGGGAG	CCCCACATACA	O=C(O)C1(NC(OCC2C3=CC=CC=C3C4=CC=	135944-07-9
107	Cycle 1	AGGGTCCTTAG	AAGGACCCTCA	O=C(O)[C@H](CC1CCC1)NC(OCC2C3=CC=C	478183-62-9
108	Cycle 1	AGCCAACTTAG	AAGTTGGCTCA	O=C(O)[C@@H]1CCC[C@H]1NC(OCC2C3=C	359586-69-9
109	Cycle 1	GCACATATCAG	GATATGTGCCA	O=C(O)CC1(NC(OCC2C3=CC=CC=C3C4=CC	282524-98-5
110	Cycle 1	AGCATCGCTAG	AGCGATGCTCA	O=C(O)CC1(CNC(OCC2C3=CC=CC=C3C4=C	882847-19-0
111	Cycle 1	GCTGCGATTAG	AATCGCAGCCA	O=C(O)[C@@H]1CC[C@H](CC1)CNC(OCC2C	167690-53-1
112	Cycle 1	CGTCTCACTAG	AGTGAGACGCA	O=[N+]([O-])C=1C=CC(=CC1)C[C@@H](C(O)	95753-55-2
113	Cycle 1	CCTGTGCATAG	ATGCACAGGCA	C1=CC=C2C(=C1)C3=CC=CC=C3C2COC(=O	86069-86-5
114	Cycle 1	CTCGACTTAAG	TAAGTCGAGCA	O=C(O)[C@@H]1CC[C@H](CC1)NC(OCC2C3	147900-46-7
115	Cycle 1	ACTTCGCACAG	GTGCGAAGTCA	CC1(OCC2=C(O1)C=CC(C[C@H](NC(OCC3C	252049-13-1
116	Cycle 1	TGTTCCGGTAG	ACCGGAACACA	IC=1C=CC(=CC1)C[C@H](CC(O)=O)NC(OCC	269396-73-8
117	Cycle 1	GCCTTAATCAG	GATTAAGGCCA	BrC=1C=CC(=CC1)C[C@@H](CC(O)=O)NC(	270062-86-7
118	Cycle 1	TGCGACGATAG	ATCGTCGCACA	ClC=1C=CC(=CC1Cl)C[C@@H](CC(O)=O)NC	270063-52-0
119	Cycle 1	AGATGAGAGAG	CTCTCATCTCA	IC=1C=CC(=CC1)C[C@@H](CC(O)=O)NC(OC	270065-72-0
120	Cycle 1	TGCCCTAGAAG	TCTAGGGCACA	O=C(O)C[C@H](CC1=CNC2=CC=CC=C12)N	353245-98-4

121	Cycle 1	TGAAGACACAG	GTGTCTTCACA	O=C(O)C[C@@H](C1=CC=C(F)C=C1)NC(OC(	479064-89-6
122	Cycle 1	TCCAGTGACAG	GTCACTGGACA	O=C(O)C[C@@H](C1=C(Cl)C(Cl)=CC=C1)NC	501015-35-6
123	Cycle 1	TTCACCACTAG	AGTGGTGAACA	O=C(O)C[C@H](C1=C(Cl)C=C(Cl)C=C1)NC(C	511272-37-0
124	Cycle 1	TAGGCATCCAG	GGATGCCTACA	O=C(O)[C@@H](NC(OCC1C2=CC=CC=C2C3	161321-36-4
125	Cycle 1	GCGTATTCGAG	CGAATACGCCA	O=C(O)[C@@H](NC(OCC1C2=CC=CC=C2C3	205526-26-7
126	Cycle 1	TAGCCTTTGAG	CAAAGGCTACA	FC=1C=CC(=CC1F)C[C@H](C(O)=O)NC(OCC	198545-59-4
127	Cycle 1	CTTCGCATCAG	GATGCGAAGCA	FC=1C=CC(=CC1)C[C@@H](C(O)=O)NC(OC(	169243-86-1
128	Cycle 1	CGAATTGCTAG	AGCAATTCGCA	C1=CC=C2CN([C@H](CC2=C1)C(=O)O)C(=O	130309-33-0
129	Cycle 1	CACGTCTCAAG	TGAGACGTGCA	O=C(O)[C@H](NC(OCC1C2=CC=CC=C2C3=(	205526-22-3
130	Cycle 1	TCATGGGTAAG	TACCCATGACA	N#CC=1C=CC(=CC1)C[C@@H](C(O)=O)NC((	173963-93-4
131	Cycle 1	GATCACCGTAG	ACGGTGATCCA	CC(C)(OC(N1CCCC(C1)CC(NC(OCC2C3=CC=	457060-97-8
132	Cycle 1	GATCCGATAAG	TATCGGATCCA	C[C@]1(CCCN1C(=O)OCC2C3=CC=CC=C3C	167275-47-0
133	Cycle 1	CACAGTTGAAG	TCAACTGTGCA	C(F)(C1=CC=C(C[C@@H](C(O)=O)NC(=O)OC	1808268-08-7
134	Cycle 1	TAGAATCCGAG	CGGATTCTACA	C1CN(C[C@@H](C(=O)O)NC(OCC2C3=C(C4=	1251903-85-1
135	Cycle 1	TGATCTGACAG	GTCAGATCACA	C1=CC=C2C(=C1)C3=CC=CC=C3C2COC(=O	193693-61-7
136	Cycle 1	CTTGCCACTAG	AGTGGCAAGCA	C1=CC=C2C(=C1)C3=CC=CC=C3C2COC(=O	374791-02-3
137	Cycle 1	CTATGTGTCAG	GACACATAGCA	O=C(O)C1(NC(OCC2C3=CC=CC=C3C4=CC=	214139-28-3
138	Cycle 1	TCTGATGCGAG	CGCATCAGACA	C1=CC=C2C(=C1)CN(C2C(=O)O)C(=O)OCC3(	204320-59-2
139	Cycle 1	CGGTTTAAGAG	CTTAAACCGCA	O=C(O)[C@@H](NC(OCC1C2=CC=CC=C2C3	159610-82-9
140	Cycle 1	GGAATCTACAG	GTAGATTCCCA	C1CC[C@H]2[C@@H](C1)C[C@@H](C(=O)O)	214750-71-7
141	Cycle 1	ACCCGAAGAAG	TCTTCGGGTCA	CC(C)(C)OC(=O)N1CCN(C1C(=O)O)C(=O)OC(	207129-12-2
142	Cycle 1	TTATCCCCCAG	GGGGGATAACA	C1(C2=C(C=CC=C2)C3=C1C=CC=C3)COC(N	683217-64-3
143	Cycle 1	CCTTCAGACAG	GTCTGAAGGCA	FC=1C=CC(=CC1F)C[C@@H](C(O)=O)NC(O(	198560-43-9
144	Cycle 1	TGACCACCAAG	TGGTGGTCACA	CC1=CC=CC=C1C[C@H](NC(OCC2C3=CC=(	211637-75-1
145	Cycle 1	CTGCTACTAAG	TAGTAGCAGCA	FC(F)(F)C=1C=CC(=CC1)C[C@H](C(O)=O)N(	238742-88-6
146	Cycle 1	CCACACTTAAG	TAAGTGTGGCA	C1=CC=C2C(=C1)C3=CC=CC=C3C2COC(=O	139262-20-7
147	Cycle 1	GCTTCACTTAG	AAGTGAAGCCA	O=C(O)[C@H]1C[C@H](CC1)NC(OCC2C3=C(	220497-67-6
148	Cycle 1	GCAAGTTGTAG	ACAACTTGCCA	CC(C)(OC(N1C[C@@H](C(O)=O)[C@H](NC(O	267230-44-4
149	Cycle 1	ACGTTACAGAG	CTGTAACGTCA	C1=CC=C2C(=C1)C3=CC=CC=C3C2COC(=O	1335206-44-4
150	Cycle 1	GTCAGTAGAAG	TCTACTGACCA	C=CCC[C@@H](NC(OCC1C2=CC=CC=C2C3	865352-21-2
151	Cycle 1	CTCGAATTCAG	GAATTCGAGCA	C1=CC=C2C(=C1)C3=CC=CC=C3C2COC(=O	942153-03-9
152	Cycle 1	ATCGTCACGAG	CGTGACGATCA	O=C(O)[C@H](C1CC1)NC(OCC2C3=CC=CC=	1212257-18-5
153	Cycle 1	AACAACTGCAG	GCAGTTGTTCA	CC(C)(OC(N1CCC(C(NC(OCC2C3=CC=CC=C	313051-96-6
154	Cycle 1	AAGAGAGCAAG	TGCTCTCTTCA	CC(C)(OC(N1CCCC(C(NC(OCC2C3=CC=CC=	372144-11-1
155	Cycle 1	ATCTCTGACAG	GTCAGAGATCA	O=C(O)C[C@@H](C1=CC=C(C#N)C=C1)NC((	507472-24-4
156	Cycle 1	GCCTAGAGTAG	ACTCTAGGCCA	CN1C=C(C2=CC=CC=C21)C[C@@H](NC(OC	168471-22-5
157	Cycle 1	AGTTTCGGGAG	CCCGAAACTCA	FC(F)(F)C=1C=CC(=CC1)C[C@@H](CC(O)=C	270065-81-1
158	Cycle 1	TTACATCCCAG	GGGATGTAACA	FC1=CC=CC(C[C@H](CC(O)=O)NC(OCC2C3	331763-67-8
159	Cycle 1	CCGTATAGTAG	ACTATACGGCA	N#CC1=CC=CC(C[C@H](CC(O)=O)NC(OCC2	269726-84-3
160	Cycle 1	GCCCAACTTAG	AAGTTGGGCCA	O=C(O)C[C@H](NC(OCC1C2=CC=CC=C2C3=	268734-29-8
161	Cycle 1	CCTATCAAGAG	CTTGATAGGCA	C1=CC=C2C(=C1)C3=CC=CC=C3C2COC(=O	193693-60-6
162	Cycle 1	ACCACCAACAG	GTTGGTGGTCA	C1=CC=C2CN([C@H](CC2=C1)CC(=O)O)C(=(	332064-67-2
163	Cycle 1	ACTGATGGGAG	CCCATCAGTCA	ClC=1C=CC(=CC1)C[C@H](CC(O)=O)NC(OC	331763-60-1
164	Cycle 1	AACGGGAATAG	ATTCCCGTTCA	ClC=1C=CC(=C(C1)Cl)C[C@@H](CC(O)=O)N	270063-49-5
165	Cycle 1	ATGTCTCAGAG	CTGAGACATCA	ClC=1C=CC(=C(C1)Cl)C[C@H](CC(O)=O)NC(	269396-54-5
166	Cycle 1	GCTGAATCAAG	TGATTCAGCCA	FC=1C=CC(=CC1)C[C@@H](CC(O)=O)NC(O(	270062-83-4
167	Cycle 1	TGTACTGGCAG	GCCAGTACACA	O=C(O)C[C@H](CC1=CC=CS1)NC(OCC2C3=	269726-90-1
168	Cycle 1	ACAGAGCCAAG	TGGCTCTGTCA	O=C(O)C[C@H](CC1=CSC2=CC=CC=C12)N(	270063-46-2
169	Cycle 1	ATAGCATGGAG	CCATGCTATCA	BrC=1C=CC(=CC1)C[C@H](CC(O)=O)NC(OC	331763-76-9
170	Cycle 1	CGCATTGGAAG	TCCAATGCGCA	ClC=1C=CC(=CC1)C[C@@H](CC(O)=O)NC(C	270596-43-5
171	Cycle 1	AAGCGAACGAG	CGTTCGCTTCA	ClC=1C=CC(=CC1Cl)C[C@H](CC(O)=O)NC((	269396-57-8
172	Cycle 1	CCGCAAAACAG	GTTTTGCGGCA	FC(F)(F)C=1C=CC(=CC1)C[C@H](CC(O)=O)N	269726-78-5
173	Cycle 1	TTCCTGCTGAG	CAGCAGGAACA	O=C(O)C[C@H](C1=CC=C(Cl)C=C1)NC(OCC	479064-92-1
174	Cycle 1	TCTGGTCTGAG	CAGACCAGACA	O=C(O)C[C@H](C1=CC(Cl)=CC=C1)NC(OCC	511272-53-0
175	Cycle 1	TTGGGCATAAG	TATGCCCAACA	C1CCC(C1)C[C@H](C(=O)O)NC(=O)OCC2C3=	1262802-59-4
176	Cycle 1	GCAGGGAATAG	ATTCCCTGCCA	C=CC[C@H](NC(OCC1C2=CC=CC=C2C3=C(	146549-21-5
177	Cycle 1	GCTACCATGAG	CATGGTAGCCA	O=[N+]([O-])C=1C=CC(=CC1)C[C@H](CC(O)=	269398-78-9
178	Cycle 1	GGTTGAAGGAG	CCTTCAACCCA	O=[N+]([O-])C=1C=CC(=CC1)C[C@@H](CC((	270062-88-9
179	Cycle 1	ACGCGTAAAAG	TTTACGCGTCA	CC(=O)NCSC[C@@H](C(=O)O)NC(=O)OCC1(	86060-81-3
180	Cycle 1	ATGCTCGTGAG	CACGAGCATCA	CC(C)(C)OC(=O)NCCCC[C@@H](C(=O)O)NC	71989-26-9

181	Cycle 1	GGTAAGTTGAG	CAACTTACCCA	C1C[C@H](N(C1)C(=O)OCC2C3=CC=CC=C3(	71989-31-6
182	Cycle 1	TCTTGCACGAG	CGTGCAAGACA	CC(C(C(=O)O)NC(=O)OCC1C2=CC=CC=C2C	71989-35-0
183	Cycle 1	TACCCGAATAG	ATTCGGGTACA	CSCCC(C(=O)O)NC(=O)OCC1C2=CC=CC=C2	71989-28-1
184	Cycle 1	TTGTAGCGCAG	GCGCTACAACA	CC(C)(C)OCC(C(=O)O)NC(=O)OCC1C2=CC=(	128107-47-1
185	Cycle 1	ATTGCGTGCAG	GCACGCAATCA	CC(C)C(C(=O)O)NC(=O)OCC1C2=CC=CC=C2	68858-20-8
186	Cycle 1	GTAGTTCCGAG	CGGAACTACCA	CC(C)CC(C(=O)O)NC(=O)OCC1C2=CC=CC=(	35661-60-0
187	Cycle 1	CAGTAGCTAAG	TAGCTACTGCA	C1=CC=C(C=C1)CC(C(=O)O)NC(=O)OCC2C3	35661-40-6
188	Cycle 1	CATACGCGTAG	ACGCGTATGCA	CC(C(=O)O)NC(=O)OCC1C2=CC=CC=C2C3=	35661-39-3
189	Cycle 1	ACAAGCACTAG	AGTGCTTGTCA	CC(C)(C)OC(=O)CCC(C(=O)O)NC(=O)OCC1C	71989-18-9
190	Cycle 1	CGACATCCTAG	AGGATGTCGCA	CC(C)(C)OC(=O)CC(C(=O)O)NC(=O)OCC1C2=	71989-14-5
191	Cycle 1	CGAGGAGTTAG	AACTCCTCGCA	C1=CC=C2C(=C1)C(C3=CC=CC=C32)COC(=	29022-11-5
192	Cycle 1	AAATCAGCCAG	GGCTGATTTCA	CCC(C)C(C(=O)O)NC(=O)OCC1C2=CC=CC=(	71989-23-6
193	Cycle 1	GATCCACATAG	ATGTGGATCCA	COC(=O)CC(C(=O)O)NC(=O)OCC1C2=CC=C(	145038-53-5
194	Cycle 1	gttaaagggAG	ccctttaacCA	CC(C)(C)OCC(C(=O)O)NC(=O)OCC1C2=CC=(	71989-33-8
195	Cycle 1	cttgaccagAG	ctggtcaagCA	CC(C(=O)O)NC(=O)OCC1C2=CC=CC=C2C3=	79990-15-1
196	Cycle 1	gggctgtaaAG	ttacagcccCA	CC(C)CC(C(=O)O)NC(=O)OCC1C2=CC=CC=(	114360-54-2
197	Cycle 1	ggtgaatgtAG	acattcaccCA	CSCCC(C(=O)O)NC(=O)OCC1C2=CC=CC=C2	112883-40-6
198	Cycle 1	actccctctAG	agagggagtCA	C1=CC=C(C=C1)CC(C(=O)O)NC(=O)OCC2C3	86123-10-6
199	Cycle 1	tacacgctgAG	cagcgtgtaCA	CCCCC(C(=O)O)NC(=O)OCC1C2=CC=CC=C	112883-41-7
200	Cycle 1	gctttgtgtAG	acacaaagcCA	CC(C)(C)OC(=O)CCC(C(=O)O)NC(=O)OCC1C	104091-08-9
201	Cycle 1	ttgaaggcaAG	tgccttcaaCA	CC(C)C(C(=O)O)NC(=O)OCC1C2=CC=CC=C2	84624-17-9
202	Cycle 1	ctgcactaaAG	ttagtgcagCA	CC(C(C(=O)O)NC(=O)OCC1C2=CC=CC=C2C	138797-71-4
203	Cycle 1	tgggctctaAG	tagagcccaCA	CC(C)(C)OC1=CC=C(C=C1)CC(C(=O)O)NC(=	118488-18-9
204	Cycle 1	agaccatctAG	agatggtctCA	C1CC(N(C1)C(=O)OCC2C3=CC=CC=C3C4=C	101555-62-8
205	Cycle 1	ccgatgattAG	aatcatcggCA	C1=CC=C(C=C1)CCC(C(=O)O)NC(=O)OCC2(	135994-09-1
206	Cycle 1	caatgtggcAG	gccacattgCA	C1=CC=C2C(=C1)C(C3=CC=CC=C32)COC(=	35737-10-1
207	Cycle 1	attagccgaAG	tcggctaatCA	C1CCC(CC1)CC(C(=O)O)NC(=O)OCC2C3=C(	135673-97-1
208	Cycle 1	tatgcgtacAG	gtacgcataCA	C	
209					
210	Cycle 2	tagcttgctGT	agcaagctaCT	C#CC[C@@H](NC(OCC1C2=CC=CC=C2C3=(	332064-94-5
211	Cycle 2	ggatgacctGT	aggtcatccCT	FC=1C=CC(=CC1)C[C@H](CC(O)=O)NC(OC(	331763-70-3
212	Cycle 2	tccatggtaGT	taccatggaCT	N#CC=1C=CC(=CC1)C[C@@H](CC(O)=O)NC	270065-90-2
213	Cycle 2	cacaaaaccGT	ggttttgtgCT	FC1=C(F)C(F)=C(F)C(F)=C1C[C@@H](CC(O)	270063-43-9
214	Cycle 2	gatgtaacgGT	cgttacatcCT	C#CC[C@H](NC(OCC1C2=CC=CC=C2C3=C(	1217669-02-7
215	Cycle 2	tgtcttggtGT	accaagacaCT	FC1=C(F)C(F)=C(F)C(F)=C1C[C@H](CC(O)=(	269398-94-9
216	Cycle 2	aagagtgccGT	ggcactcttCT	O=C(O)[C@H]1C[C@H](C=C1)NC(OCC2C3=(	220497-64-3
217	Cycle 2	ggatcctcaGT	tgaggatccCT	ClC1=CC2=C(C=C1)C(C[C@H](C(O)=O)NC(O	925916-73-0
218	Cycle 2	acattcggaGT	tccgaatgtCT	N#CC=1C=CC(=CC1)C[C@H](CC(O)=O)NC(C	269726-87-6
219	Cycle 2	ccttgggtaGT	tacccaaggCT	O=C(O)[C@@H](NC(OCC1C2=CC=CC=C2C3	269078-73-1
220	Cycle 2	agccatctgGT	cagatggctCT	C1=CC=C2CN([C@@H](CC2=C1)C(=O)O)C(=	136030-33-6
221	Cycle 2	accttctggGT	ccagaaggtCT	ClC=1C=CC(=CC1)C[C@H](C(O)=O)NC(OCC	142994-19-2
222	Cycle 2	aggccataaGT	ttatggcctCT	N#CC=1C=CC(=CC1)C[C@H](C(O)=O)NC(OC	205526-34-7
223	Cycle 2	gagaacagtGT	actgttctcCT	C1=CC=C2C(=C1)C3=CC=CC=C3C2COC(=O	101555-63-9
224	Cycle 2	acagatcacGT	gtgatctgtCT	O=C(O)[C@H](NC(OCC1C2=CC=CC=C2C3=(	198543-96-3
225	Cycle 2	acactgctcGT	gagcagtgtCT	O=C(O)[C@H](NC(OCC1C2=CC=CC=C2C3=(	269078-72-0
226	Cycle 2	ataacctccGT	ggaggttatCT	O=C([C@@H]1C[C@H](NC(OCC2C3=C(C4=C	220497-66-5
227	Cycle 2	aagcaaaggGT	cctttgcttCT	C1=CC=C2C(=C1)C3=CC=CC=C3C2COC(=O	193693-64-0
228	Cycle 2	ttgtttccgGT	cggaaacaaCT	C1=CC=C2C(=C1)C3=CC=CC=C3C2COC(=O	129223-22-9
229	Cycle 2	tcttggagcGT	gctccaagaCT	O=C(O)[C@H](CC1=CSC=C1)NC(OCC2C3=C	186320-06-9
230	Cycle 2	caatgctgtGT	acagcattgCT	ClC1=CC2=C(C=C1)C(C[C@@H](C(O)=O)NC	908847-42-7
231	Cycle 2	gacattgacGT	gtcaatgtcCT	O=C(O)[C@H](CC1=CSC=N1)NC(OCC2C3=C	205528-32-1
232	Cycle 2	ggttcaactGT	agttgaaccCT	CN([C@@H](CC1CCCCC1)C(=O)O)C(=O)OC(	148983-03-3
233	Cycle 2	ataaggtcgGT	cgaccttatCT	O=C(O)[C@H](CC1=CC=CO1)NC(OCC2C3=C	159611-02-6
234	Cycle 2	tgggagtatGT	atactcccaCT	O=C(O)[C@H](NC(OCC1C2=CC=CC=C2C3=(	205526-38-1
235	Cycle 2	taacgctgcGT	gcagcgttaCT	O=C(O)C1CCC(CC1)CNC(OCC2C3=CC=CC=	188715-40-4
236	Cycle 2	ccagtactgGT	cagtactggCT	C=CCC(C(O)=O)(NC(OCC1C2=CC=CC=C2C3	1311992-97-8
237	Cycle 2	actaaggggGT	ccccttagtCT	O=C(O)C[C@H](C1=CC([N+]([O-])=O)=CC=C1	374791-04-5
238	Cycle 2	cttctttggGT	ccaaagaagCT	NC(NCCC[C@H](C(O)=O)NC(OCC1C2=CC=C	200344-33-8
239	Cycle 2	agtcagcttGT	aagctgactCT	O=C(O)C[C@H](C1=CC=C(Br)C=C1)NC(OCC	220498-04-4
240	Cycle 2	gtctatgtcGT	gacatagacCT	CC1=CC=CC=C1[C@H](NC(OCC2C3=CC=C(	507472-27-7

241	Cycle 2	taggtgctcGT	gagcacctaCT	O=C(O)C[C@H](C1=CC=C(C(F)(F)F)C=C1)NC(	517905-88-3
242	Cycle 2	tctgggagaGT	tctcccagaCT	O=C(O)CC(C1=CC=C(Br)C=C1)NC(OCC2C3=	269078-76-4
243	Cycle 2	tgctgatgtGT	acatcagcaCT	CC1=CC=C(C(NC(OCC2C3=CC=CC=C3C4=(	284492-08-6
244	Cycle 2	ctgacatacGT	gtatgtcagCT	C1=CC=C(C=C1)C[C@@H](C(=O)N2CCC[C@	138372-76-6
245	Cycle 2	cgatgtcctGT	aggacatcgCT	C=CCC(NC(OCC1C2=CC=CC=C2C3=CC=C(	221884-63-5
246	Cycle 2	tcgcgagaaGT	ttctcgcgaCT	C1CCC2C(C1)C[C@H](C(=O)O)N2C(=O)OCC	1217512-55-4
247	Cycle 2	gaaatggggGT	ccccatttcCT	O=C(O)C[C@@H](CC1=CC=CS1)NC(OCC2C	270262-98-1
248	Cycle 2	gctaacttcGT	gaagttagcCT	C=CC[C@@H](NC(OCC1C2=CC=CC=C2C3=	170642-28-1
249	Cycle 2	caccacgttGT	aacgtggtgCT	C#CCCC[C@@H](C(=O)O)NC(=O)OCC1C2=C	1097192-05-6
250	Cycle 2	ttctagtggGT	ccactagaaCT	FC1=C(F)C(F)=C(F)C(F)=C1C[C@@H](C(O)=(	205526-32-5
251	Cycle 2	atatggtccGT	ggaccatatCT	CC1=CC=C(C[C@H](NC(OCC2C3=CC=CC=C(	199006-54-7
252	Cycle 2	ctcgcagtaGT	tactgcgagCT	CC1=C(C(C)=CC(O)=C1)C[C@H](NC(OCC2C	206060-54-0
253	Cycle 2	acaccttcaGT	tgaaggtgtCT	O=C(O)[C@H](CC1=CSC2=CC=CC=C12)NC(	177966-60-8
254	Cycle 2	catgagggaGT	tccctcatgCT	O=C([C@H]1N(C(OCC2C3=C(C4=C2C=CC=C	130309-37-4
255	Cycle 2	aggcctagaGT	tctaggcctCT	O=C(O)C1=CC=CC(CNC(OCC2C3=CC=CC=(	155369-11-2
256	Cycle 2	gttctaccaGT	tggtagaacCT	FC1=CC(C[C@H](C(O)=O)NC(OCC2C3=CC=(	205526-31-4
257	Cycle 2	catggtcgaGT	tcgaccatgCT	ClC=1C=CC(=CC1Cl)C[C@@H](C(O)=O)NC((	177966-59-5
258	Cycle 2	cctagagctGT	agctctaggCT	C1=CC=C2C(=C1)C3=CC=CC=C3C2COC(=O	885951-89-3
259	Cycle 2	ccccgtaaaGT	tttacggggCT	IC=1C=CC(=CC1)C[C@@H](C(O)=O)NC(OCC	82565-68-2
260	Cycle 2	tcggccaatGT	attggccgaCT	IC=1C=CC(=CC1)C[C@H](C(O)=O)NC(OCC2(	205526-29-0
261	Cycle 2	caaagccctGT	agggctttgCT	C1=CC=C2C(=C1)C[C@@H](C(=O)O)N2C(=O	198560-38-2
262	Cycle 2	ggctacaatGT	attgtagccCT	O=[N+]([O-])C=1C=CC(=C(C1)[N+]([O-])=O)N(	140430-54-2
263	Cycle 2	gagtcctttGT	aaaggactcCT	O=C(O)[C@@H](CC1=CSC2=CC=CC=C12)N(	177966-61-9
264	Cycle 2	ctgttgttgGT	caacaacagCT	O=C(O)[C@H](CC1CC1)NC(OCC2C3=CC=CC	214750-76-2
265	Cycle 2	gactgatcgGT	cgatcagtcCT	O=C(O)C[C@H](CC1=CC=CO1)NC(OCC2C3=	270263-07-5
266	Cycle 2	acacgacagGT	ctgtcgtgtCT	O=C(O)C1(NC(OCC2C3=CC=CC=C3C4=CC=	162648-54-6
267	Cycle 2	ttttcgctgGT	cagcgaaaaCT	FC1=CC2=C(C=C1)C(CC(C(O)=O)NC(OCC3C	1219392-55-8
268	Cycle 2	gtgttgtgtGT	acacaacacCT	ClC=1C=CC(=CC1Cl)C[C@H](C(O)=O)NC(OC	177966-58-4
269	Cycle 2	ttggcggatGT	atccgccaaCT	BrC=1C=CC(=CC1)C[C@@H](C(O)=O)NC(OC	198561-04-5
270	Cycle 2	tactaggtcGT	gacctagtaCT	O=[N+]([O-])C=1C=CC(=CC1)C[C@H](C(O)=(	177966-63-1
271	Cycle 2	cgtagcgttGT	aacgctacgCT	O=C(O)C[C@@H](NC(OCC1C2=CC=CC=C2C	1217460-65-5
272	Cycle 2	gacgaatgaGT	tcattcgtcCT	O=C(O)[C@@H](CC1=CN=CC=C1)NC(OCC2(	142994-45-4
273	Cycle 2	atggttgtgGT	cacaaccatCT	O=C(O)[C@@H](NC(OCC1C2=CC=CC=C2C3	220497-61-0
274	Cycle 2	gcagtttcaGT	tgaaactgcCT	O=C(O)C=1C=CC(=CC1)CNC(OCC2C3=CC=(	164470-64-8
275	Cycle 2	tactgagtcGT	gactcagtaCT	O=C(O)C1(CCCC1)NC(OCC2C3=CC=CC=C3(	117322-30-2
276	Cycle 2	tatgcactcGT	gagtgcataCT	O=C(O)C1(CCC1)NC(OCC2C3=CC=CC=C3C	885951-77-9
277	Cycle 2	tggcctacaGT	tgtaggccaCT	FC(F)(F)C=1C=CC(=CC1)C[C@@H](C(O)=O)I	247113-86-6
278	Cycle 2	gaggacgtaGT	tacgtcctcCT	C1=CC=C2C(=C1)C3=CC=CC=C3C2COC(=O	178432-49-0
279	Cycle 2	ggtcttttcGT	gaaaagaccCT	COC1=C(OC)C=C(C[C@H](NC(OCC2C3=CC=	184962-88-7
280	Cycle 2	gttcttgagGT	ctcaagaacCT	O=C(O)[C@H](CC1=CC=CS1)NC(OCC2C3=C	130309-35-2
281	Cycle 2	tcaccgctaGT	tagcggtgaCT	OC=1C=CC2=C(C1)C(=CN2)C[C@@H](C(O)=	178119-94-3
282	Cycle 2	ttctgctcaGT	tgagcagaaCT	O=C(O)[C@H]1CCC[C@@H]1NC(OCC2C3=C	359586-64-4
283	Cycle 2	ggggataaaGT	tttatccccCT	O=C(O)C[C@H](CC1=CSC=C1)NC(OCC2C3=	270263-01-9
284	Cycle 2	gtccggaaaGT	tttccggacCT	O=C(O)C1(CCOCC1)NC(OCC2C3=CC=CC=C	285996-72-7
285	Cycle 2	taaagagggGT	ccctctttaCT	O=C(O)[C@H](C1=CSC=C1)NC(OCC2C3=CC	1217706-09-6
286	Cycle 2	cttggcactGT	agtgccaagCT	O=C(O)C1(CC1)NC(OCC2C3=CC=CC=C3C4=	126705-22-4
287	Cycle 2	atgagtcagGT	ctgactcatCT	C1=CC=C2C(=C1)C3=CC=CC=C3C2COC(=O	185116-43-2
288	Cycle 2	tcctctggtGT	accagaggaCT	C#CC[C@@H](NC(OCC1C2=CC=CC=C2C3=(	220497-98-3
289	Cycle 2	acccgctaaGT	ttagcgggtCT	C#CC[C@H](NC(OCC1C2=CC=CC=C2C3=C(	198561-07-8
290	Cycle 2	cataggagcGT	gctcctatgCT	ClC=1C=CC(=C(C1)Cl)C[C@@H](C(O)=O)NC	352351-62-3
291	Cycle 2	tcgctagttGT	aactagcgaCT	FC1=CC(C[C@@H](C(O)=O)NC(OCC2C3=CC	205526-30-3
292	Cycle 2	acatccgcaGT	tgcggatgtCT	O=C(O)[C@H](CC1=CN=CC=C1)NC(OCC2C3	175453-07-3
293	Cycle 2	gataccaagGT	cttggtatcCT	O=C(O)[C@H](NC(OCC1C2=CC=CC=C2C3=(	136555-16-3
294	Cycle 2	cagtcacctGT	aggtgactgCT	O=C(O)[C@@H](NC(OCC1C2=CC=CC=C2C3	138775-07-2
295	Cycle 2	gctttgctcGT	gagcaaagcCT	FC(F)(F)C(NCCCC[C@@H](C(O)=O)NC(OCC	76265-69-5
296	Cycle 2	ttccgagaaGT	ttctcggaaCT	O=C(CC[C@H](NC(OCC1C2=CC=CC=C2C3=	150047-85-1
297	Cycle 2	caccgagttGT	aactcggtgCT	[N-]=[N+]=NCCC[C@@H](C(O)=O)NC(OCC1(	1097192-04-5
298	Cycle 2	cttactacgGT	cgtagtaagCT	C#CC[C@](C(O)=O)(NC(OCC1C2=CC=CC=C	1198791-65-9
299	Cycle 2	tcggaatgtGT	acattccgaCT	C[C@@H](OCC1=CC=CC=C1)[C@H](NC(OC(	117872-75-0
300	Cycle 2	gagcatcgtGT	acgatgctcCT	O=C(O)C[C@H](C1=CC=C([N+]([O-])=O)C=C	507472-26-6

301	Cycle 2	aatacgtcgGT	cgacgtattCT	COC1=CC(OC)=CC([C@H](NC(OCC2C3=CC=	511272-41-6
302	Cycle 2	ttgttcacgGT	cgtgaacaaCT	O=C(O)C[C@H](C1=CN=CC=C1)NC(OCC2C3	511272-43-8
303	Cycle 2	cttaccactGT	agtggtaagCT	O=C(O)C[C@H](C1=CC=CS1)NC(OCC2C3=C	511272-45-0
304	Cycle 2	catcagtccGT	ggactgatgCT	O=C(O)C[C@H](C1=CC=CO1)NC(OCC2C3=C	1217662-55-9
305	Cycle 2	tctctgagaGT	tctcagagaCT	CC(C1=CC=C(C[C@H](NC(OCC2C3=CC=CC	204716-07-4
306	Cycle 2	attaccggcGT	gccggtaatCT	O=C(O)C1=CC(NC(OCC2C3=CC=CC=C3C4=	1071446-05-3
307	Cycle 2	aggacaatcGT	gattgtcctCT	C1(C2=C(C=CC=C2)C3=C1C=CC=C3)COC(N	1260596-73-3
308	Cycle 2	aaggtagcaGT	tgctaccttCT	O=C(O)[C@H](CC1=CNC2=C1C=CC=N2)NC(	737007-45-3
309	Cycle 2	tagactcggGT	ccgagtctaCT	N1([C@H](C(=O)O)C[C@H](C1)F)C(=O)OCC1	1228307-81-0
310	Cycle 2	gctcacataGT	tatgtgagcCT	FC1=CC(C[C@H](C(O)=O)NC(OCC2C3=CC=(	205526-25-6
311	Cycle 2	gttaaggacGT	gtccttaacCT	FC=1C=CC(=C(C1)F)C[C@@H](C(O)=O)NC((	1032337-49-7
312	Cycle 2	ggctctagtGT	actagagccCT	C1=CC=C2C(=C1)C3=CC=CC=C3C2COC(=O	133054-21-4
313	Cycle 2	acgttcatcGT	gatgaacgtCT	C1(C2=C(C=CC=C2)C3=C1C=CC=C3)COC(N	1217716-50-1
314	Cycle 2	gacccaatcGT	gattgggtcCT	O=C(O)C1(NC(OCC2C3=CC=CC=C3C4=CC=	135944-07-9
315	Cycle 2	gcgctttatGT	ataaagcgcCT	O=C(O)[C@H](CC1CCC1)NC(OCC2C3=CC=C	478183-62-9
316	Cycle 2	gataggcgaGT	tcgcctatcCT	O=C(O)[C@@H]1CCC[C@H]1NC(OCC2C3=C	359586-69-9
317	Cycle 2	gatatgctcGT	gagcatatcCT	O=C(O)CC1(NC(OCC2C3=CC=CC=C3C4=CC	282524-98-5
318	Cycle 2	aggagtagcGT	gctactcctCT	O=C(O)CC1(CNC(OCC2C3=CC=CC=C3C4=C	882847-19-0
319	Cycle 2	gaccaggatGT	atcctggtcCT	O=C(O)[C@@H]1CC[C@H](CC1)CNC(OCC2C	167690-53-1
320	Cycle 2	cgaggttacGT	gtaacctcgCT	O=[N+]([O-])C=1C=CC(=CC1)C[C@@H](C(O)	95753-55-2
321	Cycle 2	agacaatggGT	ccattgtctCT	C1=CC=C2C(=C1)C3=CC=CC=C3C2COC(=O	86069-86-5
322	Cycle 2	tggcatgtgGT	cacatgccaCT	O=C(O)[C@@H]1CC[C@H](CC1)NC(OCC2C3	147900-46-7
323	Cycle 2	gtcaatggcGT	gccattgacCT	CC1(OCC2=C(O1)C=CC(C[C@H](NC(OCC3C	252049-13-1
324	Cycle 2	cctcctacaGT	tgtaggaggCT	IC=1C=CC(=CC1)C[C@H](CC(O)=O)NC(OCC	269396-73-8
325	Cycle 2	tgctgaggaGT	tcctcagcaCT	BrC=1C=CC(=CC1)C[C@@H](CC(O)=O)NC(C	270062-86-7
326	Cycle 2	ataccgtccGT	ggacggtatCT	ClC=1C=CC(=CC1Cl)C[C@@H](CC(O)=O)NC	270063-52-0
327	Cycle 2	tgacagaggGT	cctctgtcaCT	IC=1C=CC(=CC1)C[C@@H](CC(O)=O)NC(OC	270065-72-0
328	Cycle 2	gcgtatcatGT	atgatacgcCT	O=C(O)C[C@H](CC1=CNC2=CC=CC=C12)N(	353245-98-4
329	Cycle 2	atctacctcGT	gaggtagatCT	O=C(O)C[C@@H](C1=CC=C(F)C=C1)NC(OC(	479064-89-6
330	Cycle 2	tcgattcacGT	gtgaatcgaCT	O=C(O)C[C@@H](C1=C(Cl)C(Cl)=CC=C1)NC	501015-35-6
331	Cycle 2	tccaaaggtGT	acctttggaCT	O=C(O)C[C@H](C1=C(Cl)C=C(Cl)C=C1)NC(C	511272-37-0
332	Cycle 2	ataaccaggGT	cctggttatCT	O=C(O)[C@@H](NC(OCC1C2=CC=CC=C2C3	161321-36-4
333	Cycle 2	agcaacttgGT	caagttgctCT	O=C(O)[C@@H](NC(OCC1C2=CC=CC=C2C3	205526-26-7
334	Cycle 2	tggatcgacGT	gtcgatccaCT	FC=1C=CC(=CC1F)C[C@H](C(O)=O)NC(OCC	198545-59-4
335	Cycle 2	taccgggtaGT	tacccggtaCT	FC=1C=CC(=CC1)C[C@@H](C(O)=O)NC(OC(	169243-86-1
336	Cycle 2	gccatcaagGT	cttgatggcCT	C1=CC=C2CN([C@H](CC2=C1)C(=O)O)C(=O	130309-33-0
337	Cycle 2	ctaagccacGT	gtggcttagCT	O=C(O)[C@H](NC(OCC1C2=CC=CC=C2C3=(	205526-22-3
338	Cycle 2	tgggctttcGT	gaaagcccaCT	N#CC=1C=CC(=CC1)C[C@@H](C(O)=O)NC((	173963-93-4
339	Cycle 2	cgtaggtgaGT	tcacctacgCT	CC(C)(OC(N1CCCC(C1)CC(NC(OCC2C3=CC=	457060-97-8
340	Cycle 2	ggtattccaGT	tggaataccCT	C[C@]1(CCCN1C(=O)OCC2C3=CC=CC=C3C	167275-47-0
341	Cycle 2	tacattcccGT	gggaatgtaCT	C(F)(C1=CC=C(C[C@@H](C(O)=O)NC(=O)OC	1808268-08-7
342	Cycle 2	cgtatcaagGT	cttgatacgCT	C1CN(C[C@@H](C(=O)O)NC(OCC2C3=C(C4=	1251903-85-1
343	Cycle 2	gagtgatagGT	ctatcactcCT	C1=CC=C2C(=C1)C3=CC=CC=C3C2COC(=O	193693-61-7
344	Cycle 2	actgctaacGT	gttagcagtCT	C1=CC=C2C(=C1)C3=CC=CC=C3C2COC(=O	374791-02-3
345	Cycle 2	actctctgtGT	acagagagtCT	O=C(O)C1(NC(OCC2C3=CC=CC=C3C4=CC=	214139-28-3
346	Cycle 2	acattgcgaGT	tcgcaatgtCT	C1=CC=C2C(=C1)CN(C2C(=O)O)C(=O)OCC3(	204320-59-2
347	Cycle 2	ctattctgcGT	gcagaatagCT	O=C(O)[C@@H](NC(OCC1C2=CC=CC=C2C3	159610-82-9
348	Cycle 2	acgctagtgGT	cactagcgtCT	C1CC[C@H]2[C@@H](C1)C[C@@H](C(=O)O)	214750-71-7
349	Cycle 2	atcgggatcGT	gatcccgatCT	CC(C)(C)OC(=O)N1CCN(C1C(=O)O)C(=O)OC(	207129-12-2
350	Cycle 2	actctcgctGT	agcgagagtCT	C1(C2=C(C=CC=C2)C3=C1C=CC=C3)COC(N	683217-64-3
351	Cycle 2	taagtggctGT	agccacttaCT	FC=1C=CC(=CC1F)C[C@@H](C(O)=O)NC(O(	198560-43-9
352	Cycle 2	aaccagcttGT	aagctggttCT	CC1=CC=CC=C1C[C@H](NC(OCC2C3=CC=(	211637-75-1
353	Cycle 2	agaagtggtGT	accacttctCT	FC(F)(F)C=1C=CC(=CC1)C[C@H](C(O)=O)N(	238742-88-6
354	Cycle 2	atgaacacgGT	cgtgttcatCT	C1=CC=C2C(=C1)C3=CC=CC=C3C2COC(=O	139262-20-7
355	Cycle 2	aaggttggtGT	accaaccttCT	O=C(O)[C@H]1C[C@H](CC1)NC(OCC2C3=C(	220497-67-6
356	Cycle 2	acctactccGT	ggagtaggtCT	CC(C)(OC(N1C[C@@H](C(O)=O)[C@H](NC(O	267230-44-4
357	Cycle 2	gaggggaacaGT	tgttccctcCT	C1=CC=C2C(=C1)C3=CC=CC=C3C2COC(=O	1335206-44-4
358	Cycle 2	ctgtctaacGT	gttagacagCT	C=CCC[C@@H](NC(OCC1C2=CC=CC=C2C3	865352-21-2
359	Cycle 2	ctgccaaatGT	atttggcagCT	C1=CC=C2C(=C1)C3=CC=CC=C3C2COC(=O	942153-03-9
360	Cycle 2	cgggatacaGT	tgtatcccgCT	O=C(O)[C@H](C1CC1)NC(OCC2C3=CC=CC=	1212257-18-5

361	Cycle 2	cactacaggGT	cctgtagtgCT	CC(C)(OC(N1CCC(C(NC(OCC2C3=CC=C(	313051-96-6
362	Cycle 2	tttccatggGT	ccatggaaaCT	CC(C)(OC(N1CCCC(C(NC(OCC2C3=CC=CC=	372144-11-1
363	Cycle 2	actcacctgGT	caggtgagtCT	O=C(O)C[C@@H](C1=CC=C(C#N)C=C1)NC((	507472-24-4
364	Cycle 2	ggacgtgtaGT	tacacgtccCT	CN1C=C(C2=CC=CC=C21)C[C@@H](NC(OC	168471-22-5
365	Cycle 2	gttagggacGT	gtccctaacCT	FC(F)(F)C=1C=CC(=CC1)C[C@@H](CC(O)=C	270065-81-1
366	Cycle 2	cataggtacGT	gtacctatgCT	FC1=CC=CC(C[C@H](CC(O)=O)NC(OCC2C3=	331763-67-8
367	Cycle 2	aagctagcgGT	cgctagcttCT	N#CC1=CC=CC(C[C@H](CC(O)=O)NC(OCC2	269726-84-3
368	Cycle 2	gatcttcgtGT	acgaagatcCT	O=C(O)C[C@H](NC(OCC1C2=CC=CC=C2C3=	268734-29-8
369	Cycle 2	tgactcgcaGT	tgcgagtcaCT	C1=CC=C2C(=C1)C3=CC=CC=C3C2COC(=O	193693-60-6
370	Cycle 2	gaaagtctcGT	gagactttcCT	C1=CC=C2CN([C@H](CC2=C1)CC(=O)O)C(=(	332064-67-2
371	Cycle 2	tgagcgagtGT	actcgctcaCT	ClC=1C=CC(=CC1)C[C@H](CC(O)=O)NC(OC	331763-60-1
372	Cycle 2	actggtaccGT	ggtaccagtCT	ClC=1C=CC(=C(C1)Cl)C[C@@H](CC(O)=O)N	270063-49-5
373	Cycle 2	gcgtagcttGT	aagctacgcCT	ClC=1C=CC(=C(C1)Cl)C[C@H](CC(O)=O)NC(	269396-54-5
374	Cycle 2	cgggaaatcGT	gatttcccgCT	FC=1C=CC(=CC1)C[C@@H](CC(O)=O)NC(O(	270062-83-4
375	Cycle 2	tctgaaaggGT	cctttcagaCT	O=C(O)C[C@H](CC1=CC=CS1)NC(OCC2C3=	269726-90-1
376	Cycle 2	catccttacGT	gtaaggatgCT	O=C(O)C[C@H](CC1=CSC2=CC=CC=C12)NC	270063-46-2
377	Cycle 2	ttctgctacGT	gtagcagaaCT	BrC=1C=CC(=CC1)C[C@H](CC(O)=O)NC(OC	331763-76-9
378	Cycle 2	tgtaccagtGT	actggtacaCT	ClC=1C=CC(=CC1)C[C@@H](CC(O)=O)NC(C	270596-43-5
379	Cycle 2	tctccggttGT	aaccggagaCT	ClC=1C=CC(=CC1Cl)C[C@H](CC(O)=O)NC((	269396-57-8
380	Cycle 2	gcttttgggGT	cccaaaagcCT	FC(F)(F)C=1C=CC(=CC1)C[C@H](CC(O)=O)N	269726-78-5
381	Cycle 2	actctcaacGT	gttgagagtCT	O=C(O)C[C@H](C1=CC=C(Cl)C=C1)NC(OCC	479064-92-1
382	Cycle 2	cagttcttcGT	gaagaactgCT	O=C(O)C[C@H](C1=CC(Cl)=CC=C1)NC(OCC	511272-53-0
383	Cycle 2	cttgcttggGT	ccaagcaagCT	C1CCC(C1)C[C@H](C(=O)O)NC(=O)OCC2C3=	1262802-59-4
384	Cycle 2	gtatgttccGT	ggaacatacCT	C=CC[C@H](NC(OCC1C2=CC=CC=C2C3=C(	146549-21-5
385	Cycle 2	gccgtatatGT	atatacggcCT	O=[N+]([O-])C=1C=CC(=CC1)C[C@H](CC(O)=	269398-78-9
386	Cycle 2	ttcgagcttGT	aagctcgaaCT	O=[N+]([O-])C=1C=CC(=CC1)C[C@@H](CC(C	270062-88-9
387	Cycle 2	aaaccggtgGT	caccggtttCT	CC(=O)NCSC[C@@H](C(=O)O)NC(=O)OCC1(	86060-81-3
388	Cycle 2	acactcgttGT	aacgagtgtCT	CC(C)(C)OC(=O)NCCCC[C@@H](C(=O)O)NC	71989-26-9
389	Cycle 2	agcaaagctGT	agctttgctCT	C1C[C@H](N(C1)C(=O)OCC2C3=CC=CC=C3(	71989-31-6
390	Cycle 2	agacaacagGT	ctgttgtctCT	CC(C(C(=O)O)NC(=O)OCC1C2=CC=CC=C2C	71989-35-0
391	Cycle 2	tggatacgaGT	tcgtatccaCT	CSCCC(C(=O)O)NC(=O)OCC1C2=CC=CC=C2	71989-28-1
392	Cycle 2	tcttgcggaGT	tccgcaagaCT	CC(C)(C)OCC(C(=O)O)NC(=O)OCC1C2=CC=(	128107-47-1
393	Cycle 2	gagacatacGT	gtatgtctcCT	CC(C)C(C(=O)O)NC(=O)OCC1C2=CC=CC=C2	68858-20-8
394	Cycle 2	gttcagttgGT	caactgaacCT	CC(C)CC(C(=O)O)NC(=O)OCC1C2=CC=CC=(	35661-60-0
395	Cycle 2	tgctataccGT	ggtatagcaCT	C1=CC=C(C=C1)CC(C(=O)O)NC(=O)OCC2C3	35661-40-6
396	Cycle 2	tgtacaccgGT	cggtgtacaCT	CC(C(=O)O)NC(=O)OCC1C2=CC=CC=C2C3=	35661-39-3
397	Cycle 2	cctatctgcGT	gcagataggCT	CC(C)(C)OC(=O)CCC(C(=O)O)NC(=O)OCC1C	71989-18-9
398	Cycle 2	attgccaagGT	cttggcaatCT	CC(C)(C)OC(=O)CC(C(=O)O)NC(=O)OCC1C2=	71989-14-5
399	Cycle 2	ttcggatagGT	ctatccgaaCT	C1=CC=C2C(=C1)C(C3=CC=CC=C32)COC(=	29022-11-5
400	Cycle 2	gatgcttggGT	ccaagcatcCT	CCC(C)C(C(=O)O)NC(=O)OCC1C2=CC=CC=(	71989-23-6
401	Cycle 2	agtgagcagGT	ctgctcactCT	COC(=O)CC(C(=O)O)NC(=O)OCC1C2=CC=C(	145038-53-5
402	Cycle 2	gatgccagtGT	actggcatcCT	CC(C)(C)OCC(C(=O)O)NC(=O)OCC1C2=CC=(	71989-33-8
403	Cycle 2	atcattccgGT	cggaatgatCT	CC(C(=O)O)NC(=O)OCC1C2=CC=CC=C2C3=	79990-15-1
404	Cycle 2	tgcgttgttGT	aacaacgcaCT	CC(C)CC(C(=O)O)NC(=O)OCC1C2=CC=CC=(	114360-54-2
405	Cycle 2	caaggagtaGT	tactccttgCT	CSCCC(C(=O)O)NC(=O)OCC1C2=CC=CC=C2	112883-40-6
406	Cycle 2	acgtgcaacGT	gttgcacgtCT	C1=CC=C(C=C1)CC(C(=O)O)NC(=O)OCC2C3	86123-10-6
407	Cycle 2	acatgacgcGT	gcgtcatgtCT	CCCCC(C(=O)O)NC(=O)OCC1C2=CC=CC=C2	112883-41-7
408	Cycle 2	acgagaggaGT	tcctctcgtCT	CC(C)(C)OC(=O)CCC(C(=O)O)NC(=O)OCC1C	104091-08-9
409	Cycle 2	gactgccaaGT	ttggcagtcCT	CC(C)C(C(=O)O)NC(=O)OCC1C2=CC=CC=C2	84624-17-9
410	Cycle 2	aacgacgacGT	gtcgtcgttCT	CC(C(C(=O)O)NC(=O)OCC1C2=CC=CC=C2C	138797-71-4
411	Cycle 2	ttctcttccGT	ggaagagaaCT	CC(C)(C)OC1=CC=C(C=C1)CC(C(=O)O)NC(=	118488-18-9
412	Cycle 2	acggttgctGT	agcaaccgtCT	C1CC(N(C1)C(=O)OCC2C3=CC=CC=C3C4=C	101555-62-8
413	Cycle 2	gtagaccacGT	gtggtctacCT	C1=CC=C(C=C1)CCC(C(=O)O)NC(=O)OCC2(	135994-09-1
414	Cycle 2	cagtcagtaGT	tactgactgCT	C1=CC=C2C(=C1)C(C3=CC=CC=C32)COC(=	35737-10-1
415	Cycle 2	ggtagtagtGT	actactaccCT	C1CCC(CC1)CC(C(=O)O)NC(=O)OCC2C3=C(	135673-97-1
416	Cycle 2	tgccctaagGT	cttagggcaCT	C	
417					
418	Cycle 3	gcctttcgtGA	acgaaaggcAC	OC(=O)C1(CCC1)C2=CC=CC=C2	37828-19-6
419	Cycle 3	aacgatccaGA	tggatcgttAC	OC(=O)CC1=CC=C(F)C=C1	405-50-5
420	Cycle 3	actcctaccGA	ggtaggagtAC	OC(=O)C1CC1	1759-53-1

421	Cycle 3	aacgtaagcGA	gcttacgttAC	OC(=O)C1(CCC1)C(O)=O	5445-51-2
422	Cycle 3	tcatatccgGA	cggatatgaAC	OC(=O)C1CCC1	3721-95-7
423	Cycle 3	acataccgaGA	tcggtatgtAC	Cl.OC(=O)CC1=CC=CN=C1	6419-36-9
424	Cycle 3	agcaaggttGA	aaccttgctAC	OC(=O)CC1=CC=C(C=C1)[N+]([O-])=O	104-03-0
425	Cycle 3	ccaagctatGA	atagcttggAC	OC(=O)CC1=CC=C(C=C1)C(F)(F)F	32857-62-8
426	Cycle 3	tatcctaccGA	ggtaggataAC	OC(=O)C1CCC(CC1)C(O)=O	1076-97-7
427	Cycle 3	gccaaaactGA	agttttggcAC	OC(=O)CC1(CCCCC1)CC(O)=O	4355-11-7
428	Cycle 3	ttgtccgtgGA	cacggacaaAC	NC1=CC(=CC=C1C(O)=O)[N+]([O-])=O	619-17-0
429	Cycle 3	cgtaggttaGA	taacctacgAC	OC(=O)C1CCCO1	16874-33-2
430	Cycle 3	tctttgggaGA	tcccaaagaAC	OC(=O)C1CCC(=O)N1	4042-36-8
431	Cycle 3	atagggtcGA	gacccctatAC	OC(=O)CC1=C(Cl)C=CC=C1Cl	6575-24-2
432	Cycle 3	ctagagagaGA	tctctctagAC	COC1=CC=C(CC(O)=O)C=C1O	1131-94-8
433	Cycle 3	tgaccgtagGA	ctacggtcaAC	OC(C(O)C(O)=O)C(O)=O	147-71-7
434	Cycle 3	ccatatggcGA	gccatatggAC	OC(=O)C=CC1=CC=CC=C1	140-10-3
435	Cycle 3	atggaggagGA	ctcctccatAC	C[S](=O)(=O)CC(O)=O	2516-97-4
436	Cycle 3	tccttgactGA	agtcaaggaAC	OC(=O)C[N]1C=CN=C1	22884-10-2
437	Cycle 3	acctggttaGA	taaccaggtAC	Cl.OC(=O)CC1=NC=CC=C1	16179-97-8
438	Cycle 3	taccagtgtGA	acactggtaAC	OC(=O)C1CCC(=O)N1	98-79-3
439	Cycle 3	tctcgctatGA	atagcgagaAC	OC(=O)CC1=CC=C(Cl)C=C1	1878-66-6
440	Cycle 3	cgttctaggGA	cctagaacgAC	OC(=O)C1COC2=CC=CC=C2O1	3663-80-7
441	Cycle 3	aacccatggGA	ccatgggttAC	OC(=O)CC1=C[NH]C2=C1C=CC=C2	87-51-4
442	Cycle 3	ctctgcttcGA	gaagcagagAC	Cl.OC(=O)CC1=CC=NC=C1	6622-91-9
443	Cycle 3	caggctcatGA	atgagcctgAC	OC(=O)CC1=C(Cl)C=C(Cl)C=C1	19719-28-9
444	Cycle 3	agaaccacgGA	cgtggttctAC	CCC(C)C(O)=O	116-53-0
445	Cycle 3	agctatcacGA	gtgatagctAC	OC(=O)C1CCOCC1	5337-03-1
446	Cycle 3	ttcacggctGA	agccgtgaaAC	OC(=O)C=CC1=CC=C(Cl)C=C1	1615-02-7
447	Cycle 3	gcttcacaaGA	ttgtgaagcAC	OC(=O)C=CC1=CC=C(C=C1)C(F)(F)F	16642-92-5
448	Cycle 3	cgttatgcgGA	cgcataacgAC	OC(=O)CCC1=CC=C(O)C=C1	501-97-3
449	Cycle 3	ggtgattgcGA	gcaatcaccAC	OC(=O)C1CC=CC1	7686-77-3
450	Cycle 3	tcacctcaaGA	ttgaggtgaAC	OC(=O)CC1=CC=C(O)C=C1	156-38-7
451	Cycle 3	accgattgaGA	tcaatcggtAC	OC(=O)CC1=CC(=CC(=C1)F)F	105184-38-1
452	Cycle 3	cgtactggtGA	accagtacgAC	OC(=O)CCCCCCC(O)=O	505-48-6
453	Cycle 3	catcaacgaGA	tcgttgatgAC	OC(=O)CCC(F)(F)F	406-93-9
454	Cycle 3	actttacgcGA	gcgtaaagtAC	OC(=O)CCC1=CC=CS1	5928-51-8
455	Cycle 3	gtgttgtcgGA	cgacaacacAC	OC(=O)CC1=C(F)C(=CC=C1)F	145689-41-4
456	Cycle 3	ctcacatggGA	ccatgtgagAC	OC(=O)C1CCC=CC1	4771-80-6
457	Cycle 3	ggcaactagGA	ctagttgccAC	CCC1CCC(CC1)C(O)=O	6833-47-2
458	Cycle 3	ctacagctcGA	gagctgtagAC	CC(C)C1CCC(C)CC1OCC(O)=O	40248-63-3
459	Cycle 3	agcgcaataGA	tattgcgctAC	OC(=O)CCCC1=CC=CS1	4653-11-6
460	Cycle 3	gcatgtccaGA	tggacatgcAC	CC(C(O)=O)C(O)=O	516-05-2
461	Cycle 3	actgaagcaGA	tgcttcagtAC	OC(=O)CCC1=CC=C(F)C=C1	459-31-4
462	Cycle 3	tcaggcagtGA	actgcctgaAC	OC(=O)COC1CCCCC1	71995-54-5
463	Cycle 3	ggcttactcGA	gagtaagccAC	OC(=O)CCC(=O)C1=CC=C(Br)C=C1	6340-79-0
464	Cycle 3	agctagtcaGA	tgactagctAC	OC(=O)CC1=CC=C(C=C1)C#N	5462-71-5
465	Cycle 3	tactcgtctGA	agacgagtaAC	COC1=CC(=CC(=C1OC)OC)C=CC(O)=O	90-50-6
466	Cycle 3	cctctgaatGA	attcagaggAC	OC(=O)COC1=CC(=CC=C1)Cl	588-32-9
467	Cycle 3	aatgttgcgGA	cgcaacattAC	OC(=O)C1CC(=O)C1	23761-23-1
468	Cycle 3	cagagattcGA	gaatctctgAC	OC(=O)C1=NNC(=O)CC1	27372-38-9
469	Cycle 3	tgttgctgcGA	gcagcaacaAC	OC(=O)C=CC1=CC=C(O)C(=C1)O	331-39-5
470	Cycle 3	cacagtgacGA	gtcactgtgAC	OC(=O)C1CCC(=O)O1	21461-84-7
471	Cycle 3	gaacgtgtaGA	tacacgttcAC	OC(=O)CCCCC1CCSS1	1077-28-7
472	Cycle 3	gatagactgGA	cagtctatcAC	OC(=O)C1CCC(CC1)C(O)=O	619-82-9
473	Cycle 3	cttaagacgGA	cgtcttaagAC	OC(=O)C1(CC1)C2=CC=C(F)C=C2	773100-29-1
474	Cycle 3	cagtacacgGA	cgtgtactgAC	OC(=O)C1(CC1)C2=CC(=CC=C2)Cl	124276-34-2
475	Cycle 3	tggtgttgaGA	tcaacaccaAC	OC(=O)CC1=CC=CC(=C1)O	621-37-4
476	Cycle 3	ctagacgcaGA	tgcgtctagAC	OC(=O)C12CC3CC(CC(C3)C1)C2	828-51-3
477	Cycle 3	gaaagcgaaGA	ttcgctttcAC	OC(=O)CCC1=CC=C(Br)C=C1	1643-30-7
478	Cycle 3	cggctataaGA	ttatagccgAC	OC(=O)CCC1=NC=CC=C1	15197-75-8
479	Cycle 3	cagacgtgtGA	acacgtctgAC	OC(=O)C=CC1=CC(=CC=C1)[N+]([O-])=O	555-68-0
480	Cycle 3	agatctcagGA	ctgagatctAC	COC1=CC=C(Cl)C=C1CC(O)=O	7569-62-2

481	Cycle 3	gtgcaacatGA	atgttgcacAC	CC(C)(C)C1=CC=C(CC(O)=O)C=C1	32857-63-9
482	Cycle 3	gccaaacatGA	atgtttggcAC	OC(=O)C=CC1=CC(=CC=C1)C(F)(F)F	779-89-5
483	Cycle 3	cccattcctGA	aggaatgggAC	OC(=O)C12CC3CC(C1)CC(C3)(C2)C(O)=O	39269-10-8
484	Cycle 3	gtcctacagGA	ctgtaggacAC	OC(=O)C1CC=CCC1C(O)=O	2305-26-2
485	Cycle 3	cacatagccGA	ggctatgtgAC	OC(=O)C1(CC1)C(O)=O	598-10-7
486	Cycle 3	ctaagggctGA	agcccttagAC	OC(=O)CCC1=C[NH]C2=CC=CC=C12	830-96-6
487	Cycle 3	aggcgtagtGA	actacgcctAC	OC(=O)CC1=CC=C(O)C(=C1)O	102-32-9
488	Cycle 3	agtgaaggaGA	tccttcactAC	CN(C)C1=CC=C(C=CC(O)=O)C=C1	1552-96-1
489	Cycle 3	ctacgtctaGA	tagacgtagAC	OC(=O)CCC1=CC=CC=C1F	1643-26-1
490	Cycle 3	actcgtgctGA	agcacgagtAC	OC(=O)C1CCCO1	87392-07-2
491	Cycle 3	gttgaagccGA	ggcttcaacAC	COC1=CC=C(CC(O)=O)C=C1F	452-14-2
492	Cycle 3	agaaagggcGA	gccctttctAC	CC(C)(C(O)=O)C(O)=O	595-46-0
493	Cycle 3	agacgatcgGA	cgatcgtctAC	OC(=O)CC1=CC(=CC=C1)C(F)(F)F	351-35-9
494	Cycle 3	gctcgatacGA	gtatcgagcAC	OC(=O)CCC1=CC=CC(=C1)[N+]([O-])=O	1664-57-9
495	Cycle 3	ccgattgtcGA	gacaatcggAC	OC(C(O)=O)C1=CC=C(F)C=C1	395-33-5
496	Cycle 3	caatccaggGA	cctggattgAC	OC(=O)CC1=CC=C(I)C=C1	1798-06-7
497	Cycle 3	aaccccgatGA	atcggggttAC	OC(=O)CCC1=CC=CC(=C1)Cl	21640-48-2
498	Cycle 3	gattagcggGA	ccgctaatcAC	OC(=O)C12CC3CC(CC(O)(C3)C1)C2	42711-75-1
499	Cycle 3	tttccaaccGA	ggttggaaaAC	OC(=O)CC1=CC(=CC=C1Br)Cl	81682-38-4
500	Cycle 3	ggatgccatGA	atggcatccAC	OC(=O)CCC1=CC=CC(=C1)C(F)(F)F	585-50-2
501	Cycle 3	gatggtcagGA	ctgaccatcAC	Cl.NCC(=O)CCC(O)=O	5451-09-2
502	Cycle 3	tgccagtctGA	agactggcaAC	OC(=O)C1CCC(F)(F)CC1	122665-97-8
503	Cycle 3	atagtggcgGA	cgccactatAC	OC(=O)CC1=CC=C(Br)C=C1F	114897-92-6
504	Cycle 3	tcagcatagGA	ctatgctgaAC	OC(=O)CSC(C1=CC=CC=C1)C2=CC=CC=C2	63547-22-8
505	Cycle 3	atgtgctggGA	ccagcacatAC	OC(=O)CC1=CC=C2OCCC2=C1	69999-16-2
506	Cycle 3	ccgcatgatGA	atcatgcggAC	COC1=CC(=CC(=C1O)OC)C=CC(O)=O	530-59-6
507	Cycle 3	aactcgagaGA	tctcgagttAC	OC(=O)C1CCC(=O)CC1	874-61-3
508	Cycle 3	tggtcacctGA	aggtgaccaAC	CC(C)(C)OC(=O)CC(O)=O	40052-13-9
509	Cycle 3	agctgactcGA	gagtcagctAC	OC(=O)CC1=CC=C(F)C(=C1)Br	194019-11-9
510	Cycle 3	tcgtacagcGA	gctgtacgaAC	CC(C)(C)OC(=O)NC1CCC(CC1)C(O)=O	53292-89-0
511	Cycle 3	cggttcttaGA	taagaaccgAC	CC(C(O)=O)C1=CC=CC=C1	7782-26-5
512	Cycle 3	cacgccattGA	aatggcgtgAC	OC(=O)C=CC1=CC=C(O)C=C1	501-98-4
513	Cycle 3	ttgtcagcaGA	tgctgacaaAC	OC(=O)CC1=CC=C(F)C=C1Br	61150-59-2
514	Cycle 3	cgccattgtGA	acaatggcgAC	Cl.NC1=CC(=CC(=C1)O)C(O)=O	14206-69-0
515	Cycle 3	caagtaacgGA	cgttacttgAC	OC(=O)C1=CC=C(Cl)S1	24065-33-6
516	Cycle 3	gccgattaaGA	ttaatcggcAC	NC1=C(C=CC=N1)C(O)=O	5345-47-1
517	Cycle 3	cagaactgaGA	tcagttctgAC	OC(=O)C1=CC=C(N=C1)C(F)(F)F	231291-22-8
518	Cycle 3	gttatcagcGA	gctgataacAC	OC(=O)CC1=CC=CS1	1918-77-0
519	Cycle 3	ctaacgcgaGA	tcgcgttagAC	OC(=O)C1=CC=CC=C1I	88-67-5
520	Cycle 3	gtctaaaggGA	cctttagacAC	OC(=O)C1=CC=C(C=C1Cl)[N+]([O-])=O	99-60-5
521	Cycle 3	ttcagagcaGA	tgctctgaaAC	NC1=CC=C(Br)C=C1C(O)=O	5794-88-7
522	Cycle 3	tacggcgaaGA	ttcgccgtaAC	COC1=CC(=CC=C1O)C(O)=O	121-34-6
523	Cycle 3	ctagagatgGA	catctctagAC	OC(=O)C1=CC(=CC=C1Cl)Br	21739-92-4
524	Cycle 3	ctctgacaaGA	ttgtcagagAC	OC(=O)C1=CC=CC(=C1)Br	585-76-2
525	Cycle 3	agtaccgaaGA	ttcggtactAC	CN(C)C1=CC(=CC=C1)C(O)=O	99-64-9
526	Cycle 3	gtcgatgaaGA	ttcatcgacAC	OC(=O)C1=CC=CC(=C1)O	99-06-9
527	Cycle 3	agcccaagtGA	acttgggctAC	OC(=O)C1=CN=CC(=C1)Br	20826-04-4
528	Cycle 3	gtactcactGA	agtgagtacAC	COC1=CC=C(C=C1O)C(O)=O	645-08-9
529	Cycle 3	ttaggcttgGA	caagcctaaAC	OC(=O)C1=CSC=C1	88-13-1
530	Cycle 3	actgcaaccGA	ggttgcagtAC	NC1=CC=C(C=C1N)C(O)=O	619-05-6
531	Cycle 3	ctctggtcaGA	tgaccagagAC	OC(=O)C1=CN=C(Cl)C=C1	5326-23-8
532	Cycle 3	gtaagcaacGA	gttgcttacAC	OC(=O)C1=C(Cl)N=CC=C1	2942-59-8
533	Cycle 3	catttcacgGA	cgtgaaatgAC	CC1=CC=C(S1)C(O)=O	1918-79-2
534	Cycle 3	gtactcagtGA	actgagtacAC	NC1=CC(=CC=C1)C(O)=O	99-05-8
535	Cycle 3	ggcagcttaGA	taagctgccAC	OC(=O)C1=CC=C(Br)C=C1[N+]([O-])=O	99277-71-1
536	Cycle 3	gcttgctacGA	gtagcaagcAC	C[N]1N=C(C(O)=O)C2=C1C=CC=C2	50890-83-0
537	Cycle 3	ccataccatGA	atggtatggAC	OC(=O)C1=CC=C(C=C1O)C(F)(F)F	328-90-5
538	Cycle 3	cgttatcctGA	aggataacgAC	COC1=CC=C(C(=C1)C(O)=O)[N+]([O-])=O	1882-69-5
539	Cycle 3	gatacctacGA	gtaggtatcAC	COC1=CC(=CC=C1)C(O)=O	586-38-9
540	Cycle 3	aacaaggggGA	ccccttgttAC	OC(=O)C1=CC=CC=C1C(F)(F)F	433-97-6

540	Cycle 3	aacaaggggGA	ccccttgttAC	OC(=O)C1=CC=CC=C1C(F)(F)F	433-97-6
541	Cycle 3	tgaacctacGA	gtaggttcaAC	OC(=O)C1=CC=CC(=C1)C(F)(F)F	454-92-2
542	Cycle 3	agtcgatctGA	agatcgactAC	CC1=C(C=CC=C1C(O)=O)[N+]([O-])=O	1975-50-4
543	Cycle 3	acggcgataGA	tatcgccgtAC	OC(=O)C1=NC2=CC=CC=C2N=C1	879-65-2
544	Cycle 3	tttgacgtcGA	gacgtcaaaAC	OC(=O)C1=N[NH]C=C1[N+]([O-])=O	5334-40-7
545	Cycle 3	gaagagcagGA	ctgctcttcAC	OC(=O)C1=N[NH]C=C1Br	13745-17-0
546	Cycle 3	gttcacactGA	agtgtgaacAC	CCC1=CC=C(C=C1)C(O)=O	619-64-7
547	Cycle 3	tagtcggaaGA	ttccgactaAC	CC1=CC=C(C(=C1)C)C(O)=O	611-01-8
548	Cycle 3	tacgaggtaGA	tacctcgtaAC	OC(=O)C1=C(Cl)C=CC=C1Cl	50-30-6
549	Cycle 3	ctgtgtaacGA	gttacacagAC	OC(=O)C1=CN=C(Cl)C(=C1)Br	29241-62-1
550	Cycle 3	gaaaaccgcGA	gcggttttcAC	OC(=O)C1=C(Cl)N=CC(=C1)Br	29241-65-4
551	Cycle 3	ttgagaaggGA	ccttctcaaAC	COC1=C(C=C(N)C(=C1)C(O)=O)[N+]([O-])=O	196194-99-7
552	Cycle 3	gataacgcgGA	cgcgttatcAC	CC1=CC=C(Cl)C=C1C(O)=O	7499-06-1
553	Cycle 3	tagattcgcGA	gcgaatctaAC	OC(=O)C1=CC=C(C(=C1)[N+]([O-])=O)[N+]([C	528-45-0
554	Cycle 3	tttgtcgccGA	ggcgacaaaAC	OC(=O)C1=C(C=CC=C1F)[N+]([O-])=O	385-02-4
555	Cycle 3	ctgtcgtctGA	agacgacagAC	CC1=CC=C(C=C1I)C(O)=O	82998-57-0
556	Cycle 3	acaagtcgtGA	acgacttgtAC	OC(=O)C1=CC=C(S1)C2=CC=CC=C2	19163-24-7
557	Cycle 3	tacattcgcGA	gcgaatgtaAC	CN1CCN(CC1)C2=CC(=CC=C2)C(O)=O	215309-01-6
558	Cycle 3	cgagctattGA	aatagctcgAC	NC1=CN=C(C=N1)C(O)=O	40155-43-9
559	Cycle 3	cttagggtgGA	caccctaagAC	OC(=O)C1=NC=CC(=C1)Br	30766-03-1
560	Cycle 3	tacgcctcaGA	tgaggcgtaAC	OC(=O)C1=CN=C(Br)C=C1	6311-35-9
561	Cycle 3	ctaatgcgtGA	acgcattagAC	NC1=CC(=CC=C1O)C(O)=O	1571-72-8
562	Cycle 3	tatccatcgGA	cgatggataAC	NC1=CC=C(O)C(=C1)C(O)=O	89-57-6
563	Cycle 3	tcaaagctcGA	gagctttgaAC	COC(=O)C1=CC=CC(=C1)C(O)=O	1877-71-0
564	Cycle 3	gtgtcatcgGA	cgatgacacAC	OC(=O)C1=CC=CC(=C1Cl)[N+]([O-])=O	3970-35-2
565	Cycle 3	aagttcctgGA	caggaacttAC	OC(=O)C1=CC=CC(=C1F)Br	161957-56-8
566	Cycle 3	acaattgccGA	ggcaattgtAC	OC(=O)C1=CC=CN=C1C(O)=O	89-00-9
567	Cycle 3	cggtctctaGA	tagagaccgAC	OC(=O)C1=CC=CC=C1N2CCOCC2	42106-48-9
568	Cycle 3	catgagcacGA	gtgctcatgAC	OC(=O)C1=CC=CC=C1[N]2C=CC=N2	55317-53-8
569	Cycle 3	tccacaacgGA	cgttgtggaAC	OC(=O)C1=CC=C(C=C1)N2CCOCC2	7470-38-4
570	Cycle 3	acttggtcgGA	cgaccaagtAC	OC(=O)C1=CC=CC(=C1)N2CCCC2	72548-79-9
571	Cycle 3	tctatcgccGA	ggcgatagaAC	OC(=O)C1=CC=CC=C1N2CCCC2	78648-27-8
572	Cycle 3	ggcaagagtGA	actcttgccAC	CC1=CC=C(C=C1O)C(O)=O	586-30-1
573	Cycle 3	ctgcaagcaGA	tgcttgcagAC	OC1=CC(=CN=C1)C(O)=O	27828-71-3
574	Cycle 3	tcatgccatGA	atggcatgaAC	OC(=O)C1=CC(=CN=C1)C(O)=O	499-81-0
575	Cycle 3	tatcgcatgGA	catgcgataAC	OC(=O)C1=CC=CC(=C1Br)F	132715-69-6
576	Cycle 3	tgacaacgcGA	gcgttgtcaAC	CCOC1=CC=CC=C1C(O)=O	134-11-2
577	Cycle 3	gatcagcctGA	aggctgatcAC	C[N]1C=C(C(O)=O)C2=C1C=CC=C2	32387-21-6
578	Cycle 3	ctactgctcGA	gagcagtagAC	COC1=C(OC)C(=CC(=C1)C(O)=O)OC	118-41-2
579	Cycle 3	tgctacacgGA	cgtgtagcaAC	CC1=CN=C(C=N1)C(O)=O	5521-55-1
580	Cycle 3	ggttggactGA	agtccaaccAC	OC(=O)C1=N[NH]C2=C1C=CC=C2	4498-67-3
581	Cycle 3	ggccctattGA	aatagggccAC	NC1=CC=CC(=C1C(O)=O)[N+]([O-])=O	50573-74-5
582	Cycle 3	cgcgattacGA	gtaatcgcgAC	OC(=O)C1=C(N=CC=C1)N2CCOCC2	423768-54-1
583	Cycle 3	agggtccatGA	atggaccctAC	OC(=O)C1=NC=CC(=C1)Cl	5470-22-4
584	Cycle 3	ccatttcggGA	ccgaaatggAC	OC(=O)C1=CC(=NC=C1)Cl	6313-54-8
585	Cycle 3	agtatggccGA	ggccatactAC	CC1(C)OB(OC1(C)C)C2=CC=CC(=C2)C(O)=O	269409-73-6
586	Cycle 3	tacaacggtGA	accgttgtaAC	OB(O)C1=CC=CC(=C1)C(O)=O	25487-66-5
587	Cycle 3	acctctcctGA	aggagaggtAC	OC(=O)C1=C(F)C=CC=C1F	385-00-2
588	Cycle 3	ttcacgaccGA	ggtcgtgaaAC	OC(=O)C1=C(O)C=CC(=C1)C=O	616-76-2
589	Cycle 3	caactaaggGA	ccttagttgAC	CC1=C(C=NO1)C(O)=O	42831-50-5
590	Cycle 3	gtaaccactGA	agtggttacAC	CC1=C(C=CC(=C1)N)C(O)=O	2486-75-1
591	Cycle 3	gcgagtataGA	tatactcgcAC	NC1=CN=CC=C1C(O)=O	7579-20-6
592	Cycle 3	gatcgagacGA	gtctcgatcAC	CSC1=NC=C(Br)C(=N1)C(O)=O	50593-92-5
593	Cycle 3	cagctcctaGA	taggagctgAC	OC(=O)C1=CC=C(C(=C1)F)[N+]([O-])=O	403-21-4
594	Cycle 3	aagagccgaGA	tcggctcttAC	NC1=CC=C(C=C1[N+]([O-])=O)C(O)=O	1588-83-6
595	Cycle 3	caagtggcaGA	tgccacttgAC	CC1=CC=C(C=C1Cl)C(O)=O	5162-82-3
596	Cycle 3	cattgttgcGA	gcaacaatgAC	OC(=O)C1=CC(=CC(=C1)O)O	99-10-5
597	Cycle 3	acccatacgGA	cgtatgggtAC	OC(=O)C1=NC=C(Br)C=N1	37131-87-6
598	Cycle 3	ttgcaggtgGA	cacctgcaaAC	OC(=O)C1=CC=CC(=C1O)O	303-38-8
599	Cycle 3	tgtccttagGA	ctaaggacaAC	COC1=CC=C(O)C(=C1)C(O)=O	2612-02-4
600	Cycle 3	atacacgcgGA	cgcgtgtatAC	OC(=O)C1=CC=NC(=C1)N2CCOCC2	295349-64-3
601	Cycle 3	tggccataaGA	ttatggccaAC	OC(=O)C1=NC=C(C=C1)[N+]([O-])=O	30651-24-2
602	Cycle 3	ttcagccatGA	atggctgaaAC	OC(=O)C1=CC=C(CBr)C=C1	6232-88-8
603	Cycle 3	caagactacGA	gtagtcttgAC	CC1=CC=C(C=C1[N+]([O-])=O)C(O)=O	96-98-0
604	Cycle 3	agtcgtggtGA	accacgactAC	OC(=O)C1=CC=C2OC=CC2=C1	90721-27-0
605	Cycle 3	ctattgaccGA	ggtcaatagAC	CC1=CC(=C(C)C=C1)C(O)=O	610-72-0
606	Cycle 3	ctgactgacGA	gtcagtcagAC	OCC1=CC=C(C=C1)C(O)=O	3006-96-0
607	Cycle 3	aggtttcacGA	gtgaaacctAC	CC1=CC=C(C=C1)C(O)=O	99-94-5
608	Cycle 3	gaaagcagtGA	actgctttcAC	C[N]1C=NC(=C1)C(O)=O	41716-18-1
609	Cycle 3	atctggctaGA	tagccagatAC	OC(=O)C1=C(C=CC=C1)C2=CC=CC=C2	947-84-2
610	Cycle 3	atgttccacGA	gtggaacatAC	c	c

11. Affinity selection

HisPur™ Ni-NTA Magneitic Beads (20 µl ,Thermo Scientific 88832) were washed three times with washing buffer (200 ml; 50 mM PBS [pH 7.4], 0.1% Tween-20,10 mM imidazole).The protein was added to the magnetic beads, and incubated in 100 µl of selection buffer (50 mM PBS [pH 7.4] ,0.1% Tween-20,10 mM imidazole, 0.1 mg/mL sheared salmon sperm DNA) for 30 min With continuous gentle mixing at room temperature. The beads were washed once with 200 µl selection buffer and subsequently transferred to a solution of DEL (5 nmol) in 100 µl selection buffer. The beads were incubated for 1h with continuous gentle mixing at room temperature. The beads were washed three times with selection buffer (200 µl), incubated in a dry-bath at 95°C for 10 minutes in 100 µl of selection buffer. The elutes (90 µl) were transferred to the protein-loaded beads. The beads were incubated in 100 µl of selection buffer for 1h with continuous gentle mixing at room temperature. The beads were washed three times with selection buffer (200 µl), incubated in a dry-bath at 95°C for 10 minutes in 100 µl of selection buffer. The elutes (90 µl) were transferred to the protein-loaded beads. Beads were incubated in 100 µl of selection buffer for 1h with continuous gentle mixing at room temperature. The beads were washed three times with selection buffer (200 µl). 100 µl of ddH_2O was added and incubated in a dry-bath at 95°C for 10 minutes. The elutes were used to run qPCR and amplified by PCR. After submitted to GENEWIZ, Inc for Next-generation sequencing on Illumina.

12. Enrichment Calculation

For 3-cycle DELs: Enrichment = $\frac{C}{N} \Big/ \frac{X}{S}$

Enrichment: normalization processing of copy number

C: copy number of the molecule

N: total reads

S: library size

X: real number of the molecule

13. Radioactive acetyltransferase activity assay - by Shanghai Chem-

Partner Co., Ltd

Materials

p300: BPS, Cat. No. 50071

[3H]-Ac-CoA: PerkinElmer, Cat. No. NET290

Ac-CoA: Sigma, Cat. No.A2056

C646: Calbiochem, Cat. No. 382113

384-well Flashplate: Perkin Elmer, Cat. No. SMP410A001PK

Compounds: in 10 mM DMSO stock

Procedure

1. Prepare 1x buffer

   Prepare 1x assay buffer (modified Tris Buffer).

2. Compound serial dilution:

   Transfer compounds to assay plate by Echo in 100% DMSO. The final fraction of DMSO is 1%.

3. Prepare enzyme solution:

   Prepare enzyme solution in 1x assay buffer.

4. Prepare substrate solution:

   Add peptide and [3H]-Ac-CoA in 1x assay buffer to make the substrate solution.

5. Transfer 10 μL of enzyme solution to assay plate or for low control transfer 10 μL of 1x assay buffer. Incubate at room temperature for 15 min.
6. Add 10 μL of substrate solution to each well to start reaction. Incubate at room temperature for 60 min.
7. Prepare stop solution:

   Add cold Ac-CoA in 1x assay buffer to make the stop mix.

8. Stop reaction with addition of 10 μL per well of stop solution.
9. Transfer 25 μL of volume per well to Flashplate from assay plate. Incubate for 1 hr minimum at room temperature.
10. Wash Flashplate with ddH_2O + 0.1% Tween-20 three times.
11. Read plate on Microbeta.

12. Data process

Fit the data in Excel to obtain inhibition values using equation (1)

Equation (1): inh %= (Max-Signal)/ (Max-Min) *100

Fit the data in XL-Fit to obtain IC50 values using equation (2)

Equation (2): Y=Bottom + (Top-Bottom)/(1+(IC50/X) *HillSlope)

Y is %inhibition and X is compound concentration.

14. Supplementary notes

List of abbreviations.

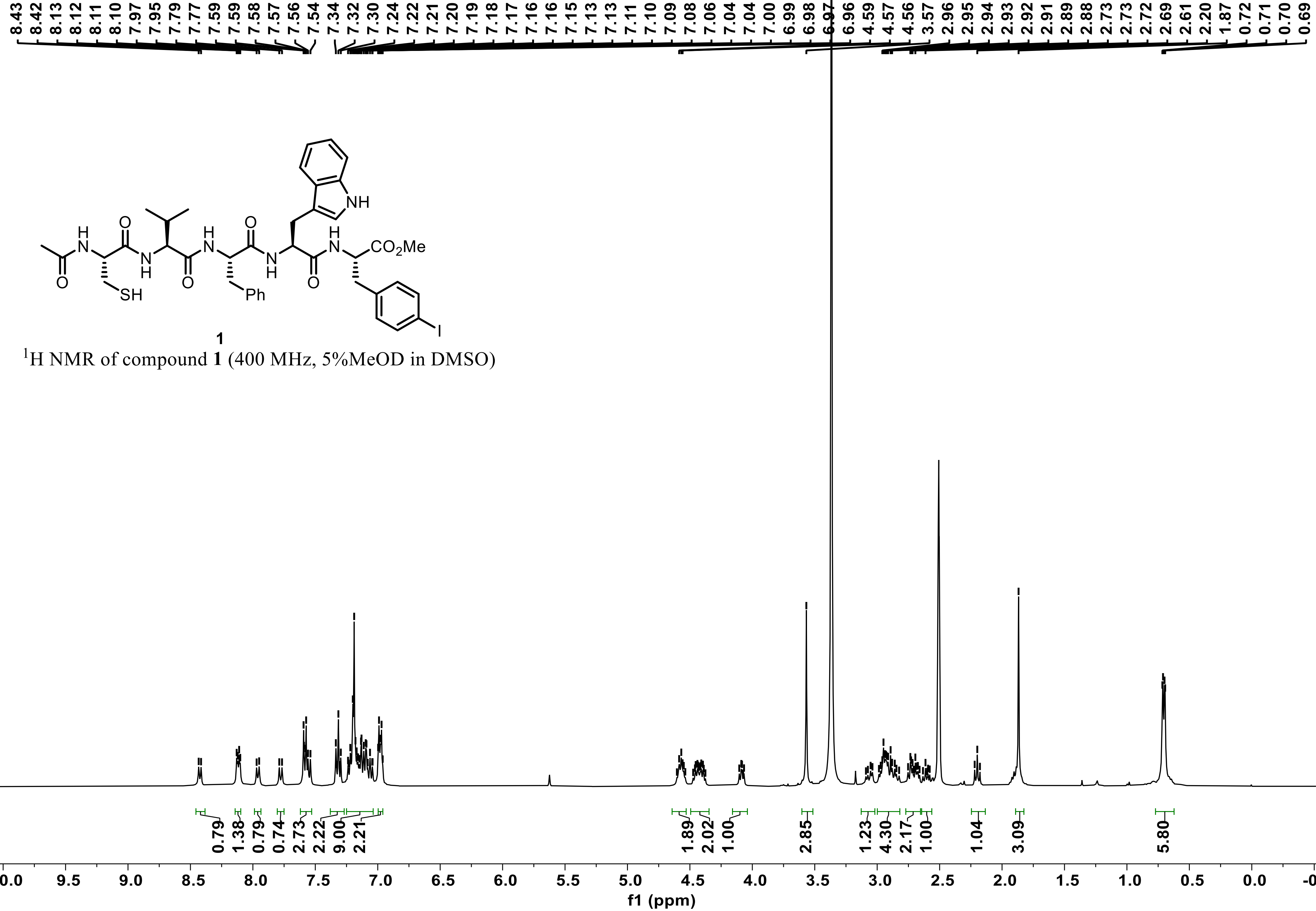
AcOH	**Acetic acid**
brine	**Saturated NaCl (aqueous)**
Boc	**t-butoxycarbonyl**
Cbz	**benzyloxycarbonyl**
DCM	**Dichloromethane**
DCE	**1,2-Dichloroethane**
ddH_2O	**double-distilled water**
DIC	**N, N'-Diisopropylcarbodiimide**
DIPEA	**N, N-Diisopropylethylamine**
DMF	**N, N-Dimethylformamide**
***t*BuOH**	**2-methyl-2-propano**
***t*-AmylOH**	**2-Methyl-2-butanol**
Fmoc-Cl	**Fluorenylmethoxycarbonyl-Cl**
HATU	***O*-(6-Chlorobenzotriazol-1-yl)-N, N, N′, N′-tetramethyluronium hexafluorophosphate**
HOAt	**1-Hydroxy-7-azabenzotriazole**
HPLC	**High-performance liquid chromatog-raphy**
HRMS	**High-resolution mass spectrometry**
LRMS	**Low-resolution mass spectrometry**

NMP	**N-Methyl-2-pyrrolidone**
NMR	**Nuclear magnetic resonance**
Oxyma	**Ethyl (hydroxyimino)cyanoacetate**
Pbf	**2,2,4,6,7-pentamethyldihydrobenzofu-ran-5-sulfonyl**
SPPS	**Solid-phase peptide synthesis**
TFA	**Trifluroacetic acid**
TFE	**Trifluoroethanol**

15. Reference

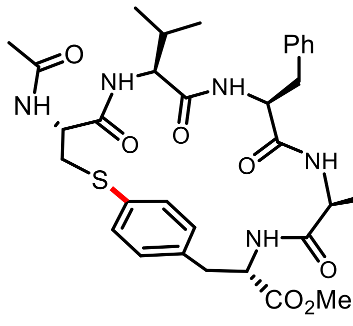
Bo Li, Xinghua Li, Boyang Han, Zhijie Chen, Xuekai Zhang, Gang He, and Gong Chen. Construction of Natural-Product-Like Cyclophane-Braced Peptide Macrocycles via sp3 C–H Arylation. *J. Am. Chem. Soc.* **2019**, 141, 23, 9401–9407.

16. NMR spectrum



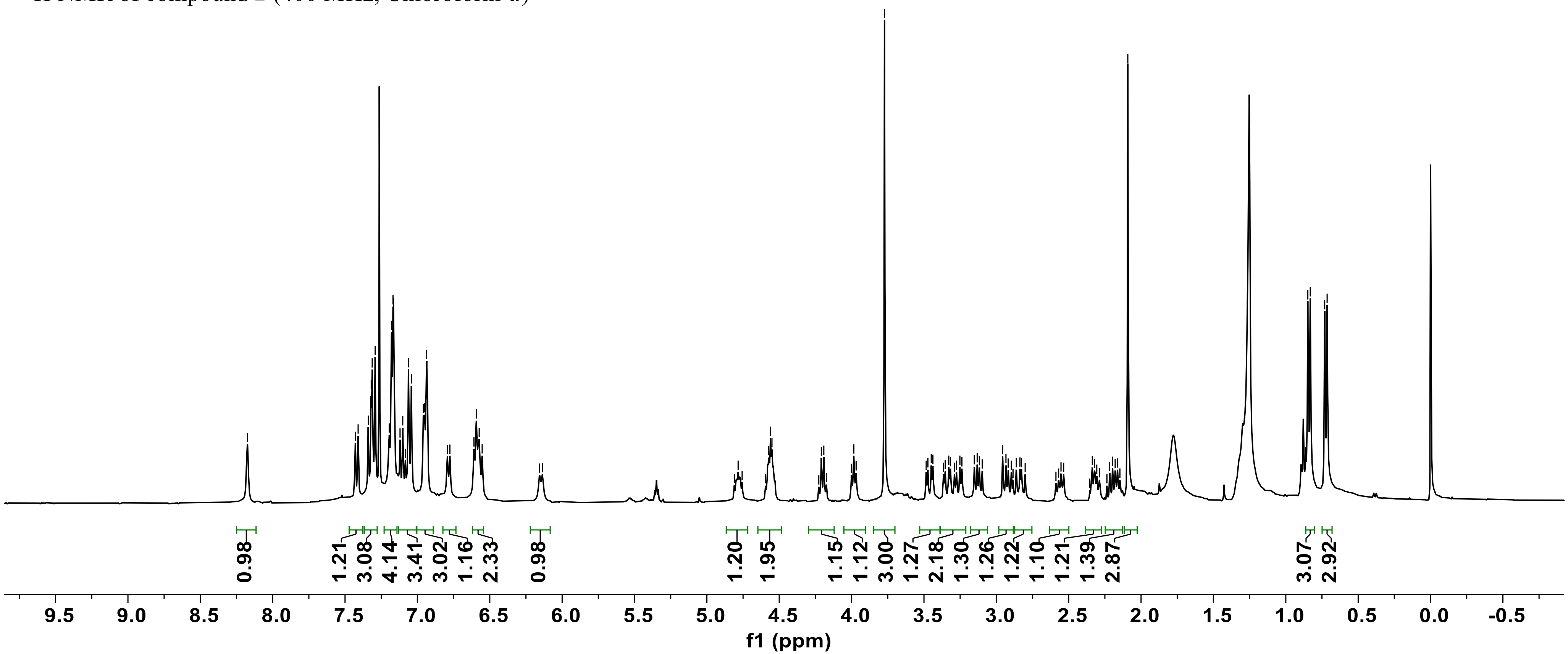
1

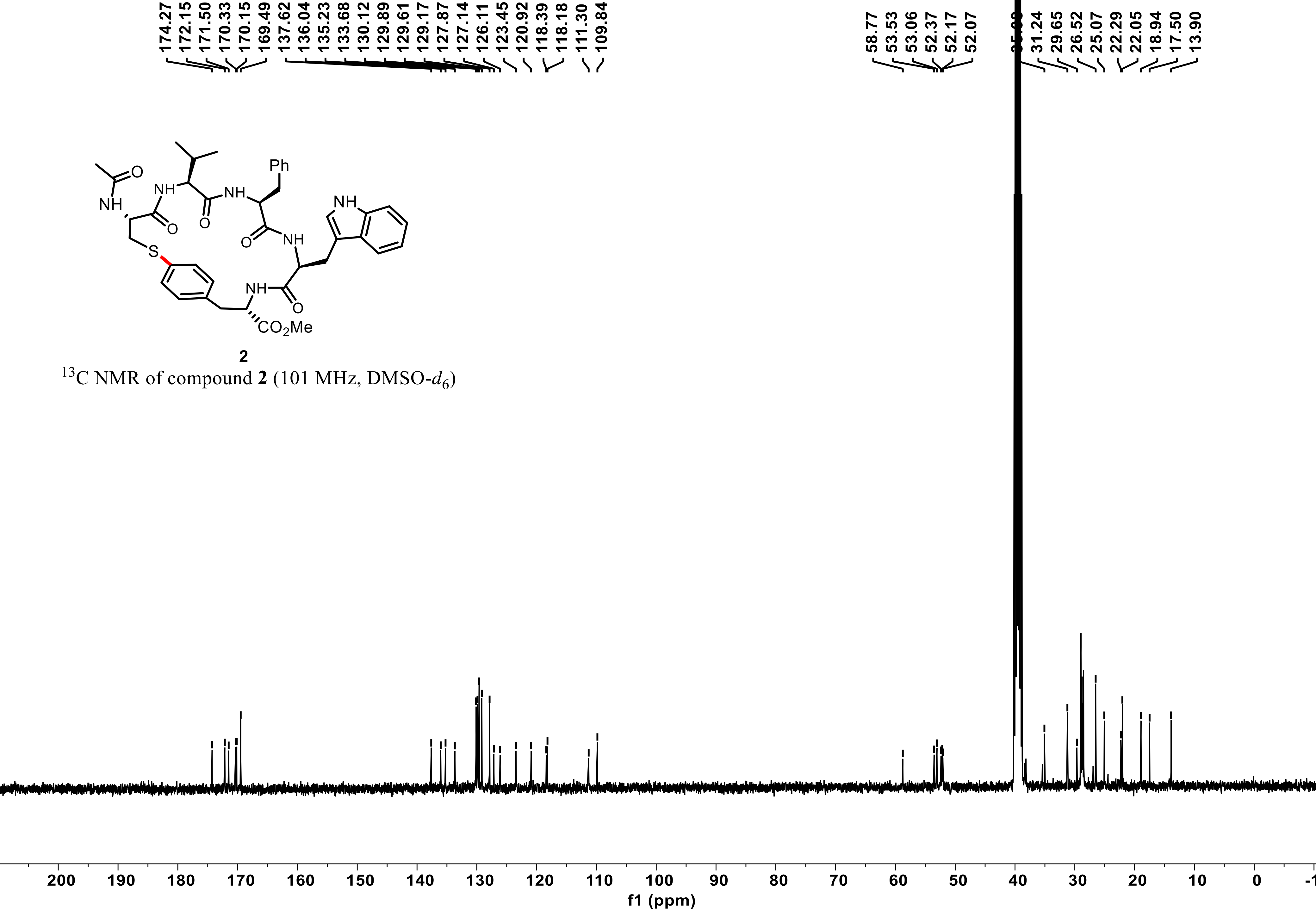
[1]H NMR of compound **1** (400 MHz, 5%MeOD in DMSO)



2

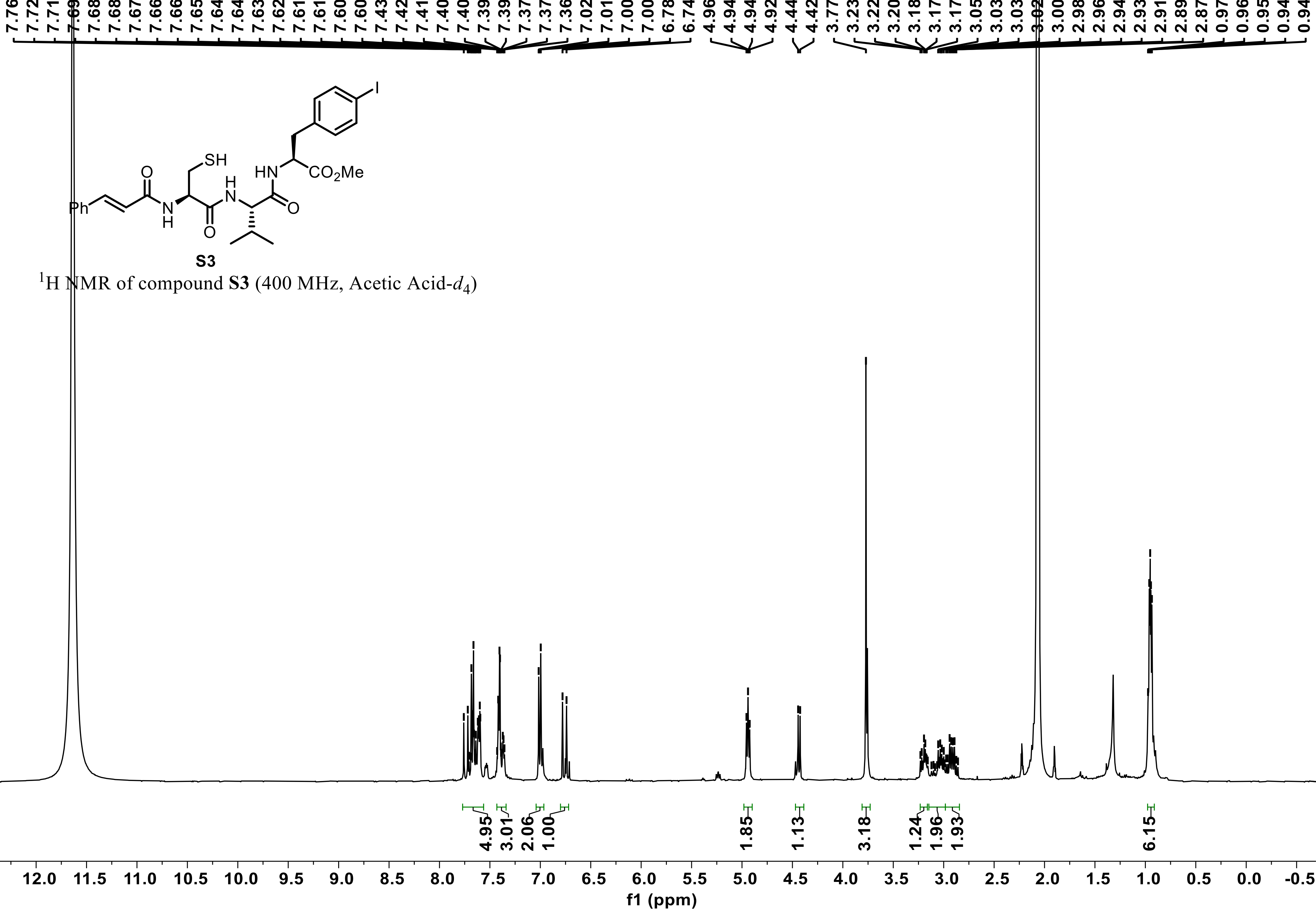
[1]H NMR of compound **2** (400 MHz, Chloroform-*d*)



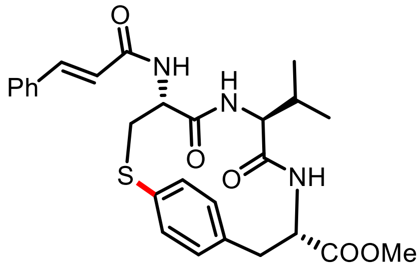


2

^{13}C NMR of compound **2** (101 MHz, DMSO-d_6)

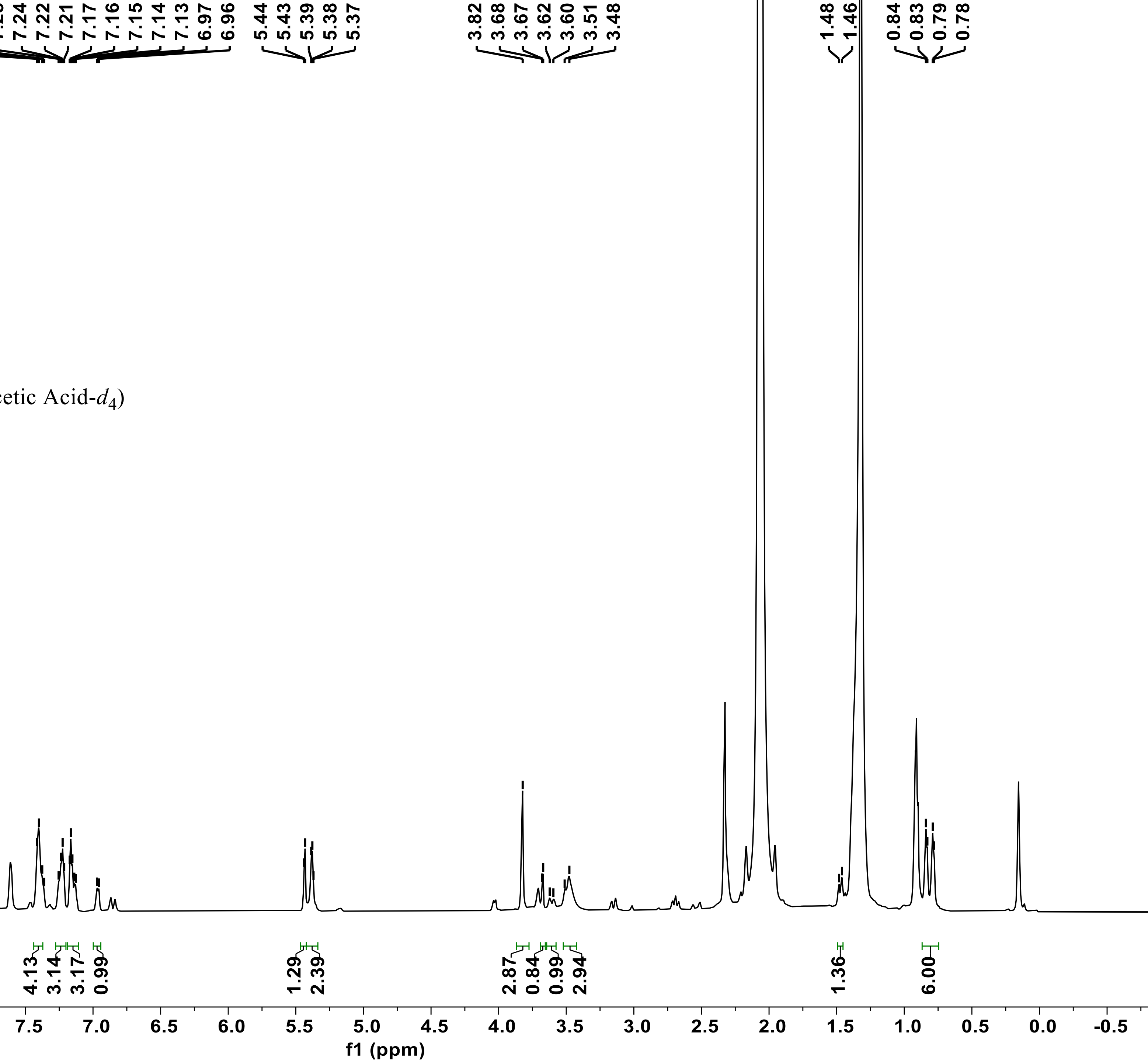


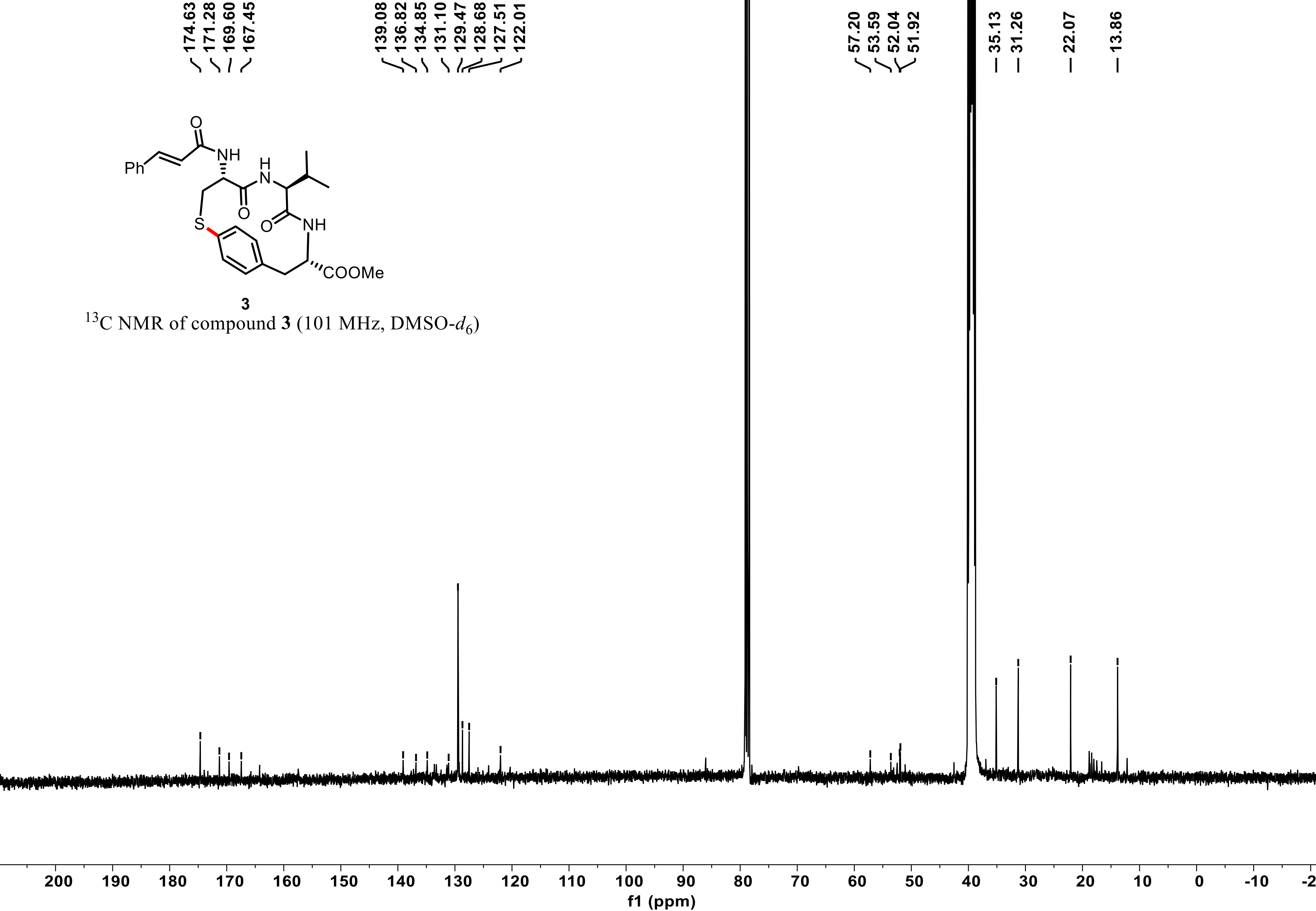
^{1}H NMR of compound **S3** (400 MHz, Acetic Acid-d_4)



3

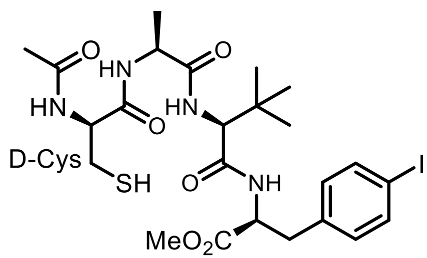
[1]H NMR of compound **3** (600 MHz, Acetic Acid-d_4)





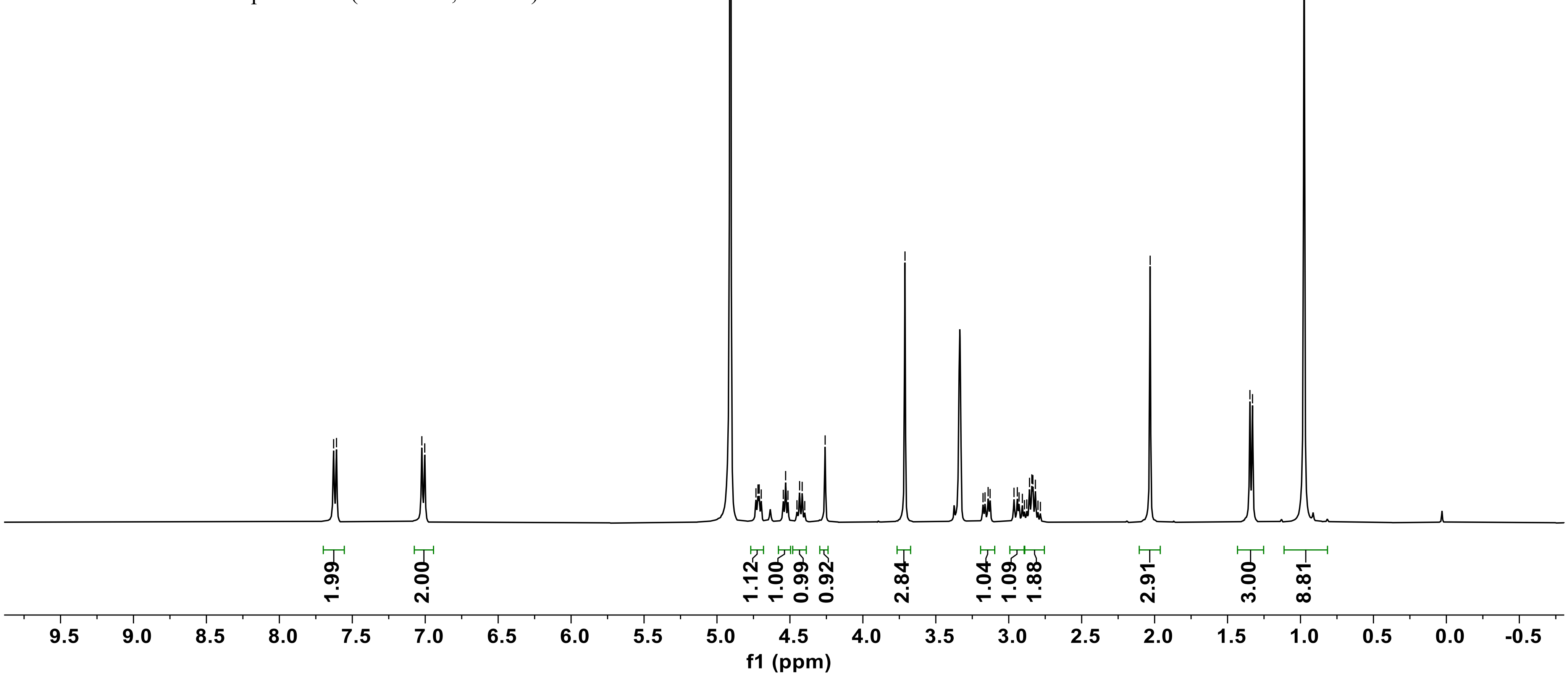
3

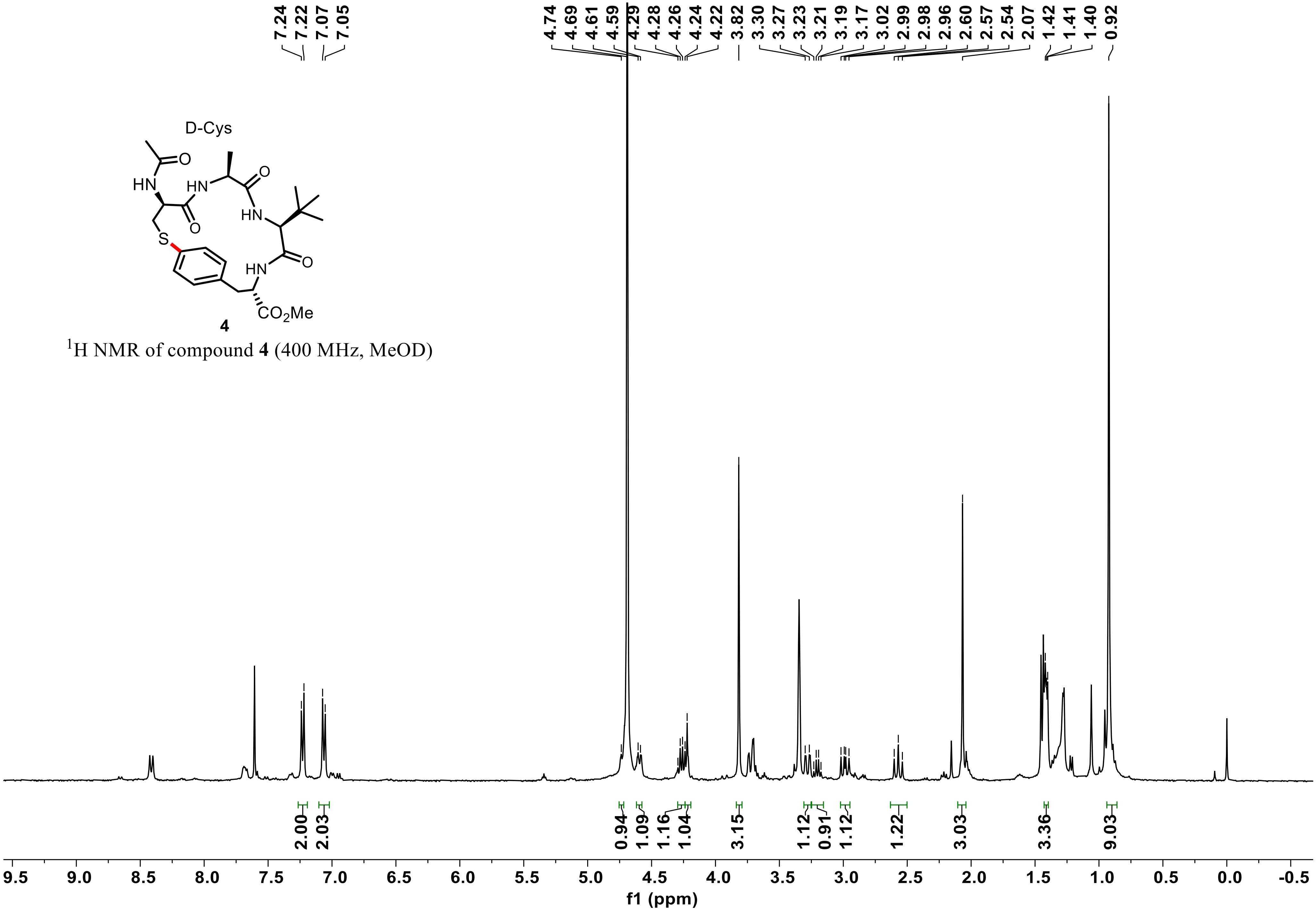
^{13}C NMR of compound **3** (101 MHz, DMSO-d_6)



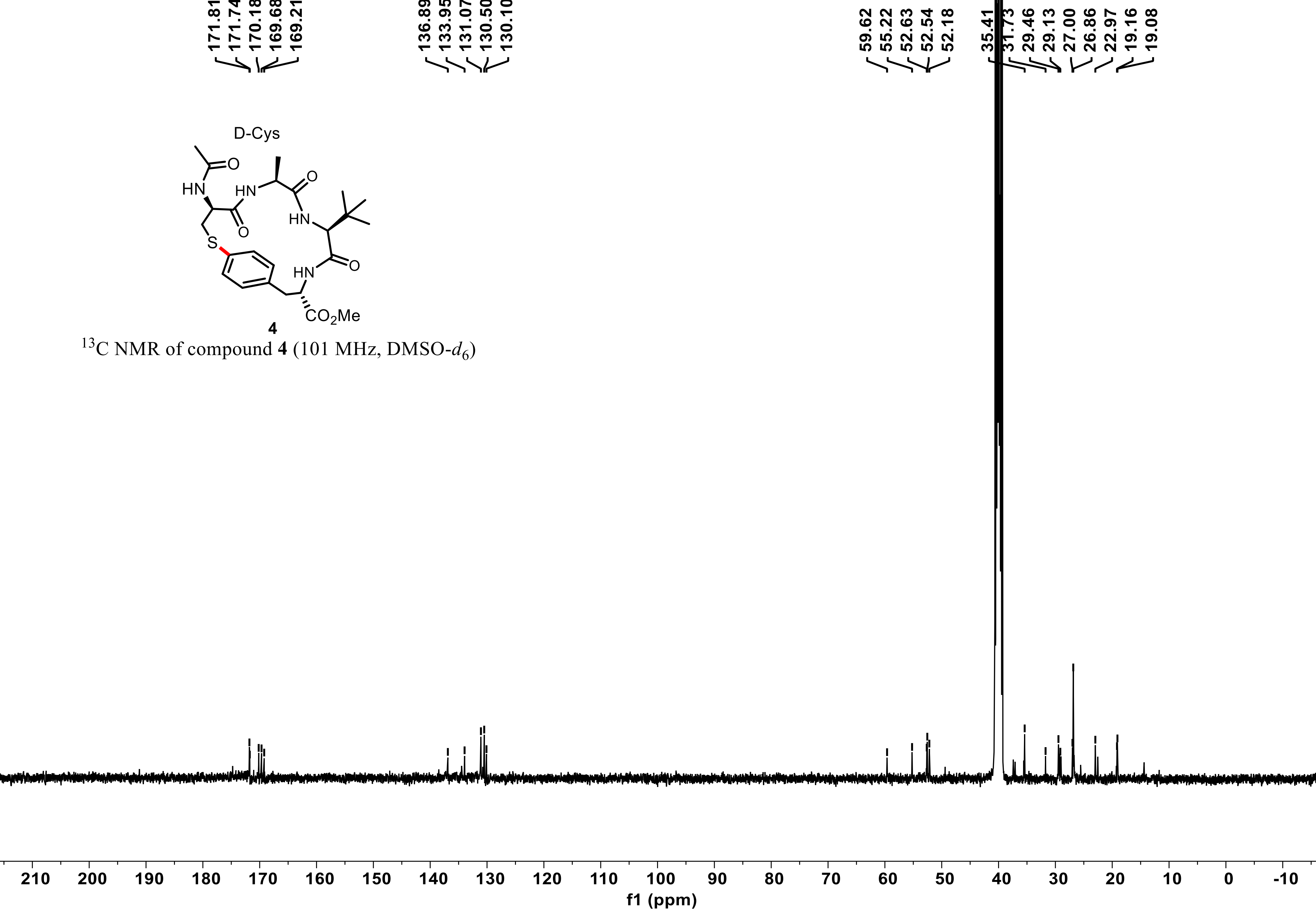
S4

^{1}H NMR of compound S**4** (400 MHz, MeOD)

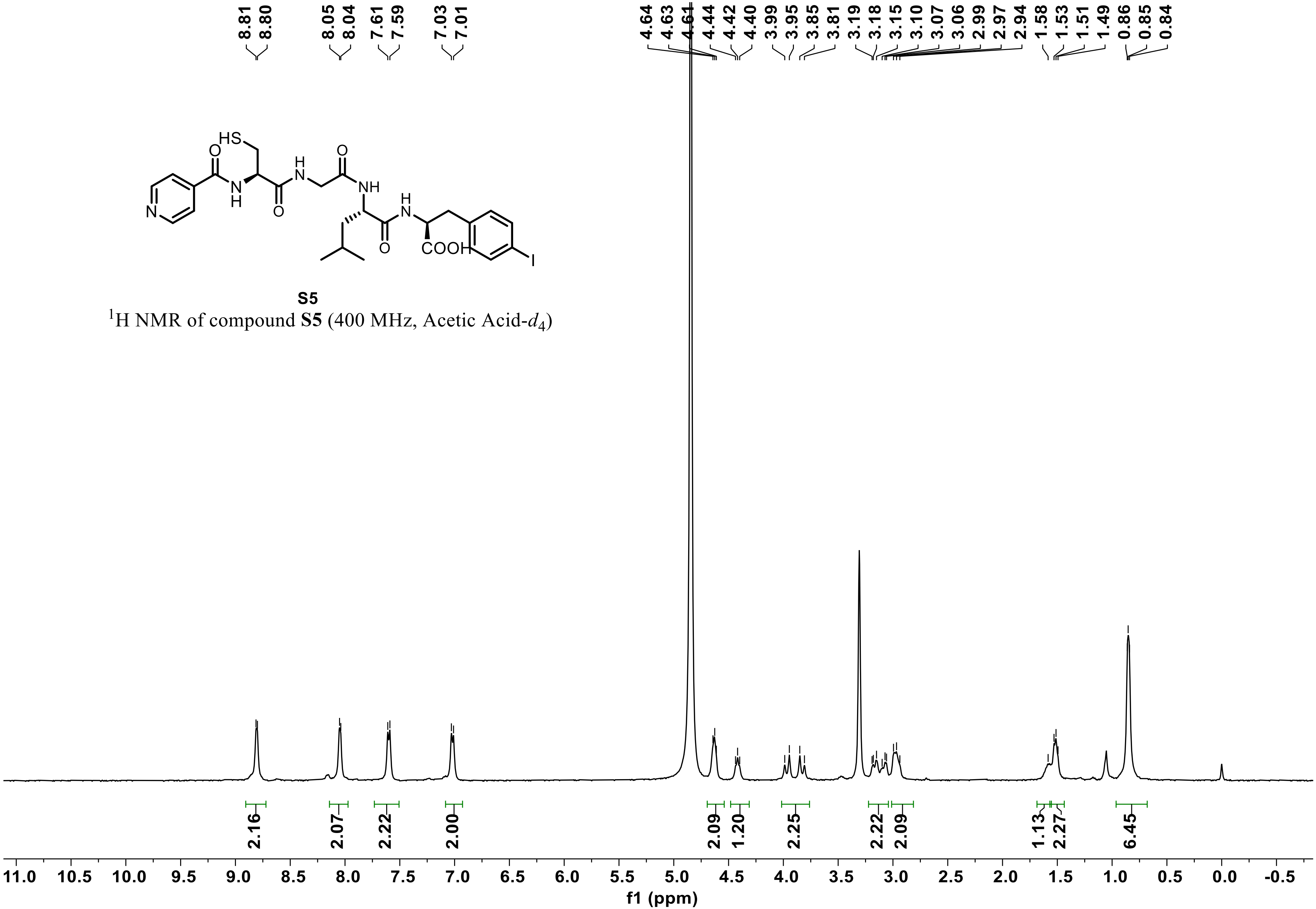




^{1}H NMR of compound **4** (400 MHz, MeOD)

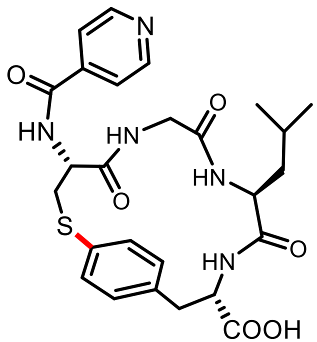


^{13}C NMR of compound **4** (101 MHz, DMSO-d_6)



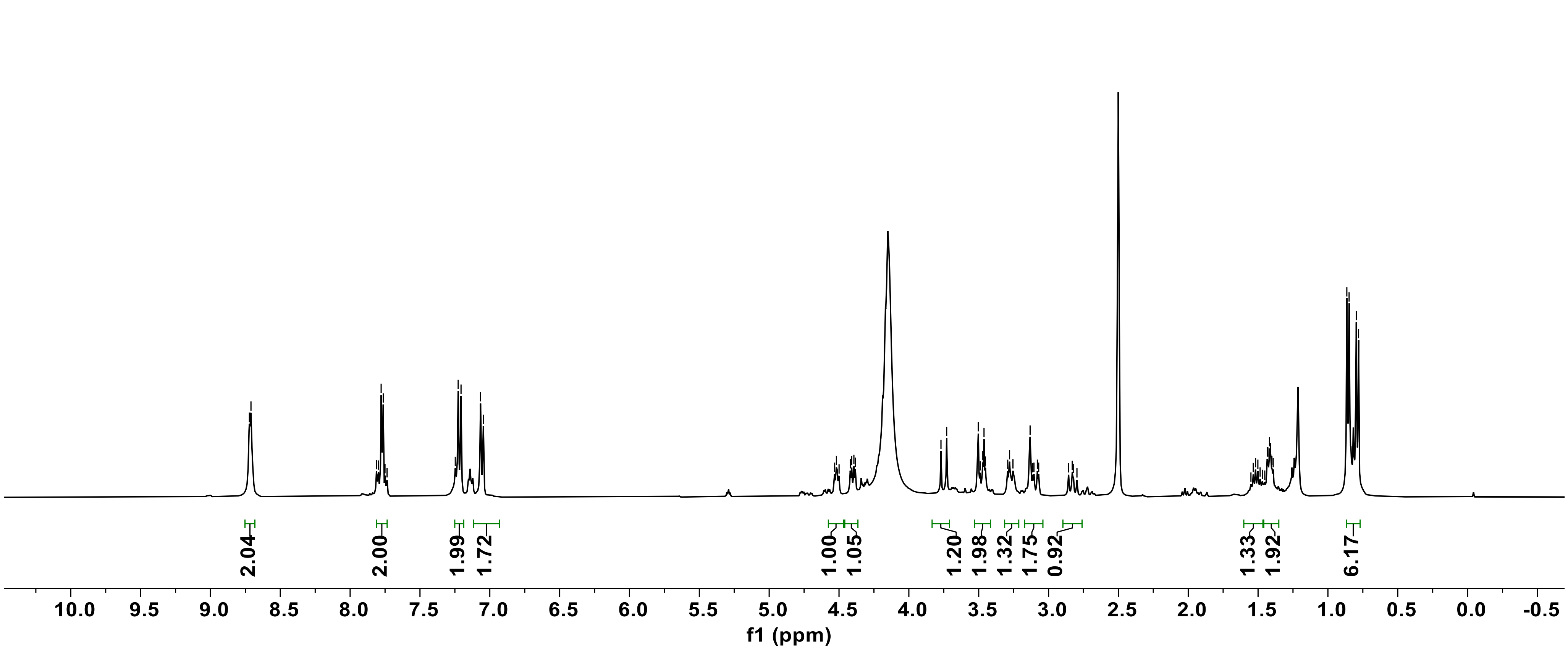
S5

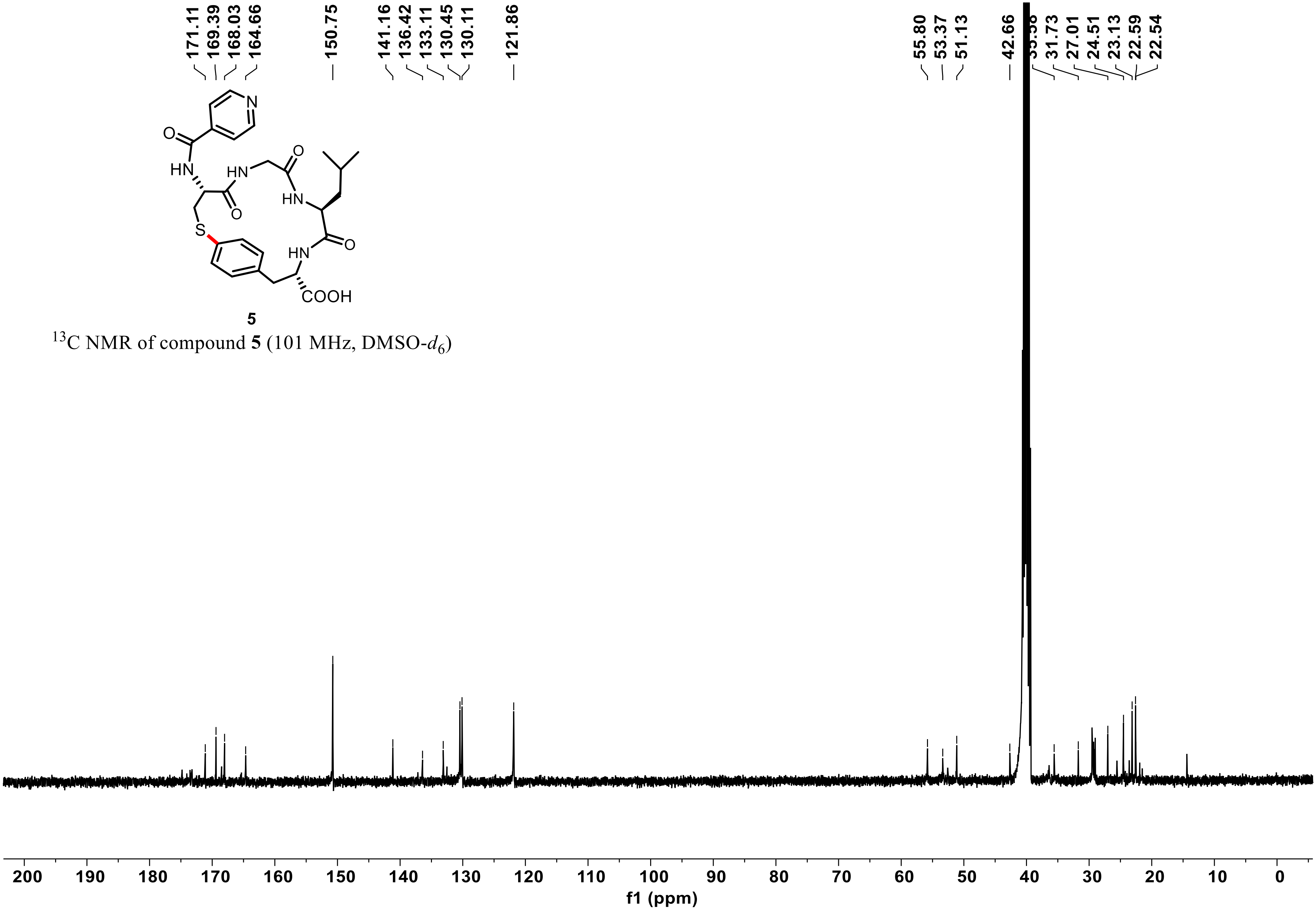
^{1}H NMR of compound **S5** (400 MHz, Acetic Acid-d_4)



5

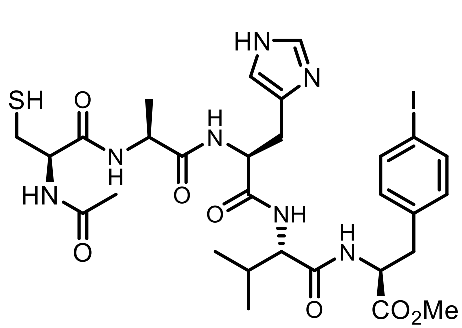
^{1}H NMR of compound **5** (400 MHz, 5%D_2O in DMSO-d_6)





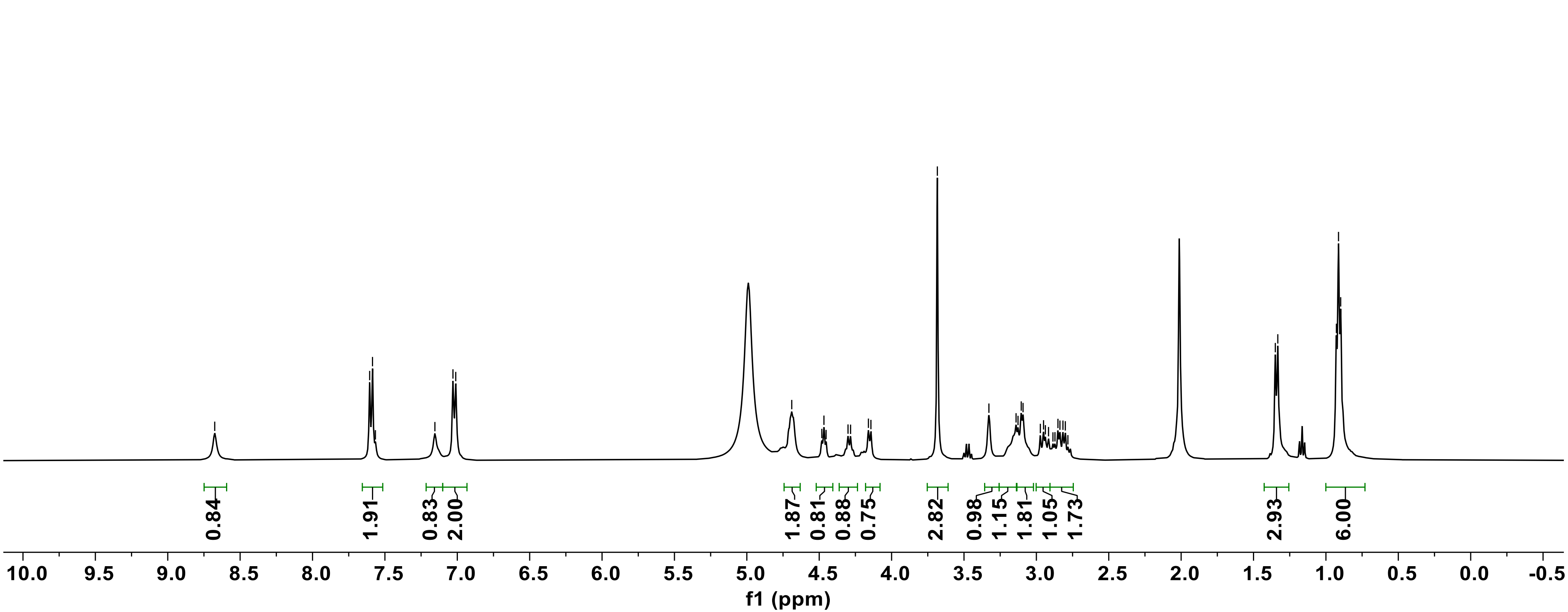
5

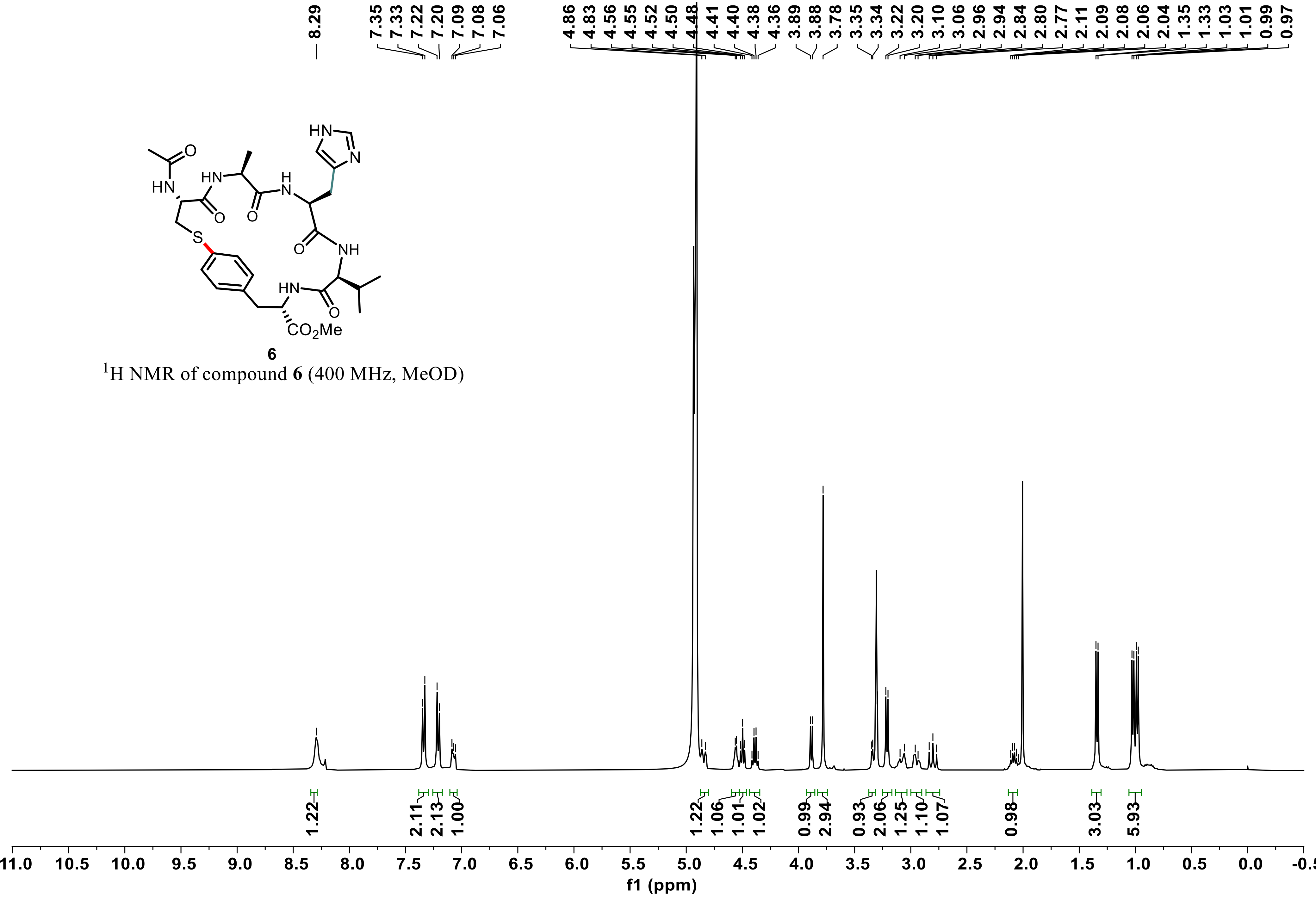
^{13}C NMR of compound **5** (101 MHz, DMSO-d_6)



S6

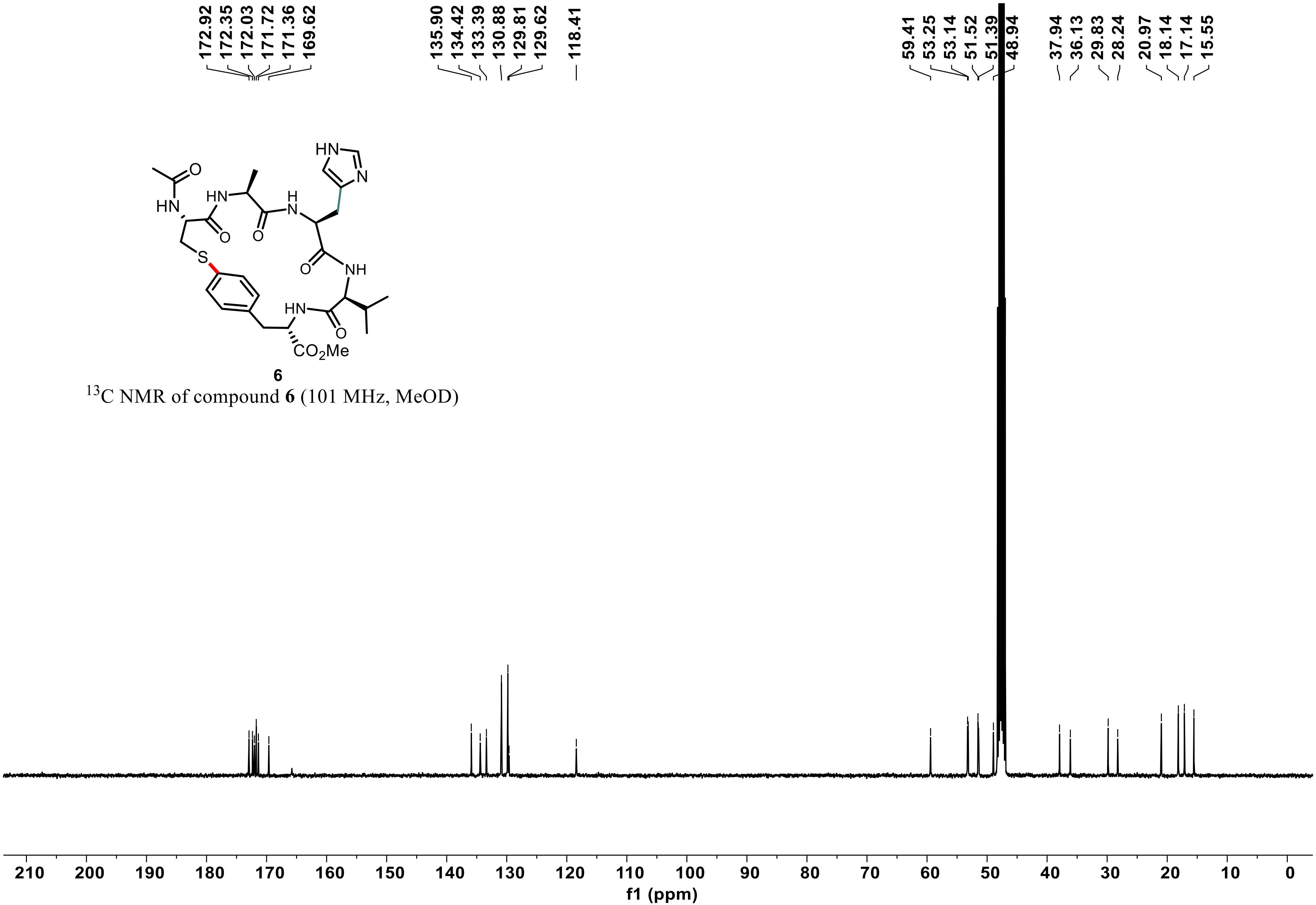
[1]H NMR of compound S**6** (400 MHz, Acetic Acid-d_4)





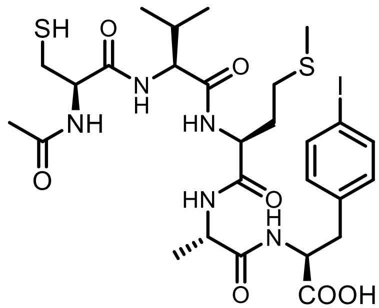
6

^{1}H NMR of compound **6** (400 MHz, MeOD)



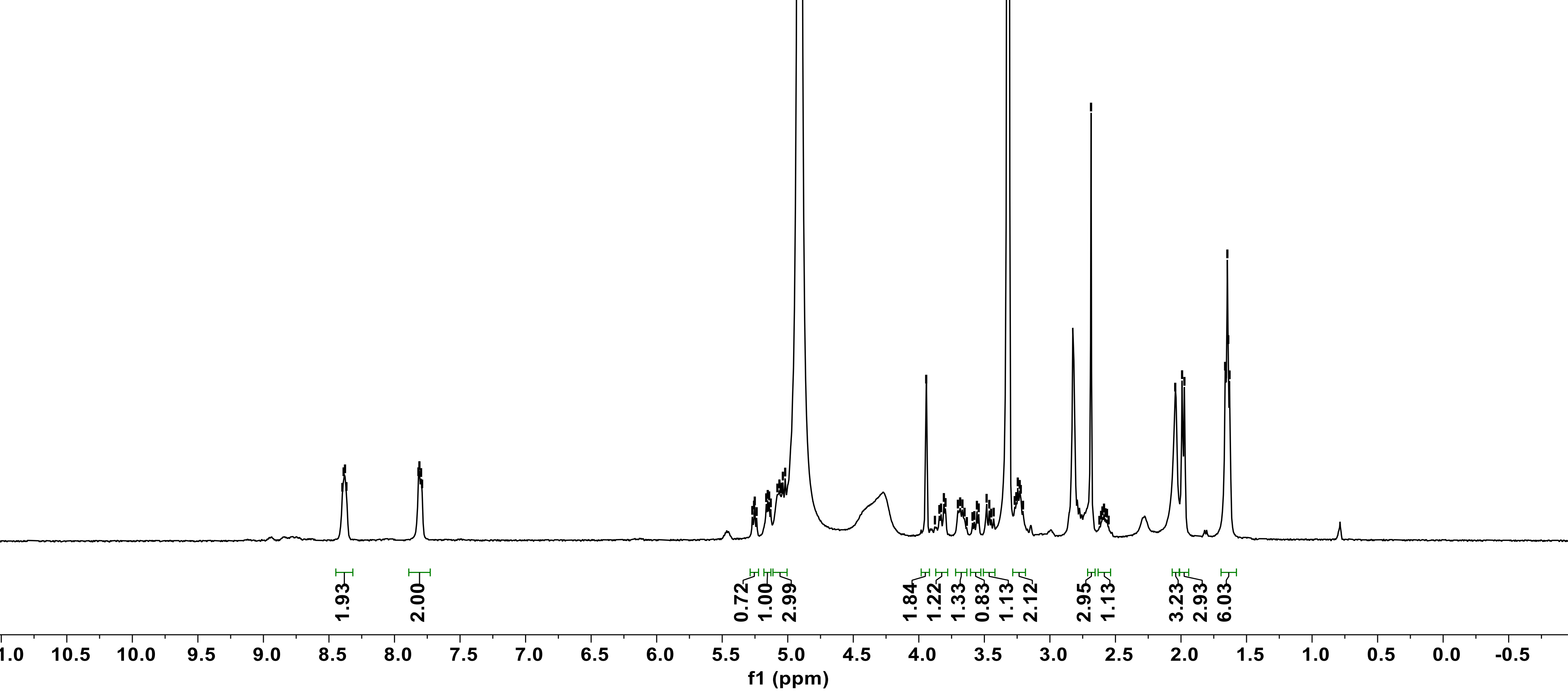
6

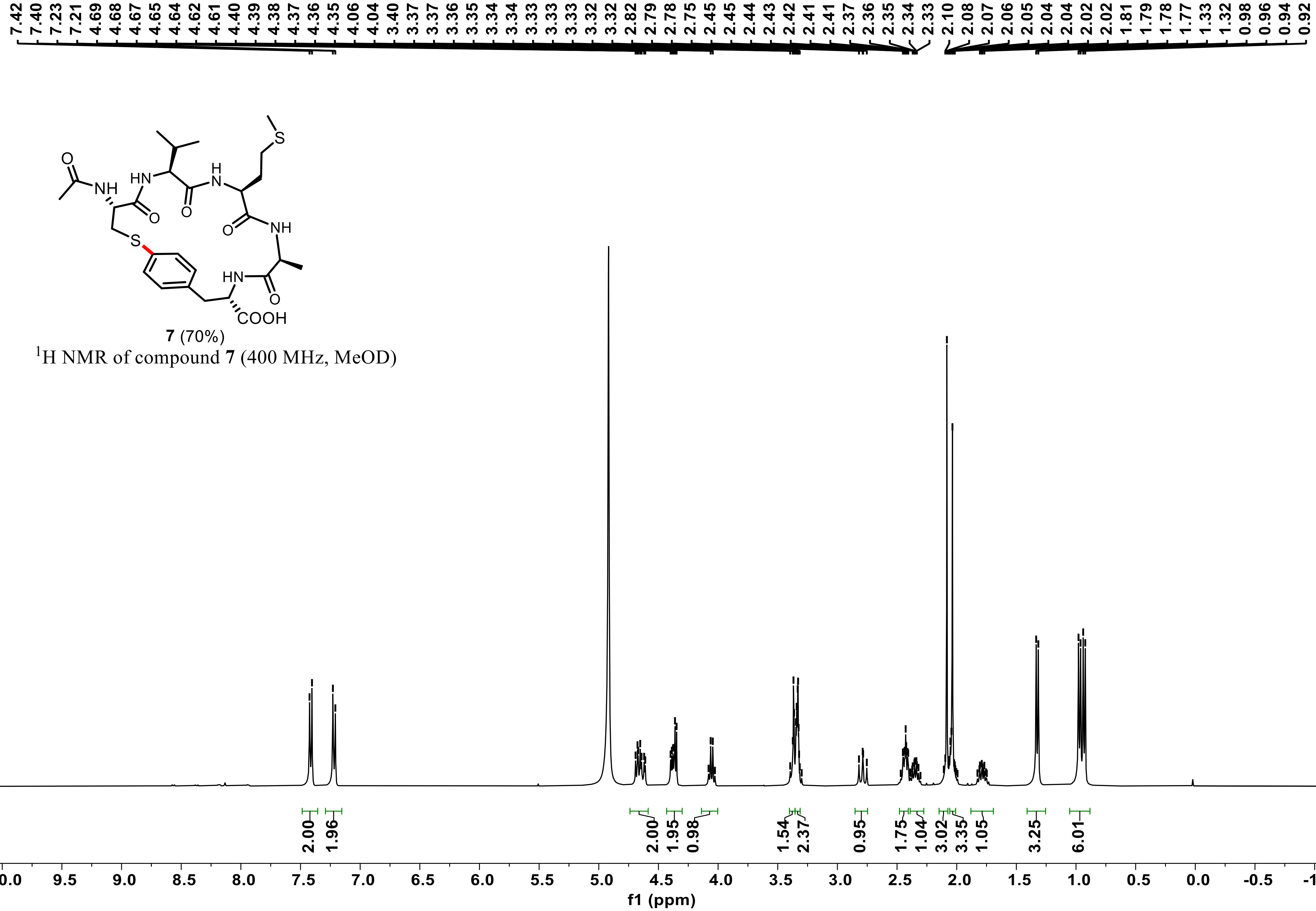
^{13}C NMR of compound **6** (101 MHz, MeOD)



S7

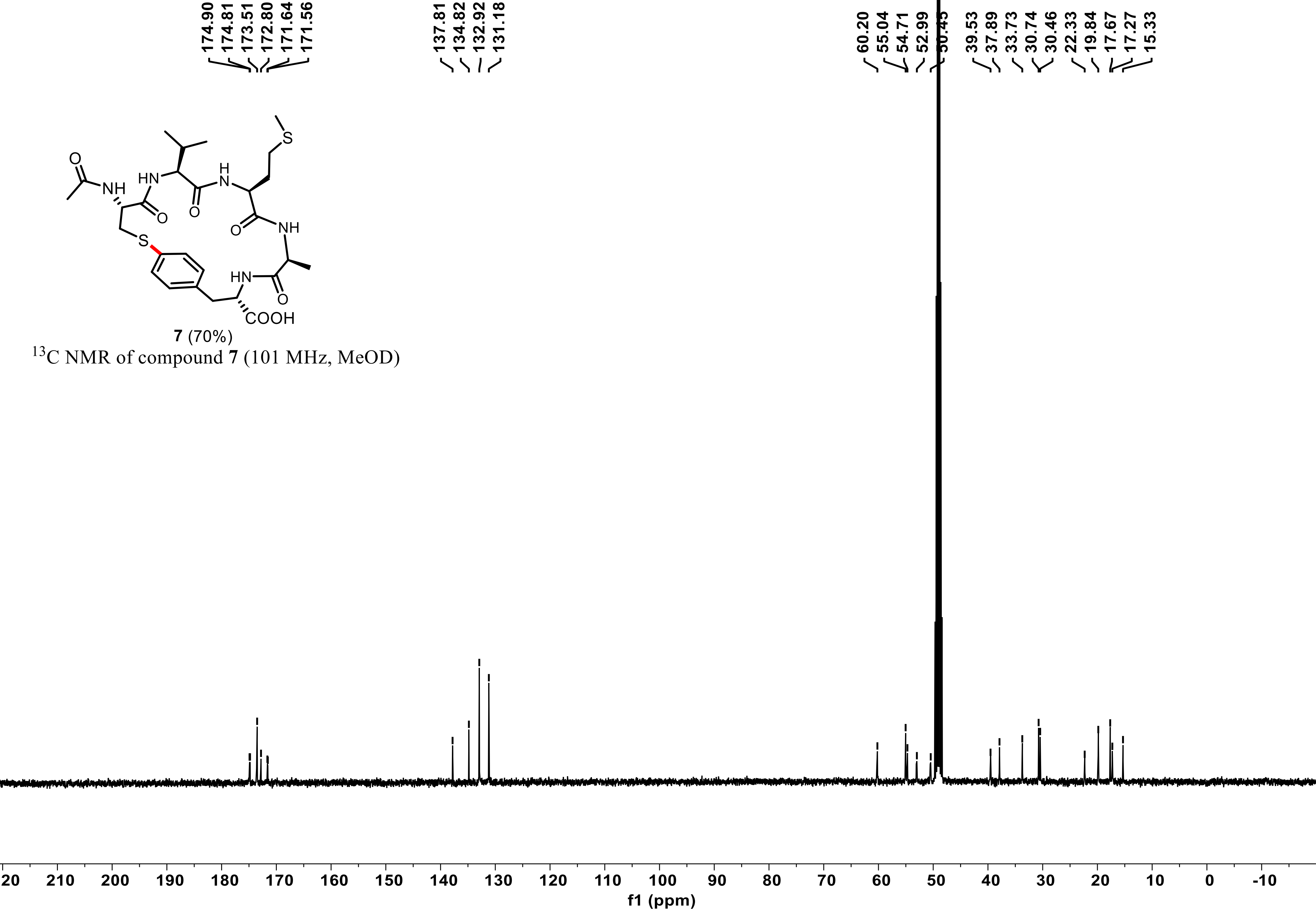
[1]H NMR of compound **S7** (400 MHz, MeOD)





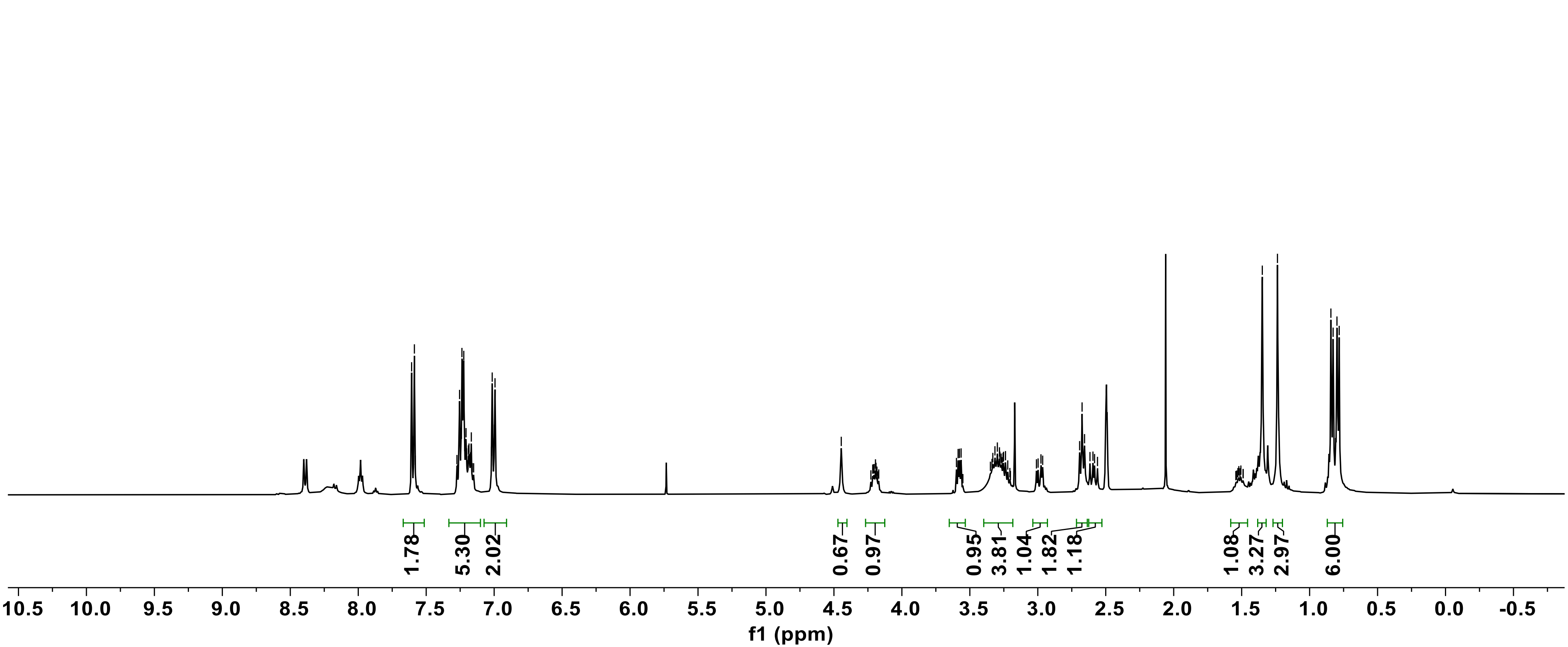
7 (70%)

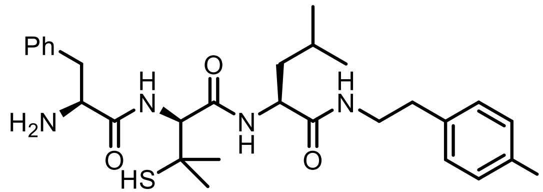
^{1}H NMR of compound **7** (400 MHz, MeOD)



7 (70%)

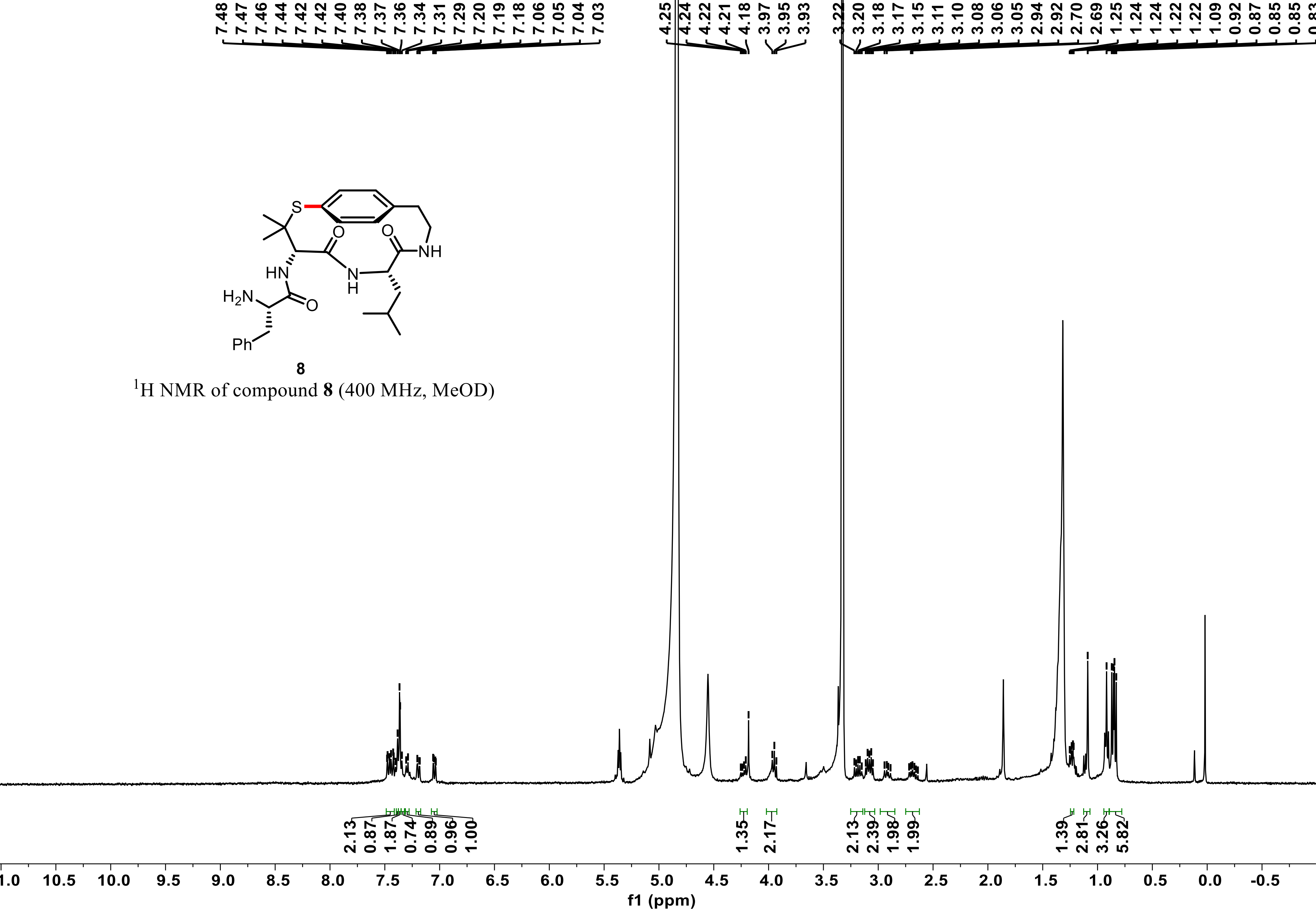
^{13}C NMR of compound **7** (101 MHz, MeOD)



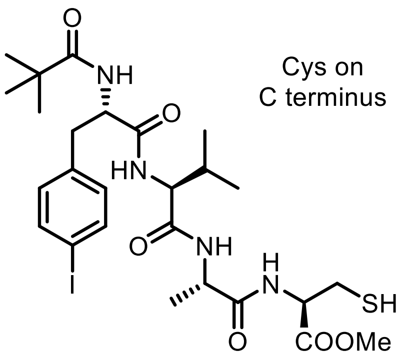


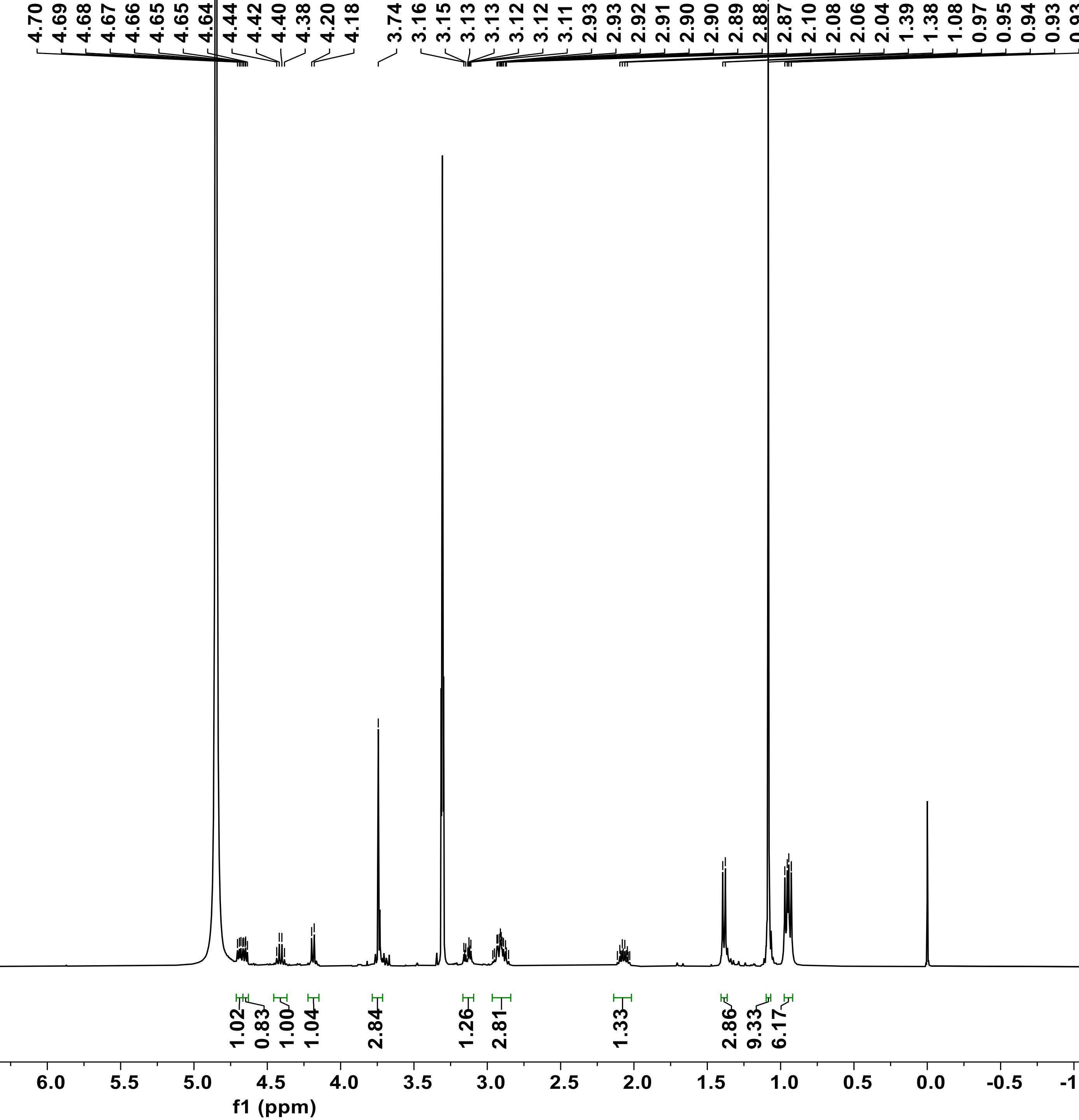
S8

^{1}H NMR of compound S**8** (400 MHz, DMSO-d_6)



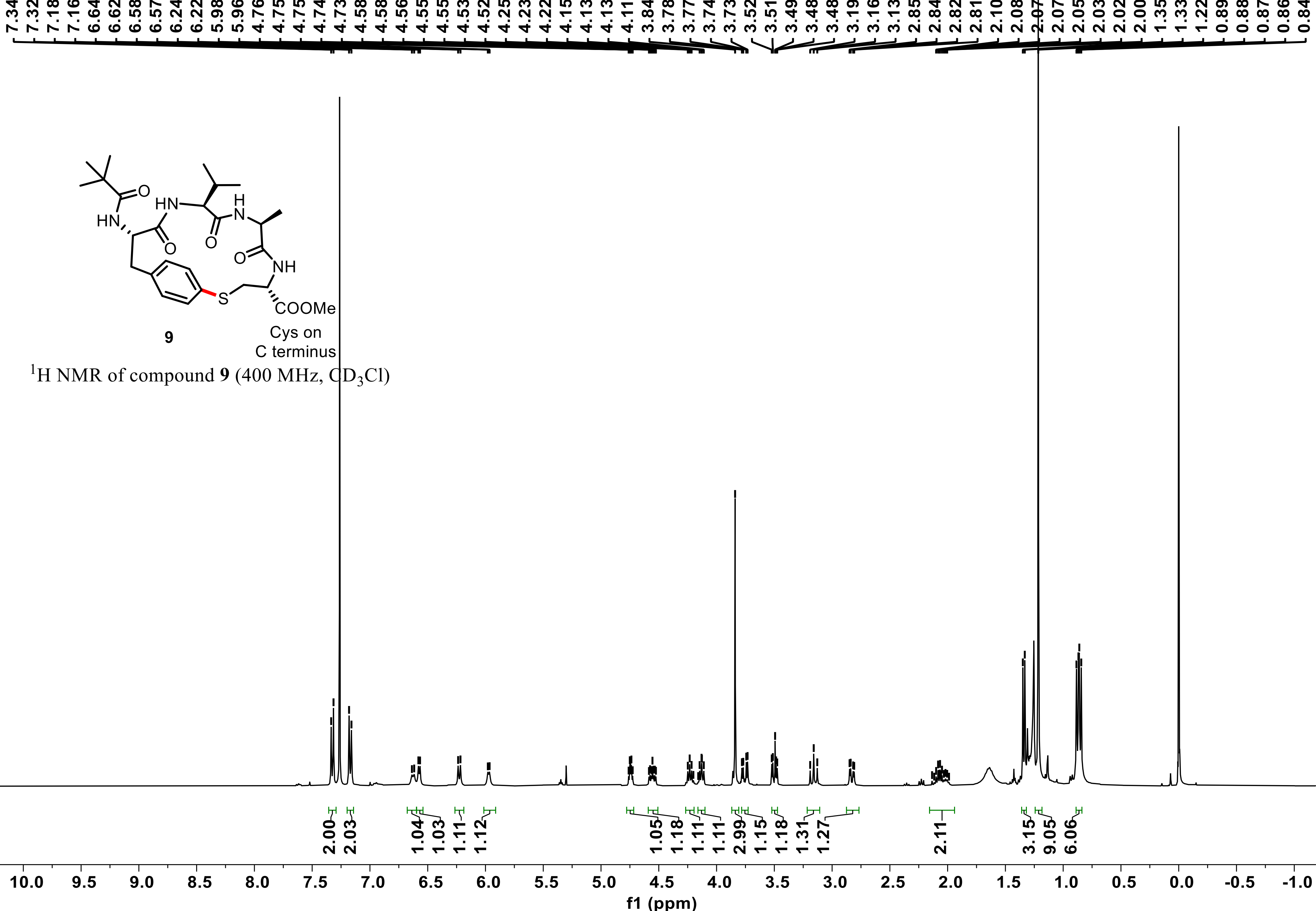
^{1}H NMR of compound **8** (400 MHz, MeOD)



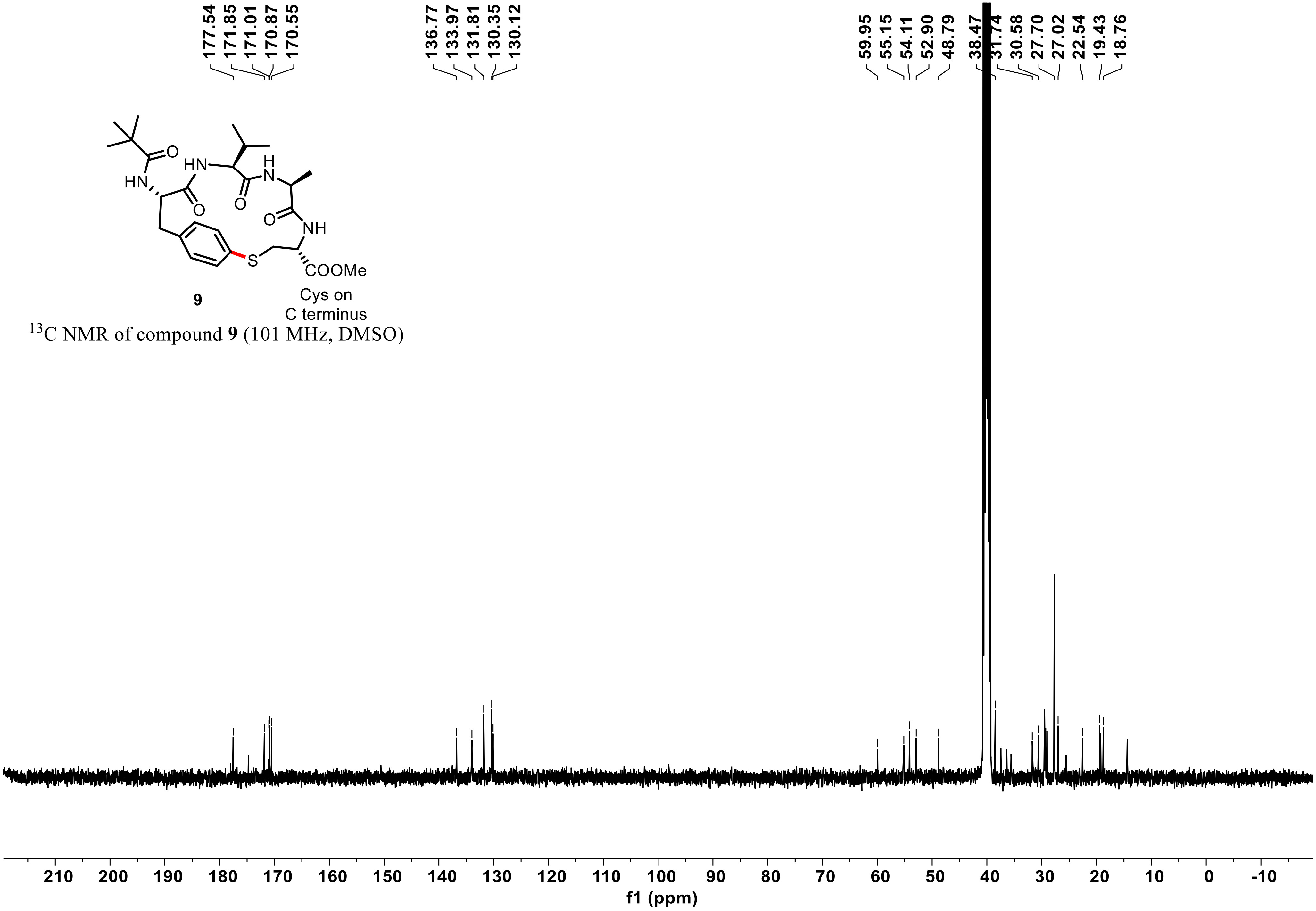


S9

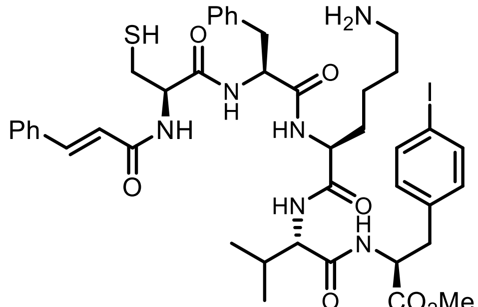
^{1}H NMR of compound **S9** (400 MHz, MeOD)



[1]H NMR of compound **9** (400 MHz, CD_3Cl)

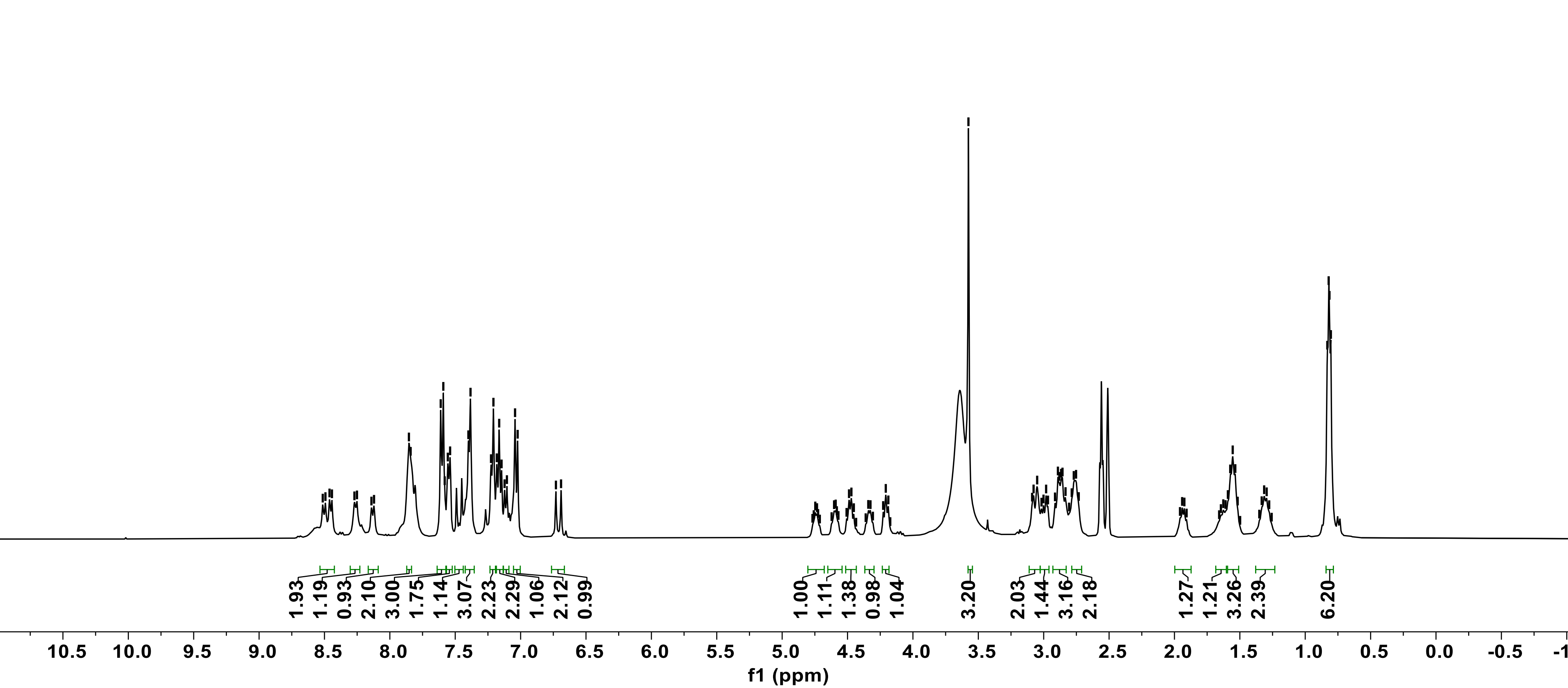


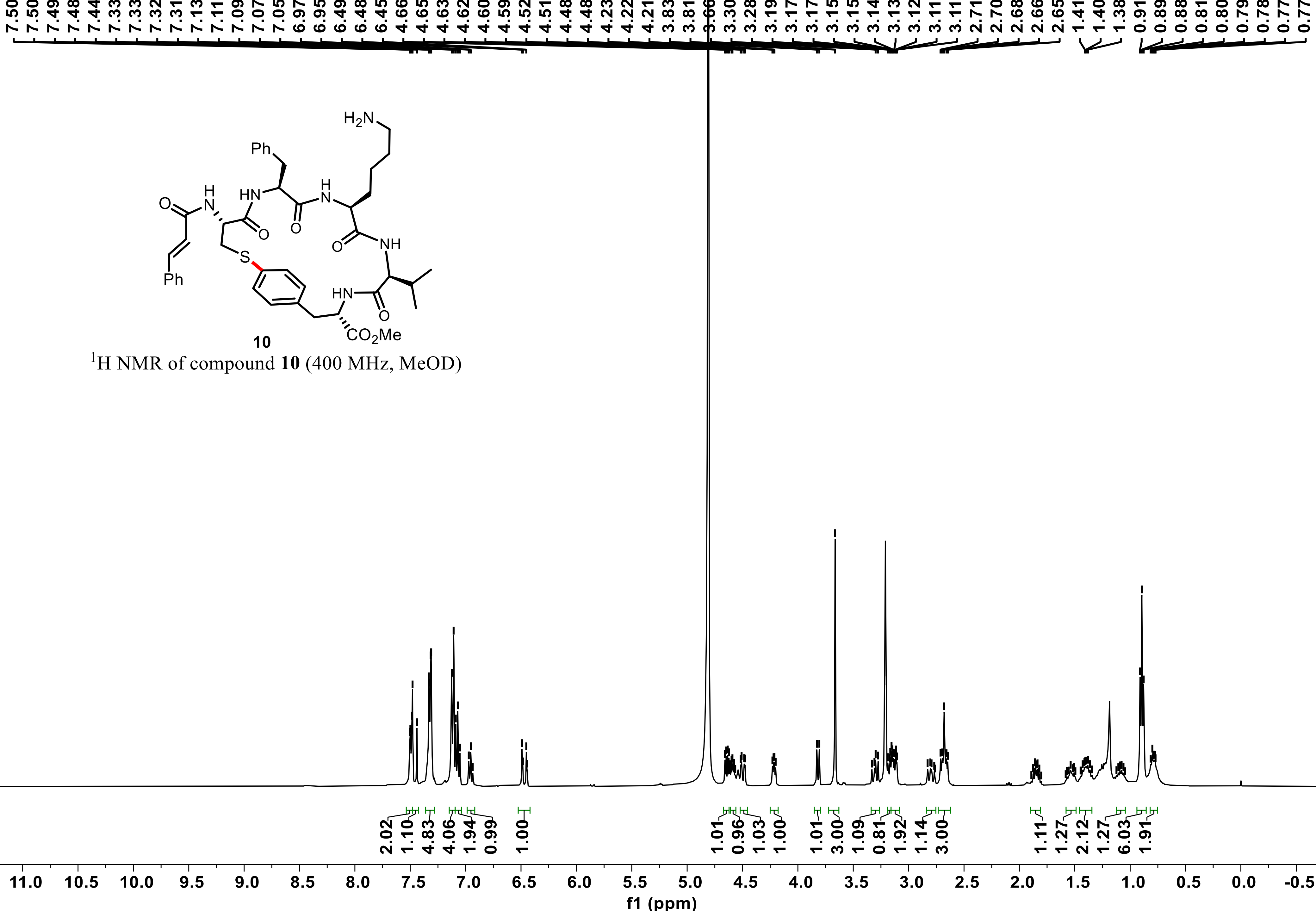
^{13}C NMR of compound **9** (101 MHz, DMSO)



S10

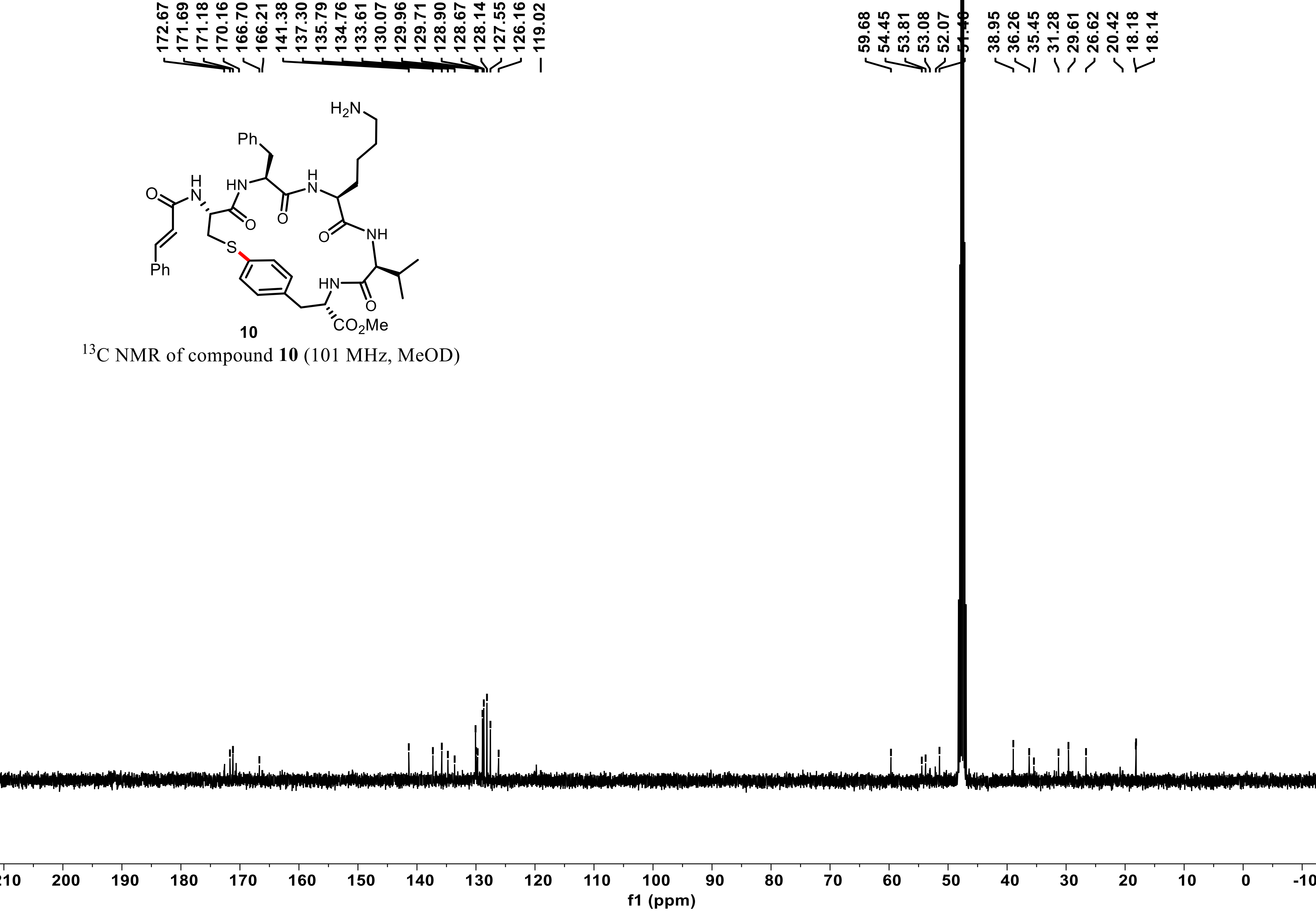
[1]H NMR of compound S**10** (400 MHz, DMSO)





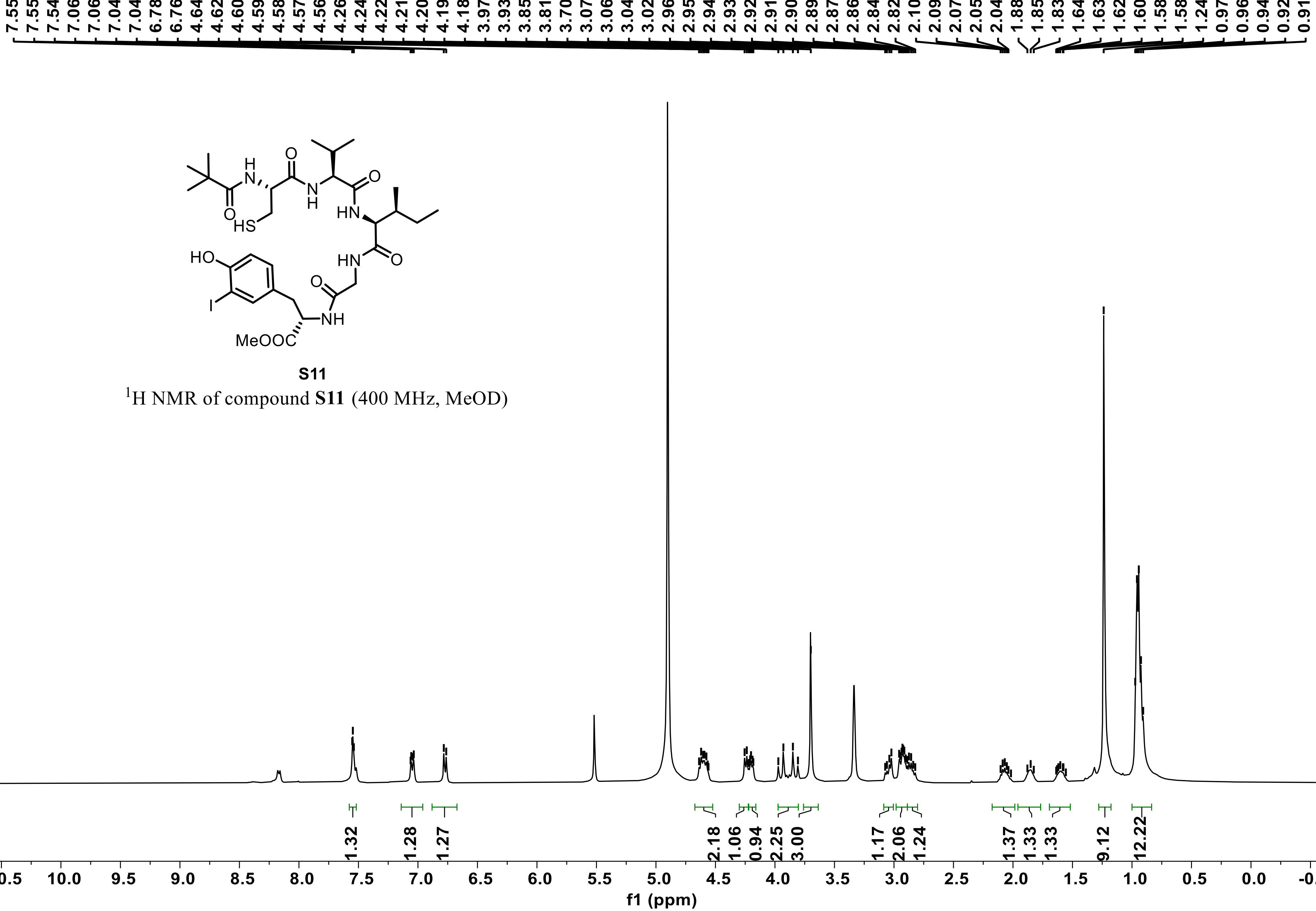
10

^{1}H NMR of compound **10** (400 MHz, MeOD)



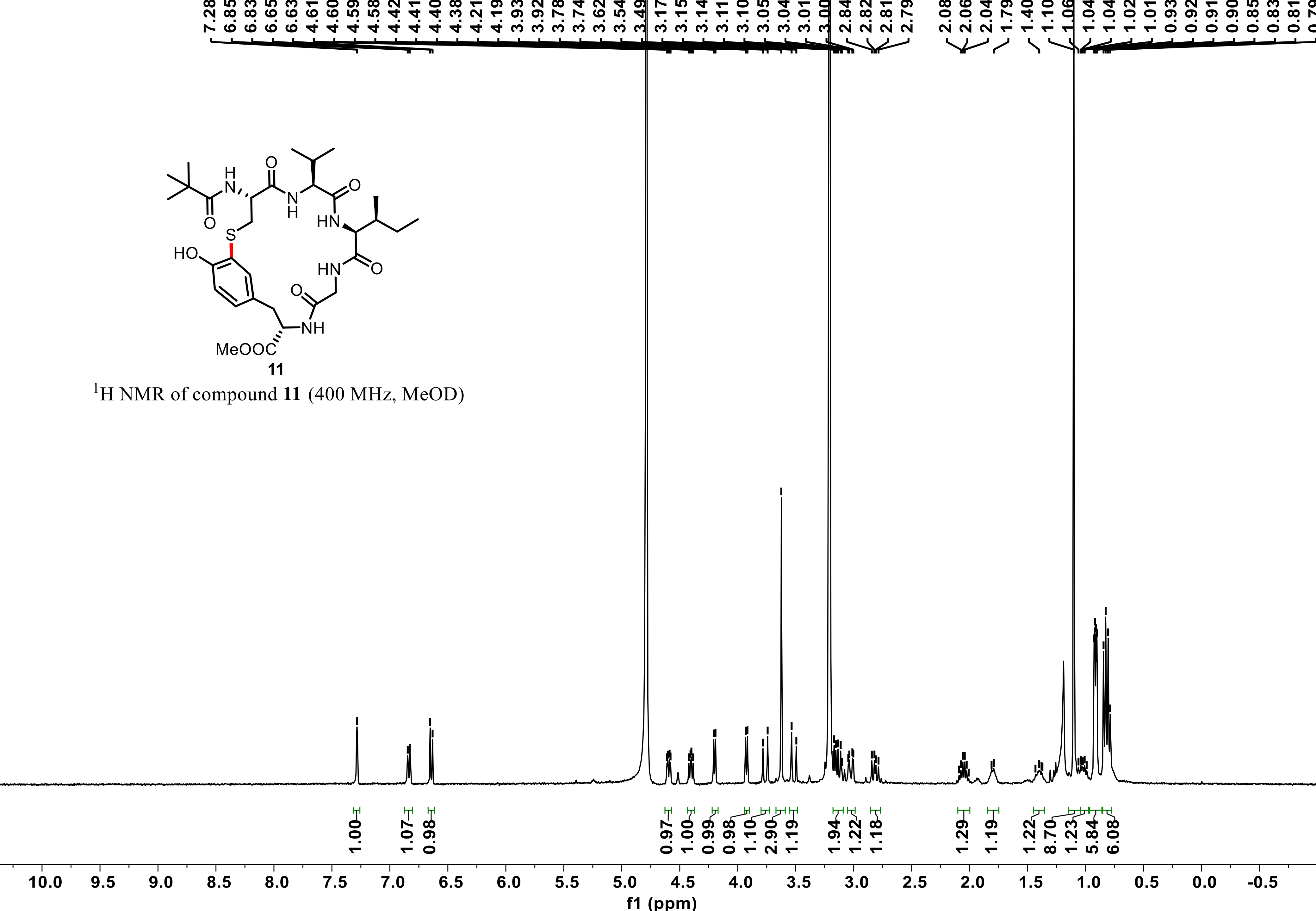
10

^{13}C NMR of compound **10** (101 MHz, MeOD)

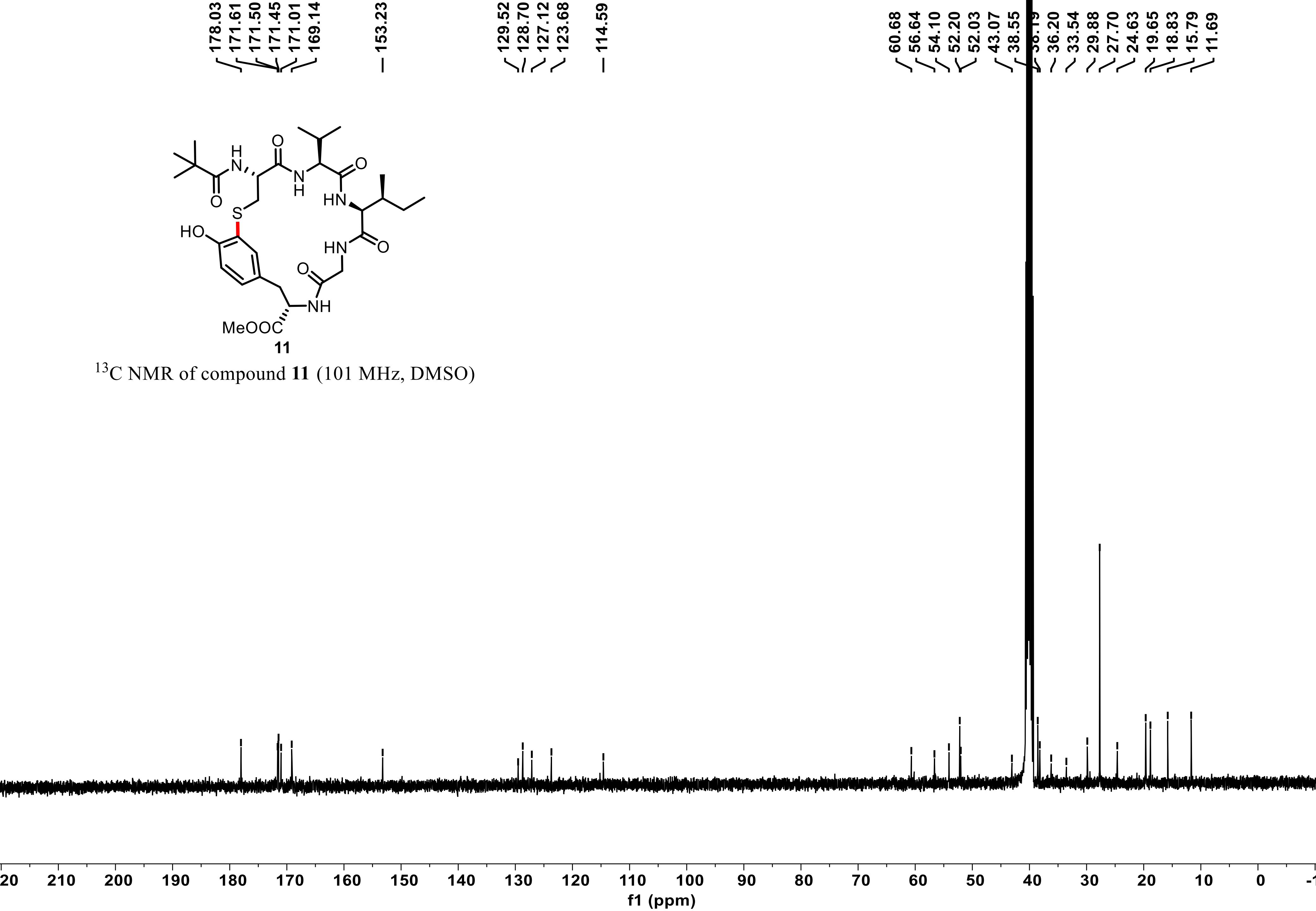


S11

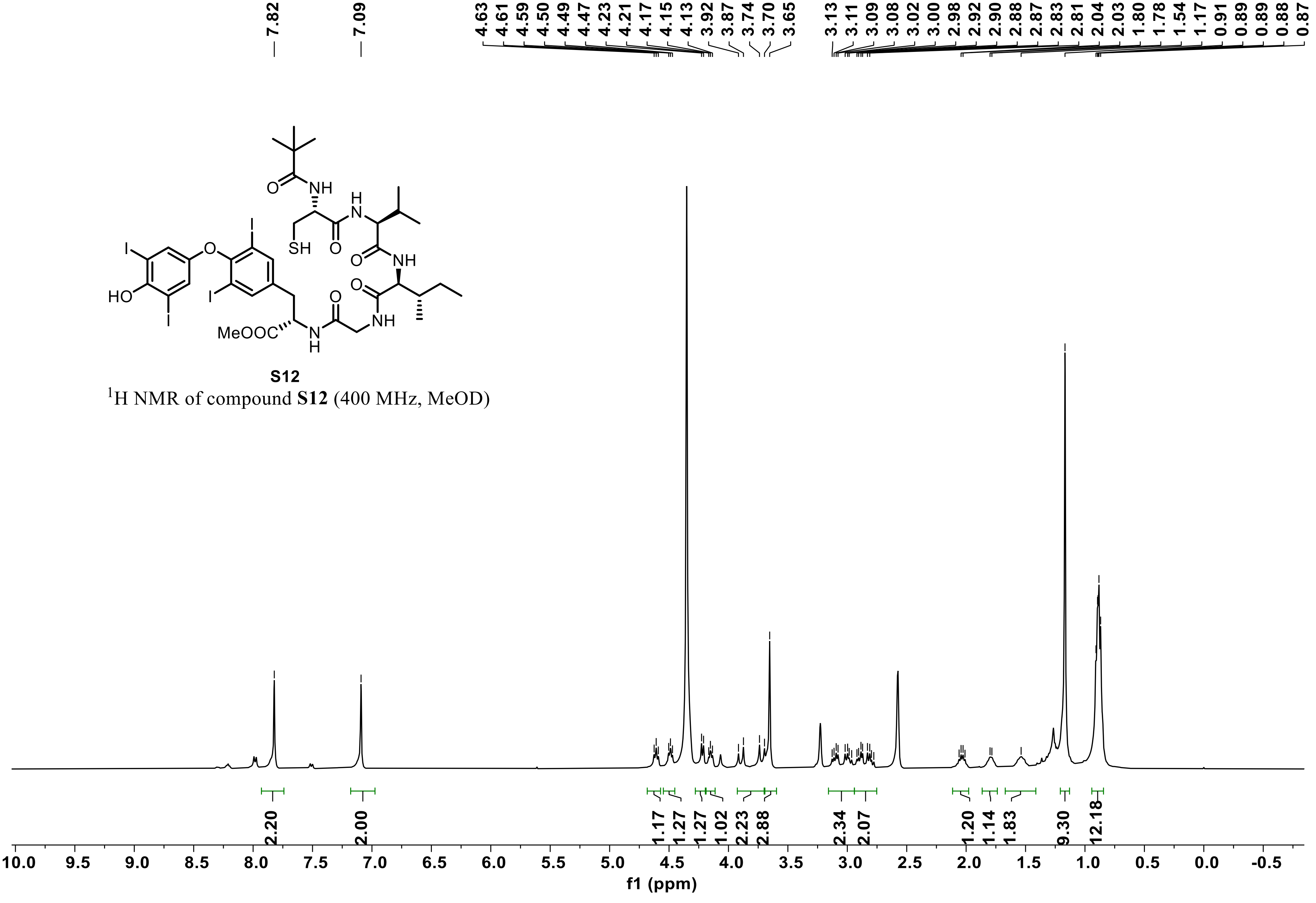
^{1}H NMR of compound **S11** (400 MHz, MeOD)



^{1}H NMR of compound **11** (400 MHz, MeOD)

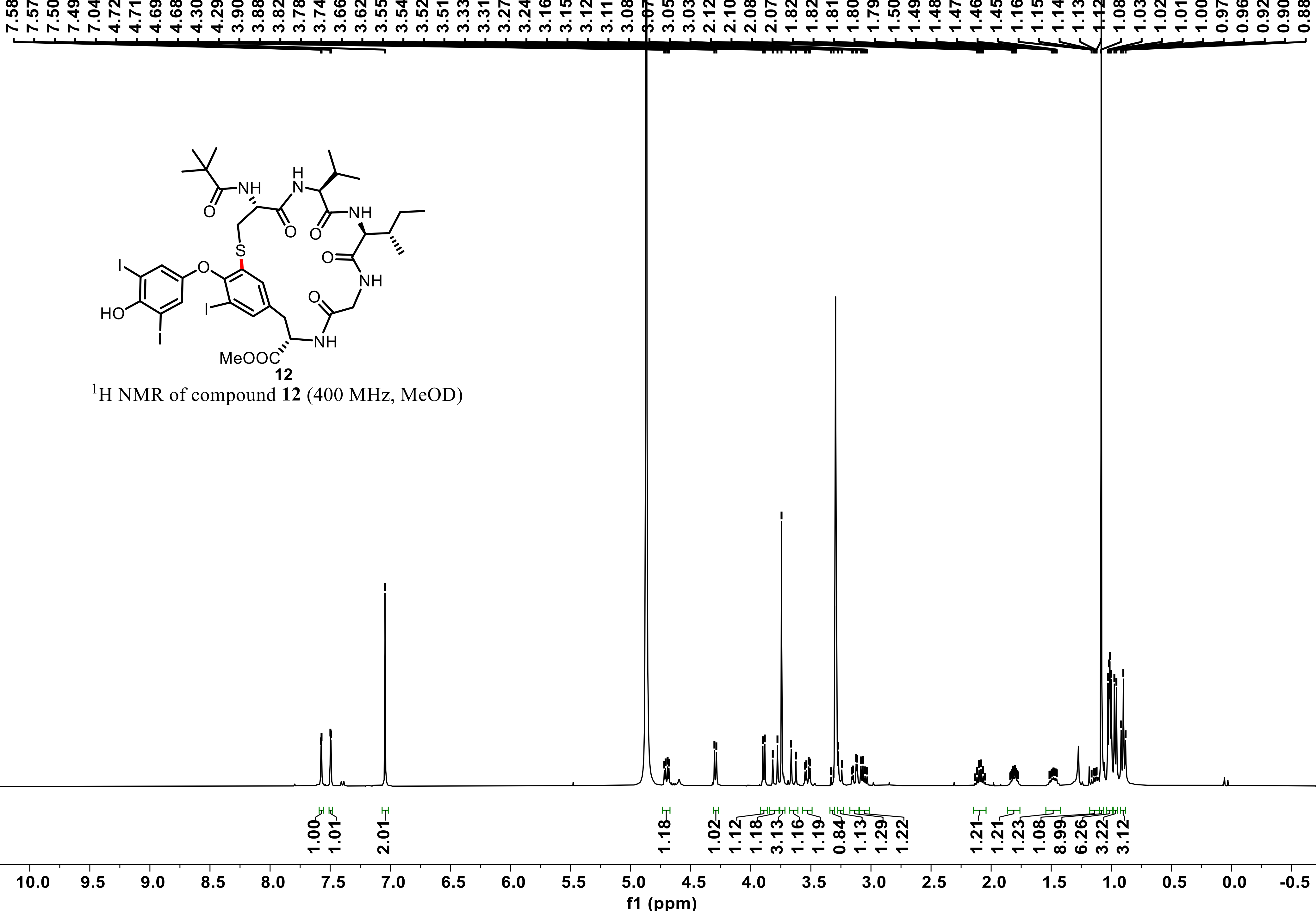


^{13}C NMR of compound **11** (101 MHz, DMSO)

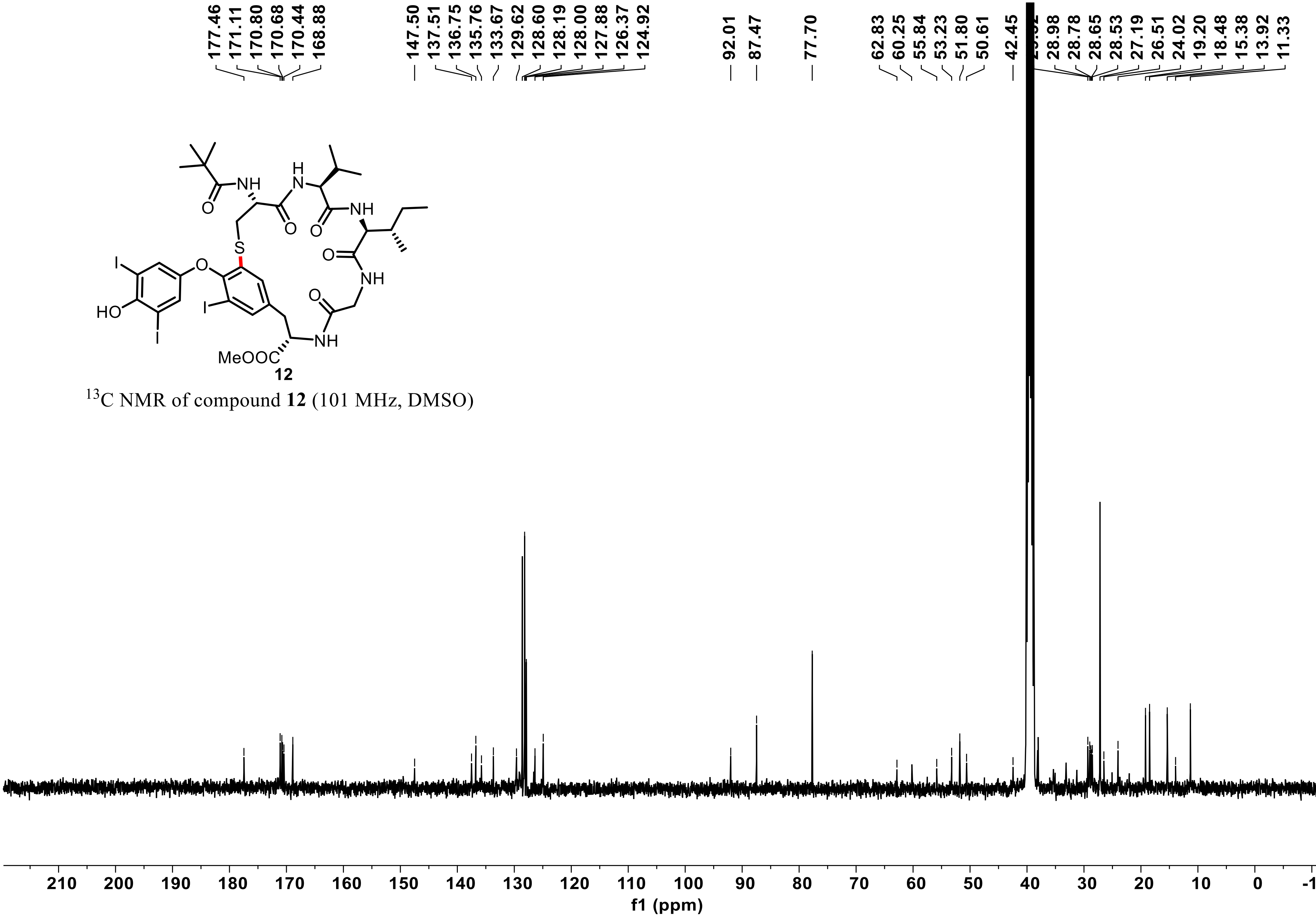


S12

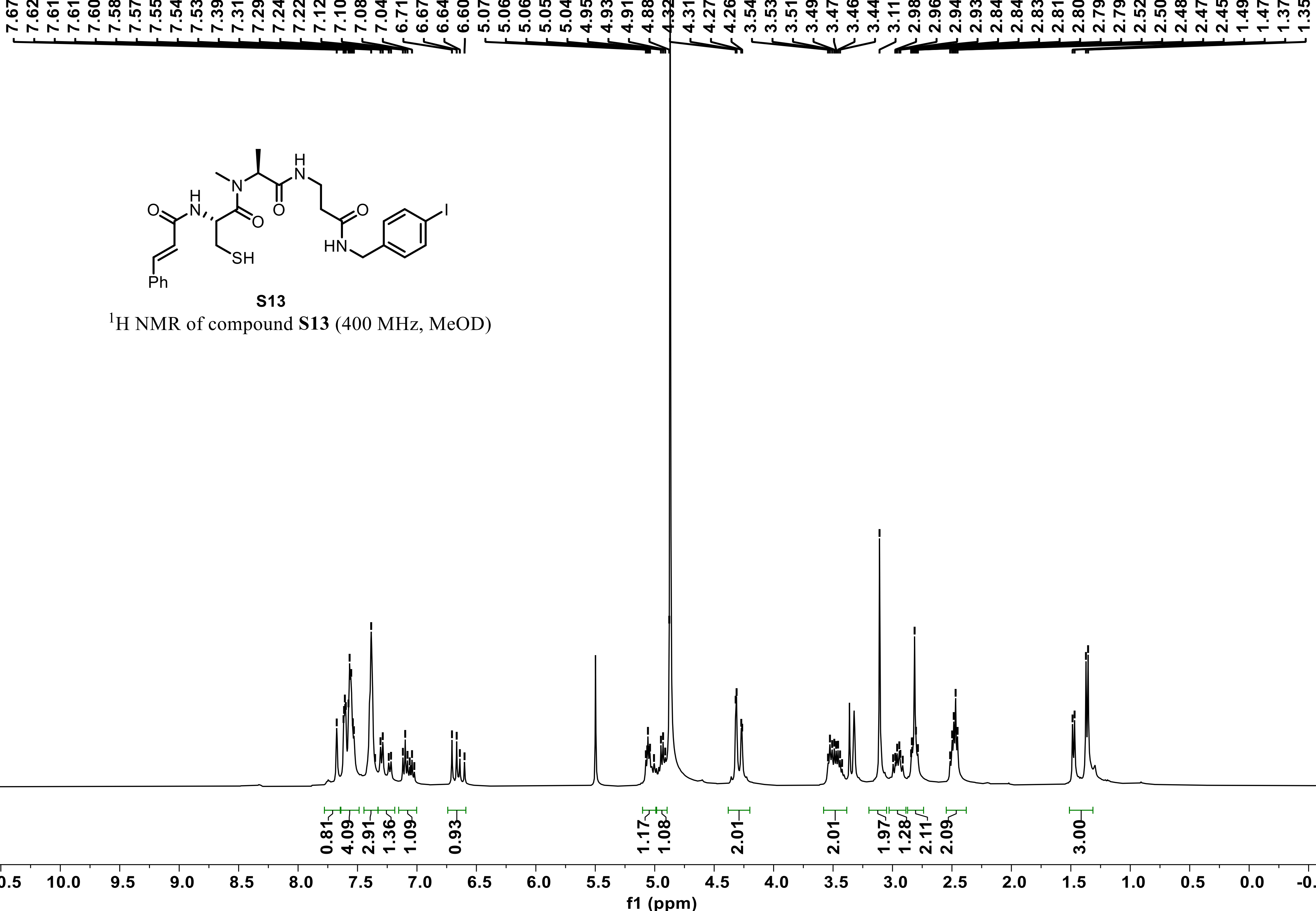
[1]H NMR of compound **S12** (400 MHz, MeOD)



^{1}H NMR of compound **12** (400 MHz, MeOD)

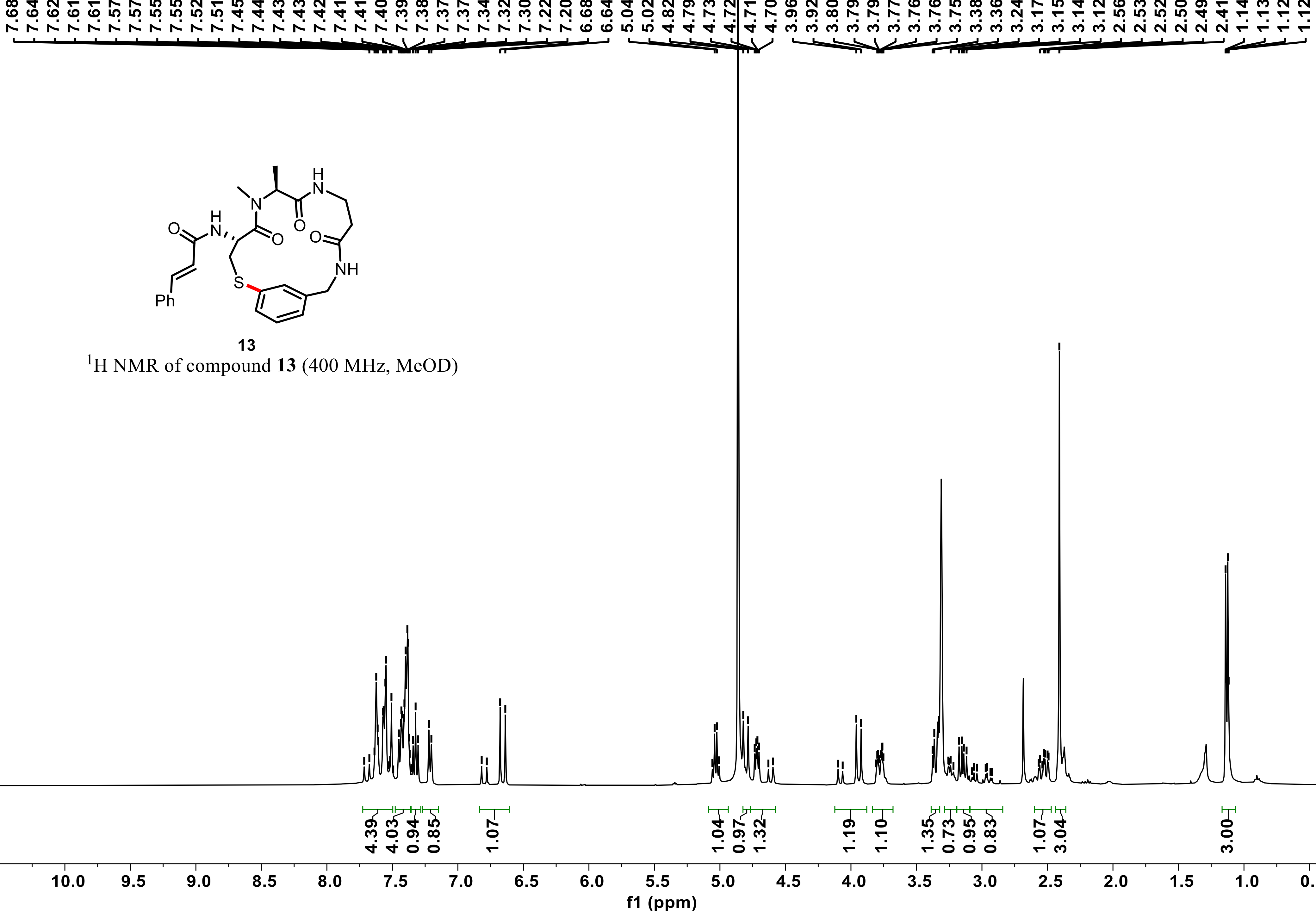


^{13}C NMR of compound **12** (101 MHz, DMSO)



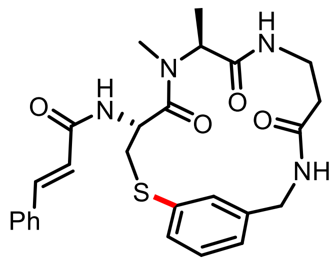
S13

^{1}H NMR of compound **S13** (400 MHz, MeOD)



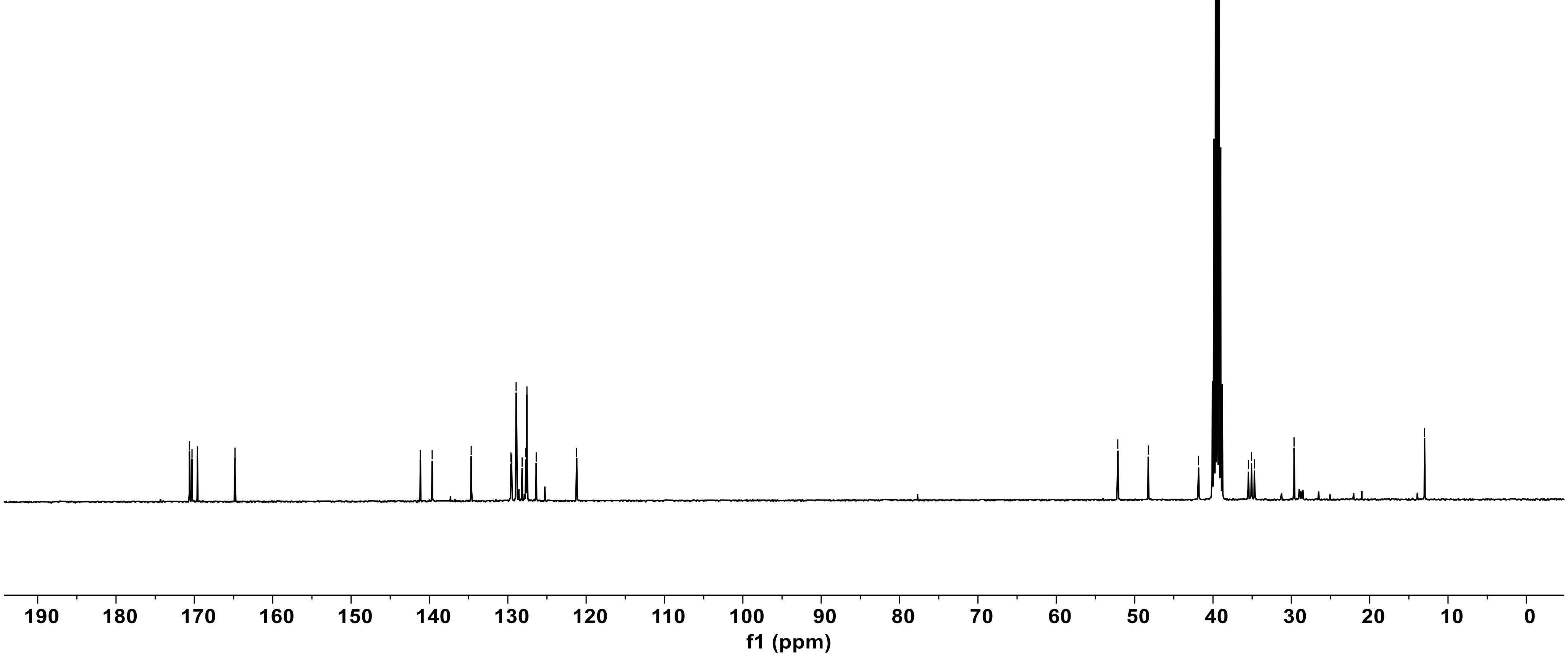
13

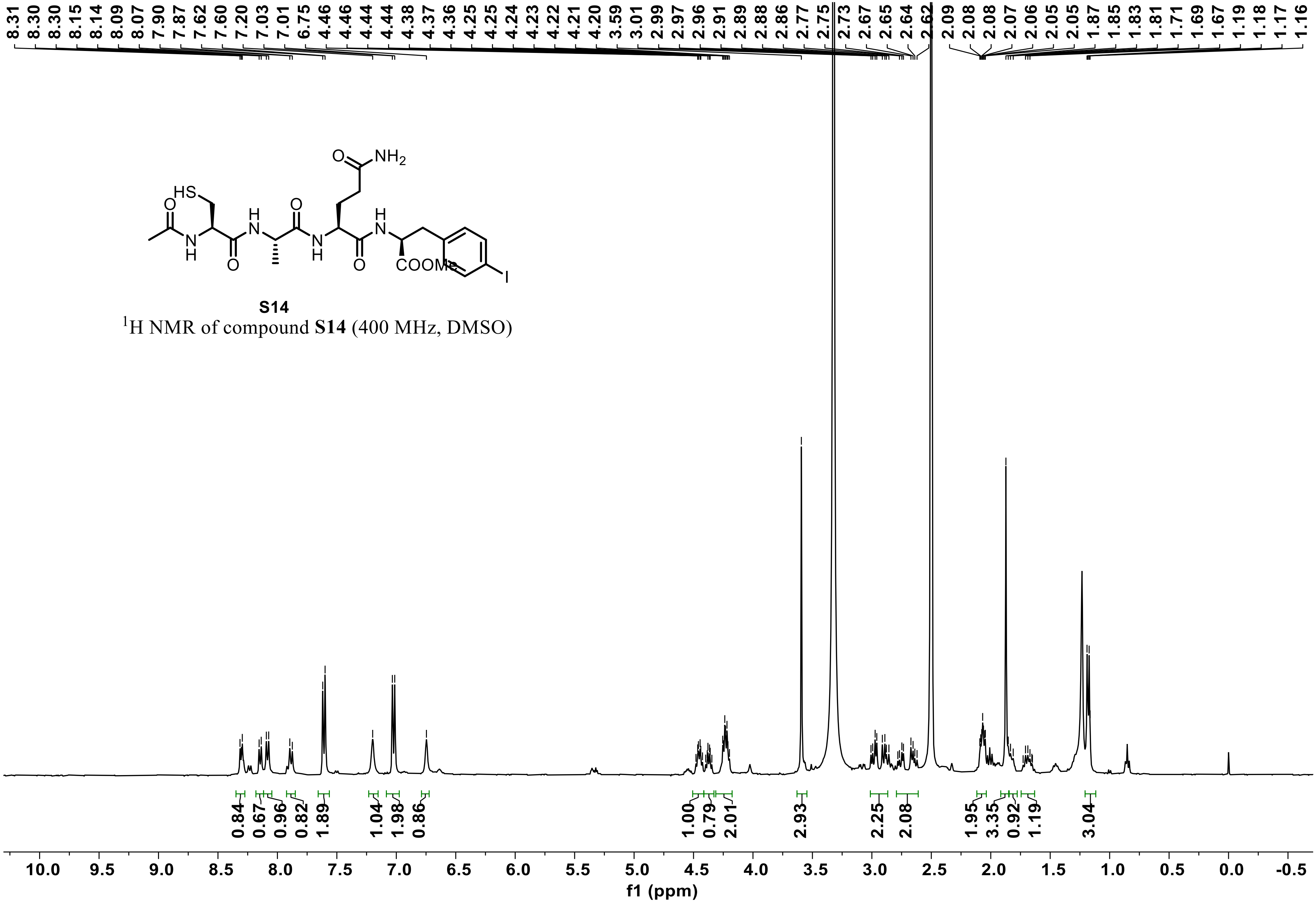
^{1}H NMR of compound **13** (400 MHz, MeOD)



13

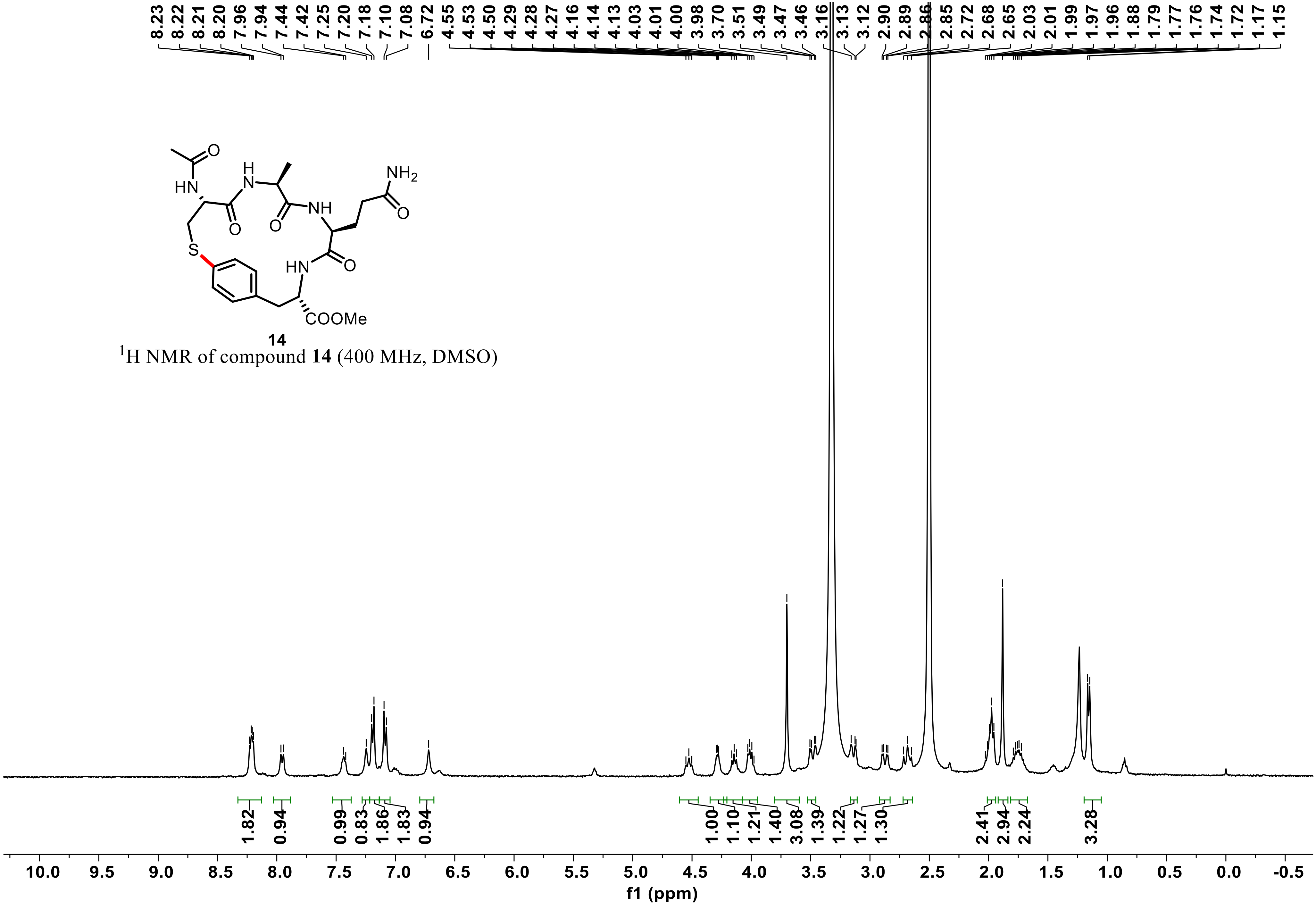
^{13}C NMR of compound **13** (101 MHz, DMSO)





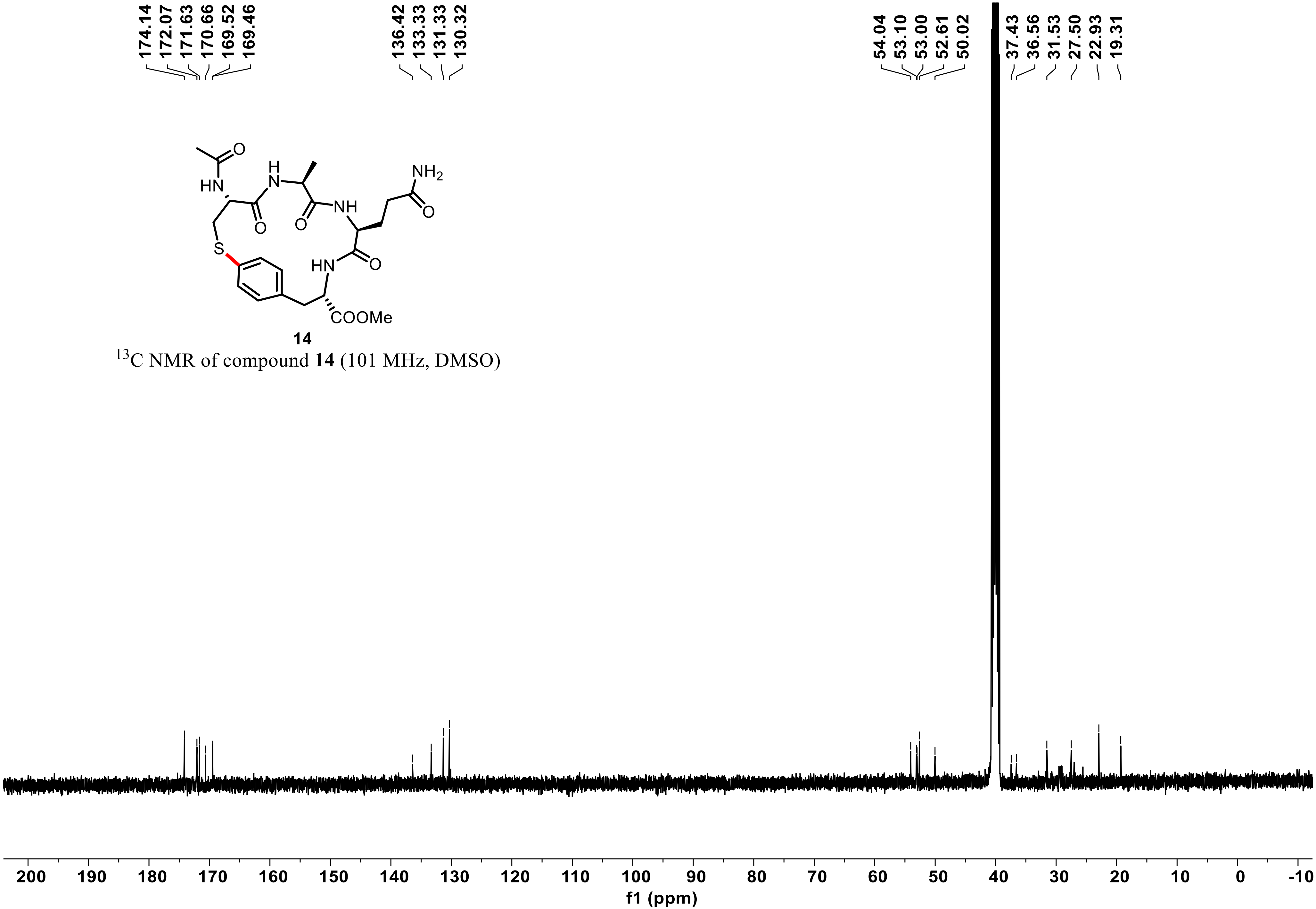
S14

^{1}H NMR of compound **S14** (400 MHz, DMSO)



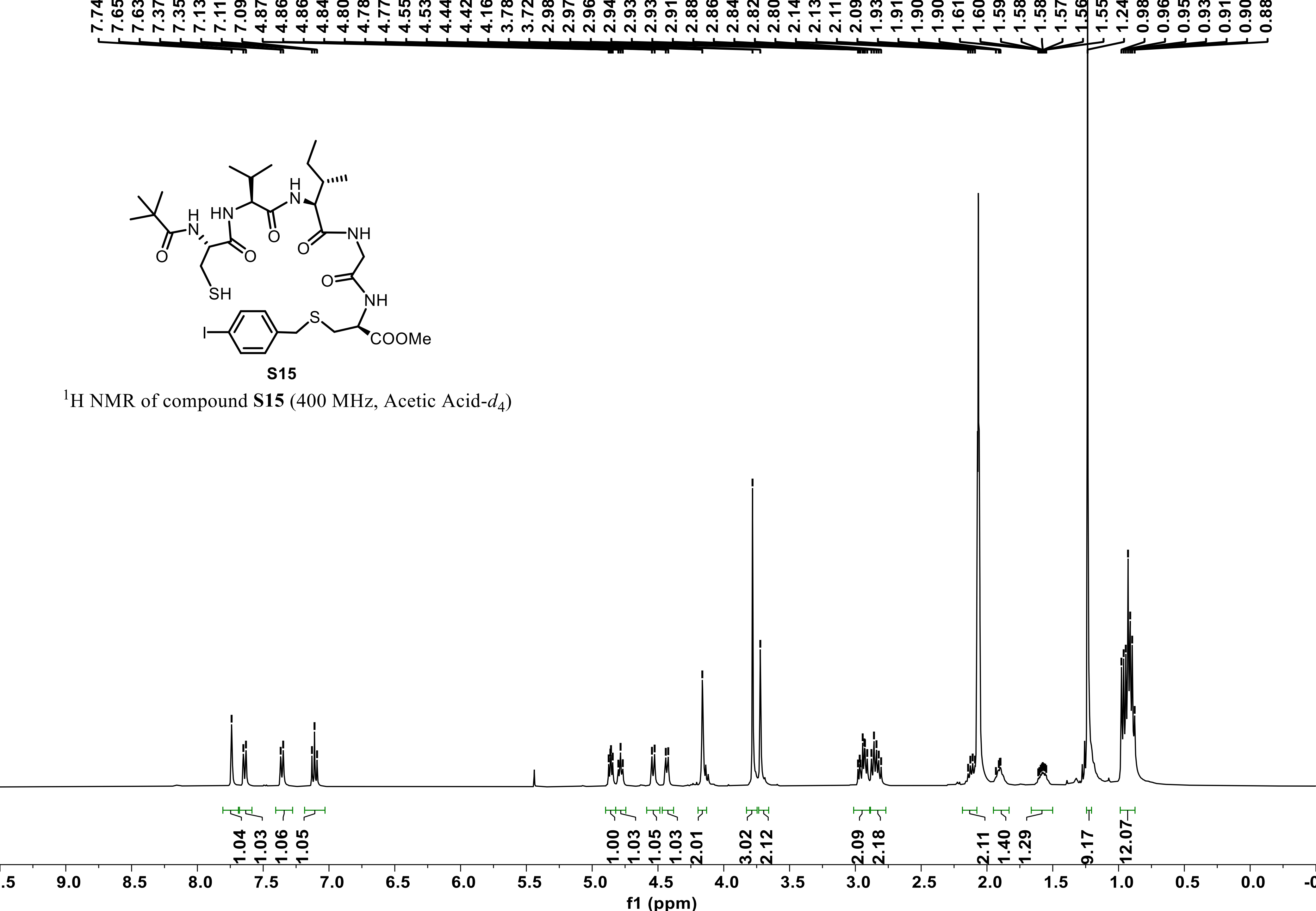
14

^{1}H NMR of compound **14** (400 MHz, DMSO)



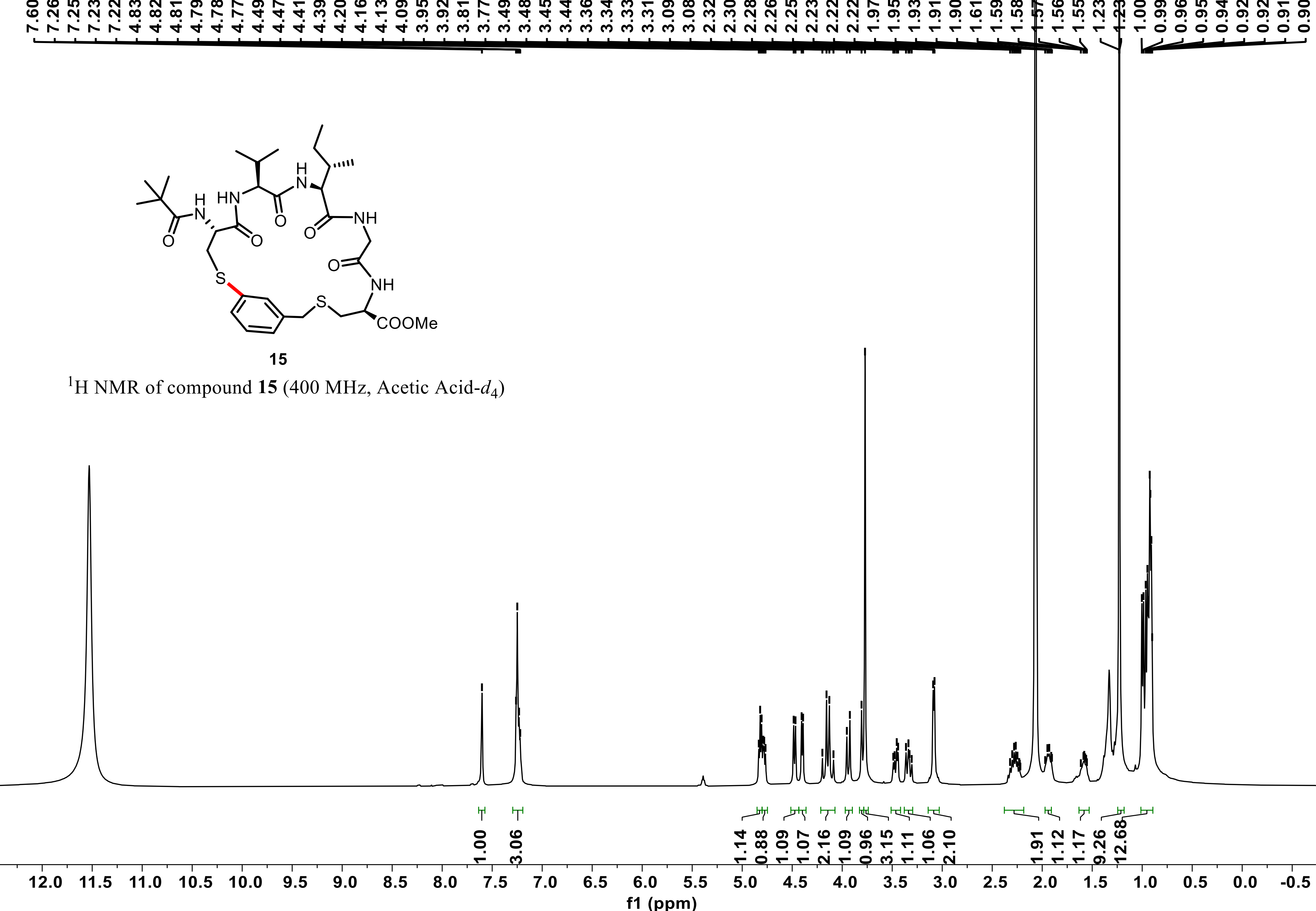
14

^{13}C NMR of compound **14** (101 MHz, DMSO)



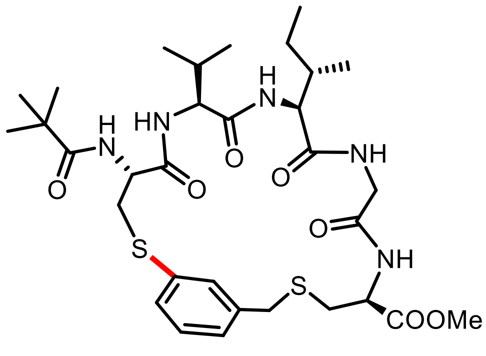
S15

^{1}H NMR of compound **S15** (400 MHz, Acetic Acid-d_4)



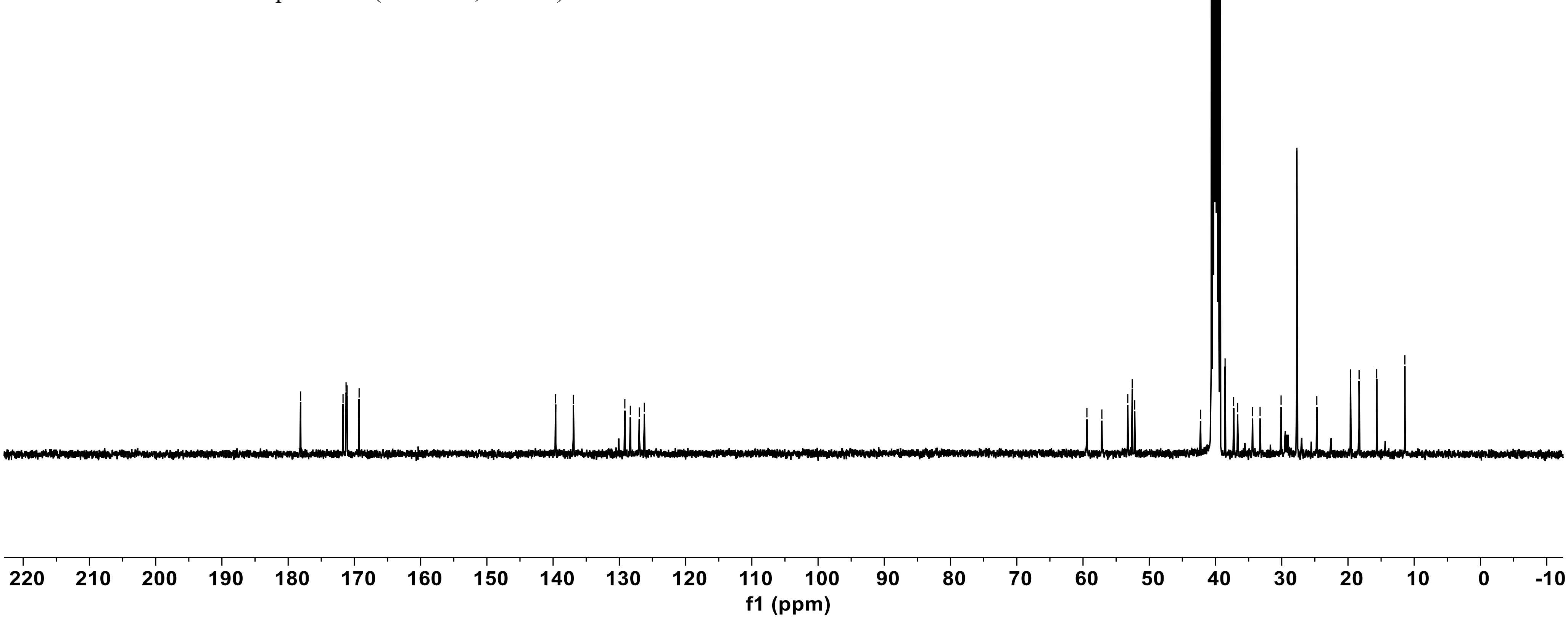
15

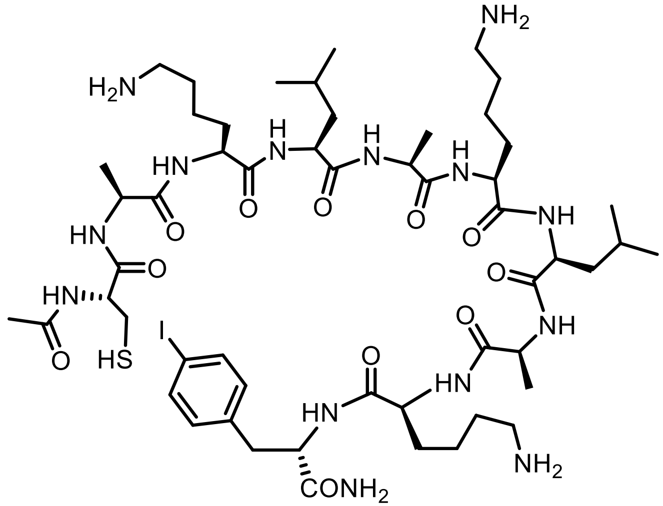
^{1}H NMR of compound **15** (400 MHz, Acetic Acid-d_4)



15

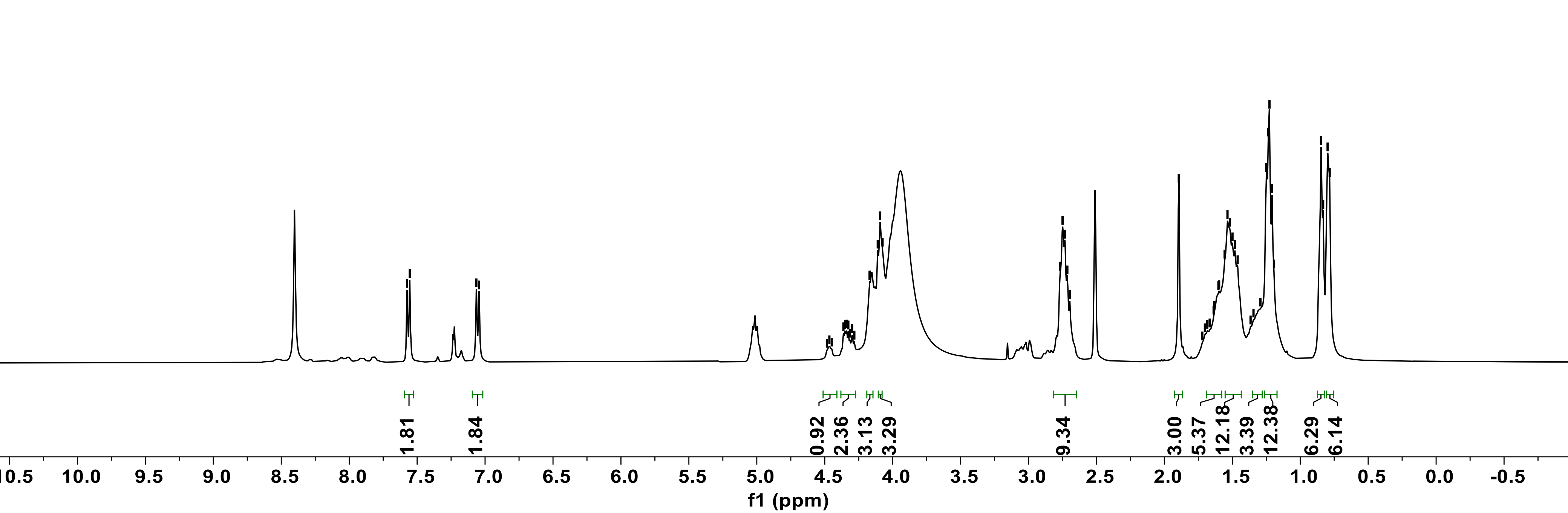
^{13}C NMR of compound **15** (101 MHz, DMSO)

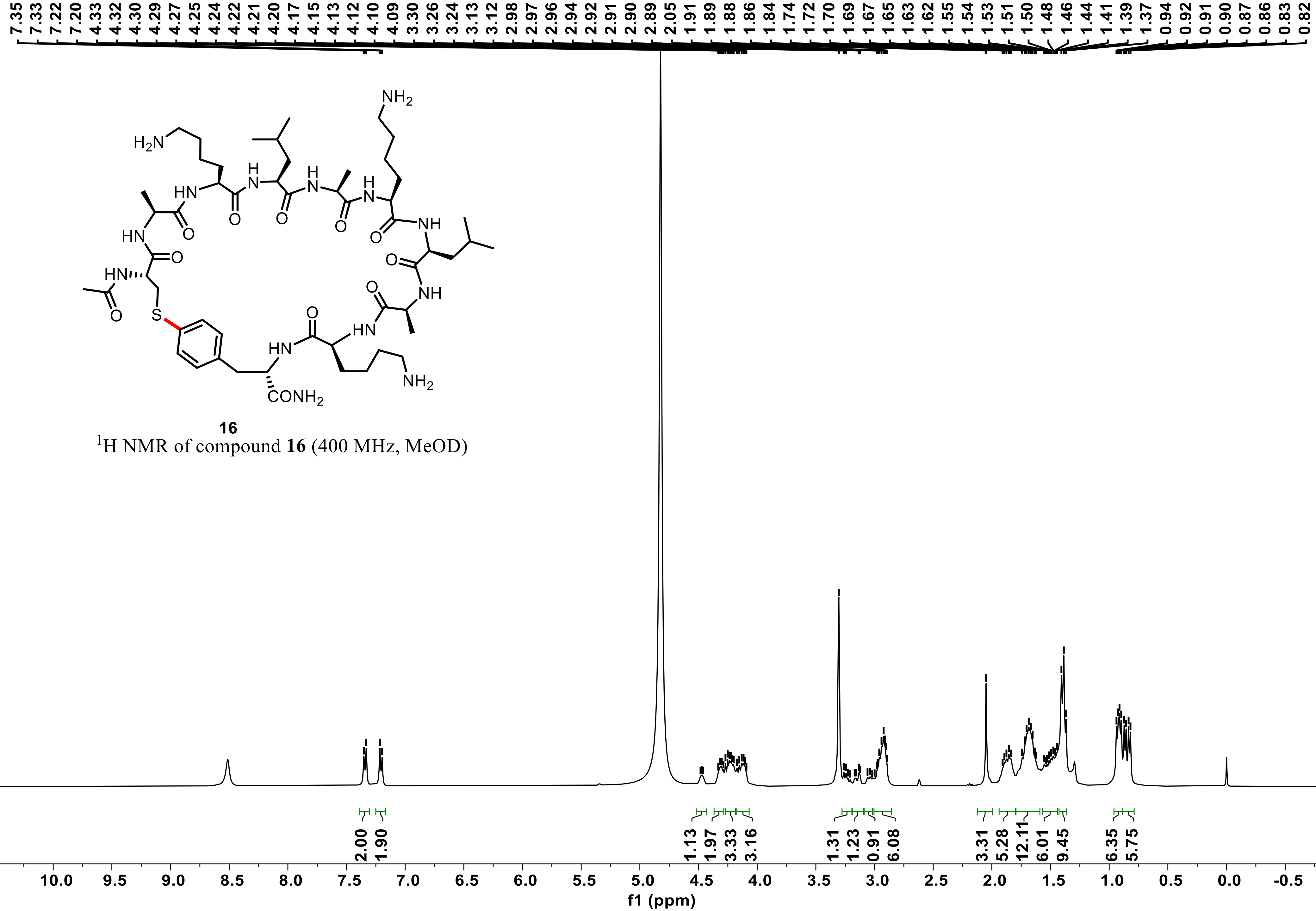




S16

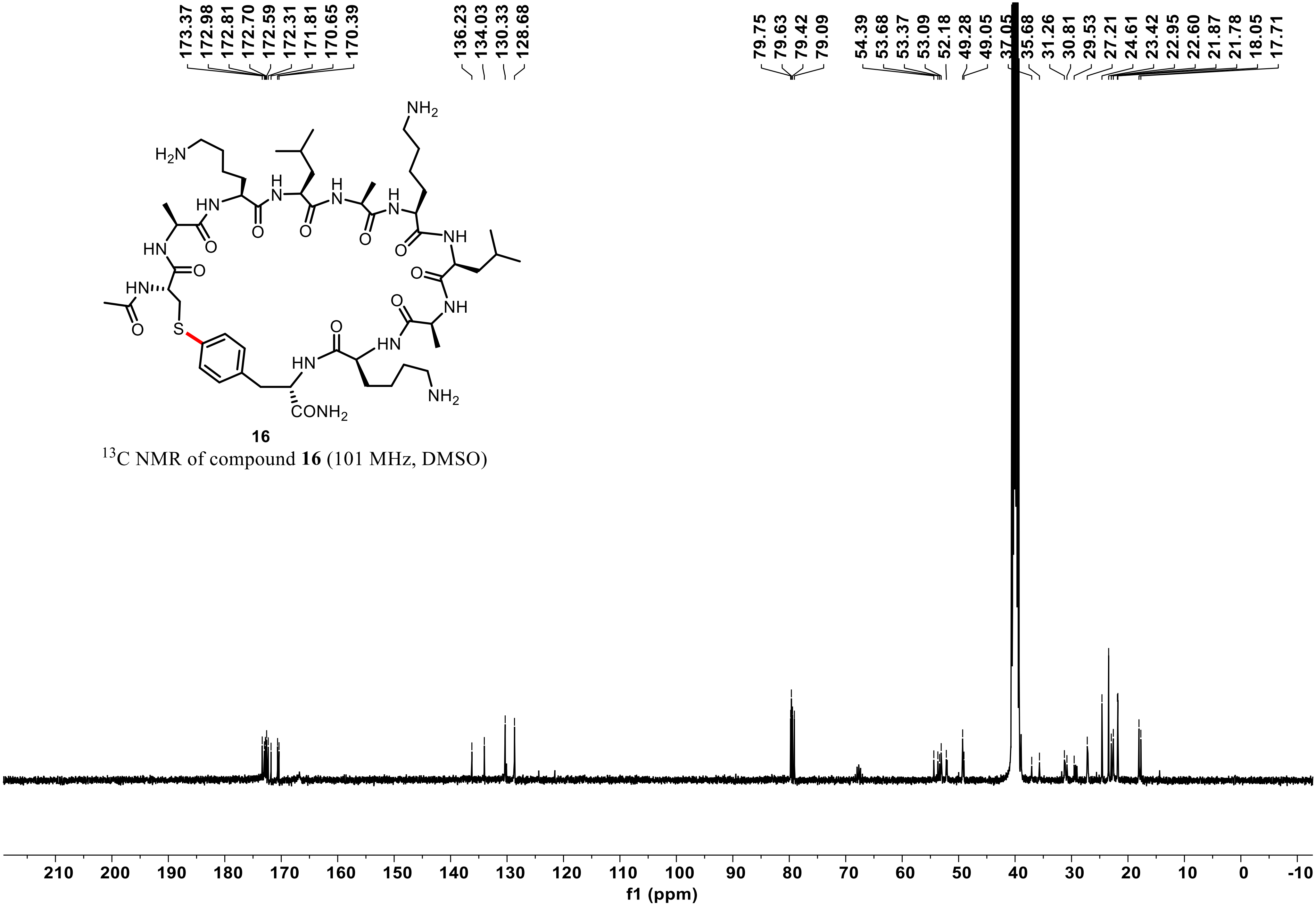
[1]H NMR of compound **S16** (400 MHz, 5%MeOD in DMSO-d_6)





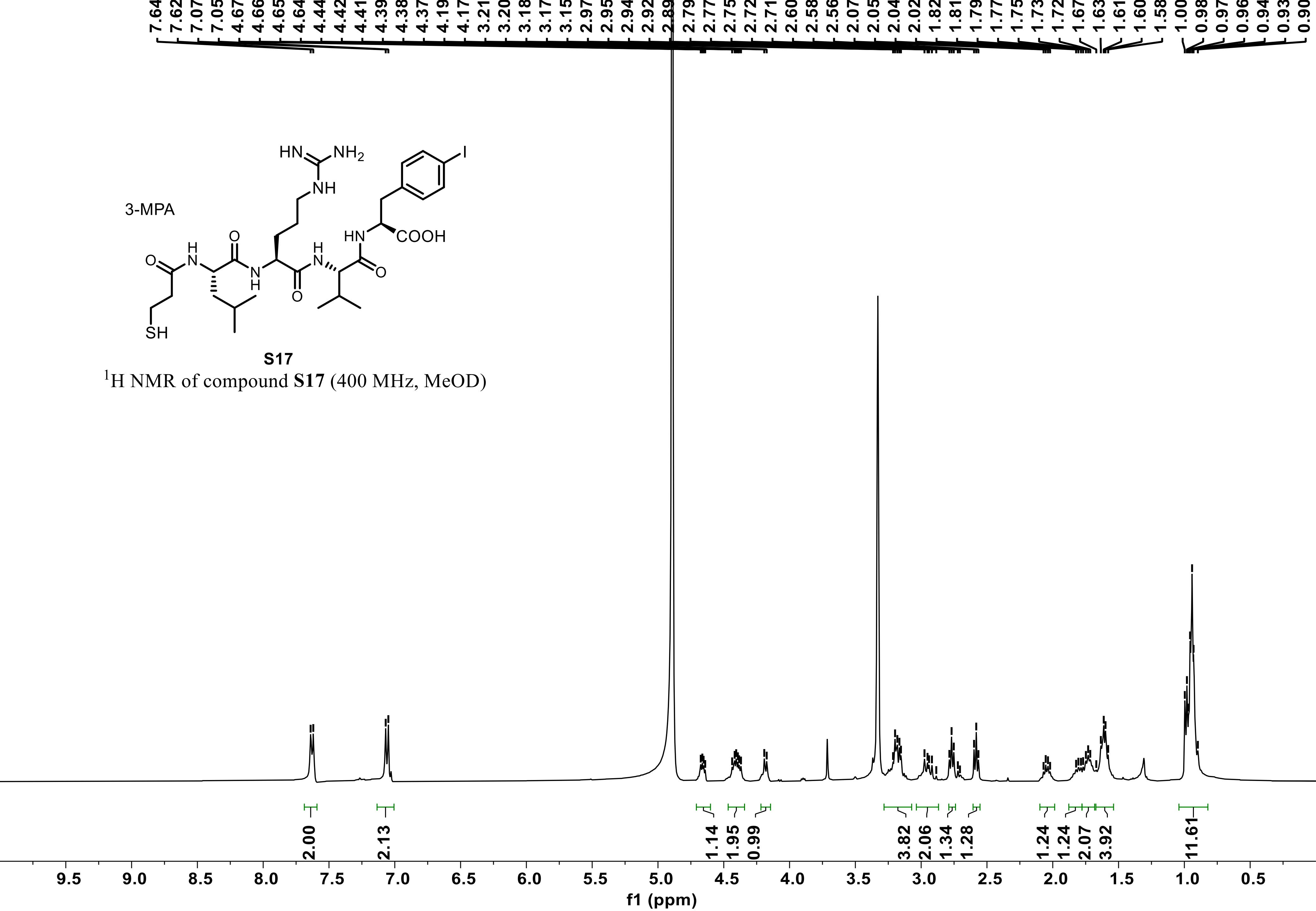
16

^{1}H NMR of compound **16** (400 MHz, MeOD)



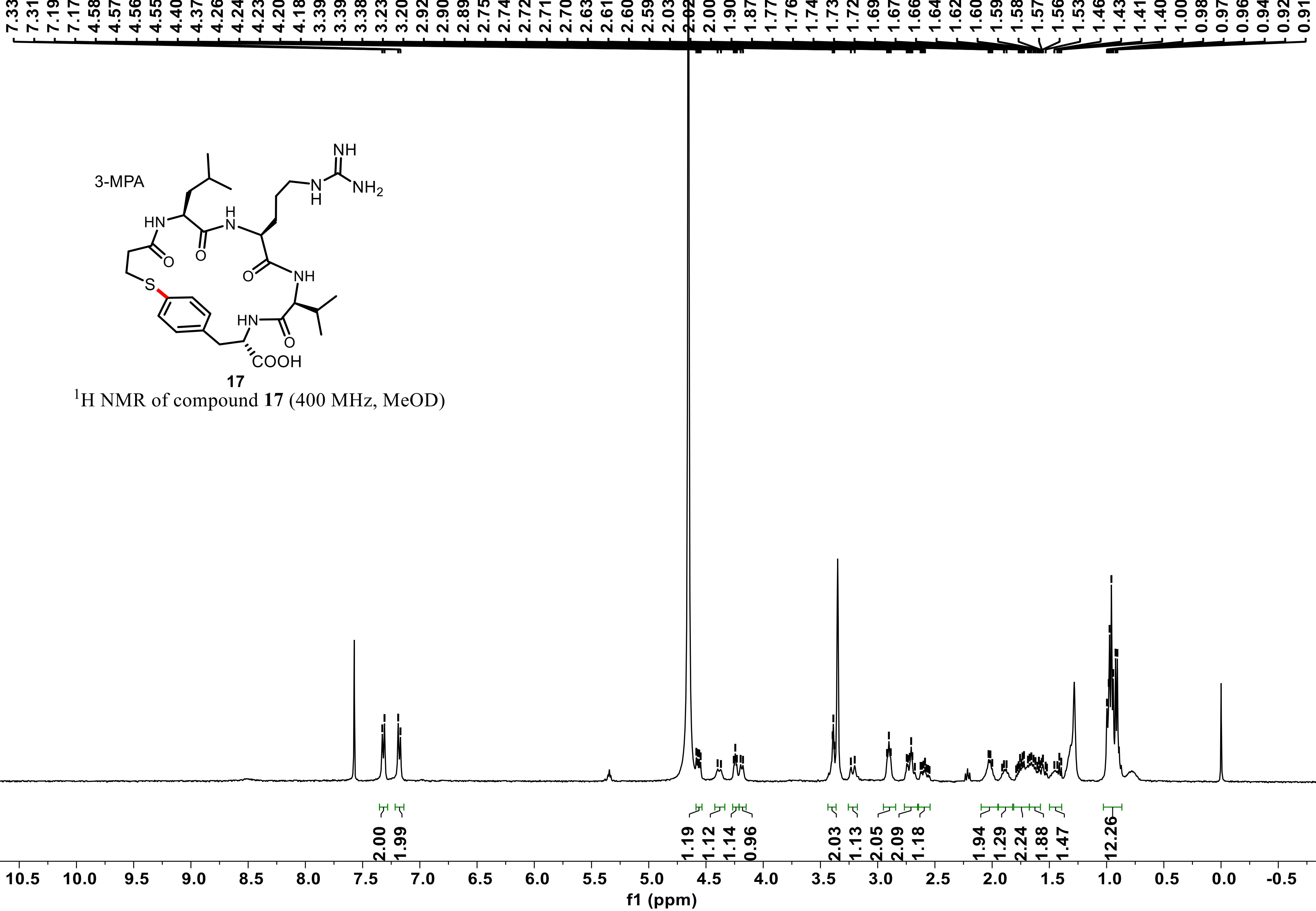
16

^{13}C NMR of compound **16** (101 MHz, DMSO)

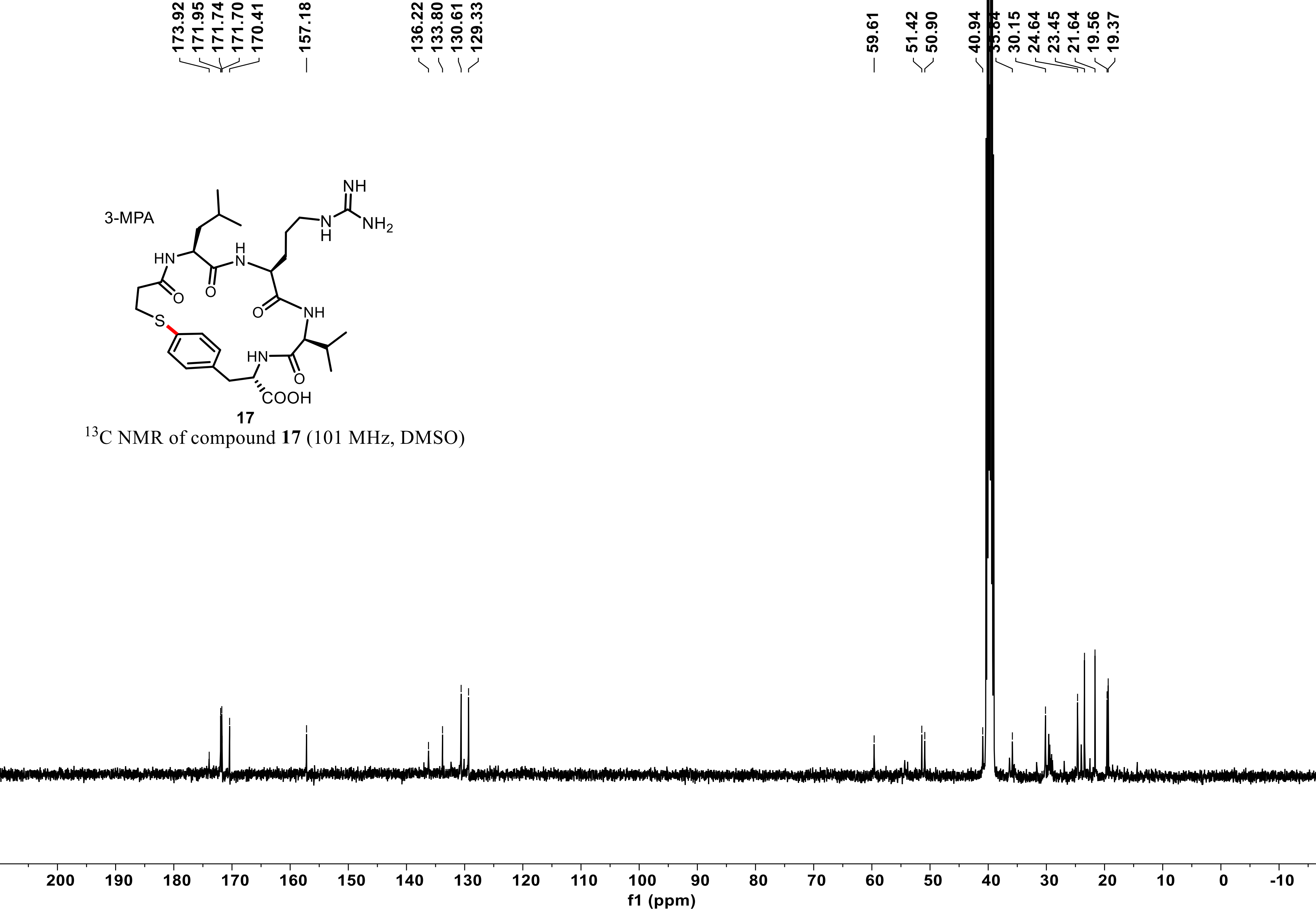


S17

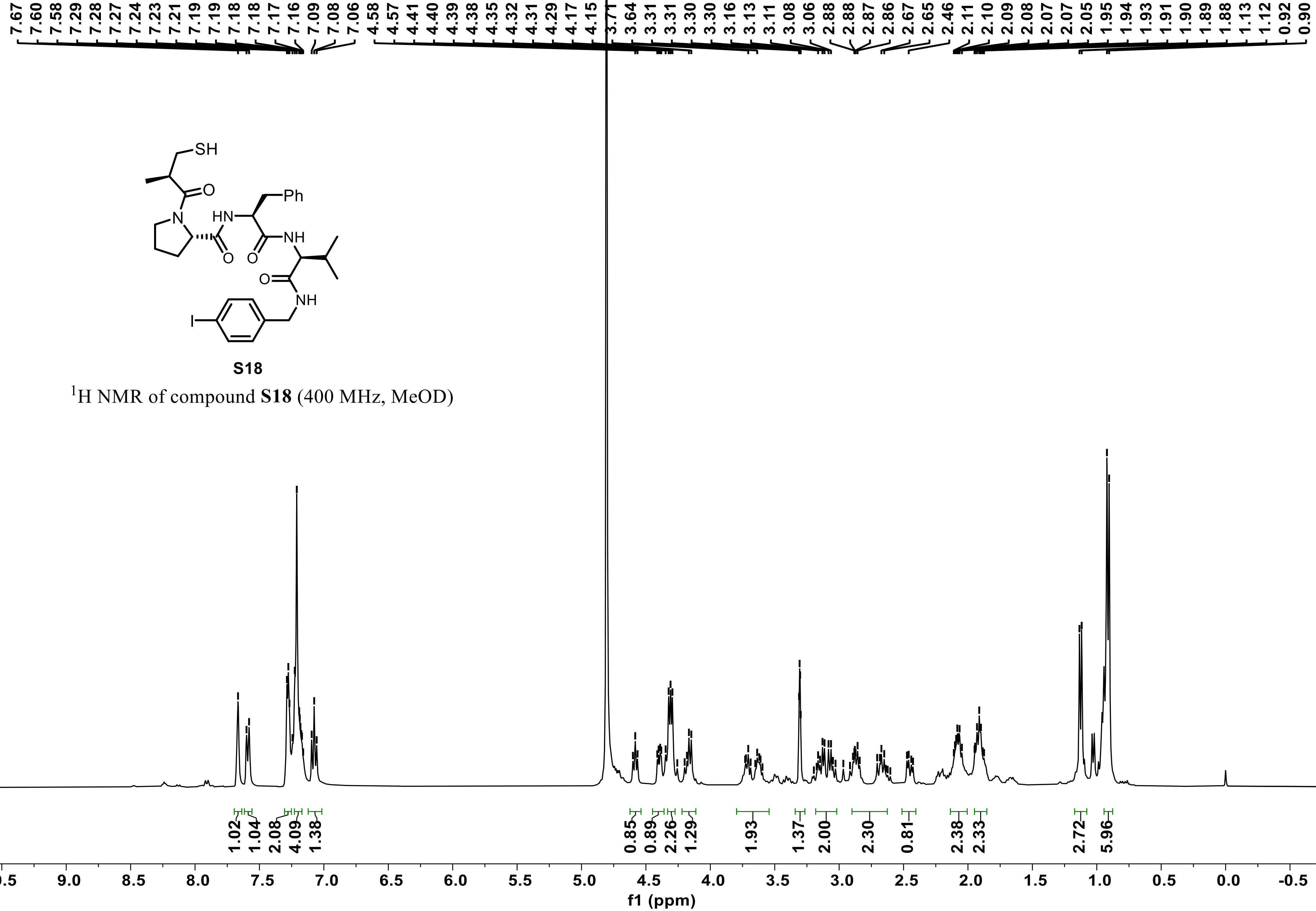
^{1}H NMR of compound **S17** (400 MHz, MeOD)



^{1}H NMR of compound **17** (400 MHz, MeOD)

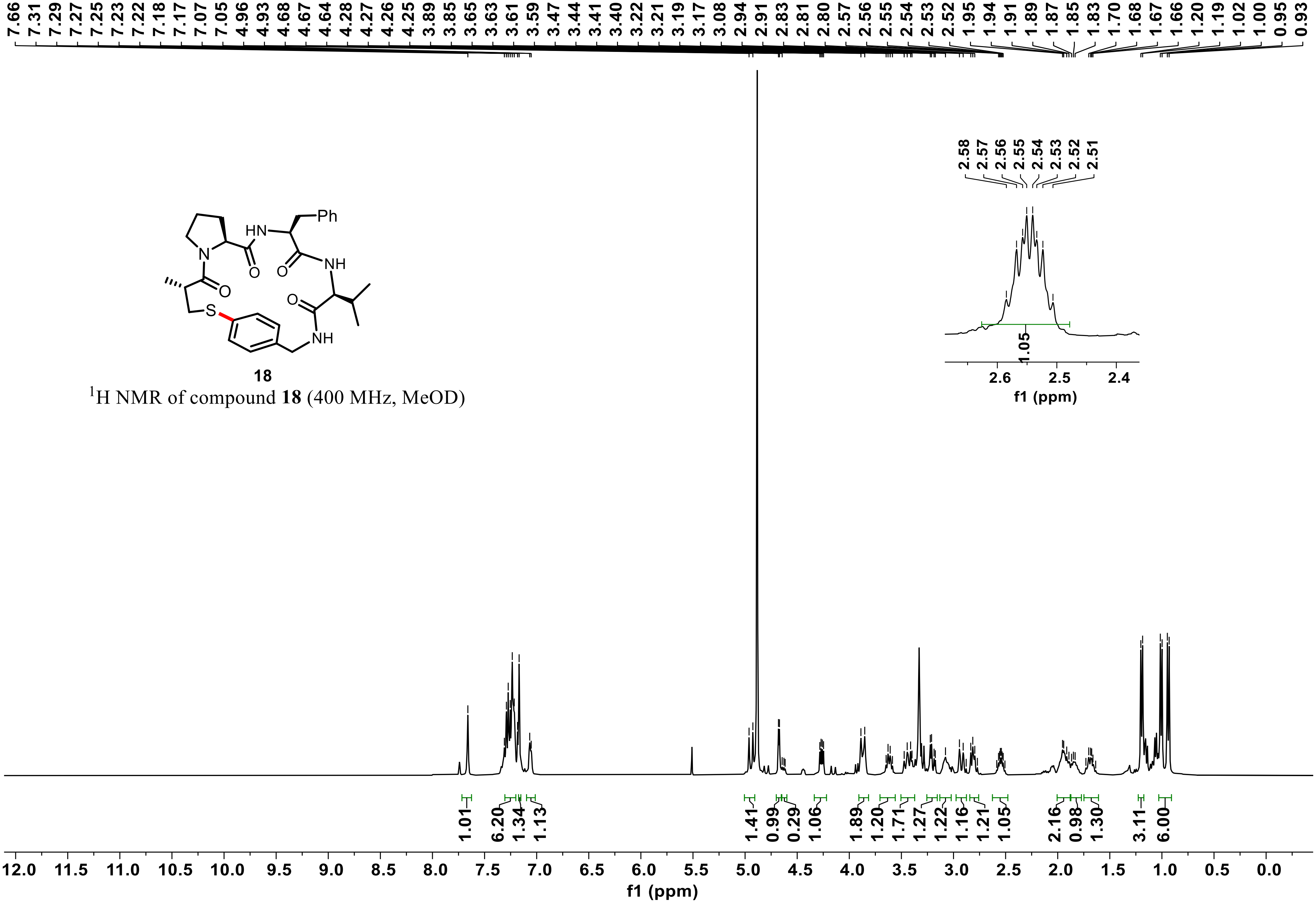


^{13}C NMR of compound **17** (101 MHz, DMSO)



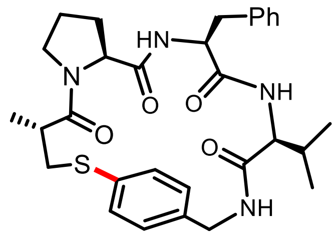
S18

^{1}H NMR of compound **S18** (400 MHz, MeOD)



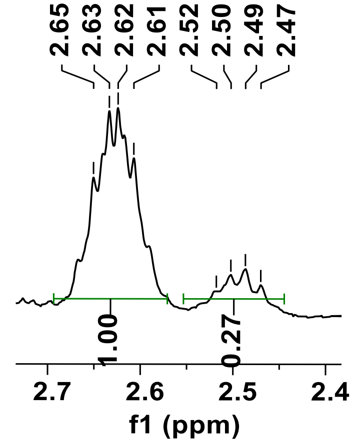
18

^{1}H NMR of compound **18** (400 MHz, MeOD)

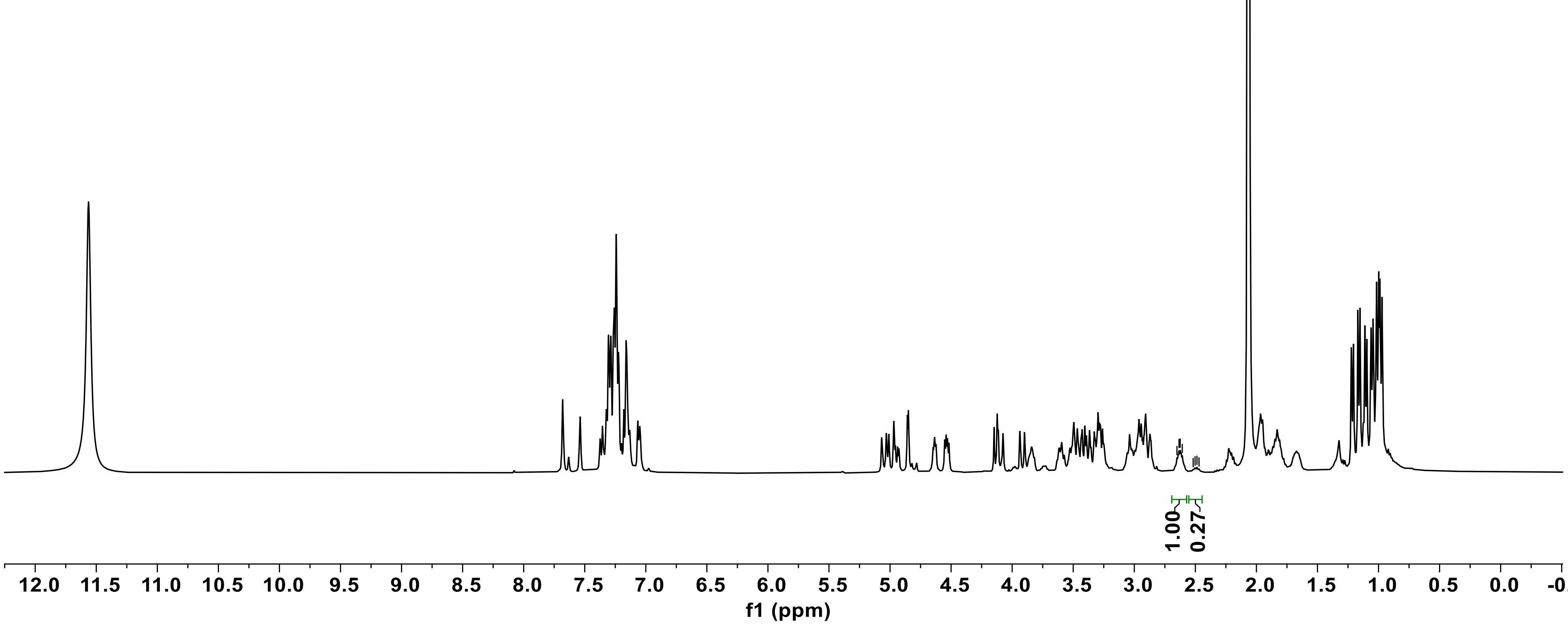


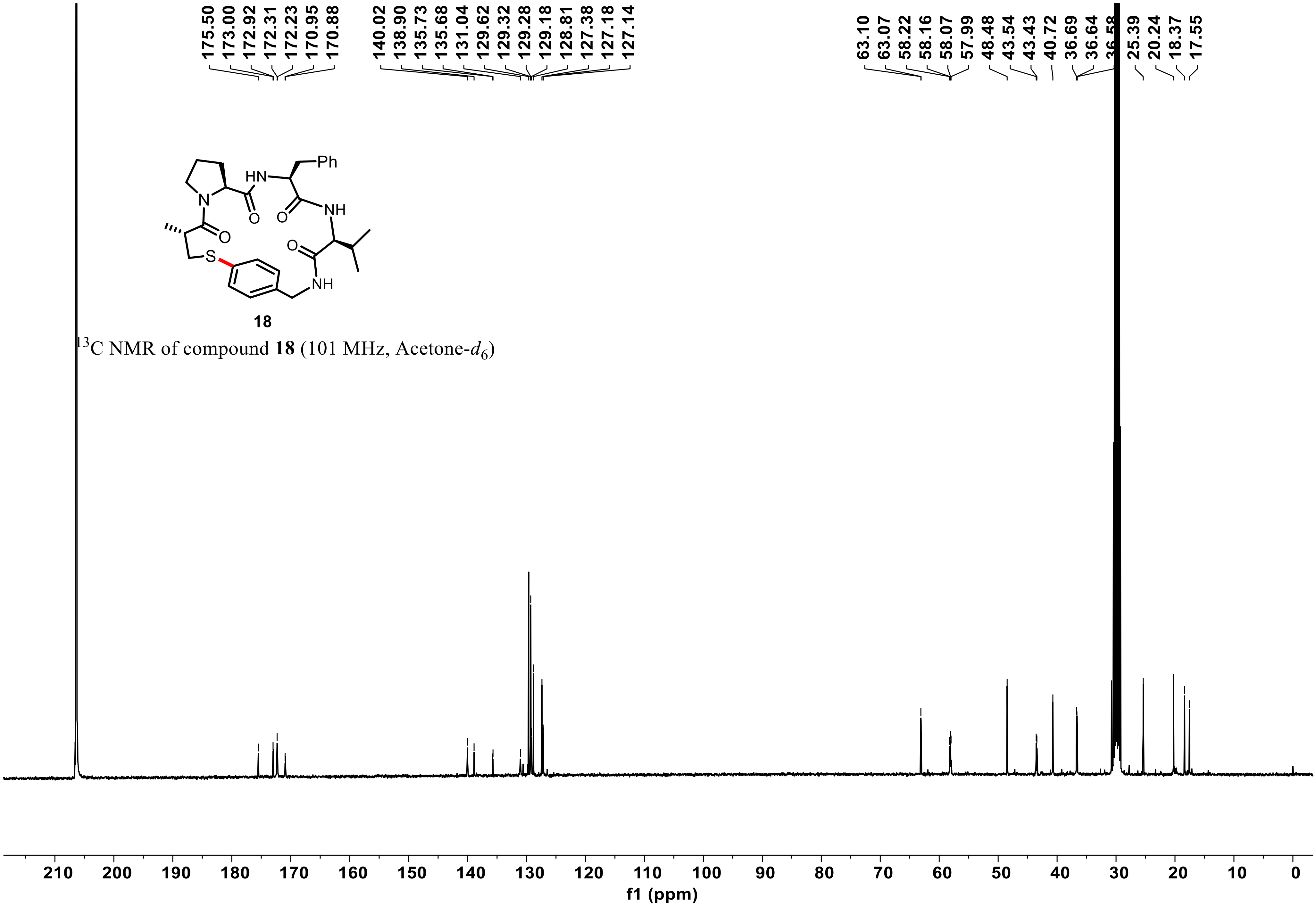
18

[1]H NMR of compound **18** (400 MHz, Acetone-d_6)



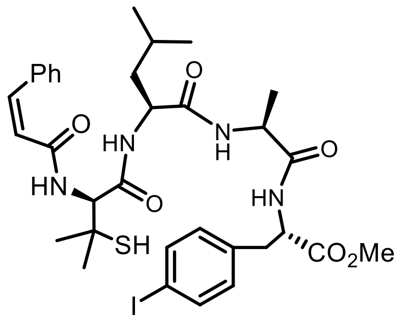
2.65
2.63
2.62
2.61
2.52
2.50
2.49
2.47





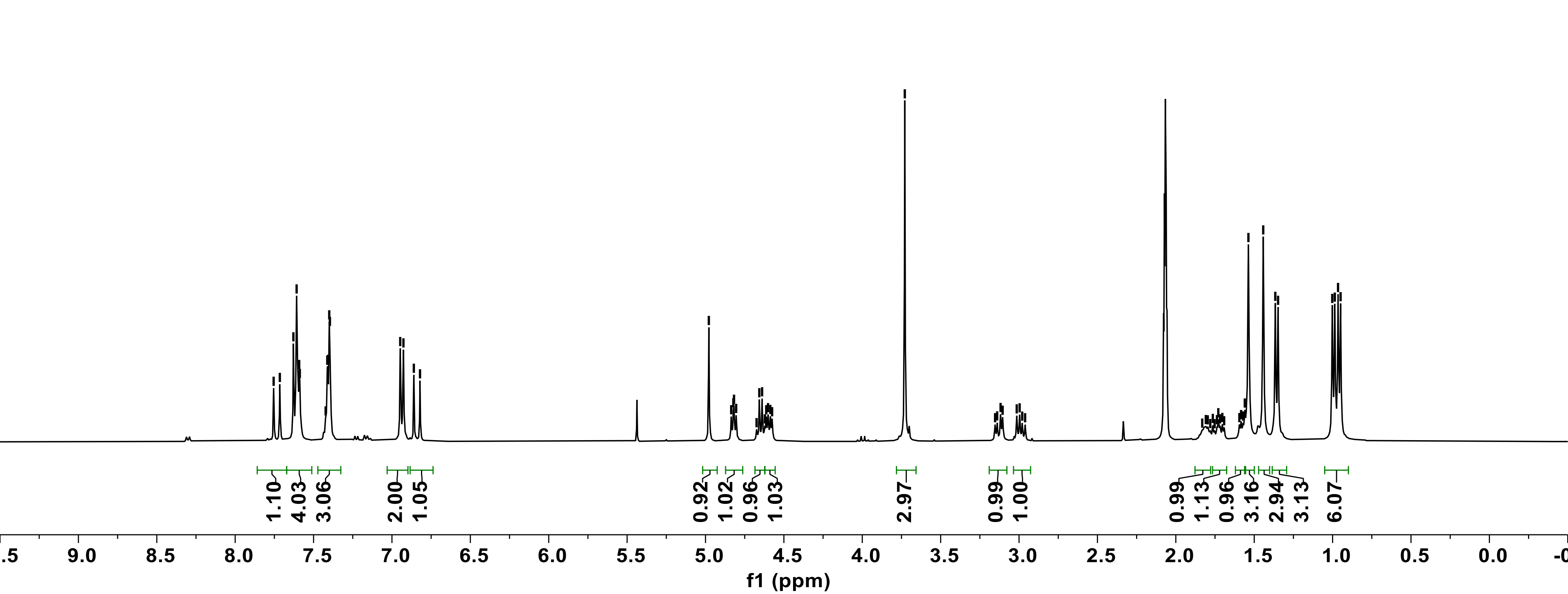
18

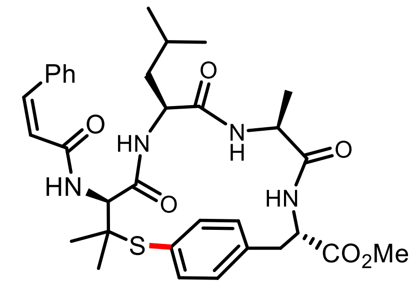
^{13}C NMR of compound **18** (101 MHz, Acetone-d_6)



S19

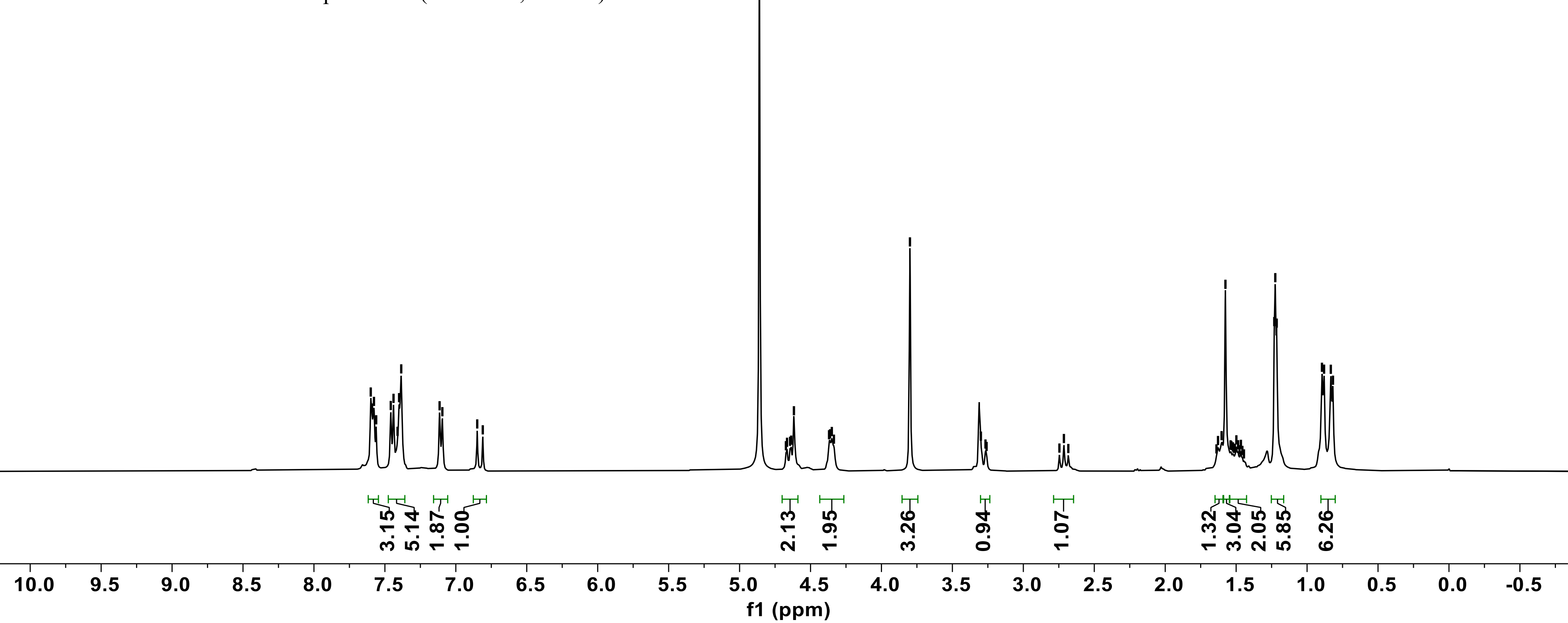
[1]H NMR of compound **S19** (400 MHz, Acetic Acid-d_4)

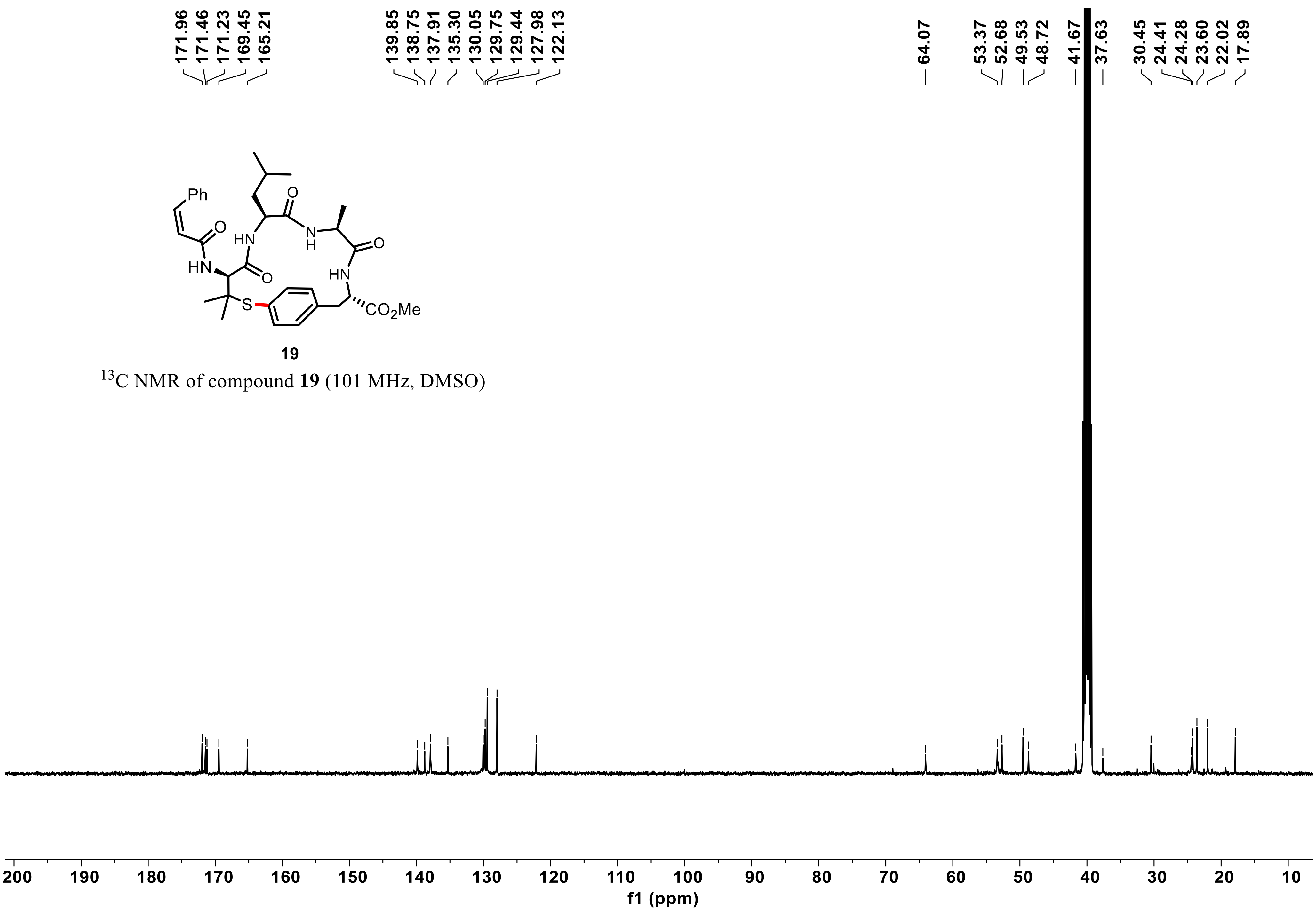




19

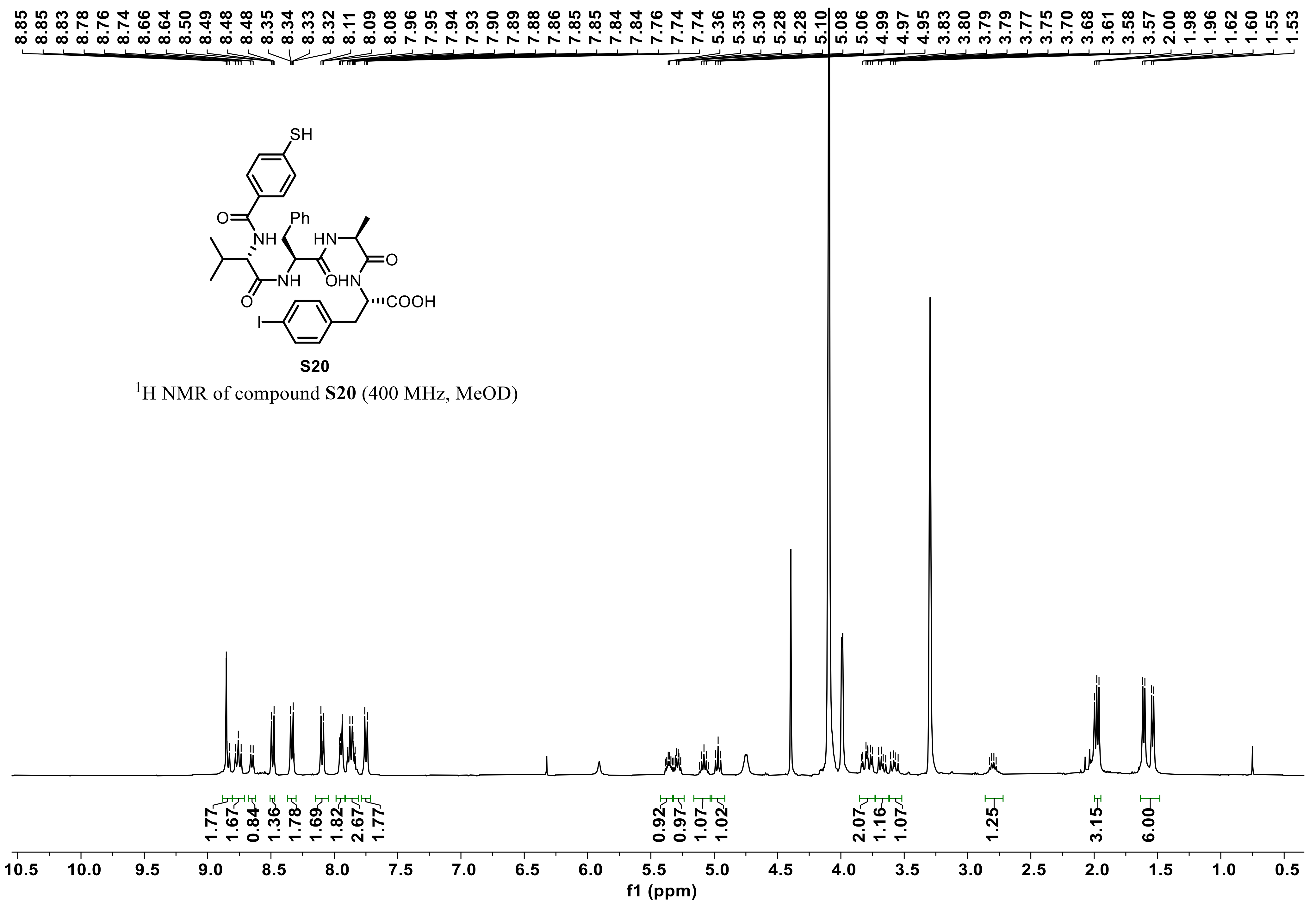
[1]H NMR of compound **19** (400 MHz, MeOD)





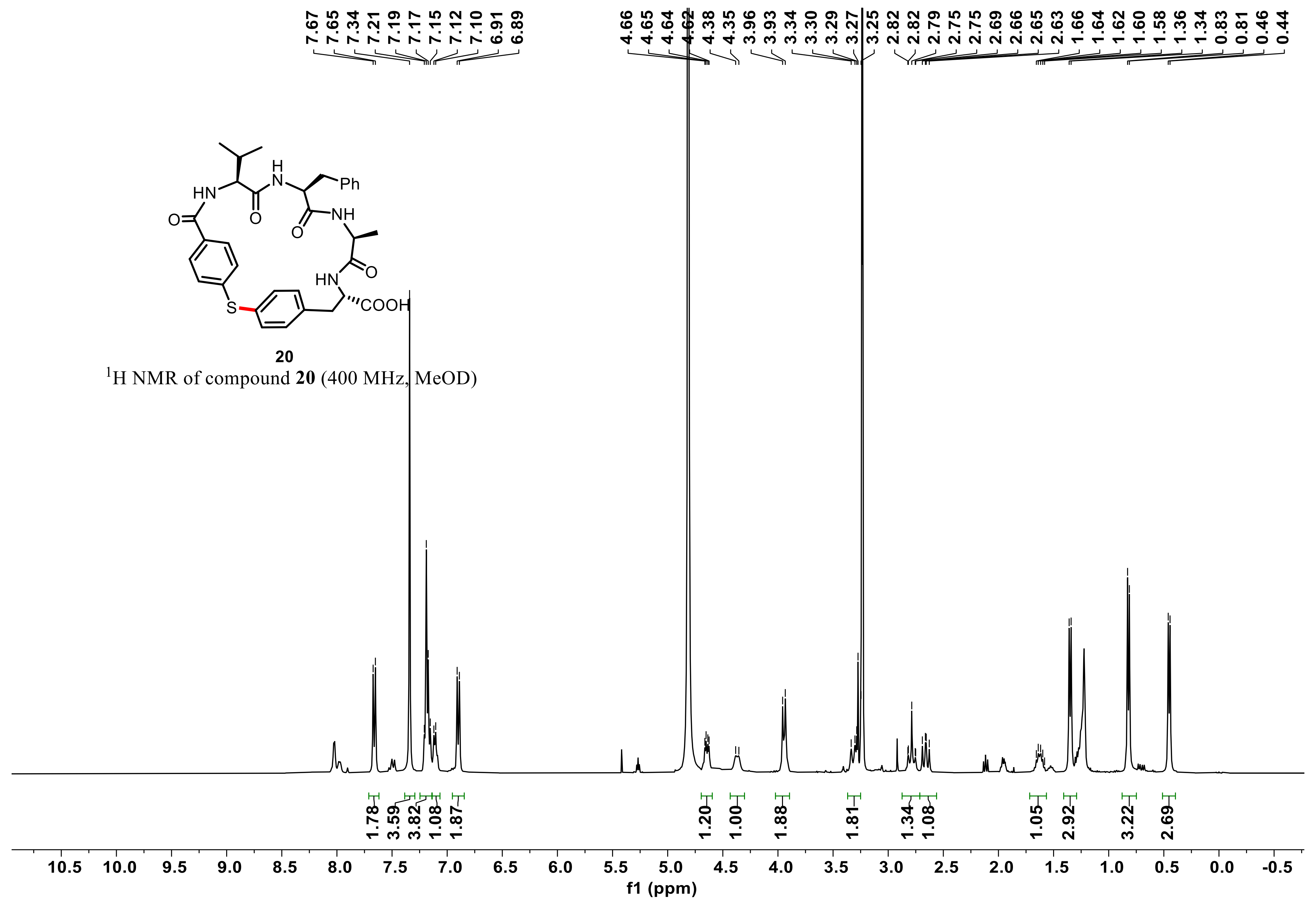
19

^{13}C NMR of compound **19** (101 MHz, DMSO)



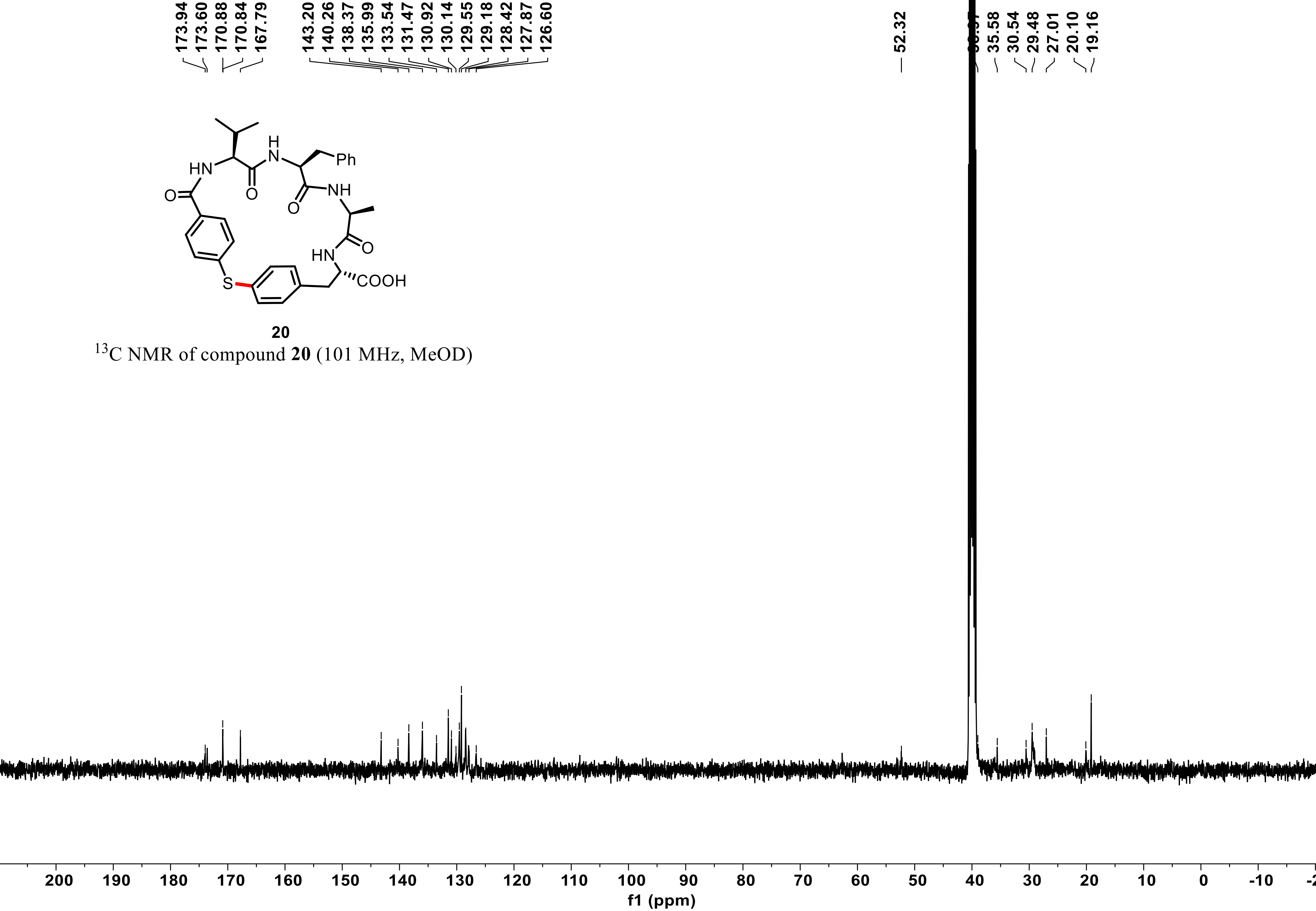
S20

^{1}H NMR of compound **S20** (400 MHz, MeOD)



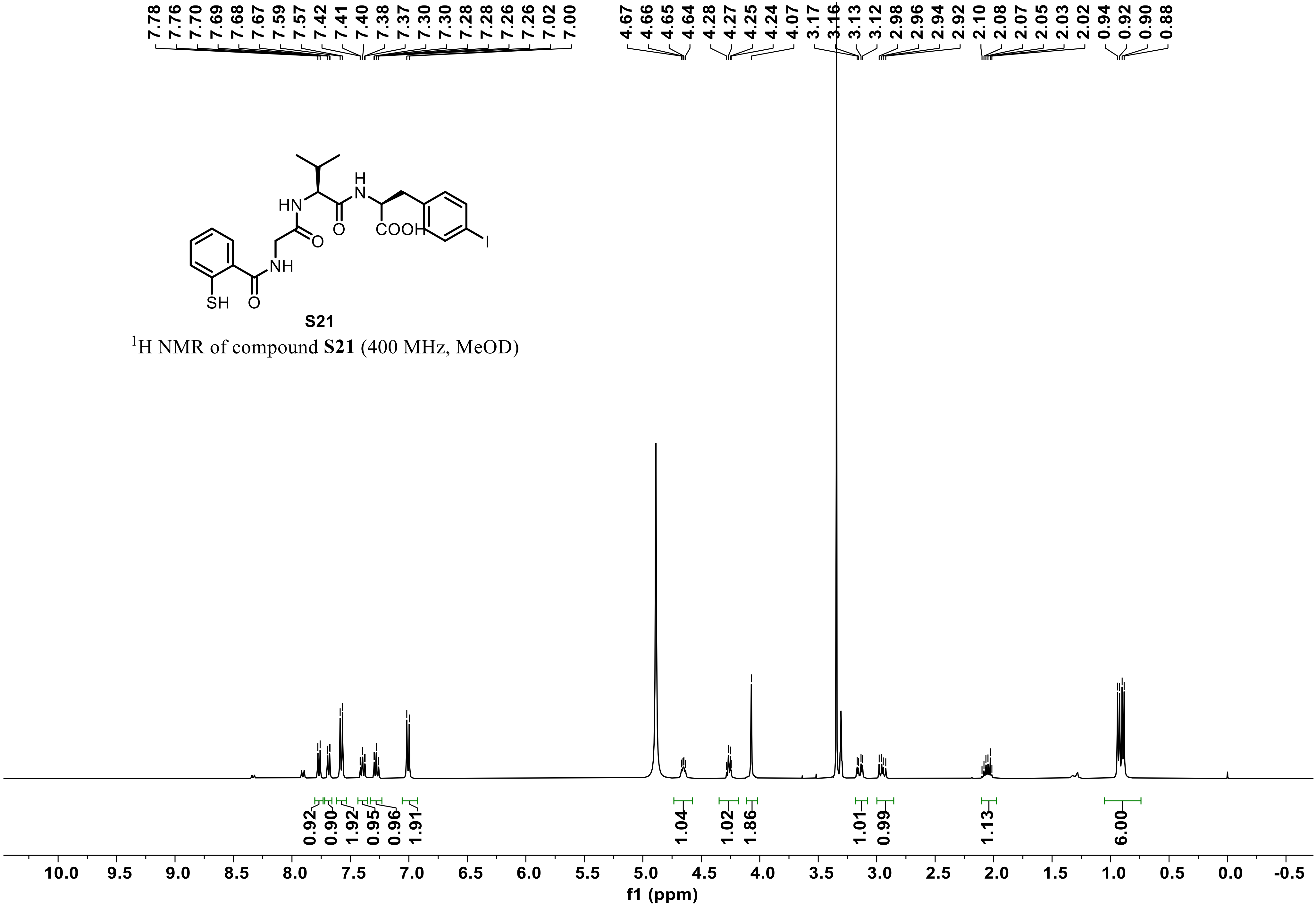
20

^{1}H NMR of compound **20** (400 MHz, MeOD)



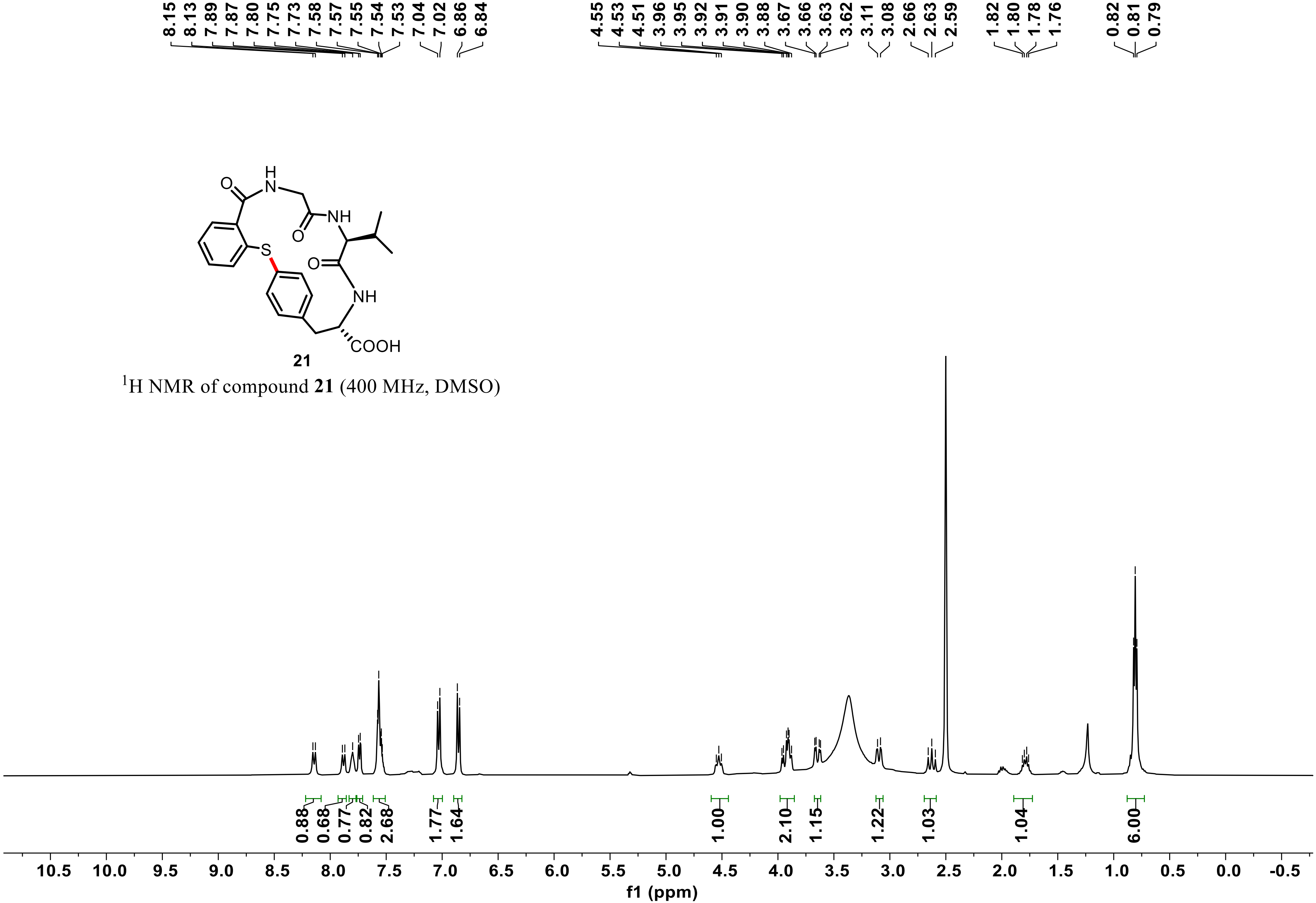
20

^{13}C NMR of compound **20** (101 MHz, MeOD)

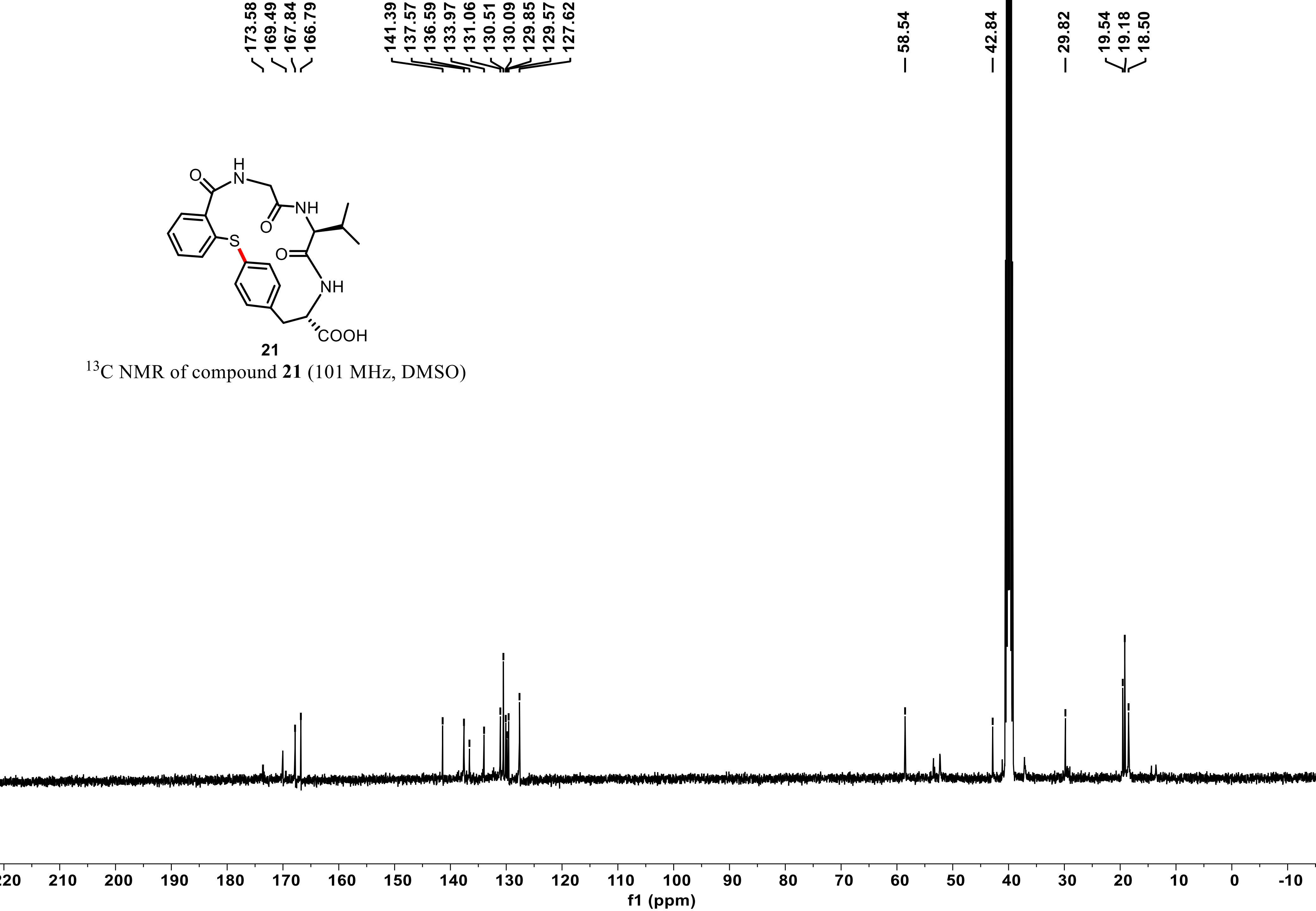


S21

[1]H NMR of compound **S21** (400 MHz, MeOD)

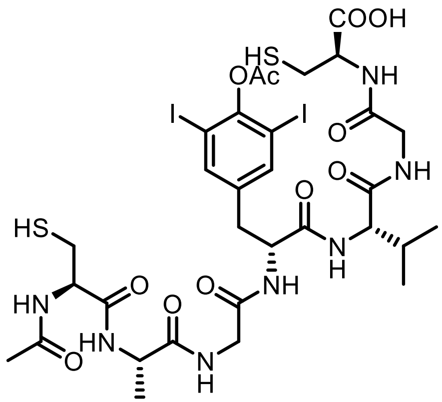


^{1}H NMR of compound **21** (400 MHz, DMSO)



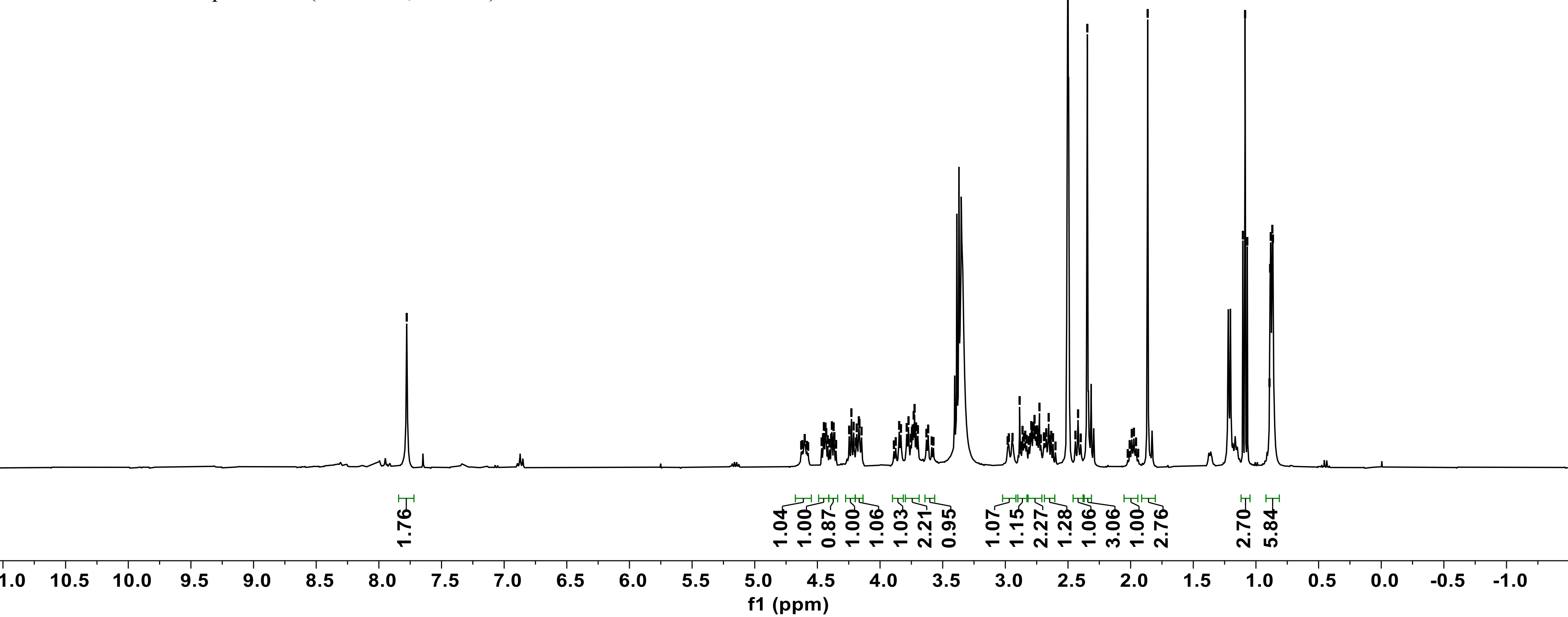
21

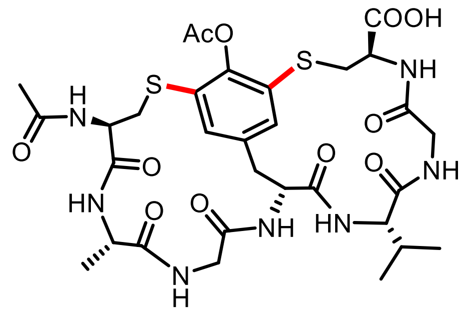
^{13}C NMR of compound **21** (101 MHz, DMSO)



22

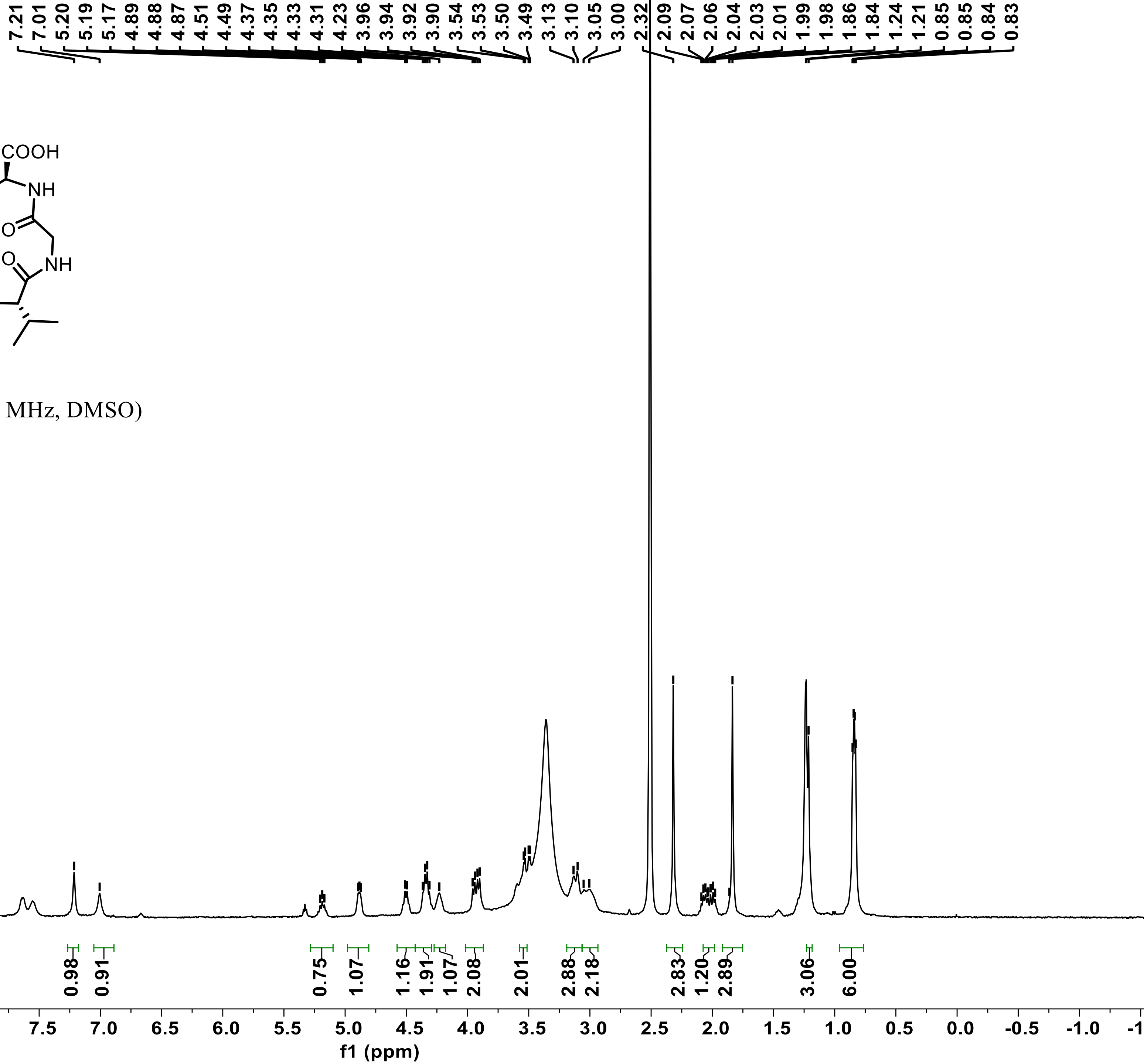
^{1}H NMR of compound **22** (400 MHz, DMSO)

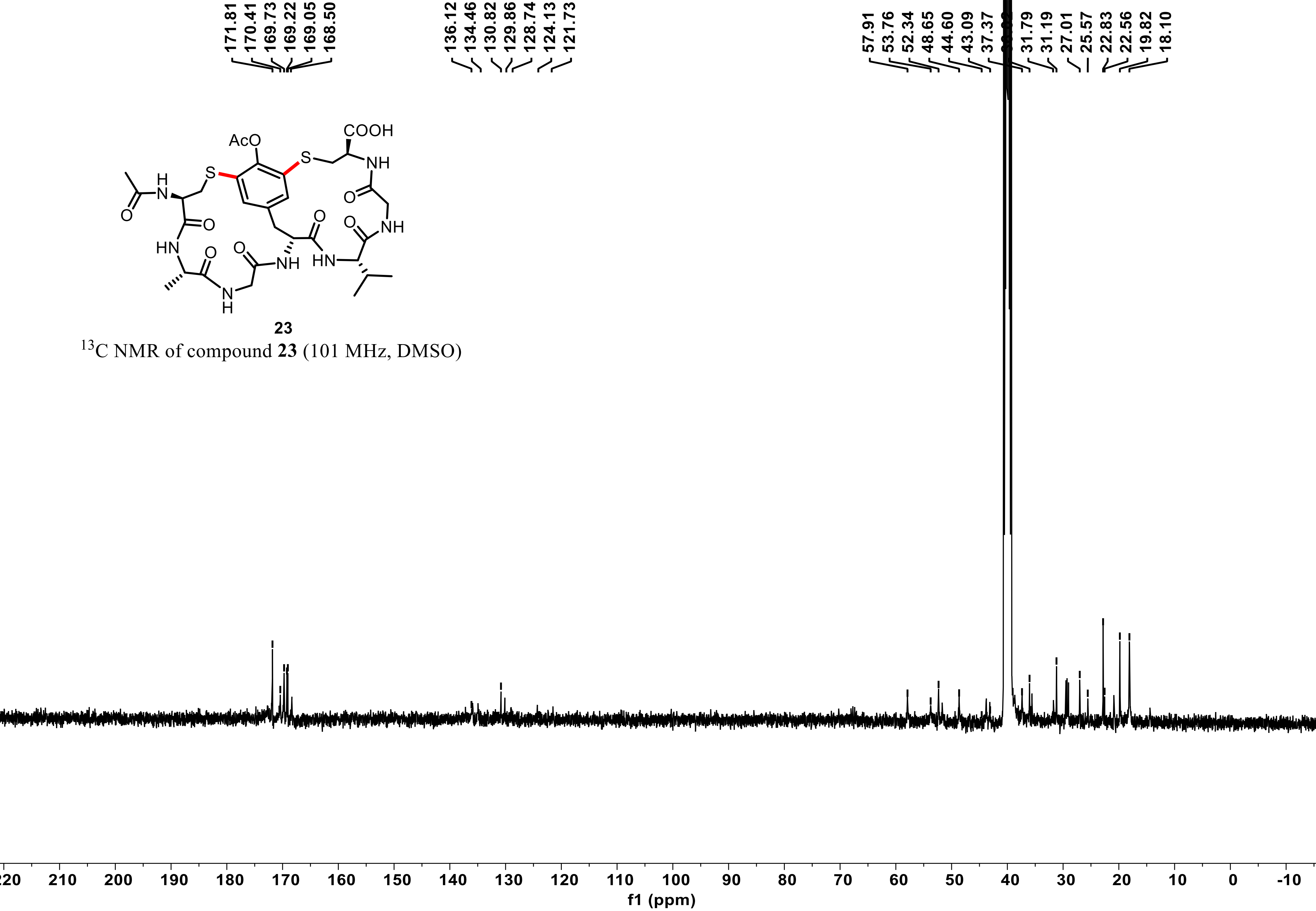




23

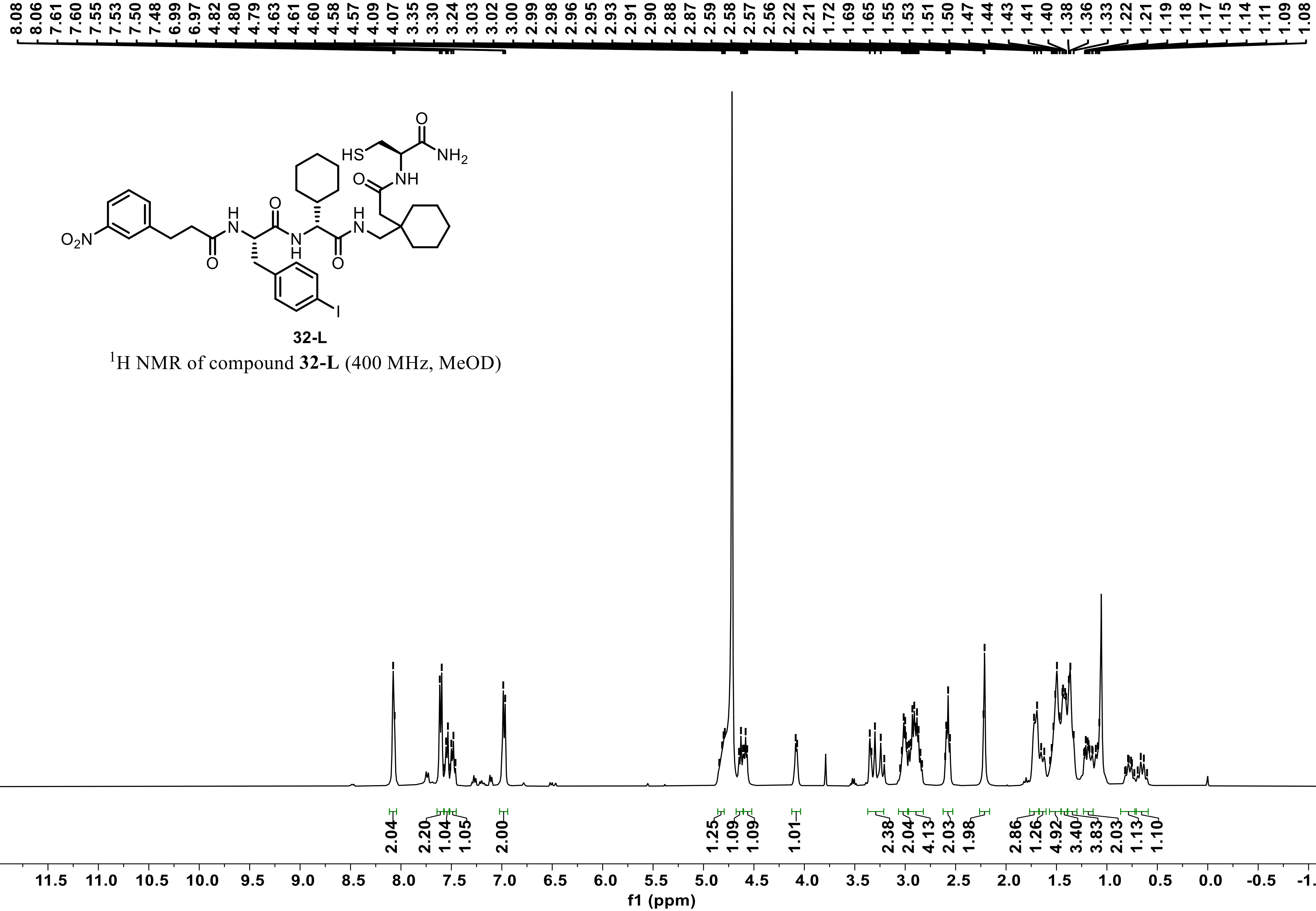
^{1}H NMR of compound **23** (400 MHz, DMSO)





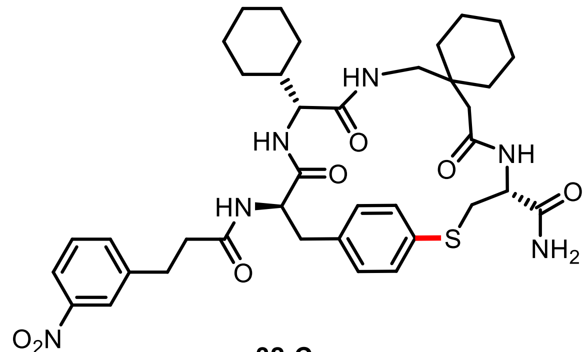
23

^{13}C NMR of compound **23** (101 MHz, DMSO)



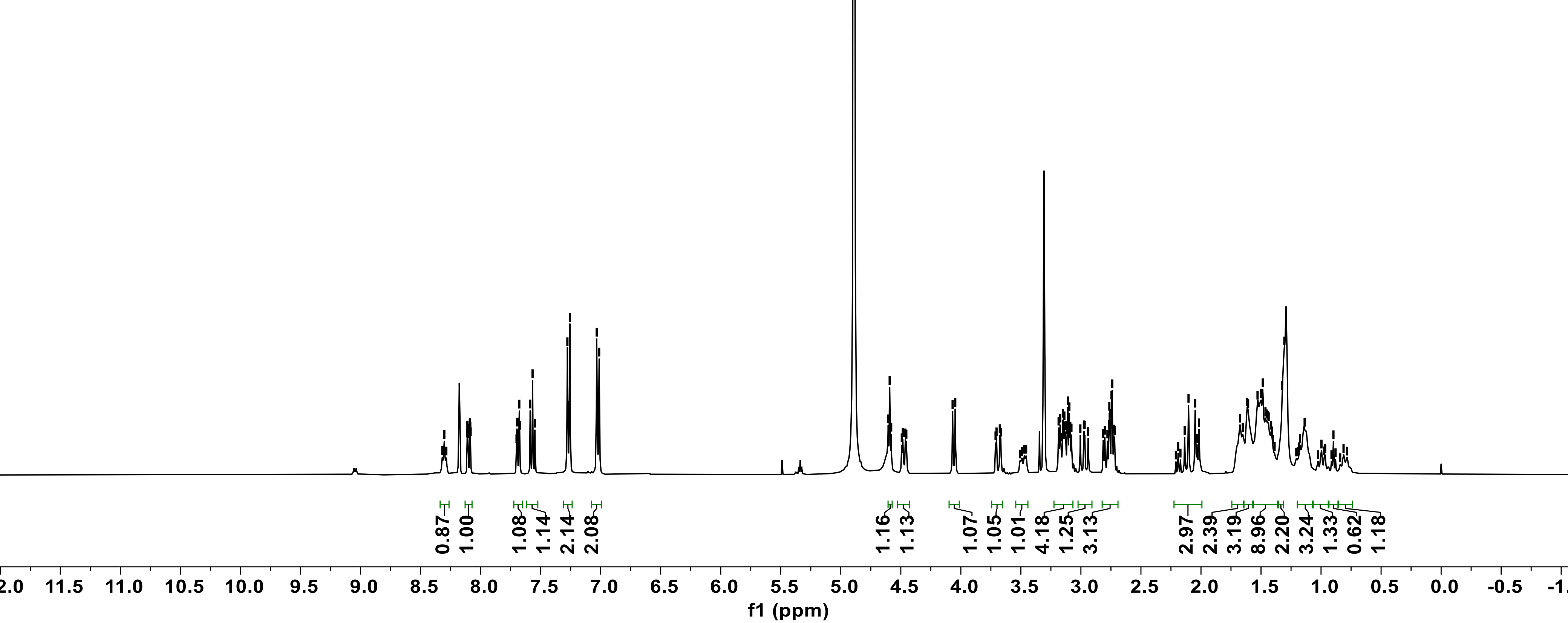
32-L

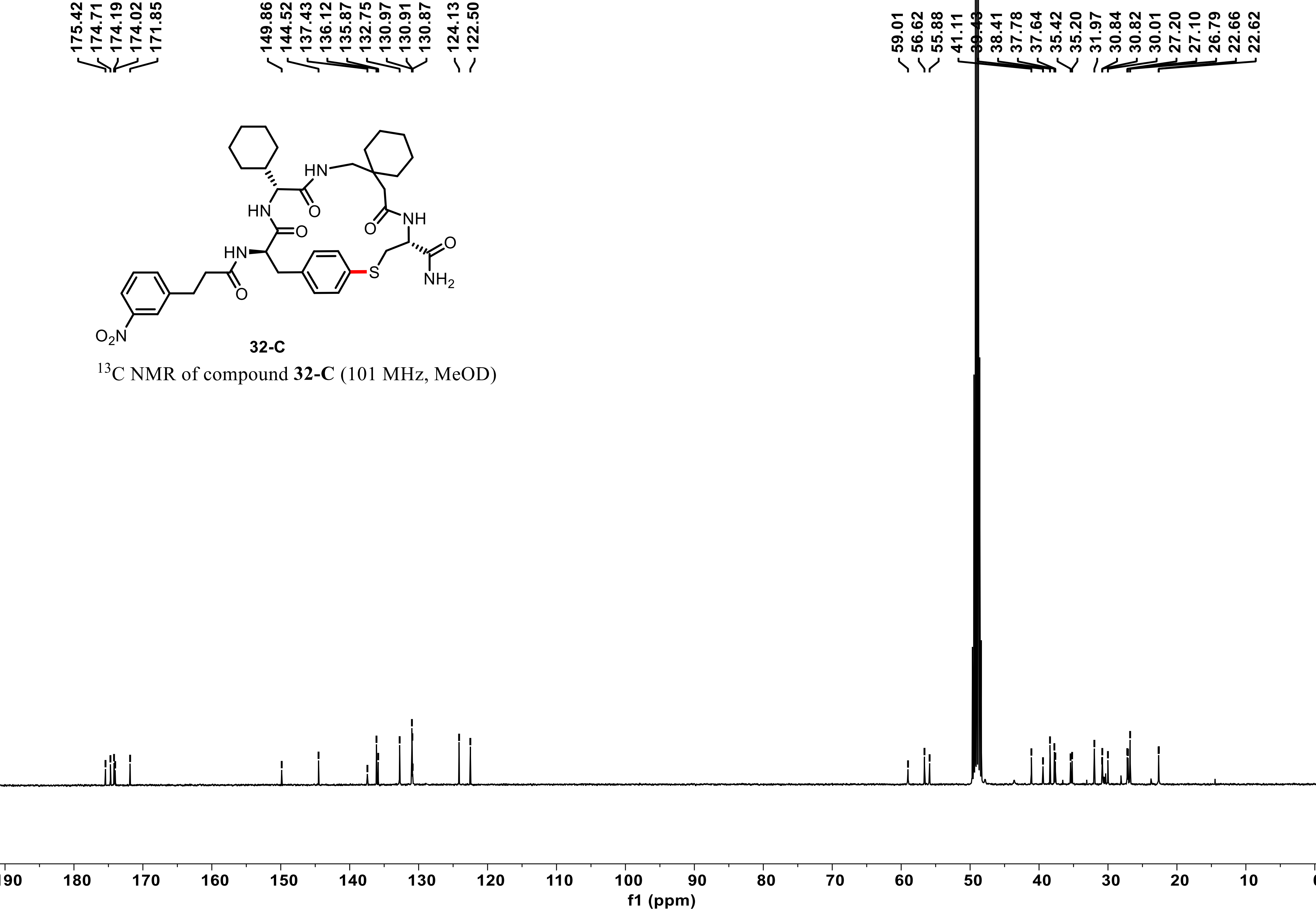
[1]H NMR of compound **32-L** (400 MHz, MeOD)



32-C

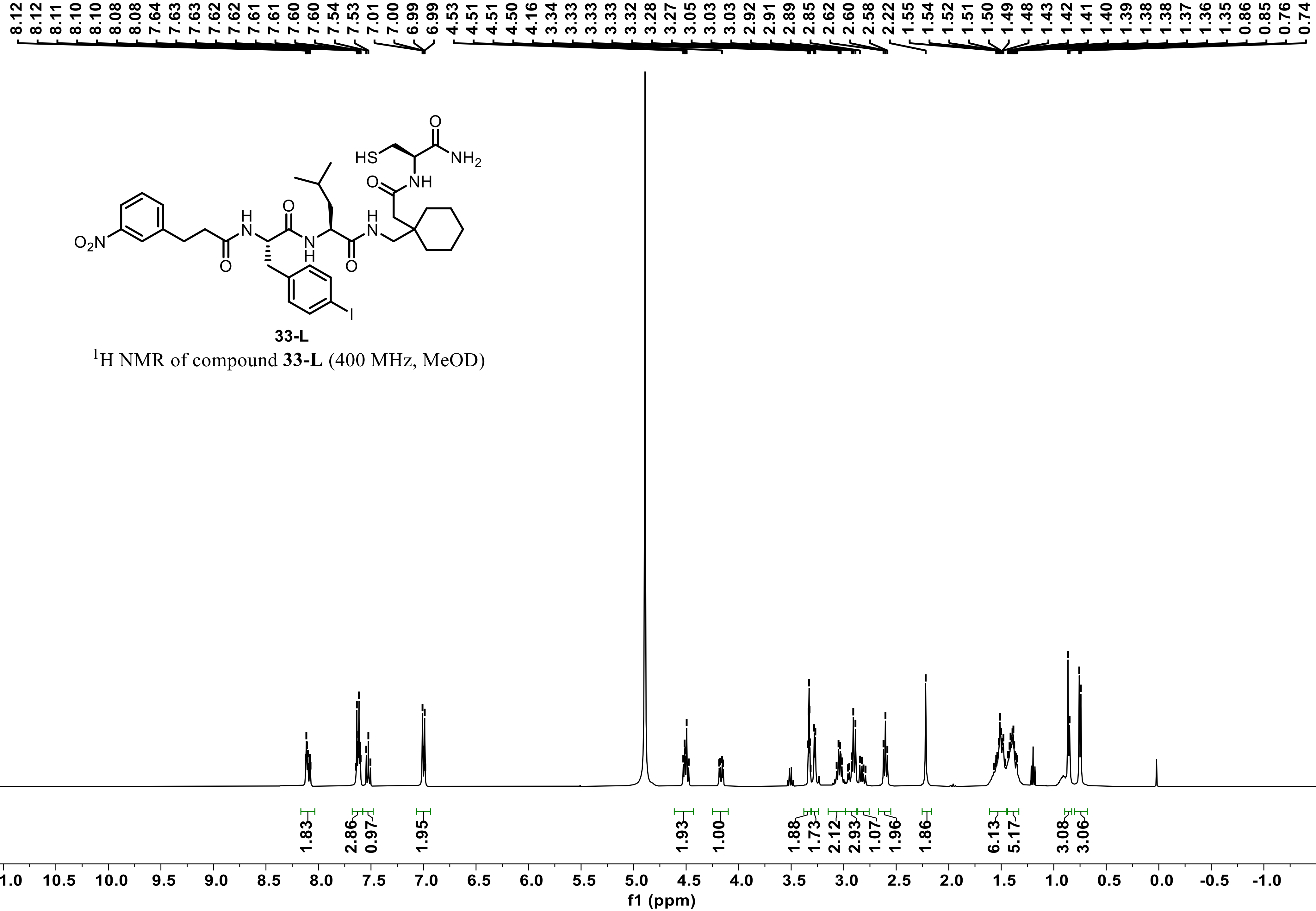
[1]H NMR of compound **32-C** (400 MHz, MeOD)





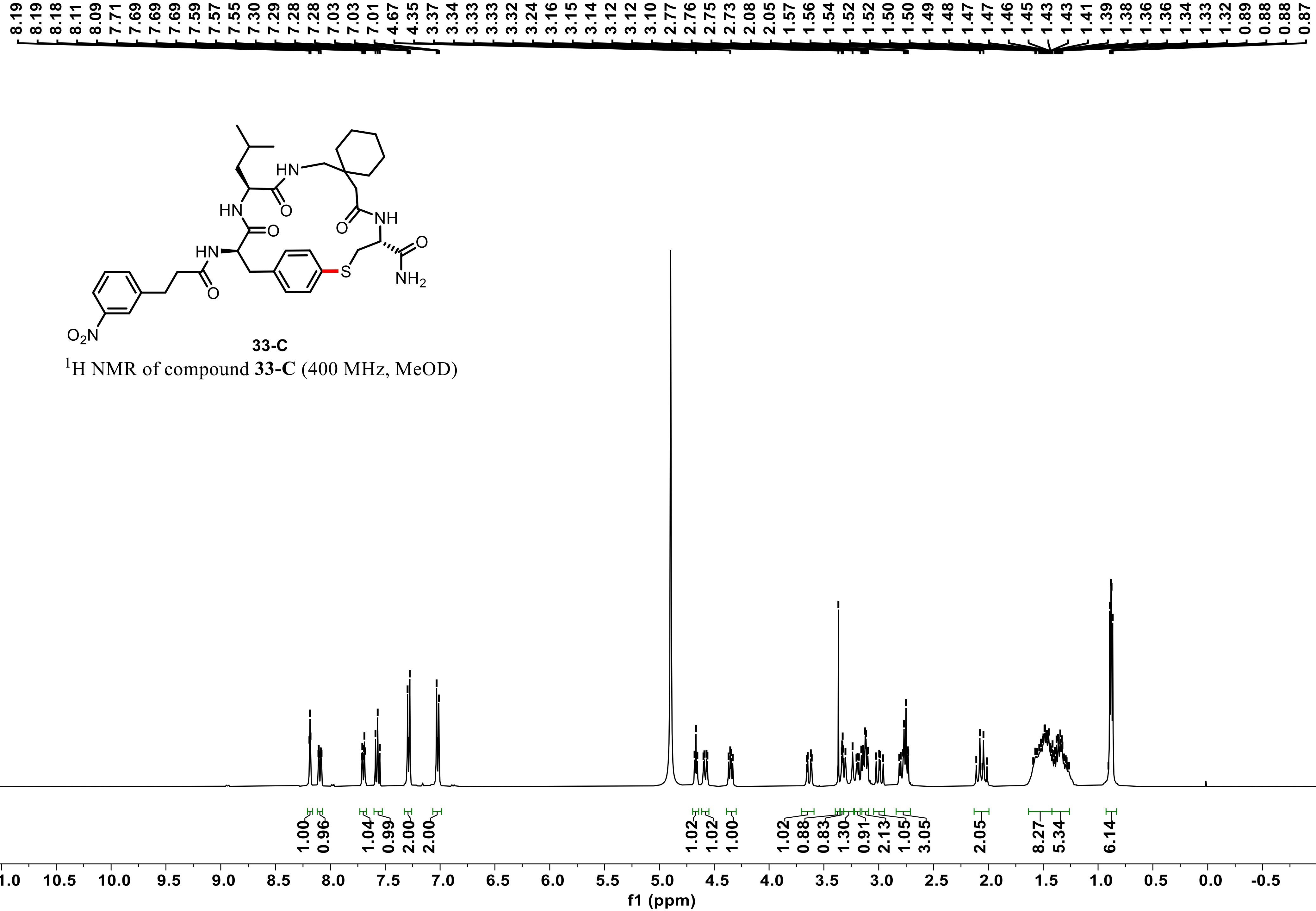
32-C

^{13}C NMR of compound **32-C** (101 MHz, MeOD)



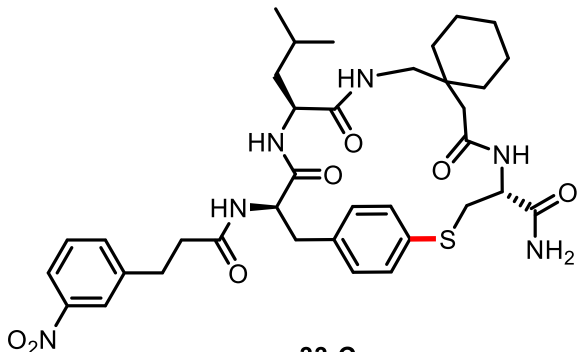
33-L

[1]H NMR of compound **33-L** (400 MHz, MeOD)



33-C

^{1}H NMR of compound **33-C** (400 MHz, MeOD)



33-C

^{13}C NMR of compound **33-C** (101 MHz, MeOD)