Electronic Supplementary Information

Total synthesis of potent anti-inflammatory natural product solomonamide A along with structural revision and biological activity evaluation

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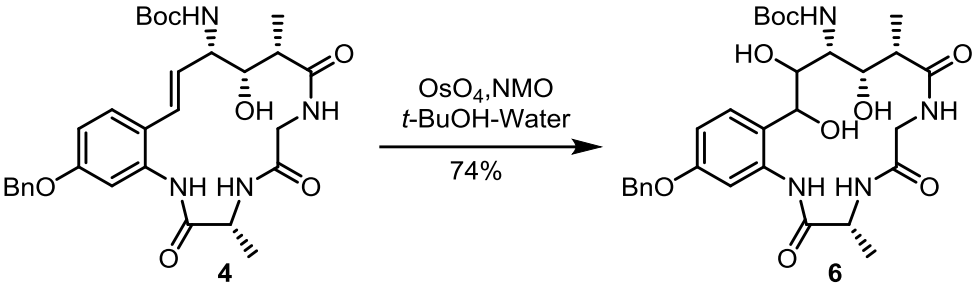
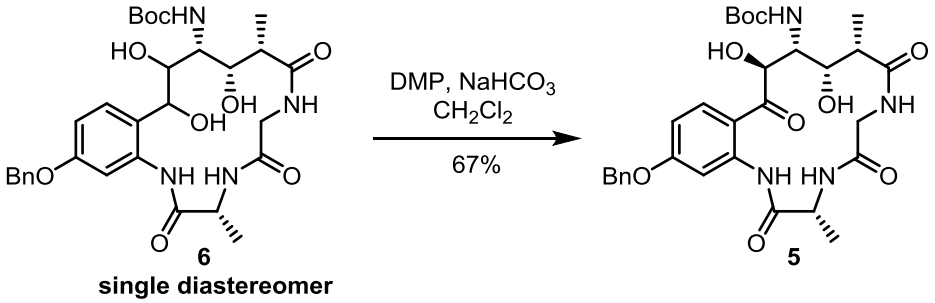
General:

All reactions were carried out in oven-dried glassware under a positive pressure of argon or nitrogen unless otherwise mentioned with magnetic stirring. Air sensitive reagents and solutions were transferred via syringe or cannula and were introduced to the apparatus *via* rubber septa. All reagents, starting materials, and solvents were obtained from commercial suppliers and used as such without further purification. Reactions were monitored by thin layer chromatography (TLC) with 0.25 mm pre-coated silica gel plates (60 F_{254}). Visualization was accomplished with either UV light, or by immersion in ethanolic solution of phosphomolybdic acid (PMA), *para*-anisaldehyde, 2,4-DNP stain, $KMnO_4$, Ninhydrin solution, Iodine adsorbed on silica gel followed by heating on a heat gun for ~15 sec. Column chromatography was performed on silica gel (100-200 or 230-400 mesh size). Deuterated solvents for NMR spectroscopic analyses were used as received. All ^{1}H NMR and ^{13}C NMR spectra were obtained using a 400 MHz, or 500 MHz spectrometer. Coupling constants were measured in Hertz. All chemical shifts were quoted in ppm, relative to DMSO and MeOD using the residual solvent peak as a reference standard. The following abbreviations were used to explain the multiplicities: s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet, br = broad. HRMS (ESI) were recorded on ORBITRAP mass analyzer (Thermo Scientific, Q Exactive). Infrared (IR) spectra were recorded on a FT-IR spectrometer as a thin film. Chemical nomenclature was generated using ChemBioDraw. Melting points of solids were measured in Buchi B-540 melting point apparatus. Optical rotation values were recorded on P-2000 polarimeter at 589 nm.

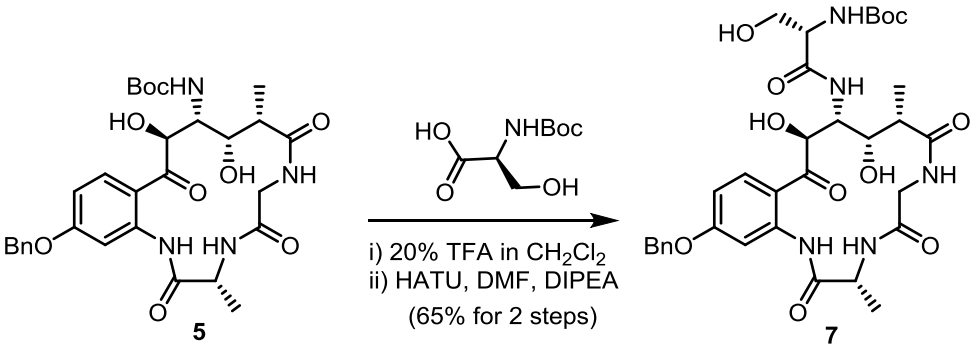
Experimental procedures:



***tert*-Butyl ((3*R*,9*S*,10*S*,11*R*)-16-(benzyloxy)-10,12,13-trihydroxy-3,9-dimethyl-2,5,8-trioxo-2,3,4,5,6,7,8,9,10,11,12,13-dodecahydro-1H-benzo[h][1,4,7]triazacyclopentadecin-11-yl)carbamate (6)[1]:** To a solution of compound **4** (175 mg, 0.308 mmol) in *t*-BuOH-H_2O (2 ml, 1:1),NMO (54.2 mg, 0.463 mmol) and OsO_4 (94 µL, 2.5 % solution in *t*-BuOH) was added at 0 °C and stirred for 6 h. After completion of reaction *t*-BuOH was removed under vacuum, reaction mixture was diluted with EtOAc (5 mL) washed with saturated sodium sulfite solution (4 mL) and brine (4 ml). Organic layer was separated, dried under vacuum. Purification by column chromatography (silica gel 230-400 mesh 4% methanol - CH_2Cl_2) yielded compound **6** (138 mg, 74%) as white solid as single diastereomer. Mp = 121 - 123 °C; $[\alpha]_D^{22}$ - 26.23 (*c* 0.81, CH_3OH); IR υ_{max}(film): cm^{-1} 3646, 3282, 2926, 1626, 1528, 1453;^{1}H NMR (400 MHz, DMSO-d_6): δ 9.89 (brs, 1H), 8.16 (brs, 1H), 7.45 - 7.31 (m, 7H), 6.87 - 6.85(d, *J* = 3.7 Hz, 1H), 5.07 (s, 2H), 5.03–5.01 (m, 1H), 4.71 (brs, 1H), 4.61 (d, *J* = 3.7 Hz, 1H), 4.54 (brs, 1H), 4.41 (brs, 1H), 4.10 (d, *J* = 6.71, 1H), 4.06 (d, *J* = 6.1 Hz, 1H), 3.97 (brs, 1H), 3.83 (d, *J* = 7.9 Hz, 1H), 3.71(d, *J* = 6.10 Hz, 1H), 3.63 - 3.59 (m, 2H), 3.26 (d, *J* = 12.2 Hz, 1H), 2.29 - 2.22 (m, 1H), 1.40 (s, 9H), 1.30 (d, *J* = 6.7 Hz, 3H), 0.98 (d, *J* = 6.1 Hz, 3H); ^{13}C NMR (100 MHz, CD_3OD): δ 178.3, 172.2, 159.8, 158.3, 138.7, 129.6, 129.0, 128.7, 81.5, 78.1, 71.2, 63.4, 59.1, 45.4, 28.9, 19.0, 14.5; HRMS calculated for $C_{30}H_{40}O_9N_4Na$ $[M+Na]^+$: 623.2679, found 623.2687.



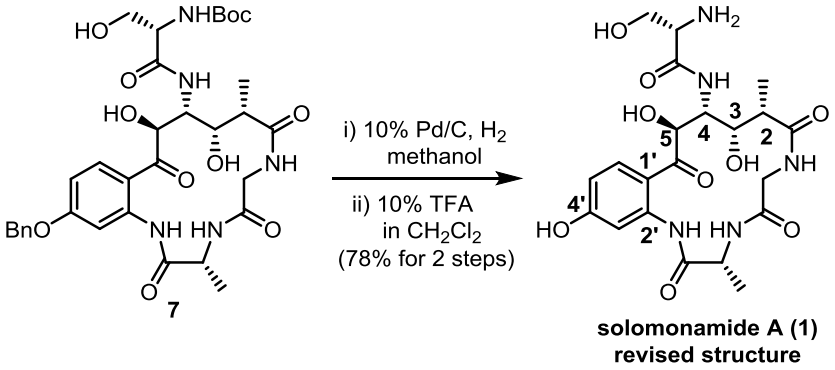
***tert*-Butyl ((3*R*,9*S*,10*S*,11*R*)-16-(benzyloxy)-10,12-dihydroxy-3,9-dimethyl-2,5,8,13-tetraoxo-2,3,4,5,6,7,8,9,10,11,12,13-dodecahydro-1H-benzo[h][1,4,7]triazacyclopentadecin-11-yl)carbamate (5):** To a solution of compound **6** (0.110 g, 0.183 mmol) in dry CH_2Cl_2 at 0 °C solid $NaHCO_3$ (0.019 g, 0.219 mmol) was added followed by addition of Dess–Martin periodinane (0.077 g, 0.183 mmol) under nitrogen atmosphere. The resulting mixture was stirred at room temperature for 3 h. After completion of the reaction (TLC analysis), saturated $NaHCO_3/Na_2SO_3$ solution (1:1, 20 mL) was added, the aqueous phase was separated and extracted with CH_2Cl_2 (2 x 20 mL). The combined organic extracts were dried over Na_2SO_4, filtered and concentrated. Purification of the residue by flash chromatography gave ketone **5** (0.074 g, 67%) as white solid. Mp = 138 - 140 °C; $[\alpha]_D^{22}$-7.12 (*c* 0.81, CH_3OH); IR υ_{max}(film): cm^{-1} 3465, 3285, 2929, 1659, 1630, 1529, 1450; ^1H NMR (400 MHz, DMSO-d_6): δ 11.49 (brs, 1H), 8.72 (d, *J* = 7.3 Hz, 1H), 8.17 (brs, 1H), 7.98 (d, *J* = 7.9 Hz, 1H), 7.91 (d, *J* = 8.5 Hz, 1H), 7.70 (d, *J* = 7.3 Hz, 1H), 7.49 - 7.35 (m, 6H), 7.25 - 7.21 (m, 1H), 6.85 (d, *J* = 8.5 Hz, 1H), 5.60 (d, *J* = 9.8 Hz, 1H), 5.53 (d, *J* = 7.9 Hz, 1H), 5.21 (s, 2H), 5.01 (d, *J* = 6.7 Hz, 1H), 4.68 (t, *J* = 8.5 Hz, 1H), 4.43 (t, *J* = 7.0 Hz, 1H), 4.13 - 4.08 (m, 1H), 3.90- 3.85 (m, 1H), 3.80 - 3.77 (m, 1H), 3.15 (t, *J* = 8.2 Hz, 1H), 2.40 - 2.33(m, 1H), 1.41 (s, 9H), 1.31 (d, *J* = 7.3 Hz, 3H), 0.97 (d, *J* = 6.7 Hz, 3H); ^{13}C NMR (125 MHz, DMSO-d_6): δ 202.1, 173.8, 171.1, 169.3, 162.6, 156.0, 141.6, 136.3, 133.4, 128.5, 128.4, 128.0, 127.7, 127.5, 117.2, 108.9, 106.1, 77.9, 71.4, 70.6, 69.5, 54.7, 49.3, 44.5, 42.8, 28.2, 15.8, 13.8; HRMS calculated for $C_{30}H_{39}O_9N_4$ $[M+H]^+$: 599.2706, found 599.2712.



5 **7**

***tert*-Butyl ((2*S*)-1-(((3*R*,9*S*,10*S*,11*R*)-16-(benzyloxy)-10,12-dihydroxy-3,9-dimethyl-2,5,8,13-tetraoxo-2,3,4,5,6,7,8,9,10,11,12,13-dodecahydro-1H-benzo[h][1,4,7]triazacyclopentadecin-11-yl)amino)-3-hydroxy-1-oxopropan-2-yl)carbamate (7):** To a solution of compound **5** (45 mg, 0.075 mmol) in CH_2Cl_2 (5 mL) trifluoro acetic acid (1.0 mL) was added at 0 °C and the resulting suspension was stirred for 2 h at the same temperature. Reaction was monitored by TLC, and then concentrated. This residue was dissolved in dry DMF (3 mL), then HATU (35 mg, 0.091 mmol), DIPEA (27 µL, 0.150 mmol) and *N*-(*tert*-Butoxycarbonyl)-L-serine (18 mg,

0.091 mmol) was added. The resulting solution was stirred at ambient temperature for 16 h. Reaction mass was diluted with ethyl acetate (15 mL), washed with saturated solution of $NaHCO_3$ (5 mL), H_2O (5 mL), 1N HCl (5 mL). The organic layer was dried over Na_2SO_4 and the crude material obtained after removal of the solvent was purified by column chromatography (silica gel 230-400 mesh 5% methanol - CH_2Cl_2) to afford **7** (34 mg, 65 %) as off white solid. Mp = 271 - 273 °C; $[\alpha]_D^{22}$ + 11.81 (*c* 0.23, CH_3OH); IR υ_{max}(film): cm^{-1} 3646, 3285, 2926, 1669, 1632, 1529, 1221; ^1H NMR (400 MHz, DMSO-d_6): δ 11.50 (s, 1H), 8.85 (d, *J* = 7.9 Hz, 1H), 8.20 (brs, 1H), 7.95 (d, *J* = 9.2 Hz, 1H), 7.48 – 7.46 (m, 3H), 7.43 – 7.39 (m, 2H), 7.36 (d, *J* = 6.7 Hz, 1H), 7.26 (d, *J* = 9.2 Hz, 1H), 6.92 (d, *J* = 6.7 Hz, 1H), 6.85 (d, *J* = 9.2 Hz, 1H), 5.32 - 5.29 (m, 1H), 5.23(s, 2H) 4.90 (brs, 1H), 4.75 (d, *J* = 8.5 Hz, 1H), 4.42 (dd, *J* = 7.9, 14.6 Hz, 2H), 4.03–4.00 (m, 1H), 3.90 (dd, *J* = 6.4, 15.0 Hz, 1H), 3.75 – 3.72 (m, 1H), 3.62 - 3.56 (m, 2H), 3.16 (d, *J* = 5.5 Hz, 1H), 2.28 (d, *J* = 7.9 Hz, 1H), 1.40 (s, 9H), 1.31 (d, *J* = 6.7 Hz, 3H), 0.93 (d, *J* = 6.7 Hz, 3H); ^{13}C NMR (125 MHz, DMSO-d_6): δ 202.1, 173.8, 171.1, 169.3, 162.6, 156.0, 140.5, 136.3, 133.4, 132.4, 130.0, 128.5, 128.4, 128.1, 128.0, 127.7, 117.2, 108.9, 106.1, 77.9, 71.4, 70.6, 69.5, 54.7, 49.3, 44.5, 42.8, 28.2, 15.7, 13.8; HRMS calculated for $C_{33}H_{43}O_{11}N_5Na$ $[M+Na]^+$: 708.2842, found 708.2851.



(2*S*)-2-Amino-3-hydroxy-N-((3*R*,9*S*,10*S*,11*R*)-10,12,16-trihydroxy-3,9-dimethyl-2,5,8,13-tetraoxo-2,3,4,5,6,7,8,9,10,11,12,13-dodecahydro-1H-benzo[h][1,4,7]triazacyclopentadecin-11-yl)propanamide (1):

To a solution of compound **7** (15 mg, 0.021 mmol) in methanol (3 mL), 10% Pd/C (~ 3 mg) was added and stirred under H_2 atmosphere for 2 h. The reaction mixture was then filtered through silica gel column, concentrated to afford phenolic compound. The phenolic compound was dissolved in CH_2Cl_2 (3 mL), TFA (0.3 mL) was added at 0 °C and the resulting suspension was stirred for 2 h at the same temperature.

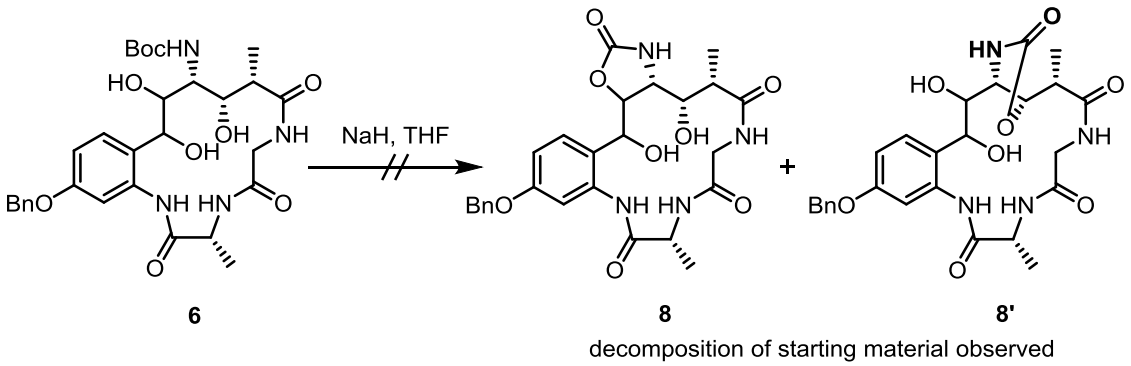
Concentrated the reaction mixture and azeotroped with diethyl ether (3 mL x 3) and dried under vacuum to afford compound **1** (8.5 mg, 78% for 2 steps) as off white solid. $[\alpha]_D^{27}$+ 3.4 (*c* 0.52, CH_3OH); IR υ_{max}(film): cm^{-1} 3439, 3067, 1669, 1578, 1529, 1221; HRMS calculated for $C_{21}H_{30}O_9N_5$ [M+H]+ : 496.2036, found 496.2041.

Table 1: ^1H and ^{13}C chemical shift comparison of natural and synthetic Solomonamide A

Comparison of ^1H NMR Values of Solomonamide A		Comparison of ^{13}C NMR Values of Solomonamide A			
Natural	**Synthetic**	**Residue**		**Natural**	**Synthetic**
0.98 (d, *J* = 7.1, 3H)	0.98 (d, *J* = 7.3 Hz, H)	**Glycine**	Carbonyl	169.2	169.1
1.31 (d, *J* = 7.0, 3H)	1.32 (d, *J* = 6.7 Hz, 3H)		CH_2	42.8	42.9
2.34 (dq, *J* = 9.7, 7.1, 1H)	2.28(dq, *J* = 9.2, 7.3, 1H)	**D-Alanine**	Carbonyl	170.7	170.9
3.17 (ovl, 1H)	3.17 (t, *J* = 6.71, 1H)		CH	49.3	49.4
3.68 (dd, *J* = 11.4, 6.9, 1H)	3.68 (m, 1H)		Methyl	15.6	15.8
3.76 (dd, *J* = 15.3, 4.7, 1H)	3.77 (m, 1H)	**L-Serine**	Carbonyl	167.5	167.6
3.81 (dd, *J* = 11.4, 6.9, 1H)	3.81 (m, 1H)		CH	54.2	54.2
3.90 (dd, *J* = 15.3, 6.6, 1H)	3.98 (brs, 1H)		CH_2	60.7	60.7
4.02 (m, 1H)	4.00 (m, 1H)	**AHMOA**	1 Carbonyl	173.4	173.4
4.43 (quint, *J* = 7.6, 1H)	4.43 (quint, *J* = 7.3, 1H)		2 CH attached to CH_3	44.5	45.0
4.54 (t, *J* = 9.6, 1H)	4.53 (t, *J*=9.77)		3 CH attached to OH	70.3	70.3
4.75 (d, *J* =9.9, 1H)	4.76 (d, J = 9.16, 1H)		4 CH attached to NH	53.5	53.6
5.26 (brs, 1H)	5.32 (brs, 1H) OH Proton		5 CH attached to OH	70.5	70.6
5.39 brs	OH Proton		6 Keto carbonyl	201.1	200.7
5.53 (brs, 1H)	5.52 (brs, 2H)		7 Methyl	13.8	13.8
6.57 (dd, *J* = 8.8, 2.3, 1H)	6.58 (d, *J* = 8.5 Hz,1H)	**Aromatic**	1'	115.2	115.0
7.49(brt, *J* = 5.5, 1H)	NH Proton		2'	141.8	142.4
7.86 (d, *J* = 8.7, 1H)	7.87 (d, *J* = 8.5, 1H)		3'	106.3	106.2
7.89 (d, *J* = 9.6, 1H)	7.89 (brs, 1H)		4'	162.8	163.2
8.02 (d, *J* = 2.3, 1H)	8.04 (brs, 1H)		5'	109.8	110.0
8.10 (brd, *J* = 4.3, 2H)	8.10 (brs, 2H)		6'	133.6	133.9
8.77 (d, *J* = 7.9, 1H)	8.75 (d, *J* = 7.93, 1H)				

Attempts towards derivatization of triol: We have planned NMR studies on a derivative of triol **6**.

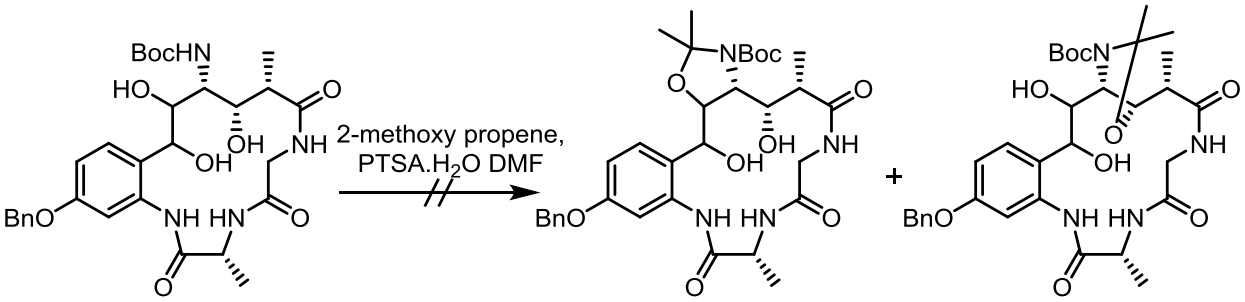
1. **Carbamate synthesis:** For this purpose, a five-membered cyclic carbamate derivative **8** and **8'** were planned from triol **6** by treatment with sodium hydride in anhydrous THF. Unfortunately we did not observed formation of carbamates.



6 **8** **8'**

decomposition of starting material observed

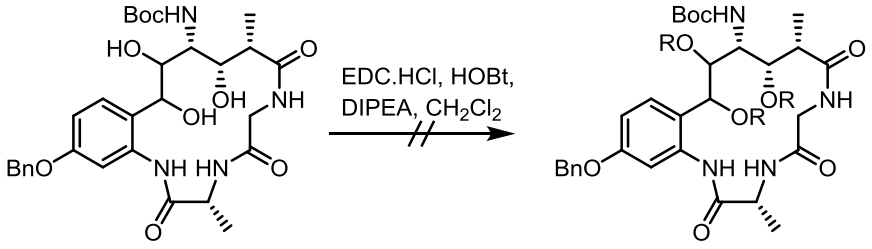
2. **Acetonide synthesis:** After unsuccessful attempts to synthesize carbamate derivative next we plan to make acetonide derivative of triol **6**, for this conversion we used 2-methoxy propene in presence of catalytic amount of PTSA.H_2O in DMF to get acetonide **9** and **9'** but we did not observed desired product instead we observed complex reaction mixture.



6 **9** **9'**

complex reaction mixture

3. **Ester formation**: for crystallization purpose we attempted esterification reaction on compound **6** by coupling with 4-Nitro benzoic acid or Ferrocene carboxylic acid respectively using coupling protocol but we failed to get required compounds, instead we recovered starting material **6**.



6 **10**

1. R = *P*-Nitro benzoic acid
2. R = Ferrocene carboxylic acid

} only starting material was observed

Biological activity

Material and Method:-

Male Swiss albino mice weighing 30-35 g were divided into 6 groups. Animals received either a sub plantar injection of either 50 µl of saline (control) or 1% carrageenan in the left hind paw.[1, 2] One hour prior to the carrageenan injection, respective group of animals was administered with a single dose of either vehicle (PEG, i.p.) or solomonamide A revised (0.03, 0.1 and 0.3 mg/kg, i.p.)[3] and dexamethasone (10 mg/kg, i.p.).[1] Plethysmometer (Ugo Basile, Italy) was used to measure the paw volume, before and after sub plantar injection of carrageenan at 4 & 6 h. The increase in paw volume was calculated as the difference between the paw volume measured at 4 & 6 h and the basal paw volume. [1, 2] Percentage inhibition was calculated by using formula Vc-Vt/Vc X 100. Where, Vc and Vt represent the mean paw volume of carrageenan and solomonamide A treated animals respectively. [4]

Statistical analysis:-

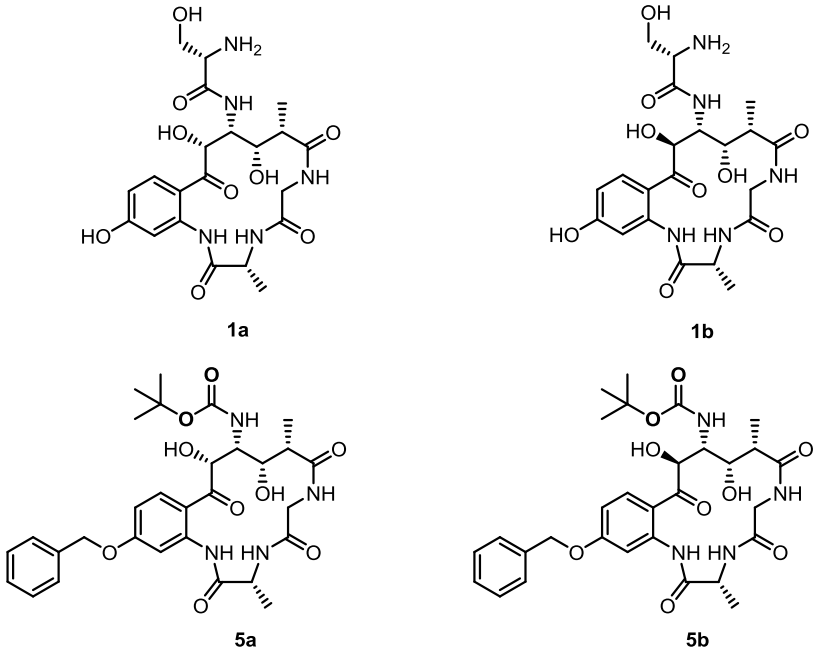
Results were expressed as Mean ± S.E.M. Statistical analysis was determined by one-way ANOVA followed by Tukey's test for multiple comparisons, using Graph Pad Prism software (Graph Pad Software Inc., San Diego, CA). Differences were considered statistically significant when $p<0.05$. $^{***}p<0.001$ control vs. carrageenan; $^{###}p<0.001$ carrageenan vs. Carrageenan + solomomnamide A or Carrageenan + Dexamethasone.

Computational details:

The starting 3D chemical structures of compounds **1a**, **1b**, **5a**, and **5b** (Chart S1) were built with Maestro11.1.[5] Optimizations of the starting 3D structures were performed using the OPLS force field[6] and the Polak-Ribier conjugate gradient algorithm (PRCG, maximum derivative less than 0.001 kcal/mol)with Macro Model 11.5.[7] For all the compounds, exhaustive conformational searches were performed at the empirical molecular mechanics (MM) level, combining Monte Carlo Multiple Minimum (MCMM) method (50000 steps) and Low Mode Conformational Search (LMCS) method (50000 steps), in order to allow a full exploration of the conformational space. Furthermore, the conformational search was also integrated with molecular dynamics simulations at 450, 600, 700, and 750 K, with a time step of 2.0 fs, an equilibration time of 0.1 ns, and a simulation time of 10 ns. For each investigated compound, all the conformers obtained

from the above reported conformational search rounds were minimized (PRCG, maximum derivative less than 0.001 kcal/mol) and superimposed. Then, the "Redundant Conformer Elimination" module of Macromodel 11.5[7] was used to select non-redundant conformers, excluding those differing more than 21.0 kJ/mol (5.02 kcal/mol) from the most energetically favoured conformation and setting a 0.5 Å RMSD (root-mean-square deviation) minimum cut-off for saving structures.

Chart S1. Chemical structures of compounds 1a, 1b, 5a and 5b.



All the subsequent QM calculations were performed using Gaussian 09 software.[8] Specifically, all the conformers obtained by MM conformational search rounds were optimized at the QM level using the MPW1PW91 functional and the 6-31G(d) basis set.[6] After the optimization of the geometries, the conformers were visually inspected in order to remove further redundant conformers. The subsequent computation of the ^{13}C NMR chemical shifts was performed on the selected conformers for the investigated compounds, using the MPW1PW91 functional and the 6-31G (d,p) basis set. Final ^{13}C NMR chemical shift sets of data for each of the diastereoisomers were extracted and computed considering the influence of each conformer on the total Boltzmann distribution taking into account the relative energies. Calibrations of calculated ^{13}C chemical shifts were performed following the multi-standard approach (MSTD) (Tables S1-S2, Supporting Information).[9,10] In particular, sp^2 ^{13}C NMR chemical shifts (with the

exception of carbonyl carbons) were computed using benzene as reference compound[9,10] while TMS was used for computing sp^3 ^{13}C chemical shift data.

Experimental and calculated ^{13}C NMR chemical shifts were compared (**1a**/**1b**, **5a**/**5b** diastereoisomeric pairs) computing the Δδ parameter (Tables S1–S2, Supporting Information):

$$\Delta\delta = |\delta_{exp} - \delta_{calc}|$$

where δ_{exp} (ppm) and δ_{calc} (ppm) are the ^{13}Cexperimental and calculated chemical shifts, respectively.

The mean absolute errors (MAEs) for all the considered diastereoisomers were computed using the following equation:

$$\mathrm{MAE} = \frac{\sum(\Delta\delta)}{n}$$

Defined as the summation (Σ) of the n computed absolute error values (Δδ), normalized to the number of chemical shifts considered (n) (Tables S1–S2, Supporting Information).

Table S1. ^{13}C experimental and calculated NMR chemical shifts for **1a** and **1b**, with [a]|Δδ|(^{13}C) and [c] MAE values. Chemical shift data here reported were produced using benzene as reference compound for sp^2 carbons, and tetramethylsilane (TMS) for sp^3 carbons.

Residue		**δ_{exp} (^{13}C), ppm**	**δ_{calc} (^{13}C), ppm**		**|Δδ| (^{13}C), ppm[a]**	
			1a	**1b**	**1a**	**1b**
Glycine	Carbonyl	169.1	166.3	166.0	2.84	3.11
	CH_2	42.9	43.1	45.0	0.17	2.09
D-Alanine	Carbonyl	170.9	165.2	168.5	5.73	2.42
	CH	49.4	51.5	51.4	2.14	2.01
	Methyl	15.8	16.2	18.3	0.39	2.54
L-Serine	Carbonyl	167.6	173.1	173.0	5.50	5.35
	CH	54.2	58.4	53.9	4.18	0.26
	CH_2	60.7	65.5	66.3	4.82	5.59
AHMOA	1 Carbonyl	173.4	169.3	172.0	4.09	1.42
	2 CH attached to CH_3	45.0	47.6	43.7	2.58	1.26
	3 CH attached to OH	70.3	73.6	72.3	3.32	2.01
	4 CH attached to NH	53.6	59.0	57.0	5.37	3.39
	5 CH attached to OH	70.6	80.0	72.9	9.37	2.30
	6 Keto carbonyl	200.7	202.9	199.8	2.15	0.87
	7 Methyl	13.8	15.4	11.6	1.60	2.24
Aromatic	1'	115.0	118.1[b]	117.3[b]	3.07	2.28

	2'	142.4	142.7[b]	145.0[b]	0.30	2.55
	3'	106.2	107.3[b]	107.2[b]	1.06	1.04
	4'	163.2	160.6[b]	163.4[b]	2.64	0.23
	5'	110.0	109.2[b]	110.5[b]	0.78	0.53
	6'	133.9	136.9[b]	137.3[b]	2.96	3.40
MAE, ppm[c]					3.10	**2.23**

[a] **$|\Delta\delta|(^{13}C)$** = $|\delta_{exp} - \delta_{calc}|$ (^{13}C), ppm: absolute differences for experimental versus calculated ^{13}C NMR chemical shifts

[b] ^{13}C chemical shifts calculated using benzene as reference compound; all the remaining values calculated using TMS as reference compound.

[c] **MAE** = $(\Sigma[|(\delta_{exp} - \delta_{calc})|])/n$, summation through n of the absolute error values (difference of the absolute values between corresponding experimental and ^{13}C chemical shifts), normalized to the number of the chemical shifts.

Table S 2. ^{13}C experimental and calculated NMR chemical shifts for **5a** and **5b**, with [a]$|\Delta\delta|(^{13}C)$ and [c] MAE values. Chemical shift data here reported were produced using tetramethylsilane (TMS).

Residue		**δ_{exp} (^{13}C), ppm**	**δ_{calc} (^{13}C), ppm**		**$|\Delta\delta|$ (^{13}C), ppm[a]**	
			5a	**5b**	**5a**	**5b**
Glycine	Carbonyl	169.3	164.9	166.8	4.42	2.50
	CH_2	40.0	46.5	45.2	6.52	5.23
D-Alanine	Carbonyl	171.1	168.2	166.6	2.90	4.50
	CH	49.3	48.0	51.1	1.27	1.79
	Methyl	15.7	18.3	15.5	2.60	0.16
Boc	Carbonyl	156.0	151.8	153.8	4.17	2.19
	C	77.9	79.5	79.7	1.62	1.81
	CH_3	28.2	27.5	27.4	0.68	0.76
AHMOA	1 Carbonyl	173.8	170.1	170.9	3.67	2.88
	2 CH attached to CH_3	39.8	45.2	46.1	5.38	6.35
	3 CH attached to OH	69.5	71.3	72.0	1.81	2.45
	4 CH attached to NH	54.7	56.8	58.5	2.14	3.80
	5 CH attached to OH	70.5	77.7	70.5	7.25	0.03
	6 Keto carbonyl	202.1	198.0	199.8	4.1	2.30
	7 Methyl	13.8	14.7	15.6	0.85	1.82
Aromatic	1'					
	2'					

	3'				
	4'				
	5'				
	6'				
	CH_2				
	1''				
	2''				
	3''				
	4''				
	5''				
	6''				
MAE, ppm[b]				3.29	2.57

[a] **$\Delta\delta|(^{13}C)$** = $|\delta_{exp} - \delta_{calc}|$ (^{13}C), ppm: absolute differences for experimental versus calculated ^{13}C NMR chemical shifts

[b] **MAE** = $(\Sigma[|(\delta_{exp} - \delta_{calc})|])/n$, summation through n of the absolute error values (difference of the absolute values between corresponding experimental and ^{13}C chemical shifts), normalized to the number of the chemical shifts

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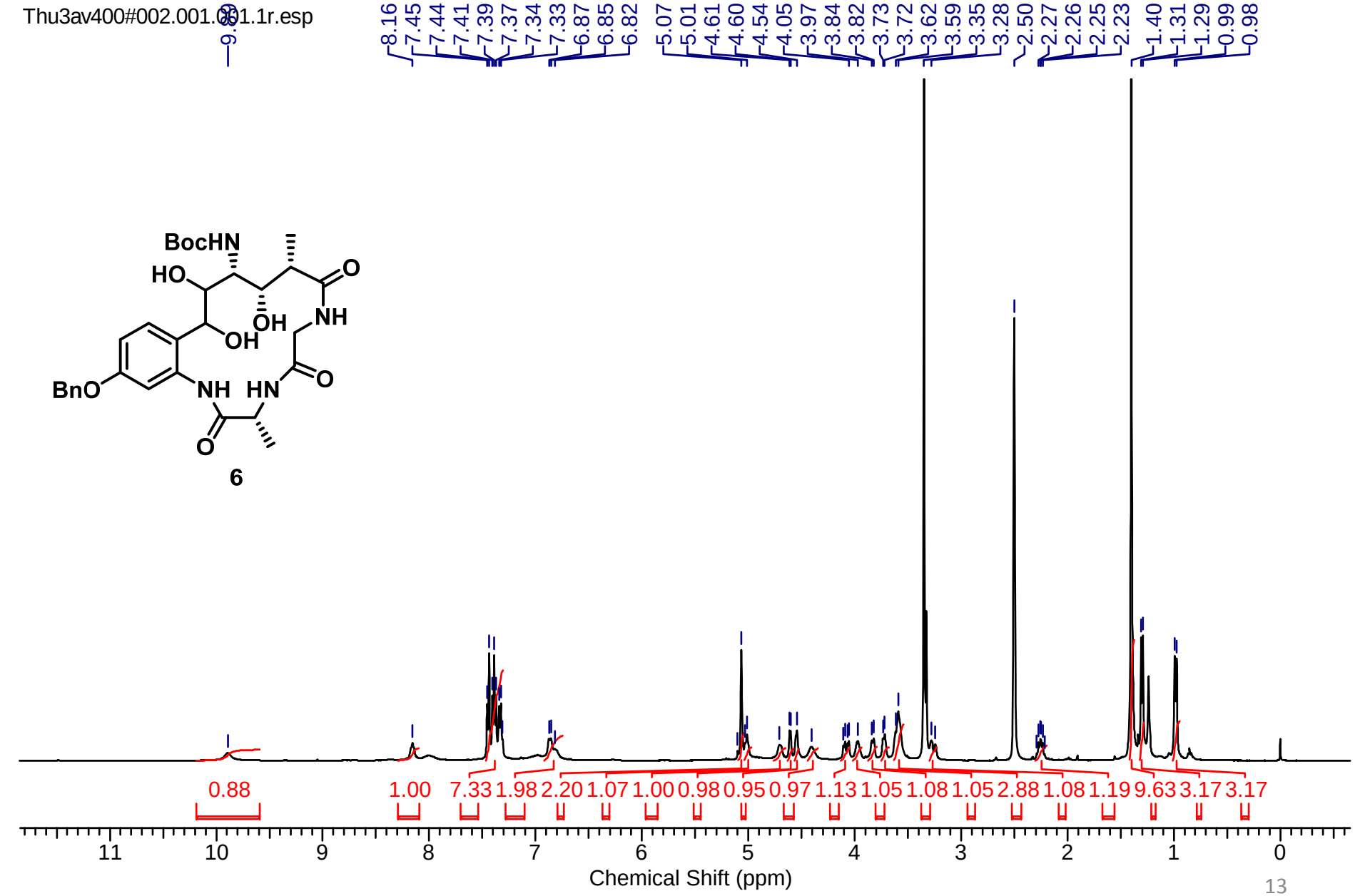
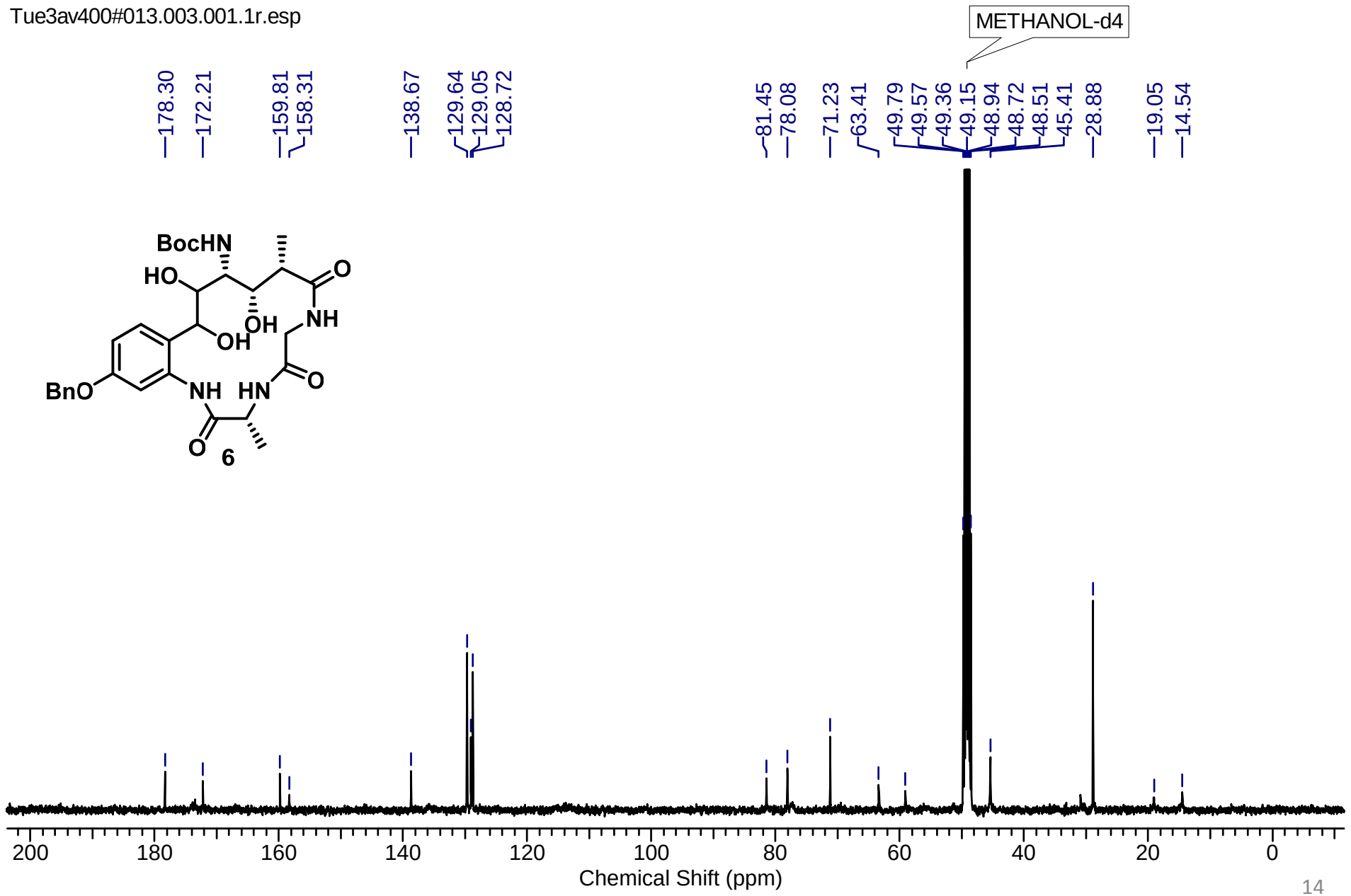
^{1}H NMR spectrum of compound 6 in CD_3OD at 400 MHz

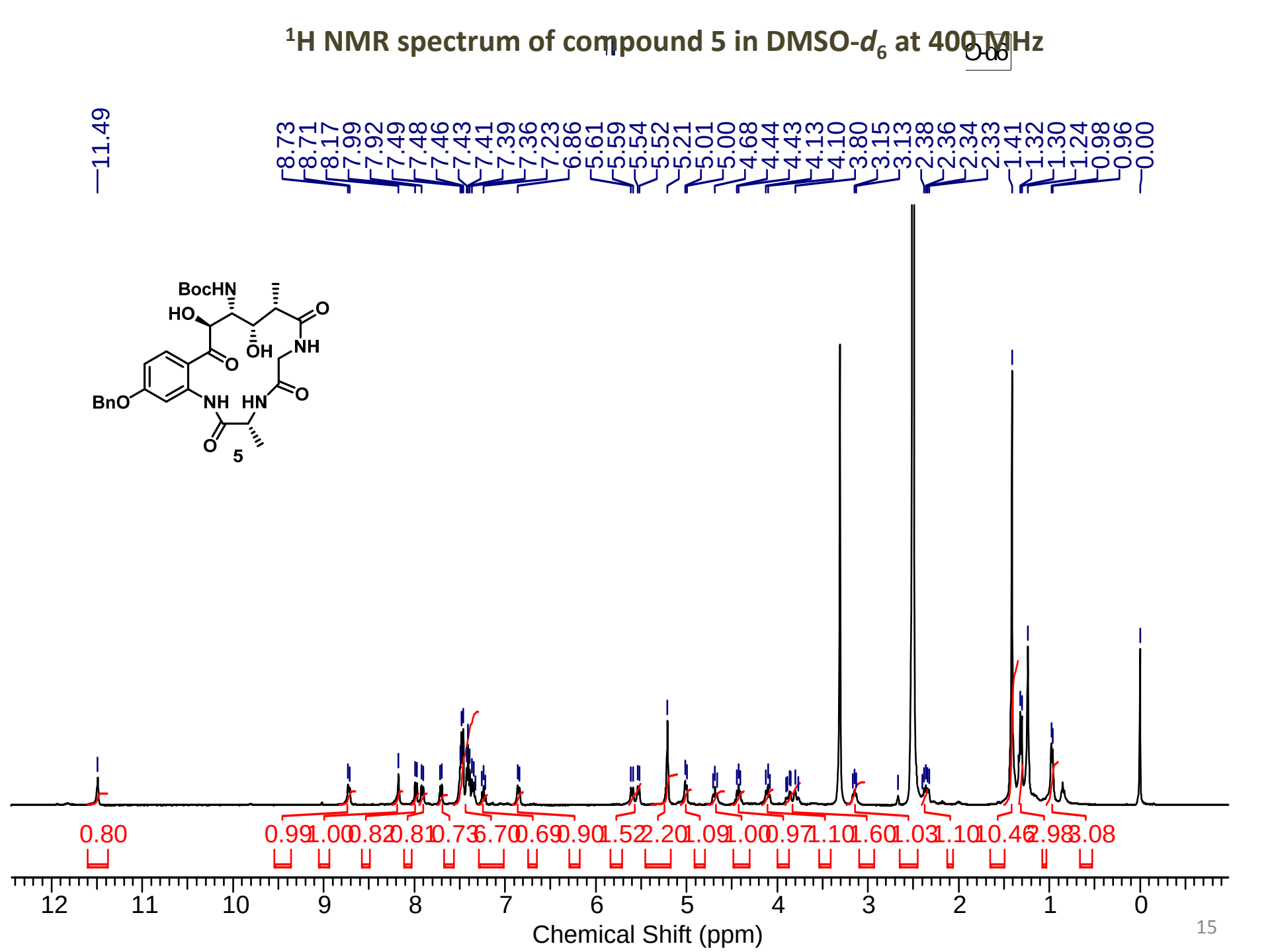


6

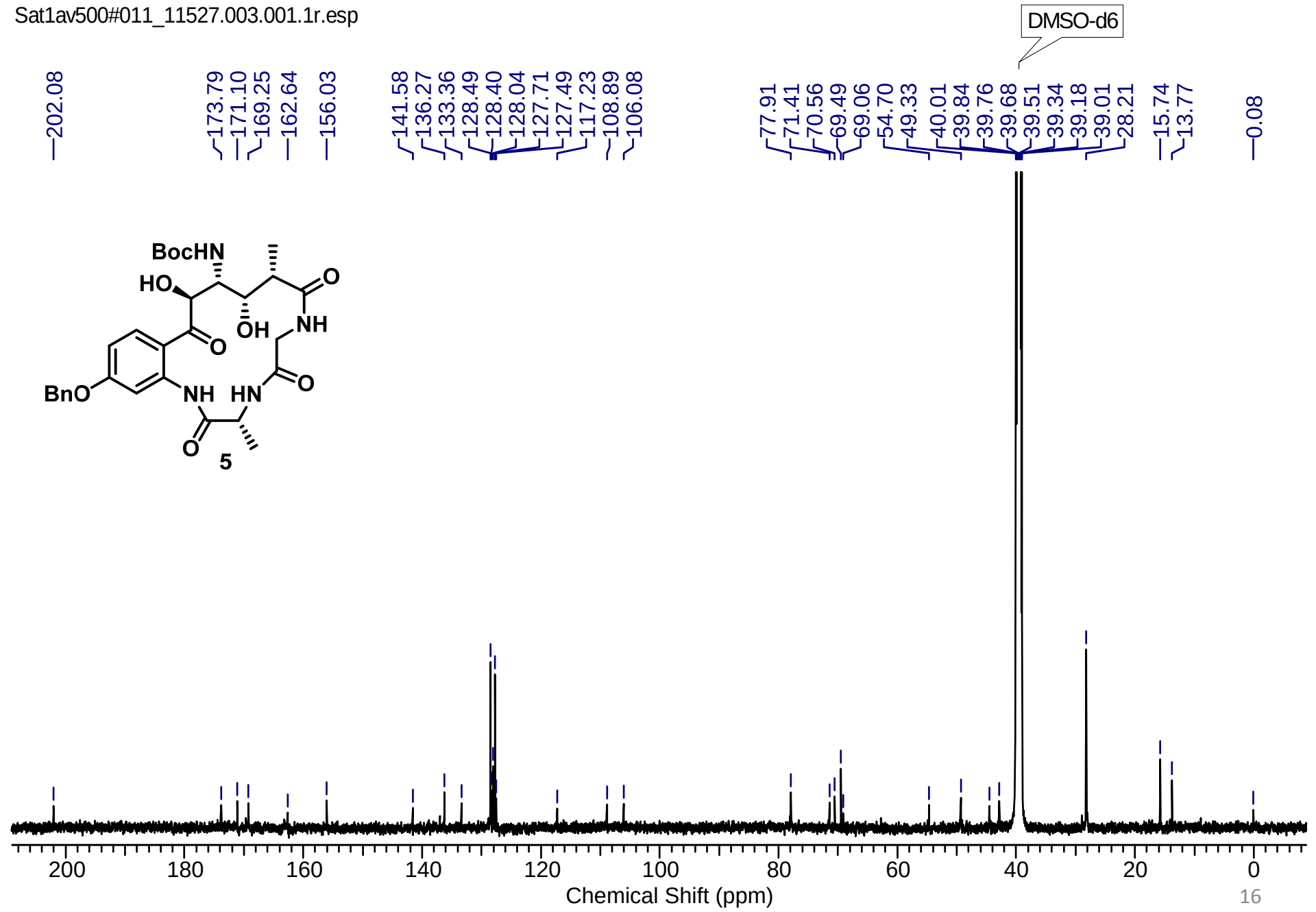
^{13}C NMR spectrum of compound 6 in CD_3OD at 100 MHz



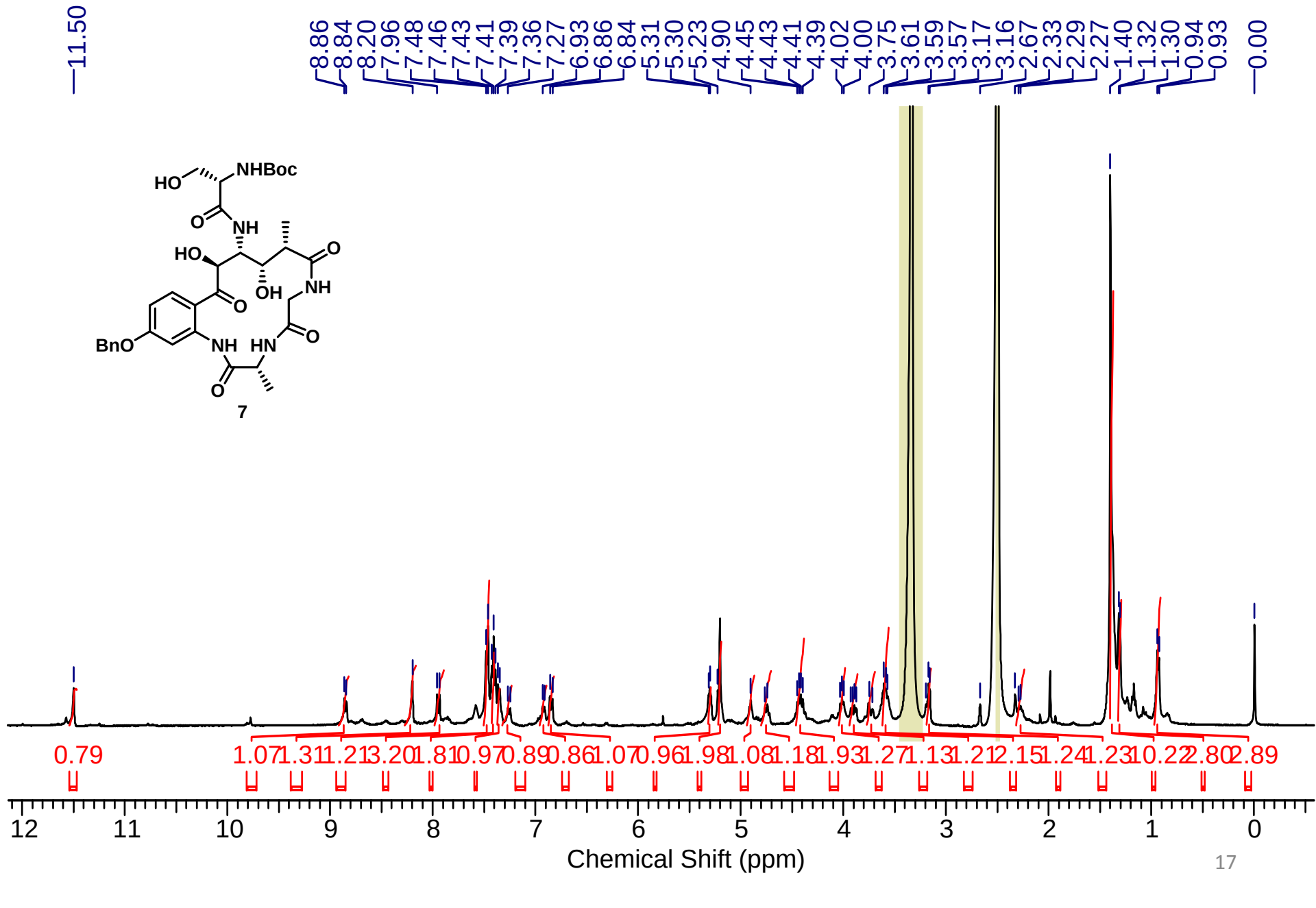
^{1}H NMR spectrum of compound 5 in DMSO-d_6 at 400 MHz



^{13}C NMR spectrum of compound 5 in DMSO-d_6 at 125 MHz



^{1}H NMR spectrum of compound 7 in DMSO-d_6 at 400 MHz



^{13}C NMR spectrum of compound 7 in DMSO-d_6 at 125 MHz

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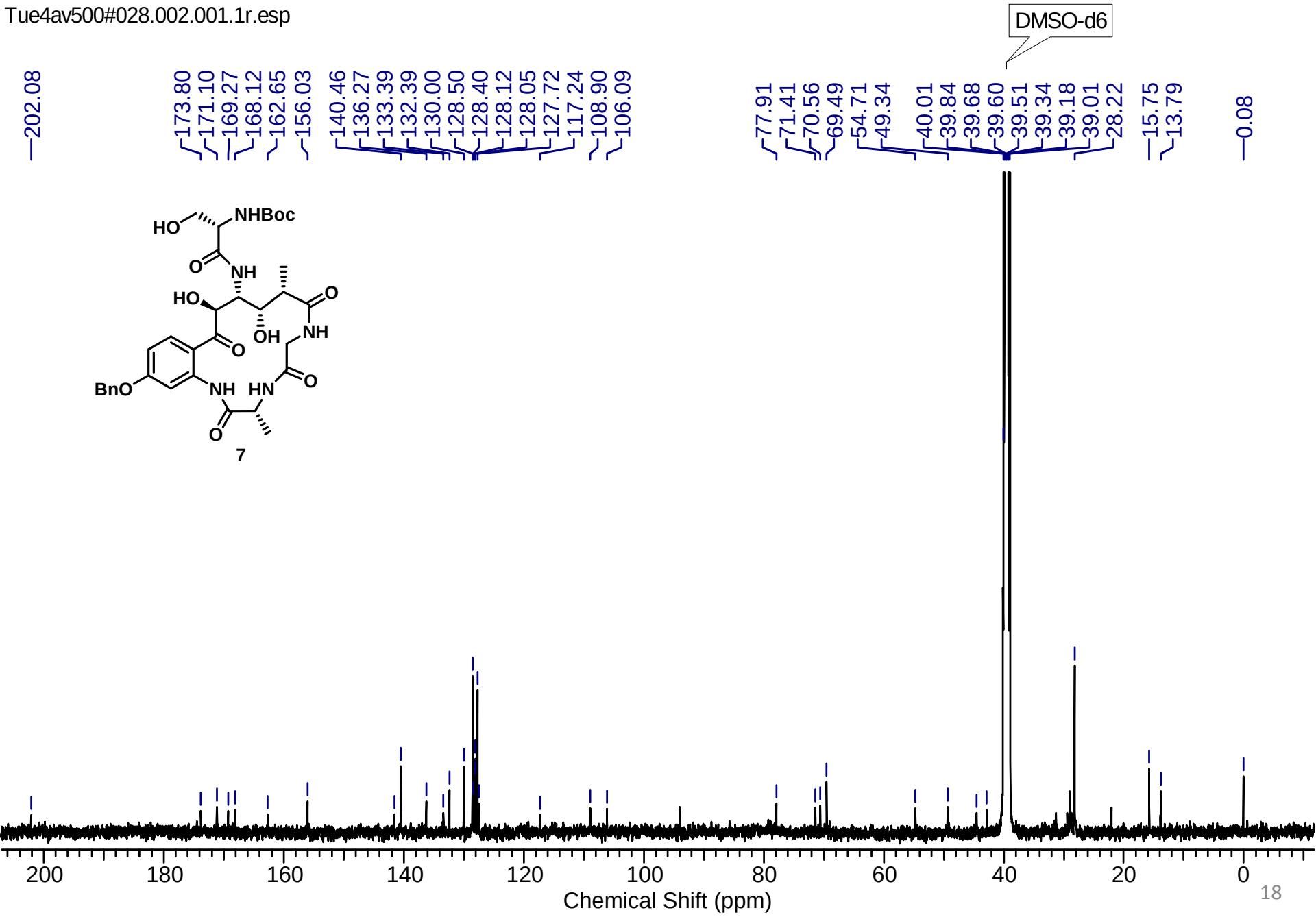
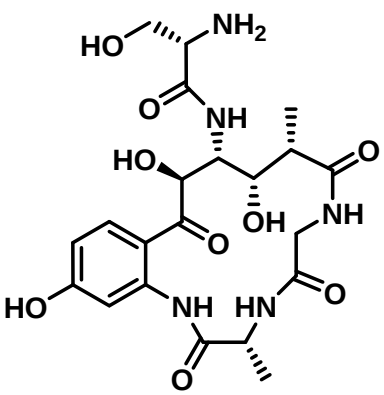


^{1}H NMR spectrum of Solomonamide A (1) in DMSO-d_6 at 400 MHz



Solomonamide A (1)

^{13}C NMR spectrum of Solomonamide A (1) in DMSO-d_6 at 100 MHz

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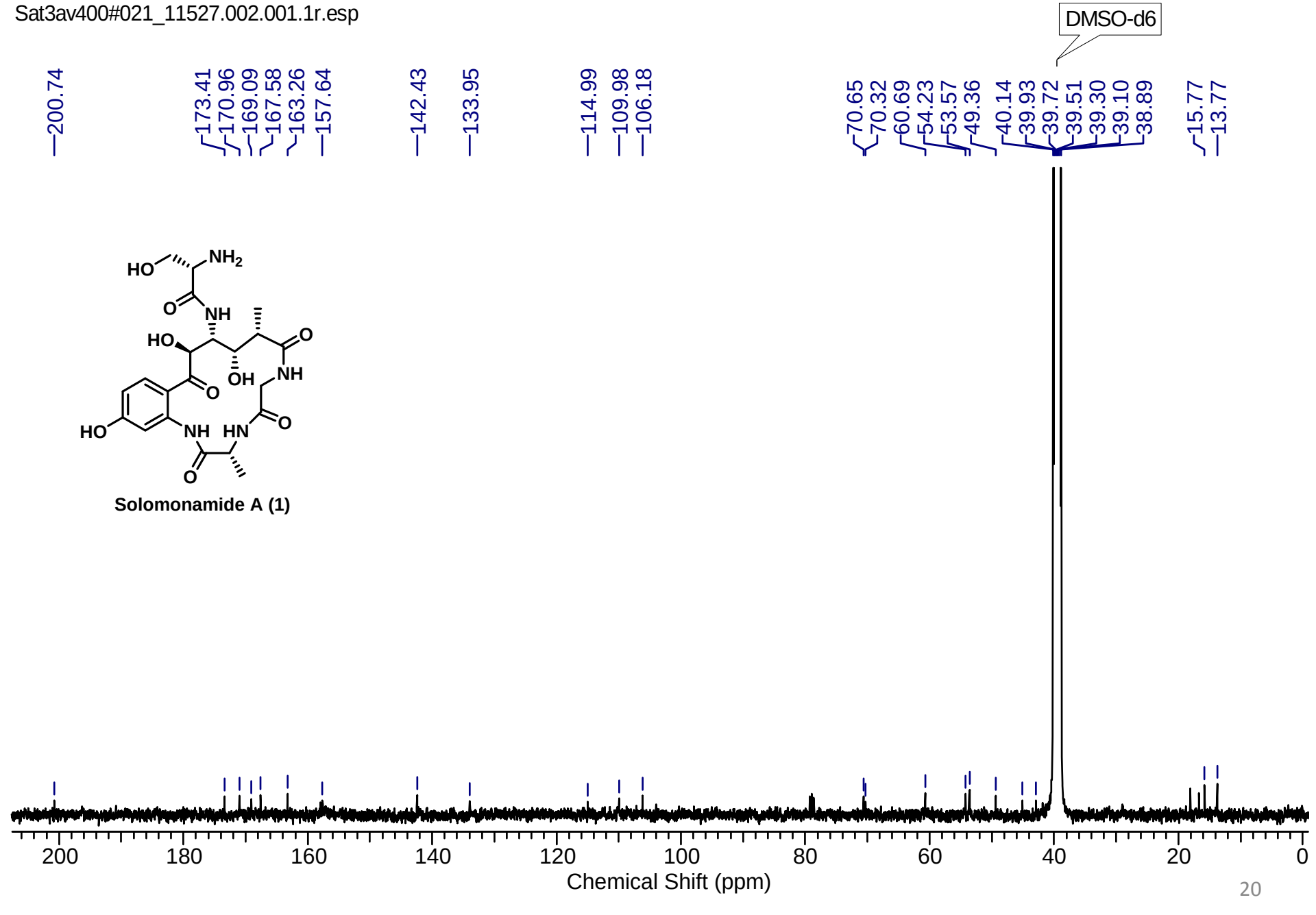

Solomonamide A (1)