-Supplementary data-

Merocyclophanes A and B, Antiproliferative Cyclophanes from the Cultured Terrestrial Cyanobacterium *Nostoc* sp.

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Table of Contents

S1. Morphological description of the strain UIC 10062

S2. X-ray crystallographic data of **1**

S3. ^{1}H NMR spectrum (600 MHz, MeOH-d_4) of **1**

S4. COSY spectrum (600 MHz, MeOH-d_4) of **1**

S5. HSQC spectrum (600 MHz, MeOH-d_4) of **1**

S6. HMBC spectrum (600 MHz, MeOH-d_4) of **1**

S7. ^{1}H NMR spectrum (600 MHz, DMSO-d_6) of **2**

S8. COSY spectrum (600 MHz, DMSO-d_6) of **2**

S9. HSQC spectrum (600 MHz, DMSO-d_6) of **2**

S10. HMBC spectrum (600 MHz, DMSO-d_6) of **2**

S11. CD spectra of **1** and **2**

S12. Torsion energy profile of the hydroxyquinone ring in **2**

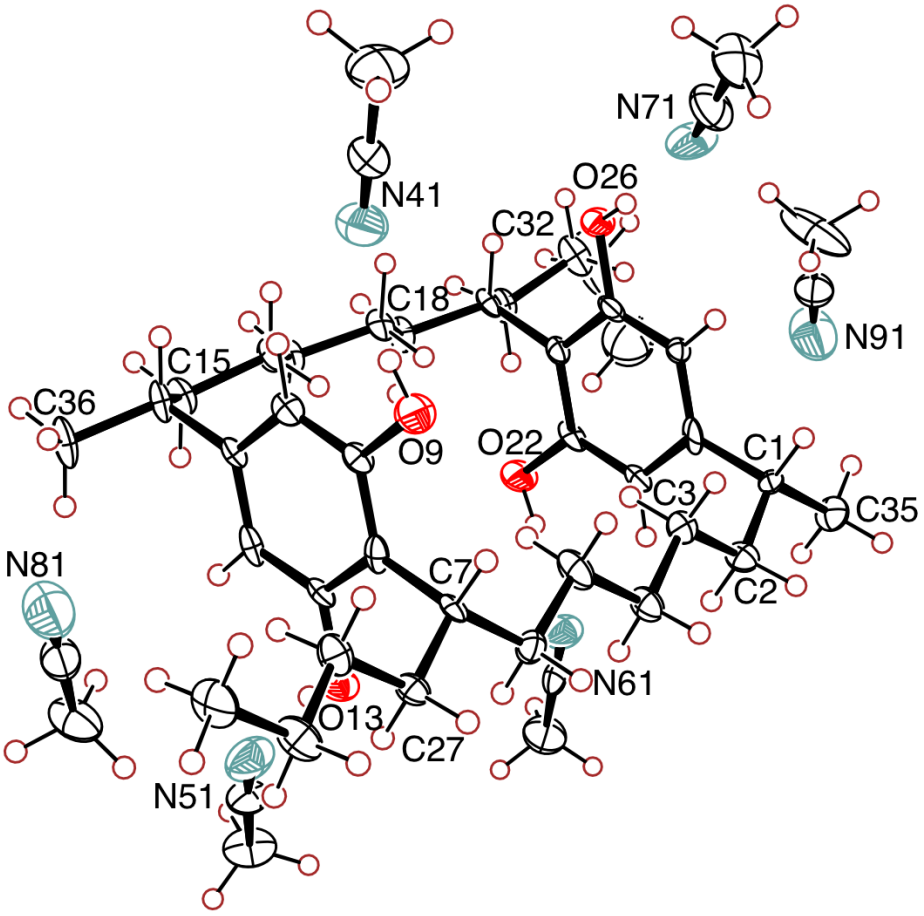
S1. Morphological description of the strain UIC 10062

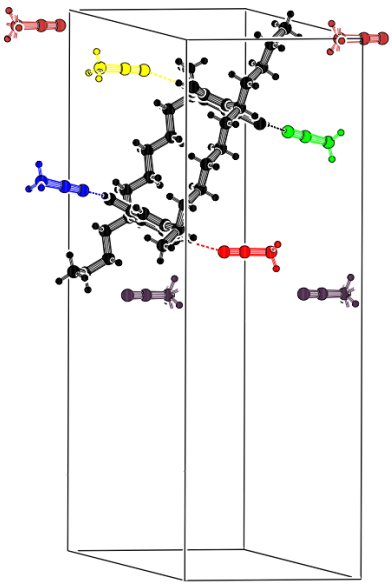
Photomicrograph (400x, bright field) of *Nostoc* sp. UIC10062

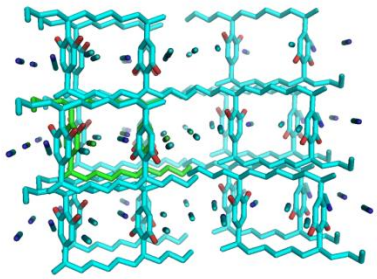
Morphological description of *Nostoc* sp. UIC10062

The thalli occurred as macroscopic, irregular mats in clusters. The filaments were isopolar with solitary, intercalary heterocysts, intermittent akinetes, and cylindrical with cells organized in trichomes. The trichomes were long, straight or irregularly waved, and covered with a thin, barely visible, muscilageous sheath. The cells were barrel-shaped with a cell length (2-3 µm) to width (1.5-2 µm). Constrictions at the cell cross-walls were observed in which cells were divided perpendicularly to the trichome axis.

S2. X-ray crystallographic data of **1**







Crystal data and structure refinement for JOMac.

Empirical formula	$C_{36}\ H_{56}O_4\ .5CH_3CN$
Formula weight	758.10
Temperature	100(1) K
Wavelength	0.800 Å
Crystal system, space group	Monoclinic, C2 (No. 5)
Unit cell dimensions	a = 14.735(2) Å b = 10.840(5) Å β = 95.226(4)° c = 29.842(3) Å
Volume	4747(2) $Å^3$
Z, Calculated density	4, 1.061 Mg/m^3
Absorption coefficient	0.057 mm^{-1}
F(000)	1656
Crystal size	0.03 × 0.03 × 0.03 mm
Theta range for data collection	1.54 to 27.73°
Limiting indices	-15≤h≤15, -11≤k≤11, -32≤l≤33
Reflections collected / unique	13719 / 5724 [R(int) = 0.0815]
Completeness to θ = 27.73°	79.2 %
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	5724 / 1 / 505
Goodness-of-fit on F^2	1.072
Final R indices [I>2sigma(I)]	R1 = 0.0882, wR2 = 0.2285
R indices (all data)	R1 = 0.1311, wR2 = 0.2572
Absolute structure parameter	-2(2) [invert 3(2)]
Extinction coefficient	0.0145(15)
Largest diff. peak and hole	0.43 and -.59 e $Å^{-3}$

Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($Å^2 \times 10^3$) for JOMac. U(eq) is defined as one third of the trace of the Orthogonalized Uij tensor.

	x	y	z	U(eq)
C(1)	6833(4)	1672(7)	6321(2)	17(2)
C(2)	7333(4)	1700(7)	6795(2)	22(2)
C(3)	7060(4)	2767(8)	7073(2)	25(2)
C(4)	7521(4)	2806(7)	7554(2)	25(2)
C(5)	7146(5)	3845(8)	7825(2)	29(2)
C(6)	7538(4)	3892(7)	8317(2)	24(2)
C(7)	7122(4)	4941(7)	8578(2)	16(2)
C(8)	6098(4)	4888(7)	8570(2)	19(2)
C(9)	5555(4)	5865(7)	8392(2)	18(2)
O(9)	6000(3)	6833(5)	8214(2)	35(1)
C(10)	4615(4)	5871(7)	8391(2)	21(2)
C(11)	4163(4)	4891(7)	8571(2)	16(2)
C(12)	4679(4)	3878(7)	8743(2)	23(2)
C(13)	5623(4)	3915(7)	8738(2)	17(2)
O(13)	6139(3)	2928(5)	8909(1)	31(1)
C(14)	3142(4)	4893(7)	8573(2)	24(2)
C(15)	2691(4)	3863(7)	8297(2)	23(2)
C(16)	2912(4)	3861(7)	7806(2)	22(2)
C(17)	2518(4)	2771(7)	7534(2)	21(2)
C(18)	2826(4)	2713(7)	7061(2)	20(2)
C(19)	2508(4)	1575(7)	6799(2)	20(2)
C(20)	2833(4)	1541(7)	6322(2)	17(2)
C(21)	3876(4)	1557(7)	6338(2)	18(2)
C(22)	4435(4)	620(7)	6530(2)	20(2)
O(22)	3997(3)	-340(5)	6724(2)	34(1)
C(23)	5378(4)	652(7)	6530(2)	23(2)
C(24)	5790(4)	1624(8)	6336(2)	24(2)
C(25)	5269(4)	2588(7)	6162(2)	15(2)
C(26)	4328(4)	2547(7)	6159(2)	23(2)
O(26)	3789(3)	3487(5)	5970(1)	28(1)
C(27)	7585(4)	5022(7)	9055(2)	21(2)
C(28)	7256(4)	6101(8)	9327(2)	28(2)
C(29)	7799(5)	6272(8)	9787(2)	33(2)
C(30)	7436(5)	7301(8)	10054(2)	39(2)
C(31)	2429(4)	451(7)	6046(2)	26(2)
C(32)	2524(5)	579(8)	5540(2)	32(2)
C(33)	2210(6)	-558(11)	5260(2)	72(4)
C(34)	2838(7)	-1608(12)	5321(3)	82(3)
C(35)	7157(4)	590(7)	6039(2)	27(2)
C(36)	2864(4)	4877(8)	9058(2)	36(2)
N(41)	5050(5)	9066(9)	8005(2)	53(2)
C(41)	5021(5)	10066(10)	7912(3)	39(2)
C(42)	4999(6)	11390(9)	7801(3)	60(3)
N(51)	5252(4)	738(9)	9173(2)	55(2)
C(51)	5161(5)	-279(9)	9196(3)	36(2)
C(52)	5086(6)	-1631(8)	9214(3)	47(2)
N(61)	4992(4)	-2531(8)	6944(2)	43(2)
C(61)	4979(4)	-3566(10)	7018(2)	31(2)
C(62)	4964(6)	-4862(9)	7113(3)	50(2)
N(71)	4748(4)	5675(8)	5774(2)	49(2)
C(71)	5043(6)	6634(11)	5789(3)	48(2)
C(72)	5404(6)	7875(8)	5801(3)	54(2)
N(81)	5000	6112(13)	10000	60(3)
C(81)	5000	5066(14)	10000	37(3)
C(82)	5000	3693(12)	10000	47(3)
N(91)	5000	23(13)	5000	70(4)
C(91)	5000	1042(15)	5000	36(3)
C(92)	5000	2342(13)	5000	81(5)

Bond lengths [Å] for JOMac.

C(1)-C(2)	1.536(8)
C(1)-C(24)	1.541(8)
C(1)-C(35)	1.545(9)
C(2)-C(3)	1.498(9)
C(3)-C(4)	1.534(8)
C(4)-C(5)	1.518(10)
C(5)-C(6)	1.529(8)
C(6)-C(7)	1.537(9)
C(7)-C(8)	1.508(8)
C(7)-C(27)	1.524(7)
C(8)-C(13)	1.383(9)
C(8)-C(9)	1.403(9)
C(9)-O(9)	1.370(8)
C(9)-C(10)	1.384(8)
C(10)-C(11)	1.387(9)
C(11)-C(12)	1.406(9)
C(11)-C(14)	1.506(8)
C(12)-C(13)	1.393(8)
C(13)-O(13)	1.383(8)
C(14)-C(15)	1.505(9)
C(14)-C(36)	1.539(7)
C(15)-C(16)	1.530(7)
C(16)-C(17)	1.519(9)
C(17)-C(18)	1.522(7)
C(18)-C(19)	1.510(9)
C(19)-C(20)	1.545(7)
C(20)-C(31)	1.529(9)
C(20)-C(21)	1.533(8)
C(21)-C(26)	1.395(10)
C(21)-C(22)	1.397(9)
C(22)-O(22)	1.379(8)
C(22)-C(23)	1.390(9)
C(23)-C(24)	1.371(10)
C(24)-C(25)	1.371(10)
C(25)-C(26)	1.386(8)
C(26)-O(26)	1.381(8)
C(27)-C(28)	1.527(9)
C(28)-C(29)	1.538(8)
C(29)-C(30)	1.498(10)
C(31)-C(32)	1.535(8)
C(32)-C(33)	1.537(12)
C(33)-C(34)	1.467(15)
N(41)-C(41)	1.120(11)
C(41)-C(42)	1.472(13)
N(51)-C(51)	1.114(11)
C(51)-C(52)	1.471(12)
N(61)-C(61)	1.144(11)
C(61)-C(62)	1.434(13)
N(71)-C(71)	1.126(12)
C(71)-C(72)	1.445(14)
N(81)-C(81)	1.134(16)
C(81)-C(82)	1.488(18)
N(91)-C(91)	1.105(16)
C(91)-C(92)	1.409(18)

Bond angles [°] for JOMac.

C(2)-C(1)-C(24)	111.7(4)
C(2)-C(1)-C(35)	111.7(5)
C(24)-C(1)-C(35)	110.4(6)
C(3)-C(2)-C(1)	113.2(5)
C(2)-C(3)-C(4)	114.9(6)
C(5)-C(4)-C(3)	111.5(6)
C(4)-C(5)-C(6)	114.2(6)
C(5)-C(6)-C(7)	112.2(5)
C(8)-C(7)-C(27)	112.2(4)
C(8)-C(7)-C(6)	114.2(5)
C(27)-C(7)-C(6)	110.5(5)
C(13)-C(8)-C(9)	115.0(6)
C(13)-C(8)-C(7)	124.2(6)
C(9)-C(8)-C(7)	120.8(6)
O(9)-C(9)-C(10)	120.7(6)
O(9)-C(9)-C(8)	116.6(5)
C(10)-C(9)-C(8)	122.7(6)
C(9)-C(10)-C(11)	120.7(7)
C(10)-C(11)-C(12)	118.5(6)
C(10)-C(11)-C(14)	121.1(6)
C(12)-C(11)-C(14)	120.4(6)
C(13)-C(12)-C(11)	118.8(6)
O(13)-C(13)-C(8)	116.3(5)
O(13)-C(13)-C(12)	119.4(6)
C(8)-C(13)-C(12)	124.3(7)
C(15)-C(14)-C(11)	112.8(6)
C(15)-C(14)-C(36)	111.3(5)
C(11)-C(14)-C(36)	110.9(5)
C(14)-C(15)-C(16)	113.8(5)
C(17)-C(16)-C(15)	114.2(5)
C(16)-C(17)-C(18)	113.4(5)
C(19)-C(18)-C(17)	114.1(5)
C(18)-C(19)-C(20)	112.9(5)
C(31)-C(20)-C(21)	111.5(5)
C(31)-C(20)-C(19)	112.1(5)
C(21)-C(20)-C(19)	111.3(5)
C(26)-C(21)-C(22)	115.6(6)
C(26)-C(21)-C(20)	120.6(6)
C(22)-C(21)-C(20)	123.9(6)
O(22)-C(22)-C(23)	121.6(6)
O(22)-C(22)-C(21)	116.1(6)
C(23)-C(22)-C(21)	122.3(6)
C(24)-C(23)-C(22)	120.1(7)
C(25)-C(24)-C(23)	119.4(6)
C(25)-C(24)-C(1)	119.3(7)
C(23)-C(24)-C(1)	121.3(7)
C(24)-C(25)-C(26)	120.2(6)
O(26)-C(26)-C(25)	121.1(6)
O(26)-C(26)-C(21)	116.6(5)
C(25)-C(26)-C(21)	122.3(6)
C(7)-C(27)-C(28)	113.8(5)
C(27)-C(28)-C(29)	113.7(6)
C(30)-C(29)-C(28)	112.6(6)
C(20)-C(31)-C(32)	113.1(6)
C(31)-C(32)-C(33)	114.4(7)
C(34)-C(33)-C(32)	113.5(8)
N(41)-C(41)-C(42)	178.4(10)
N(51)-C(51)-C(52)	177.0(9)
N(61)-C(61)-C(62)	179.7(10)
N(71)-C(71)-C(72)	178.6(11)
N(81)-C(81)-C(82)	180.000
N(91)-C(91)-C(92)	180.000

Anisotropic displacement parameters ($Å^2 \times 10^3$) for JOMac. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U11 + ... + 2hka^*b^*U12]$

	U11	U22	U33	U23	U13	U12
C(1)	20(4)	11(4)	20(3)	2(3)	7(2)	7(3)
C(2)	29(4)	15(5)	23(3)	0(3)	2(2)	0(3)
C(3)	27(4)	30(5)	19(3)	0(3)	4(2)	3(3)
C(4)	35(4)	22(5)	17(3)	-3(3)	3(3)	-1(3)
C(5)	47(4)	27(5)	14(3)	-4(3)	4(3)	-3(4)
C(6)	21(4)	32(5)	19(3)	-3(3)	2(2)	6(3)
C(7)	30(4)	6(4)	12(3)	3(3)	6(2)	0(3)
C(8)	16(3)	30(5)	11(3)	-9(3)	3(2)	-7(3)
C(9)	22(4)	12(5)	20(3)	4(3)	4(2)	-6(3)
O(9)	29(3)	32(4)	45(3)	12(3)	8(2)	-3(2)
C(10)	35(4)	8(5)	19(3)	-3(3)	6(3)	-1(3)
C(11)	20(3)	18(5)	11(3)	2(3)	3(2)	-5(3)
C(12)	28(4)	30(6)	13(3)	-4(3)	9(2)	-11(4)
C(13)	27(4)	14(5)	10(3)	3(3)	4(2)	-3(3)
O(13)	30(3)	27(4)	35(2)	12(3)	2(2)	-4(2)
C(14)	29(4)	29(5)	14(3)	-6(3)	11(2)	-9(4)
C(15)	29(4)	19(5)	20(3)	-2(3)	6(2)	-11(3)
C(16)	30(4)	20(5)	16(3)	-4(3)	7(2)	-2(3)
C(17)	32(4)	12(5)	21(3)	-3(3)	12(3)	-5(3)
C(18)	32(4)	7(5)	23(3)	2(3)	10(3)	-5(3)
C(19)	31(3)	7(4)	22(3)	-7(3)	10(2)	-9(3)
C(20)	31(4)	10(5)	12(3)	0(3)	6(2)	-5(3)
C(21)	23(4)	18(5)	13(3)	0(3)	5(2)	0(3)
C(22)	39(4)	5(4)	18(3)	2(3)	10(3)	-4(3)
O(22)	35(3)	24(4)	44(3)	17(3)	8(2)	-2(3)
C(23)	26(4)	28(5)	14(3)	8(3)	4(2)	0(4)
C(24)	25(4)	41(6)	7(3)	-7(3)	7(2)	-2(4)
C(25)	18(4)	12(5)	16(3)	1(3)	4(2)	0(3)
C(26)	34(4)	23(5)	13(3)	7(3)	7(2)	5(4)
O(26)	28(2)	17(4)	39(2)	11(2)	8(2)	1(2)
C(27)	27(4)	16(5)	19(3)	3(3)	2(2)	-2(3)
C(28)	33(4)	31(6)	19(3)	-4(3)	4(3)	-3(4)
C(29)	44(4)	32(6)	20(3)	-3(4)	-3(3)	-9(4)
C(30)	63(5)	34(6)	21(3)	-12(4)	2(3)	8(4)
C(31)	29(4)	29(5)	20(3)	-3(3)	6(3)	-4(3)
C(32)	43(4)	32(6)	22(3)	-3(4)	5(3)	-17(4)
C(33)	88(7)	97(10)	32(4)	-18(5)	15(4)	-60(7)
C(35)	32(4)	23(5)	26(3)	-8(3)	4(3)	5(3)
C(36)	43(4)	50(7)	17(3)	-11(4)	16(3)	-10(4)
N(41)	48(4)	57(7)	56(4)	23(5)	7(3)	6(5)
C(41)	43(5)	39(7)	37(4)	11(4)	11(3)	4(5)
C(42)	82(7)	33(7)	66(5)	11(5)	9(5)	13(5)
N(51)	32(4)	52(7)	81(5)	18(5)	9(3)	2(4)
C(51)	33(4)	21(6)	54(5)	18(4)	7(3)	-1(4)
C(52)	67(5)	6(5)	68(5)	9(4)	3(4)	5(4)
N(61)	35(4)	33(6)	60(4)	15(4)	5(3)	2(4)
C(61)	17(4)	45(7)	32(4)	4(4)	10(3)	0(4)
C(62)	60(5)	33(7)	57(5)	14(5)	9(4)	1(5)
N(71)	42(4)	18(5)	87(5)	16(4)	6(3)	1(4)
C(71)	42(5)	55(8)	47(5)	17(5)	7(4)	-14(5)
C(72)	67(6)	29(6)	68(5)	3(5)	20(4)	-18(5)
N(81)	76(8)	54(10)	50(6)	0	15(5)	0
C(81)	37(6)	42(11)	31(6)	0	6(4)	0
C(82)	76(8)	31(10)	32(6)	0	-3(5)	0
N(91)	98(9)	45(10)	70(7)	0	29(6)	0
C(91)	36(6)	40(10)	31(6)	0	-3(4)	0
C(92)	198(16)	14(9)	29(6)	0	6(8)	0

Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($Å^2 \times 10^3$) for JOMac.

	x	y	z	U(eq)
H(1)	6981	2455	6166	20
H(2A)	7208	923	6952	27
H(2B)	7998	1742	6769	27
H(3A)	6392	2739	7087	30
H(3B)	7204	3542	6918	30
H(4A)	7424	2010	7705	30
H(4B)	8186	2922	7545	30
H(5A)	6476	3753	7815	35
H(5B)	7273	4640	7680	35
H(6A)	8206	4008	8329	29
H(6B)	7421	3095	8463	29
H(7)	7269	5725	8424	19
H(9)	5647	7441	8181	52
H(10)	4276	6555	8267	25
H(12)	4389	3182	8860	28
H(13)	5793	2341	8962	46
H(14)	2915	5686	8433	28
H(15A)	2022	3932	8305	27
H(15B)	2883	3066	8436	27
H(16A)	2677	4632	7661	26
H(16B)	3583	3859	7799	26
H(17A)	1844	2822	7512	26
H(17B)	2700	1999	7695	26
H(18A)	2595	3452	6892	24
H(18B)	3500	2742	7082	24
H(19A)	1834	1545	6775	24
H(19B)	2739	834	6967	24
H(20)	2607	2311	6164	21
H(22)	4379	-885	6810	51
H(23)	5737	-1	6664	27
H(25)	5553	3286	6043	18
H(26)	4115	4105	5928	42
H(27A)	8251	5101	9039	25
H(27B)	7474	4244	9215	25
H(28A)	6606	5969	9373	33
H(28B)	7298	6868	9150	33
H(29A)	7780	5495	9961	39
H(29B)	8444	6444	9741	39
H(30A)	7801	7369	10345	59
H(30B)	6800	7130	10105	59
H(30C)	7470	8077	9888	59
H(31A)	1775	375	6093	31
H(31B)	2737	-316	6157	31
H(32A)	3171	745	5497	39
H(32B)	2164	1301	5425	39
H(33A)	1603	-816	5343	86
H(33B)	2144	-326	4938	86
H(34A)	2606	-2294	5130	124
H(34B)	2888	-1867	5637	124
H(34C)	3440	-1363	5238	124
H(35A)	7820	637	6030	40
H(35B)	6860	639	5732	40
H(35C)	6998	-194	6176	40
H(36A)	2197	4881	9051	54
H(36B)	3111	5607	9219	54
H(36C)	3105	4131	9212	54
H(42A)	5459	11825	8000	90
H(42B)	4394	11724	7843	90
H(42C)	5128	11501	7488	90
H(52A)	5190	-1908	9527	71
H(52B)	5542	-2004	9036	71
H(52C)	4475	-1883	9090	71
H(62A)	4909	-4987	7435	75
H(62B)	5529	-5242	7031	75
H(62C)	4443	-5243	6938	75
H(72A)	5464	8158	5493	81
H(72B)	6003	7884	5973	81
H(72C)	4988	8424	5944	81
H(82A)	5626	3391	9997	70
H(82B)	4632	3391	9732	70
H(82C)	4742	3391	10271	70
H(92A)	4377	2643	5018	121
H(92B)	5230	2643	4722	121
H(92C)	5392	2643	5260	121

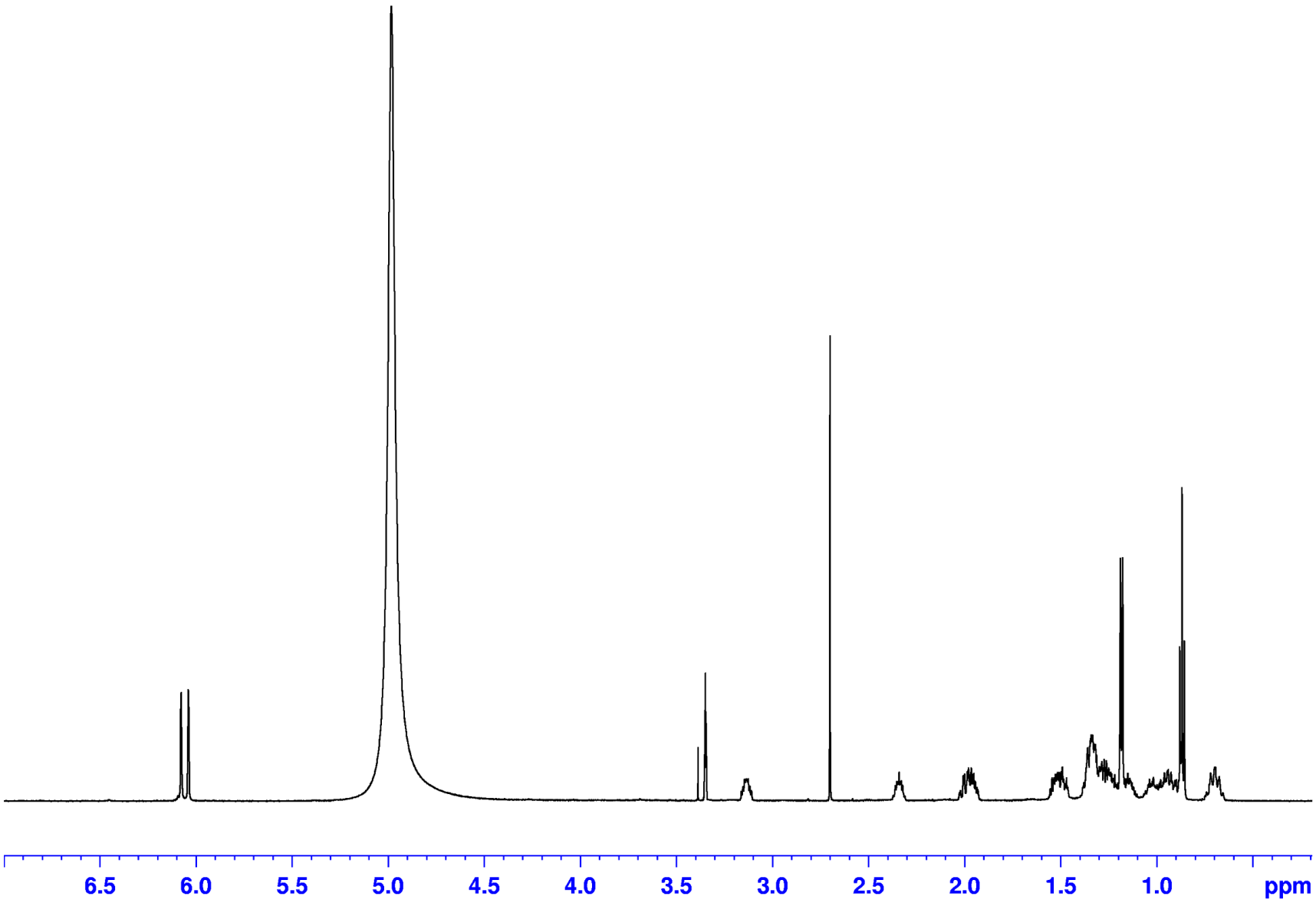
Torsion angles [deg] for JOMac.

C(24)-C(1)-C(2)-C(3)	-57.9(8)
C(35)-C(1)-C(2)-C(3)	177.8(6)
C(1)-C(2)-C(3)-C(4)	178.1(6)
C(2)-C(3)-C(4)-C(5)	-174.9(6)
C(3)-C(4)-C(5)-C(6)	176.7(6)
C(4)-C(5)-C(6)-C(7)	-178.8(5)
C(5)-C(6)-C(7)-C(8)	57.0(8)
C(5)-C(6)-C(7)-C(27)	-175.4(5)
C(27)-C(7)-C(8)-C(13)	-66.2(8)
C(6)-C(7)-C(8)-C(13)	60.5(7)
C(27)-C(7)-C(8)-C(9)	112.9(6)
C(6)-C(7)-C(8)-C(9)	-120.4(6)
C(13)-C(8)-C(9)-O(9)	-178.8(5)
C(7)-C(8)-C(9)-O(9)	2.1(8)
C(13)-C(8)-C(9)-C(10)	1.3(8)
C(7)-C(8)-C(9)-C(10)	-177.9(6)
O(9)-C(9)-C(10)-C(11)	180.0(5)
C(8)-C(9)-C(10)-C(11)	-0.1(9)
C(9)-C(10)-C(11)-C(12)	-1.5(8)
C(9)-C(10)-C(11)-C(14)	179.8(5)
C(10)-C(11)-C(12)-C(13)	1.8(8)
C(14)-C(11)-C(12)-C(13)	-179.5(5)
C(9)-C(8)-C(13)-O(13)	178.8(5)
C(7)-C(8)-C(13)-O(13)	-2.0(8)
C(9)-C(8)-C(13)-C(12)	-1.0(8)
C(7)-C(8)-C(13)-C(12)	178.2(5)
C(11)-C(12)-C(13)-O(13)	179.7(5)
C(11)-C(12)-C(13)-C(8)	-0.5(9)
C(10)-C(11)-C(14)-C(15)	117.1(7)
C(12)-C(11)-C(14)-C(15)	-61.6(7)
C(10)-C(11)-C(14)-C(36)	-117.2(7)
C(12)-C(11)-C(14)-C(36)	64.1(8)
C(11)-C(14)-C(15)-C(16)	-56.8(8)
C(36)-C(14)-C(15)-C(16)	177.8(6)
C(14)-C(15)-C(16)-C(17)	175.7(6)
C(15)-C(16)-C(17)-C(18)	-174.1(5)
C(16)-C(17)-C(18)-C(19)	174.8(6)
C(17)-C(18)-C(19)-C(20)	-179.9(5)
C(18)-C(19)-C(20)-C(31)	-174.4(6)
C(18)-C(19)-C(20)-C(21)	60.0(8)
C(31)-C(20)-C(21)-C(26)	118.2(6)
C(19)-C(20)-C(21)-C(26)	-115.8(6)
C(31)-C(20)-C(21)-C(22)	-62.3(7)
C(19)-C(20)-C(21)-C(22)	63.7(8)
C(26)-C(21)-C(22)-O(22)	177.4(5)
C(20)-C(21)-C(22)-O(22)	-2.1(9)
C(26)-C(21)-C(22)-C(23)	-2.0(9)
C(20)-C(21)-C(22)-C(23)	178.5(6)
O(22)-C(22)-C(23)-C(24)	-179.6(6)
C(21)-C(22)-C(23)-C(24)	-0.2(9)
C(22)-C(23)-C(24)-C(25)	3.1(9)
C(22)-C(23)-C(24)-C(1)	-178.6(5)
C(2)-C(1)-C(24)-C(25)	116.3(6)
C(35)-C(1)-C(24)-C(25)	-118.7(6)
C(2)-C(1)-C(24)-C(23)	-62.1(8)
C(35)-C(1)-C(24)-C(23)	63.0(7)
C(23)-C(24)-C(25)-C(26)	-3.6(9)
C(1)-C(24)-C(25)-C(26)	178.0(5)
C(24)-C(25)-C(26)-O(26)	-177.4(5)
C(24)-C(25)-C(26)-C(21)	1.3(9)
C(22)-C(21)-C(26)-O(26)	-179.8(5)
C(20)-C(21)-C(26)-O(26)	-0.2(8)
C(22)-C(21)-C(26)-C(25)	1.4(9)
C(20)-C(21)-C(26)-C(25)	-179.0(5)
C(8)-C(7)-C(27)-C(28)	-55.4(8)
C(6)-C(7)-C(27)-C(28)	175.9(5)
C(7)-C(27)-C(28)-C(29)	-173.3(6)
C(27)-C(28)-C(29)-C(30)	-177.5(6)
C(21)-C(20)-C(31)-C(32)	-69.9(7)
C(19)-C(20)-C(31)-C(32)	164.5(5)
C(20)-C(31)-C(32)-C(33)	174.2(7)
C(31)-C(32)-C(33)-C(34)	-73.0(9)

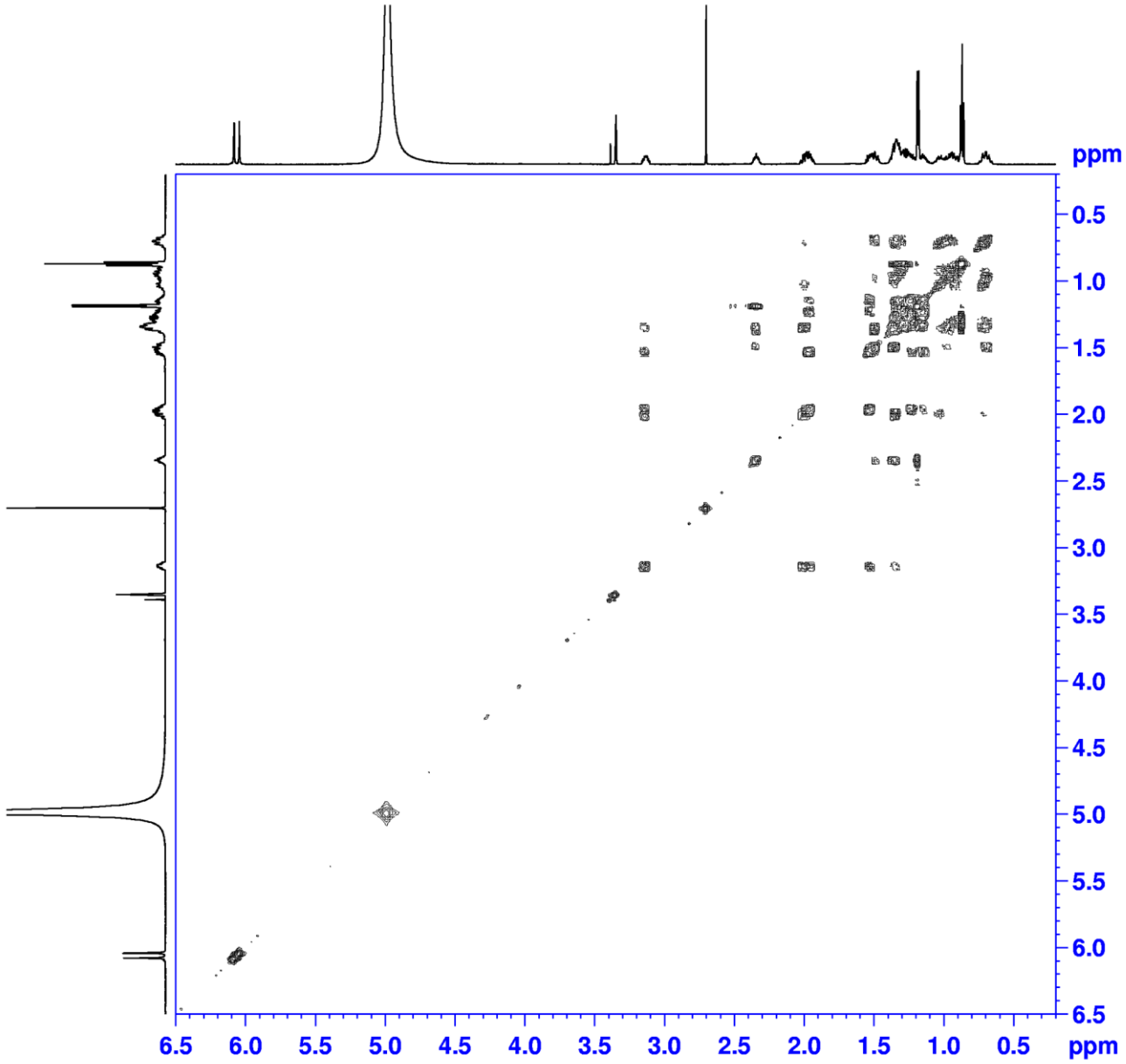
Hydrogen bonds for JOMac [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(1)-H(1)...N(57)	0.82	2.05	2.857(10)	166
O(2)-H(2A)...N(53)	0.82	2.04	2.838(10)	166
O(3)-H(3)...N(51)	0.82	2.03	2.849(10)	172
O(4)-H(4A)...N(55)	0.82	2.04	2.837(10)	163

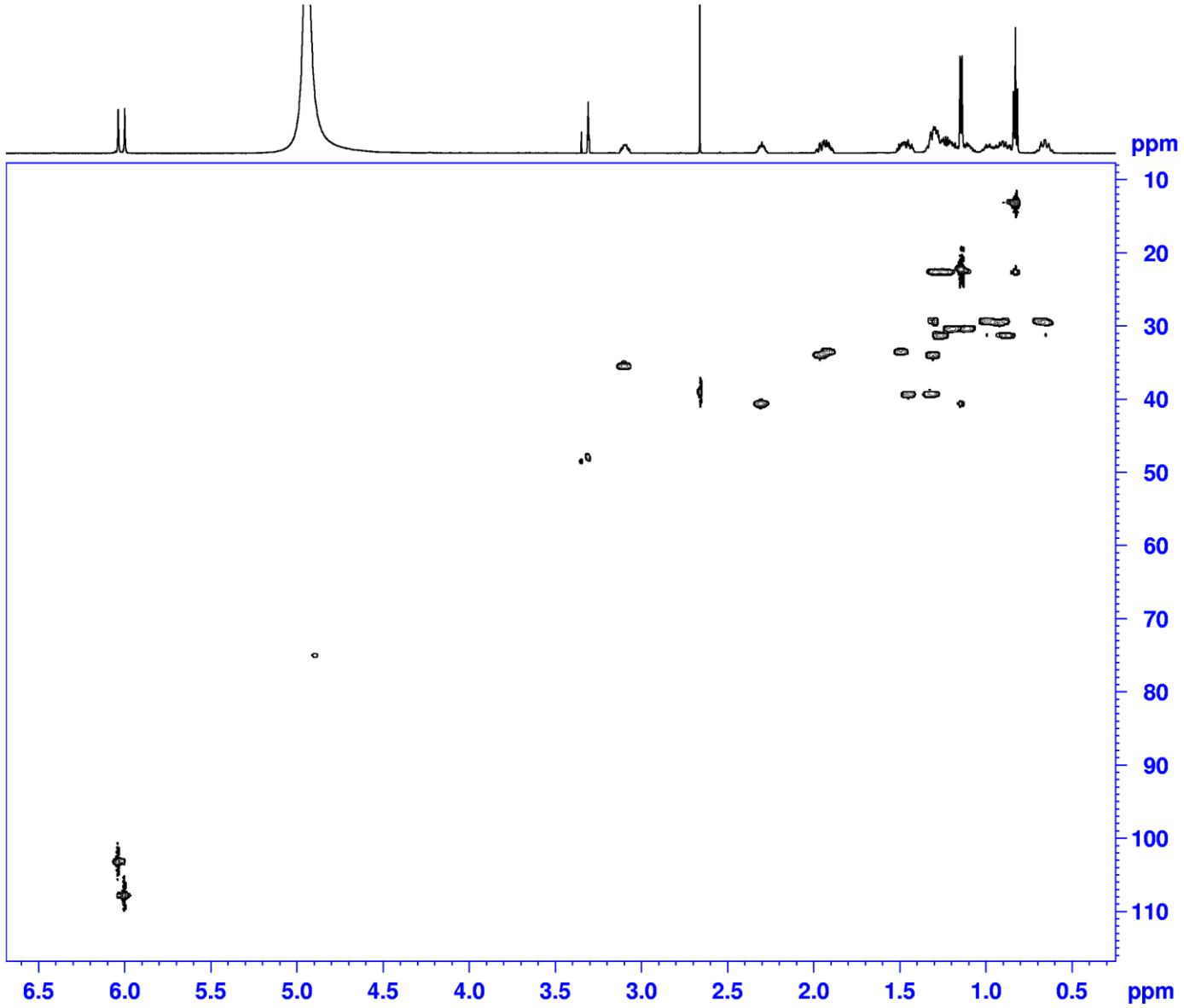
S3. ^{1}H NMR spectrum (600 MHz, MeOH-d_4) of **1**



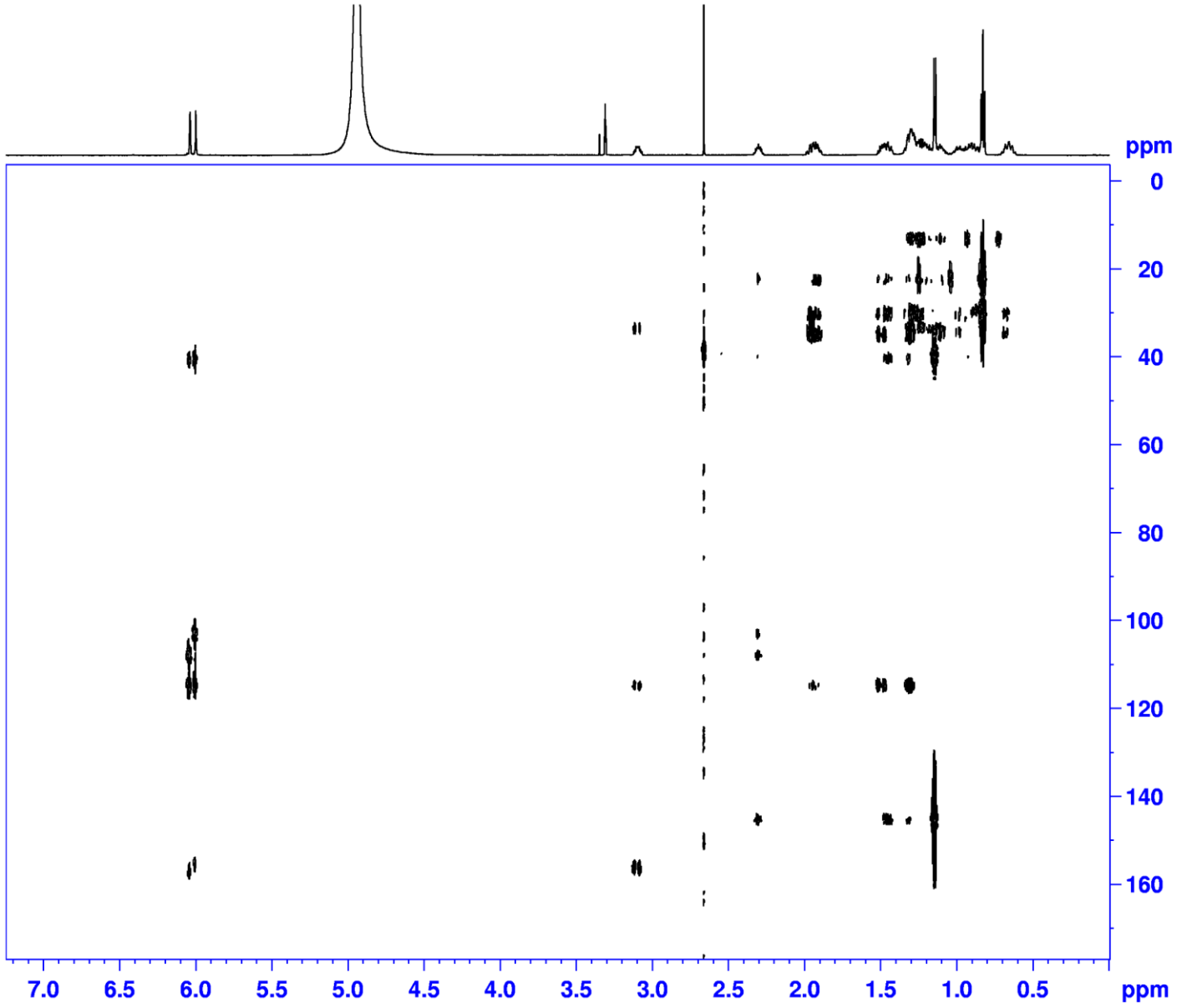
S4. COSY spectrum (600 MHz, MeOH-d_4) of **1**



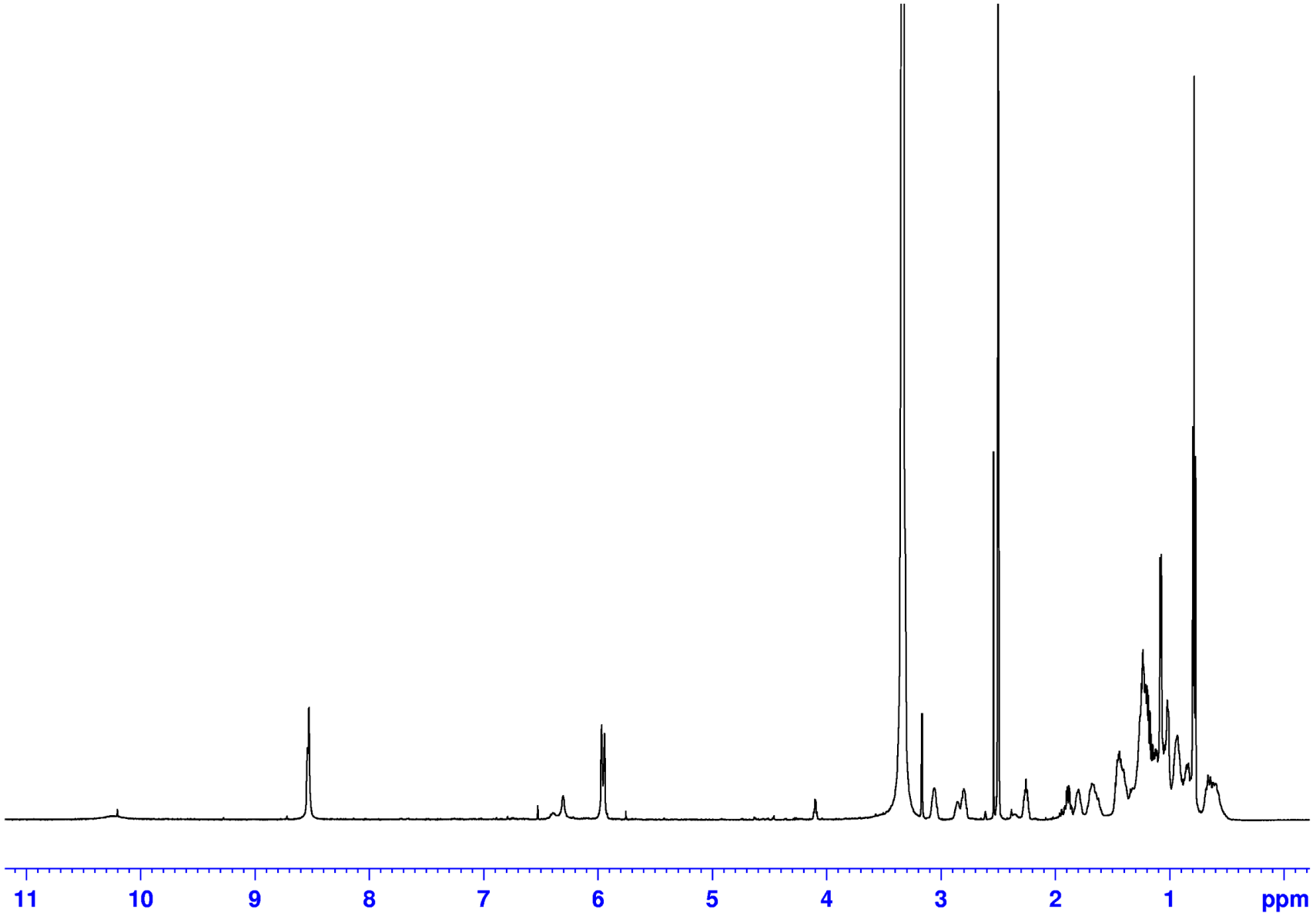
S5. HSQC spectrum (600 MHz, MeOH-d_4) of **1**



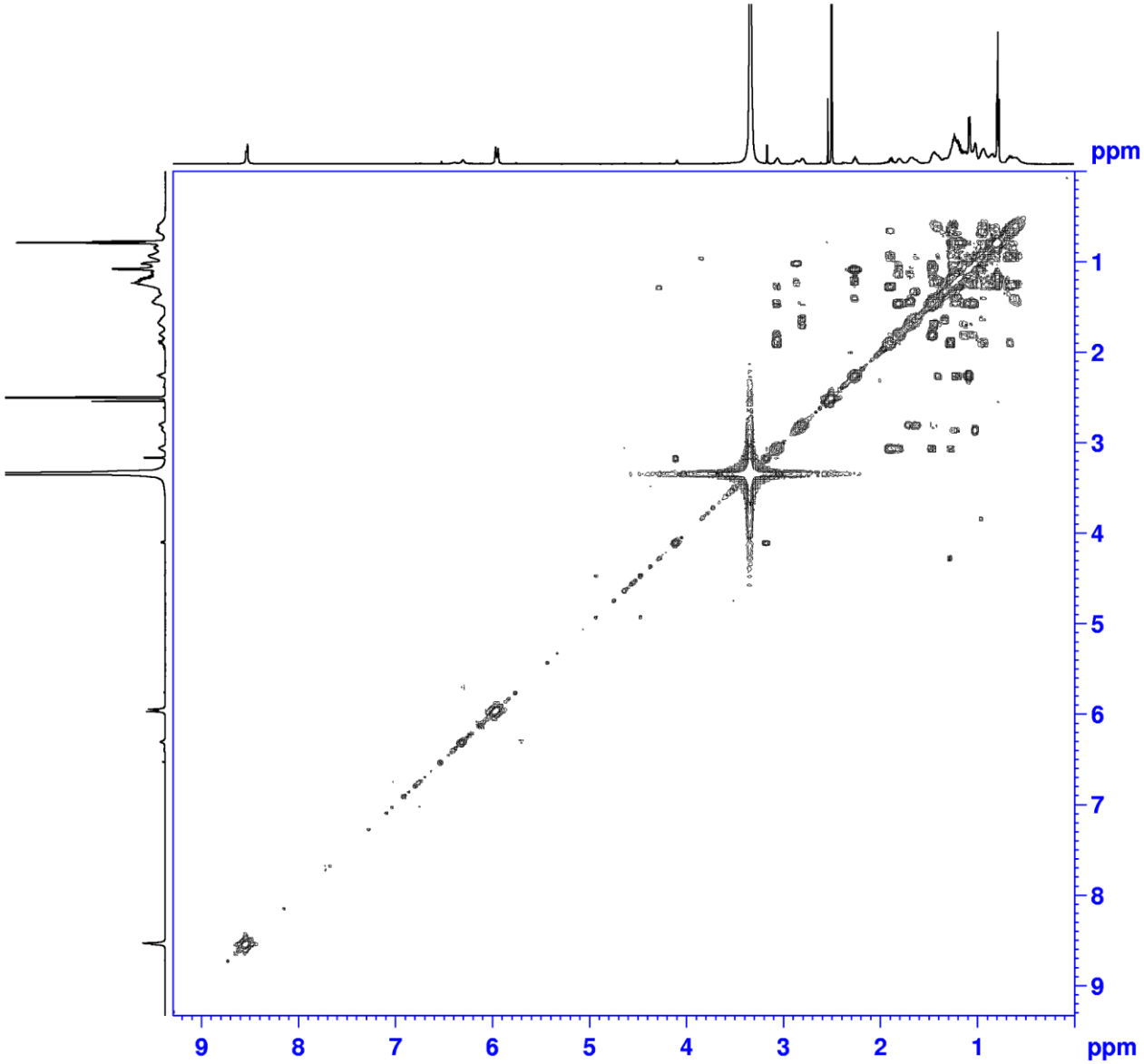
S6. HMBC spectrum (600 MHz, MeOH-d_4) of **1**



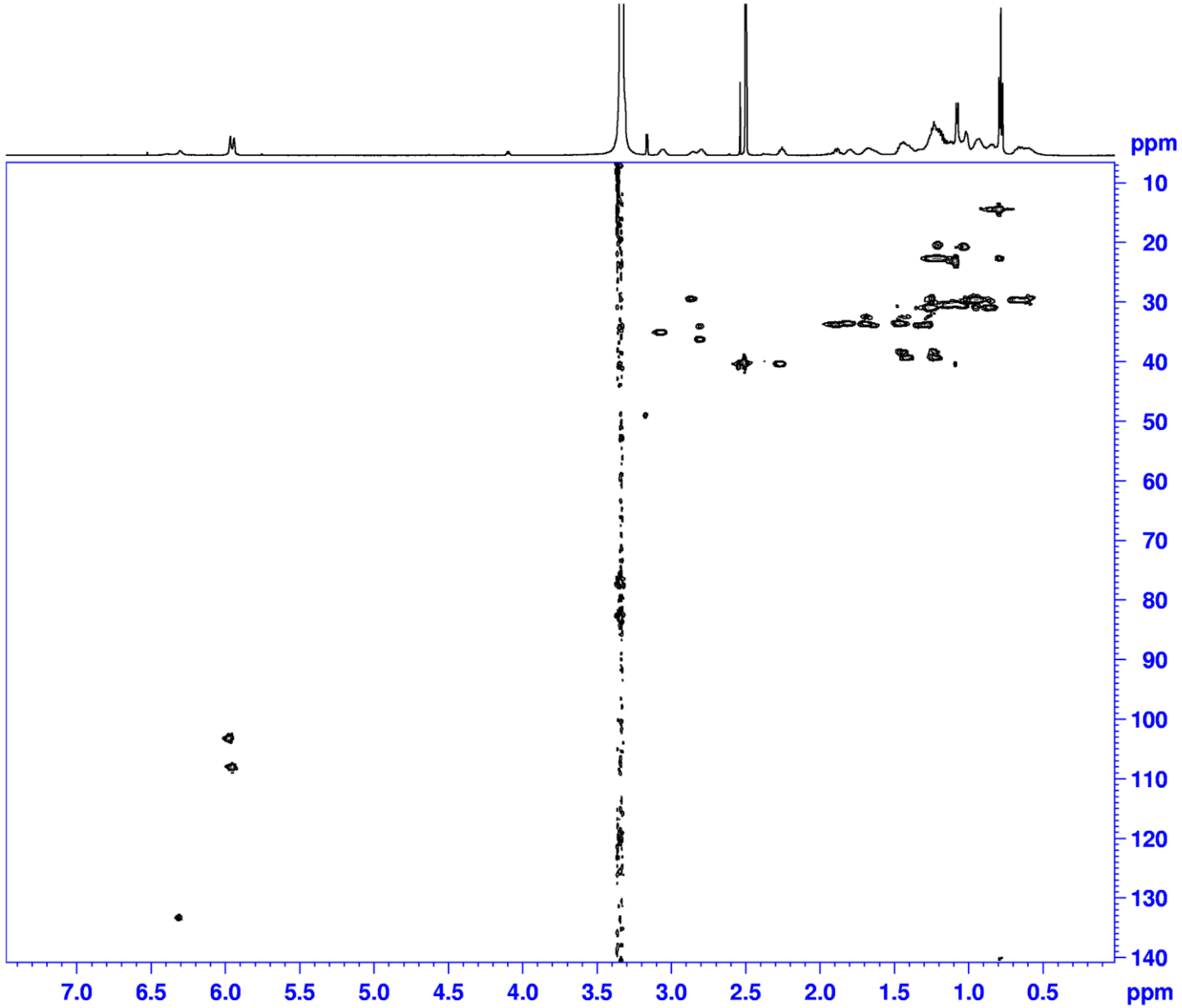
S7. ^{1}H NMR spectrum (600 MHz, DMSO-d_6) of **2**



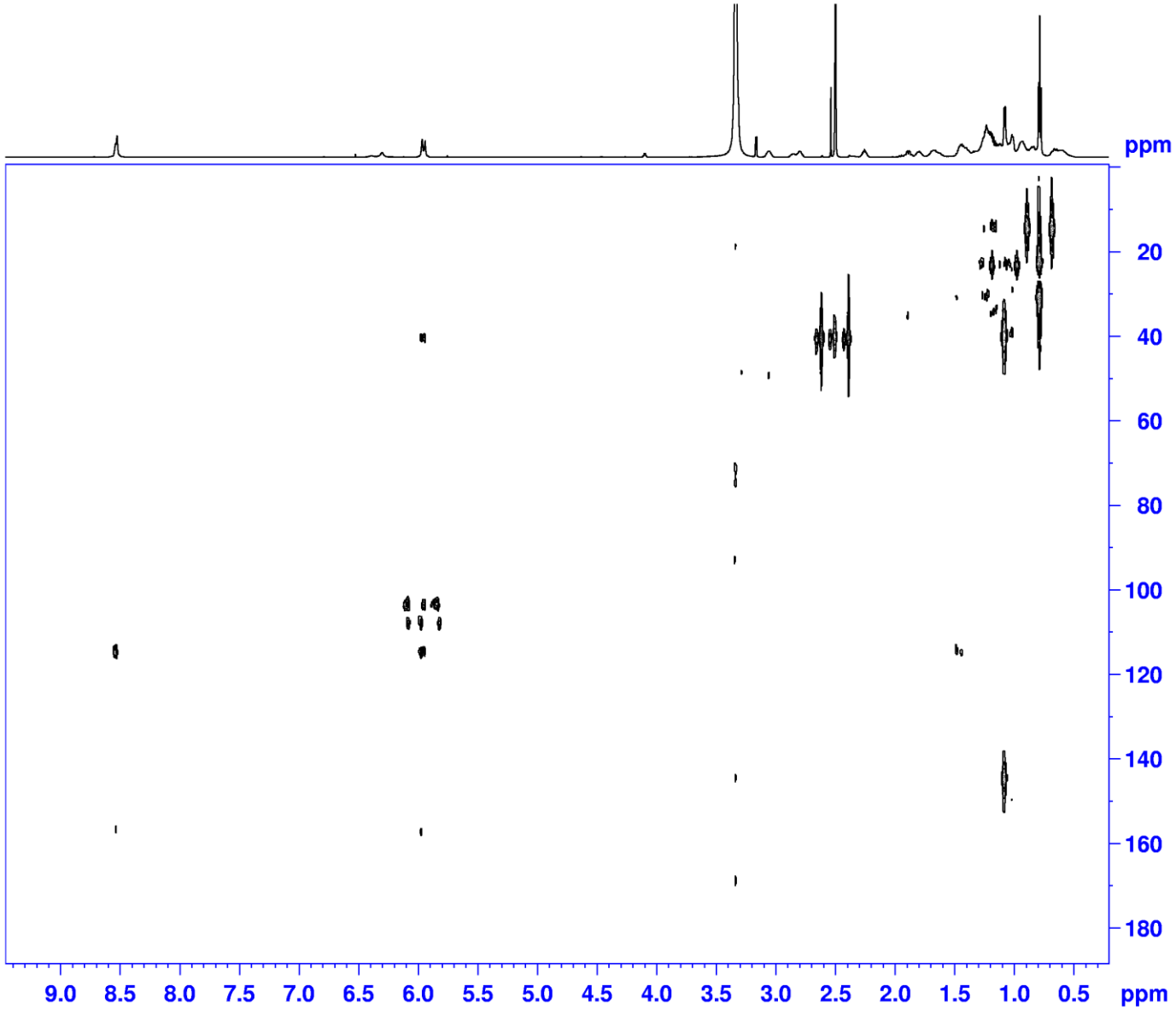
S8. COSY spectrum (600 MHz, DMSO-d_6) of **2**



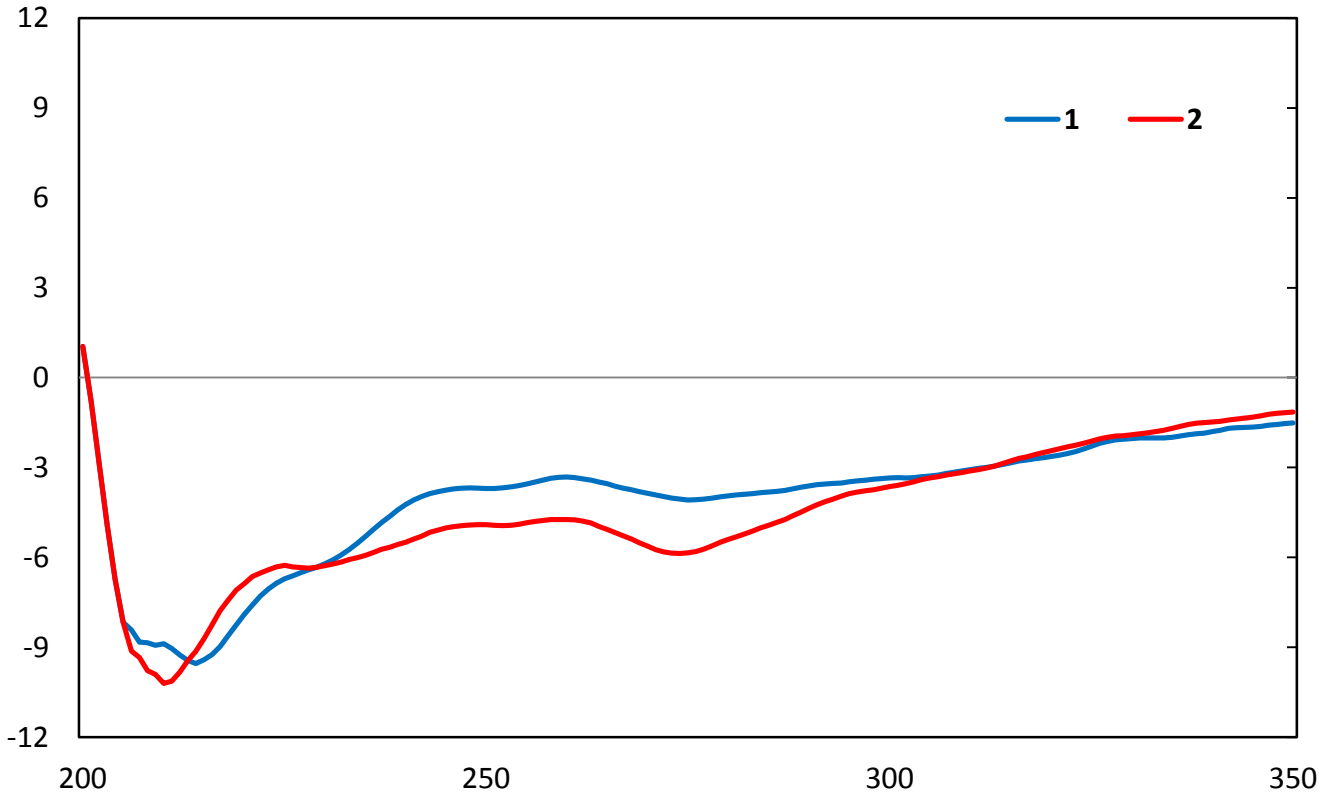
S9. HSQC spectrum (600 MHz, DMSO-d_6) of **2**



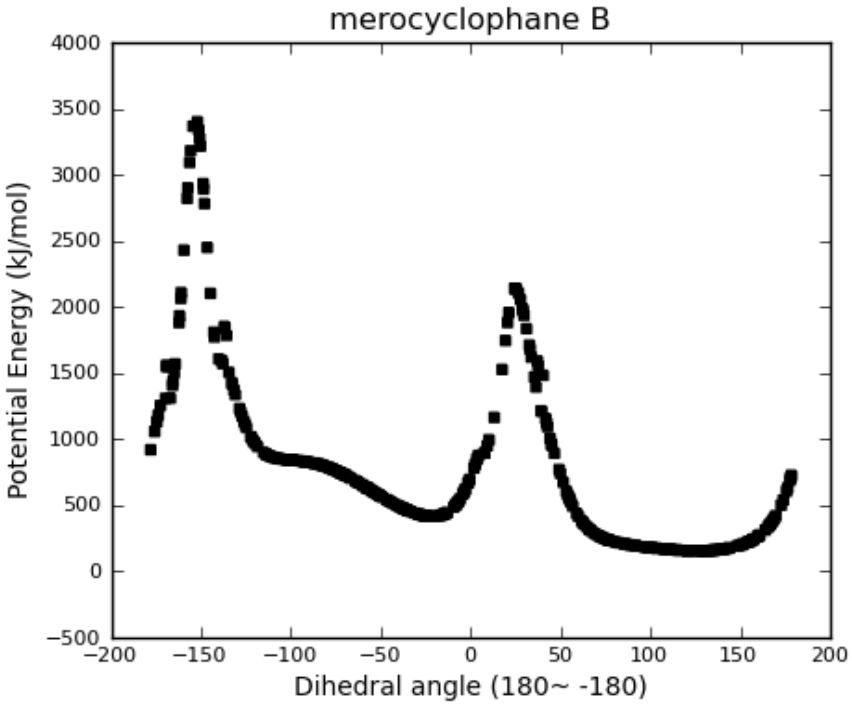
S10. HMBC spectrum (600 MHz, DMSO-d_6) of **2**



S11. CD spectra of **1** and **2**



S12. Torsion energy profile of the hydroxyquinone ring in **2**



The hydroxyquinone ring was rotated 360 degree with 1 degree increment while freezing the remaining atoms. The total energy was calculated *in vacuo* at each degree increment using Maestro 9.2 with the MM3 force field.

- Maestro, version 9.2, Schrödinger, LLC, New York, NY, 2011.
- Norman L. Allinger; Young H. Yuh; Jenn Huei Lii *J. Am. Chem. Soc.*, 1989, 111 (23), pp 8551–8566 **DOI:** 10.1021/ja00205a001