

Pyrrole-Containing Alkaloids from a Marine-Derived Actinobacterium *Streptomyces zhaozhouensis* and Their Antimicrobial and Cytotoxic Activities

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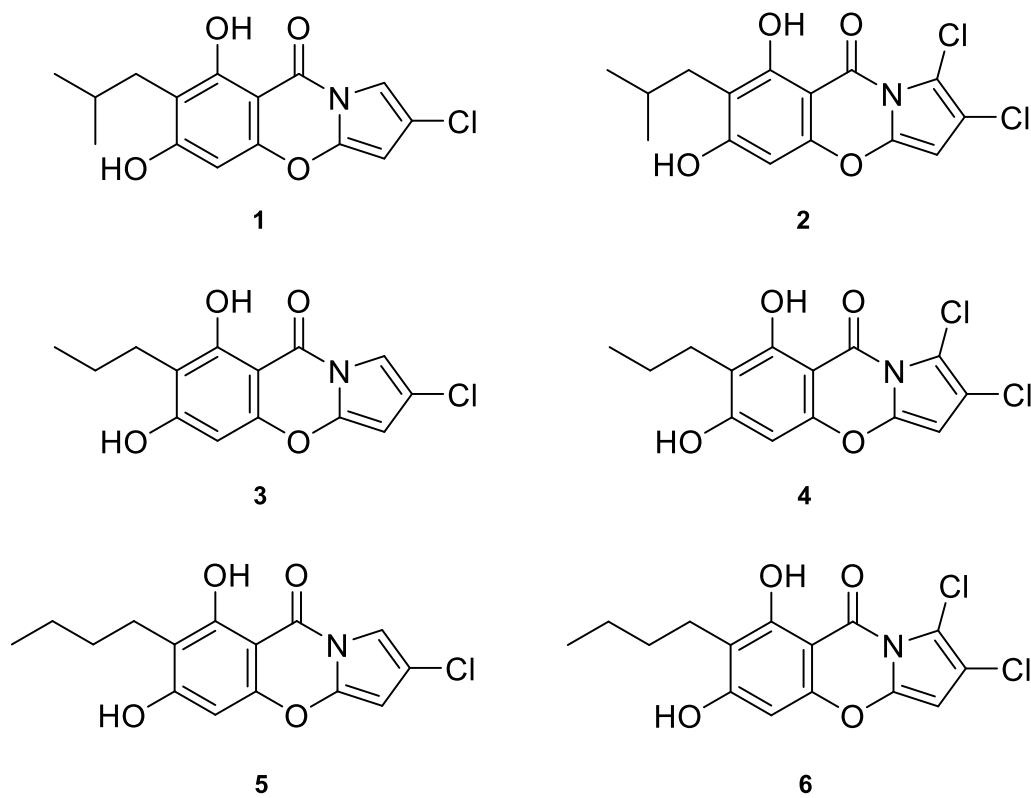


Figure S1. Structures of **1-6** isolated from *Streptomyces zhaozhouensis* 208DD-064.

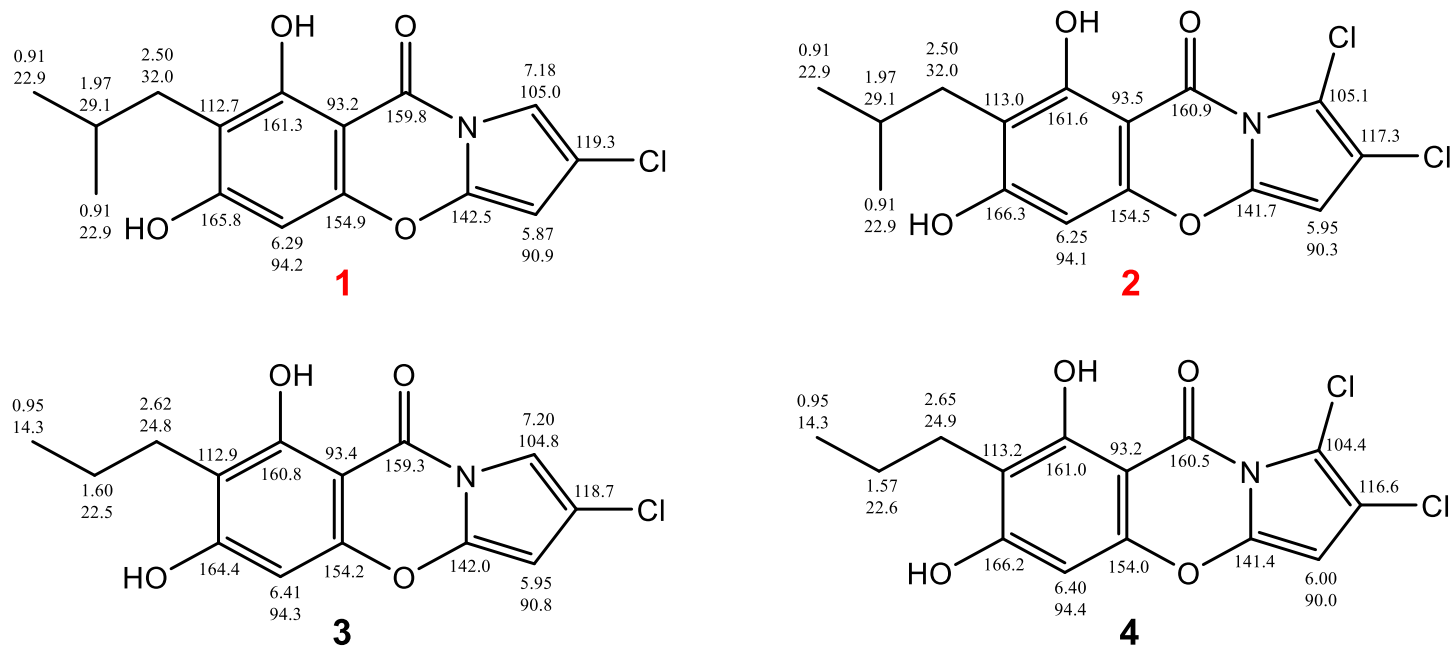


Figure S2. Comparison of chemical shifts between the new compounds (**1** and **2** in CD₃OD) and known analogs (**3** and **4** in acetone-*d*₆).

NMR data for compounds **3**, **4** were adopted from Ref. “Novel streptopyrroles from *Streptomyces rimosus* with bacterial protein histidine kinase inhibitory and antimicrobial activities”. *J. Antibiot.* **2000**, 53, 1-11.

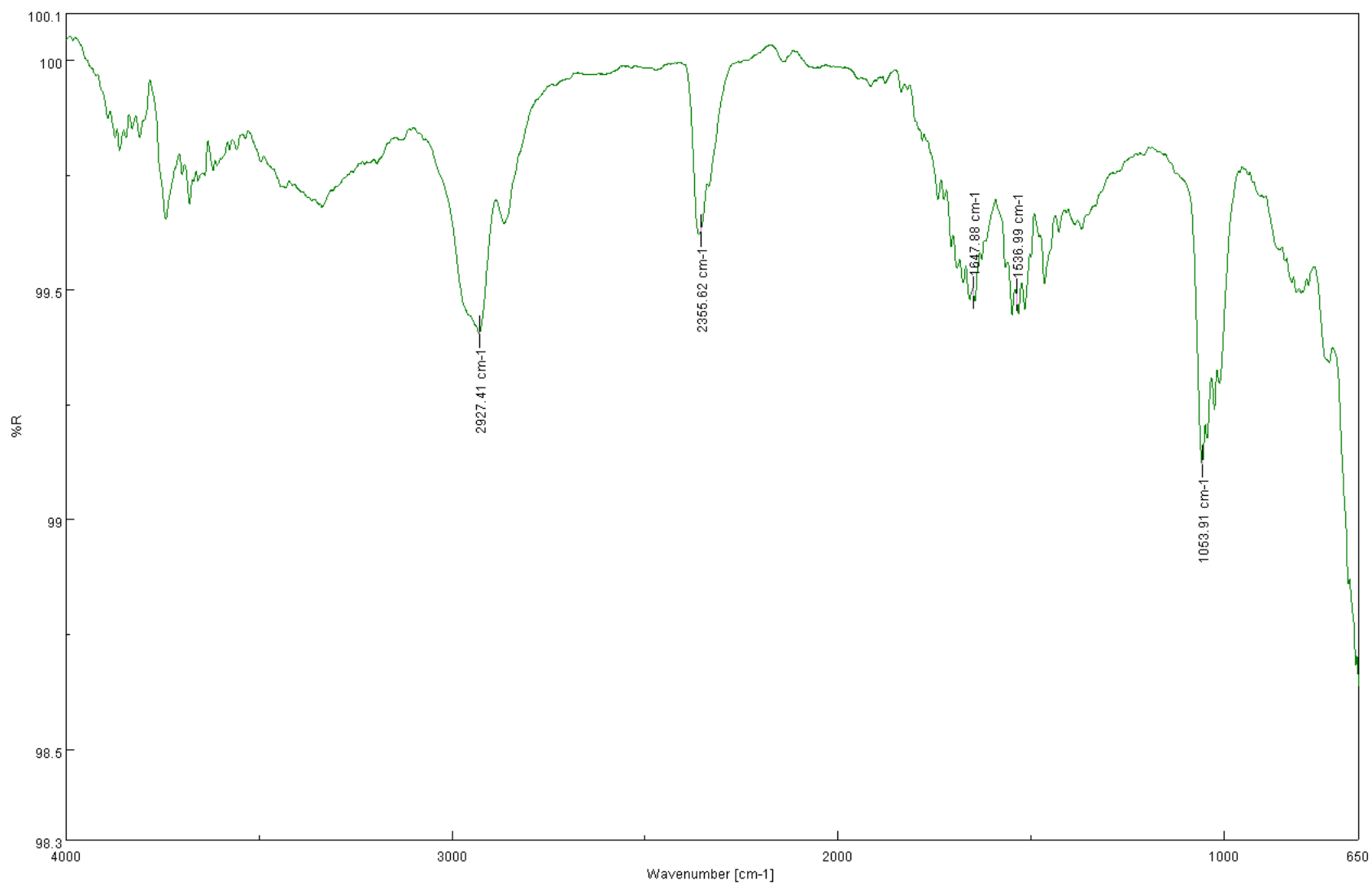
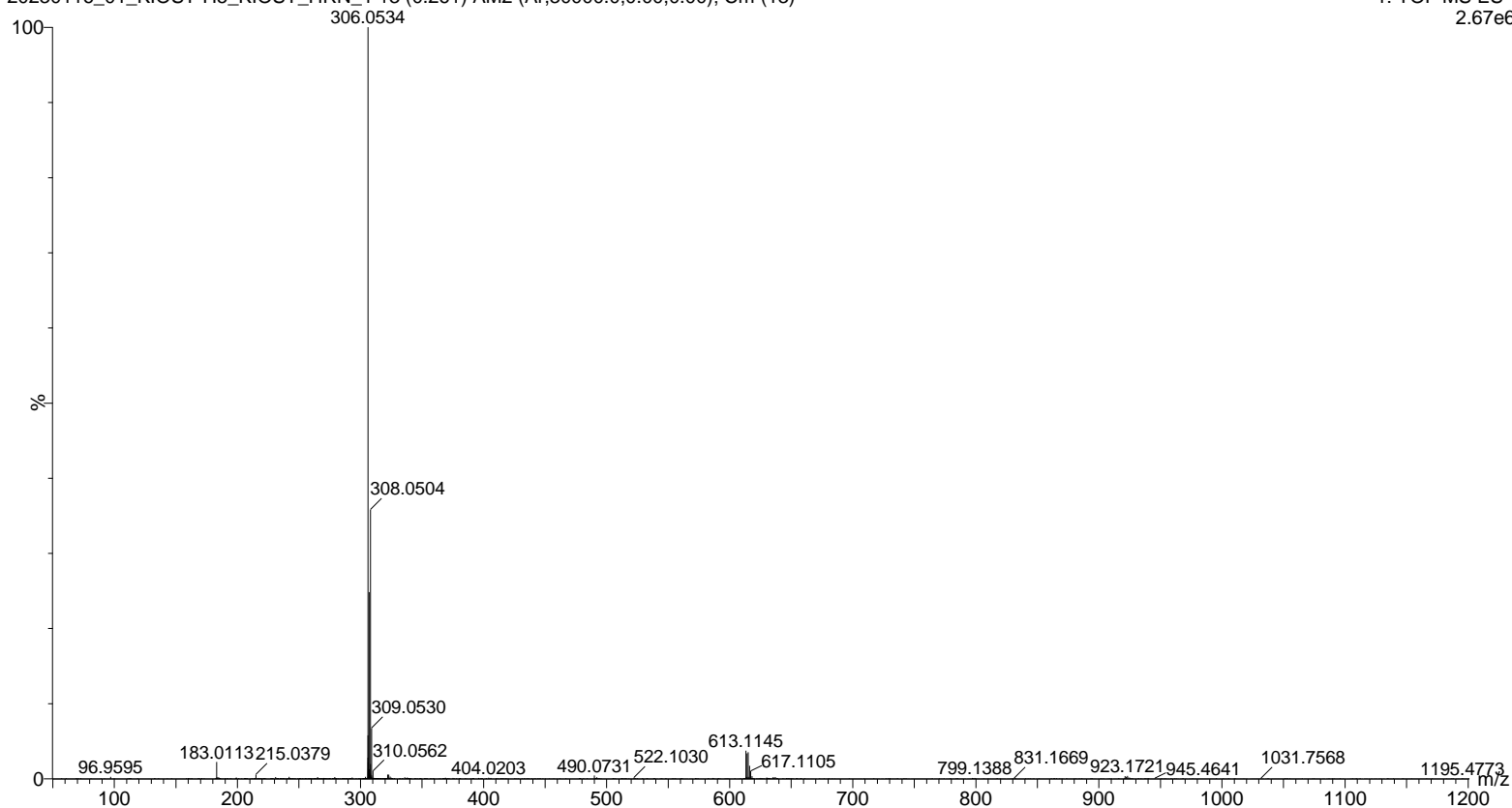


Figure S3. IR spectrum of **1**.

20230116_01_KIOST-H5_KIOST_HRN_1 13 (0.261) AM2 (Ar,30000.0,0.00,0.00); Cm (13)

1: TOF MS ES-
2.67e6



Elements Used:

C: 0-20 H: 0-180 N: 0-2 O: 0-5 Cl: 0-2

Minimum: -9.0

Maximum: 5.0 5.0 100.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
306.0534	306.0533	0.1	0.3	9.5	1496.9	n/a	n/a	C15 H13 N O4 Cl

Figure S4. HRESMS data of **1**.

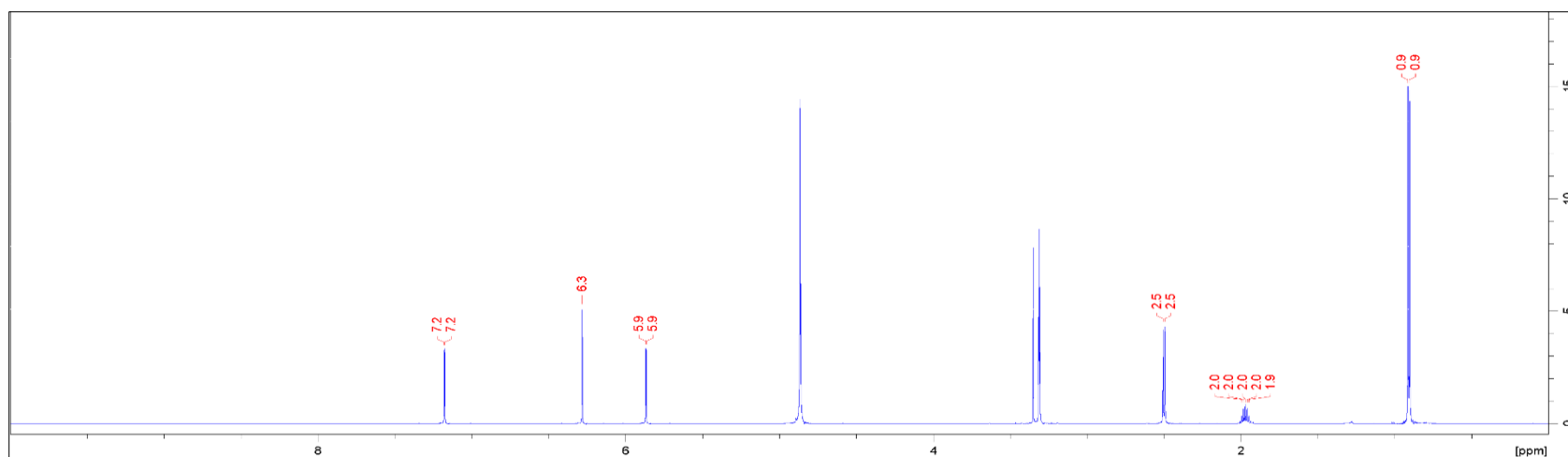


Figure S5. ¹H NMR spectrum of **1** (CD₃OD).

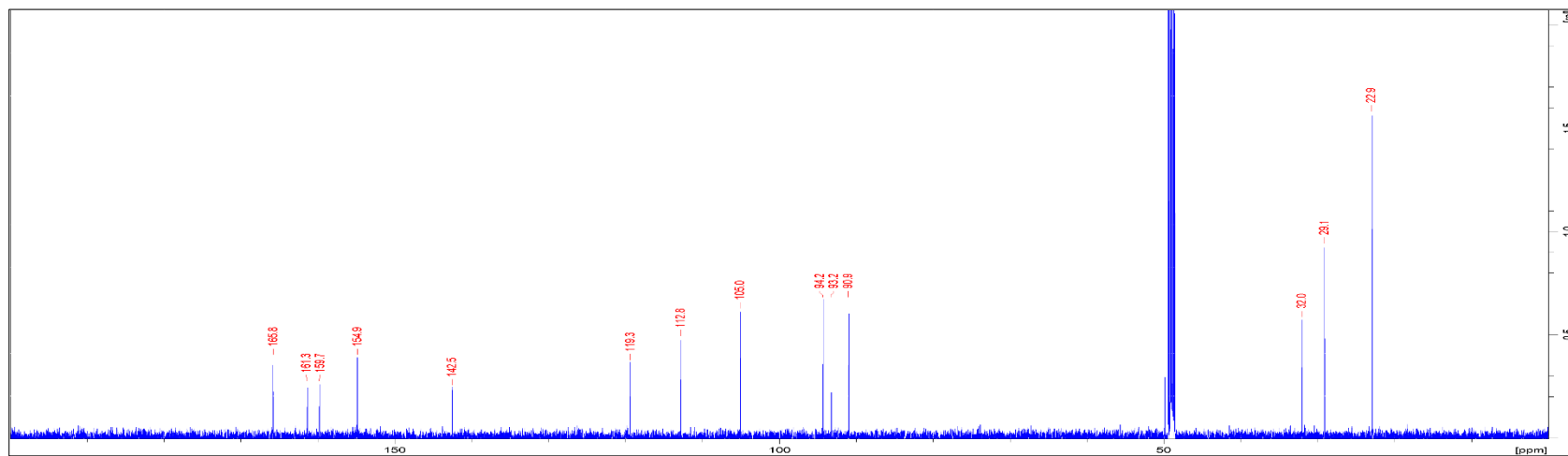


Figure S6. ¹³C NMR spectrum of **1** (CD₃OD).

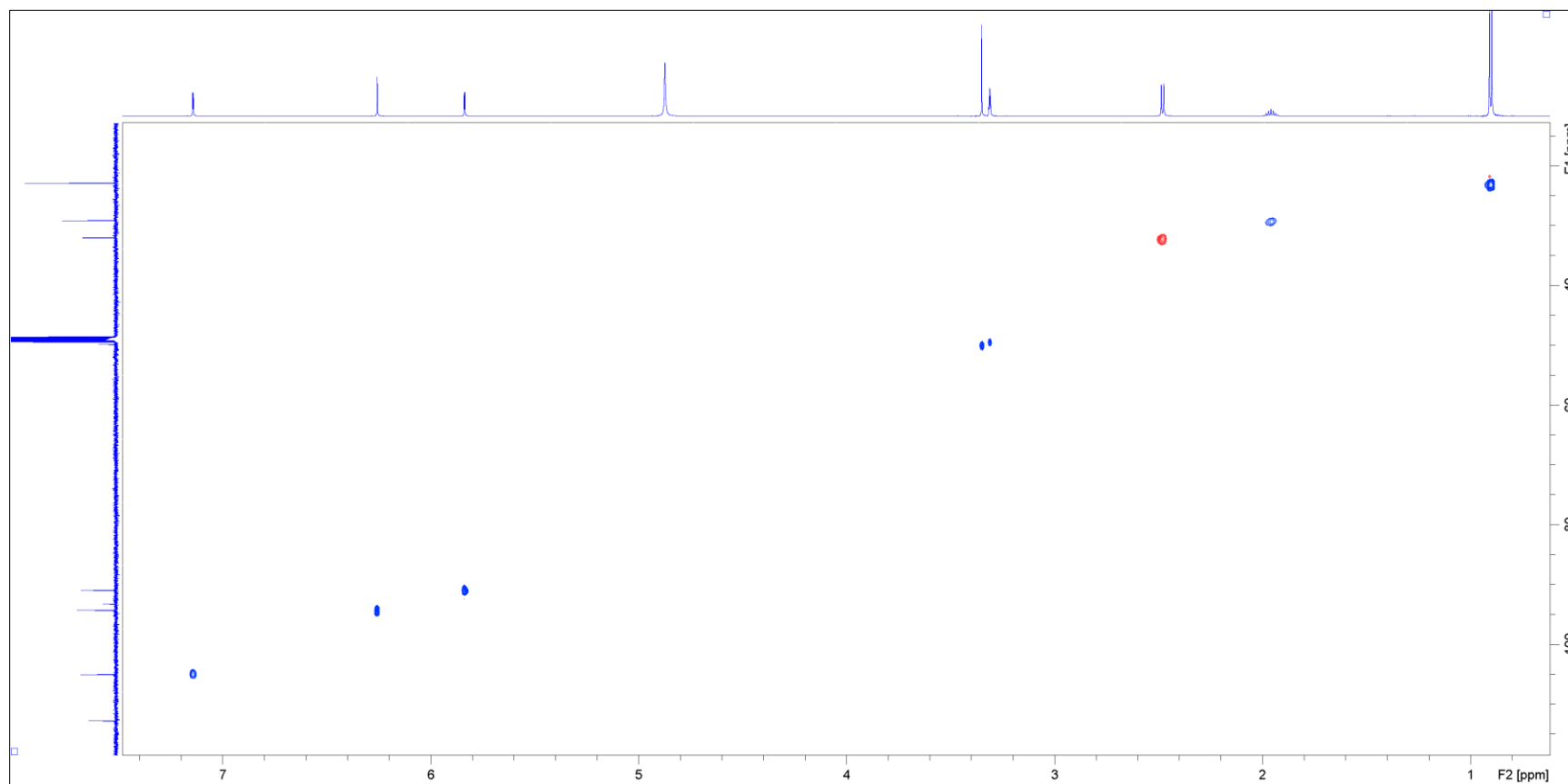


Figure S7. HSQC spectrum of **1** (CD₃OD).

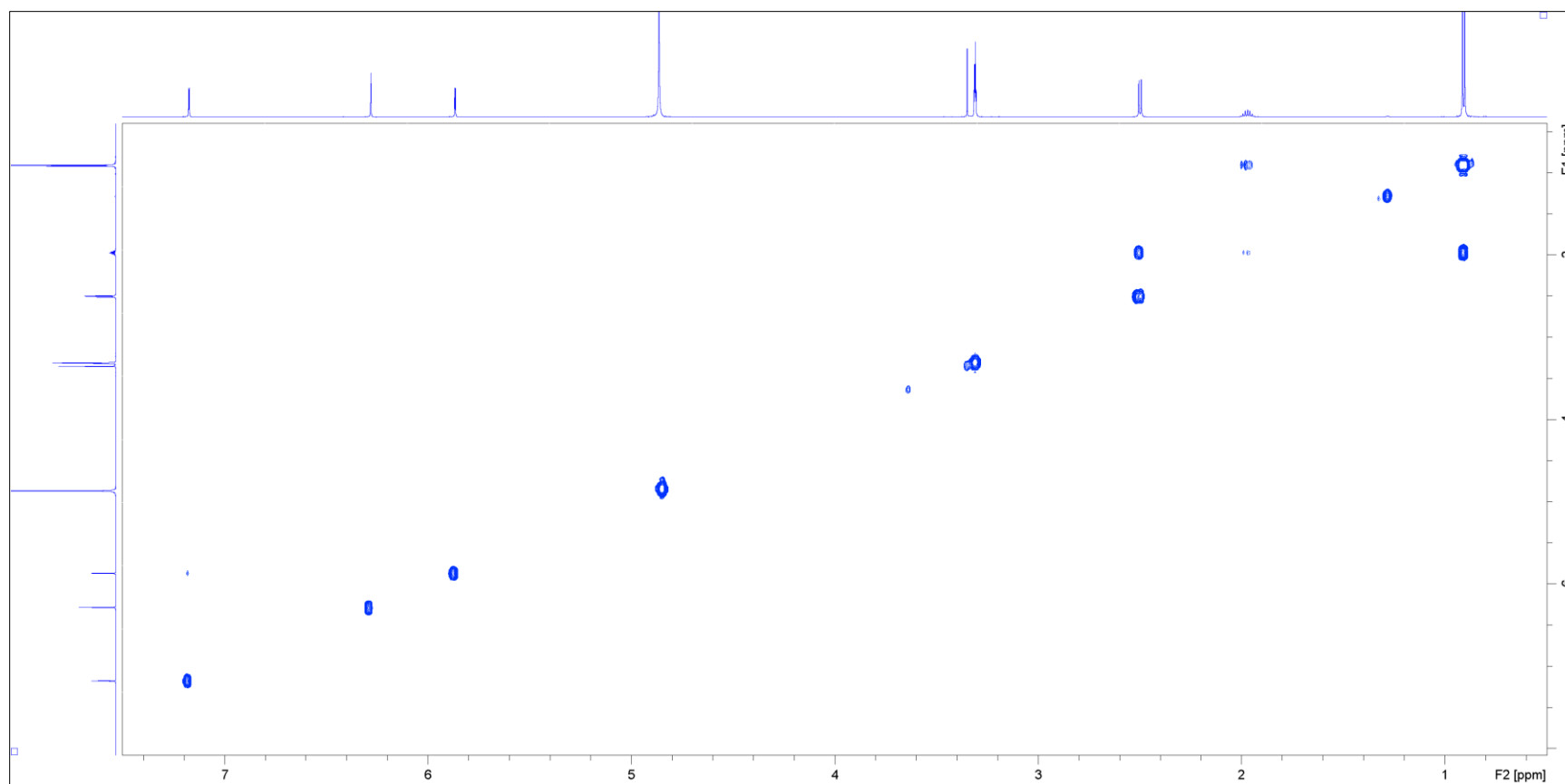


Figure S8. ^1H - ^1H COSY spectrum of **1** (CD_3OD).

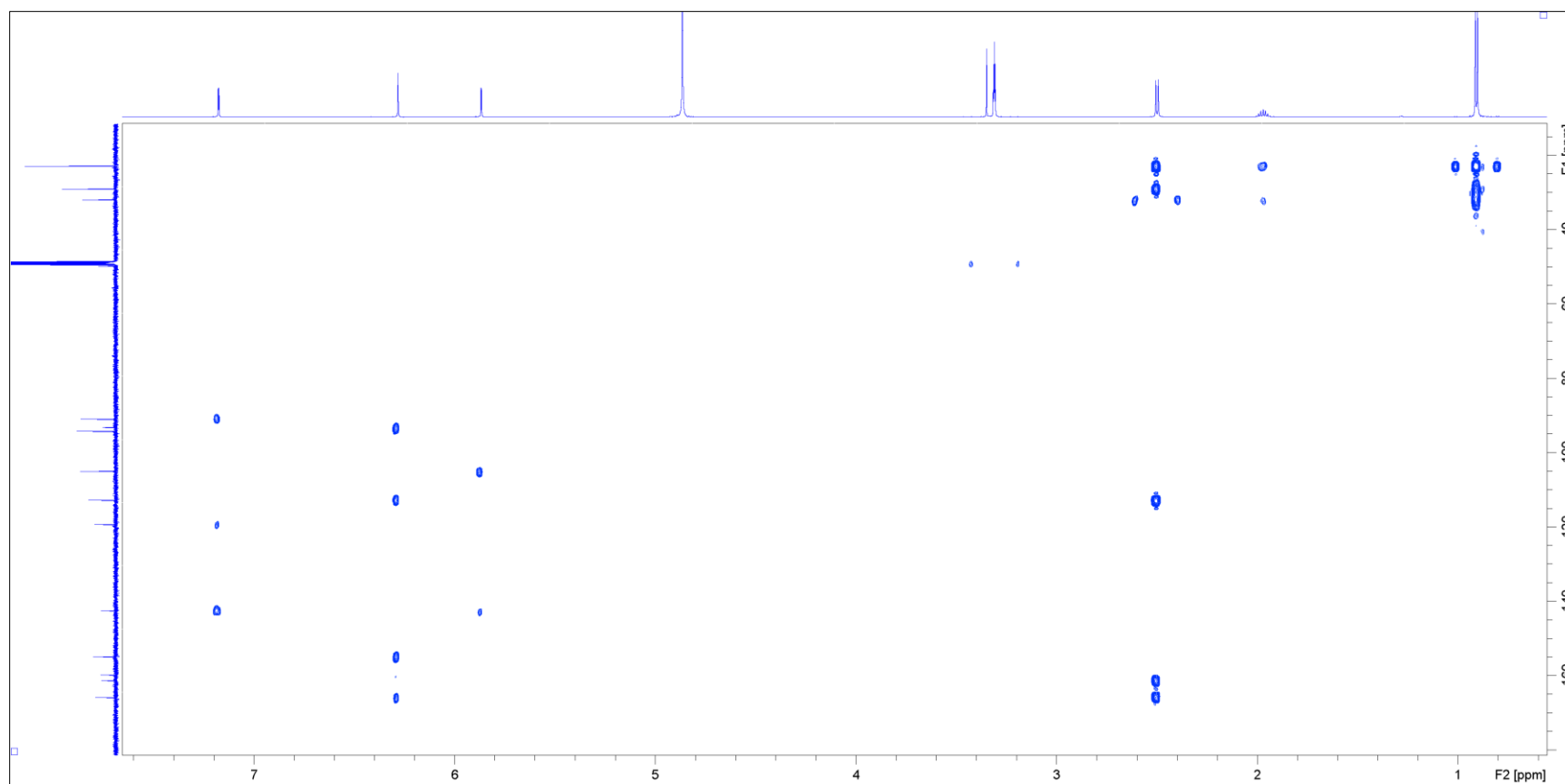


Figure S9. HMBC spectrum of **1** (CD₃OD).

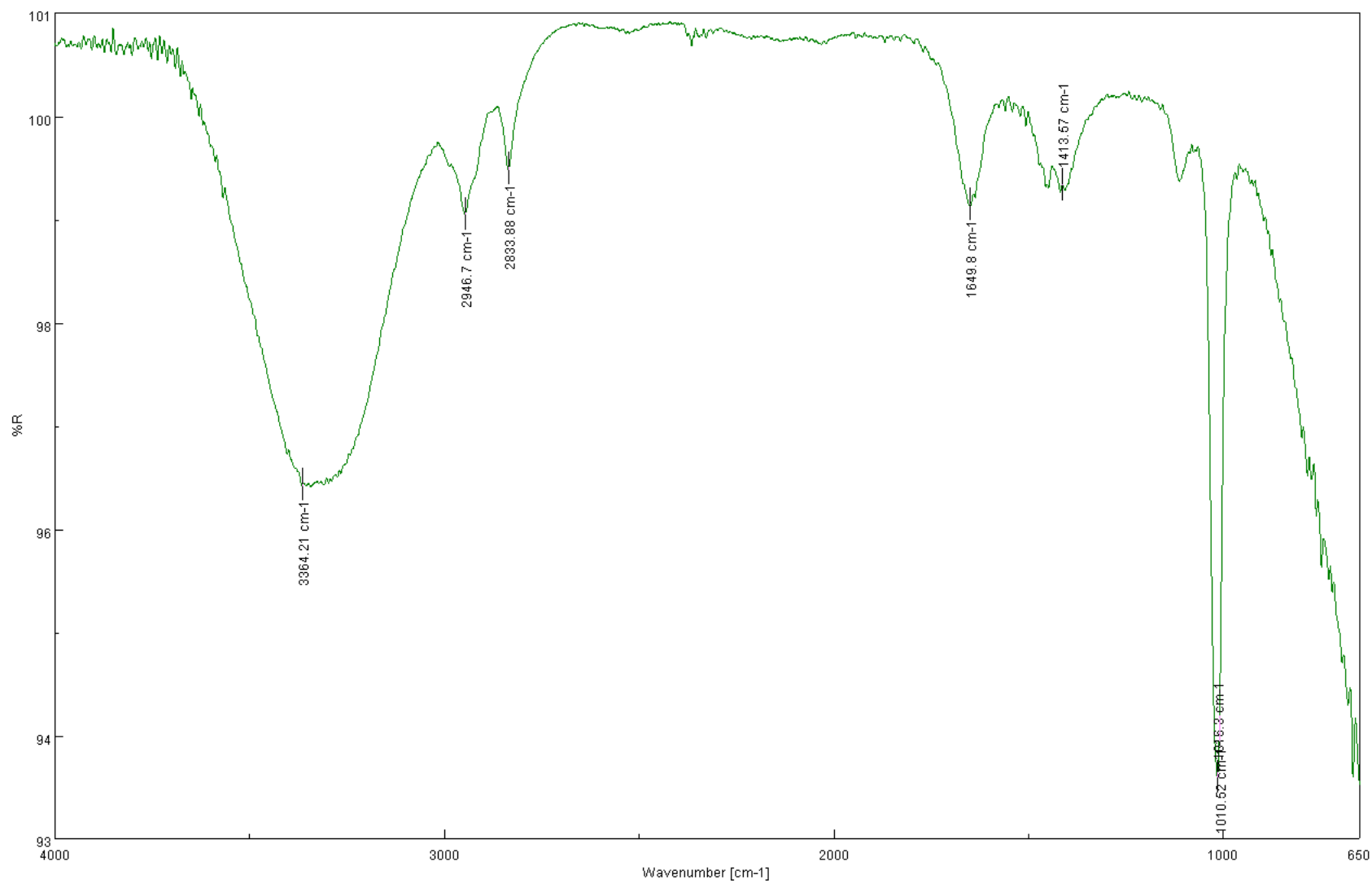
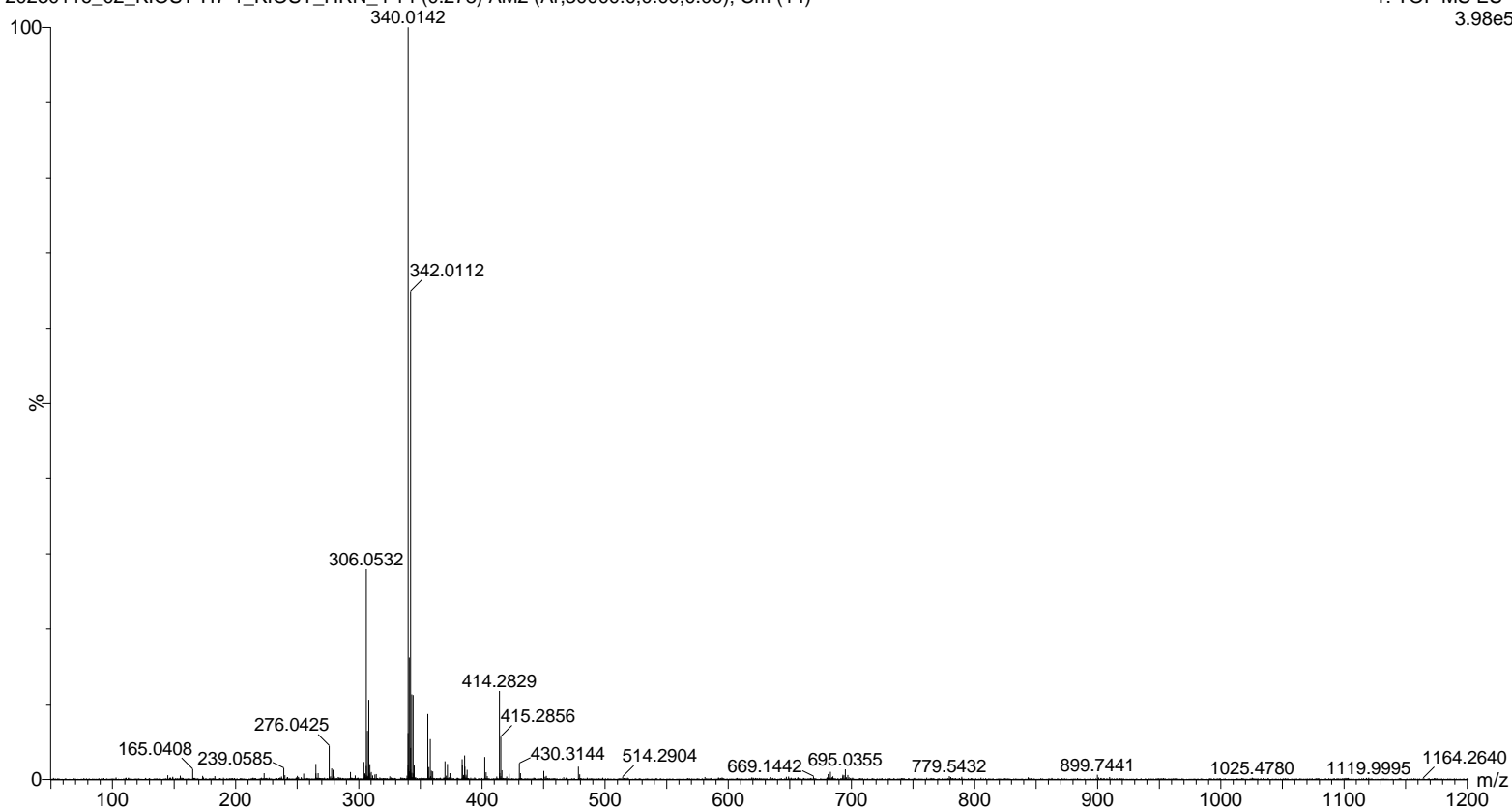


Figure S10. IR spectrum of **2**.

20230116_02_KIOST-H7-1_KIOST_HRN_4 14 (0.278) AM2 (Ar,30000.0,0.00,0.00); Cm (14)

1: TOF MS ES-
3.98e5



Elements Used:

C: 0-20 H: 0-180 N: 0-2 O: 0-5 Cl: 0-2

Minimum: -9.0

Maximum: 5.0 5.0 100.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
340.0142	340.0143	-0.1	-0.3	9.5	991.2	n/a	n/a	C15 H12 N O4 Cl2

Figure S11. HRESIMS data of **2**.

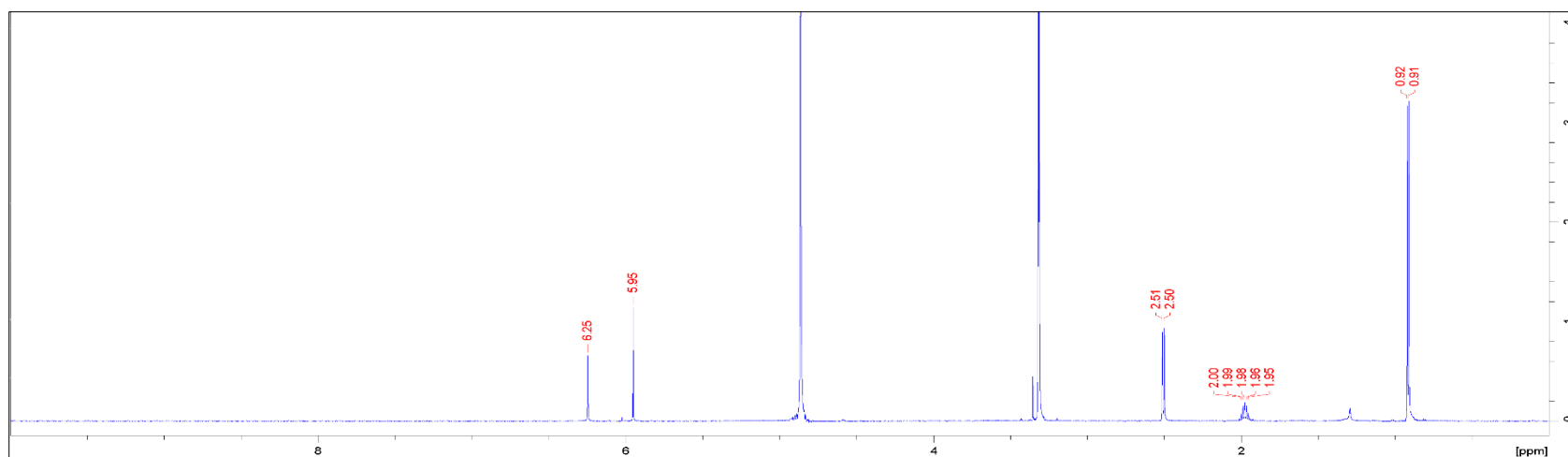


Figure S12. ¹H NMR spectrum of **2** (CD₃OD).

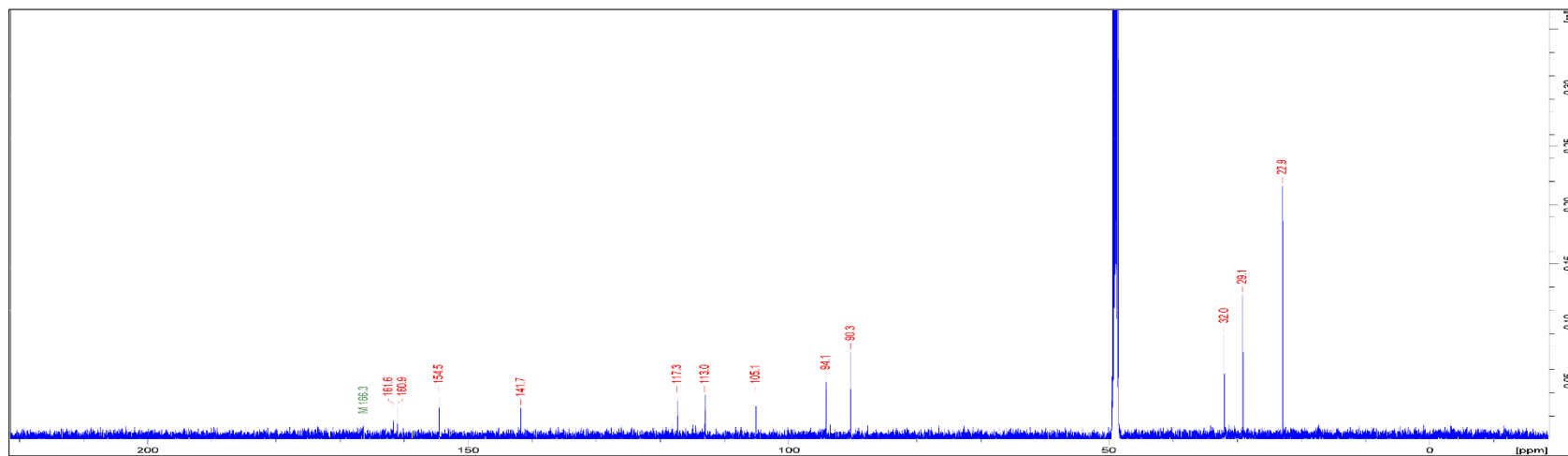


Figure S13. ¹³C NMR spectrum of **2** (CD₃OD).

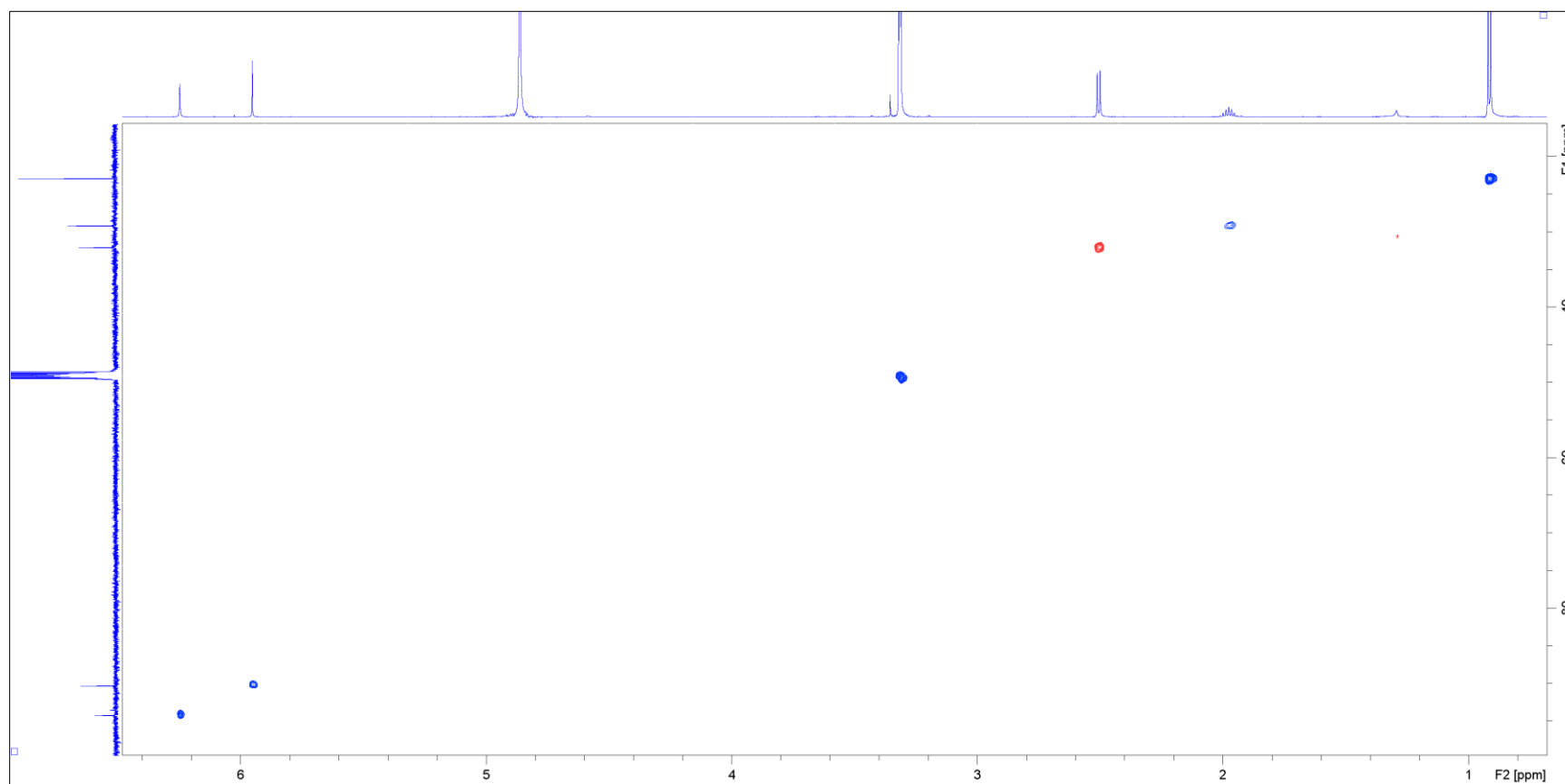


Figure S14. HSQC spectrum of **2** (CD₃OD).

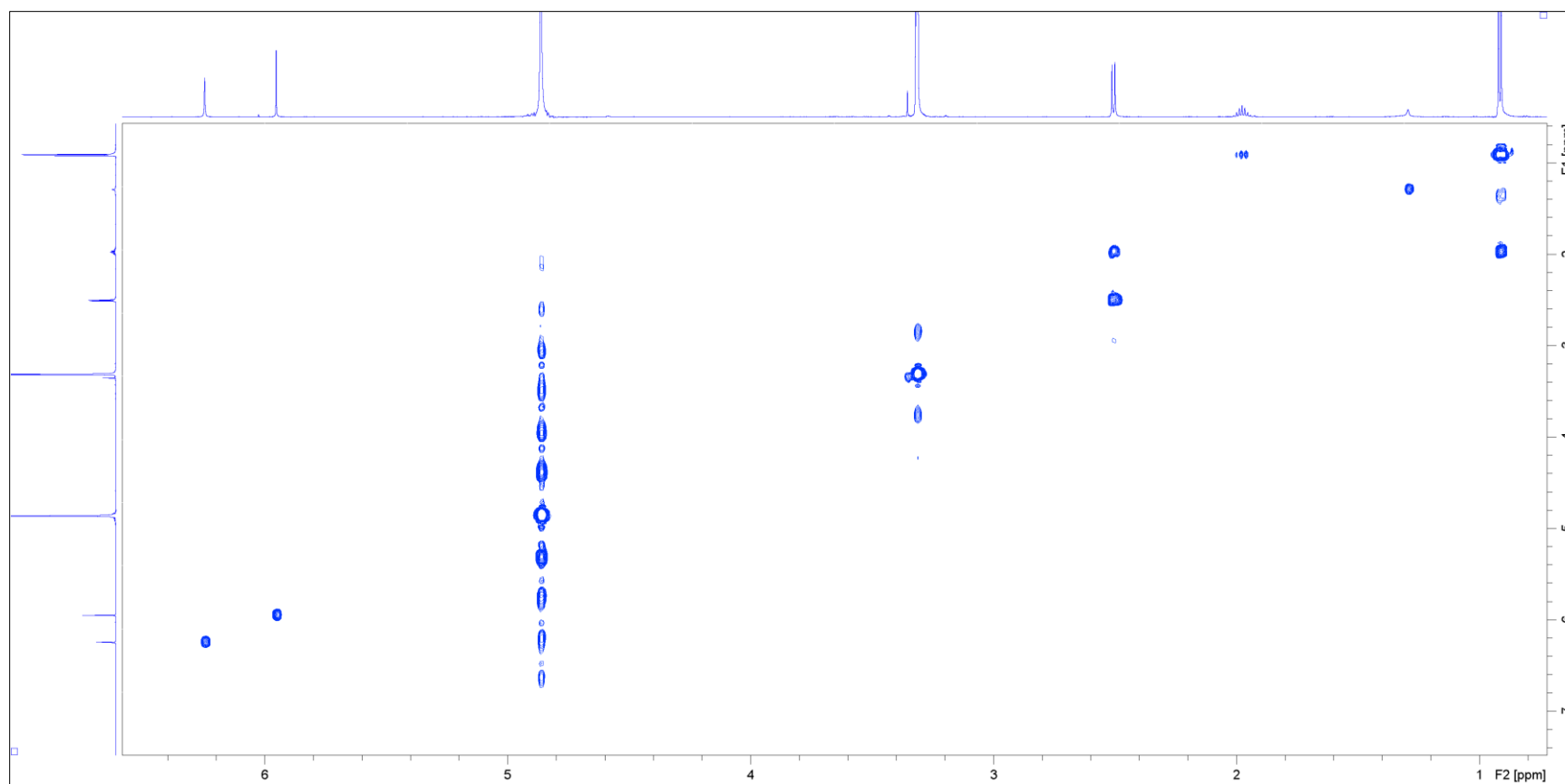


Figure S15. ^1H - ^1H COSY spectrum of **2** (CD_3OD).

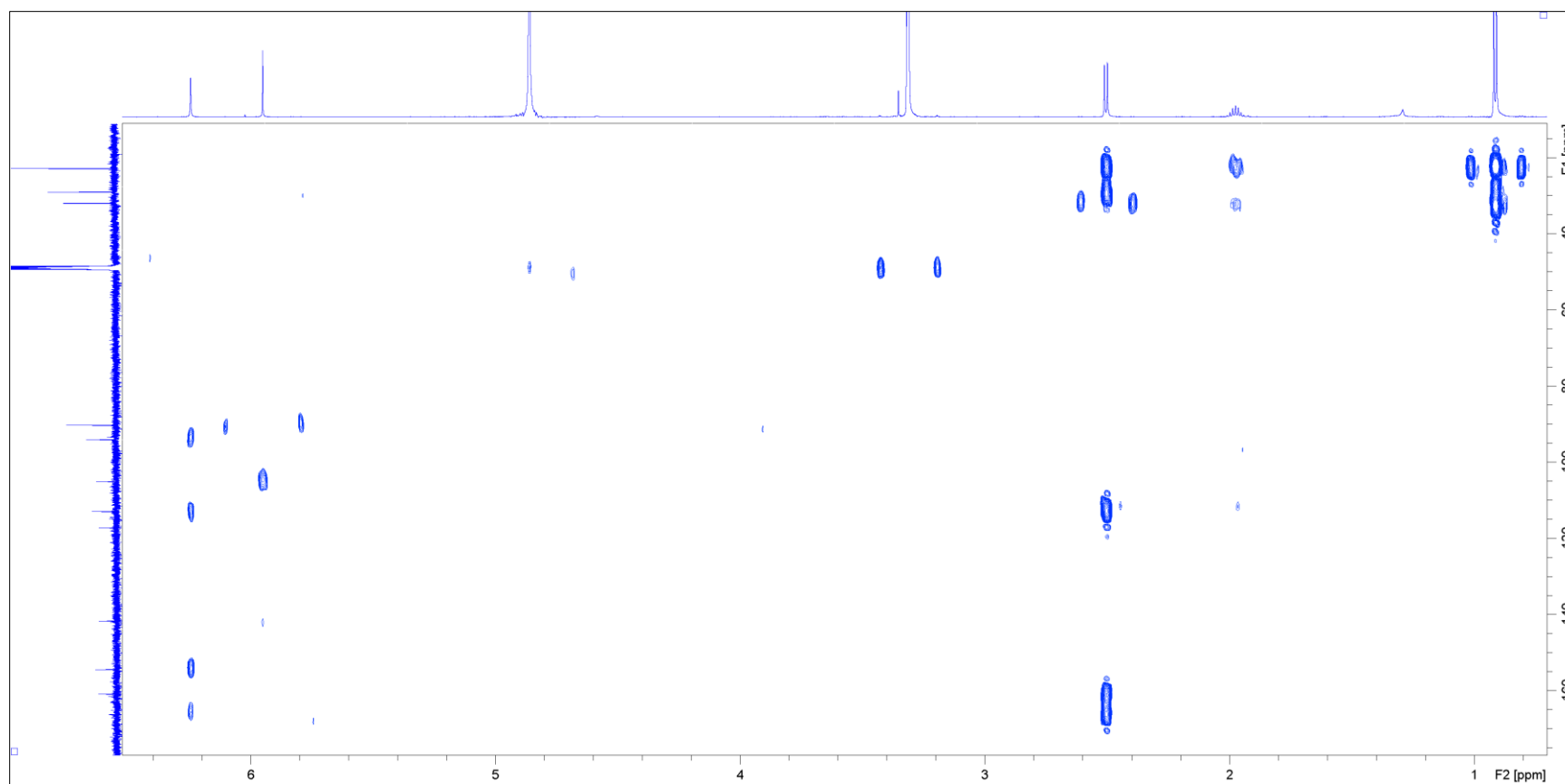


Figure S16. HMBC spectrum of **2** (CD₃OD).

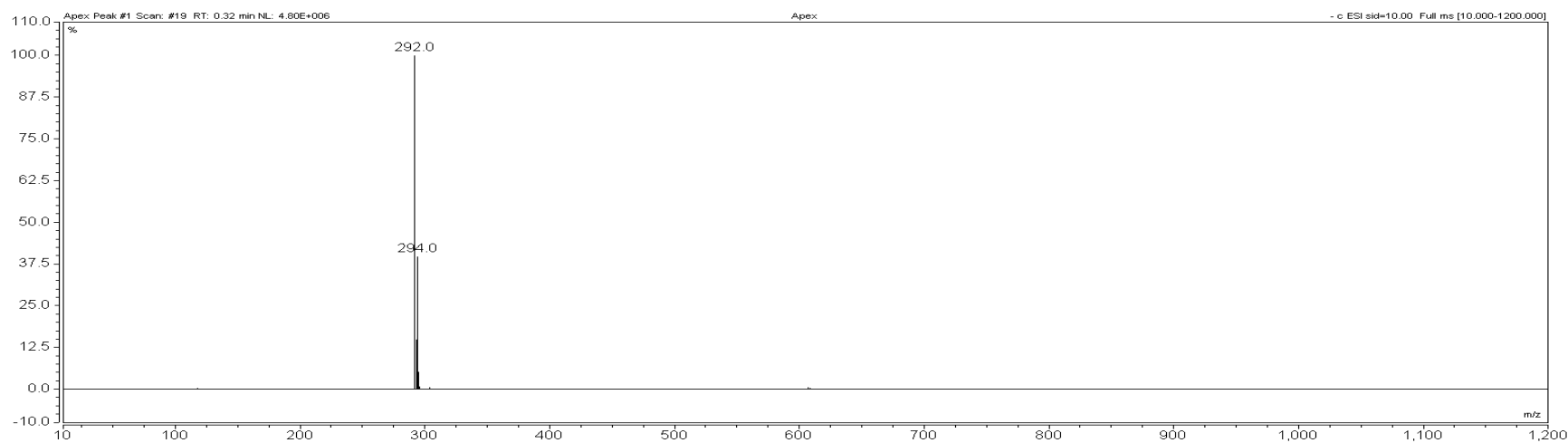


Figure S17. LRESIMS data of **3**.

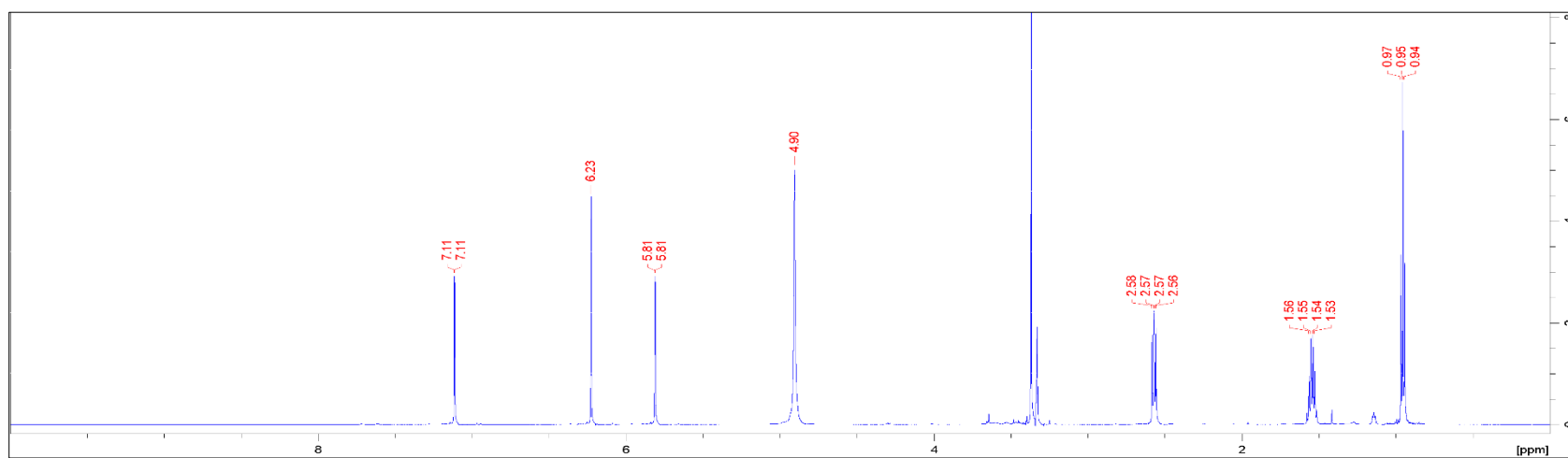


Figure S18. ^1H NMR spectrum of **3** (CD_3OD).

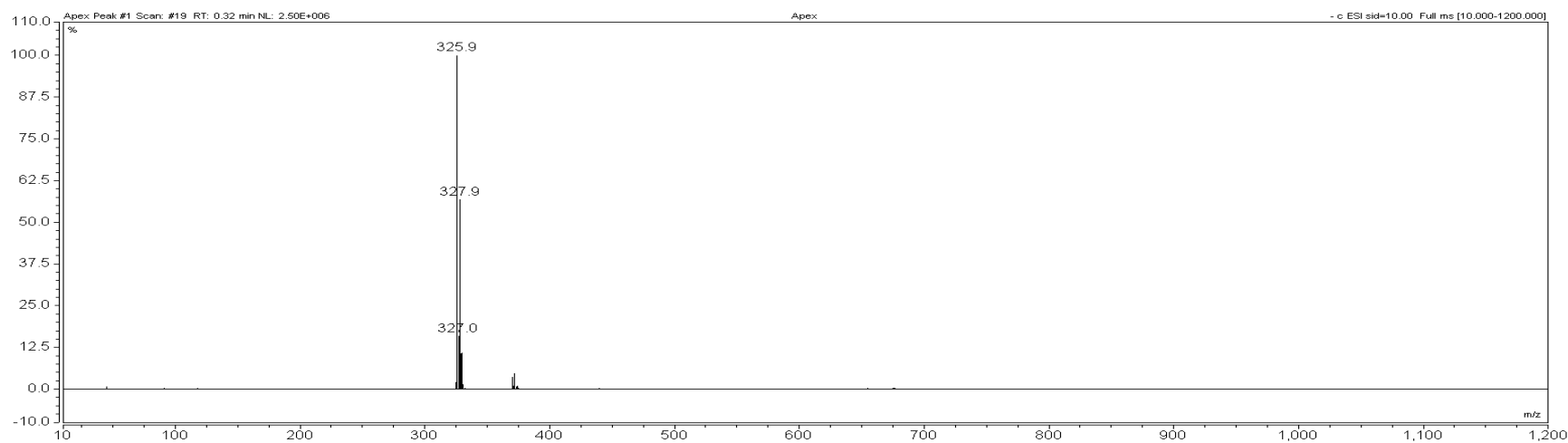


Figure S19. LRESIMS data of **4**.

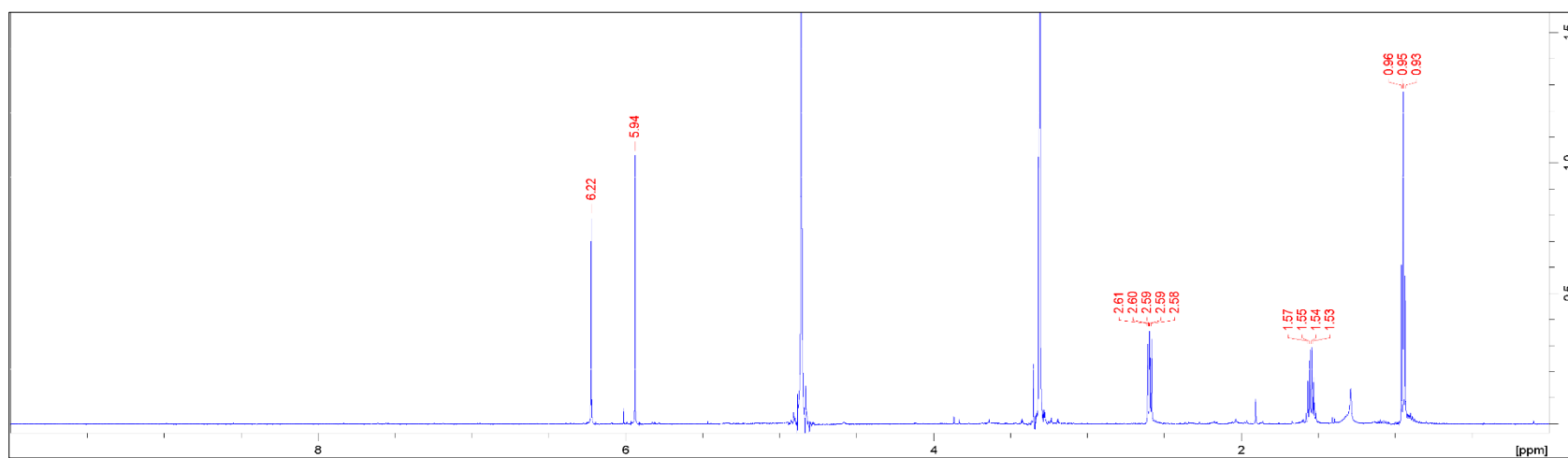


Figure S20. ^1H NMR spectrum of **4** (CD_3OD).

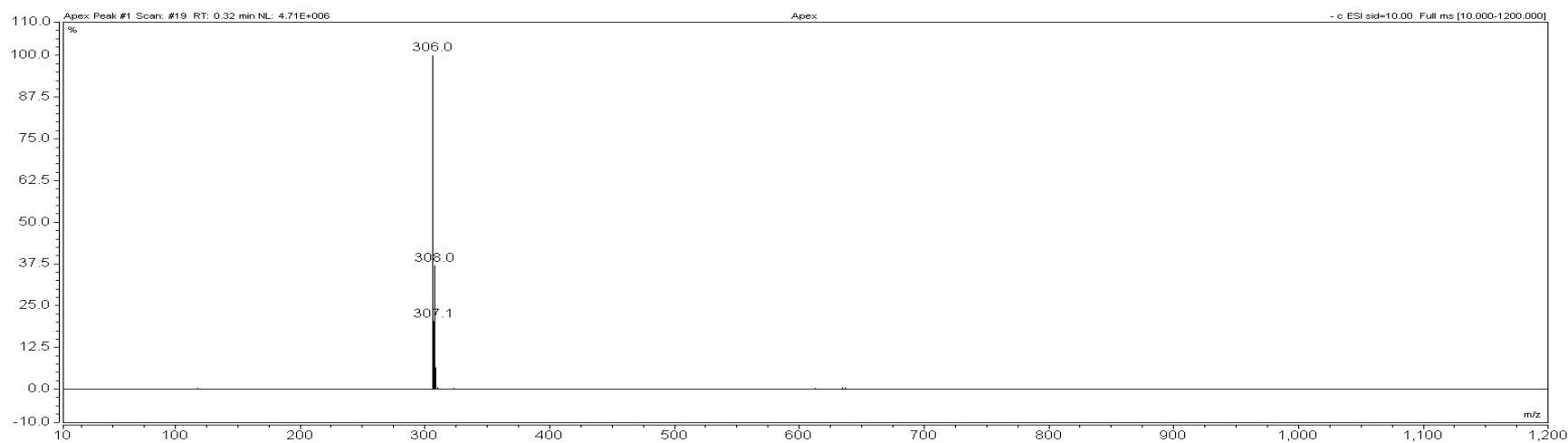


Figure S21. LRESIMS data of **5**.

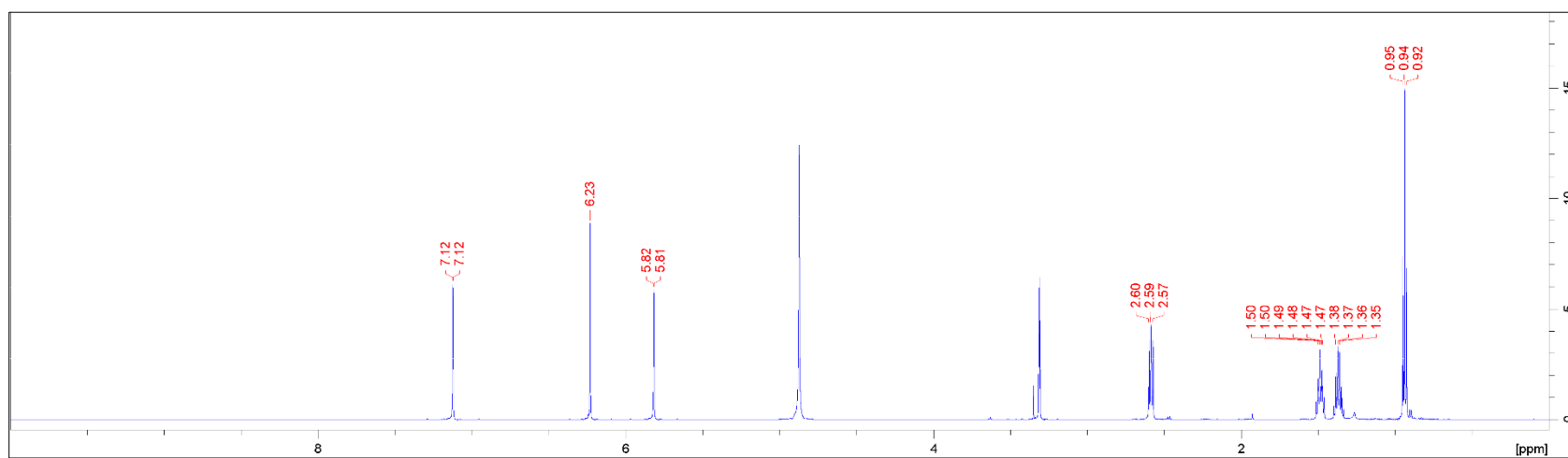


Figure S22. ^1H NMR spectrum of **5** (CD_3OD).

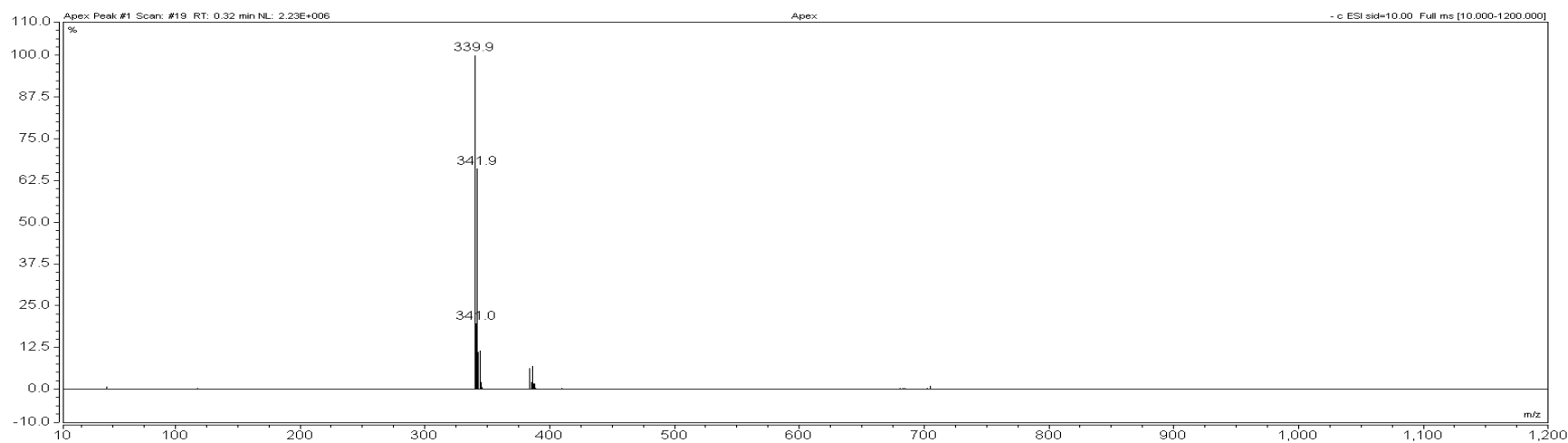


Figure S23. LRESIMS data of **6**.

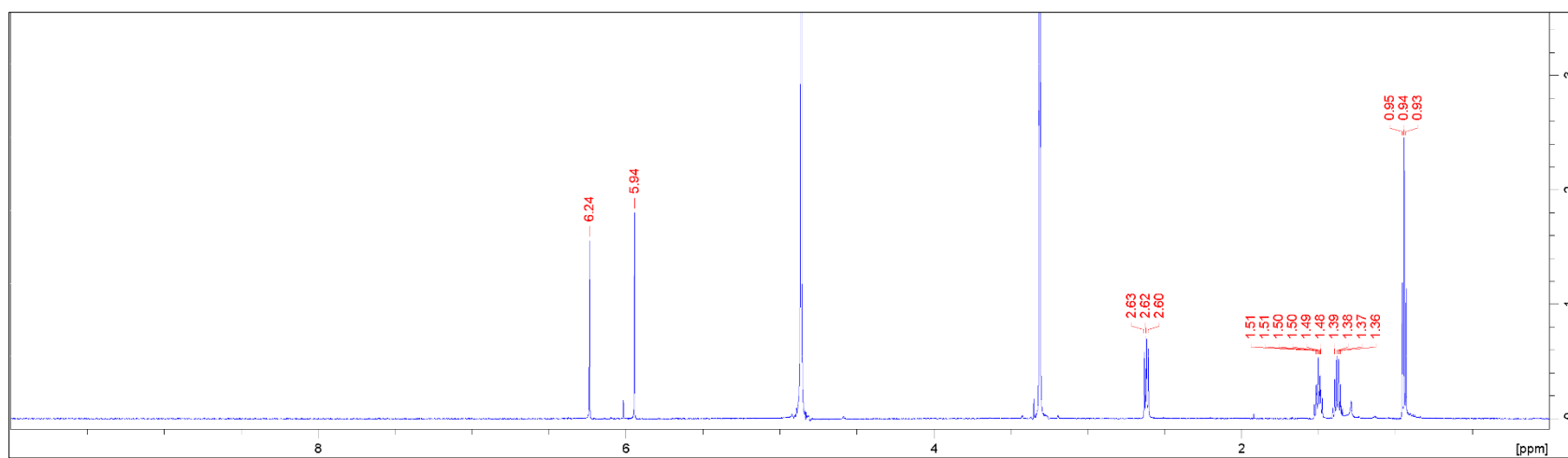


Figure S24. ^1H NMR spectrum of **6** (CD_3OD).

	1			3			5			Adriamycin		
	Conc.(ug/ml)	Mean	SD	Mean	SD		Mean	SD		Conc.(ug/ml)	Mean	SD
ACHN	30	-28.74	5.55	-29.22	4.16		-30.03	4.21		3	-7.74	5.15
	10	-4.22	2.35	0.21	7.58		-9.07	5.72		1	-5.83	3.55
	3	21.67	7.28	19.01	4.65		61.02	7.53		0.3	25.55	3.87
	1	68.73	7.02	82.14	6.25		87.32	3.88		0.1	37.90	3.82
	0.3	93.82	1.63	96.65	4.13		99.22	4.66		0.03	96.14	4.93
	GI ₅₀	1.490		1.751			3.222			GI ₅₀	0.093	
	GI ₅₀ (μM)	4.853		5.976			10.495			GI ₅₀ (μM)	0.171	
	1			3			5			Adriamycin		
	Conc.(ug/ml)	Mean	SD	Mean	SD		Mean	SD		Conc.(ug/ml)	Mean	SD
PC-3	30	-31.83	3.48	-28.51	4.28		-30.61	4.62		3	-9.55	1.82
	10	-2.76	2.21	1.84	9.77		-6.32	1.20		1	-4.42	4.11
	3	26.11	6.74	33.93	3.44		60.15	6.97		0.3	19.99	8.62
	1	82.66	1.89	86.48	2.56		91.92	9.13		0.1	32.49	5.50
	0.3	97.38	3.62	99.98	2.70		98.51	3.37		0.03	95.70	4.63
	GI ₅₀	1.920		2.244			3.207			GI ₅₀	0.080	
	GI ₅₀ (μM)	6.253		7.659			10.446			GI ₅₀ (μM)	0.147	
	1			3			5			Adriamycin		
	Conc.(ug/ml)	Mean	SD	Mean	SD		Mean	SD		Conc.(ug/ml)	Mean	SD
NCI-H23	30	-28.94	7.58	-24.36	6.08		-34.25	5.35		3	-14.08	3.85
	10	-3.66	3.18	-8.39	3.72		-8.72	3.68		1	-3.76	3.44
	3	22.53	7.88	21.86	5.63		63.95	4.15		0.3	17.16	2.00
	1	83.98	4.64	89.50	9.52		84.30	5.92		0.1	25.42	4.80
	0.3	97.69	6.02	95.48	5.90		97.62	3.90		0.03	96.66	6.95
	GI ₅₀	1.870		1.989			3.306			GI ₅₀	0.073	
	GI ₅₀ (μM)	6.090		6.788			10.769			GI ₅₀ (μM)	0.133	
	1			3			5			Adriamycin		
	Conc.(ug/ml)	Mean	SD	Mean	SD		Mean	SD		Conc.(ug/ml)	Mean	SD
MDA-MB-231	30	-29.49	4.55	-31.21	1.43		-30.78	5.54		3	-10.35	3.72
	10	-4.42	8.20	0.22	6.90		-10.99	4.83		1	-3.01	3.69
	3	29.00	2.54	38.85	6.95		66.67	4.04		0.3	17.16	9.01
	1	83.30	5.26	76.13	10.41		85.46	4.33		0.1	28.58	8.16
	0.3	95.06	6.10	93.22	6.77		97.80	1.24		0.03	95.99	4.65
	GI ₅₀	2.000		2.080			3.290			GI ₅₀	0.075	
	GI ₅₀ (μM)	6.514		7.099			10.717			GI ₅₀ (μM)	0.138	
	1			3			5			Adriamycin		
	Conc.(ug/ml)	Mean	SD	Mean	SD		Mean	SD		Conc.(ug/ml)	Mean	SD
NUGC-3	30	-30.32	5.20	-33.45	6.28		-38.09	4.87		3	-11.43	5.75
	10	0.89	8.76	-5.92	6.87		-13.38	6.39		1	-4.75	6.54
	3	19.21	5.82	27.13	4.36		57.31	4.16		0.3	17.63	6.64
	1	76.37	6.79	80.05	5.94		80.91	8.04		0.1	34.07	7.02
	0.3	97.61	0.71	97.74	4.02		96.33	4.64		0.03	97.35	2.44
	GI ₅₀	1.630		1.877			3.189			GI ₅₀	0.082	
	GI ₅₀ (μM)	5.309		6.406			10.388			GI ₅₀ (μM)	0.151	
	1			3			5			Adriamycin		
	Conc.(ug/ml)	Mean	SD	Mean	SD		Mean	SD		Conc.(ug/ml)	Mean	SD
HCT-15	30	-20.09	5.80	-24.34	5.12		-31.36	9.41		3	-13.83	4.65
	10	-5.12	9.49	-0.66	5.47		-7.96	7.10		1	-8.68	4.34
	3	26.21	4.51	30.04	2.46		65.71	4.08		0.3	19.48	8.19
	1	87.29	4.72	92.17	6.01		84.54	8.37		0.1	38.73	2.13
	0.3	100.05	3.75	99.55	3.86		98.21	3.63		0.03	97.25	4.40
	GI ₅₀	2.040		2.270			3.290			GI ₅₀	0.089	
	GI ₅₀ (μM)	6.644		7.747			10.717			GI ₅₀ (μM)	0.164	

Table S1. Results of the cytotoxicity test of **1,3** and **5**.