

## *Supporting Information*

# **Antibacterial Kaneoheic acids A-F from a Hawaiian Fungus**

## ***Fusarium* sp. FM701**

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**Figure S1: HRESIMS of compound 1**

KH Ahammad Zaman ZS 5

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1: TOF MS ES-  
5.64e5

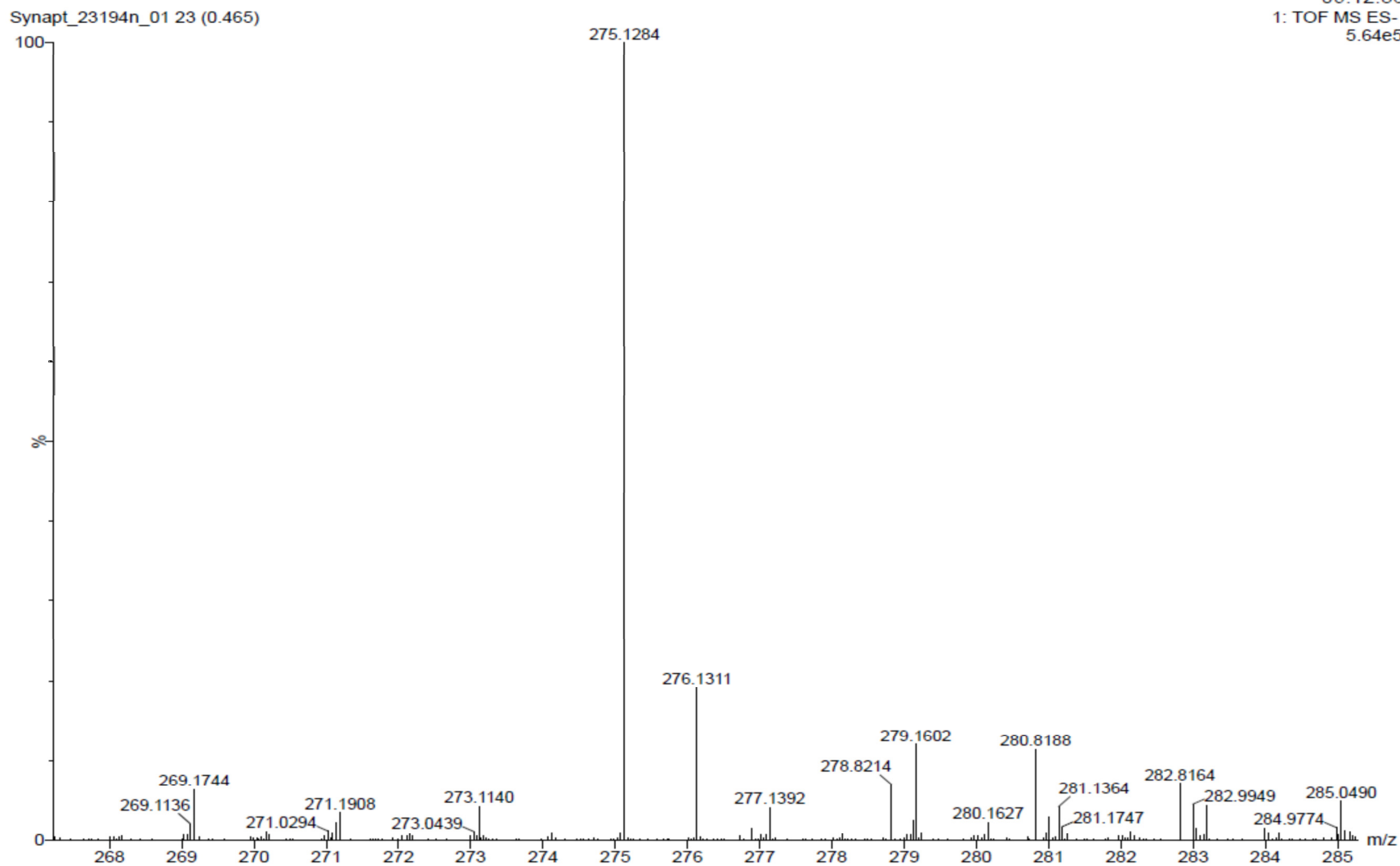


Figure S2:  $^1\text{H}$  NMR spectrum of compound 1 in  $\text{CD}_3\text{OD}$  (400MHz)

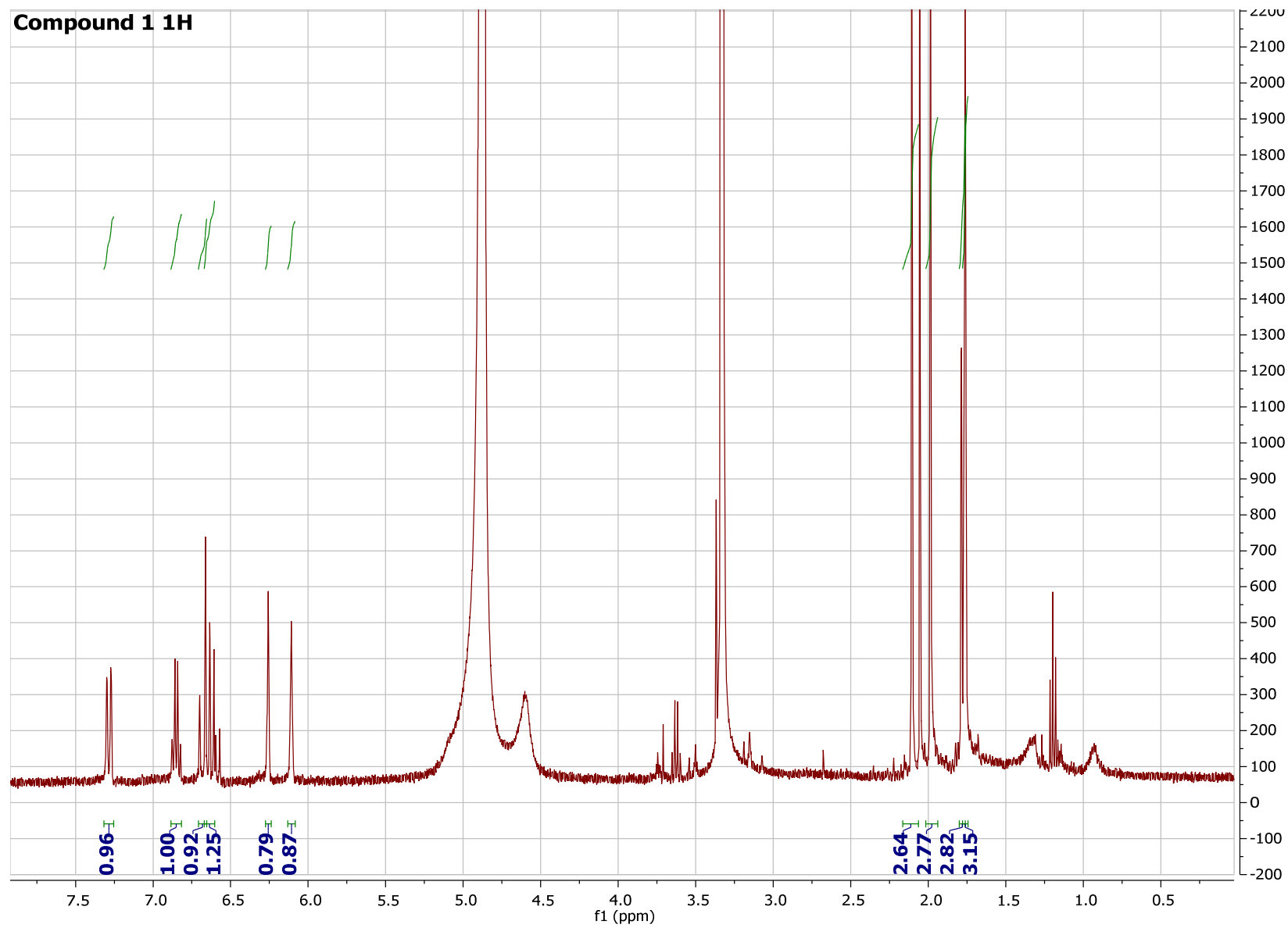


Figure S3: HSQC spectrum of compound 1 in CD<sub>3</sub>OD (400MHz)

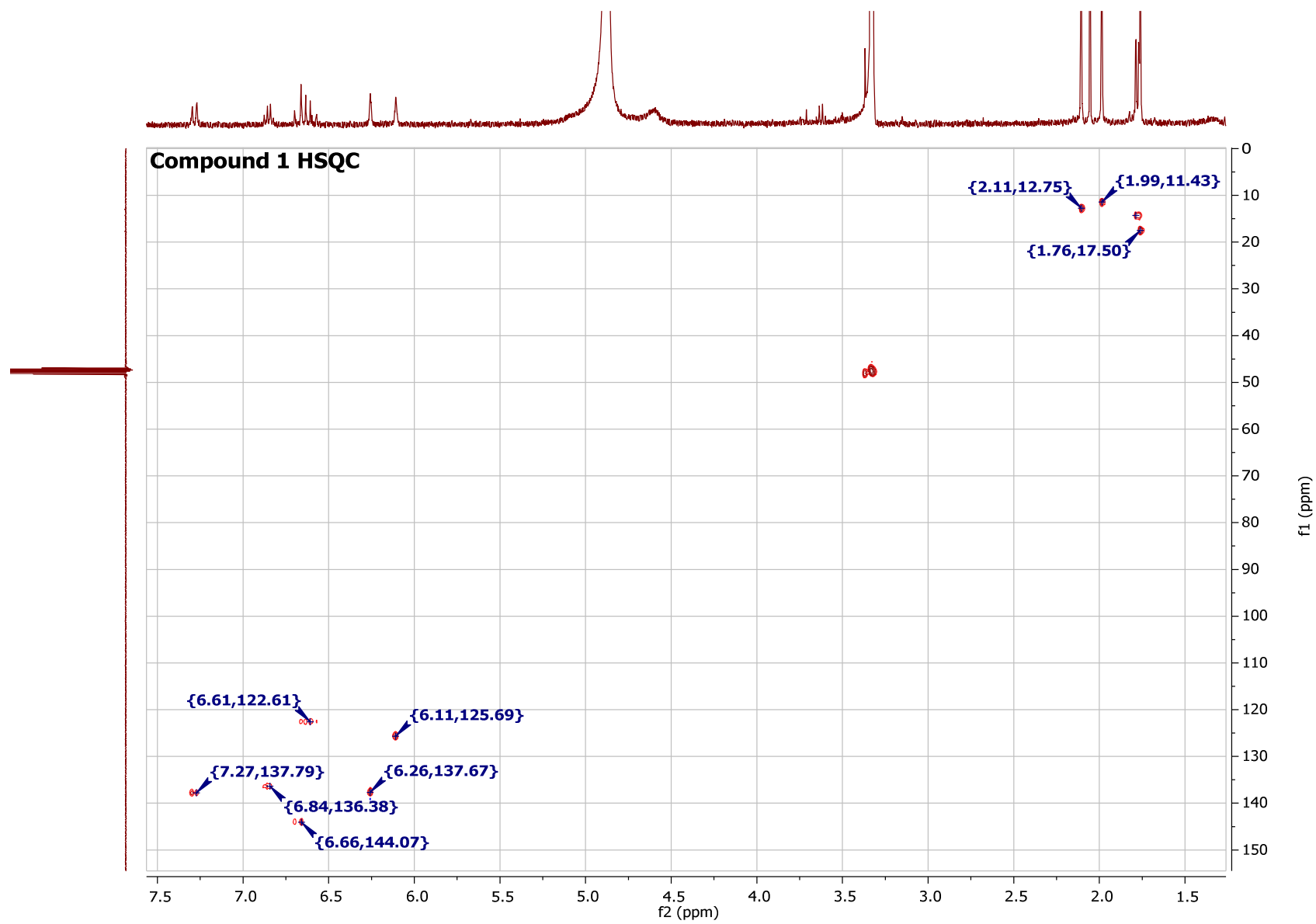


Figure S4: COSY spectrum of compound 1 in CD<sub>3</sub>OD (400MHz)

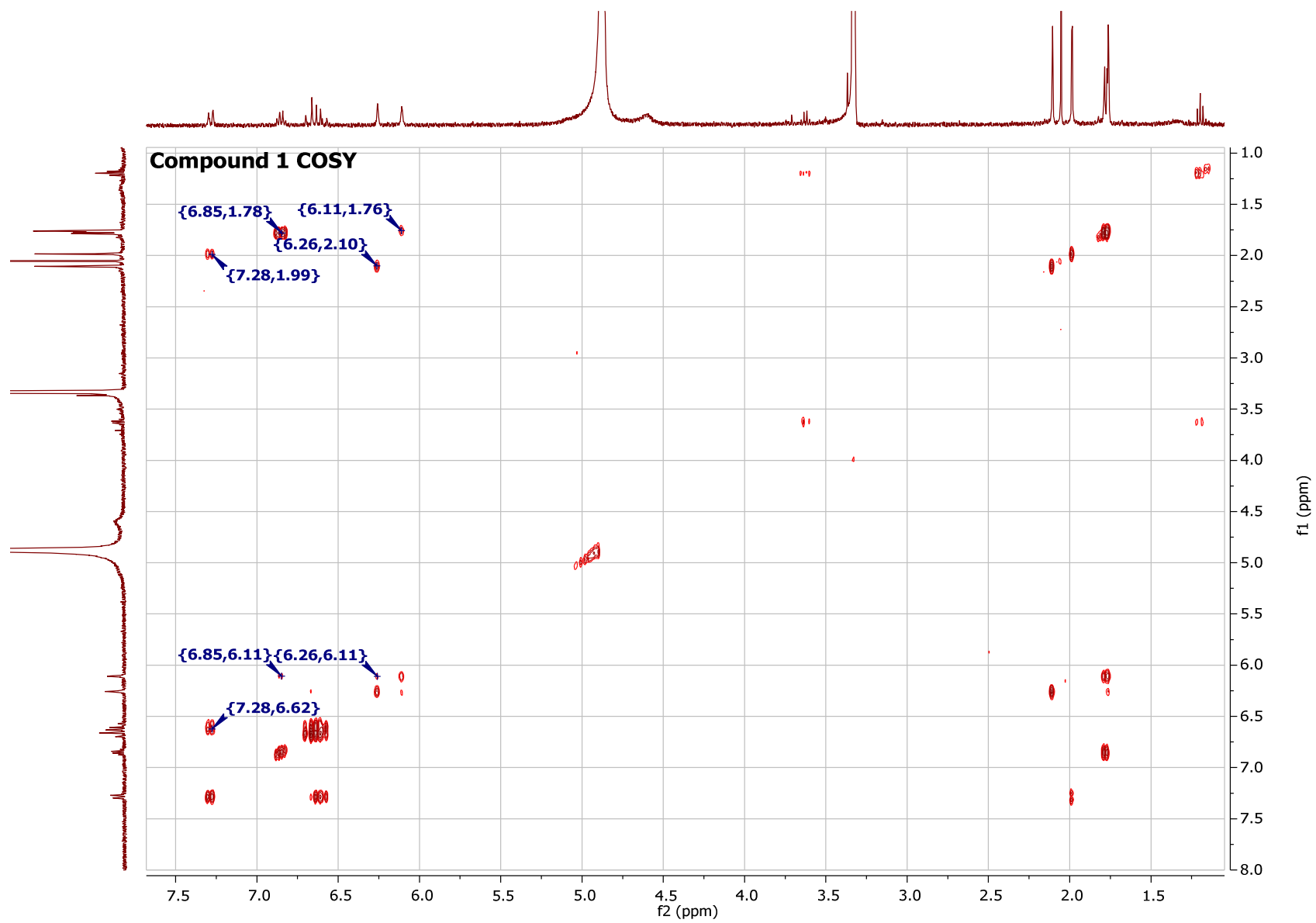
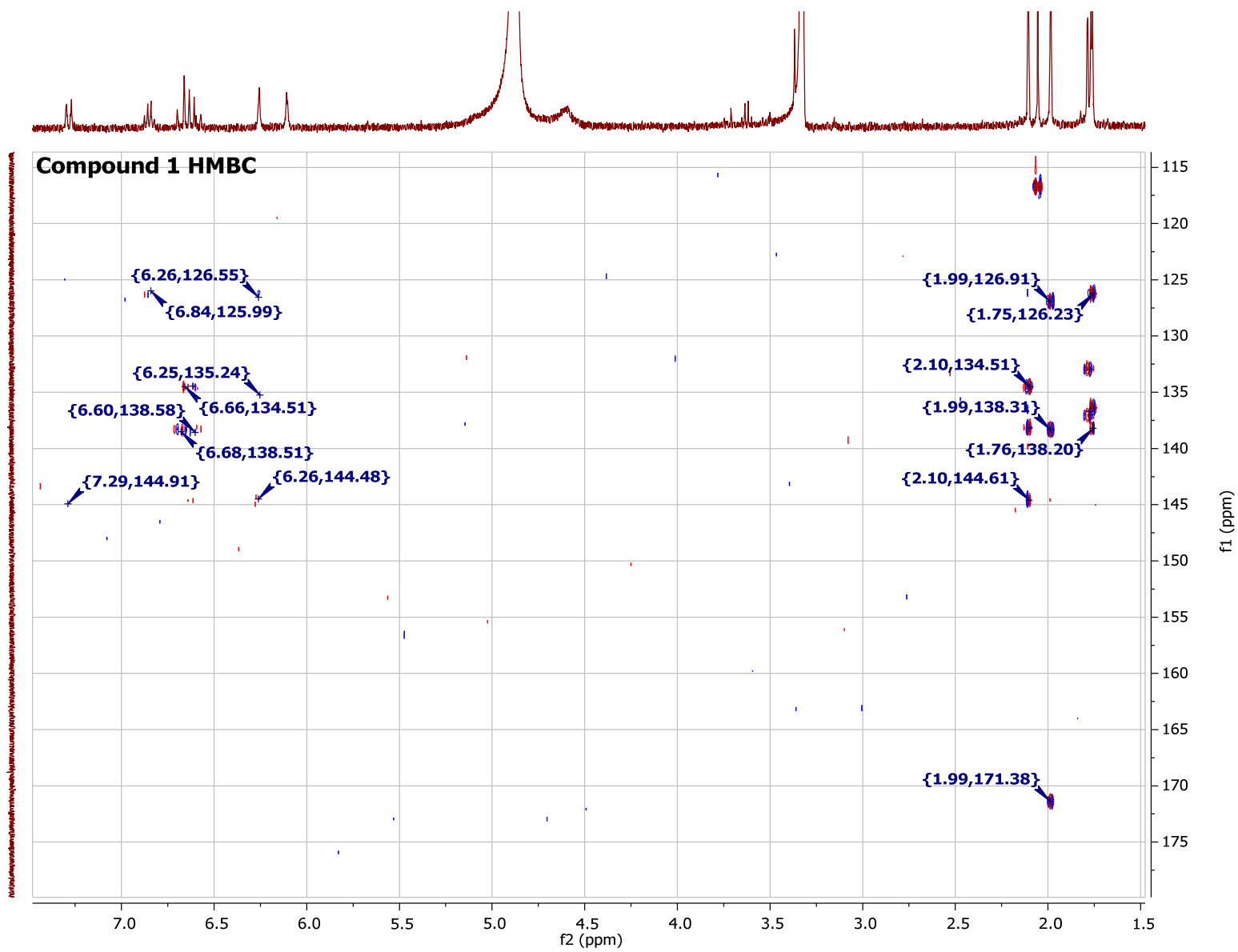


Figure S5: HMBC spectrum of compound 1 in CD<sub>3</sub>OD (400MHz)





**Figure S6: HRESIMS of compound 2**

KH Ahammad Zaman ZS 3

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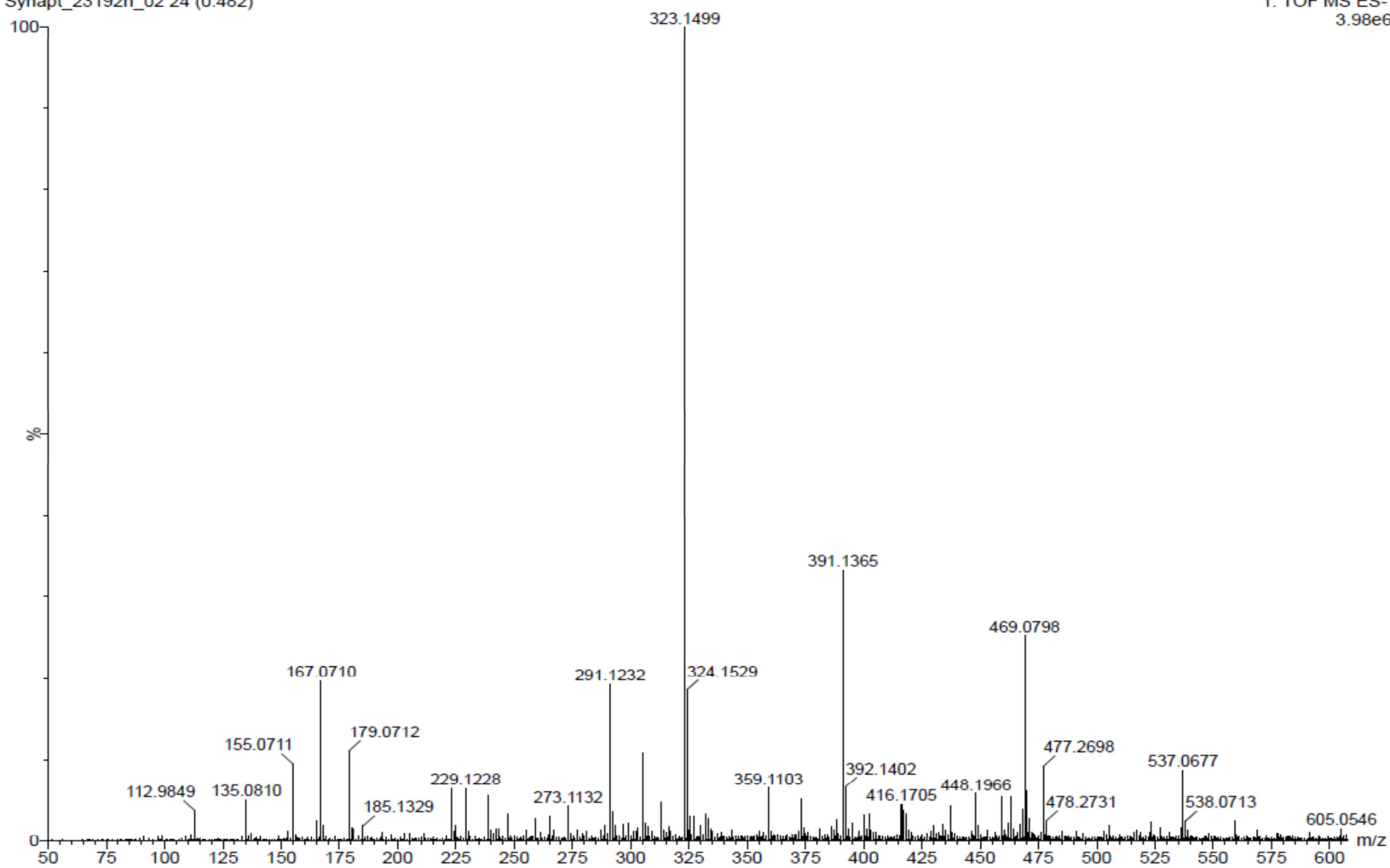


Figure S7:  $^1\text{H}$  NMR spectrum of compound 2 in  $\text{CD}_3\text{OD}$  (400MHz)

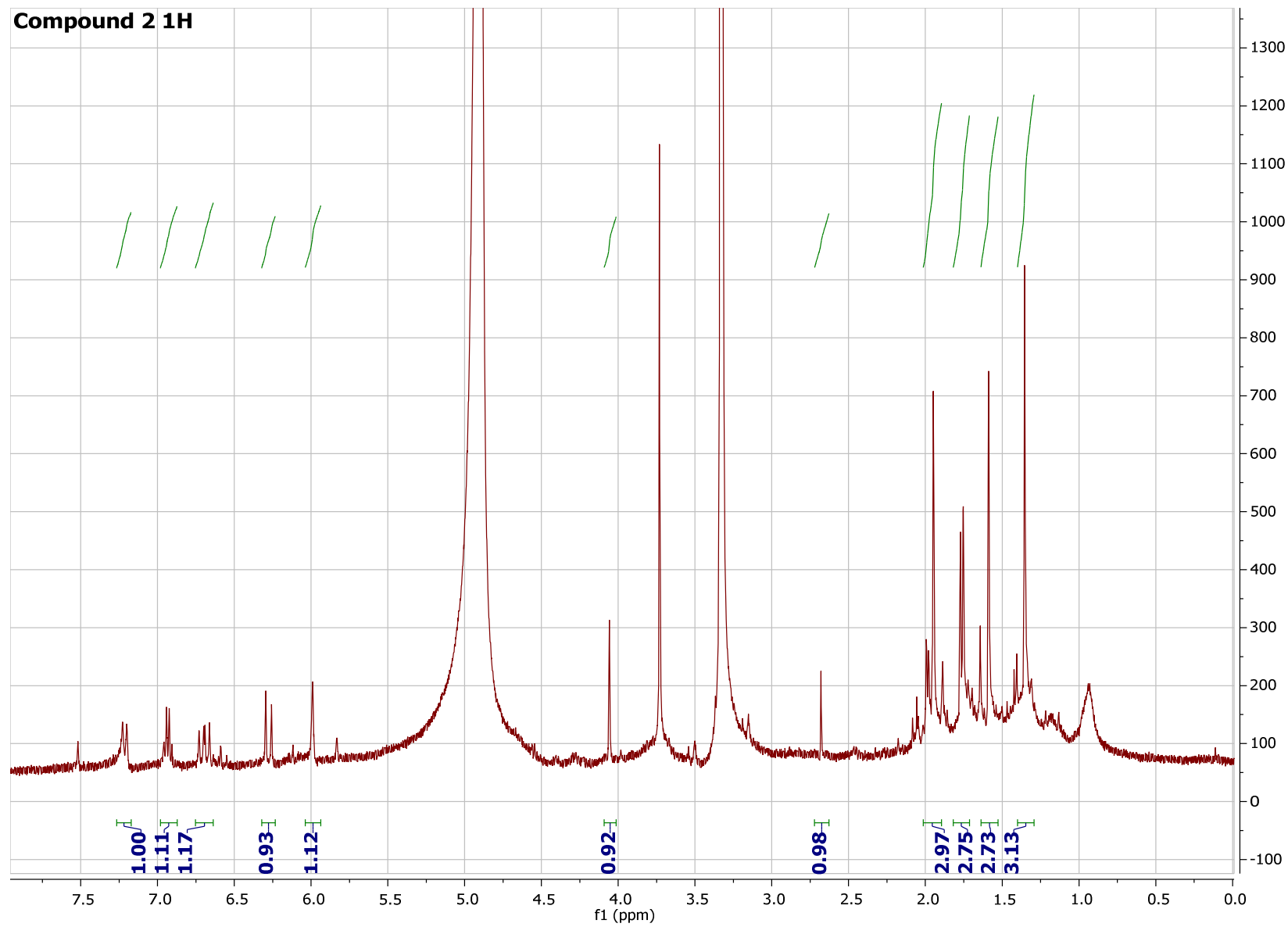


Figure S8: HSQC spectrum of compound 2 in CD<sub>3</sub>OD (400MHz)

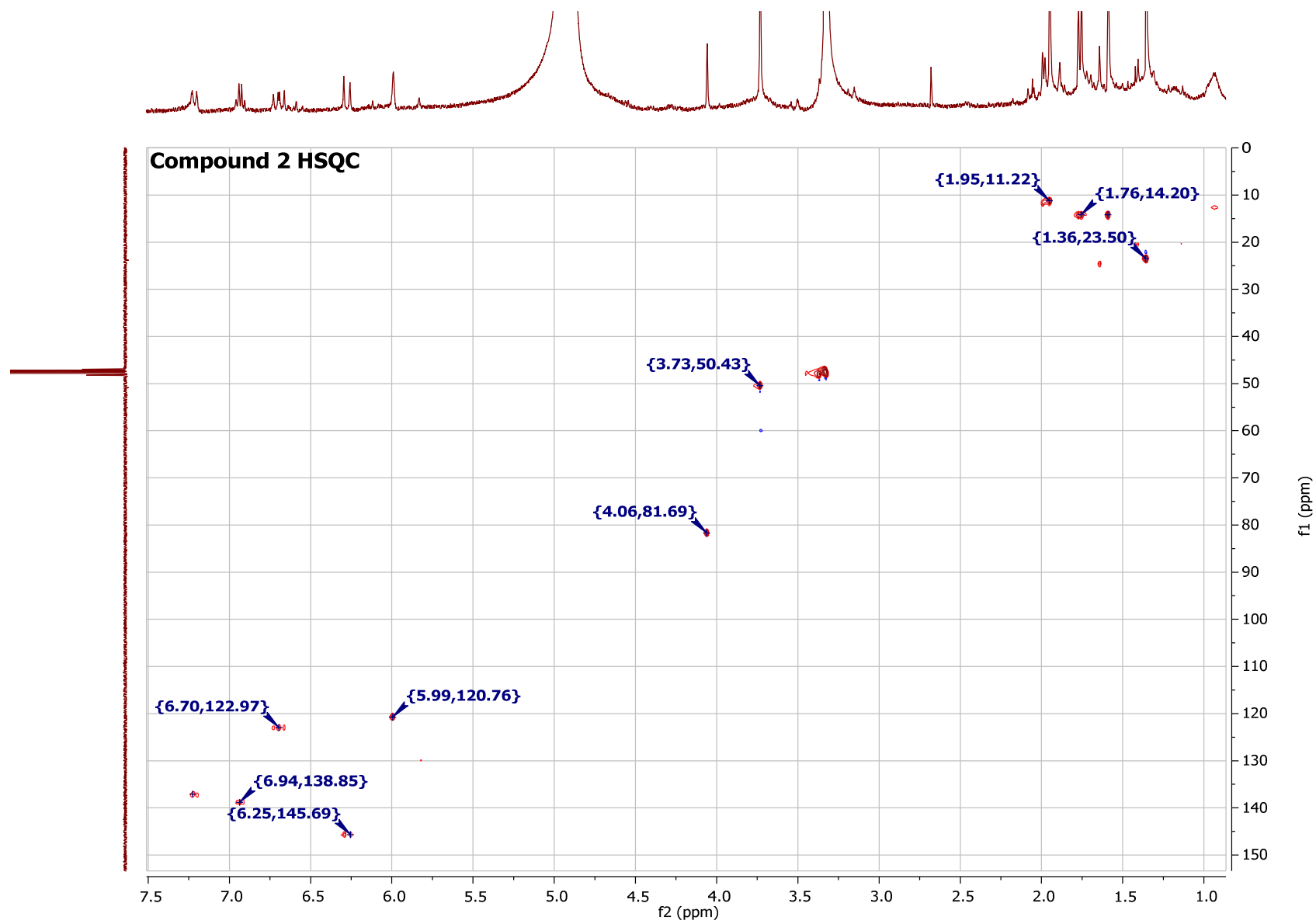


Figure S9: COSY spectrum of compound 2 in CD<sub>3</sub>OD (400MHz)

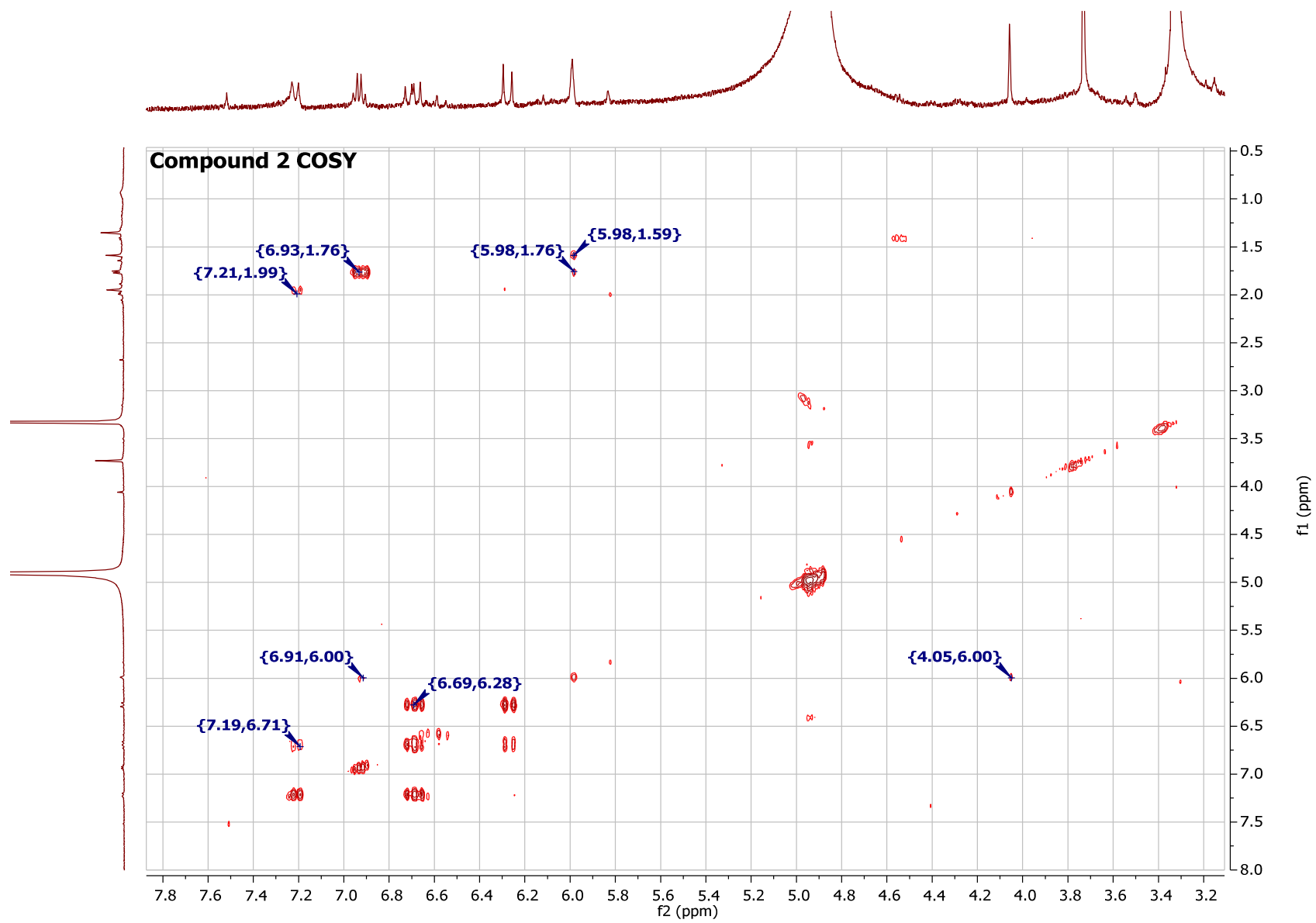


Figure S10: HMBC spectrum of compound 2 in CD<sub>3</sub>OD (400MHz)

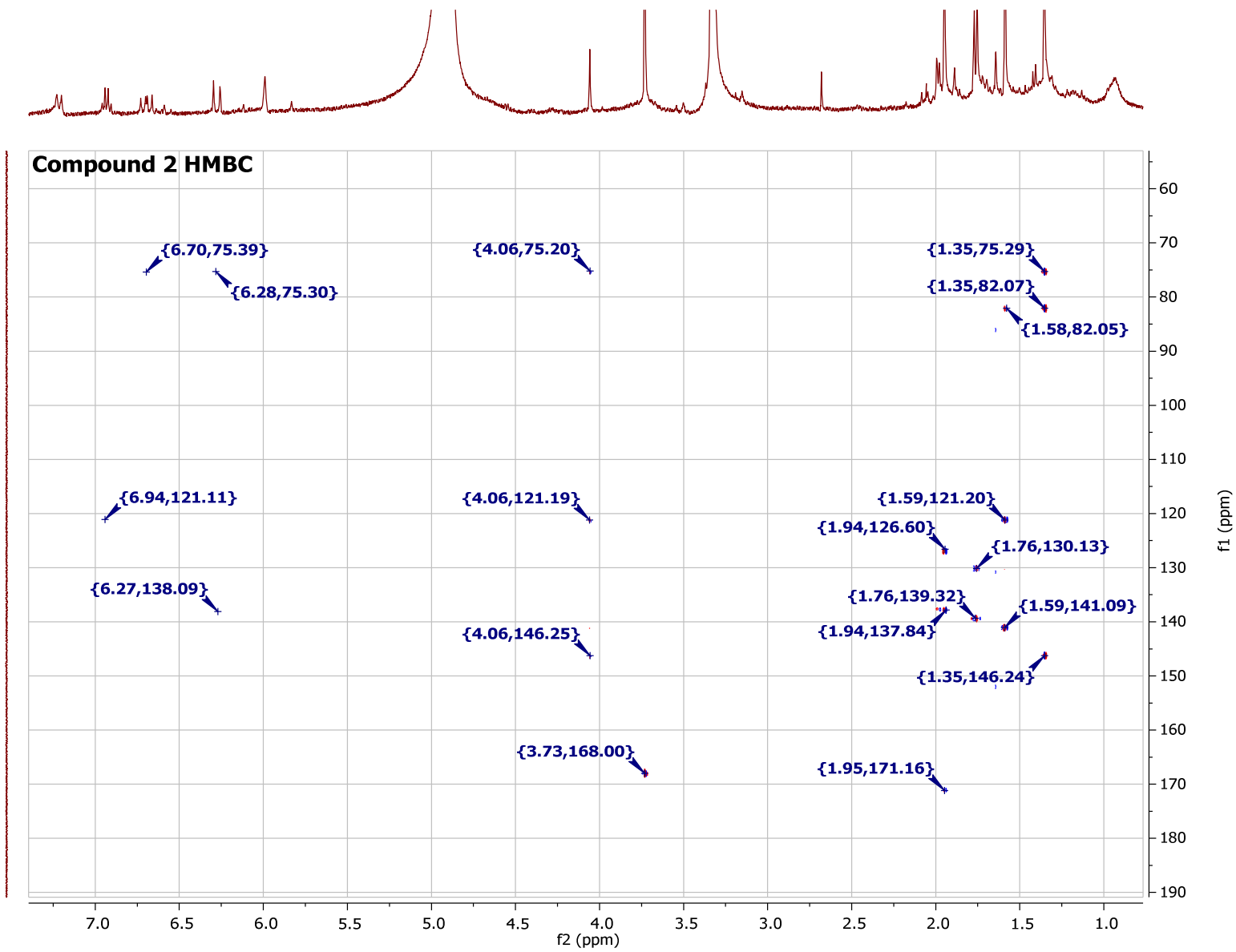
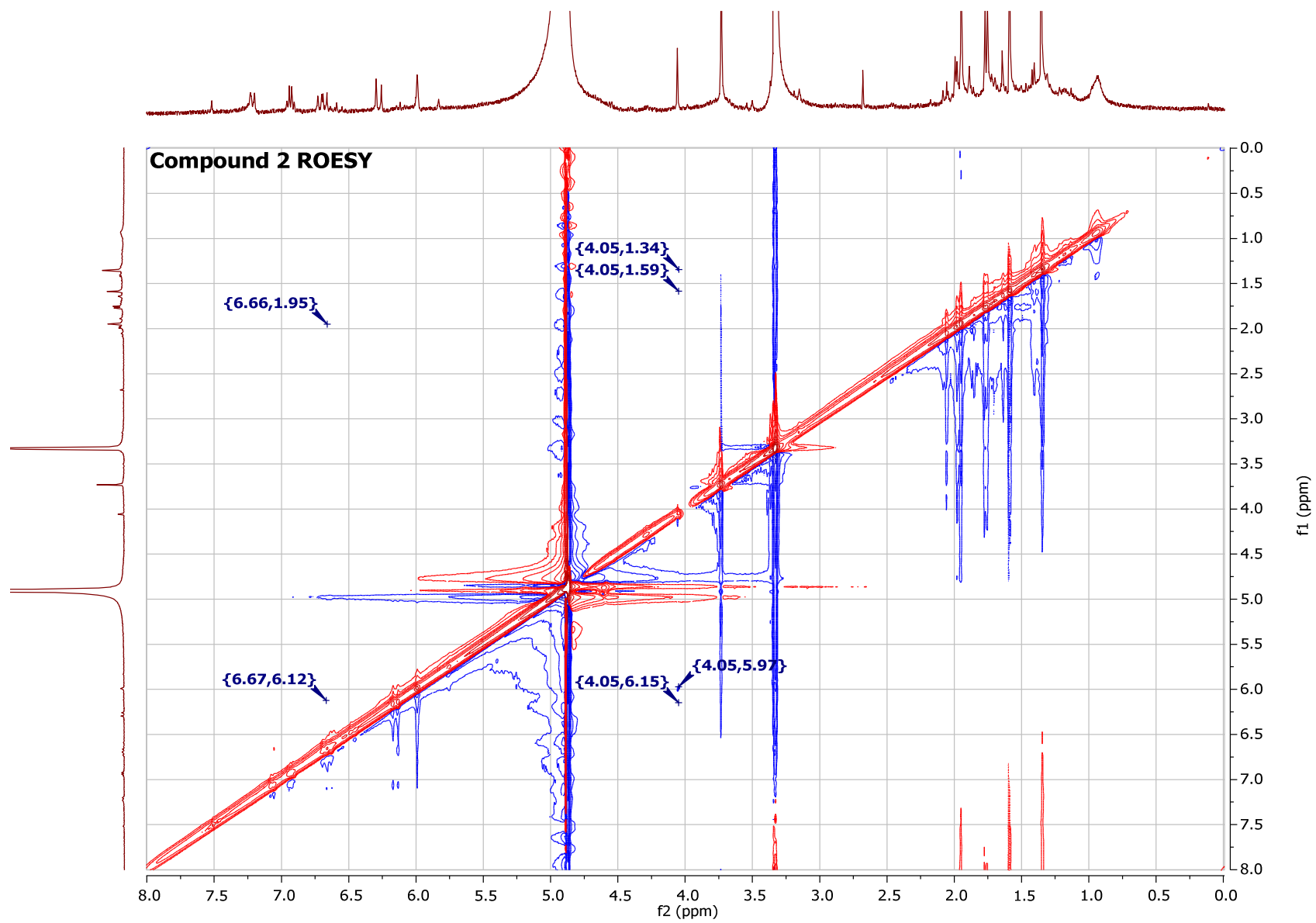


Figure S11: ROESY spectrum of compound 2 in CD<sub>3</sub>OD (400MHz)



**Table S1: Calculated and experimental NMR of compound 2 in CD<sub>3</sub>OD (400MHz)**

Atom numbers	Calculated NMR				Experimental NMR	
	2SS		2SR		Original	
	13C	1H	13C	1H	13C	1H
1	169.98		170.02		171.1	
2	126.42		126.13		126.6	
3	142.96	7.43	143.10	7.35	137	7.23
4	124.93	6.94	122.99	6.88	138.8	6.7
5	156.15	6.48	151.26	6.23	145.7	6.25
6	79.77		79.20		75.2	
7	86.24	4.07	84.93	4.06	81.7	4.06
8	141.57		143.41		141	
9	131.45	6.24	130.72	6.18	120.7	5.99
10	128.65		128.28		130.1	
11	154.45	6.44	154.99	6.27	138.8	6.94
12	16.78	2.45	16.67	2.42	14.2	1.76
13	12.88	1.92	12.96	1.90	11.2	1.95
15	23.26	1.17	27.79	1.41	23.5	1.36
16	13.51	1.85	12.69	1.73	14.1	1.59
17	169.52		169.54		168	
19	51.60	3.63	51.45	3.60	50.4	3.73

**Figure S12: HRESIMS of compound 3**

KH Ahammad Zaman ZS 4

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1: TOF MS ES-  
2.28e5

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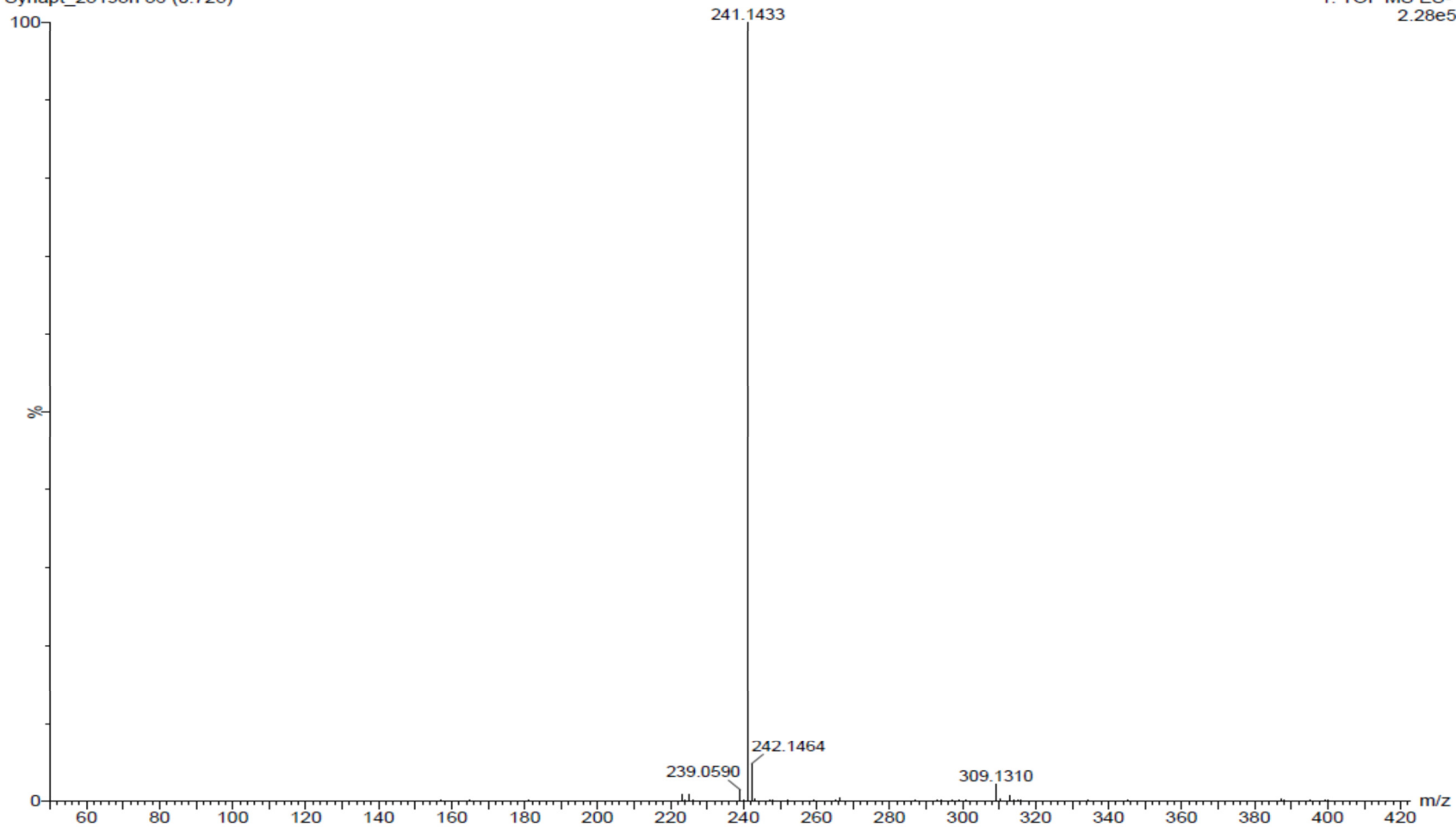




Figure S13:  $^1\text{H}$  NMR spectrum of compound 3 in  $\text{CD}_3\text{OD}$  (400MHz)

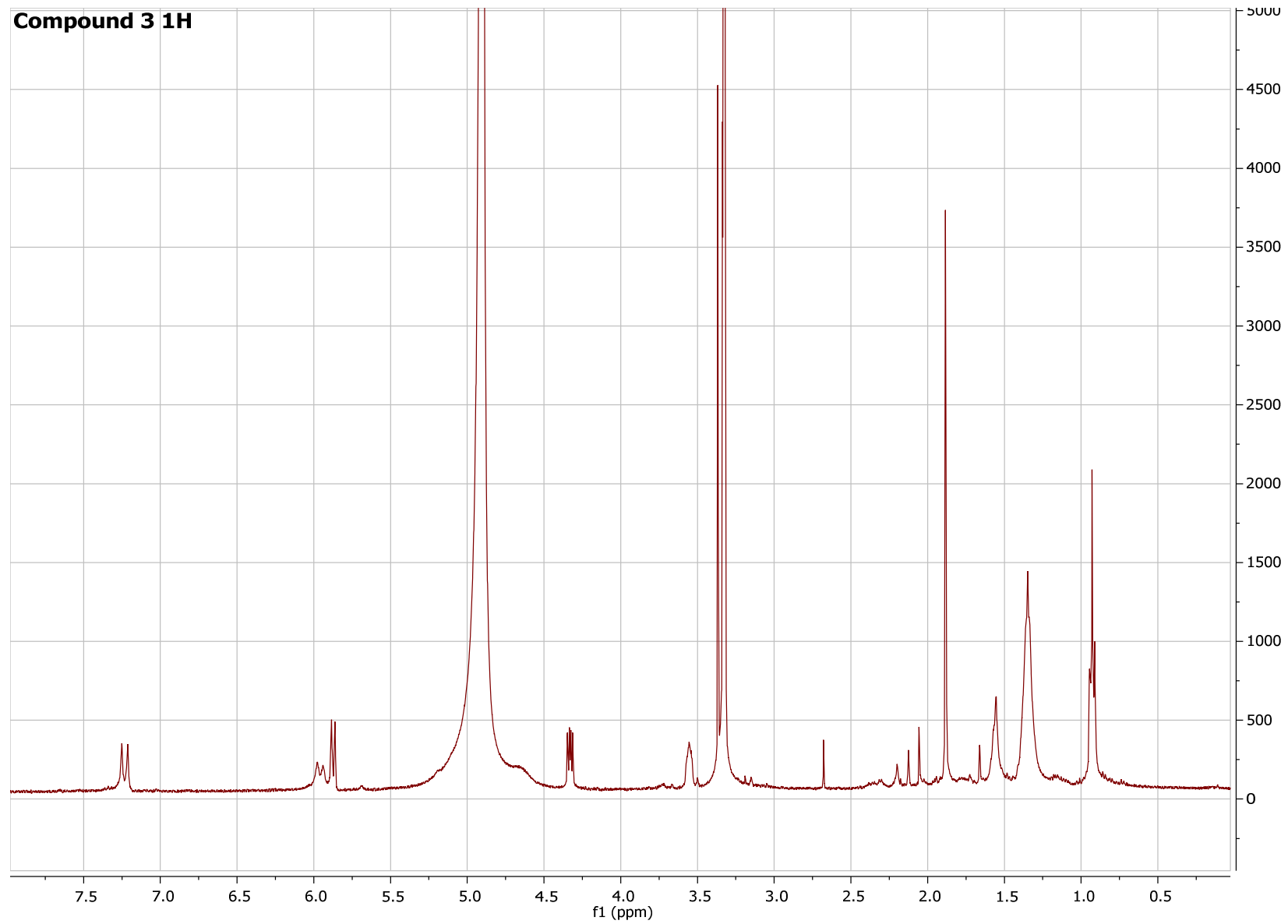


Figure S14: HSQC spectrum of compound 3 in CD<sub>3</sub>OD (400MHz)



Figure S15: COSY spectrum of compound 3 in CD<sub>3</sub>OD (400MHz)

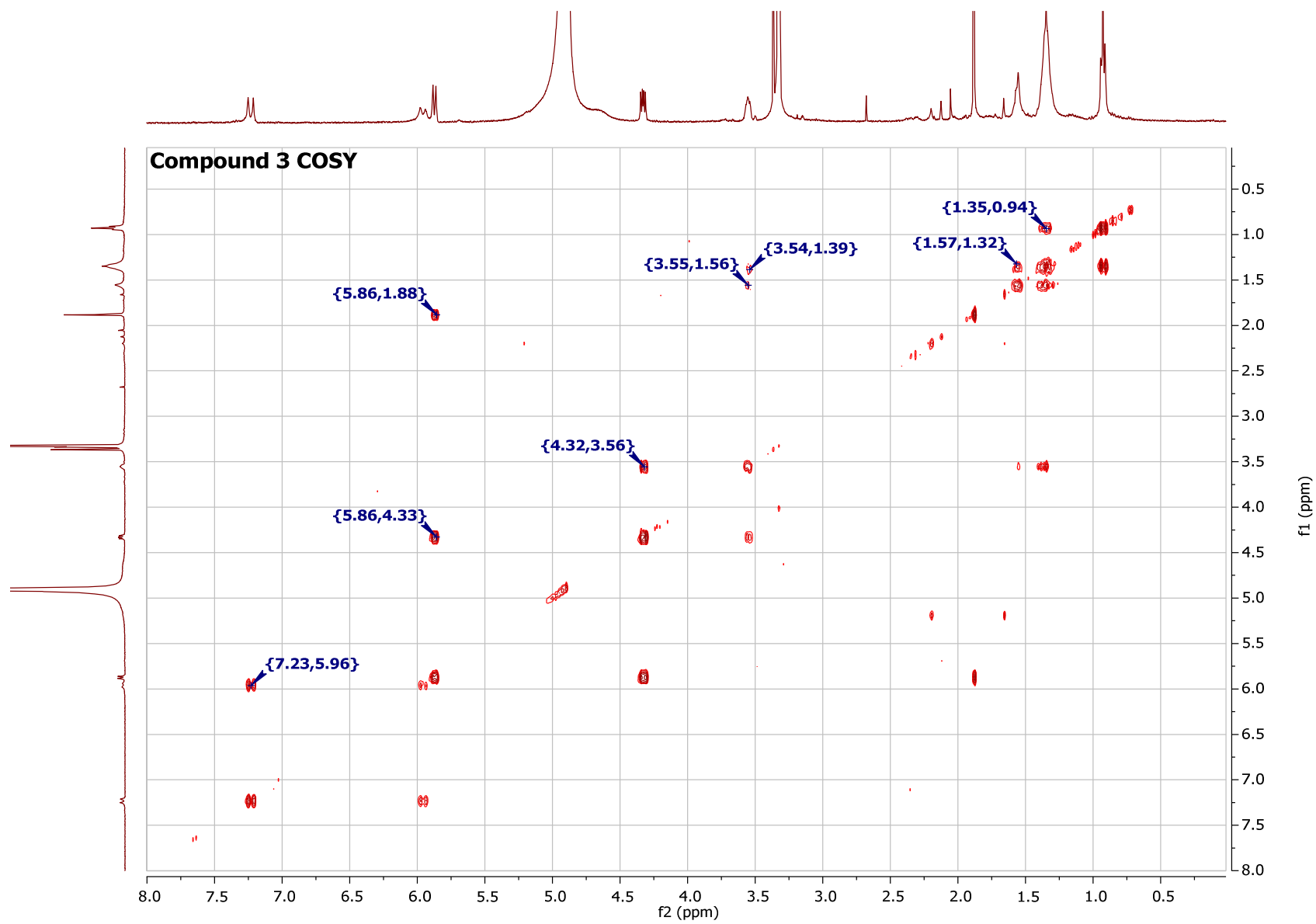


Figure S16: HMBC spectrum of compound 3 in CD<sub>3</sub>OD (400MHz)

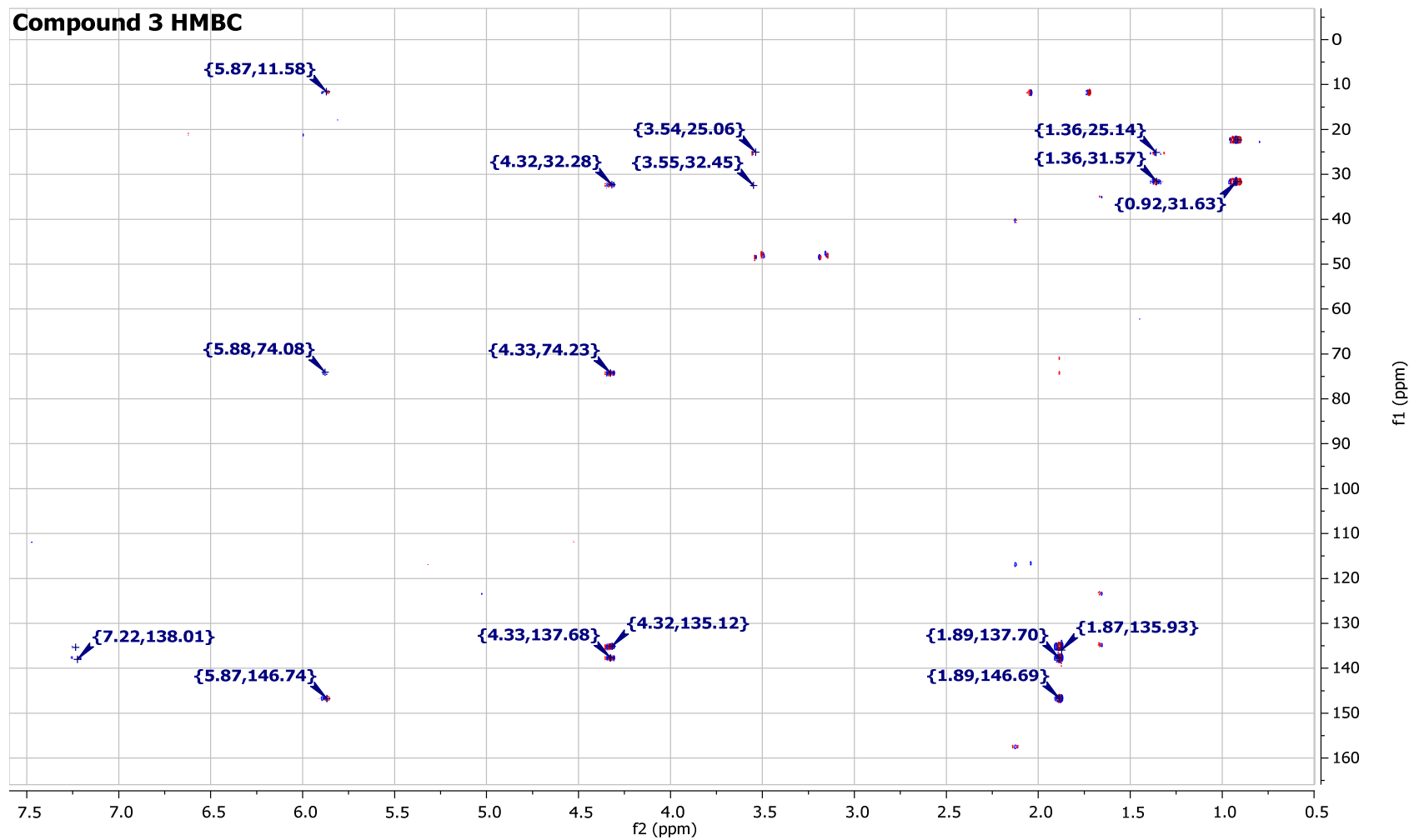
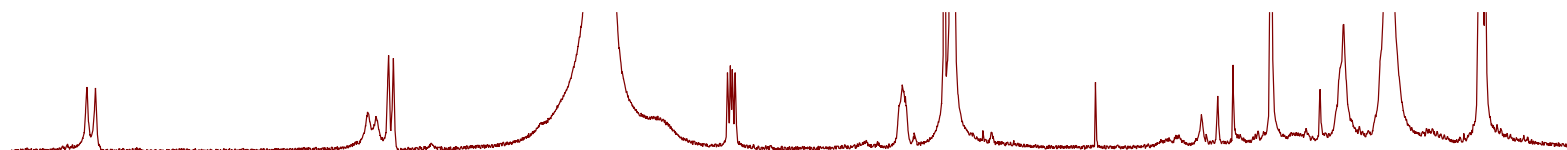
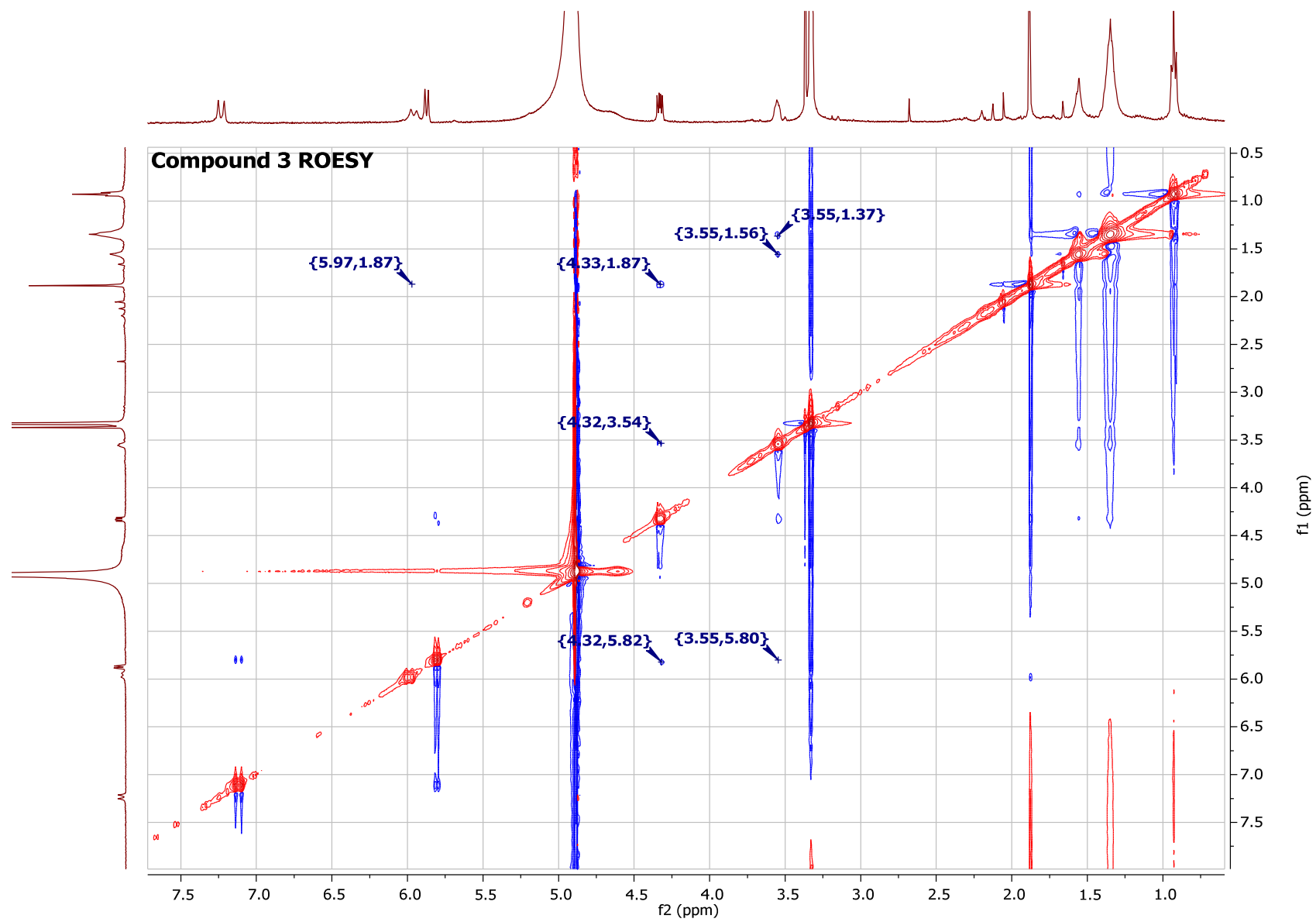


Figure S17: ROESY spectrum of compound 3 in CD<sub>3</sub>OD (400MHz)



**Figure S18: HRESIMS of compound 4**

KH Ahammad Zaman ZS 4

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1: TOF MS ES-  
2.28e5

Synapt\_23193n 36 (0.725)

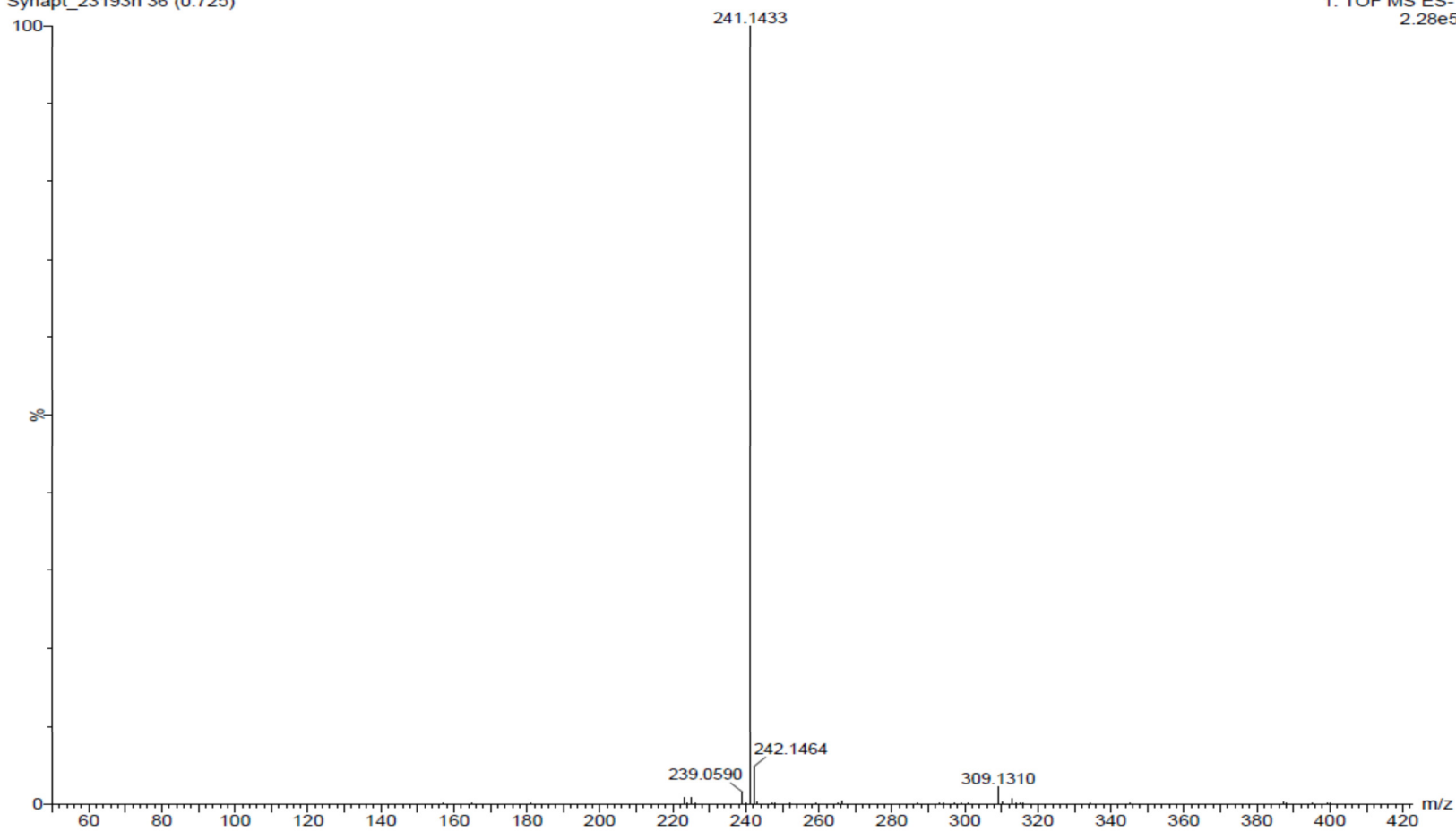


Figure S19:  $^1\text{H}$  NMR spectrum of compound 4 in  $\text{CD}_3\text{OD}$  (400MHz)

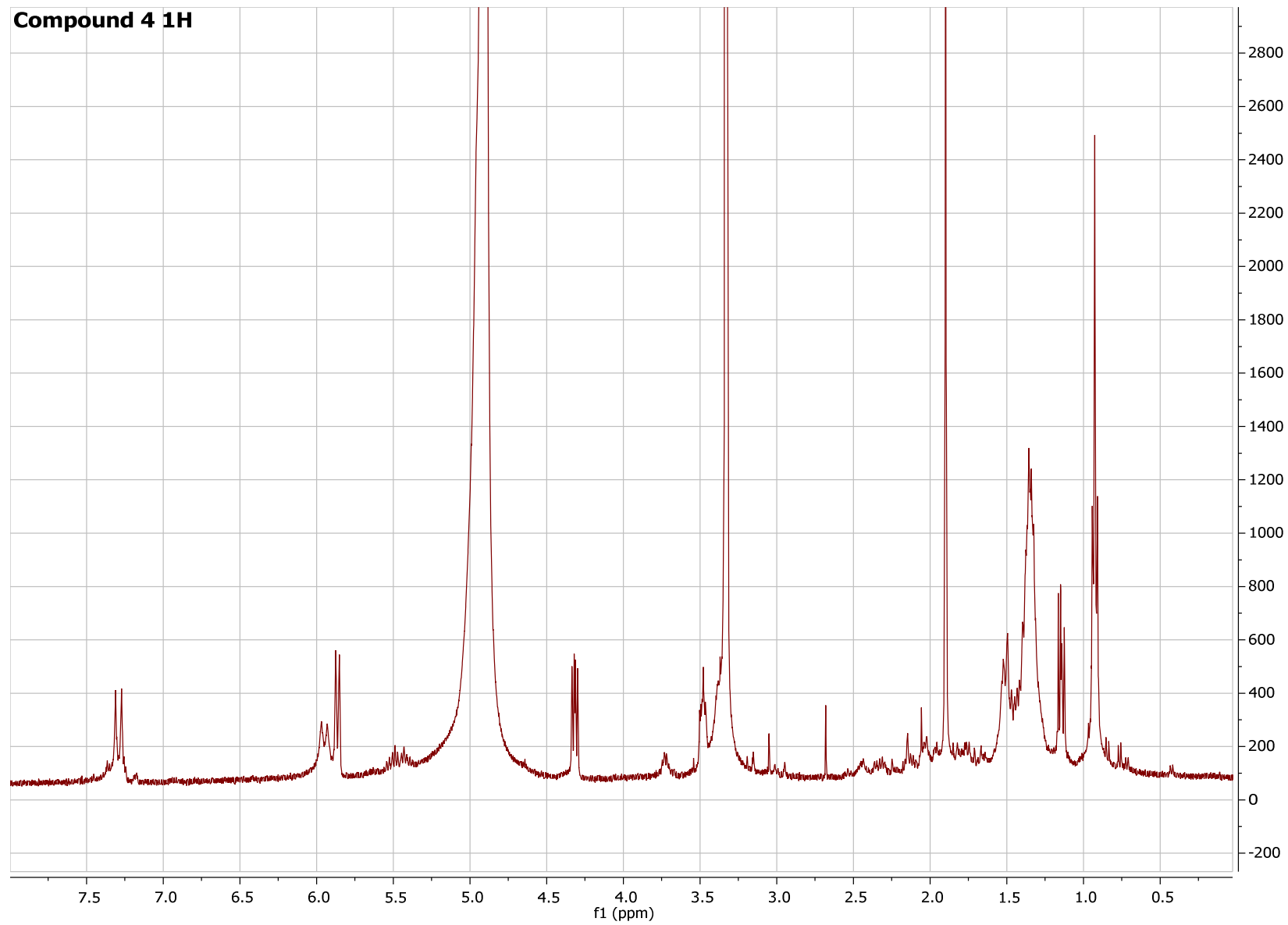


Figure S20: HSQC spectrum of compound 4 in CD<sub>3</sub>OD (400MHz)

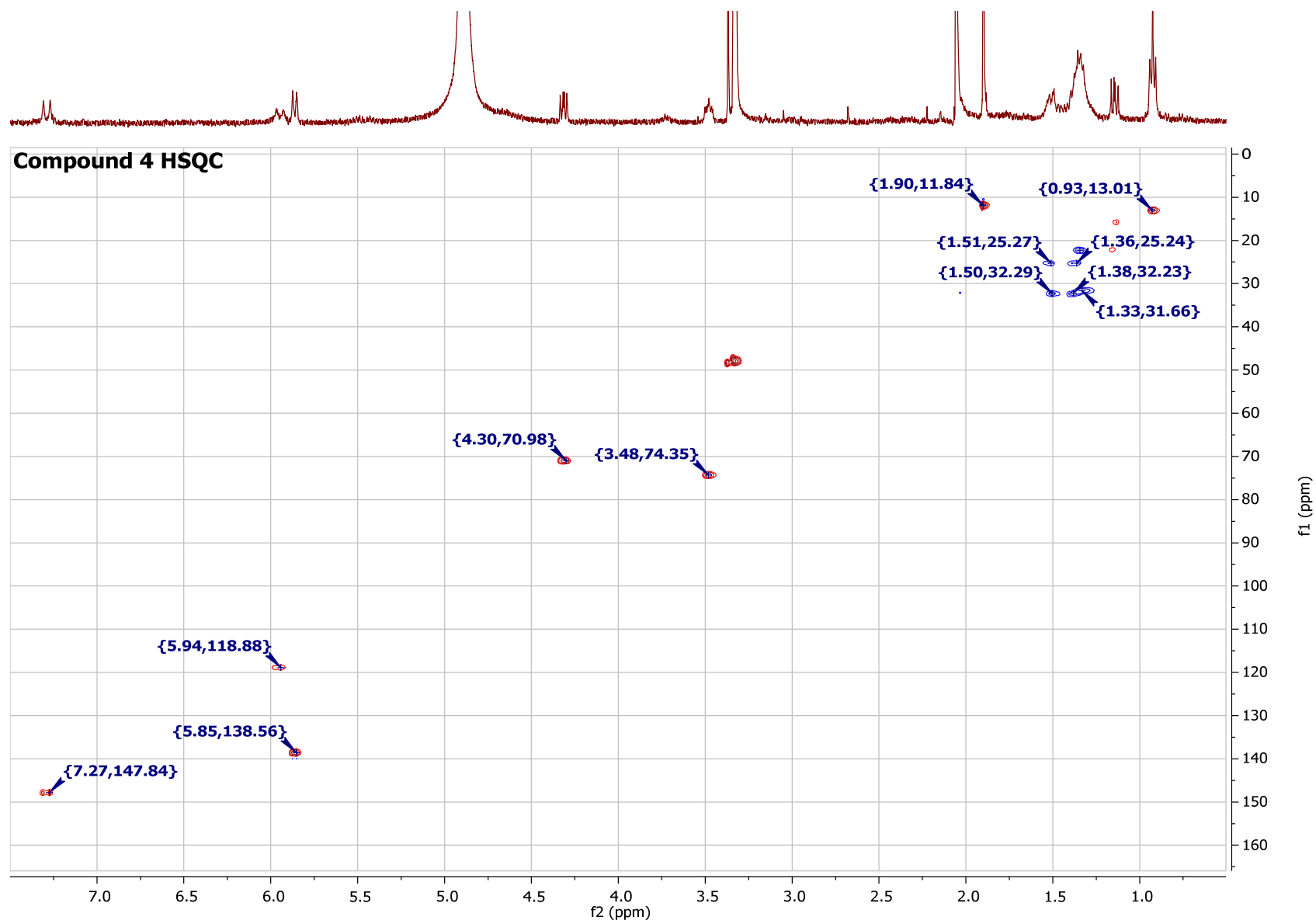




Figure S21: COSY spectrum of compound 4 in CD<sub>3</sub>OD (400MHz)

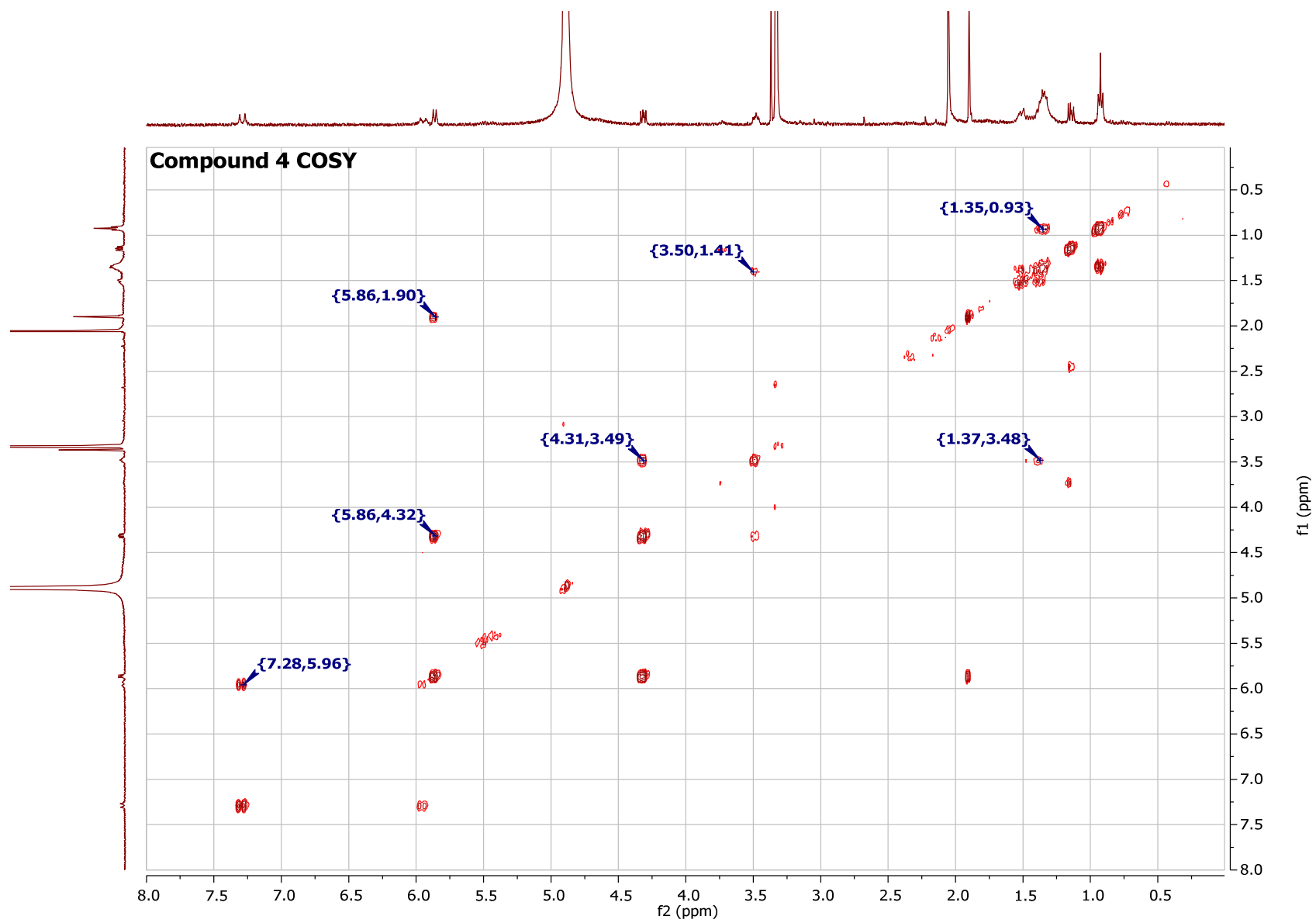


Figure S22: HMBC spectrum of compound 4 in CD<sub>3</sub>OD (400MHz)

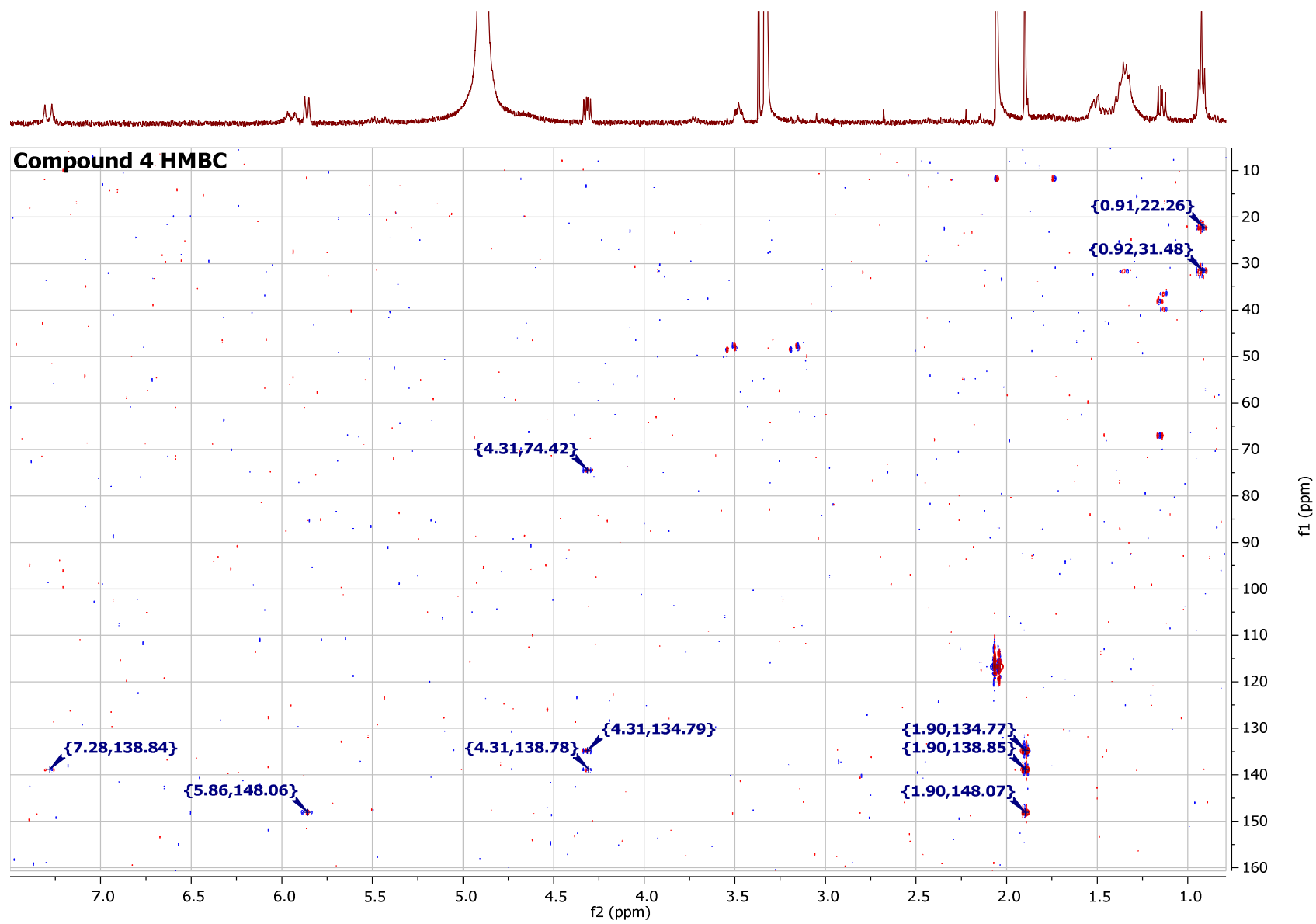
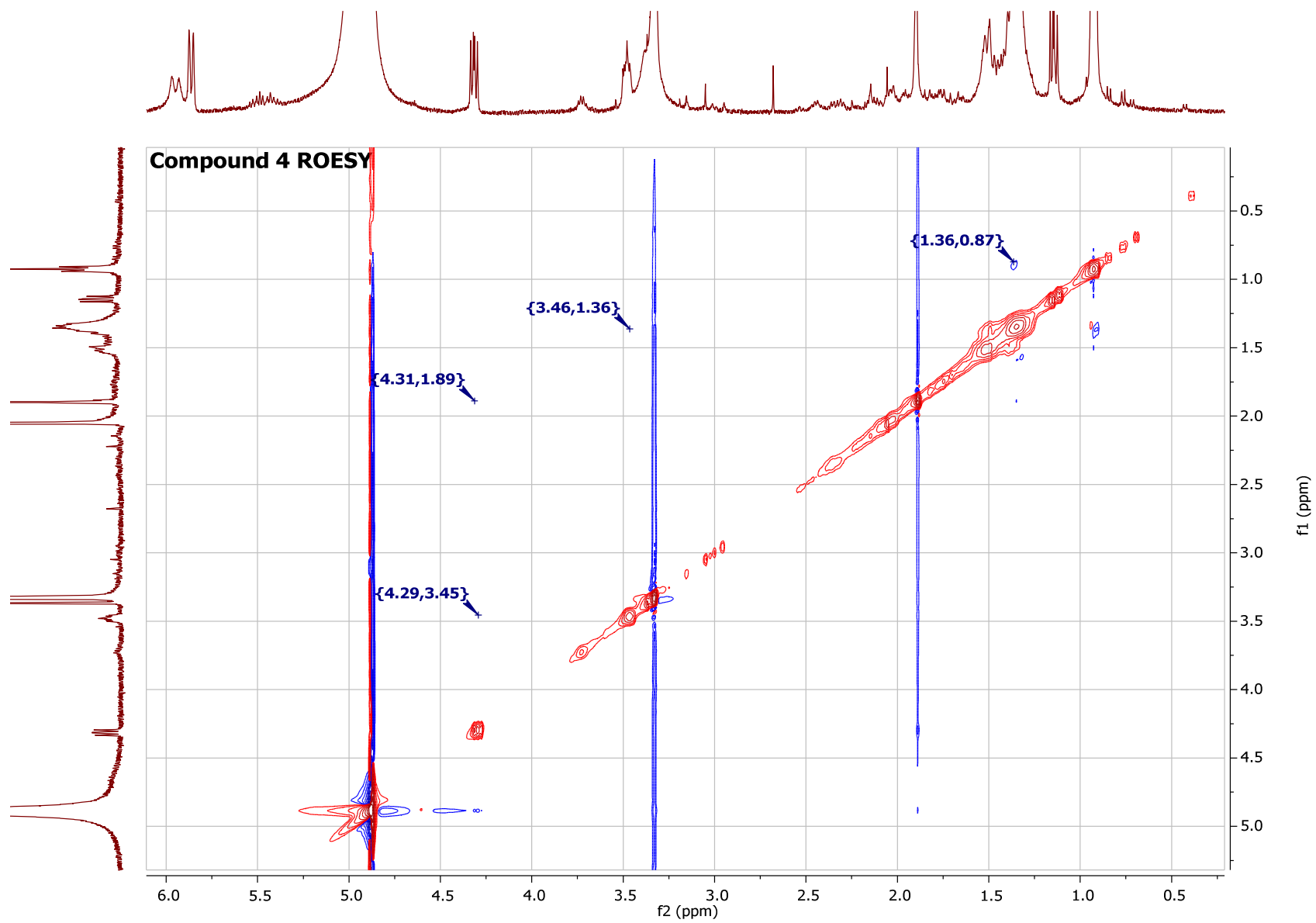


Figure S23: ROESY spectrum of compound 4 in CD<sub>3</sub>OD (400MHz)



**Figure S24: HRESIMS of compound 5**

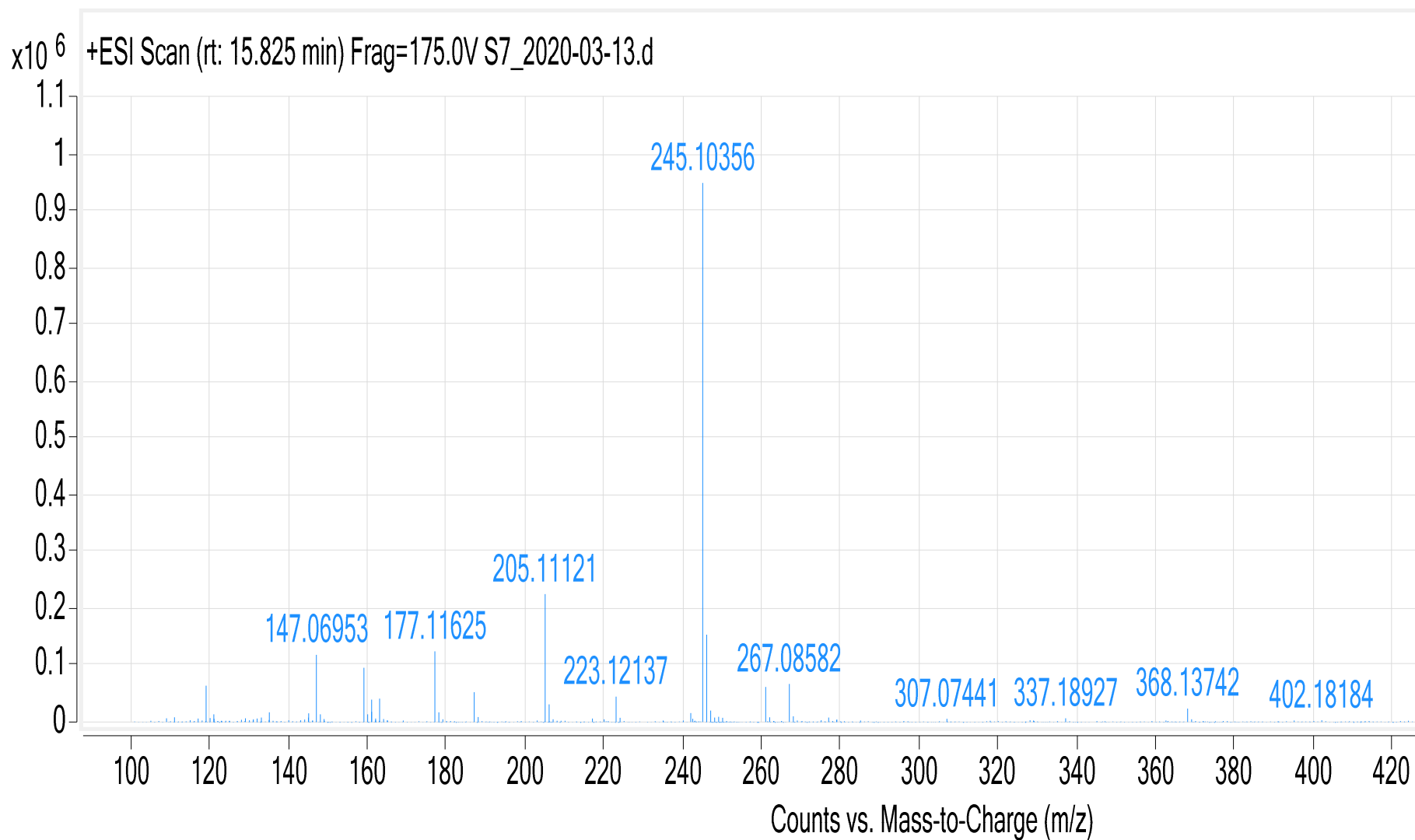


Figure S25:  $^1\text{H}$  spectrum of compound 5 in  $\text{CD}_3\text{OD}$  (400MHz)

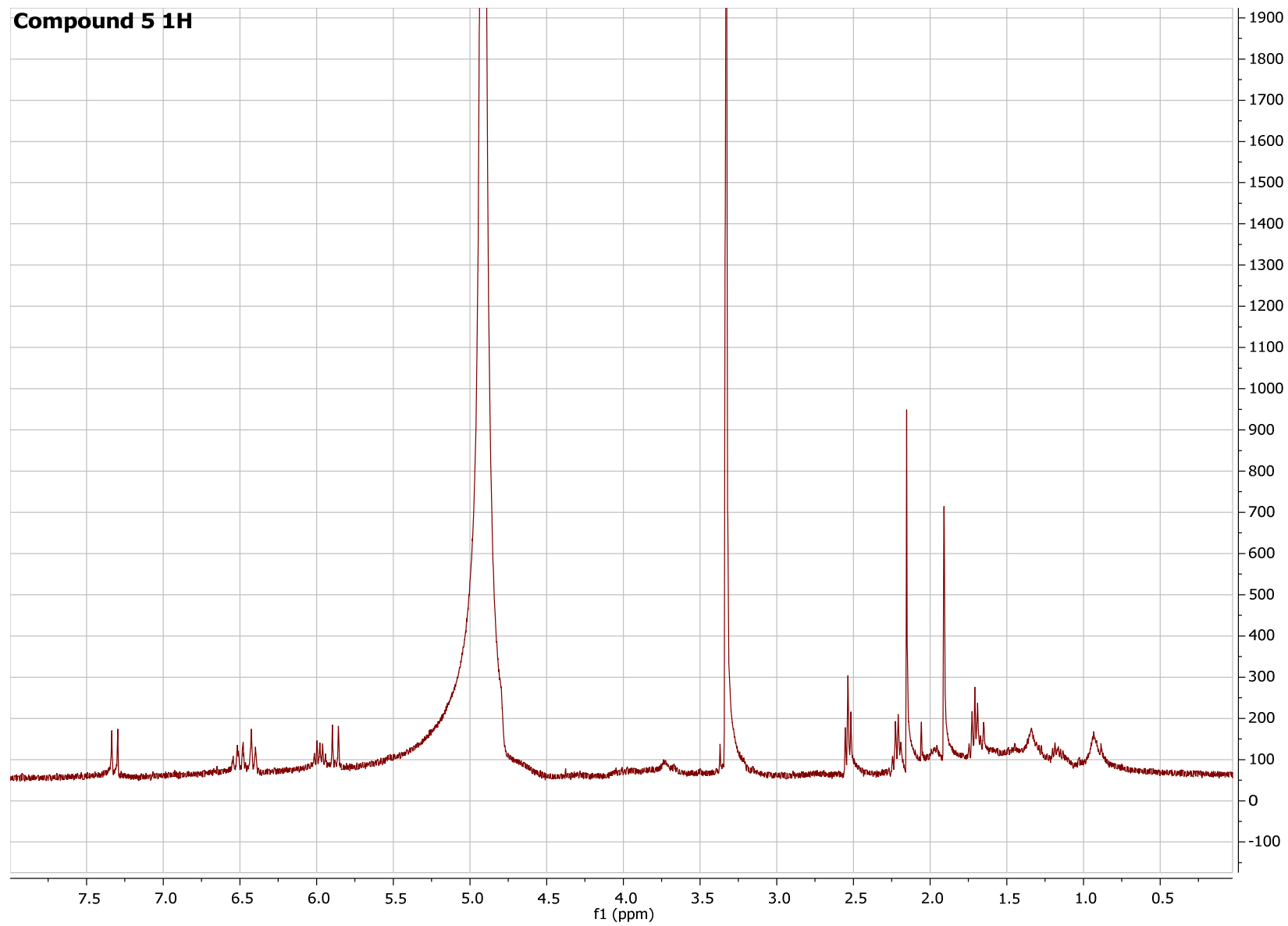


Figure S26: HSQC spectrum of compound 5 in CD<sub>3</sub>OD (400MHz)

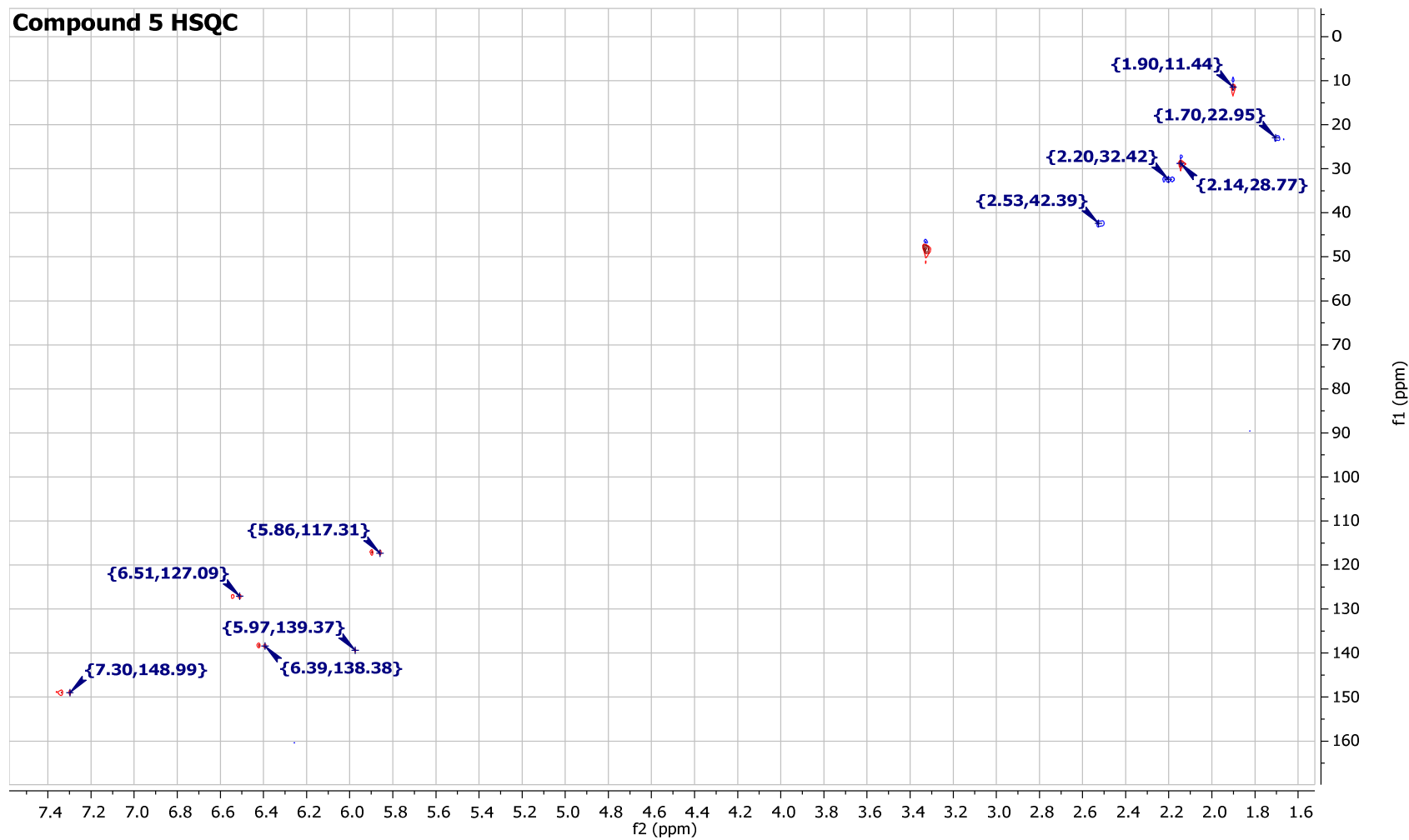
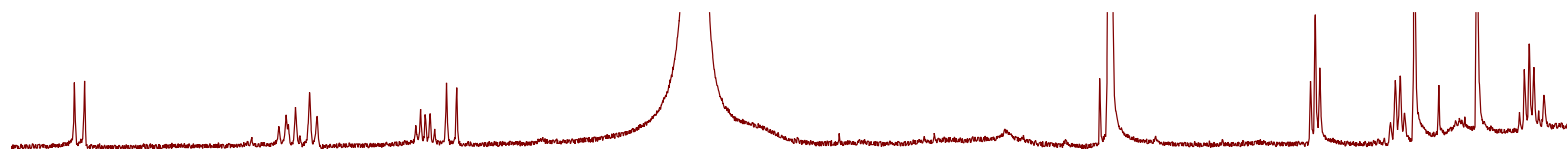


Figure S27: COSY spectrum of compound 5 in CD<sub>3</sub>OD (400MHz)

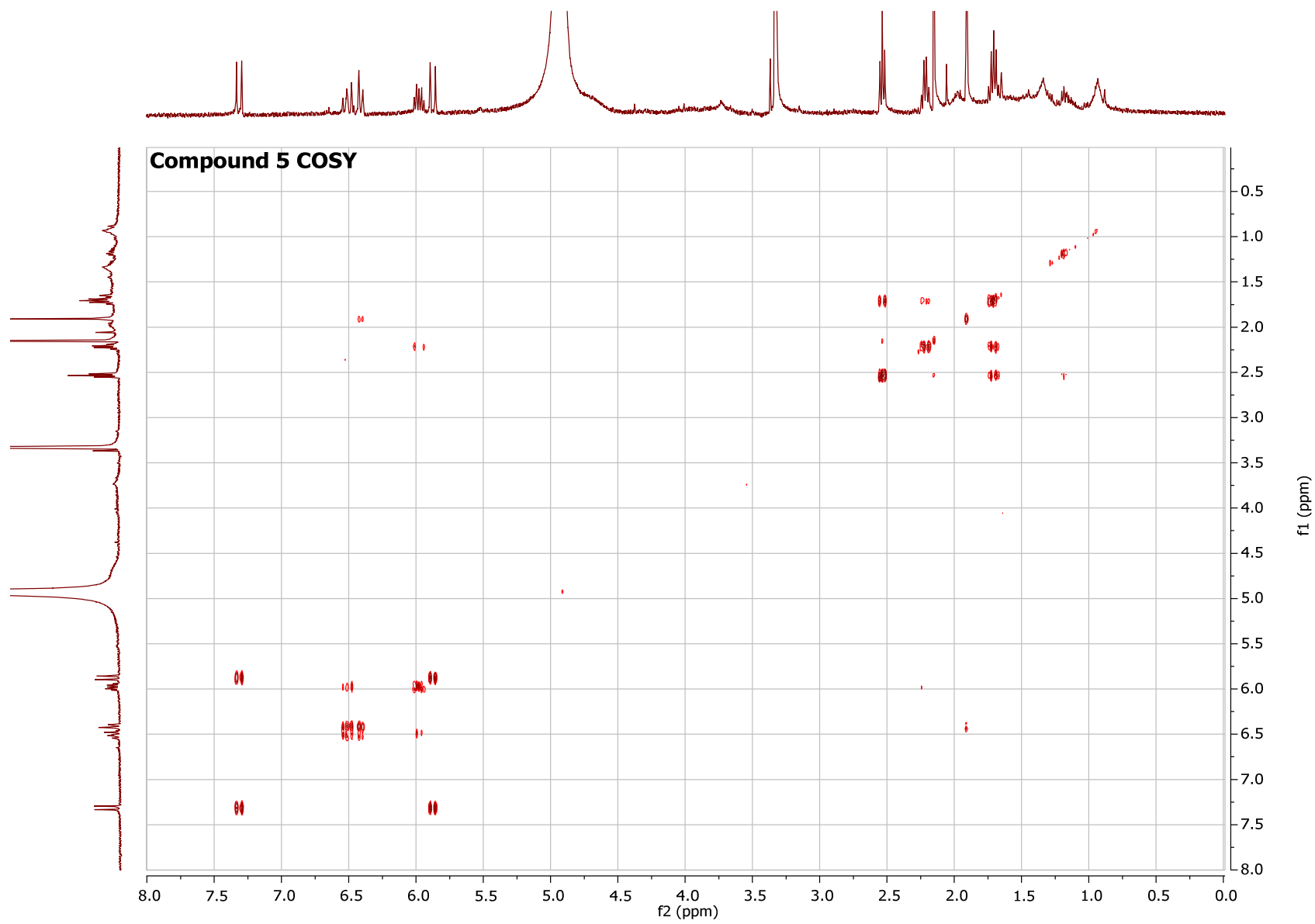
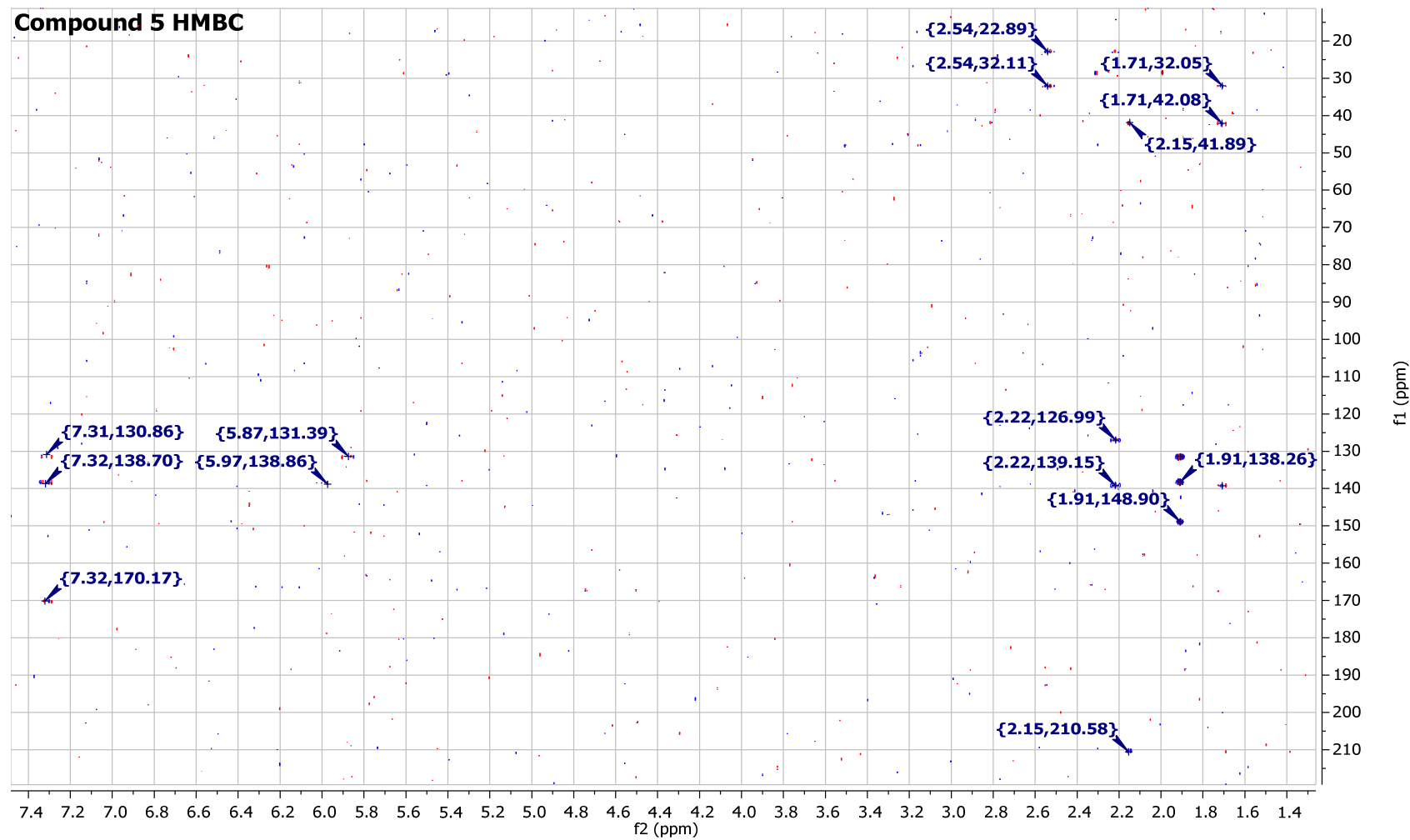


Figure S28: HMBC spectrum of compound 5 in CD<sub>3</sub>OD (400MHz)





**Figure S29: HRESIMS of compound 6**

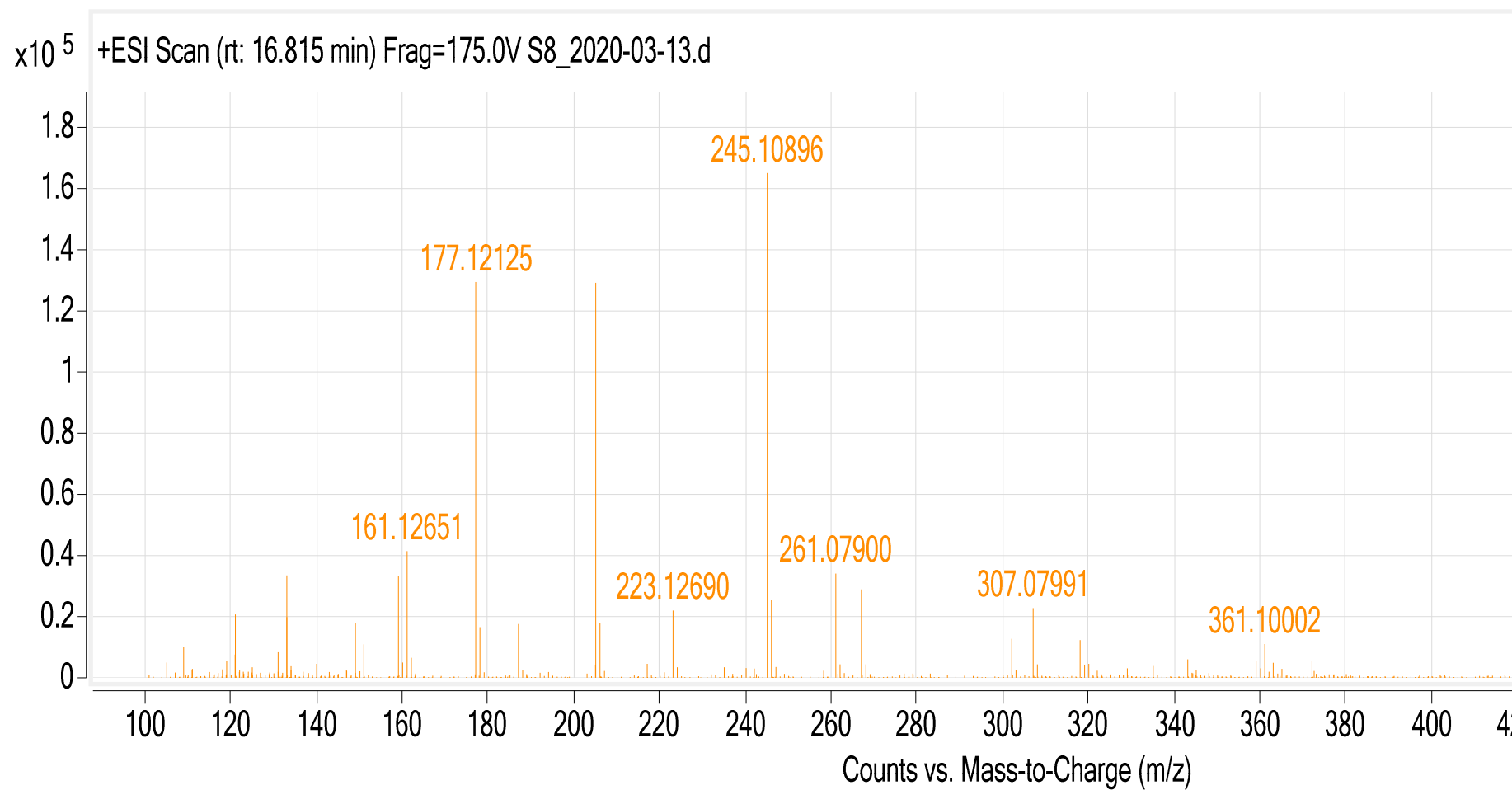


Figure S30: <sup>1</sup>H spectrum of compound 6 in CD<sub>3</sub>OD (400MHz)

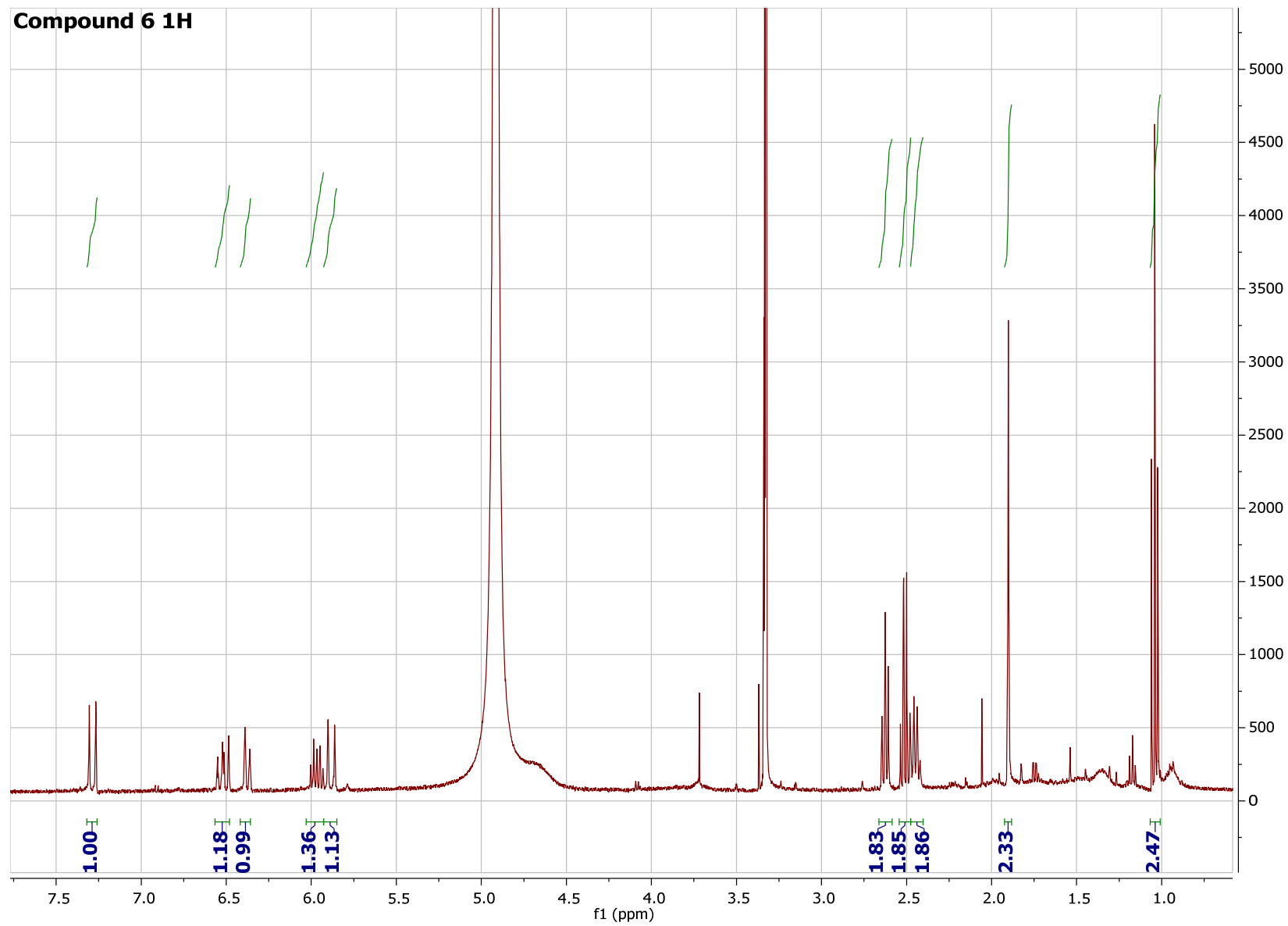


Figure S31: HSQC spectrum of compound 6 in CD<sub>3</sub>OD (400MHz)

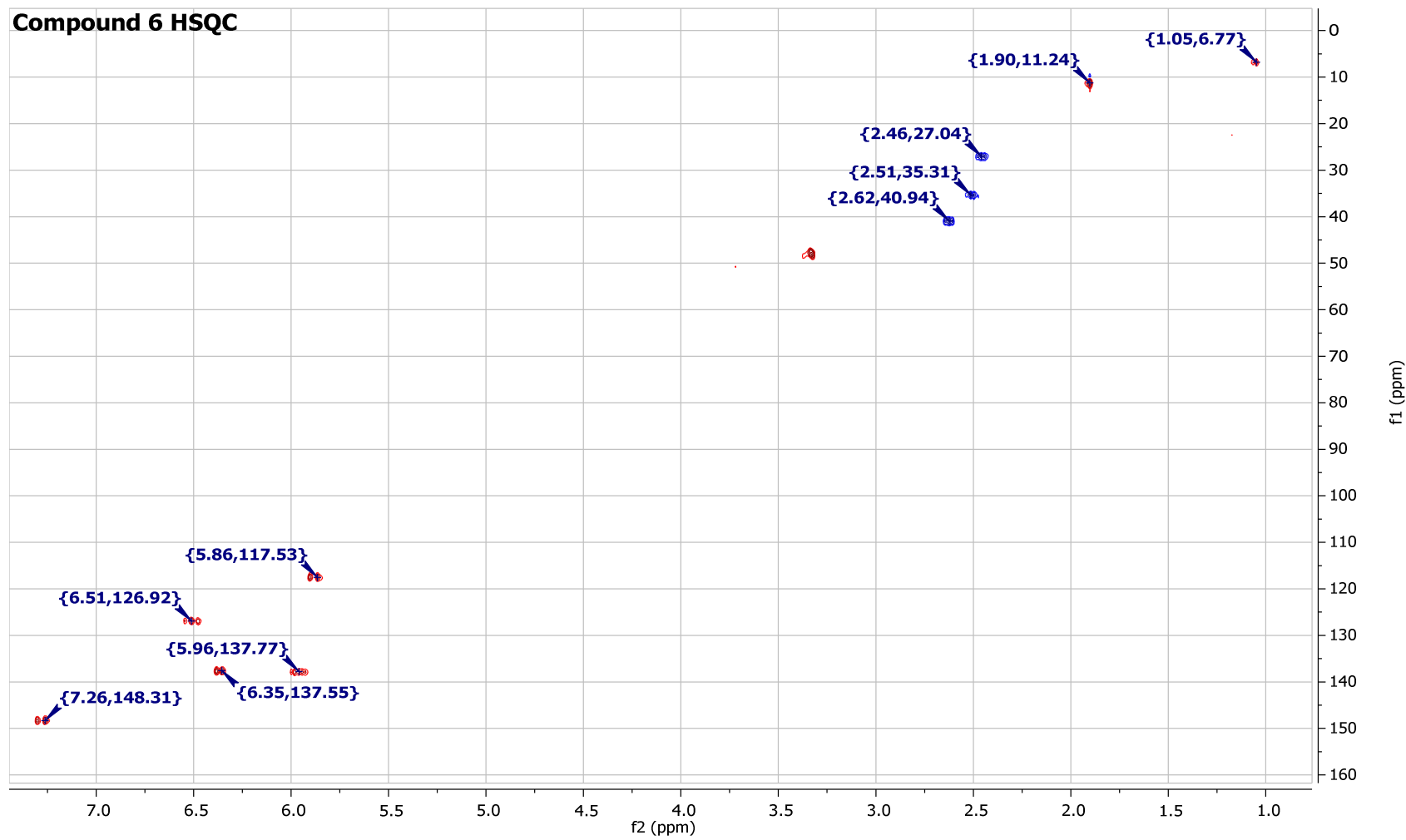


Figure S32: COSY spectrum of compound 6 in CD<sub>3</sub>OD (400MHz)

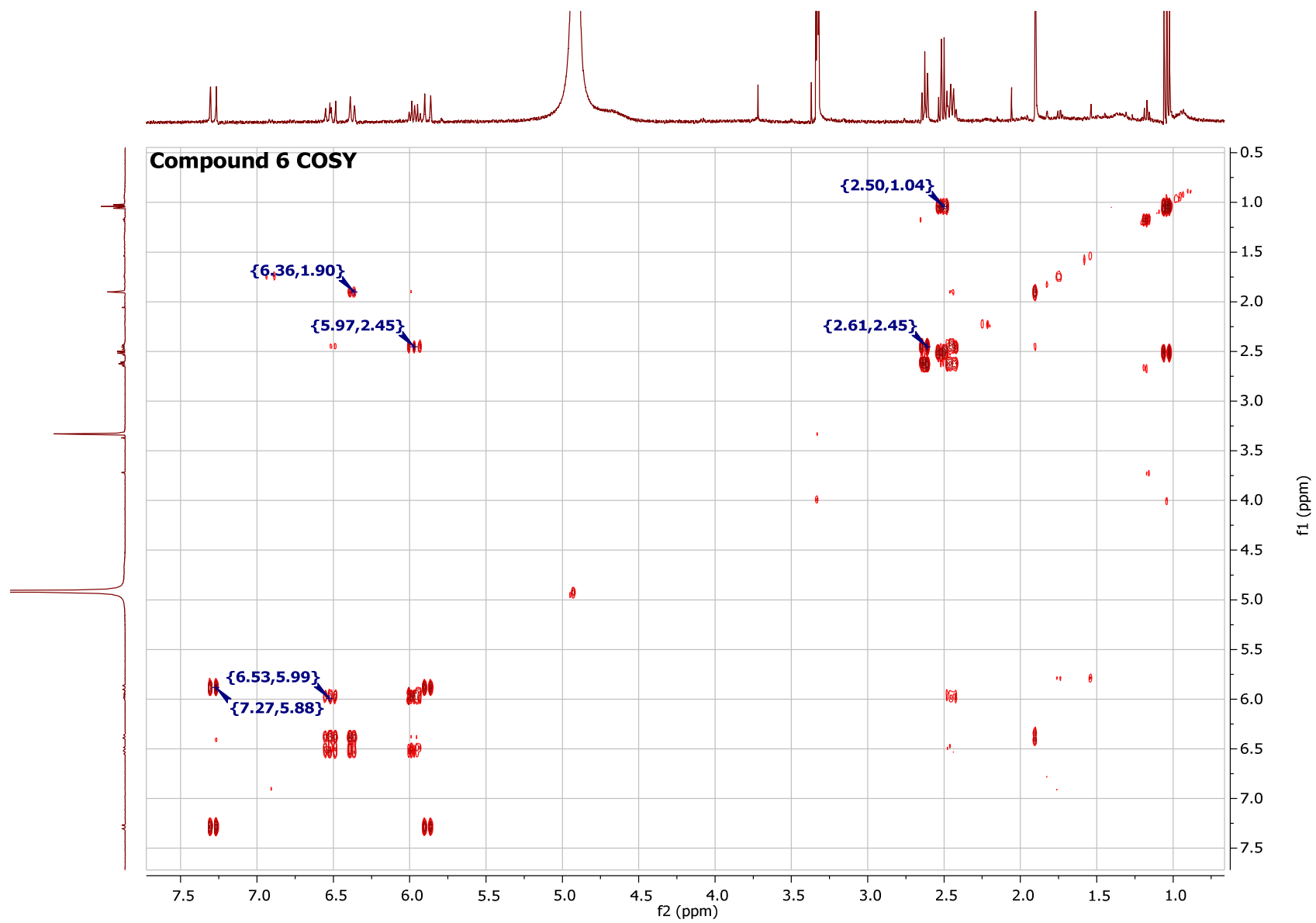
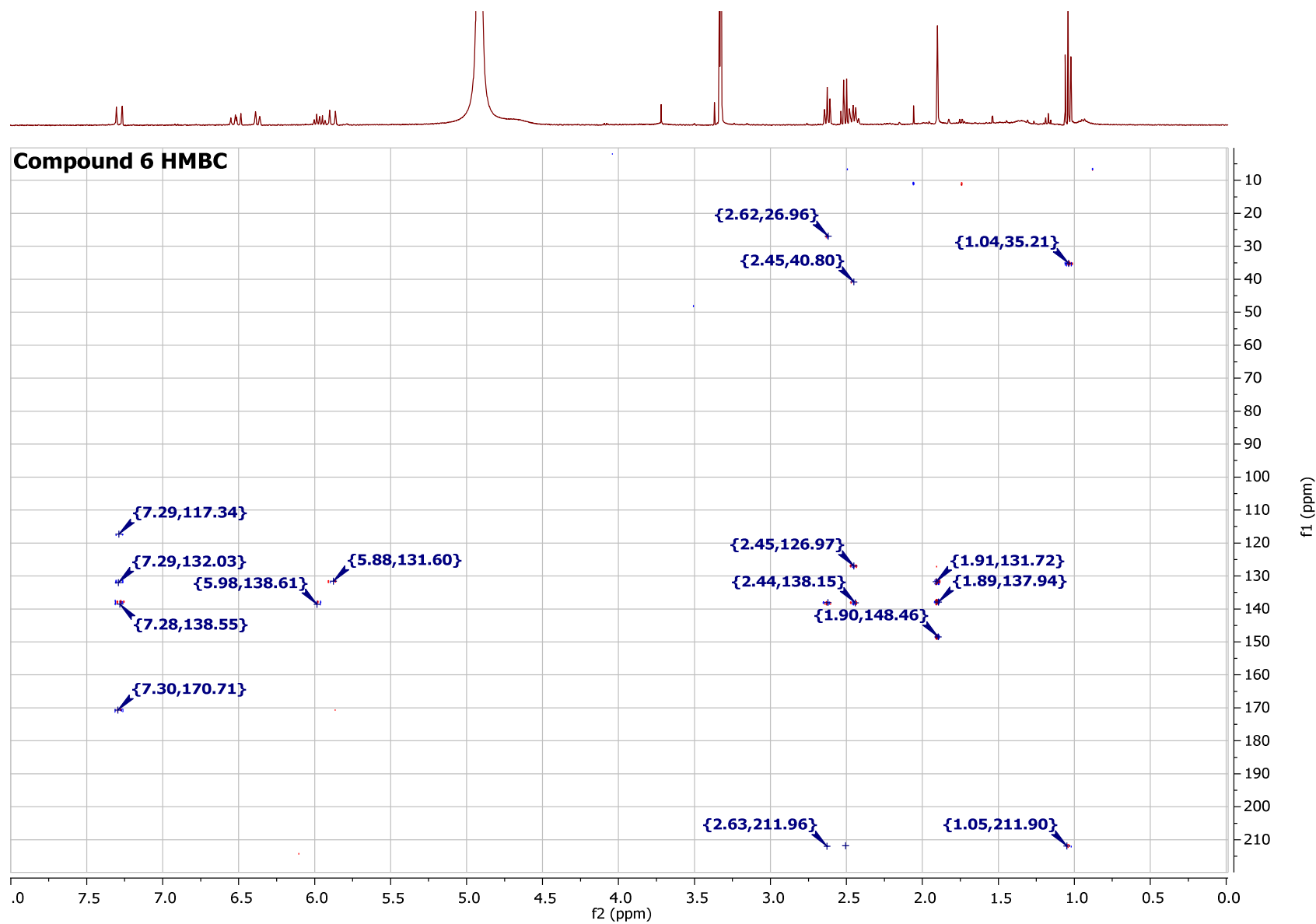


Figure S33: HMBC spectrum of compound 6 in CD<sub>3</sub>OD (400MHz)



**Table S2: Activities of Kaneoheic acids A-F against *S. aureus* (ATCC® 12600™) and *Bacillus subtilis* (ATCC® 6633™)**

	MIC found from Assay [µg/mL]					
	<i>S. aureus</i>			<i>Bacillus subtilis</i>		
	Compound alone	Compound + Disulfiram [6 µg/mL ]	Compound + Chloramphenicol [1µg/mL]	Compound alone	Compound + Disulfiram [6 µg/mL ]	Compound + Chloramphenicol [1µg/mL]
<b>Kaneoheic acid A</b>	NA	20	NA	NA	NA	NA
<b>Kaneoheic acid B</b>	NA	40	NA	NA	80	80
<b>Kaneoheic acid C</b>	NA	40	NA	NA	40	40
<b>Kaneoheic acid D</b>	NA	10	NA	NA	80	80
<b>Kaneoheic acid E</b>	NA	10	NA	NA	40	80
<b>Kaneoheic acid F</b>	NA	20	NA	NA	40	40

**NA → Not Active**

**Table S3: Activities of Small to medium chain fatty acids against *S. aureus* (ATCC® 12600<sup>TM</sup>) and *B. subtilis* (ATCC® 6633<sup>TM</sup>)**

#	Fatty Acids	MIC found from Assay [µg/mL]					
		<i>S. aureus</i>			<i>Bacillus subtilis</i>		
		Compound alone	Compound + Disulfiram [6 µg/mL ]	Compound + Chloramphenicol [1µg/mL]	Compound alone	Compound + Disulfiram [6 µg/mL ]	Compound + Chloramphenicol [1µg/mL]
1	<b>Butyric acid [Na salt] MW 110</b>	1100	550	550	550	137.5	137.5
2	<b>Capric acid [Na salt] MW 194</b>	121.2	121.2	121.2	485	242.5	242.5
3	<b>Lauric acid MW 200</b>	63	63	63	126	63	63
4	<b>Myristic acid MW 228</b>	570	285	570	285	142.5	142.5
5	<b>Linoleic acid MW 280</b>	700	88.2	350	215.6	215.6	215.6