Supplementary data

New ophiobolins from the deep-sea derived fungus *Aspergillus sp*. WHU0154 and their anti-inflammatory effects

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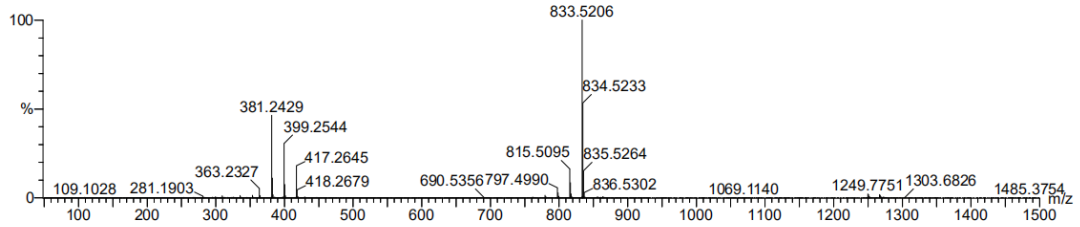
Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
849 formula(e) evaluated with 2 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 0-50 H: 0-100 N: 0-10 O: 0-100
0154-78-67-5-5
20191216009 172 (1.388)

1: TOF MS ES+
1.45e+006



Minimum:				-1.5				
Maximum:		5.0	5.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
417.2645	417.2641	0.4	1.0	7.5	384.9	0.219	80.36	C25 H37 O5
	417.2654	-0.9	-2.2	12.5	386.4	1.628	19.64	C26 H33 N4 O

Fig. S1 HR ESI-Q-TOF-MS spectrum of compound **1**

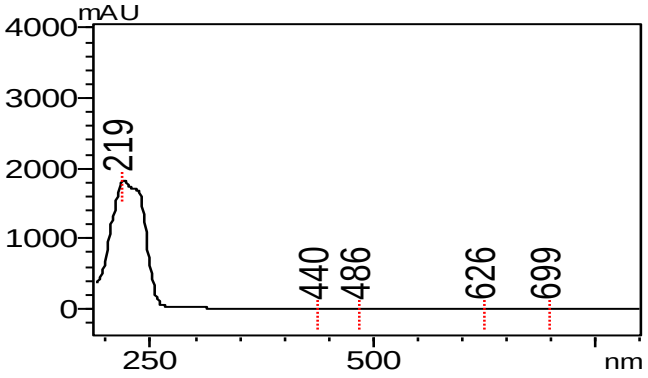


Fig. S2 UV spectrum of compound **1**

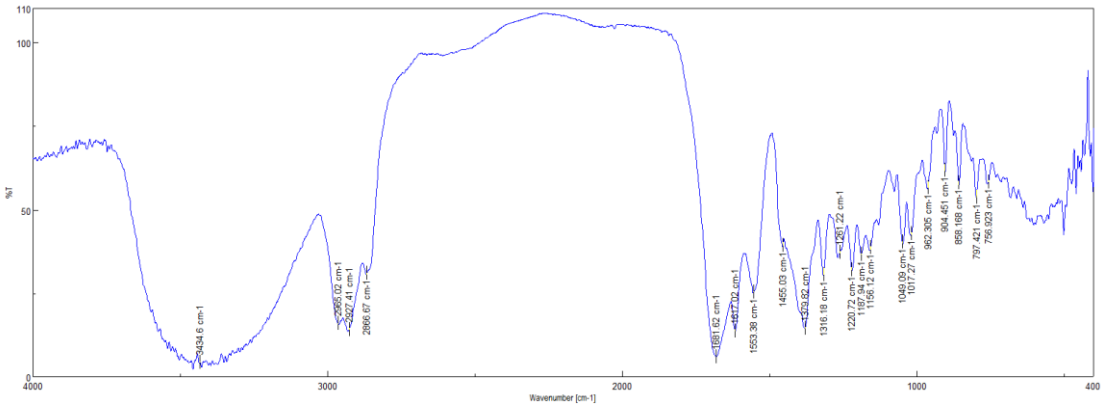


Fig. S3 IR spectrum of compound **1**

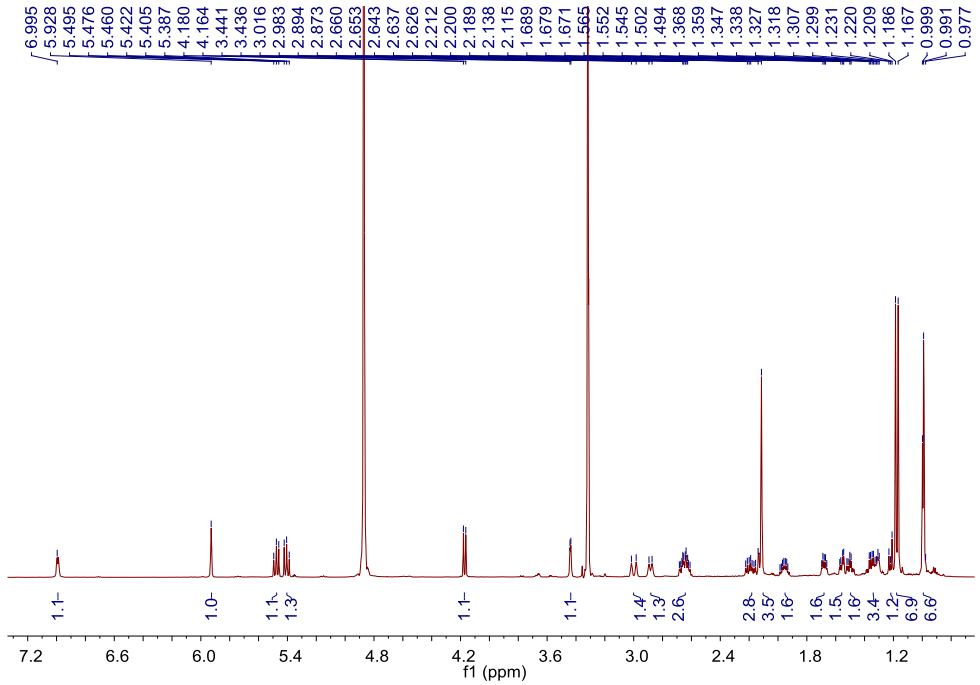


Fig. S4 ^{1}H-NMR spectrum of compound **1** (in CD_3OD)

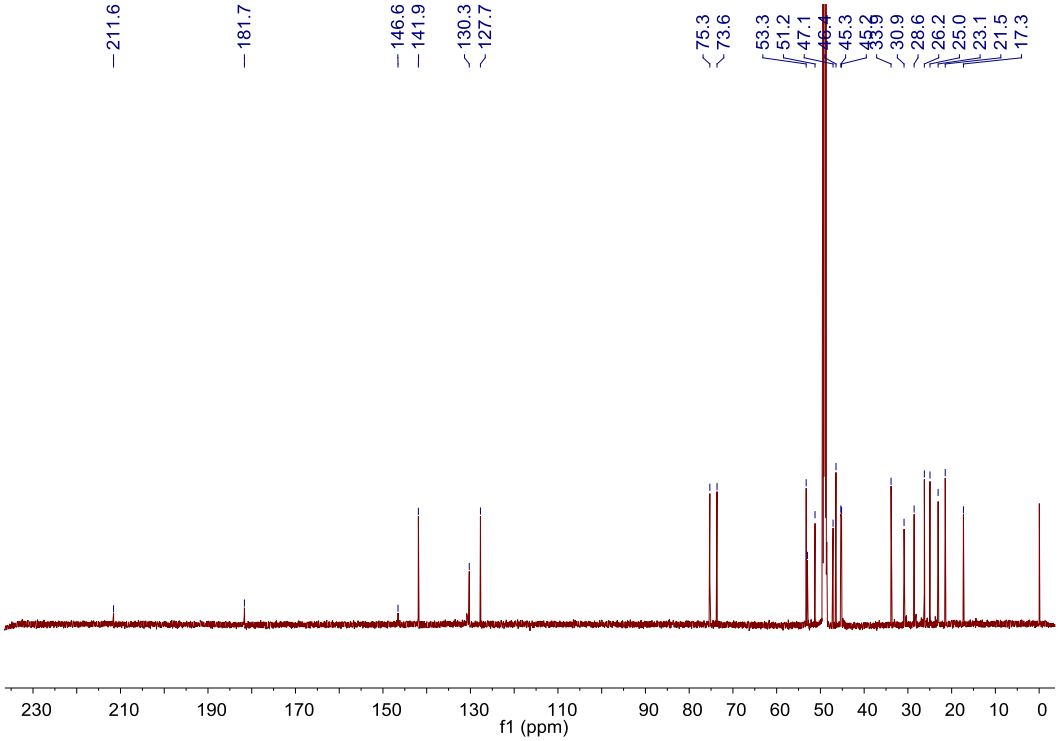


Fig. S5 ^{13}C-NMR spectrum of compound **1** (in CD_3OD)

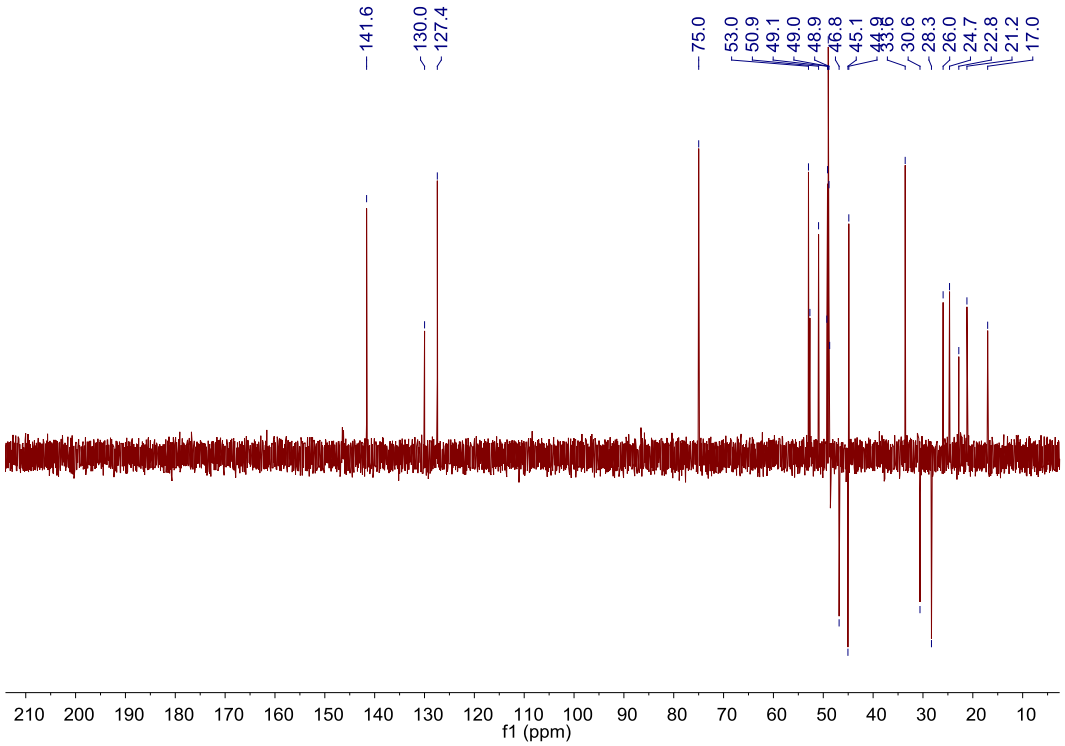


Fig. S6 DEPT135 spectrum of compound **1** (in CD_3OD)

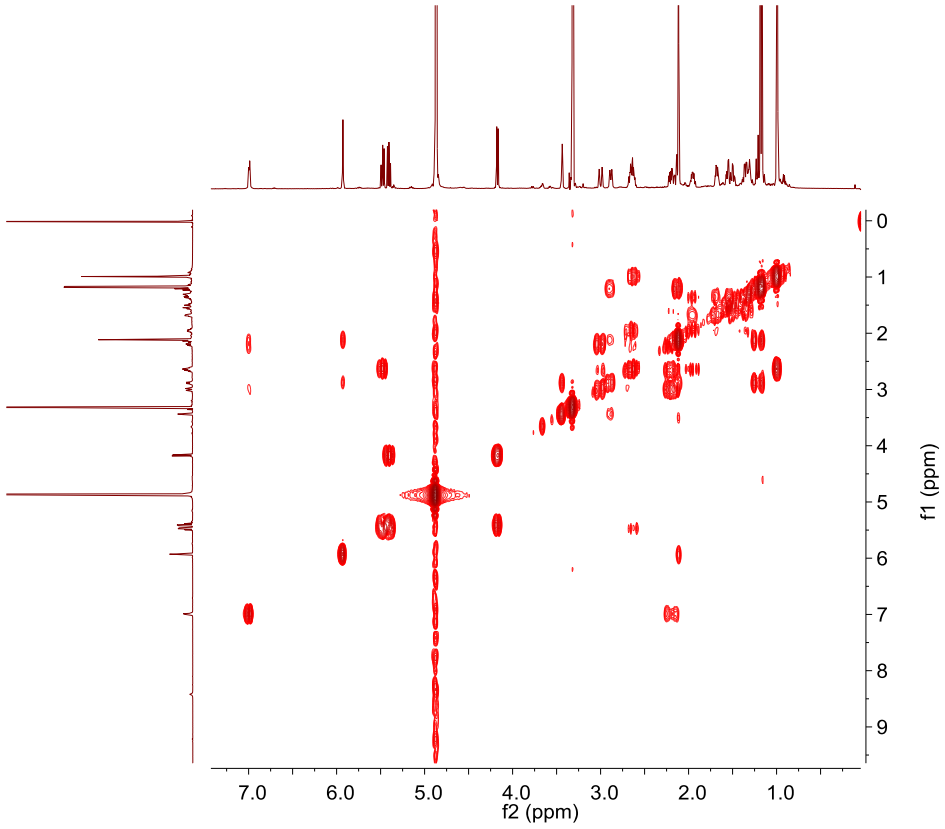


Fig. S7 ^{1}H-^{1}H COSY spectrum of compound **1** (in CD_3OD)

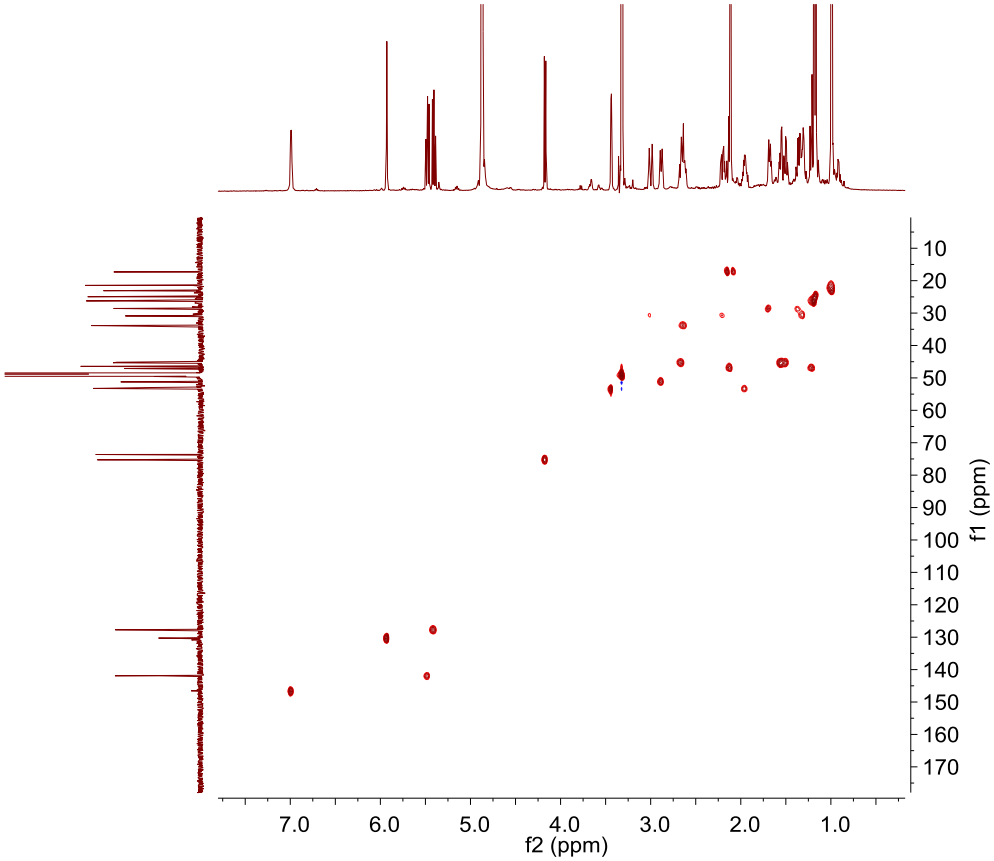


Fig. S8 HSQC spectrum of compound **1** (in CD_3OD)

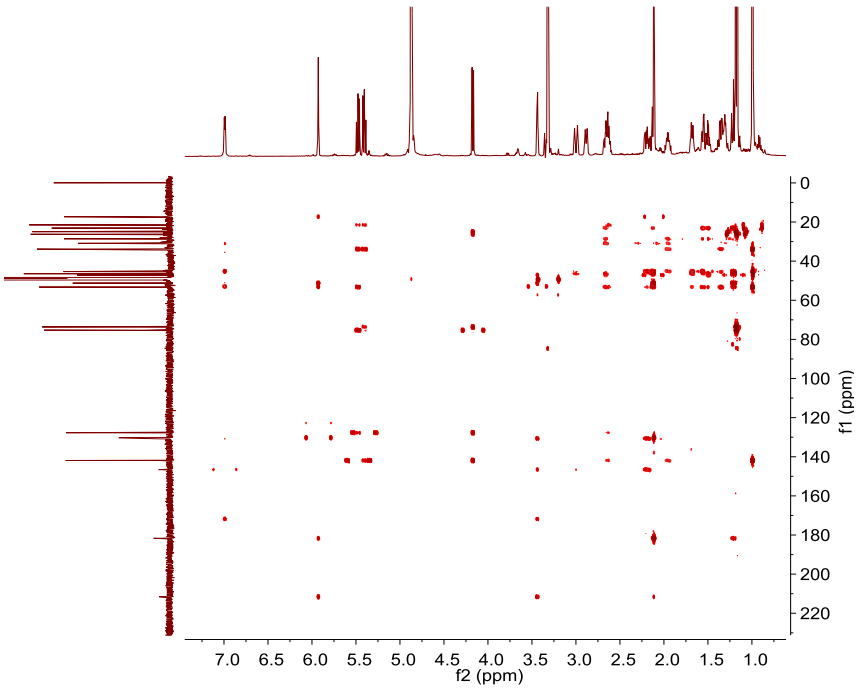


Fig. S9 HMBC spectrum of compound **1** (in CD3OD).

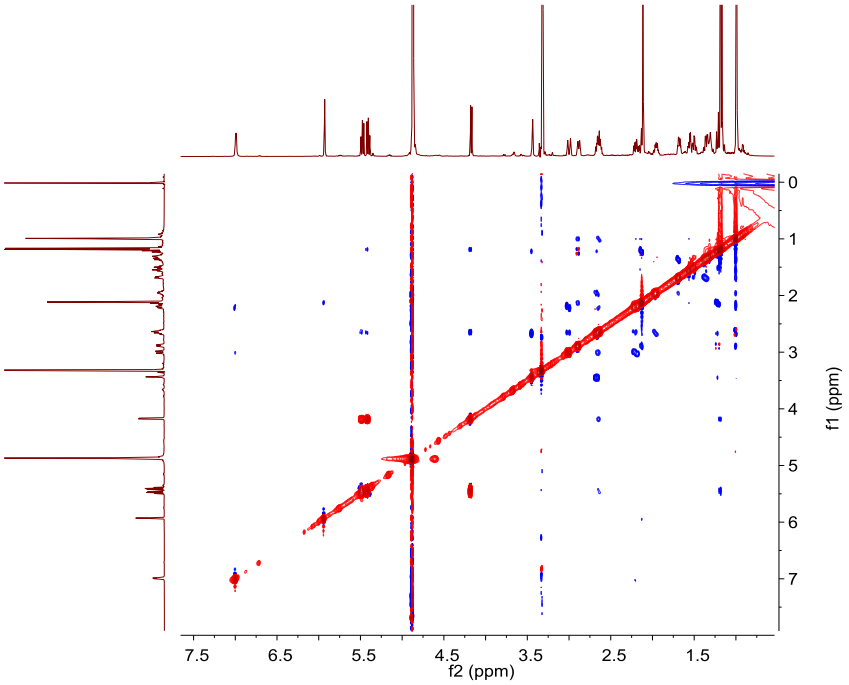


Fig. S10 ROESY spectrum of compound **1** (in CD3OD).

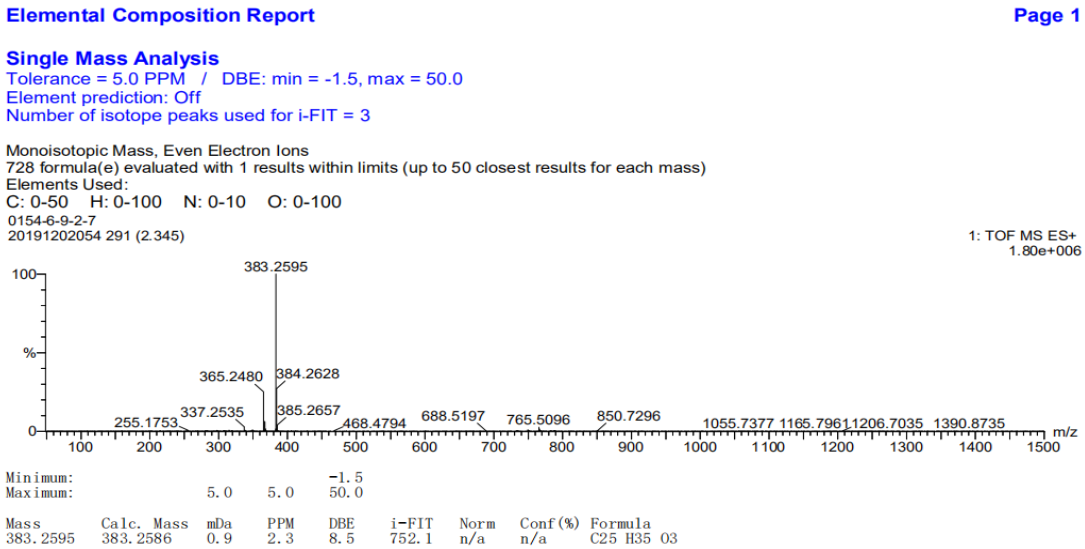


Fig. S11 HR ESI-Q-TOF-MS spectrum of compound **2**

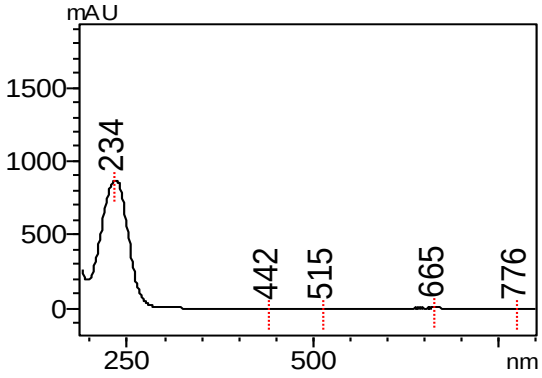


Fig. S12 UV spectrum of compound **2**

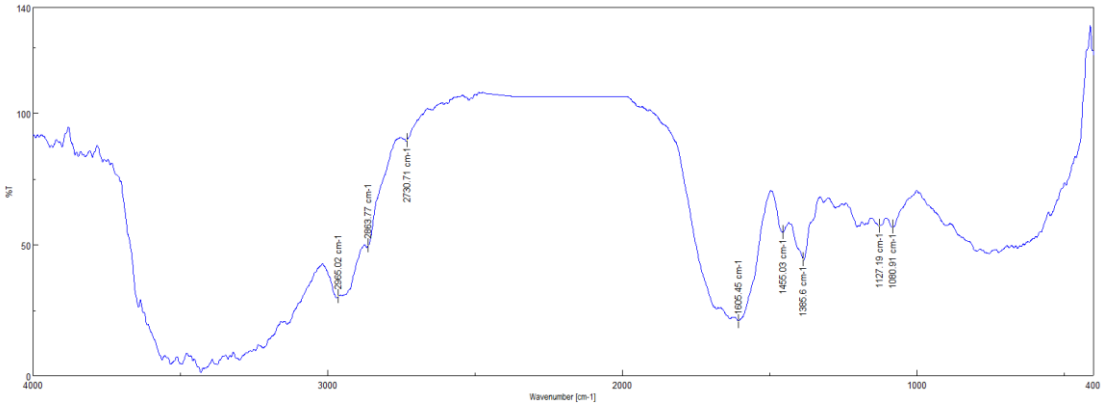


Fig. S13 IR spectrum of compound **2**

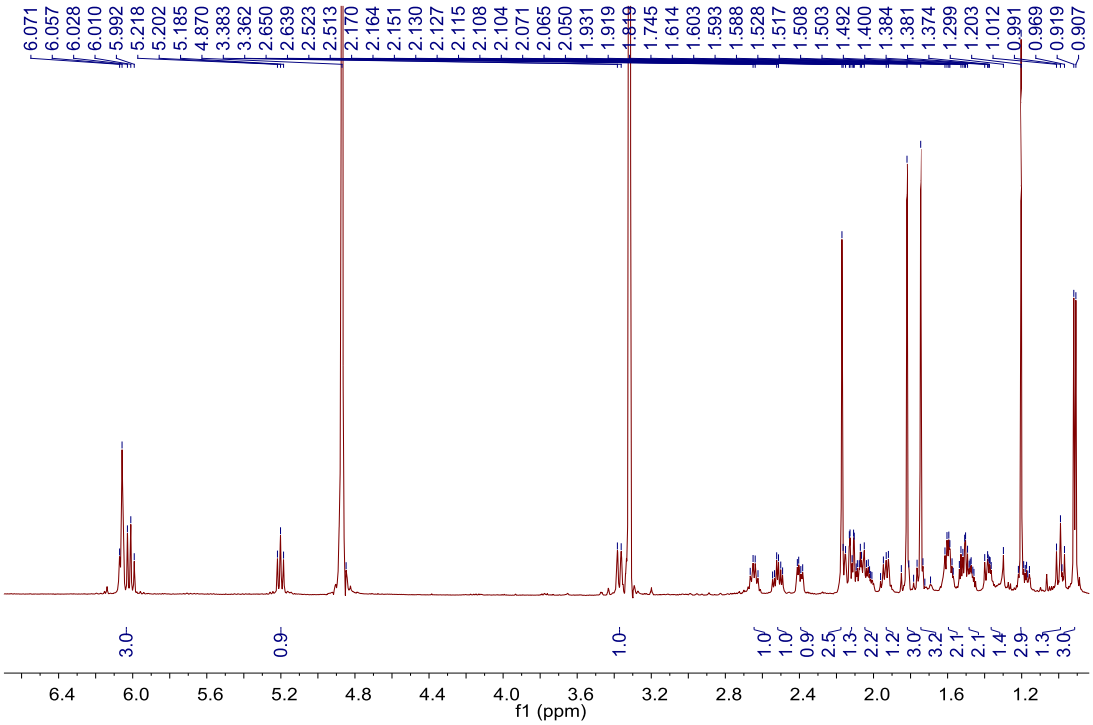


Fig. S14 ^{1}H-NMR spectrum of compound **2** (in CD_3OD)

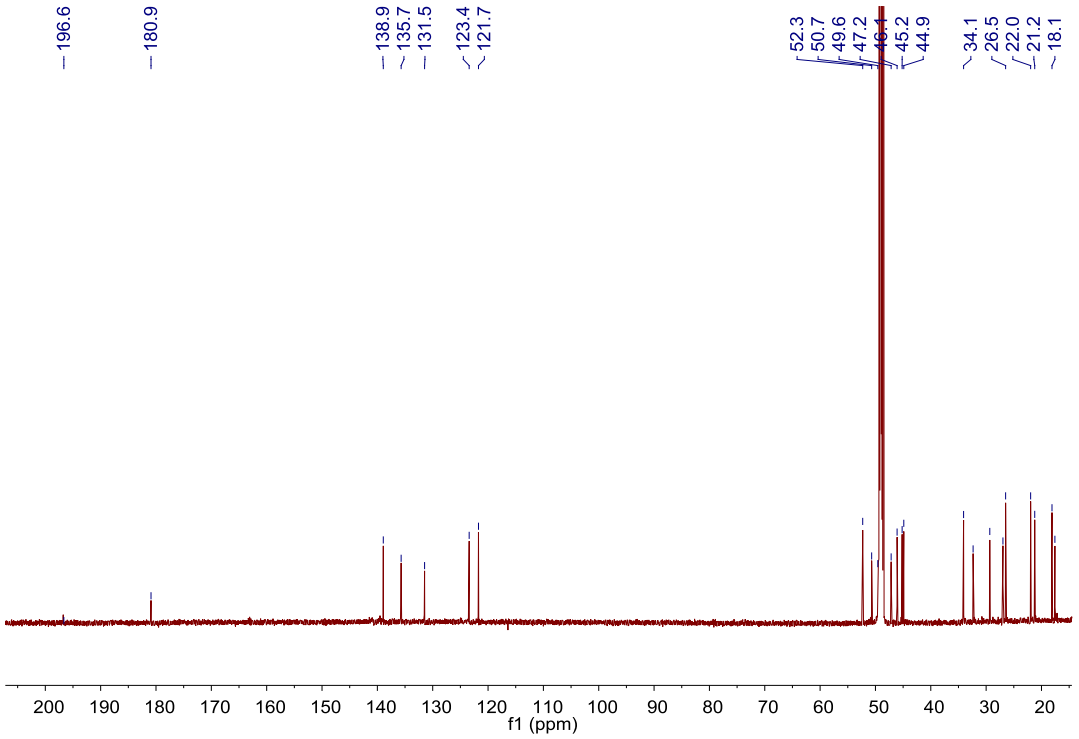


Fig. S15 ^{13}C-NMR spectrum of compound **2** (in CD_3OD)

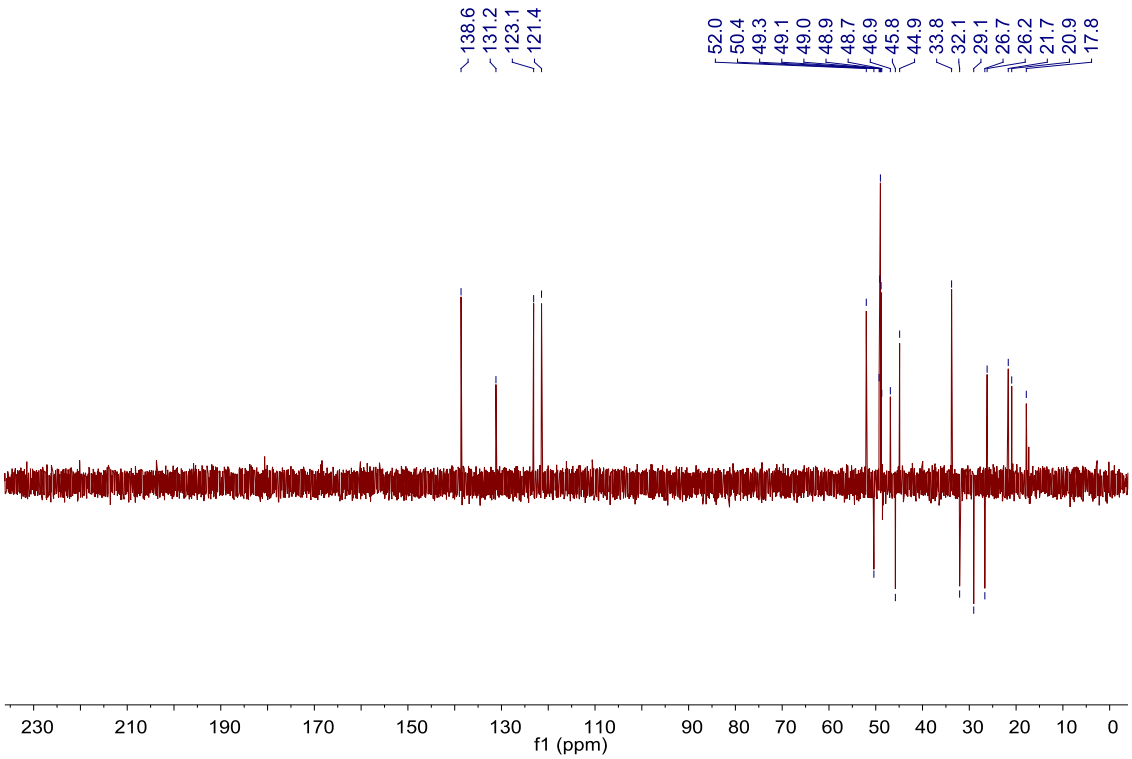


Fig. S16 DEPT135 spectrum of compound **2** (in CD_3OD)

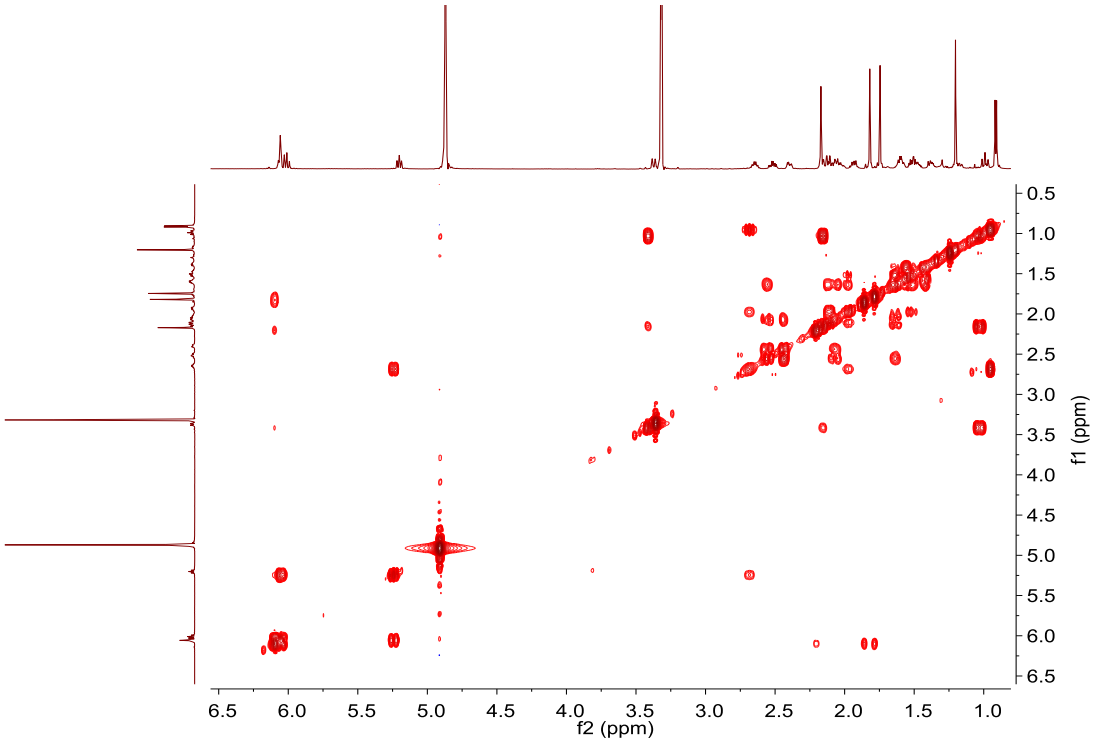


Fig. S17 ^{1}H-^{1}H COSY spectrum of compound **2** (in CD_3OD)

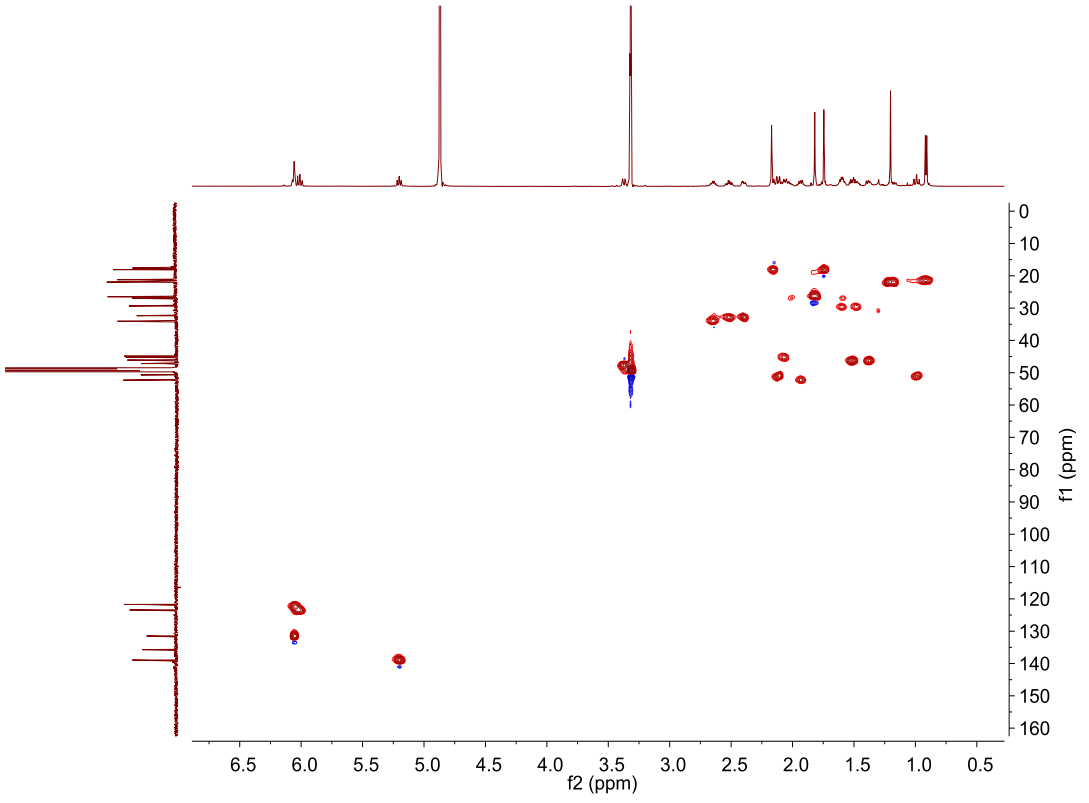


Fig. S18 HSQC spectrum of compound **2** (in CD_3OD)

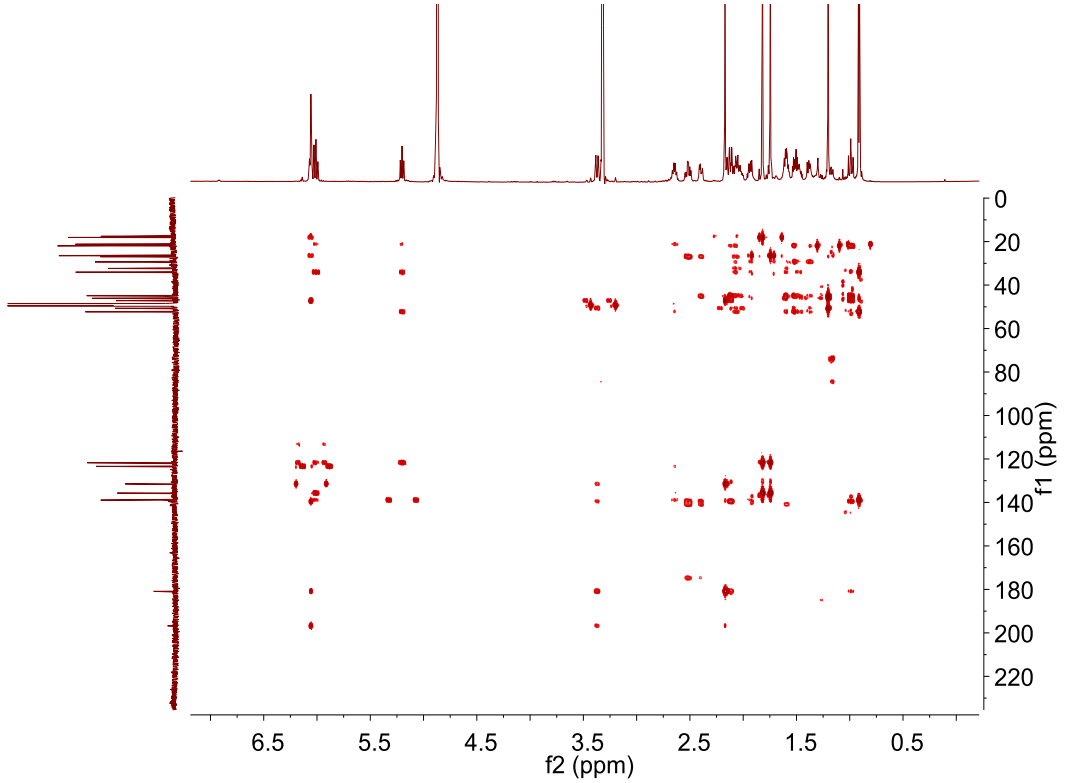


Fig. S19 HMBC spectrum of compound **2** (in CD3OD)

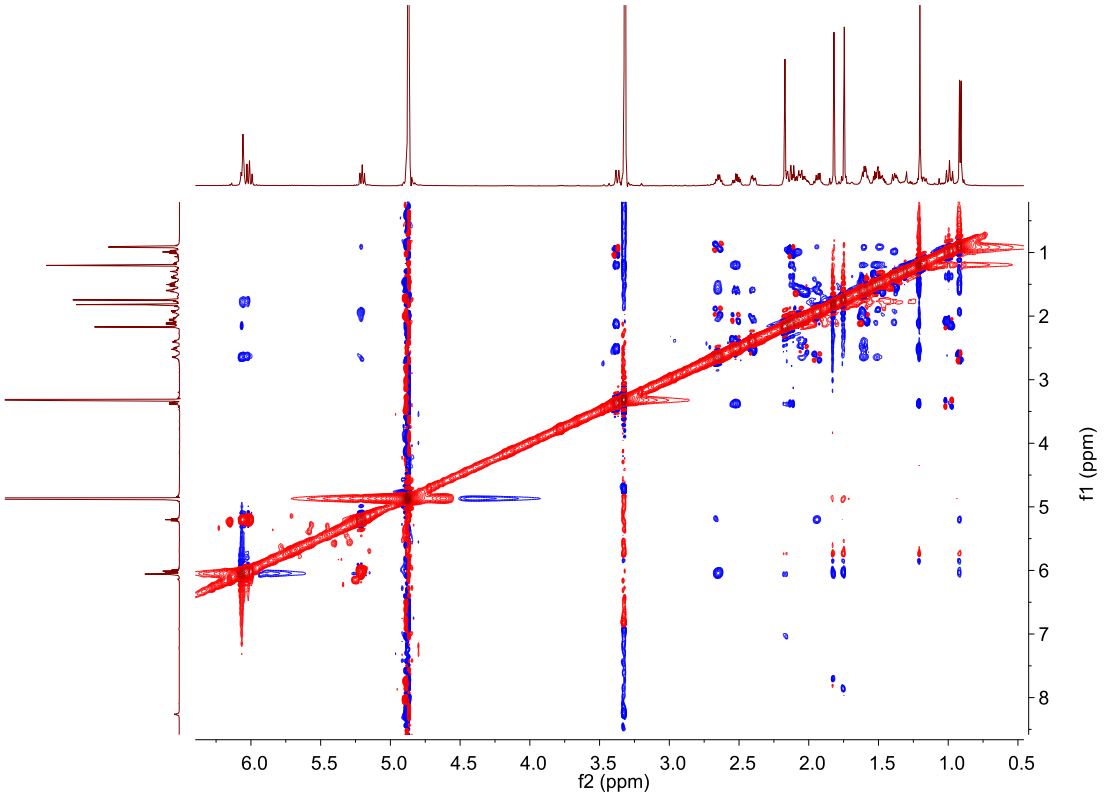


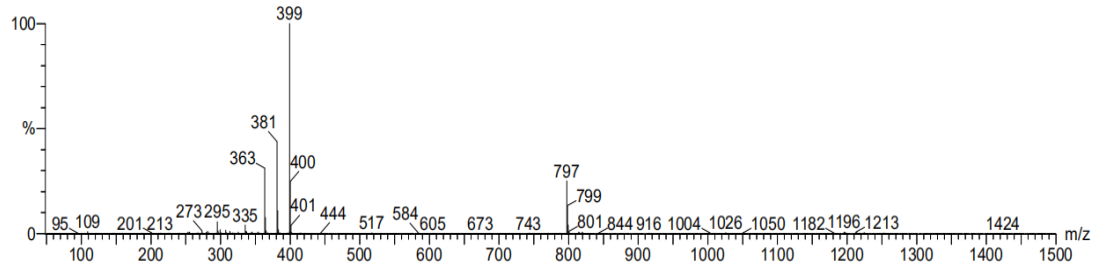
Fig. S20 ROESY spectrum of compound **2** (in CD3OD).

Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
89 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 0-500 H: 0-1000 O: 0-200
0154-78-8-2
20191104042 255 (2.053)

1: TOF MS ES+
9.83e+005



Minimum:				-1.5			
Maximum:		5.0	10.0	50.0			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
399.2537	399.2535	0.2	0.5	8.5	599.0	n/a	n/a	C25 H35 O4

Fig. S21 HR ESI-Q-TOF-MS spectrum of compound **3**

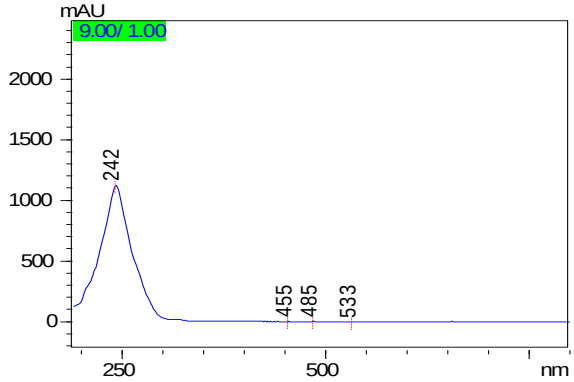


Fig. S22 UV spectrum of compound **3**

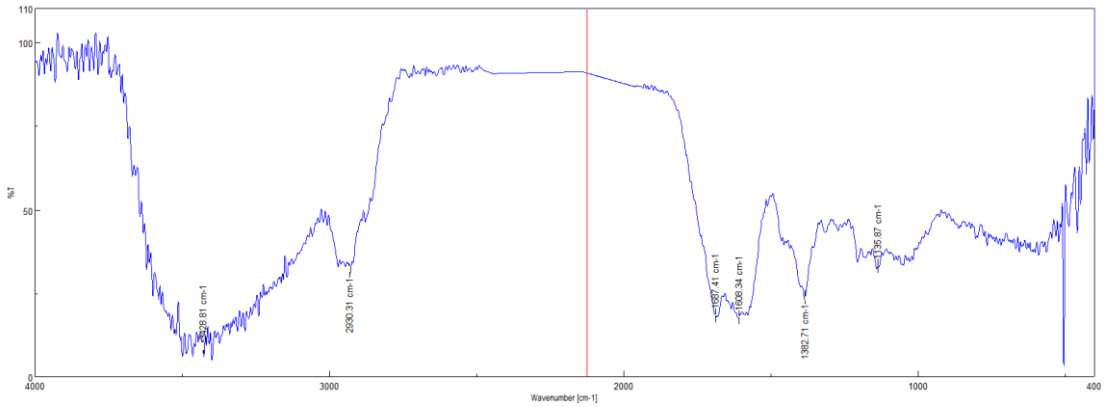


Fig. S23 IR spectrum of compound **3**

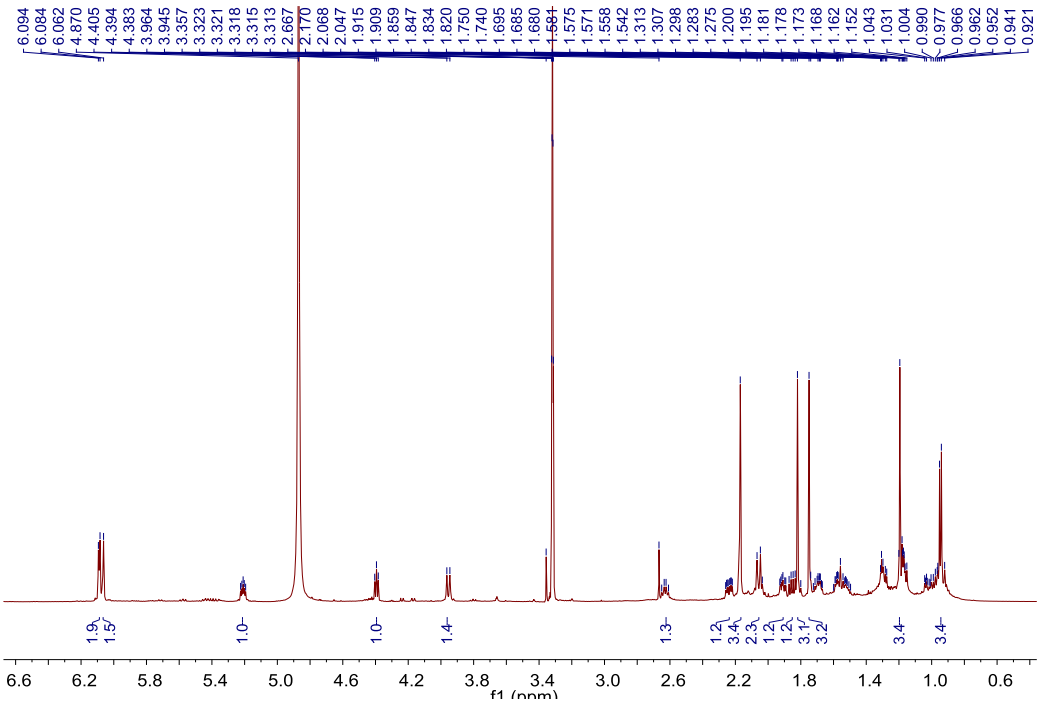


Fig. S24 ^{1}H-NMR spectrum of compound **3** (in CD_3OD)

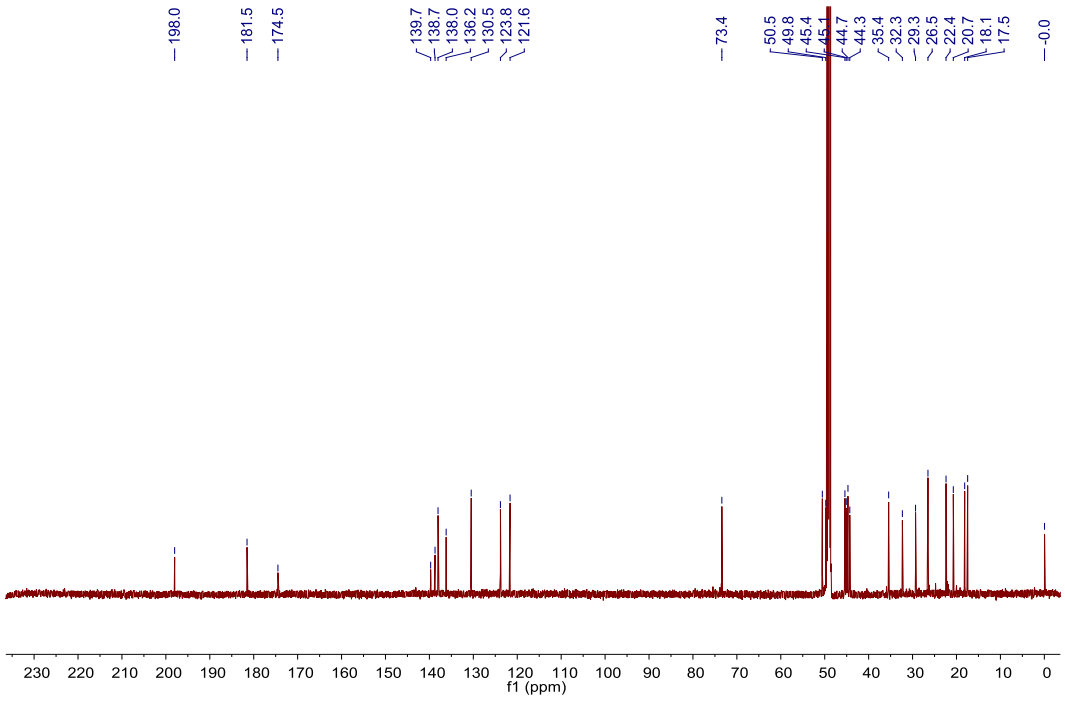


Fig. S25 ^{13}C-NMR spectrum of compound **3** (in CD_3OD)

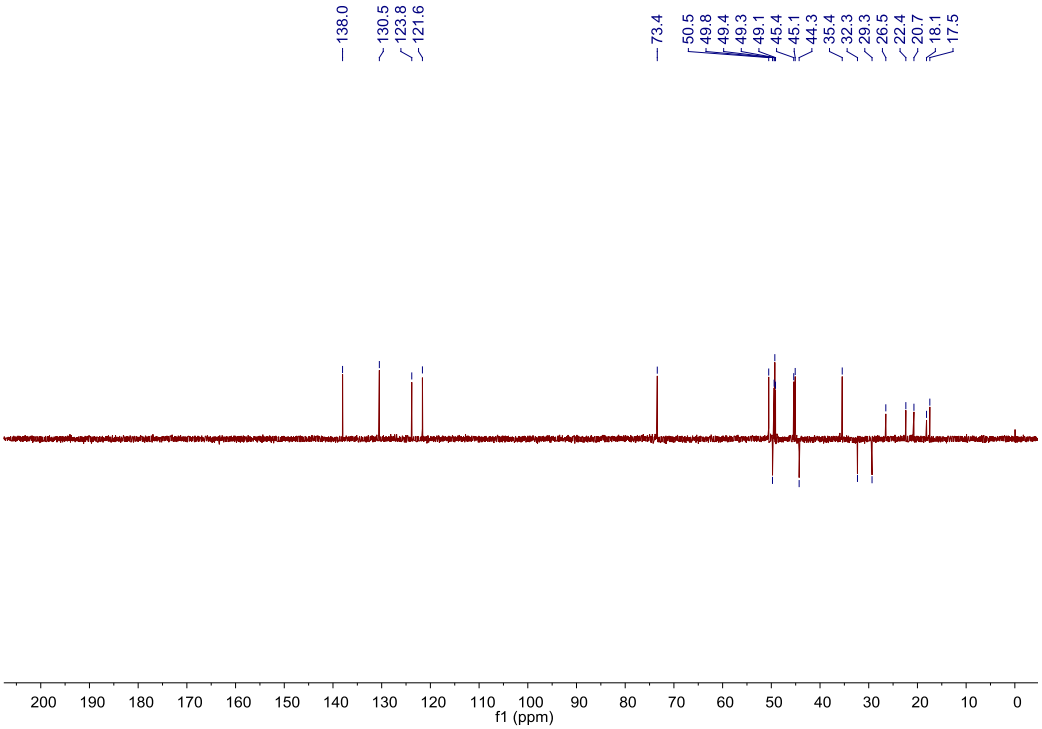


Fig. S26 DEPT135 spectrum of compound **3** (in CD_3OD)

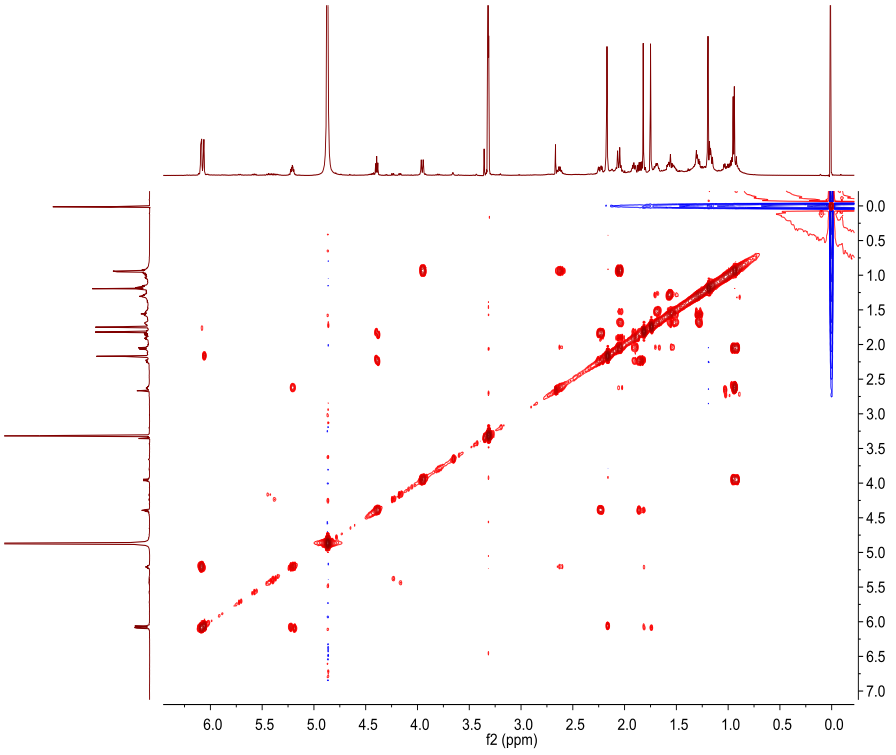


Fig. S27 ^{1}H-^{1}H COSY spectrum of compound **3** (in CD_3OD)

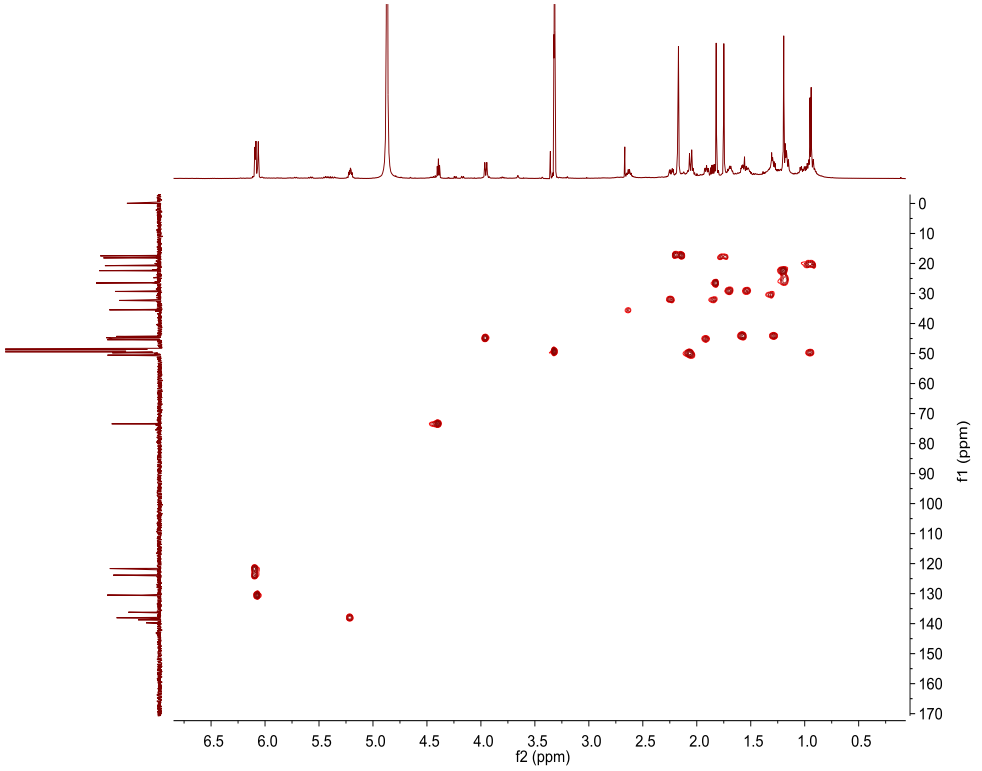


Fig. S28 HSQC spectrum of compound **3** (in CD_3OD)

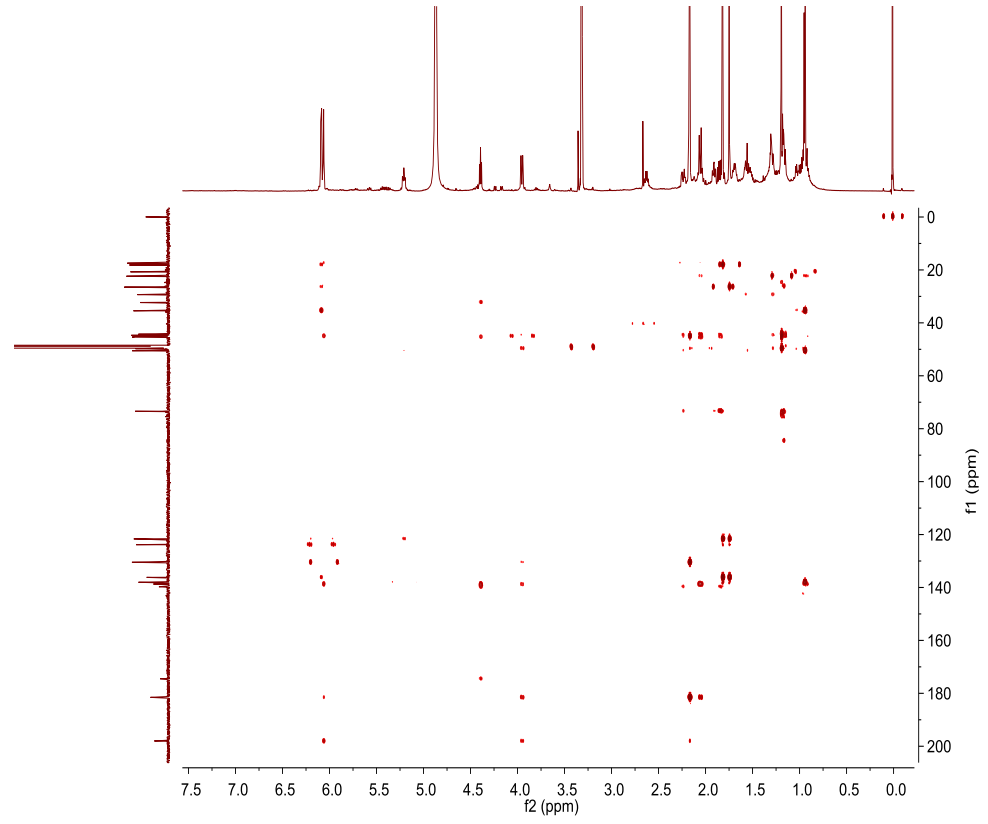


Fig. S29 HMBC spectrum of compound **3** (in CD3OD).

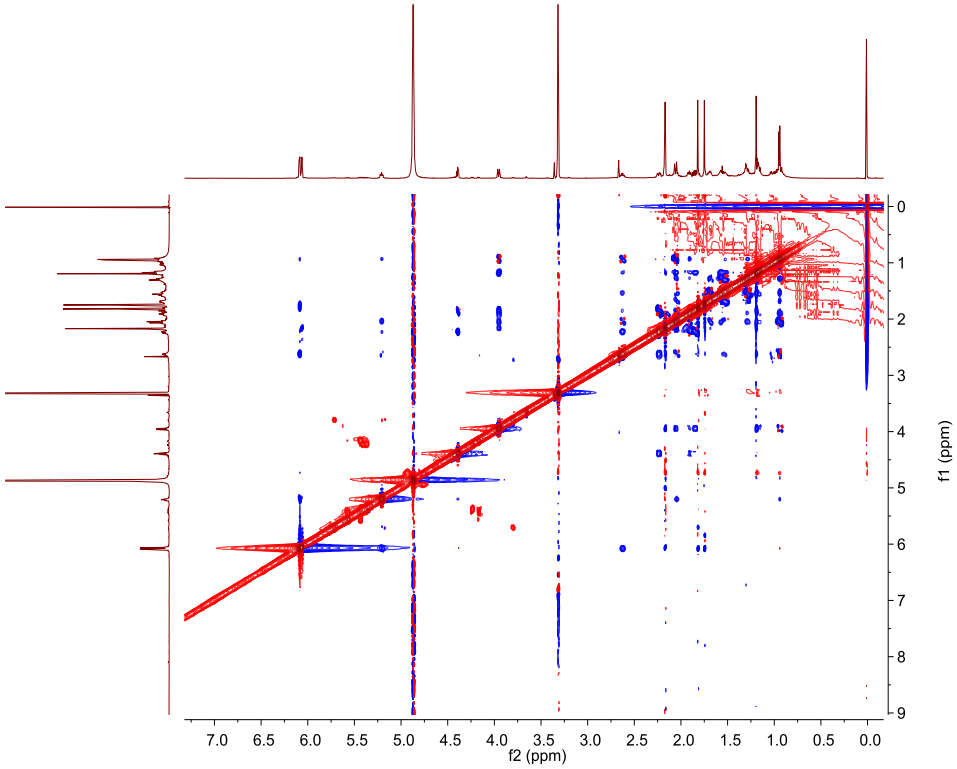


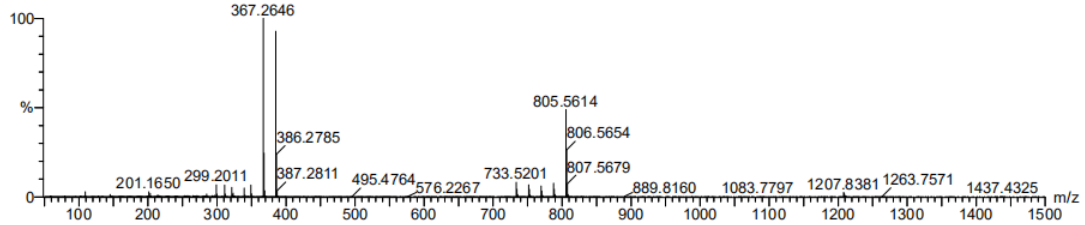
Fig. S30 ROESY spectrum of compound **3** (in CD3OD).

Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
2369 formula(e) evaluated with 7 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 0-50 H: 0-100 N: 0-10 O: 0-100
0154-78-8-4
20191104041 255 (2.053)

1: TOF MS ES+
5.14e+005



Minimum:				-1.5				
Maximum:		5.0	5.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
805.5614	805.5605	0.9	1.1	18.5	417.0	1.874	15.35	C47 H69 N10 02
	805.5592	2.2	2.7	13.5	415.3	0.199	81.97	C46 H73 N6 06
	805.5618	-0.4	-0.5	12.5	418.9	3.819	2.19	C50 H77 08
	805.5578	3.6	4.5	8.5	420.5	5.399	0.45	C45 H77 N2 010
	805.5650	-3.6	-4.5	4.5	424.2	9.084	0.01	C39 H77 N6 011
	805.5610	0.4	0.5	0.5	424.7	9.620	0.01	C34 H77 N8 013
	805.5637	-2.3	-2.9	-0.5	423.8	8.753	0.02	C38 H81 N2 015

Fig. S31 HR ESI-Q-TOF-MS spectrum of compound **4**

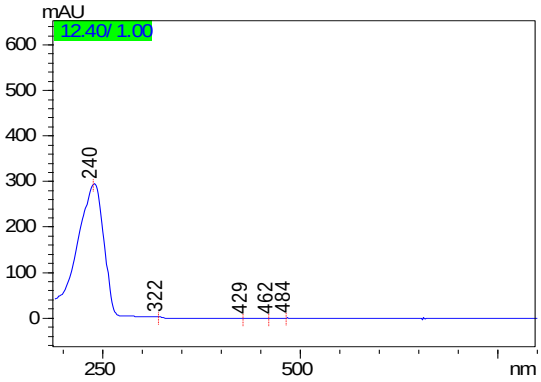


Fig. S32 UV spectrum of compound **4**

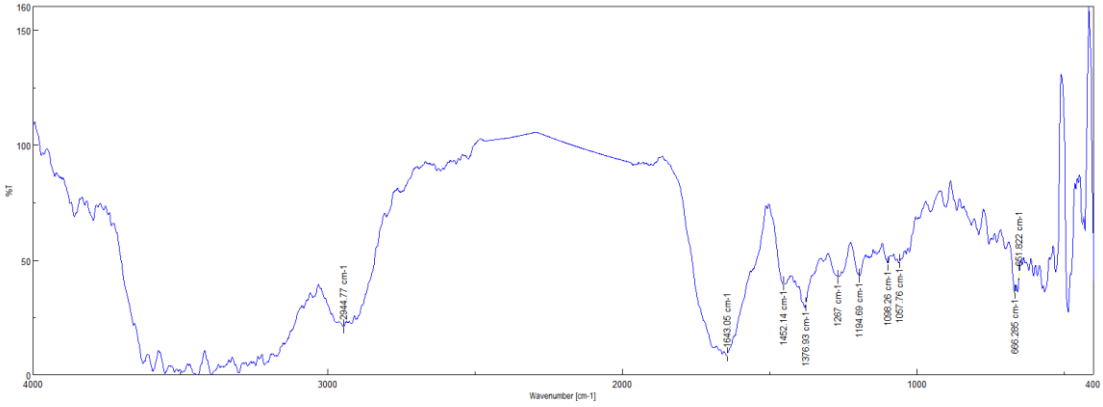


Fig. S33 IR spectrum of compound **4**

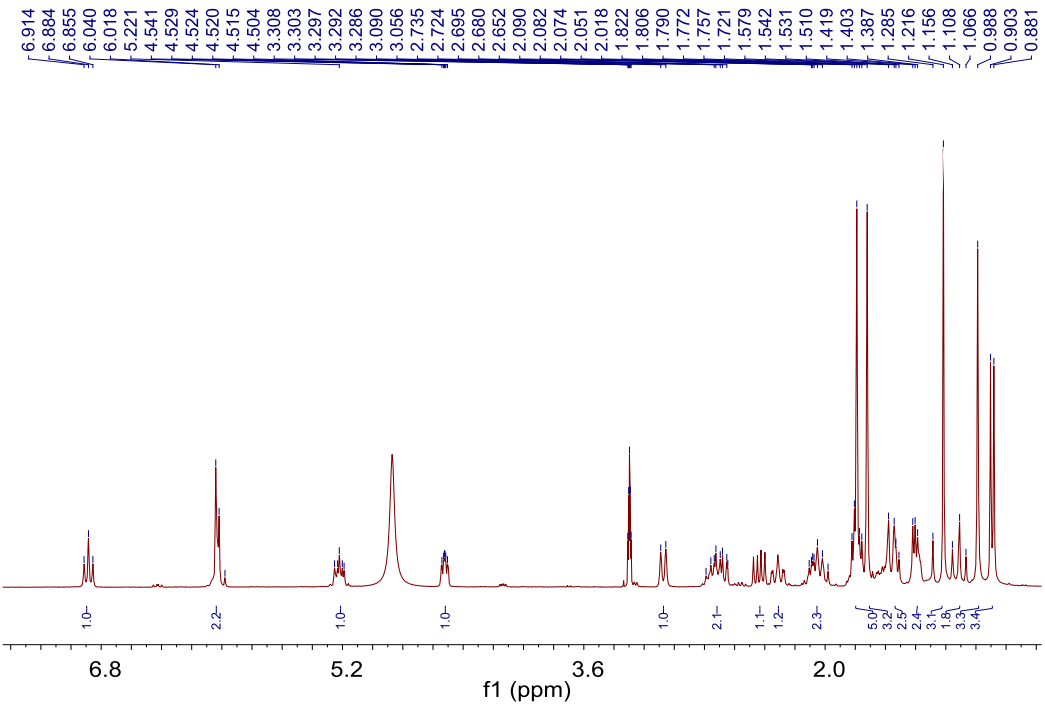


Fig. S34 ^{1}H-NMR spectrum of compound **4** (in CD_3OD)

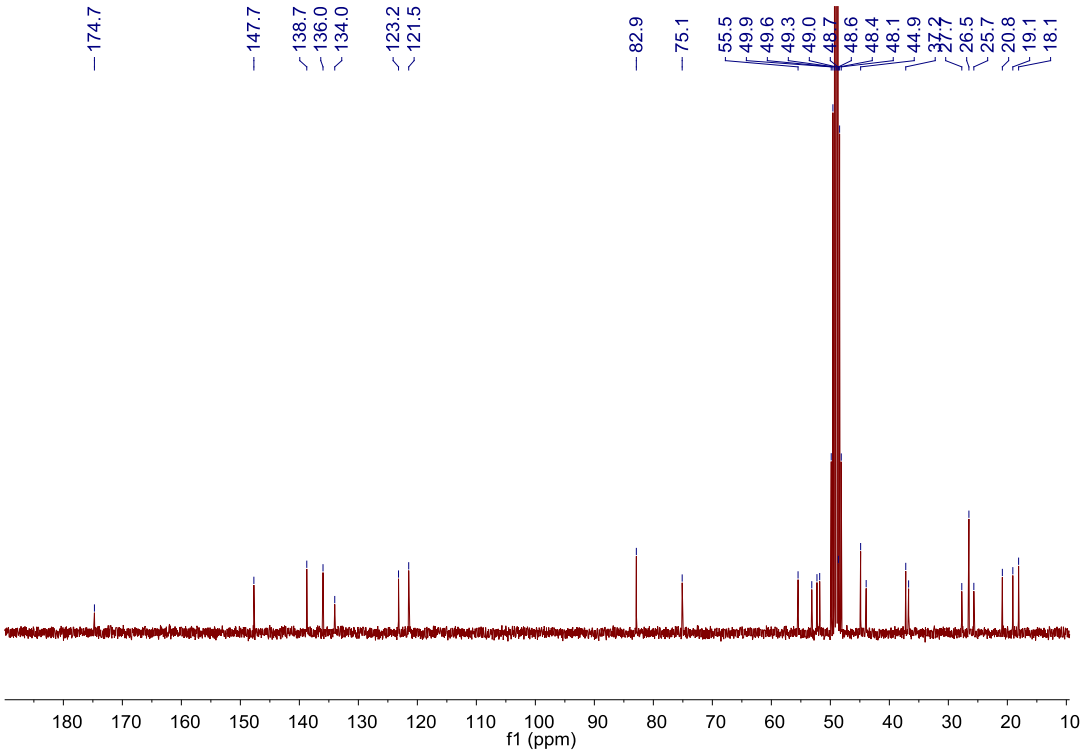


Fig. S35 ^{13}C-NMR spectrum of compound **4** (in CD_3OD)

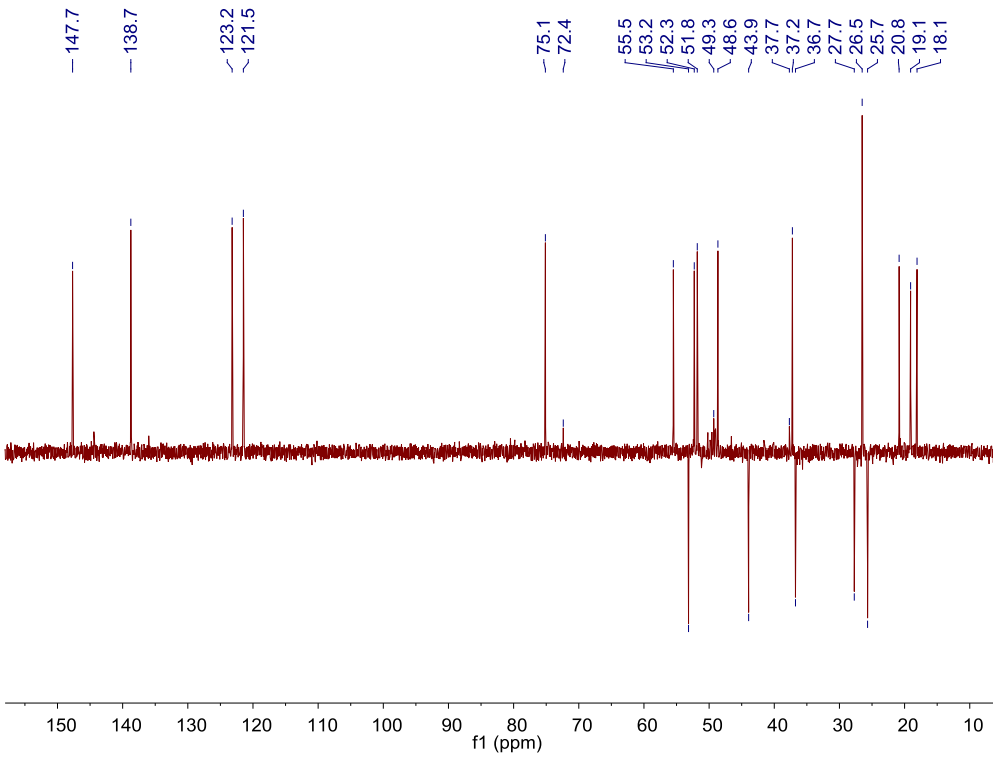


Fig. S36 DEPT135 spectrum of compound **4** (in CD_3OD)

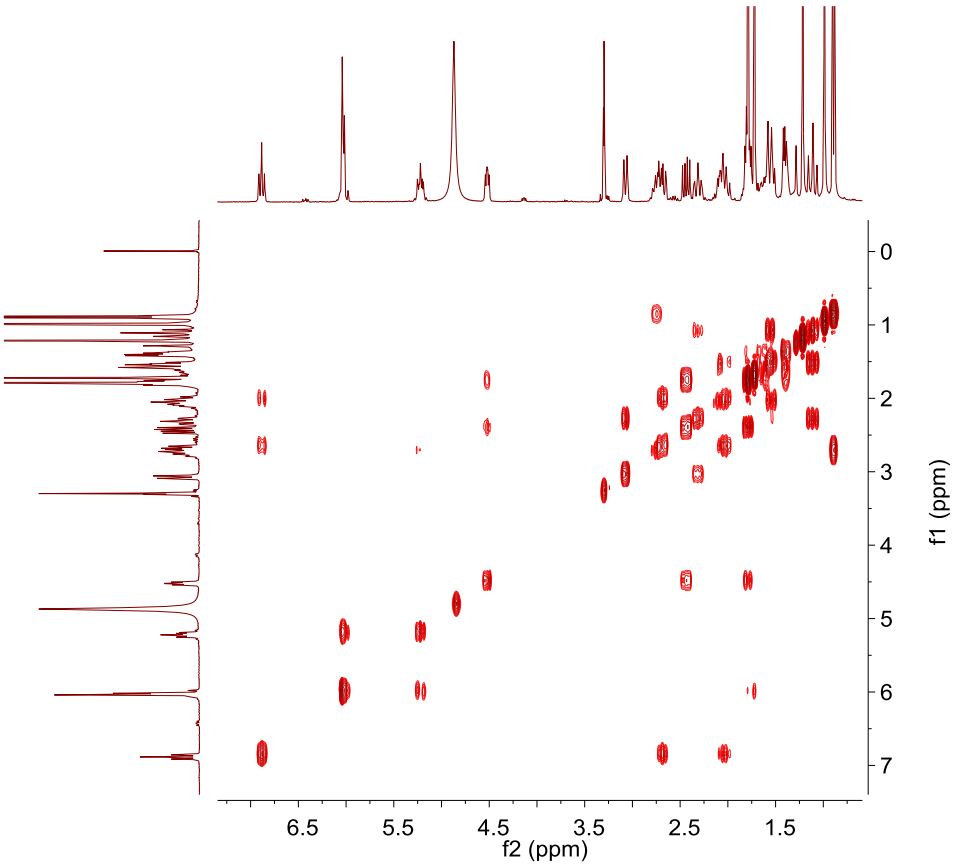


Fig. S37 ^{1}H-^{1}H COSY spectrum of compound **4** (in CD_3OD)

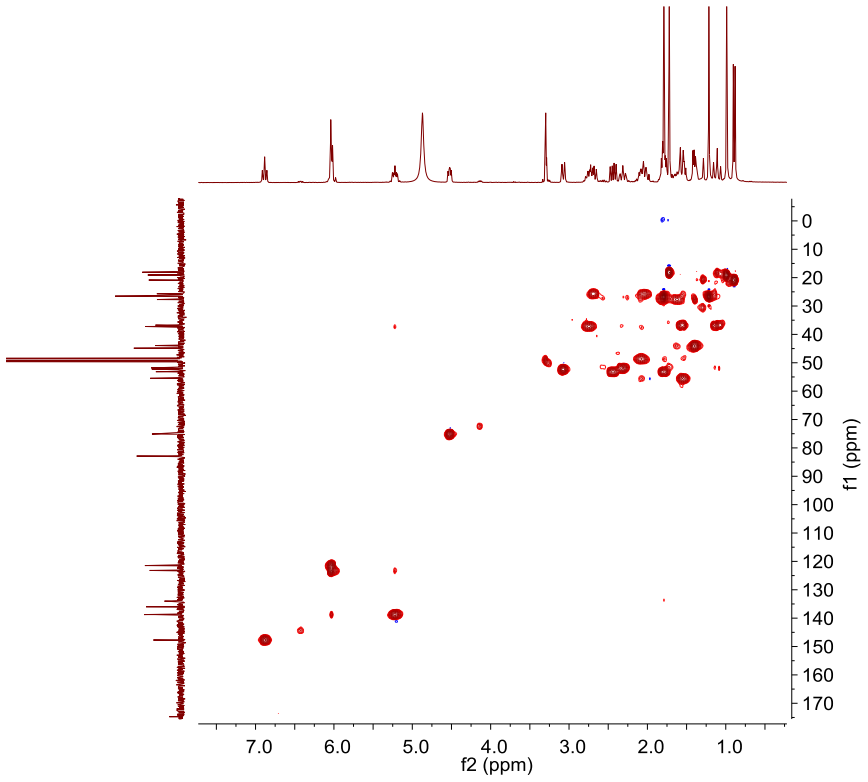


Fig. S38 HSQC spectrum of compound **4** (in CD_3OD)

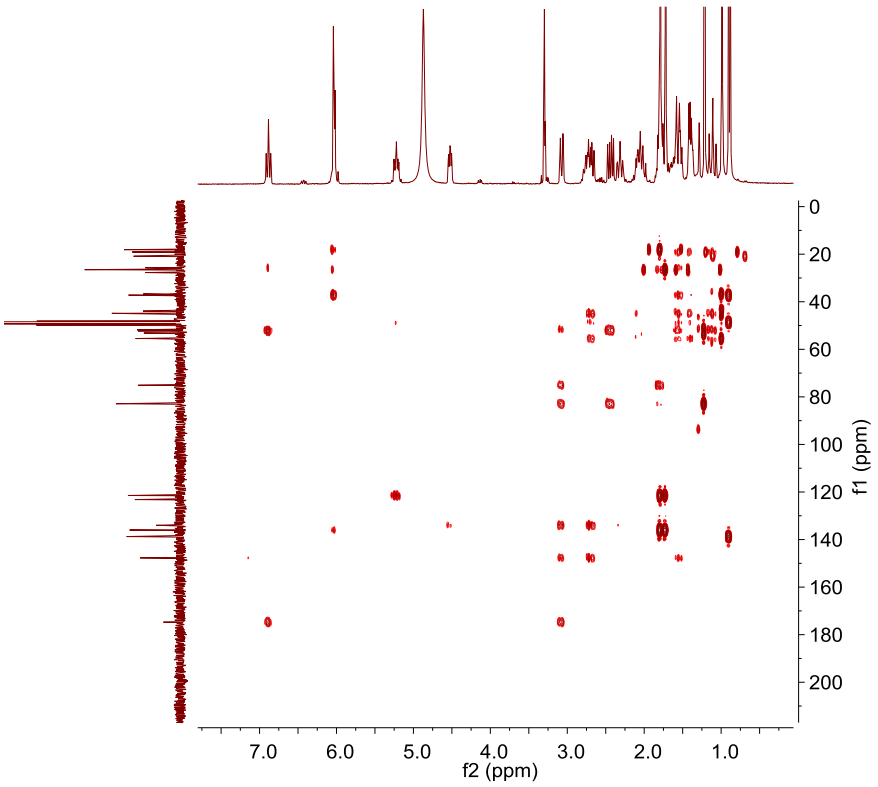


Fig. S39 HMBC spectrum of compound **4** (in CD3OD).

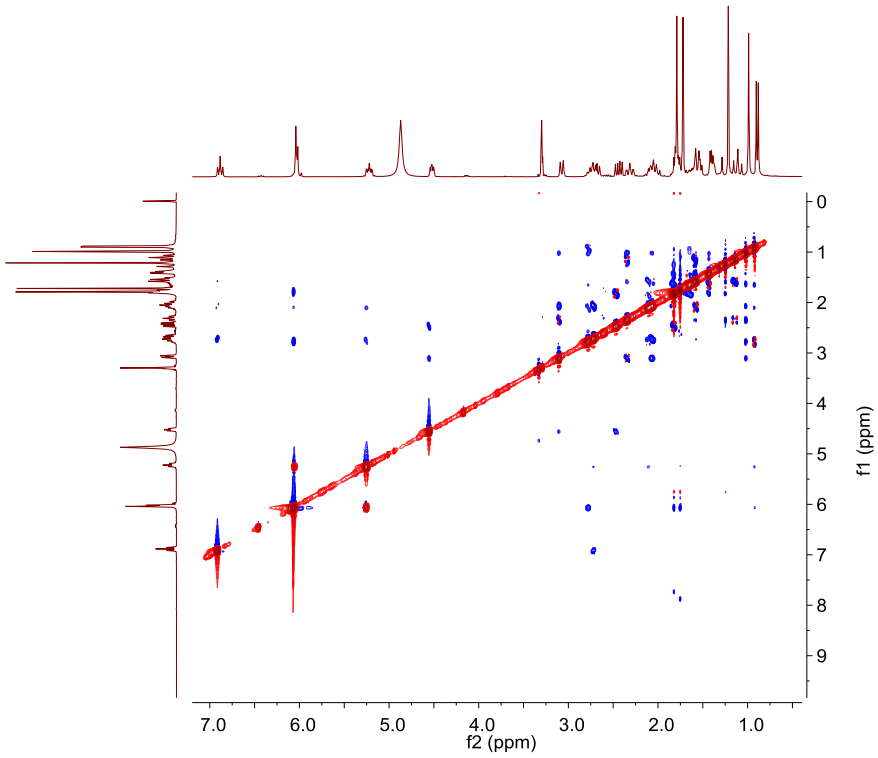
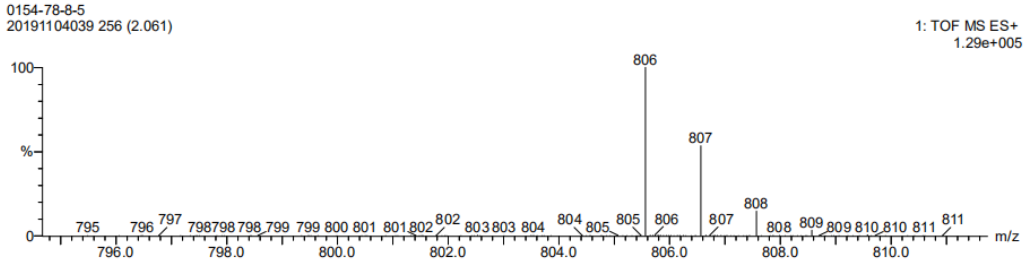


Fig. S40 ROESY spectrum of compound **4** (in CD3OD).

Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
4513 formula(e) evaluated with 11 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 0-50 H: 0-200 N: 0-20 O: 0-100
0154-78-8-5
20191104039 256 (2.061)



Minimum:				-1.5				
Maximum:		5.0	5.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
805.5621	805.5623	-0.2	-0.2	5.5	343.2	7.886	0.04	C35 H73 N12 09
	805.5618	0.3	0.4	12.5	340.1	4.842	0.79	C50 H77 08
	805.5610	1.1	1.4	0.5	344.0	8.765	0.02	C34 H77 N8 013
	805.5637	-1.6	-2.0	10.5	343.0	7.749	0.04	C36 H69 N16 05
	805.5637	-1.6	-2.0	-0.5	344.4	9.107	0.01	C38 H81 N2 015
	805.5605	1.6	2.0	18.5	337.2	1.943	14.33	C47 H69 N10 02
	805.5597	2.4	3.0	6.5	345.9	10.624	0.00	C31 H69 N18 07
	805.5650	-2.9	-3.6	15.5	343.4	8.100	0.03	C37 H65 N20 0
	805.5650	-2.9	-3.6	4.5	344.5	9.200	0.01	C39 H77 N6 011

Fig. S41 HR ESI-Q-TOF-MS spectrum of compound **5**

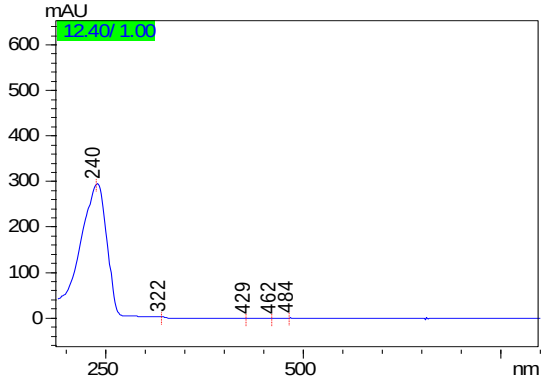


Fig. S42 UV spectrum of compound **5**

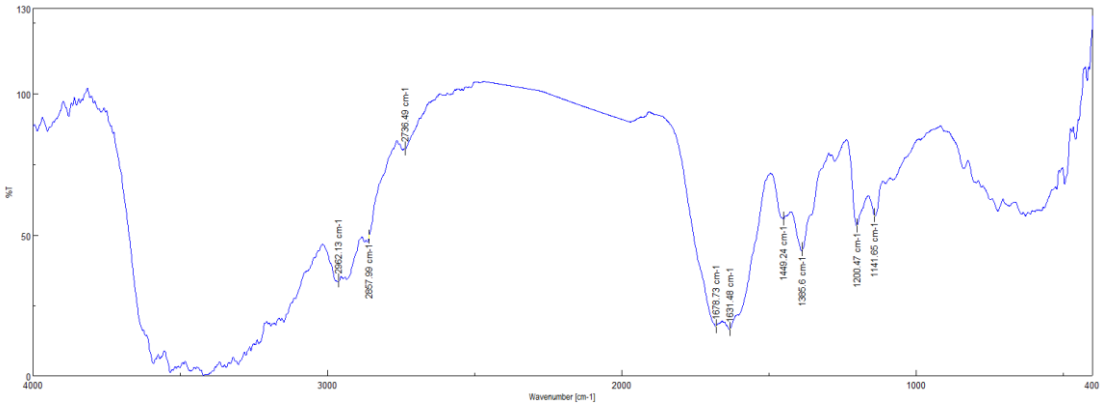


Fig. S43 IR spectrum of compound **5**

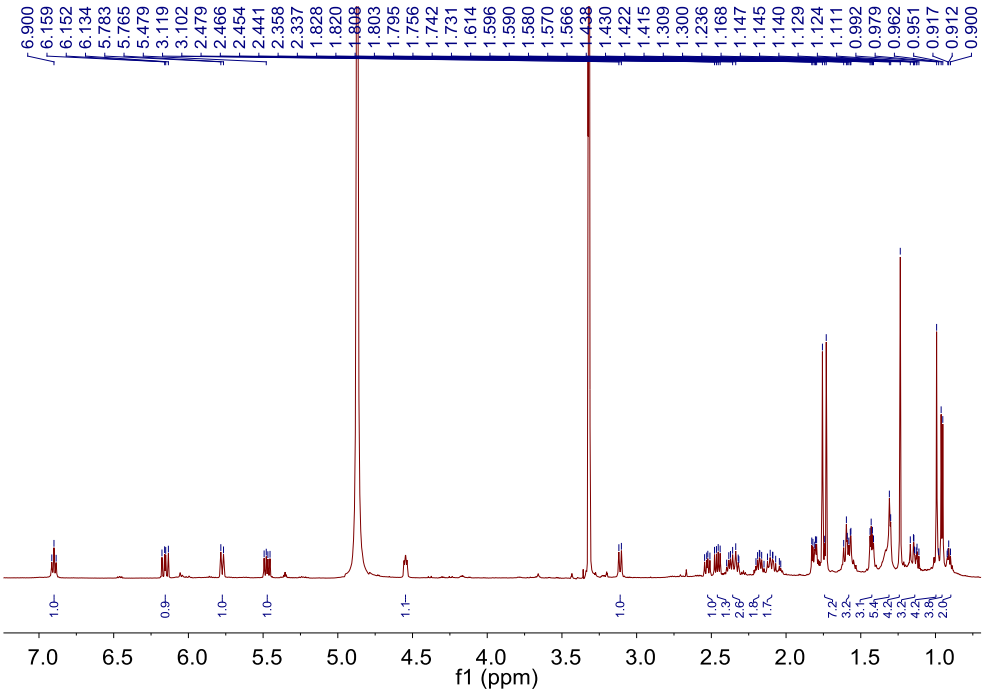


Fig. S44 ^{1}H-NMR spectrum of compound **5** (in CD_3OD)

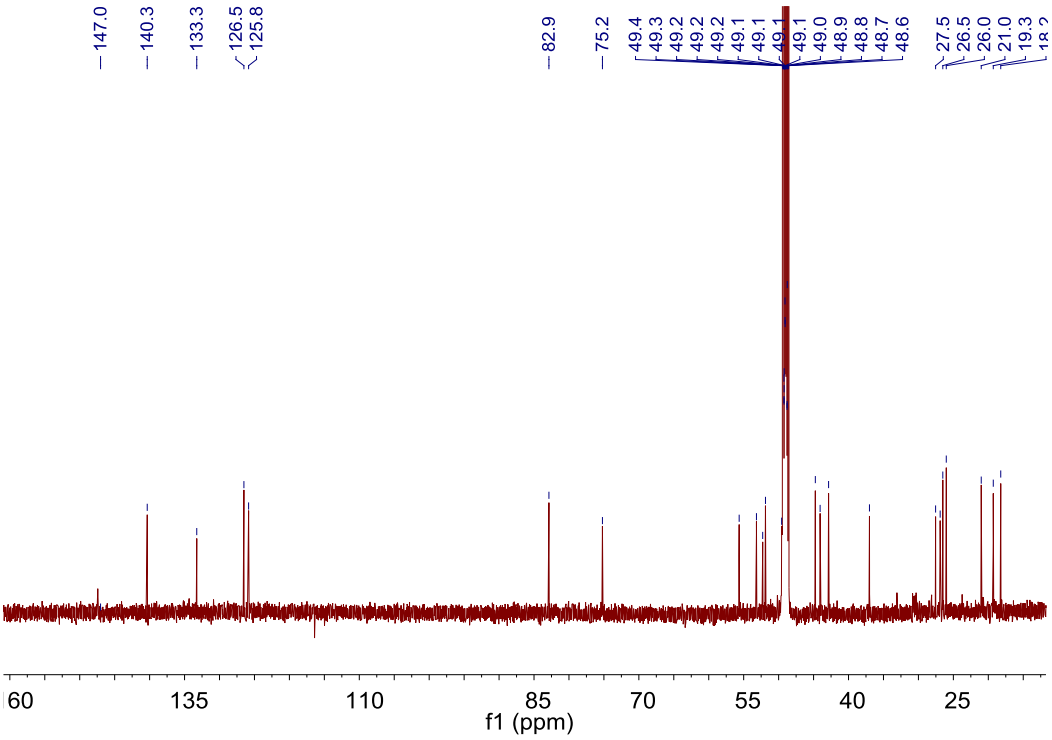


Fig. S45 ^{13}C-NMR spectrum of compound **5** (in CD_3OD)

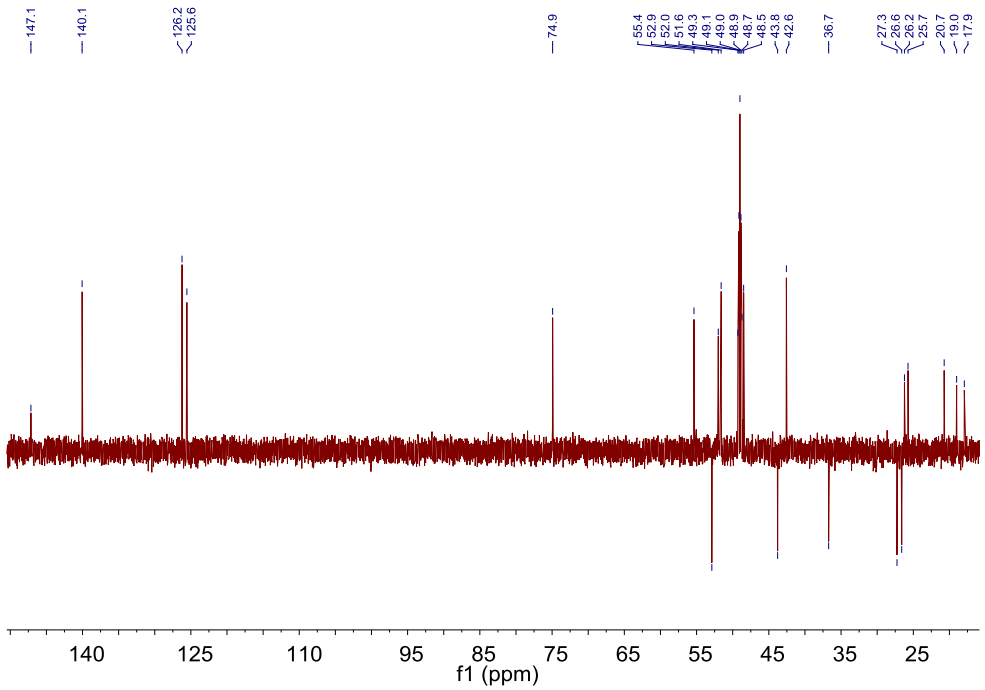


Fig. S46 DEPT135 spectrum of compound **5** (in CD_3OD)

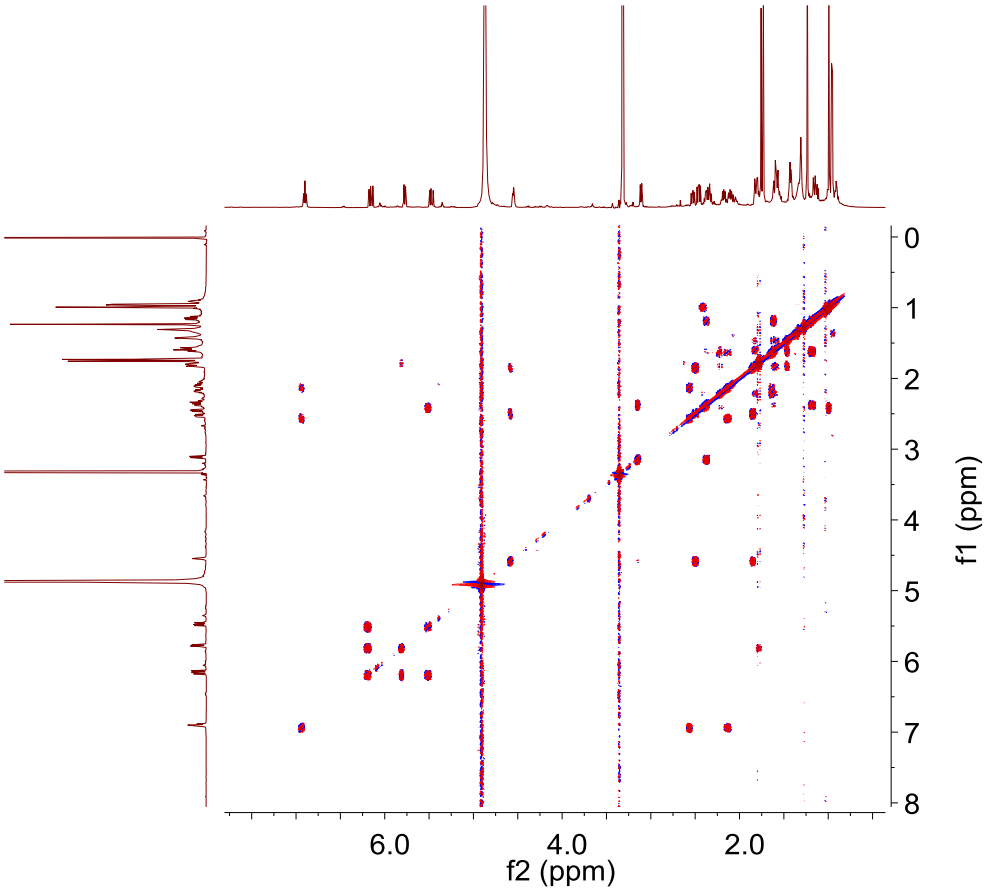


Fig. S47 ^{1}H-^{1}H COSY spectrum of compound **5** (in CD_3OD)

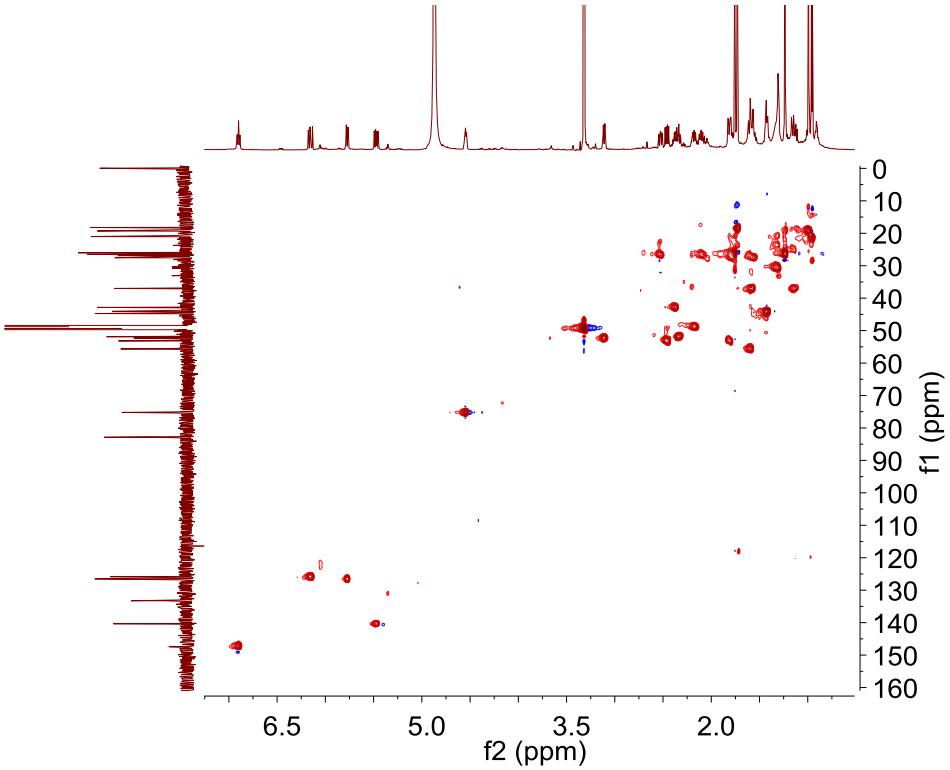


Fig. S48 HSQC spectrum of compound **5** (in CD_3OD).

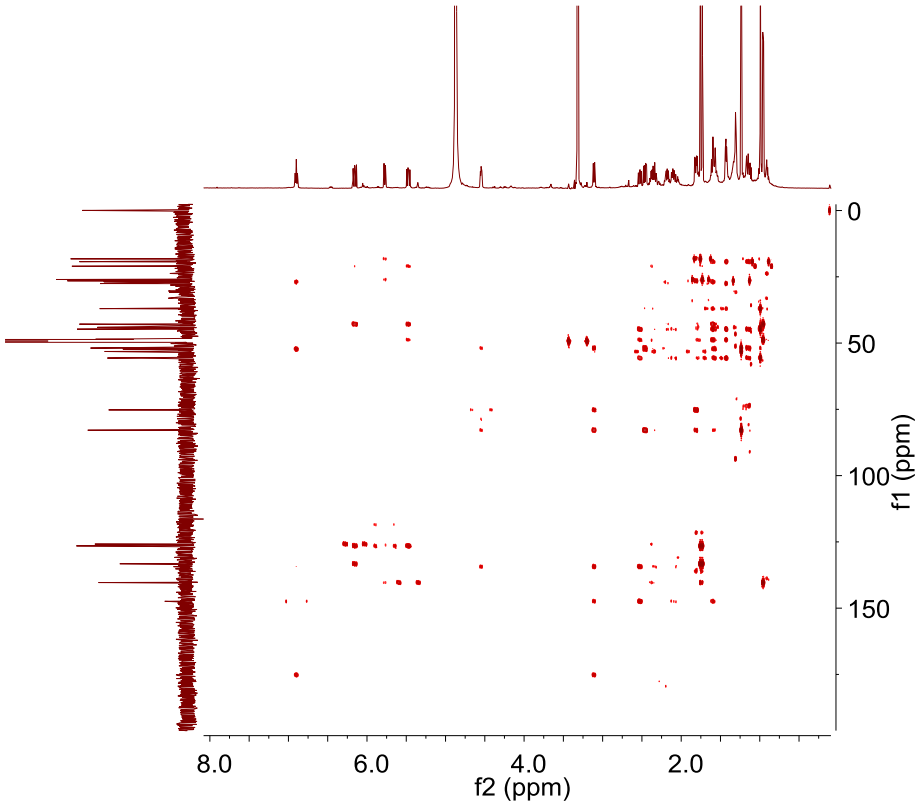


Fig. S49 HMBC spectrum of compound **5** (in CD3OD).

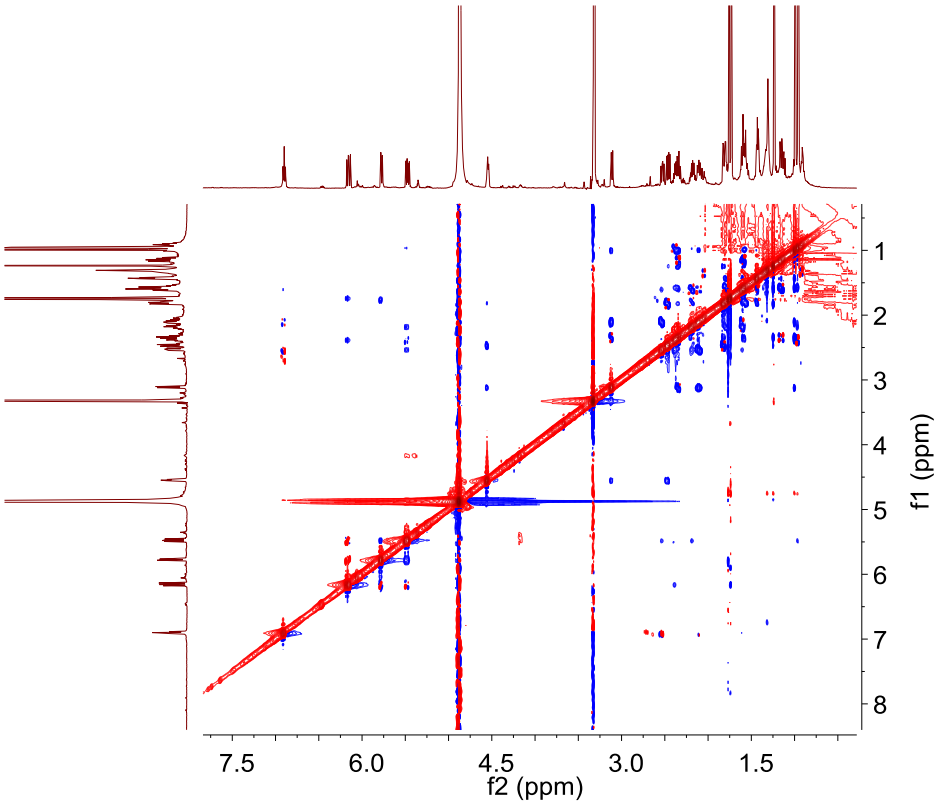


Fig. S50 ROESY spectrum of compound **5** (in CD3OD).

Fig. S51 Cultural and microscopic morphology of strain WHU0154
a. Cultural characteristics (7 days, front) of strain WHUF0154 on a Potato Dextrose Agar medium at 28 °C. The diameter of the colony is 60~65mm. The front of the colony is white, velvety texture, no exudate, and the center of the colony turns light brown-gray when grow old. The reverse side of the colony is gray.
b. The conidiogenous structures of strain WHU0154 (400×). The conidiophore originates from aerial hyphae, with a diameter of 3.8-5 μm, smooth, and the top is slightly enlarged to form a flask-shaped vesicle with a diameter of 7.5-8.8 μm. The upper part to 3/4 of the surface is fertile; the sporulation structure is double-layered, the stem base is 3-4×2-3μm; the bottle stem is 6-7×3-4μm; the conidia are spherical, with a diameter of 2-3μm, smooth.