Electronic Supplementary Material (ESI) for RSC Advances.

Notoamide-type alkaloids induced apoptosis and autophagy via P38/JNK signaling pathway in hepatocellular carcinoma cells

Supporting Information

List of Supporting Information

Table S1. ^{1}H NMR data for compounds **5-11** in DMSO-d_6

position	**5**	**6**	**7**	**8**	**9**	**10**	**11a**	**11b**
				δ_H（*J* in Hz）				
1	3.18, m	3.18, m	3.21, m	3.36, m	3.26, m	3.46, m	3.19, m	3.42, m
	3.30, m	3.29, m	3.31, m			3.49, m	3.32, m	1.98, m
2	1.84, m	1.84, m	1.84, m	1.88, m	1.84, m	1.95, m	1.86, m	2.10, m
	1.97, m	1.96, m	1.98, m	2.04, m	1.99, m	2.11, m	2.13, m	2.66, m
3	1.84, m	1.85, m	1.84, m	1.87, m	1.85, m	1.94, m	2.11, m	2.02, m
	2.54, m	2.53, m	2.54, m	2.54, m	2.55, m	2.70, m	2.55, m	
5	2.03, d (7.4)	2.05, m	2.02, d (6.7)	2.12, m	2.06, dd(10.0,12.4)	2.23, m	2.13, m	2.76, d (9.5)
					2.43, q (4.8,10.0)	2.11, m	2.55, m	
6	2.68, t (7.4,7.8)	2.72, m	2.66, t（6.7, 7.5）	2.84, dd, (5.5,10.2)	2.66, dd (4,8, 10.1)	2.66, dd (6.5,10.0)	3.14, m	3.14, m
9-H/OH	10.74, s	7.26, d (9.2)	10.58, s	11.66, s	10.44, s		10.87, s	
12	6.97, d (9.8)	5.72, d (9.2)	6.95, d, (9.3)	7.01, d, (9.9)	6.94, d (9.8)	7.89, d (10.1)	7.47, d, (9.9)	7.07, d (9.9)
13	5.76, d (9.8)	6.58, d (7.9)	5.74, d, (9.3)	5.86, d, (9.9)	5.73, d (9.8)	5.93, d (10.1)	5.66, d, (9.9)	5.60, d (9.9)
17	6.54, d (8.4)	7.42, d (7.9)	6.52 d (8.6Hz)	6.71, d, (8.5)	6.48, d (8.2)	6.86, d (8.0)	6.53, d (8.1)	6.38, d (8.6)
18	7.36, d (8.4)	4.77, s	7.28,d (8.6Hz)	7.77, d, (8.5)	7.10, d (8.2)	7.58, d (8.0)	7.58, d (8.1)	6.98, d (8.6)
21	4.76, s	8.08, s	5.04, d (8.4)		3.34, overlapped	6.80, s	4.86, s	5.30, s
					2.64, d (15.2)			
25-NH	8.07,s	1.41, s	7.67, s	8.72, s	8.78, s	8.07, s		7.64, s
27	1.33, s	1.09, s	1.31, s	1.43, s	1.30, s	1.65, s	1.02, s	1.54, s
28	1.00, s	1.41, s	1.01, s	1.25, s	1.01, s	1.23, s	1.37, s	1.67, s
29	1.39, s	1.41, s	1.38, s	1.41, s	1.39, s	1.47, s	1.25, s	1.32, s
30	1.39, s	3.36, s	1.39, s	1.41, s	1.38, s	1.47, s	1.14, s	1.31, s
31	3.38, s	10.99, s	5.18, d (8.4)					

Table S2. ^{13}C NMR data for compounds **5-11** in DMSO-d_6

position	**5**	**6**	**7**	**8**	**9**	**10**	**11a**	**11b**
	δ_C (ppm)							
1	43.9	43.8	43.9	43.7	43.5	43.8	44.1	44.4
2	24.4	24.4	24.6	24.1	24.0	24.2	24.8	24.5
3	29.0	29.0	29.1	28.4	28.7	28.9	29.6	29.4
4	66.8	66.6	62.8	67.0	65.9	66.9	64.4	65.7
5	29.9	29.7	30.1	30.6	30.1	30.6	29.6	29.4
6	45.1	45.6	44.6	51.1	49.2	52.9	46.5	43.2
7	35.4	35.9	46.2	35.6	34.6	35.9	34.9	38.0
8	142.3	139.4	141.4	158.0	139.6	144.4	140.3	151.8
10	133.2	130.1	133.3	133.0	132.8	139.9	140.9	130.4
11	105.3	104.9	105.4	110.0	104.8	111.5	111.6	104.4
12	118.4	118.5	118.6	118.6	118.1	115.8	116.1	118.6
13	129.6	129.0	130.7	130.4	128.9	132.6	132.2	128.6
14	75.6	75.4	75.5	75.6	75.0	76.6	76.4	75.4
16	148.1	149.0	148.2	149.0	147.4	155.2	153.0	148.8
17	109.7	110.5	109.5	112.1	108.6	115.9	115.2	110.2
18	119.1	119.4	118.8	120.6	117.5	120.2	123.0	119.4
19	122.4	117.8	109.1	117.2	103.8	117.5	130.0	116.2
20	106.6	102.8	105.4	105.9	121.5	132.5	116.3	98.2
21	69.2	68.9	59.8	184.0	23.8	122.2	43.3	58.2
22	62.8	62.6	66.8	67.0	59.6	62.7	70.1	61.7
23	167.7	167.6	168.5	166.7	168.4	167.3	167.6	167.0
26	173.0	173.0	172.7	171.8	173.0	172.0	173.8	174.9
27	28.9	27.6	28.5	21.1	27.9	22.7	19.6	16.4
28	22.9	20.4	22.3	26.7	21.5	14.8	26.6	26.5
29	27.7	27.7	27.5	27.2	27.1	27.2	27.5	27.5
30	27.6	27.3	27.5	27.1	27.0	27.1	27.9	27.1
31	57.5	57.4						

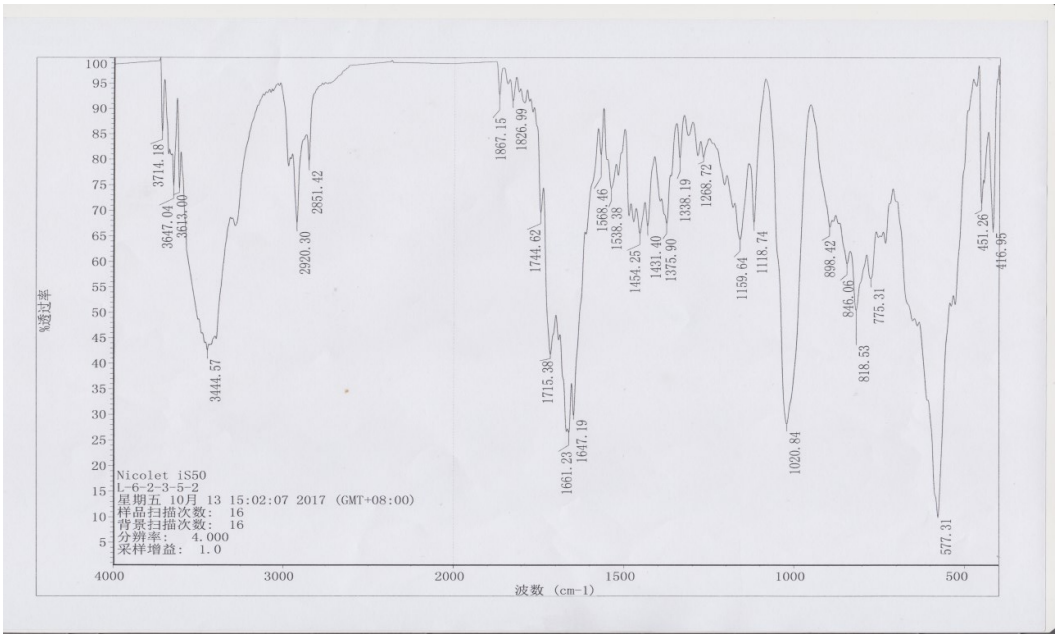


Figure S1. IR spectrum of compound **1**

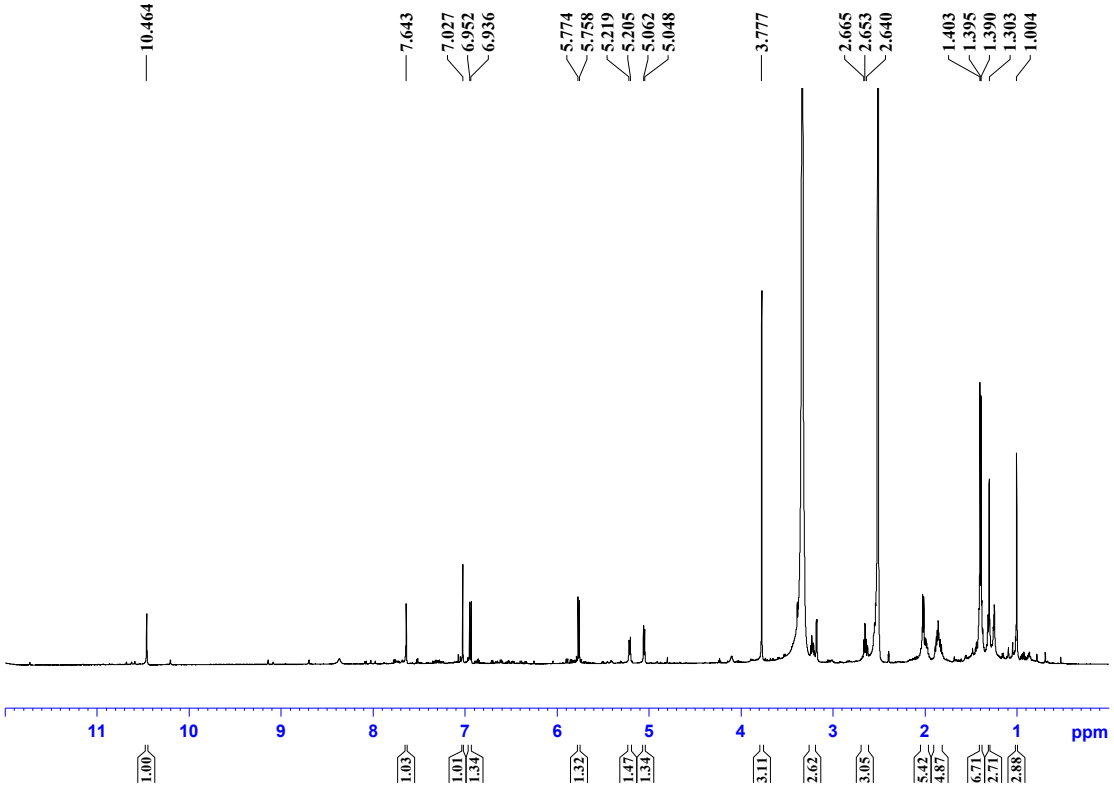


Figure S2.[1]H NMR spectrum of **1**

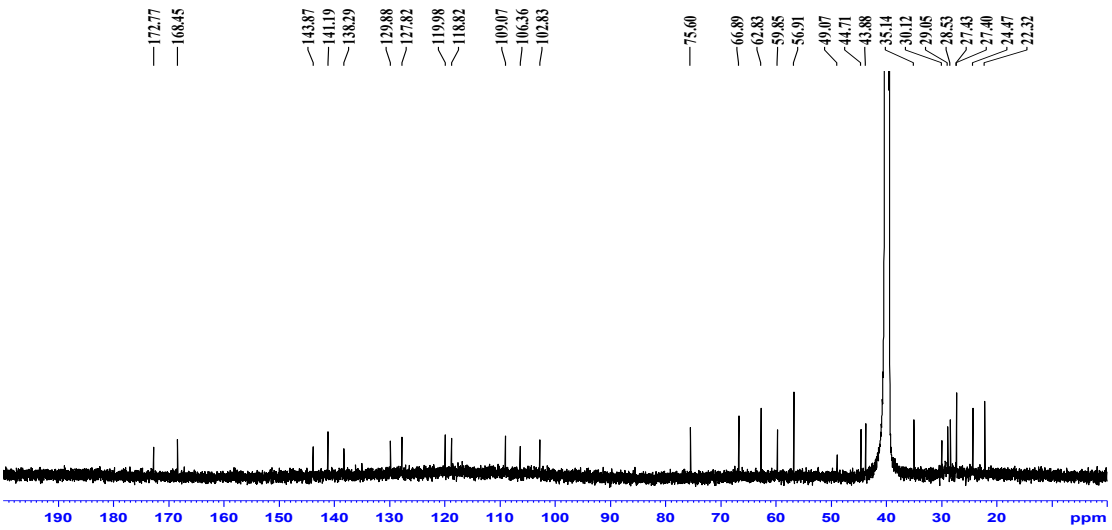


Figure S3. ^{13}C NMR spectrum of **1**

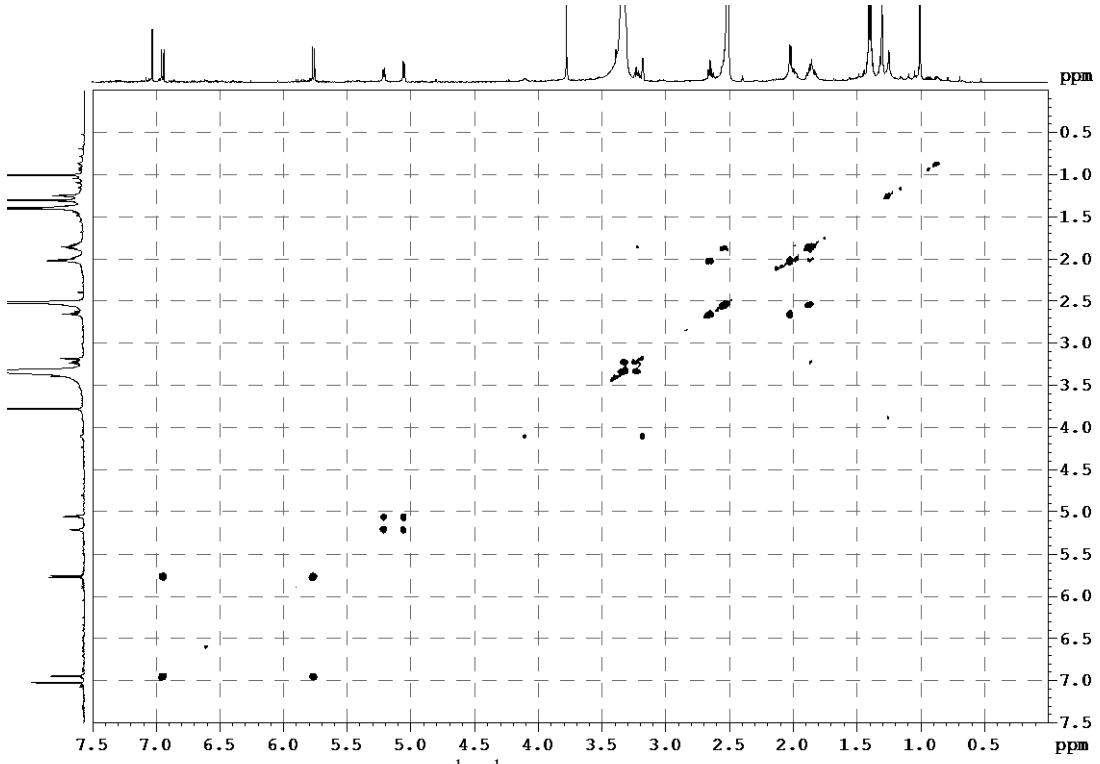


Figure S4. ^{1}H-^{1}H COSY spectrum of **1**

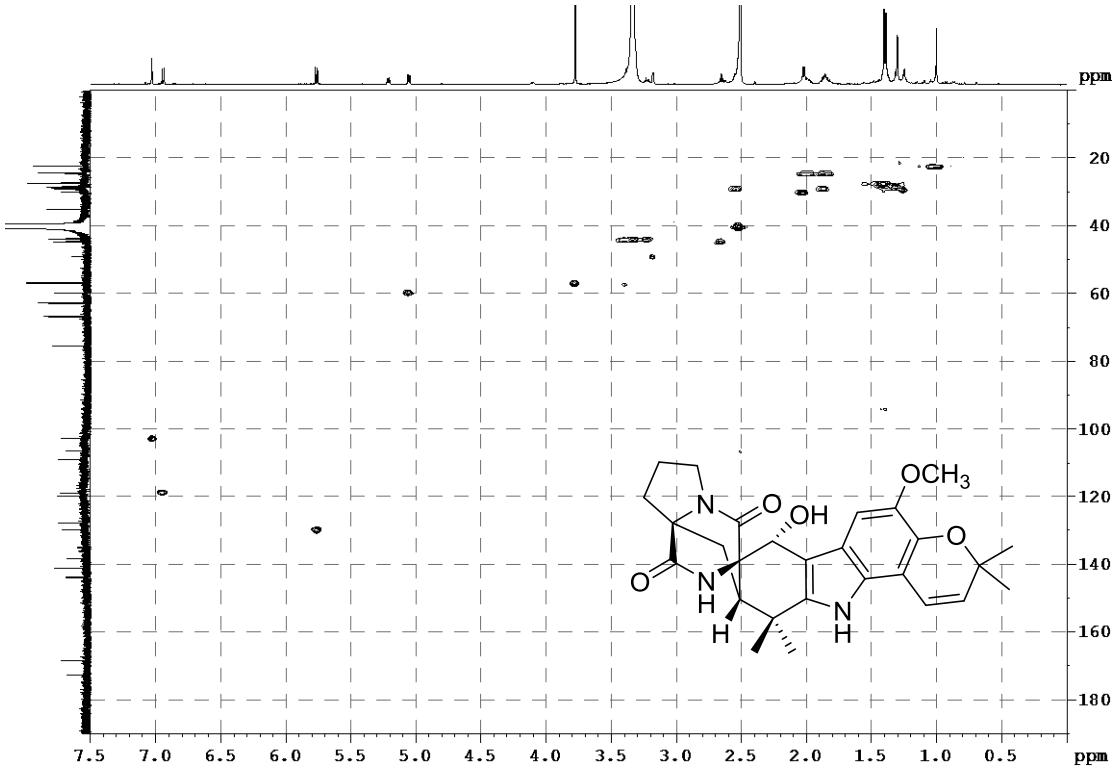


Figure S5. HSQC spectrum of **1**

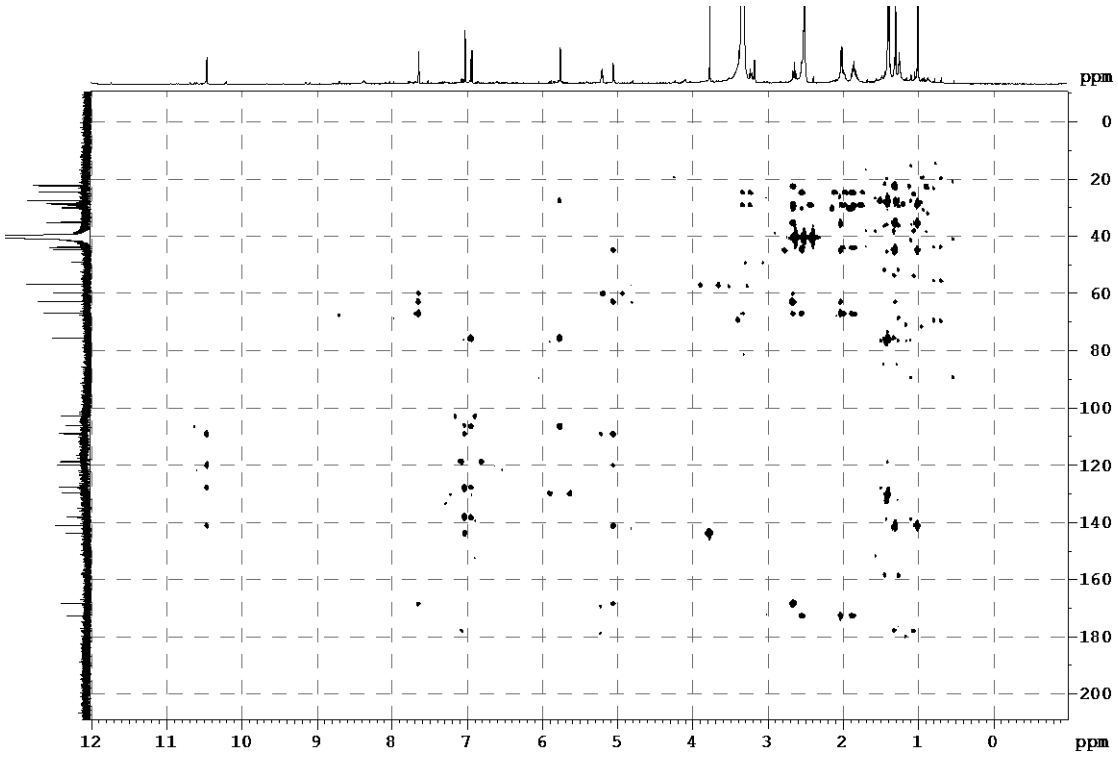


Figure S6. HMBC spectrum of **1**

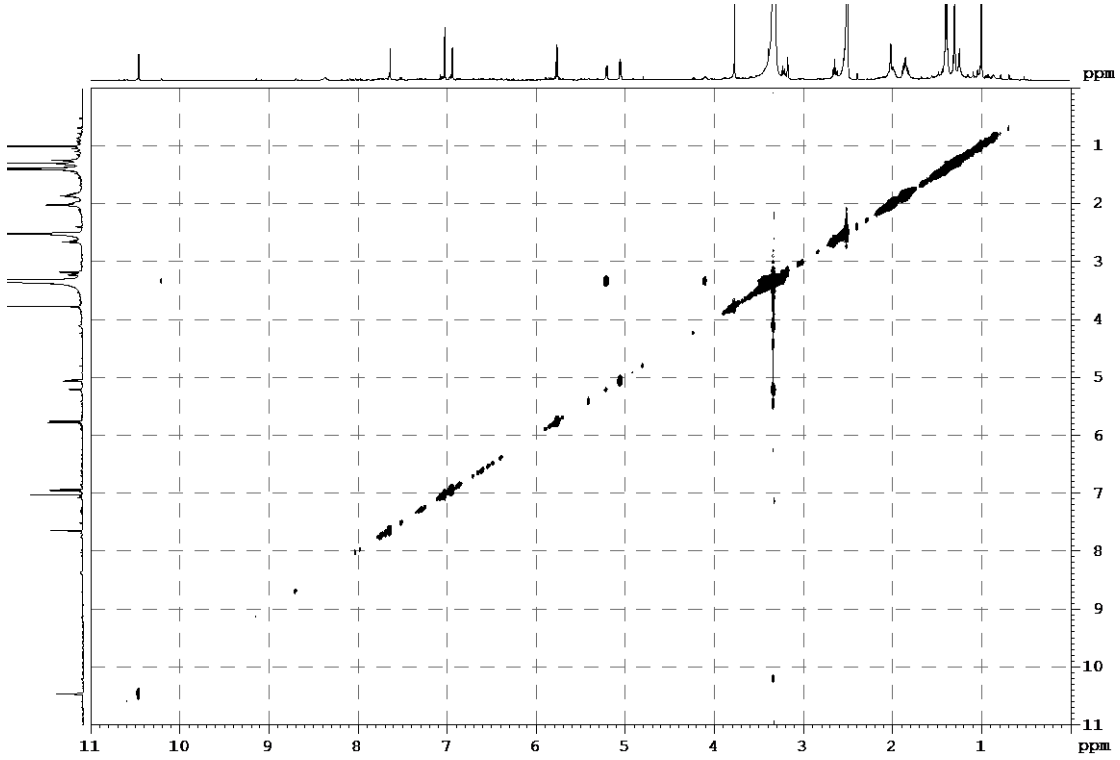


Figure S7. NOESY spectrum of **1**

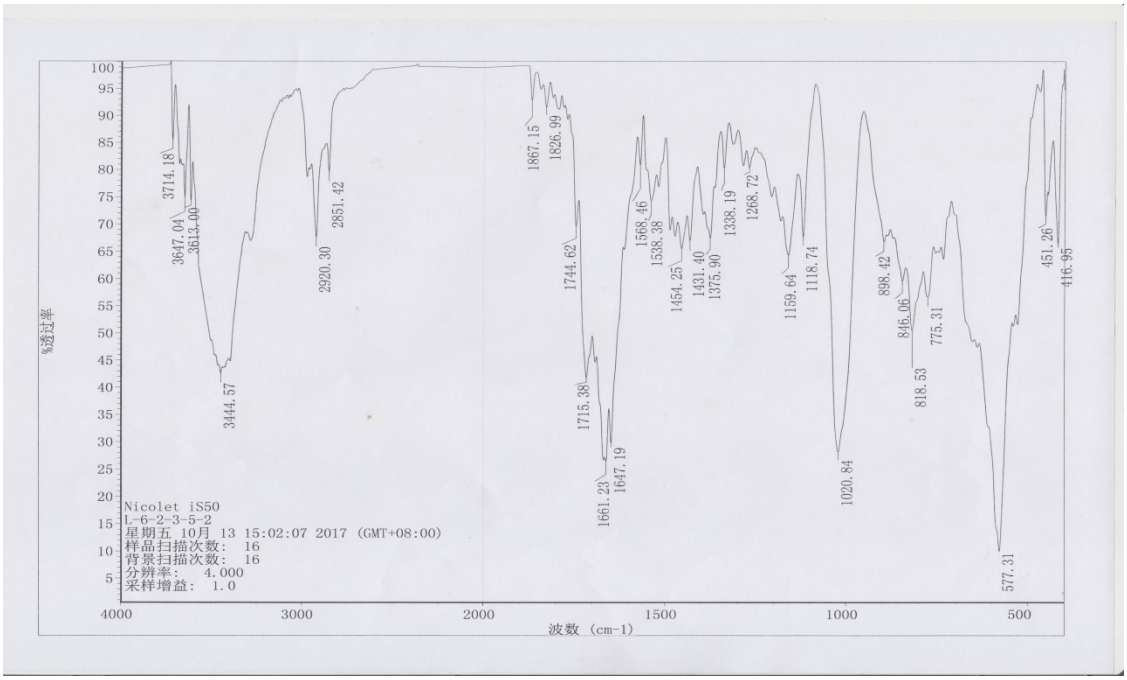


Figure S8. IR spectrum of **2**

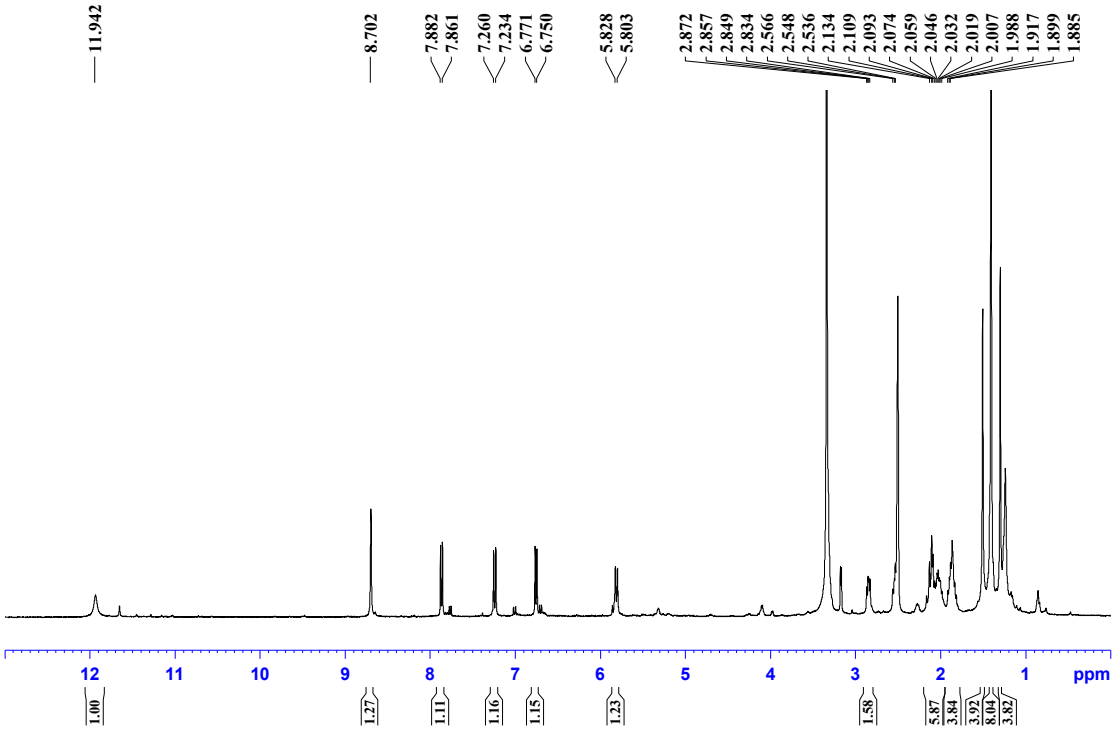


Figure S9. ^{1}H NMR spectrum of **2**

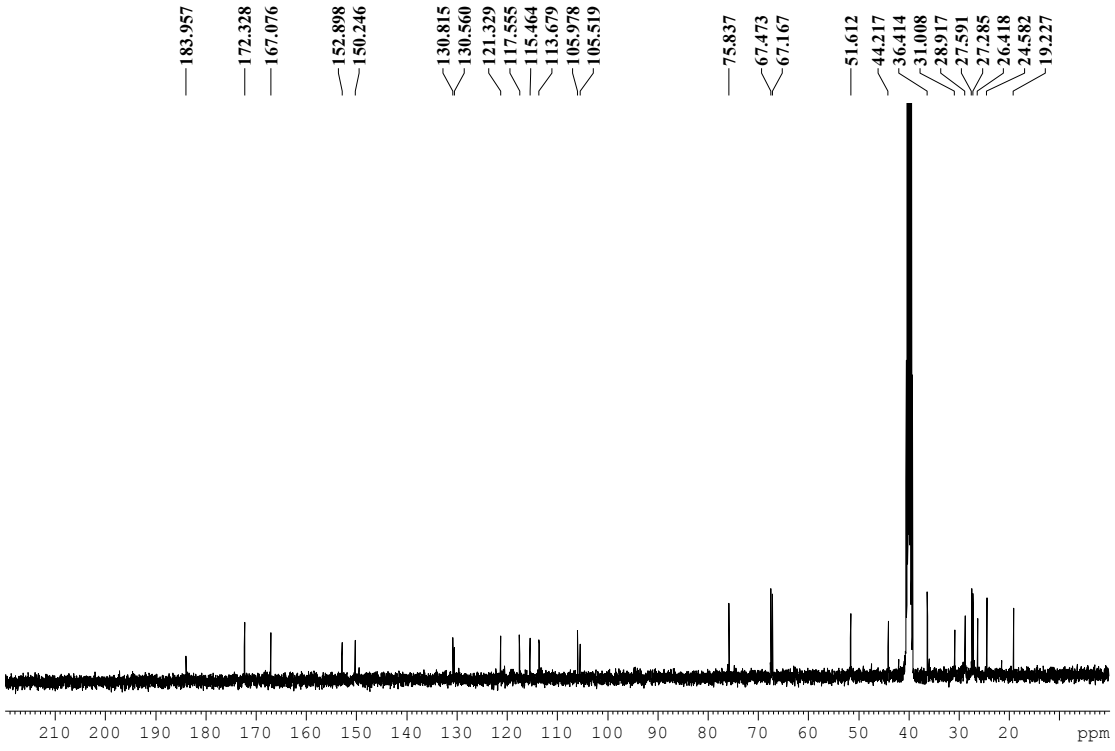


Figure S10. ^{13}C NMR spectrum of **2**

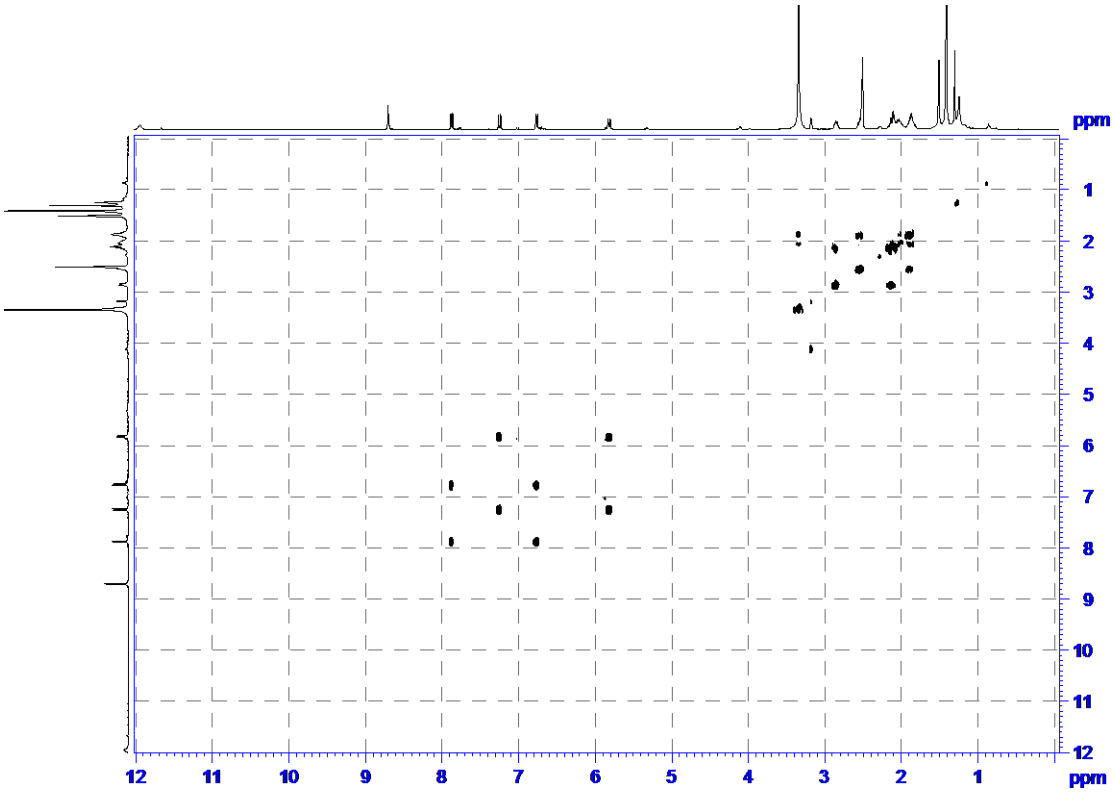


Figure S11. ^{1}H-^{1}H-COSY spectrum of **2**

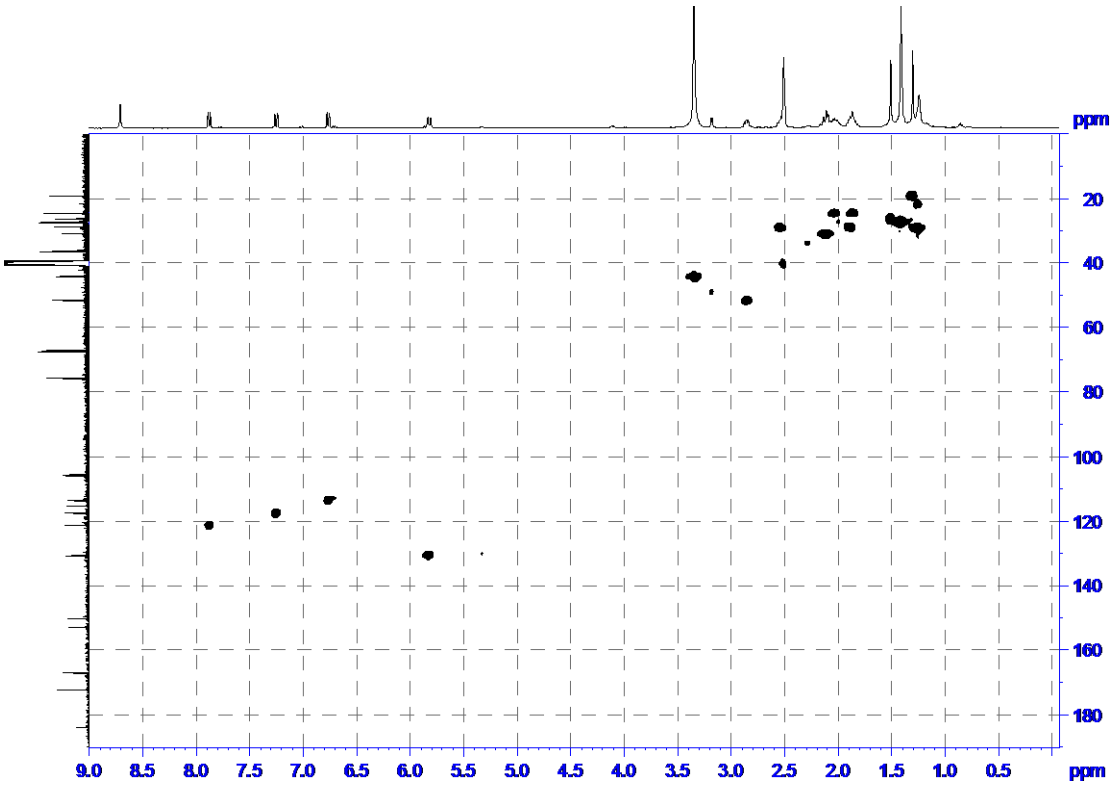


Figure S12. HSQC spectrum of **2**

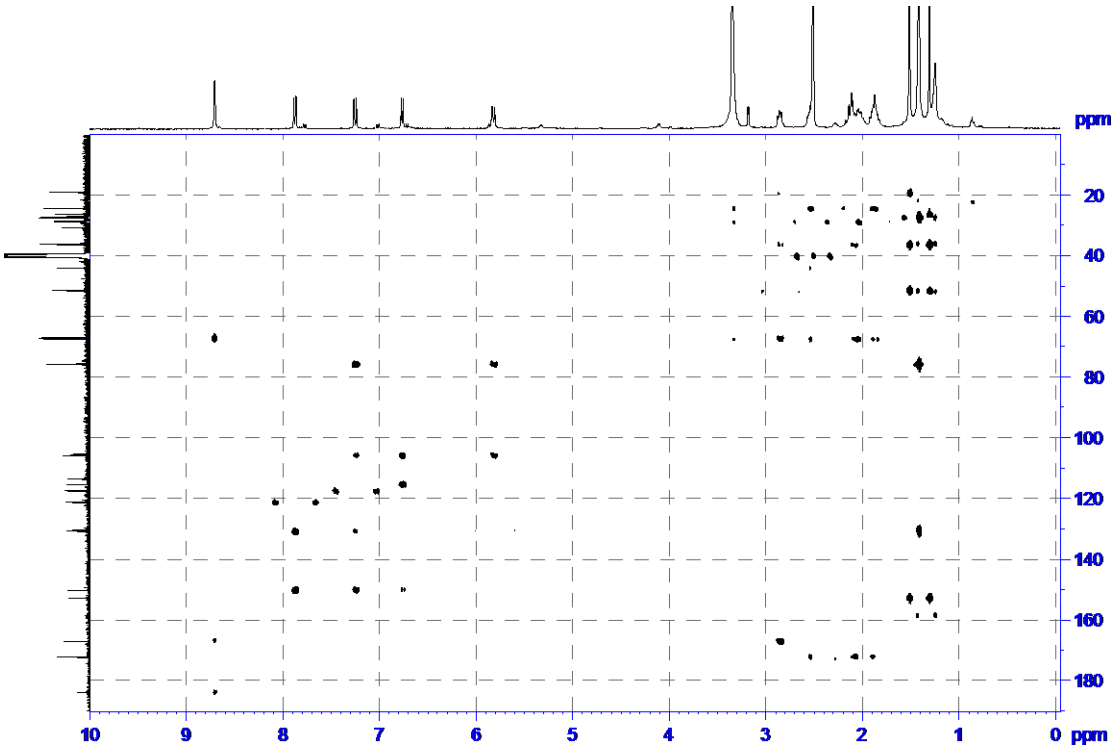


Figure S13. HMBC spectrum of **2**

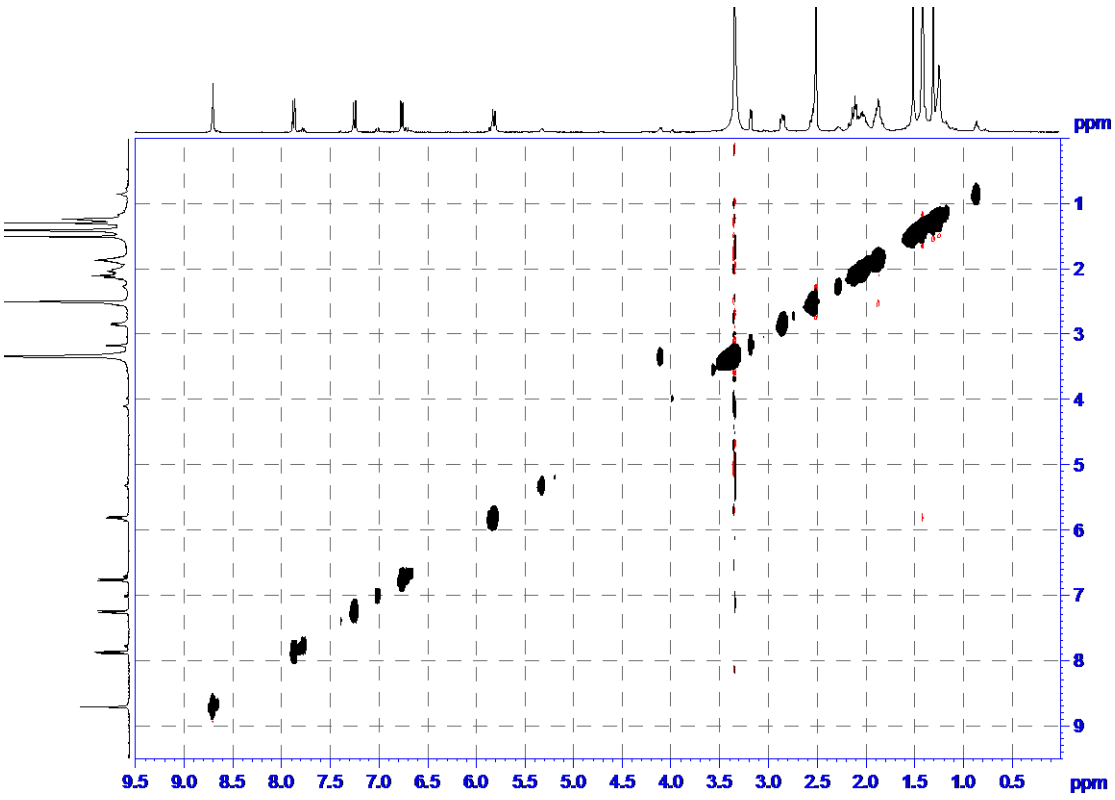
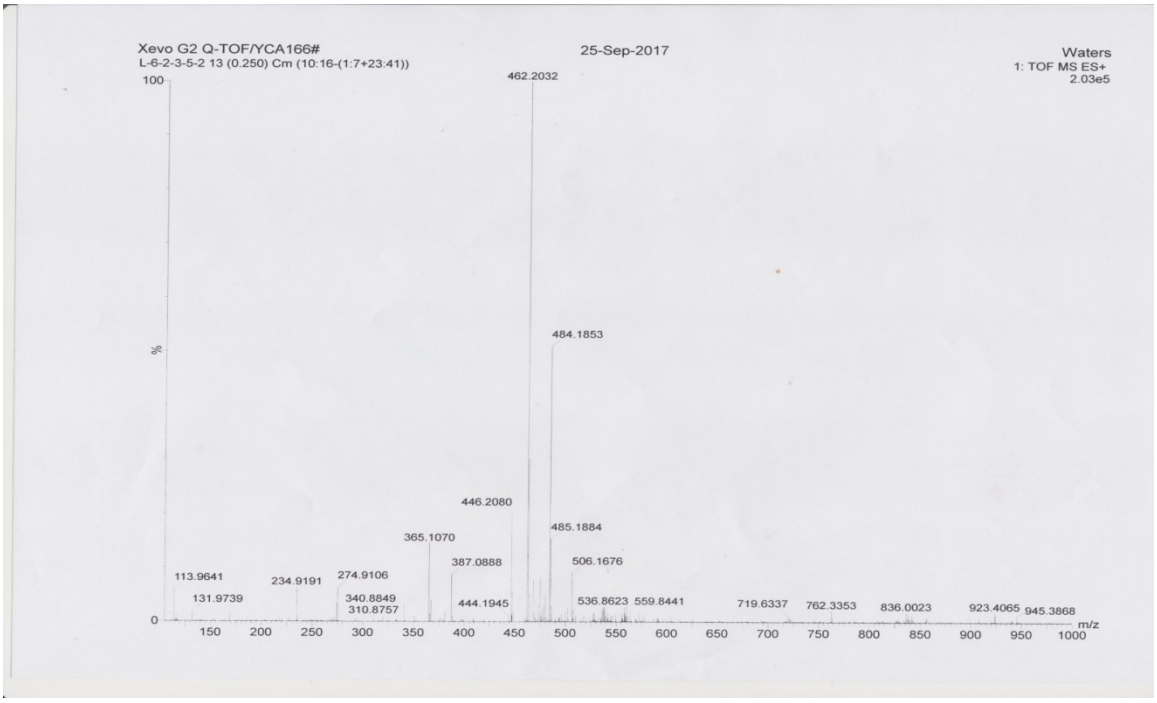


Figure S14. NOESY spectrum of **2**

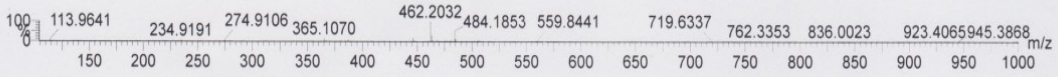


Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 1.0 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
1336 formula(e) evaluated with 2 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 0-100 H: 0-200 N: 0-15 O: 0-50

Xevo G2 Q-TOF/YCA166#
L-6-2-3-5-2 13 (0.250) Cm (10:16-(1:7+23:41))
25-Sep-2017
Waters
1: TOF MS ES+
2.03e+005



Minimum:				-1.5				
Maximum:		6.0	1.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
462.2032	462.2034	-0.2	-0.4	7.5	131.3	16.445	0.00	C11 H24 N15 O6
	462.2029	0.3	0.6	14.5	114.9	0.000	100.00	C26 H28 N3 O5

Figure S15. HRESIMS of 2

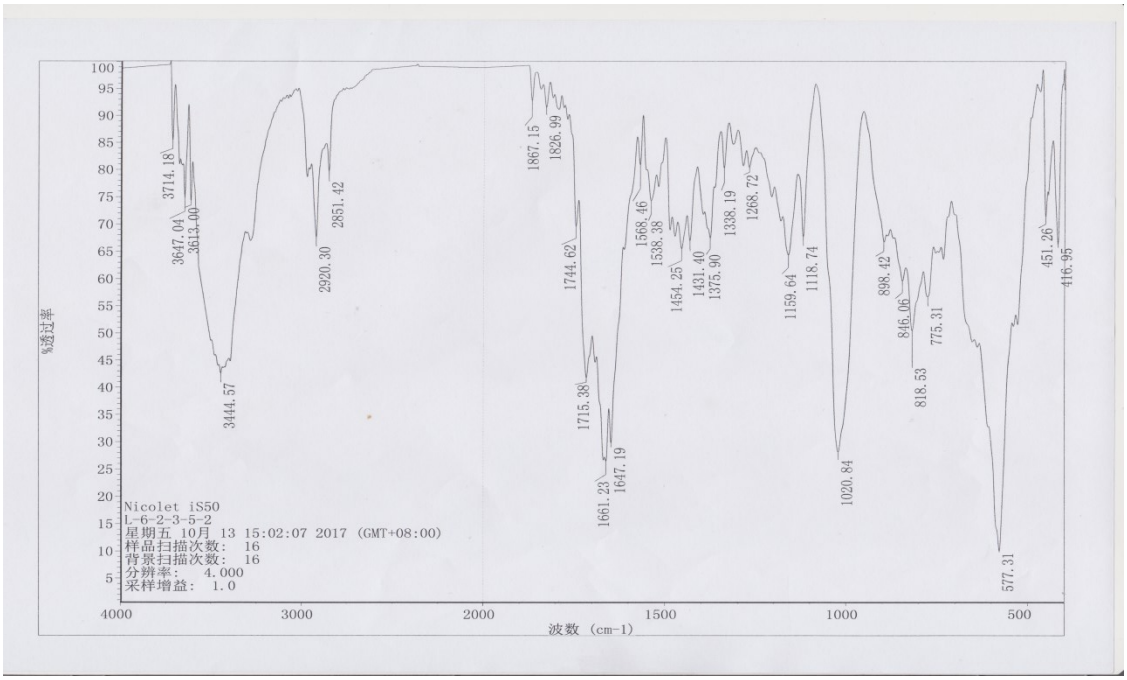


Figure S16. IR spectrum of **3**

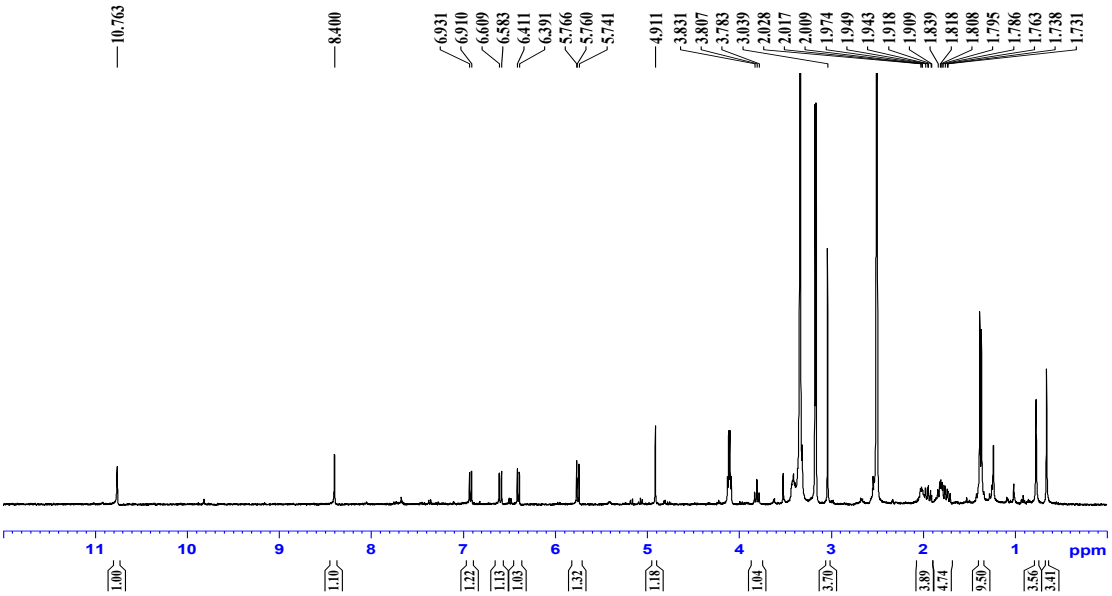


Figure S17. ^{1}H NMR spectrum of **3**

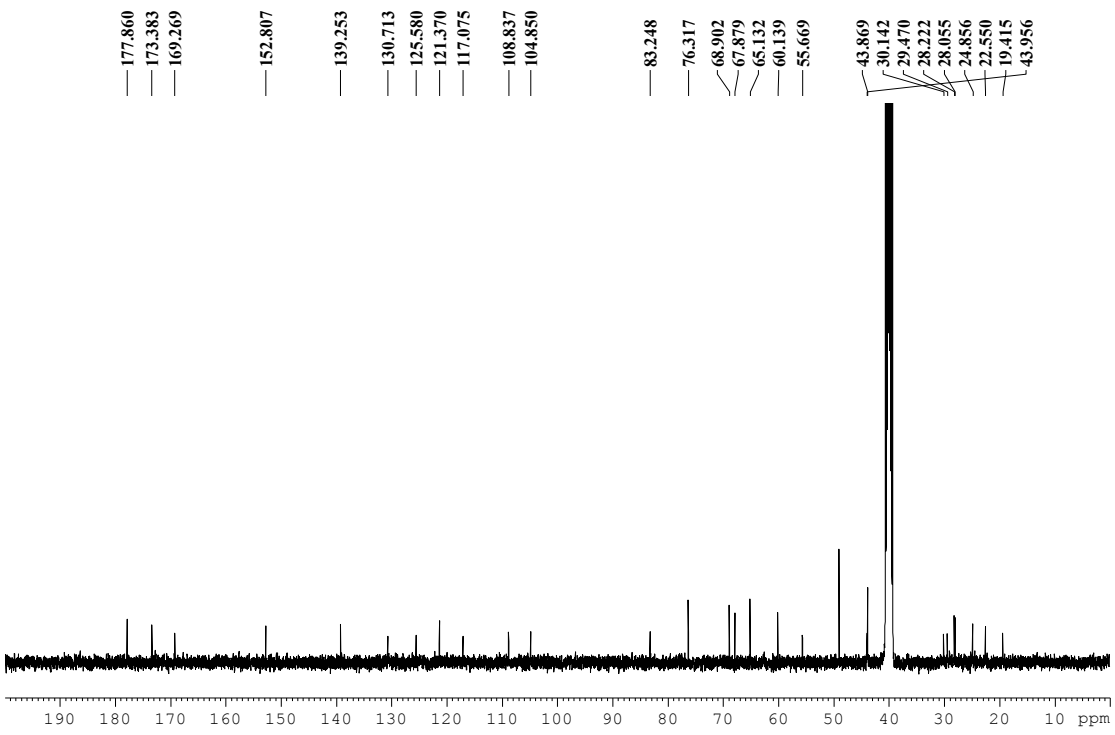


Figure S18. ^{13}C NMR spectrum of **3**

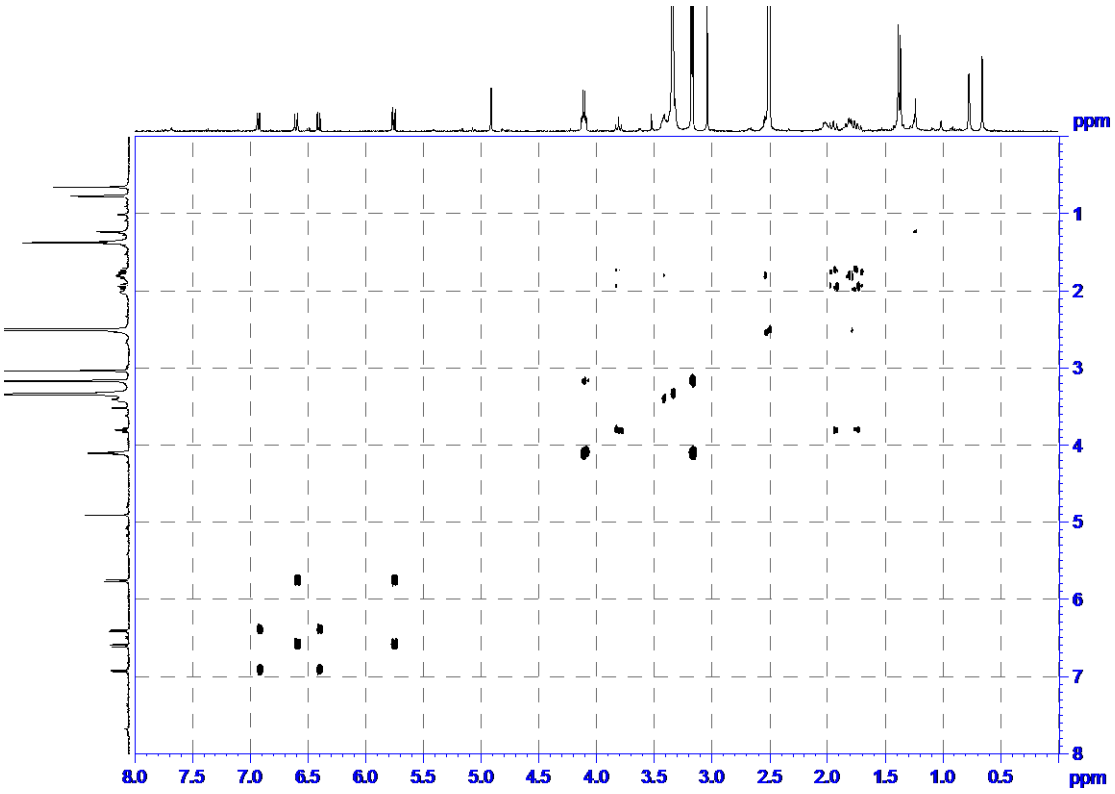


Figure S19. ^{1}H-^{1}H COSY spectrum of **3**

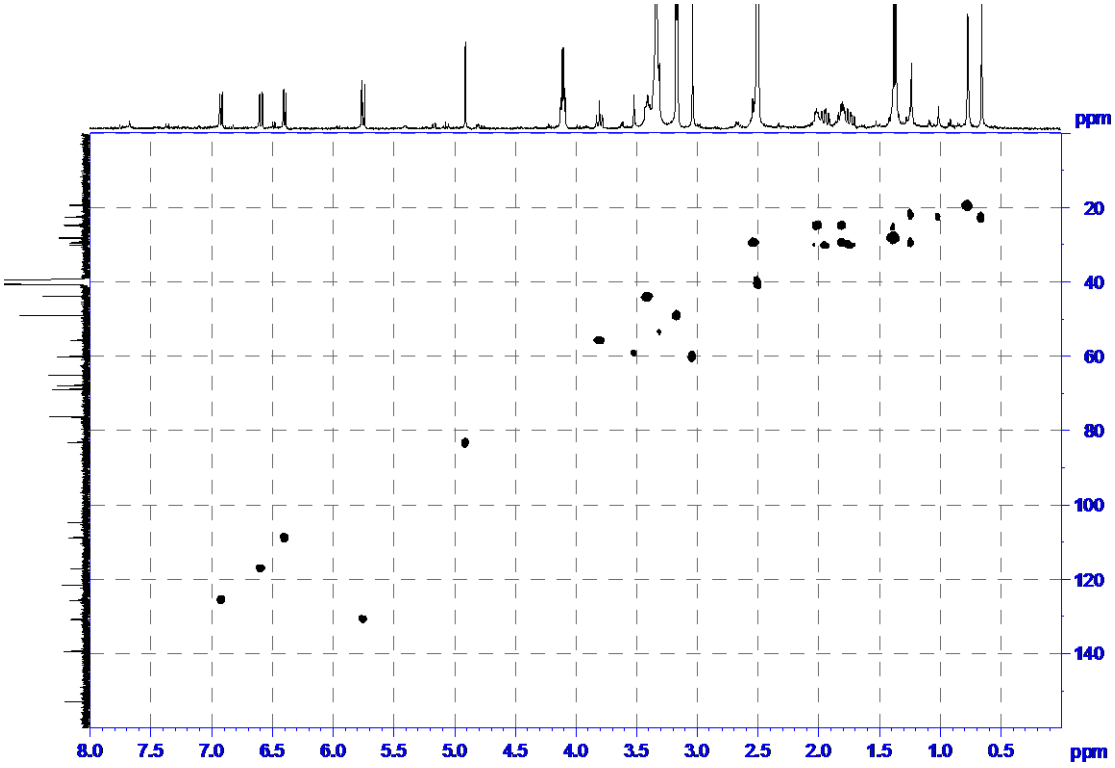


Figure S20. HSQC spectrum of **3**

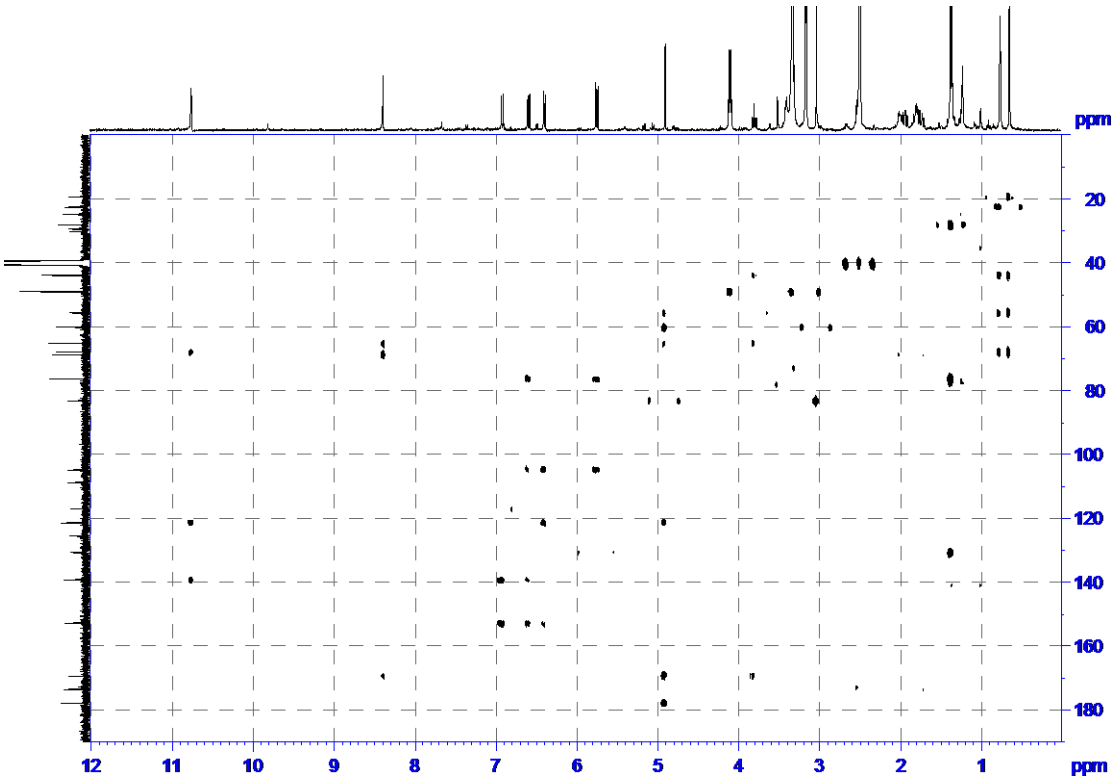


Figure S21.HMBC spectrum of **3**

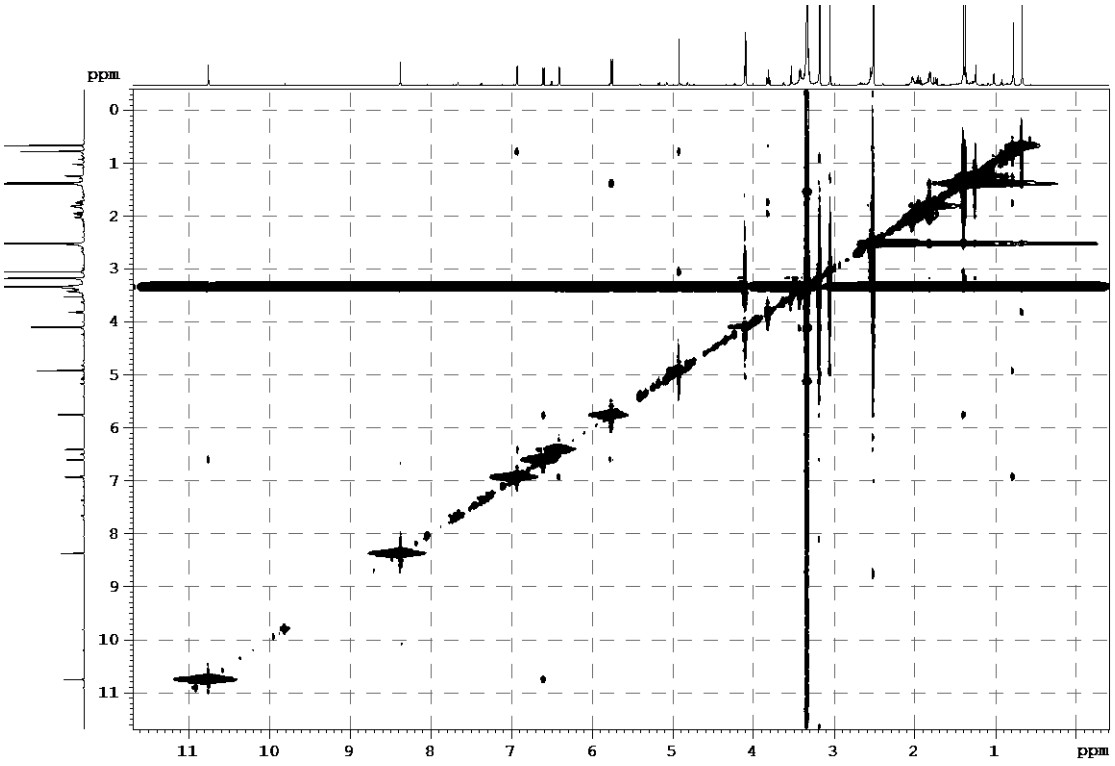


Figure S22. NOESY spectrum of **3**

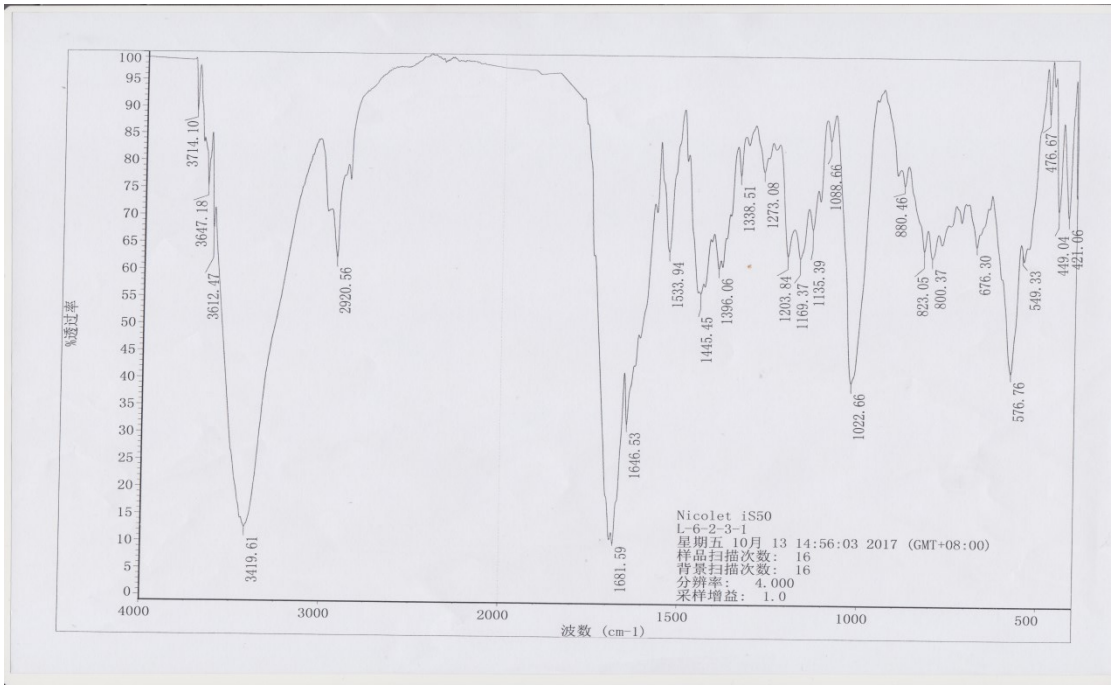


Figure S23. IR spectrum of **4**

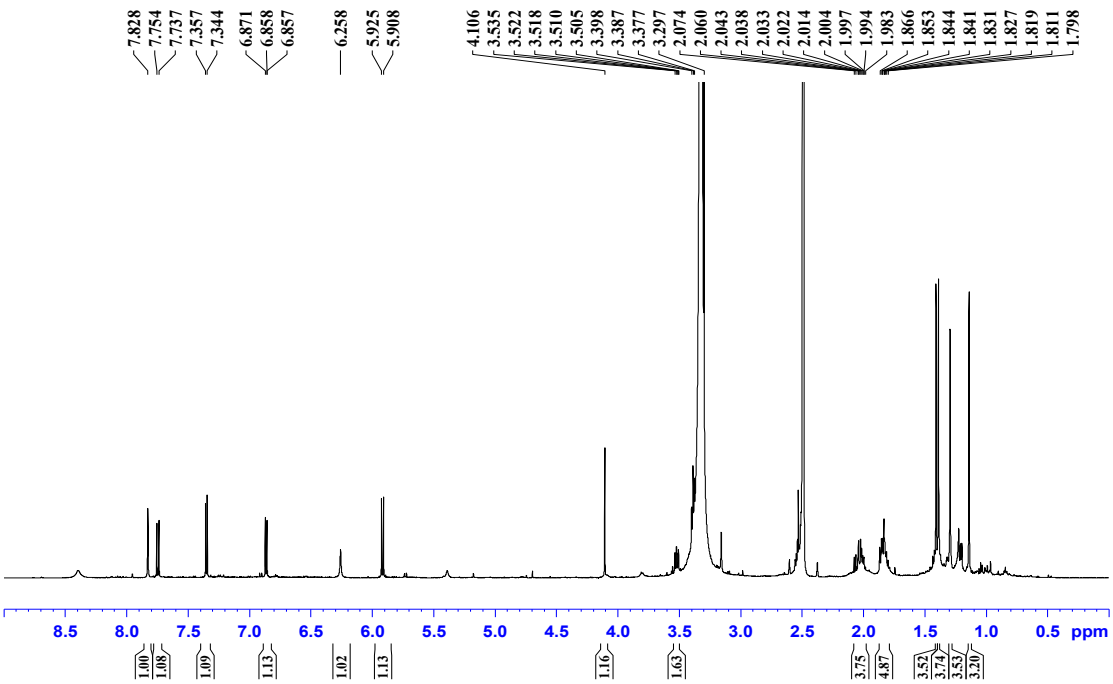


Figure S24. ^{1}H NMR spectrum of **4**

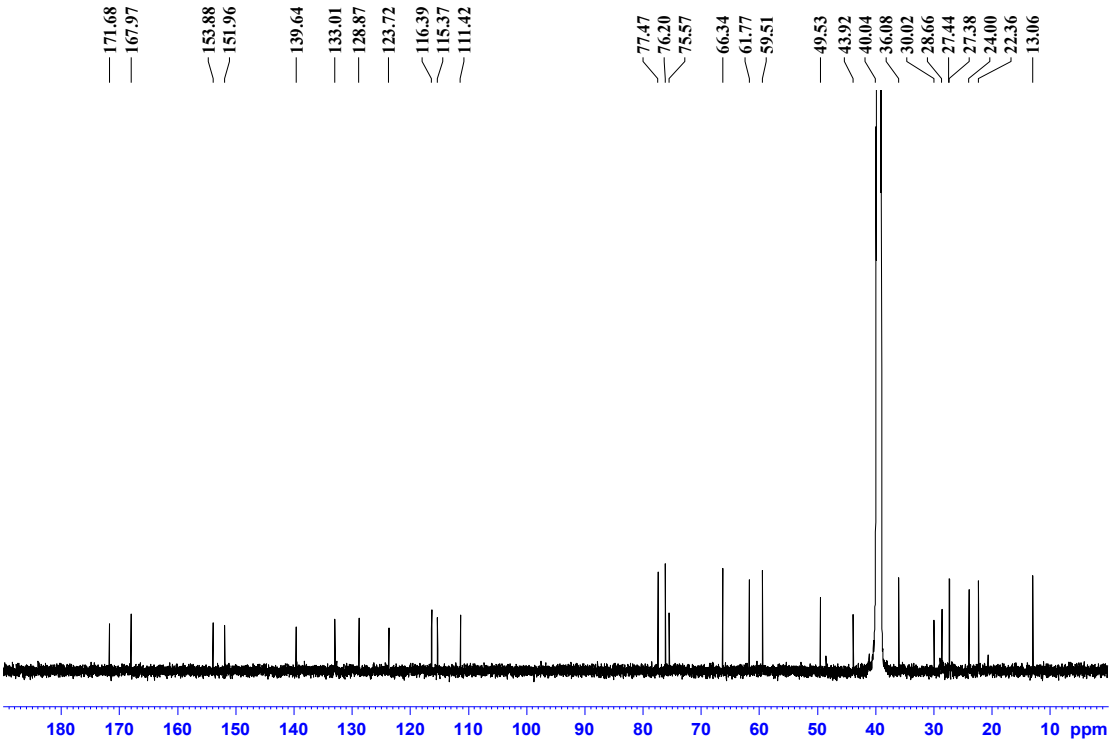


Figure S25. ^{12}C NMR spectrum of **4**

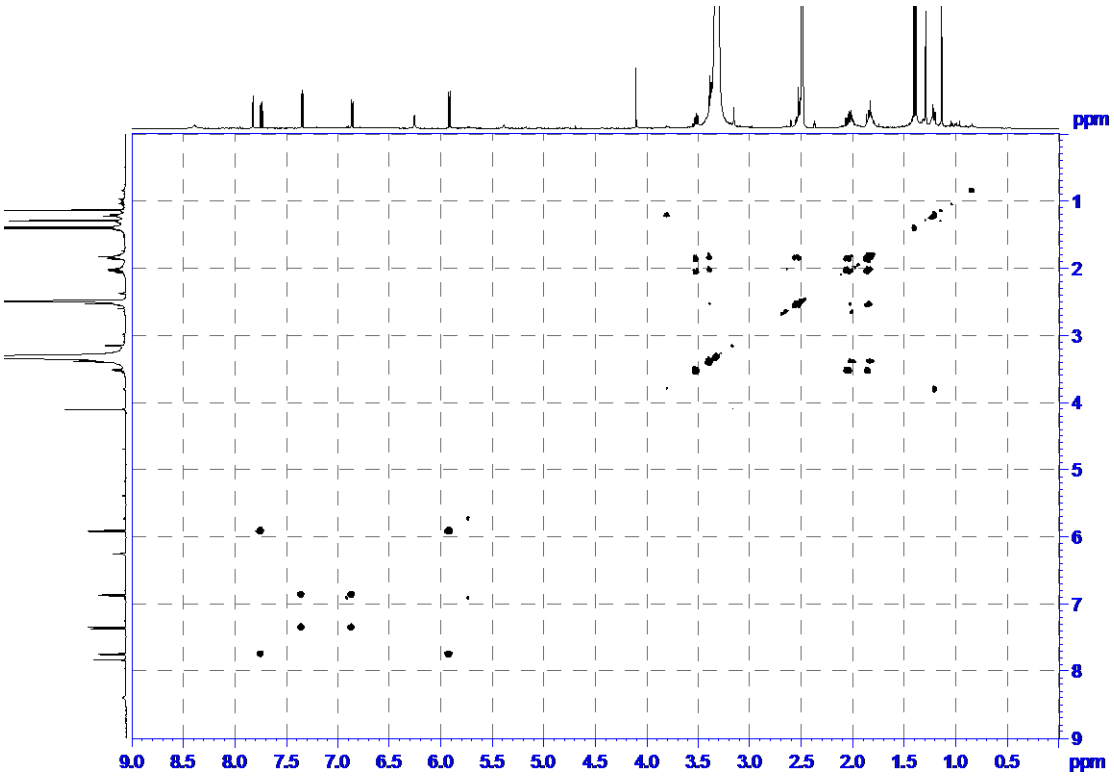


Figure S26. ^{1}H-^{1}H COSY spectrum of **4**

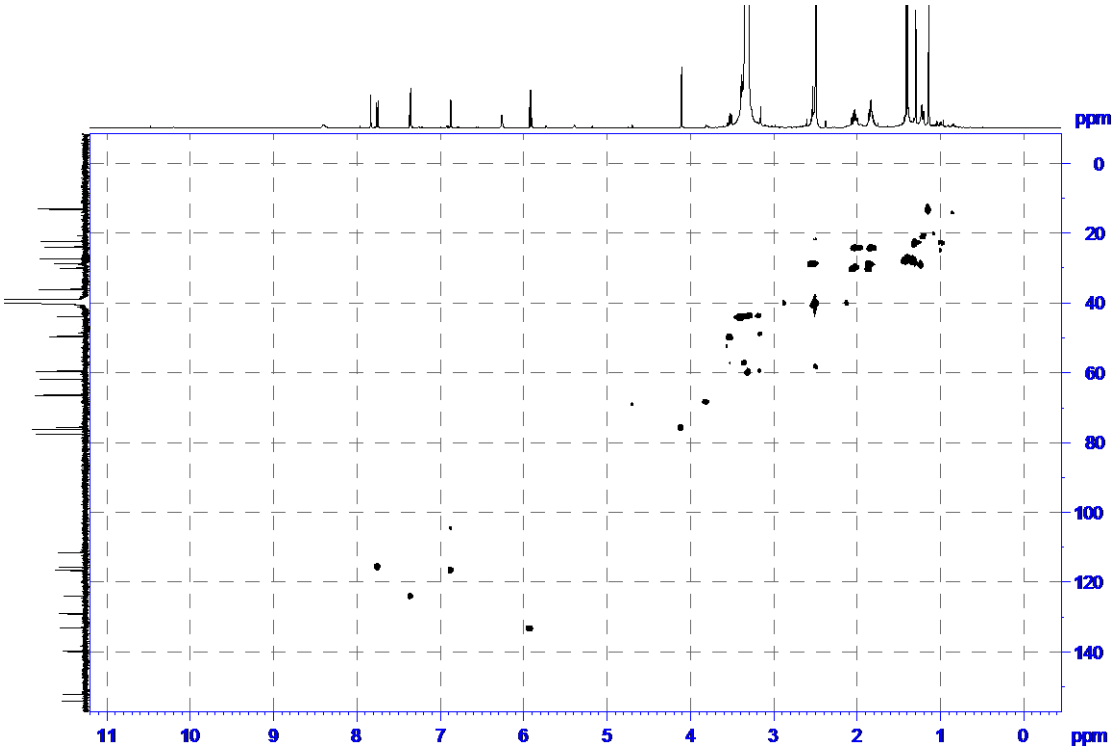


Figure S27. HSQC spectrum of **4**

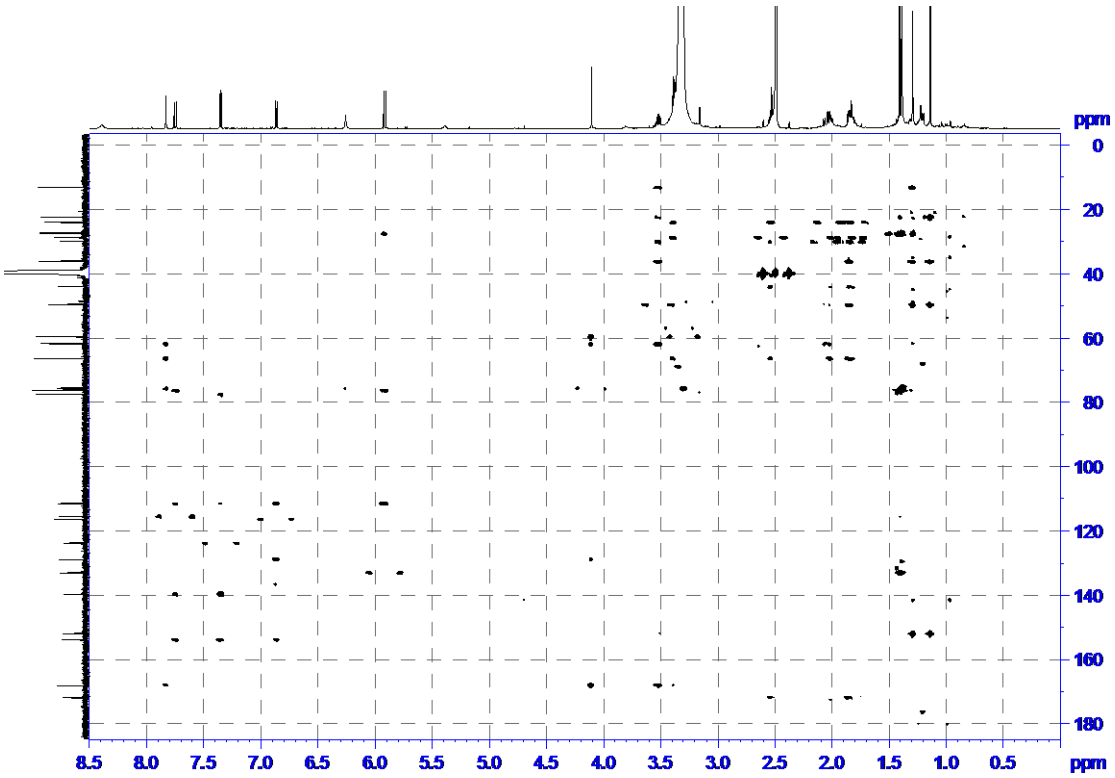


Figure S28. HMBC spectrum of **4**

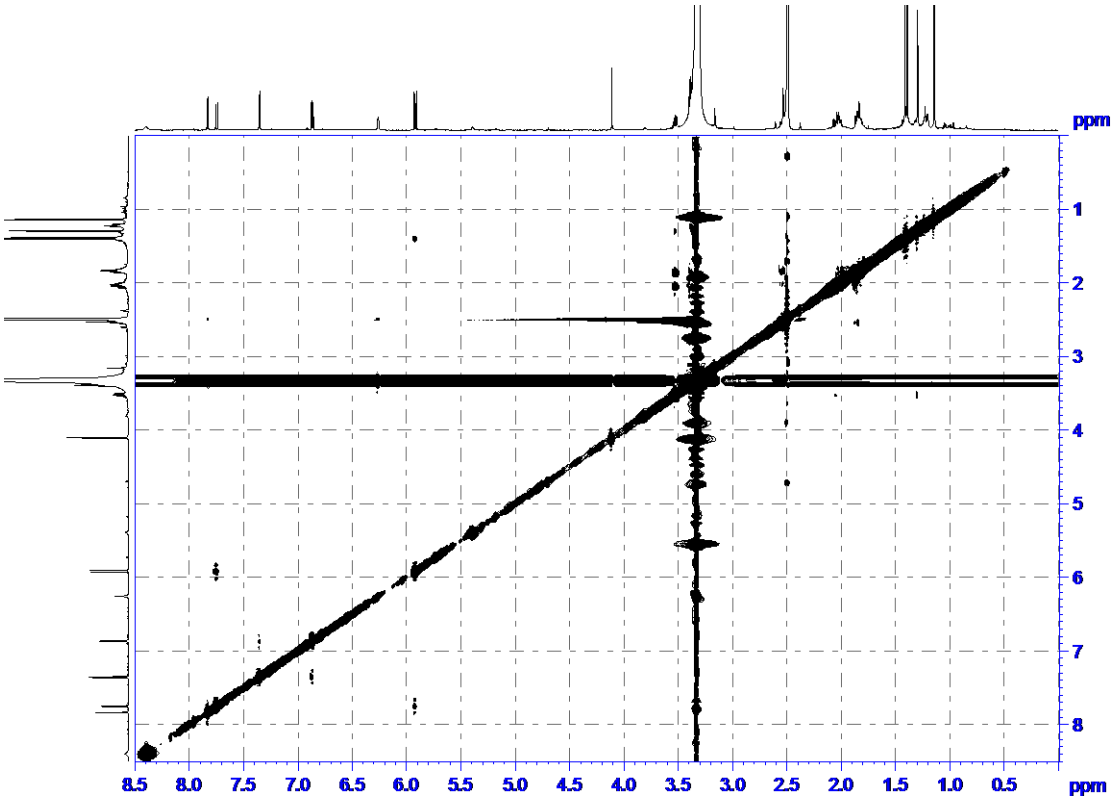


Figure S29. NOESY spectrum of **4**

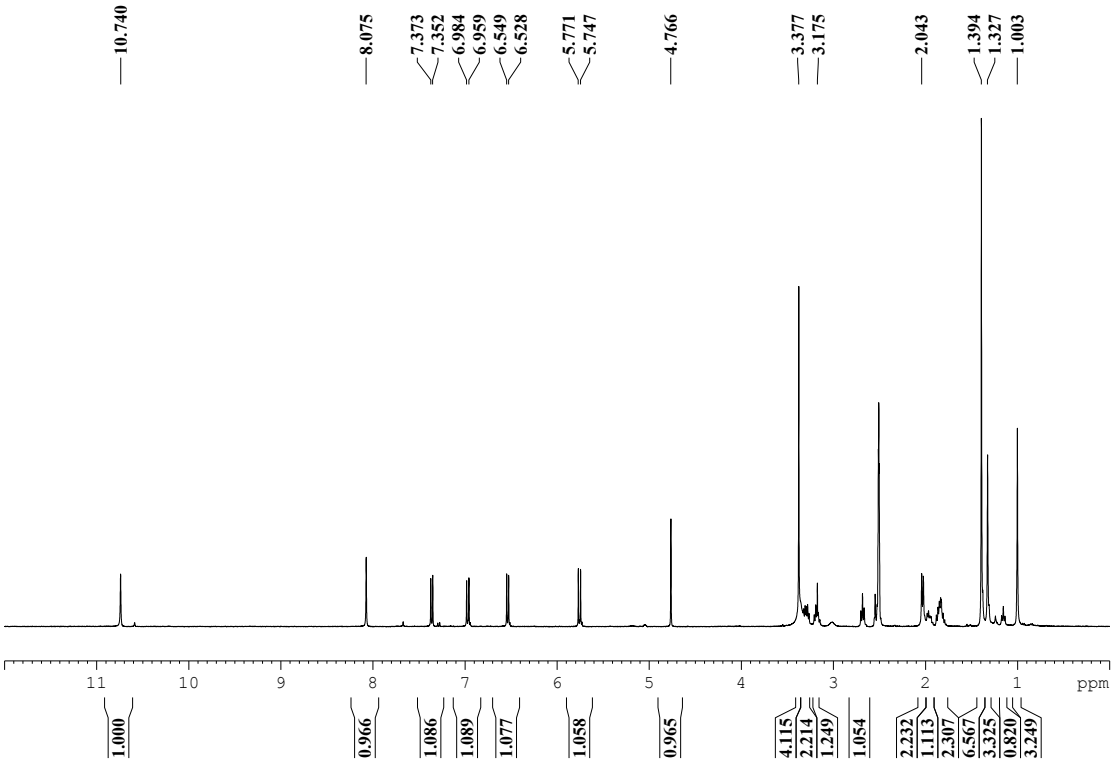


Figure S30. ^{1}H NMR spectrum of **5**

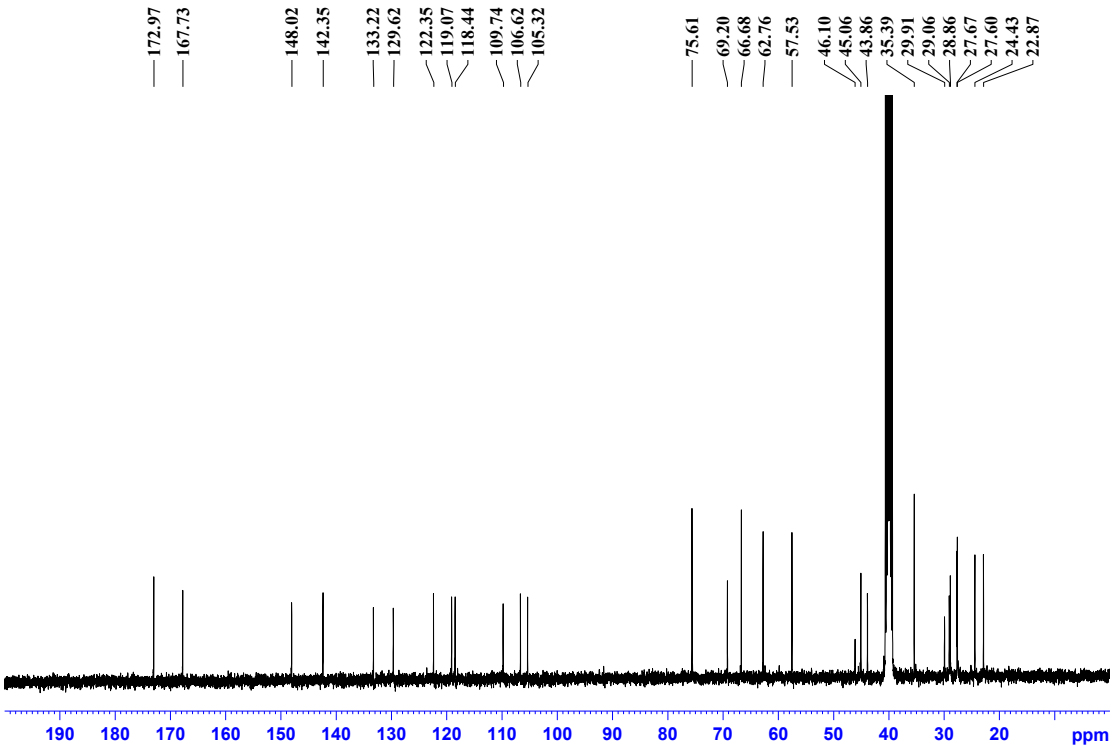


Figure S31. ^{13}C NMR spectrum of **5**

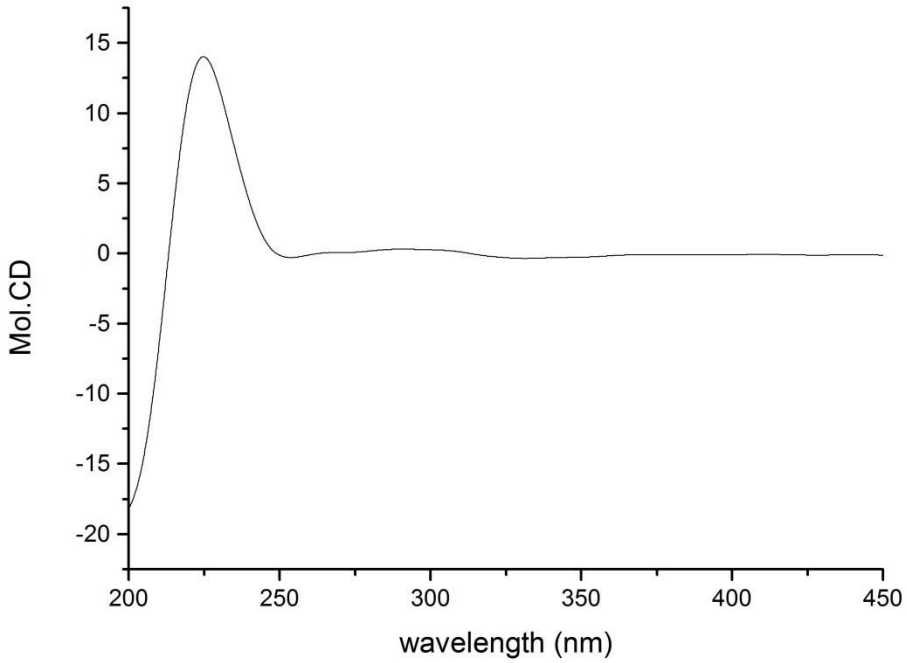


Figure S32. CD spectrum of **5**

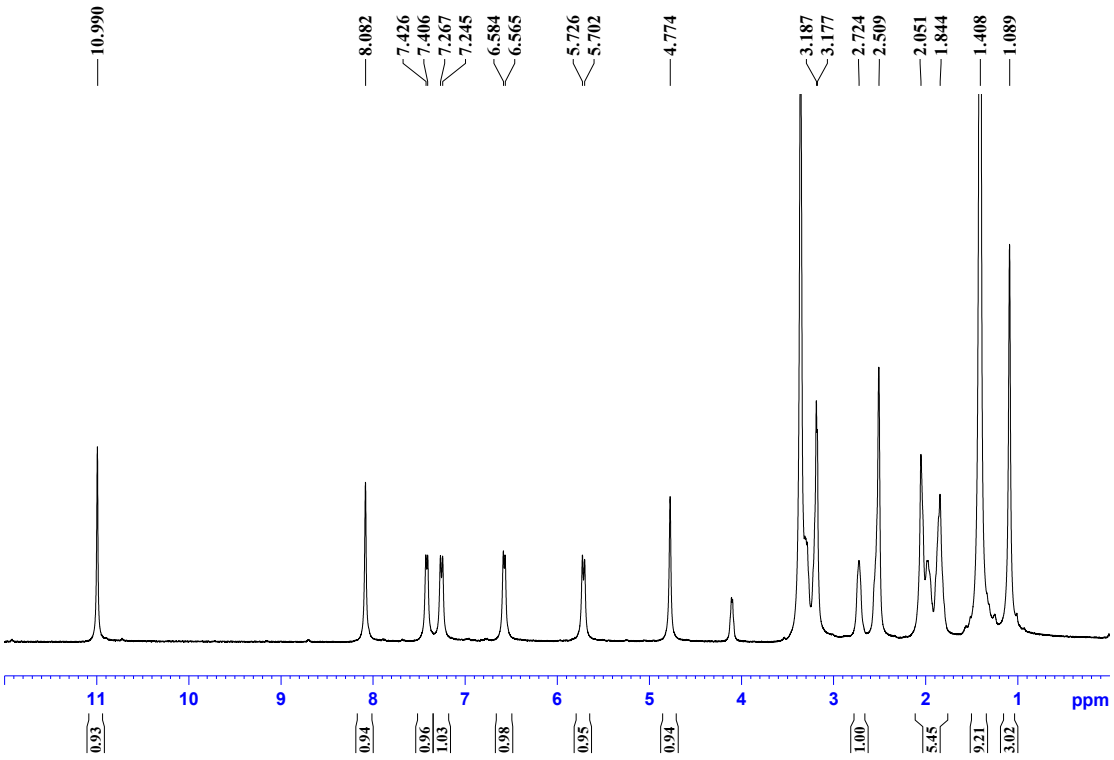


Figure S33. ^{1}H NMR spectrum of **6**

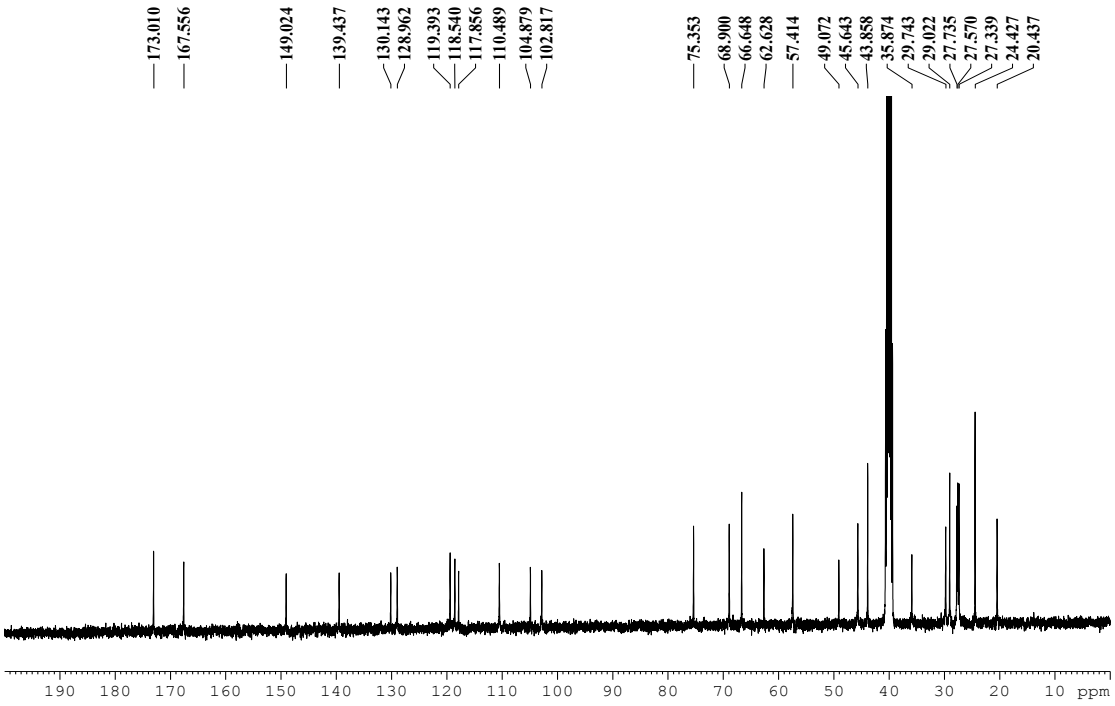


Figure S34. ^{13}C NMR spectrum of **6**

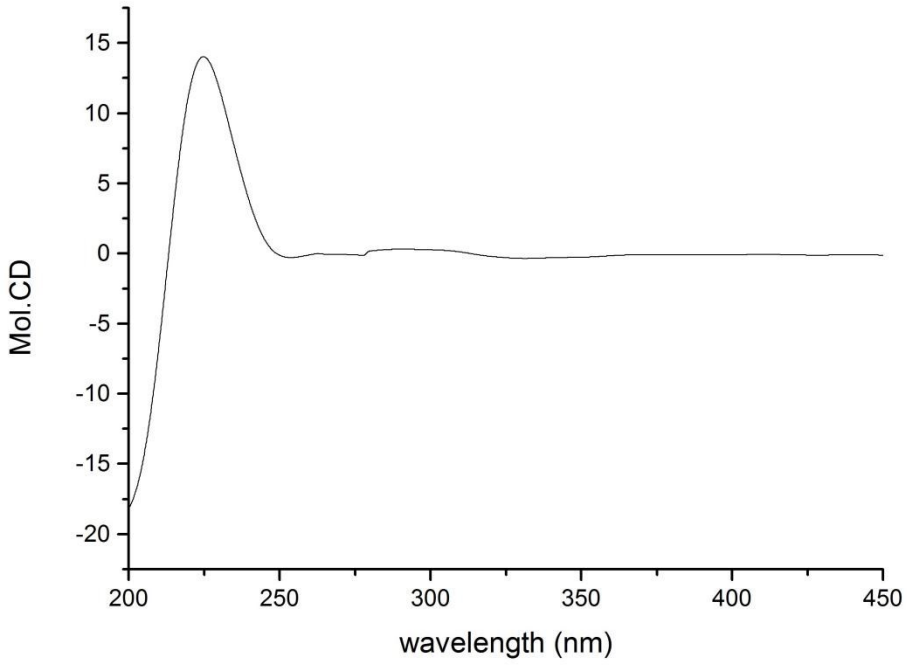


Figure S35. CD spectrum of **6**

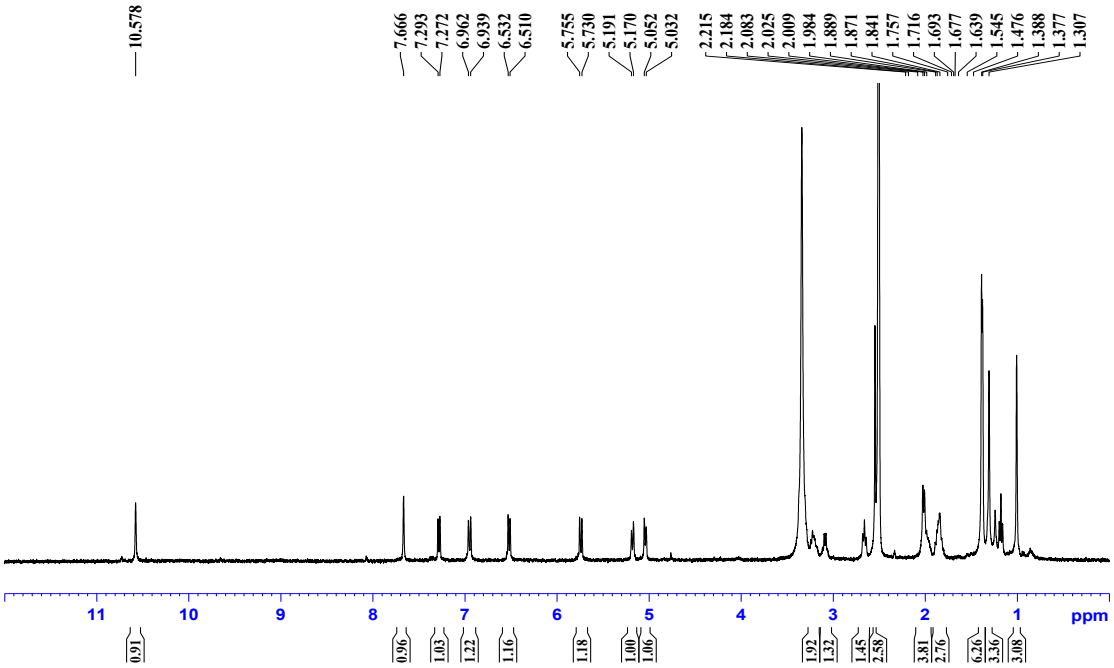


Figure S36. ^{1}H NMR spectrum of **7**

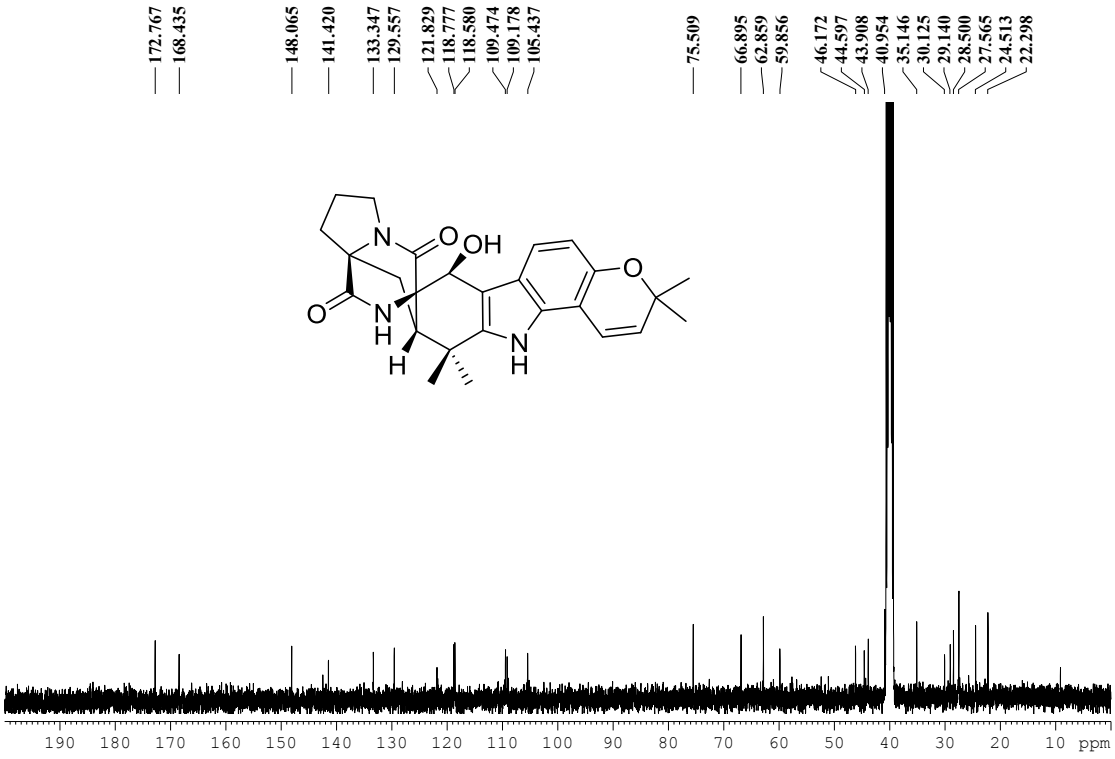


Figure S37. ^{13}C NMR spectrum of **7**

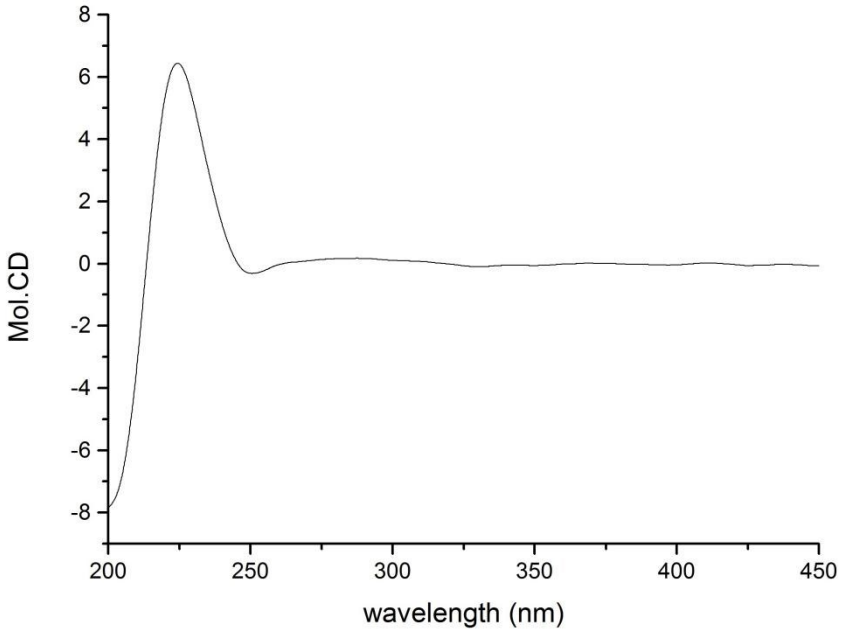


Figure S38. CD spectrum of **7**

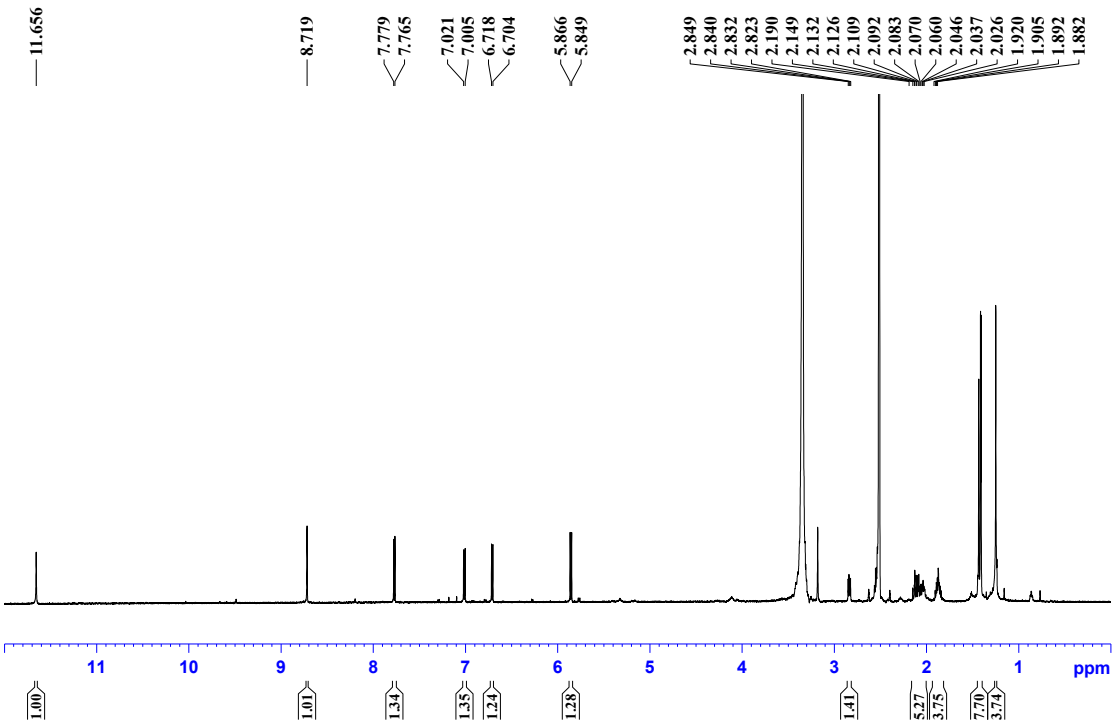


Figure S39. ^{1}H NMR spectrum of **8**

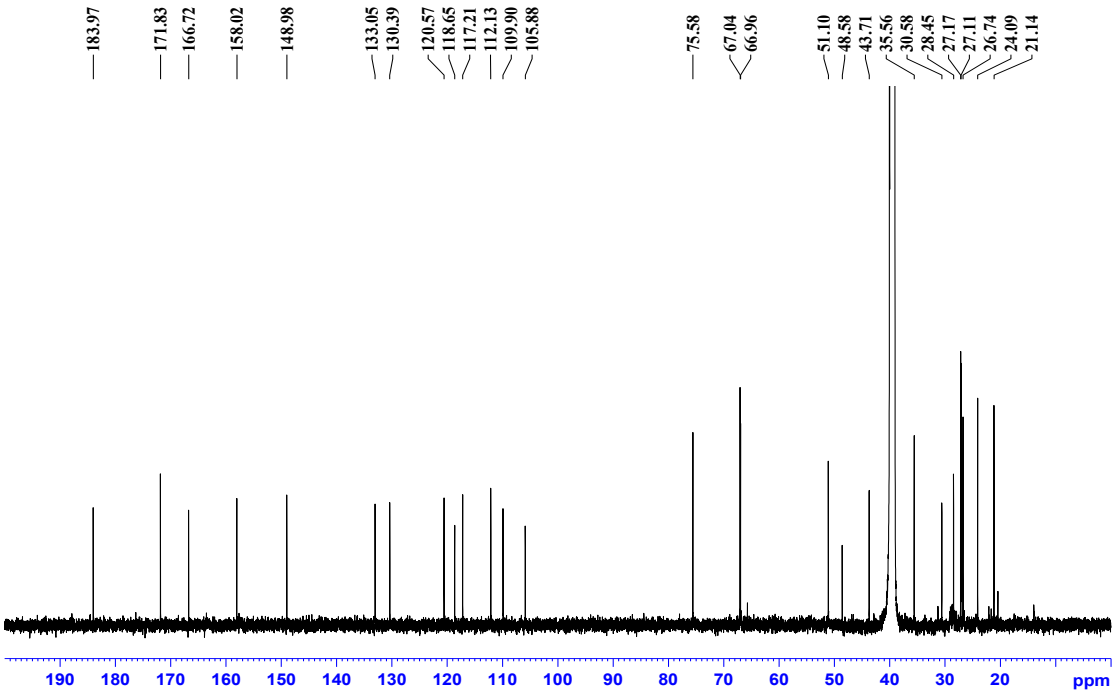


Figure S40. ^{13}C NMR spectrum of **8**

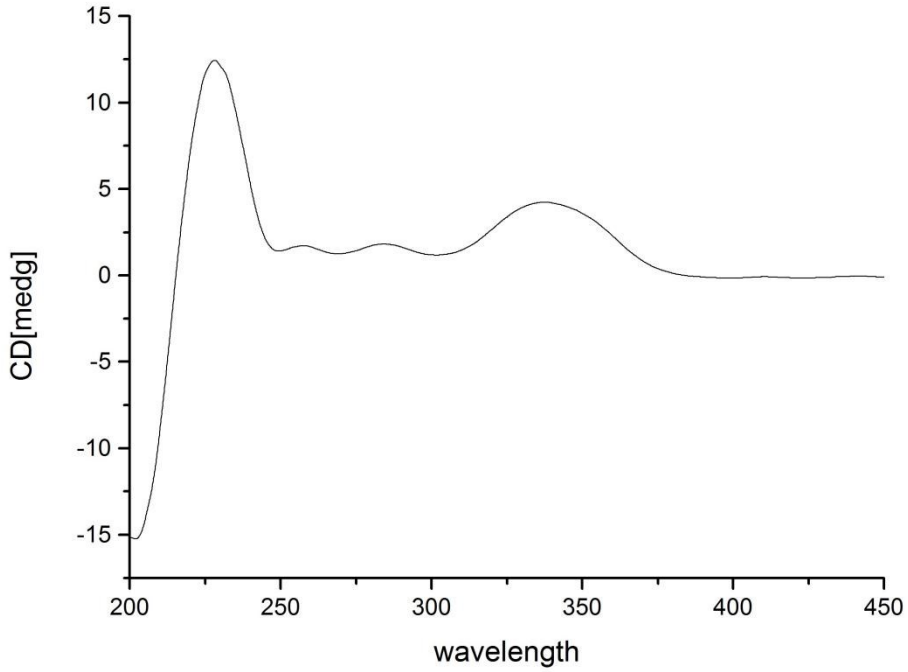


Figure S41. CD spectrum of **8**

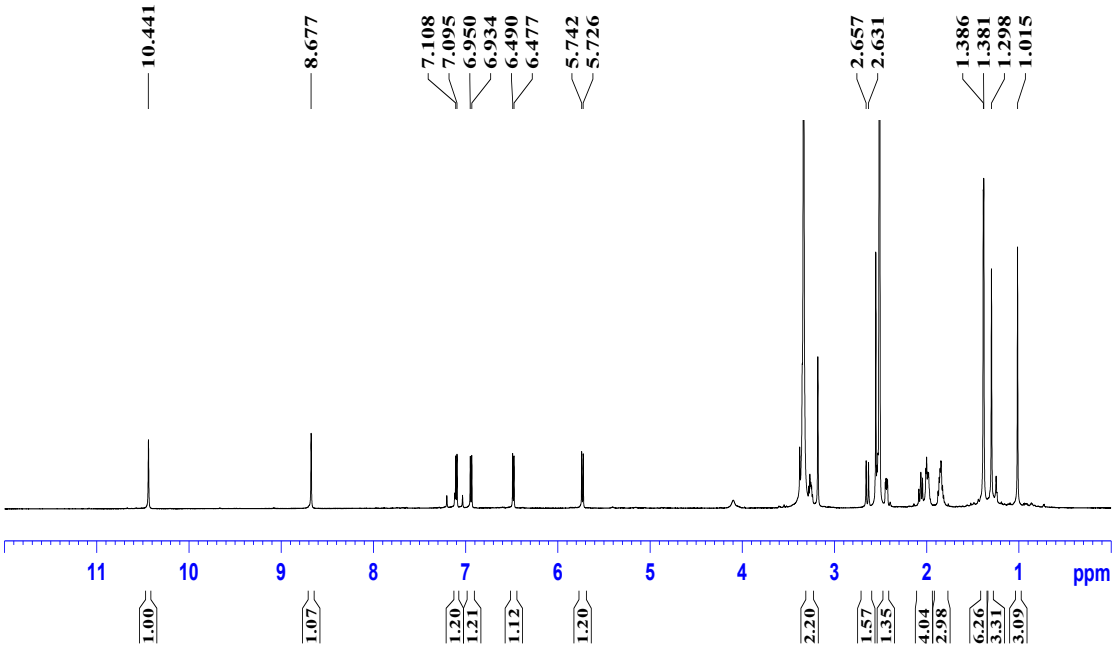


Figure S42. ^{1}H NMR spectrum of **9**

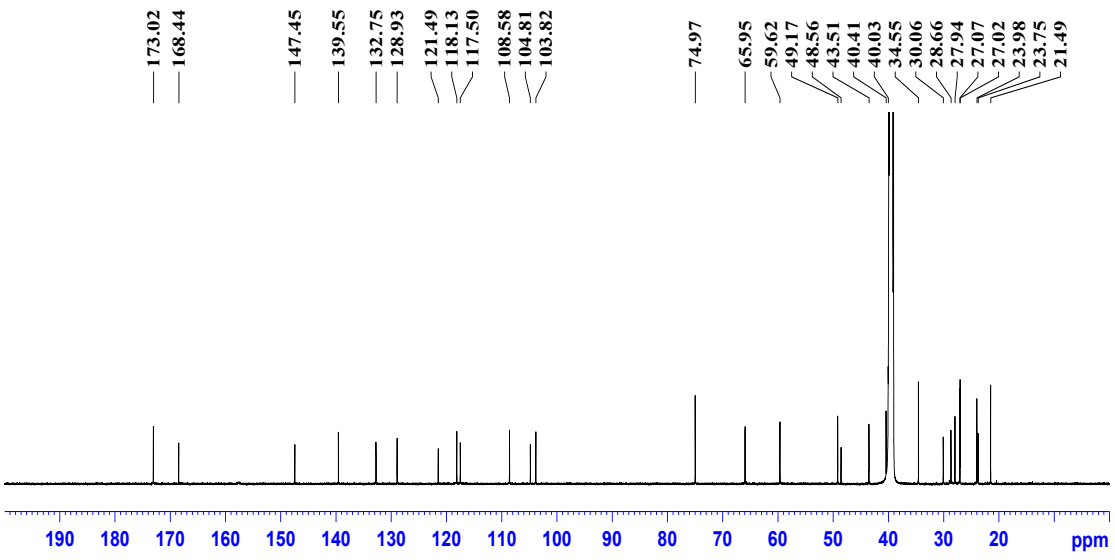


Figure S43. ^{13}C NMR spectrum of **9**

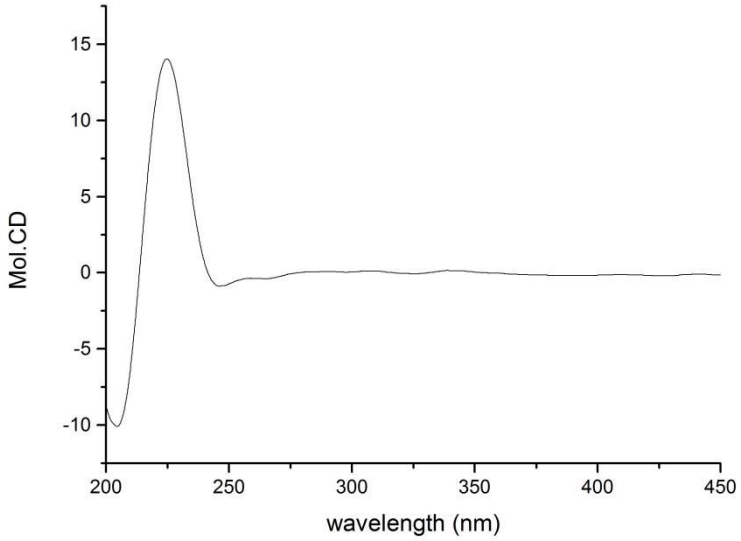


Figure S44. CD spectrum of **9**

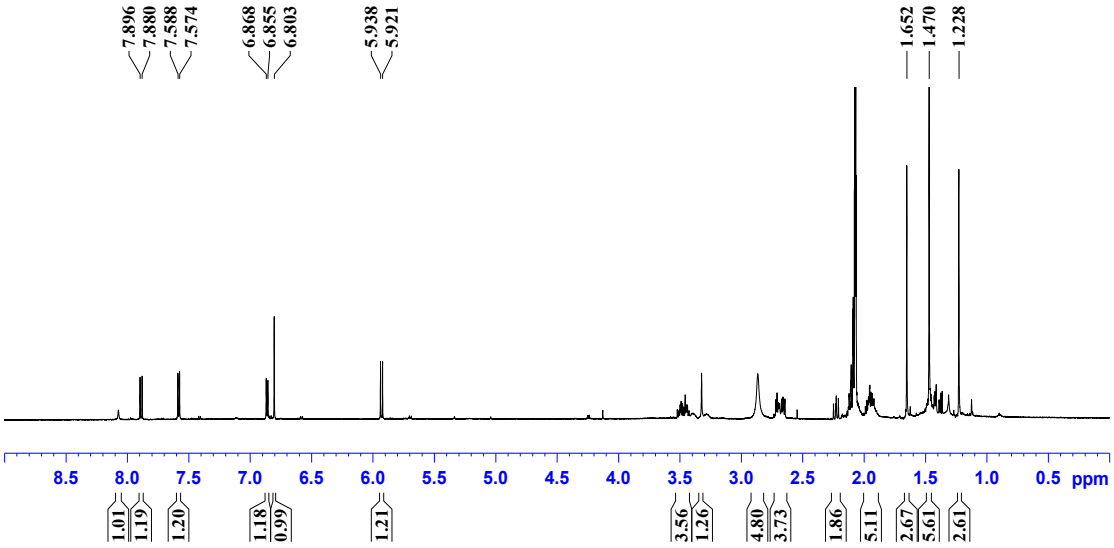


Figure S45. ^{1}H NMR spectrum of **10**

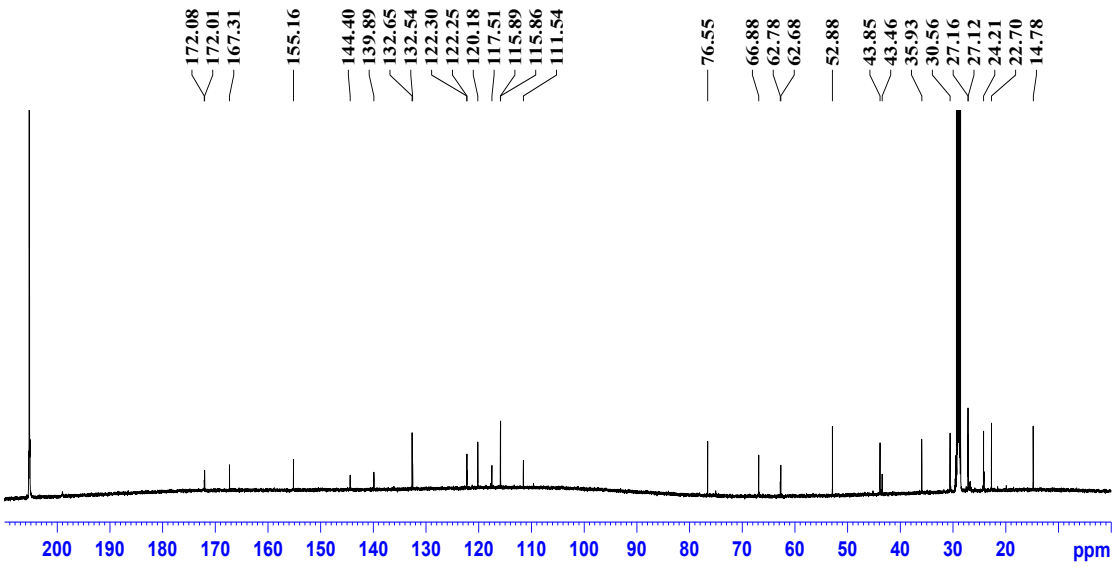


Figure S46. ^{13}C NMR spectrum of **10**

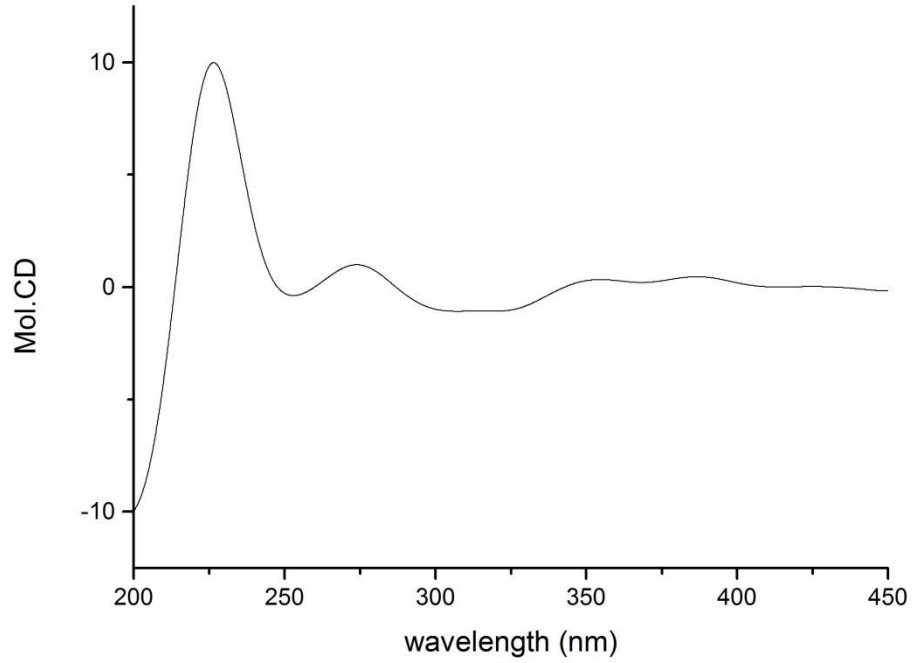


Figure S47. CD spectrum of **10**

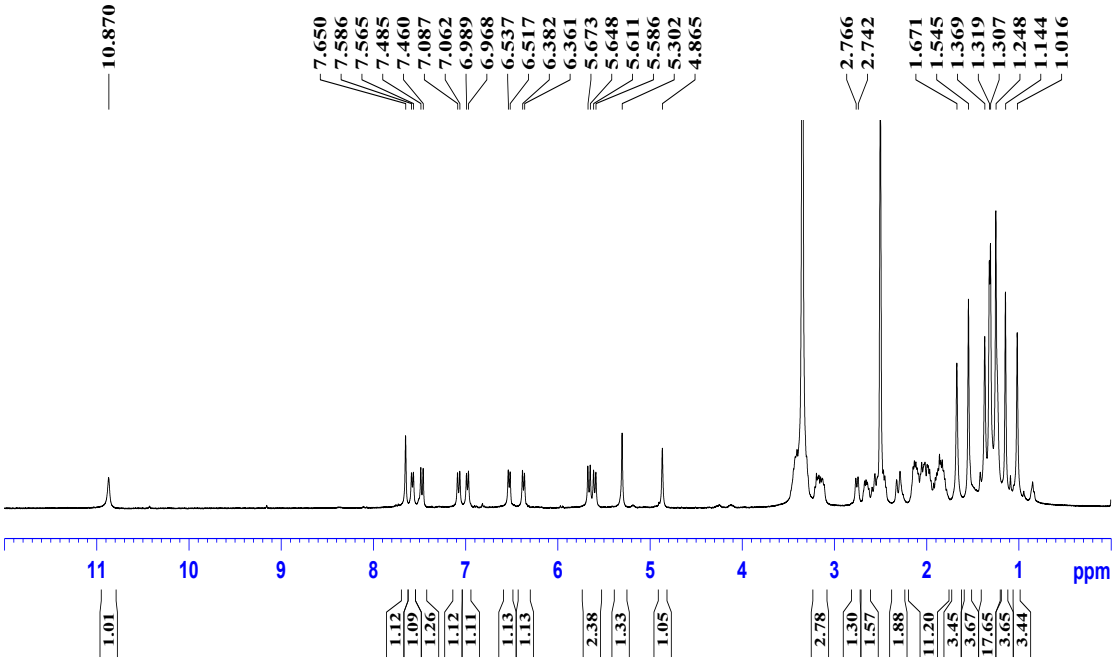


Figure S48. ^{1}H NMR spectrum of **11**

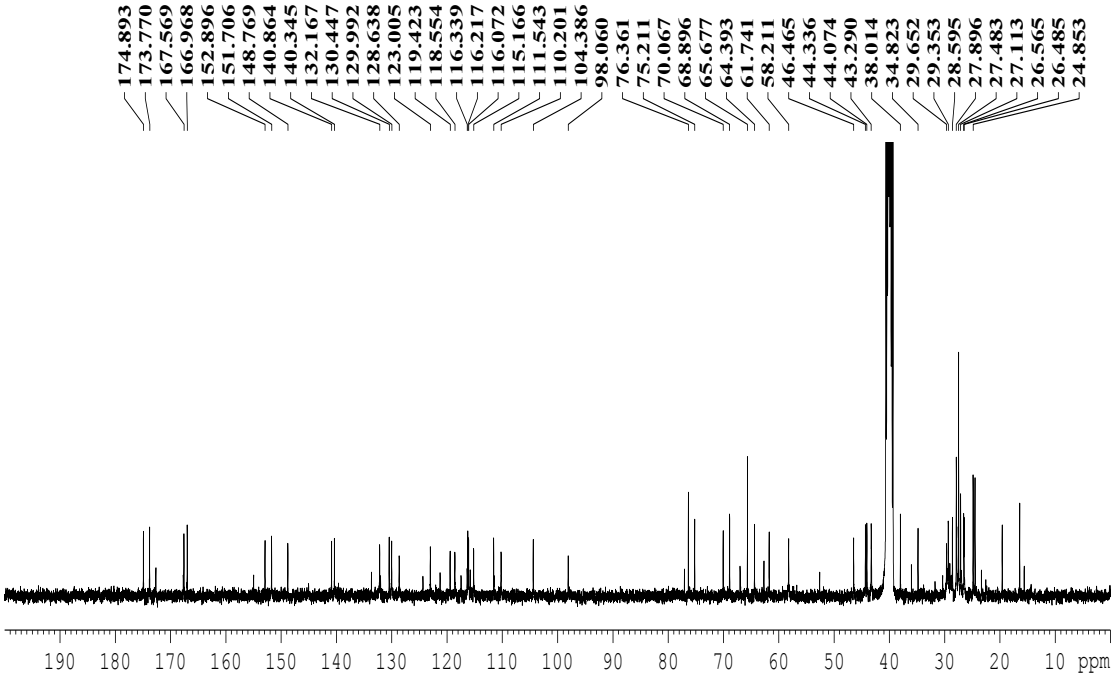


Figure S49. ^{13}C NMR spectrum of **11**

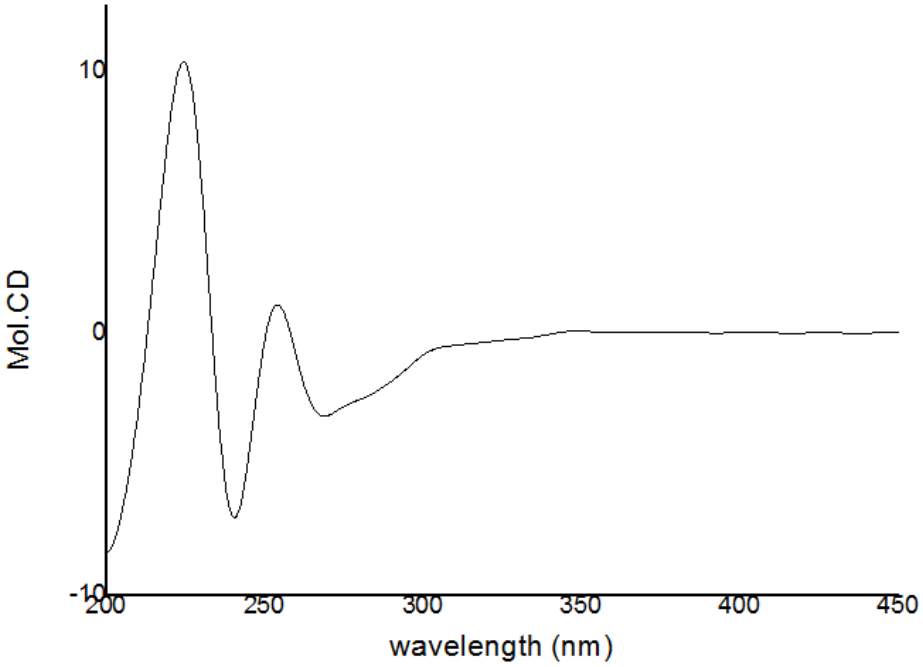


Figure S50. CD spectrum of **11**