

FIGURE LEGENDS

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Figure S26. ^{13}C NMR (150 MHz, CD_3OD) spectrum of the new compound 4

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Figure S28. HMQC NMR (600 MHz, CD_3OD) spectrum of the new compound 4

Figure S29. HMBC NMR (600 MHz, CD_3OD) spectrum of the new compound 4

Figure S30. HRESIMS spectrum of the new compound 4

Figure S31. HRESIMS data of the new compound 4

Figure S32. ESIMS (in-source fragmentation) spectrum of compound 4

Figure S33. ^1H NMR (600 MHz, DMSO) spectrum of the new compound 5

Figure S34. ^{13}C NMR (150 MHz, DMSO) spectrum of the new compound 5

Figure S35. HRESIMS spectrum of the new compound 5

Figure S36. HRESIMS data of the new compound 5

Figure S1. ^1H NMR (600 MHz, CD_3OD) spectrum of the new compound 1

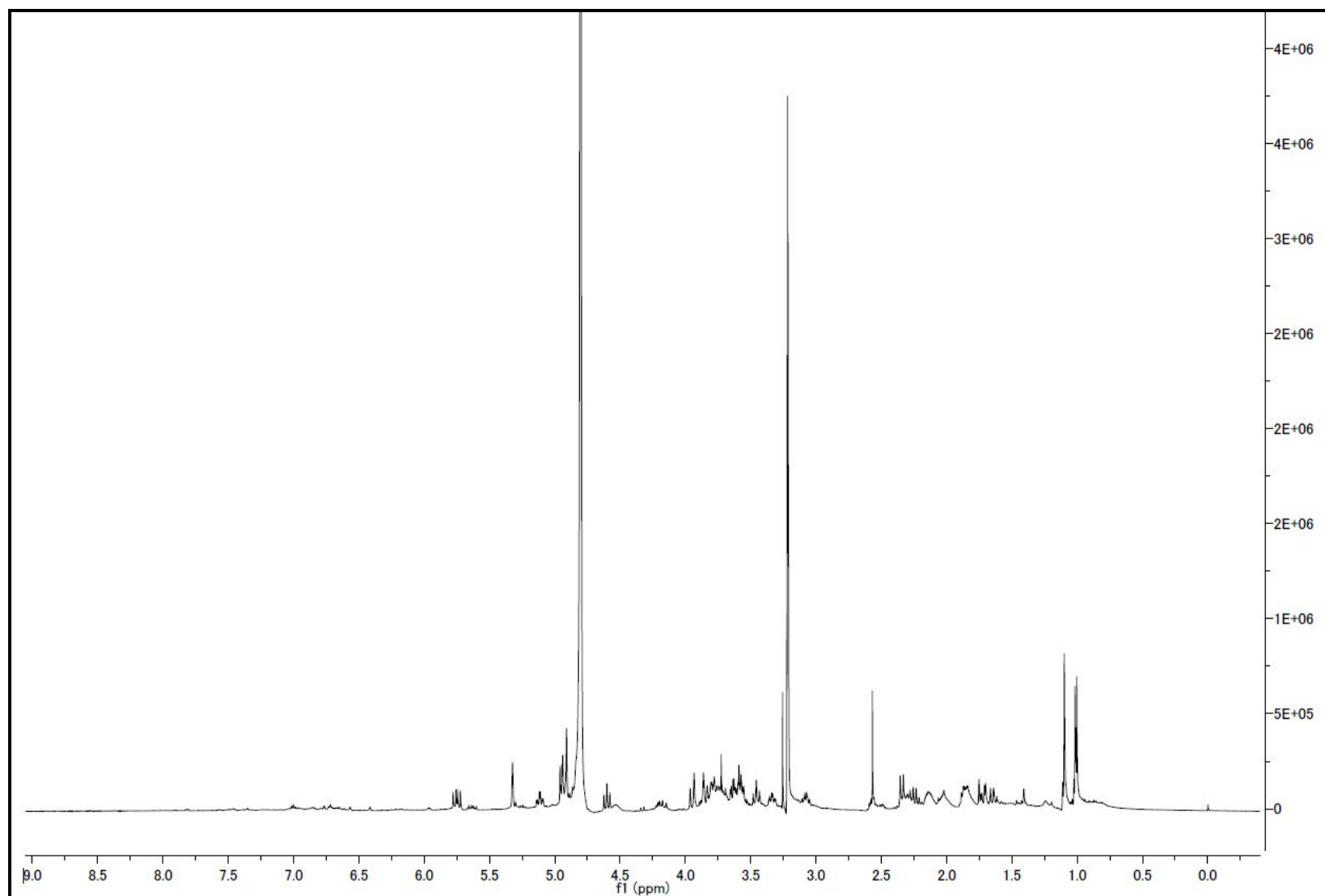


Figure S2. ^{13}C NMR (150 MHz, CD_3OD) spectrum of the new compound 1

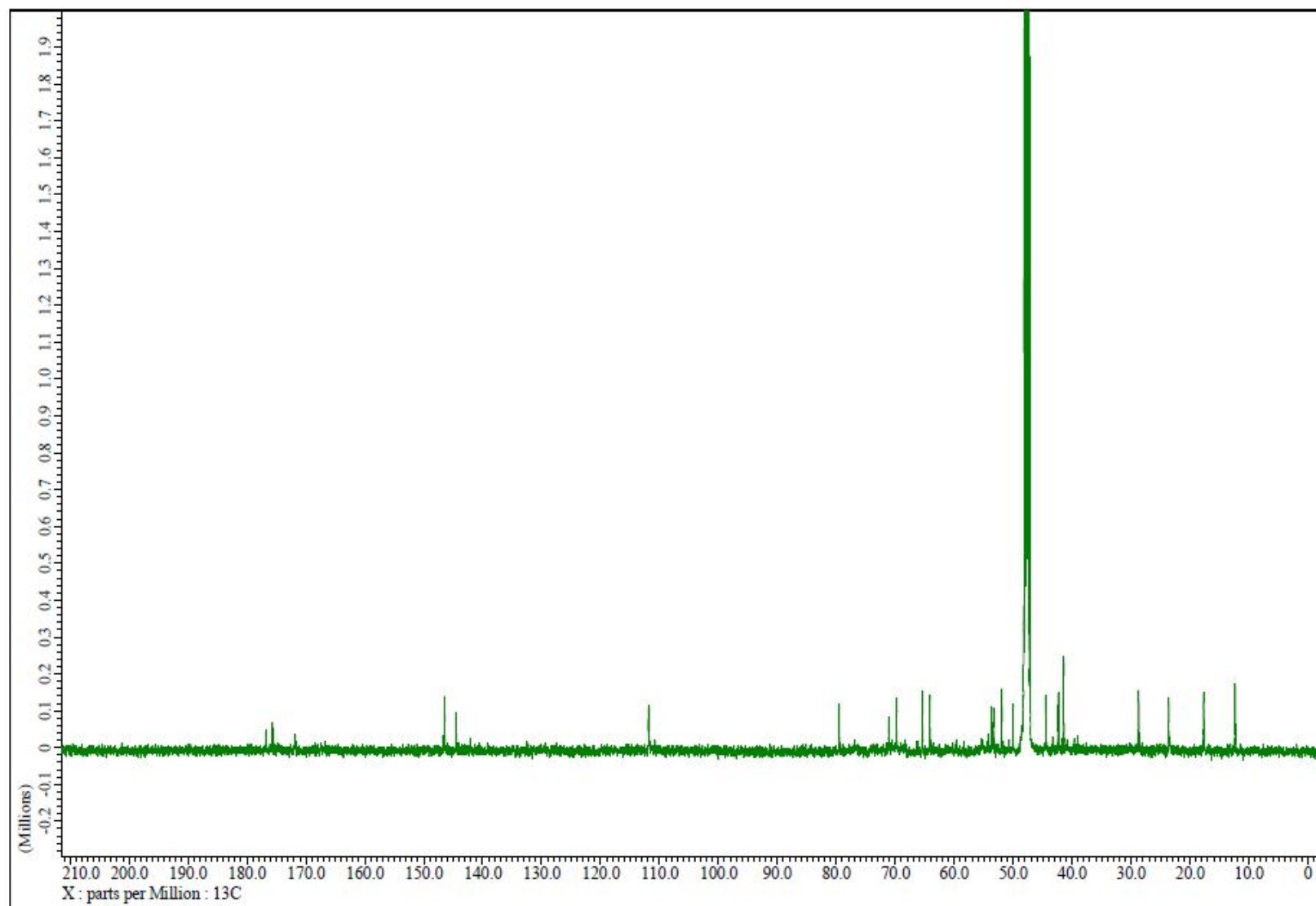


Figure S3. ^1H - ^1H COSY NMR (600 MHz, CD_3OD) spectrum of the new compound 1

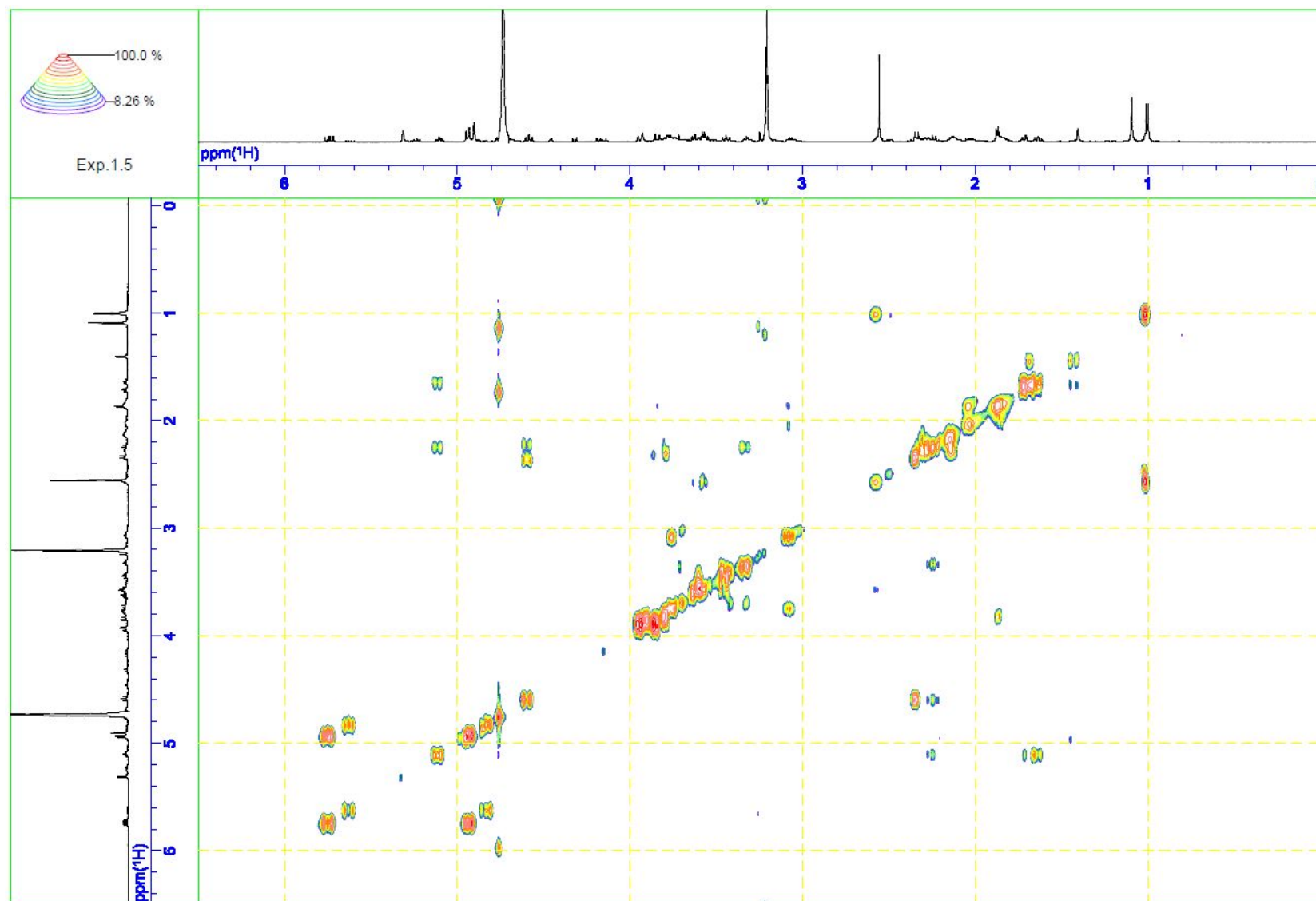


Figure S4. HMQC NMR (600 MHz, CD₃OD) spectrum of the new compound 1

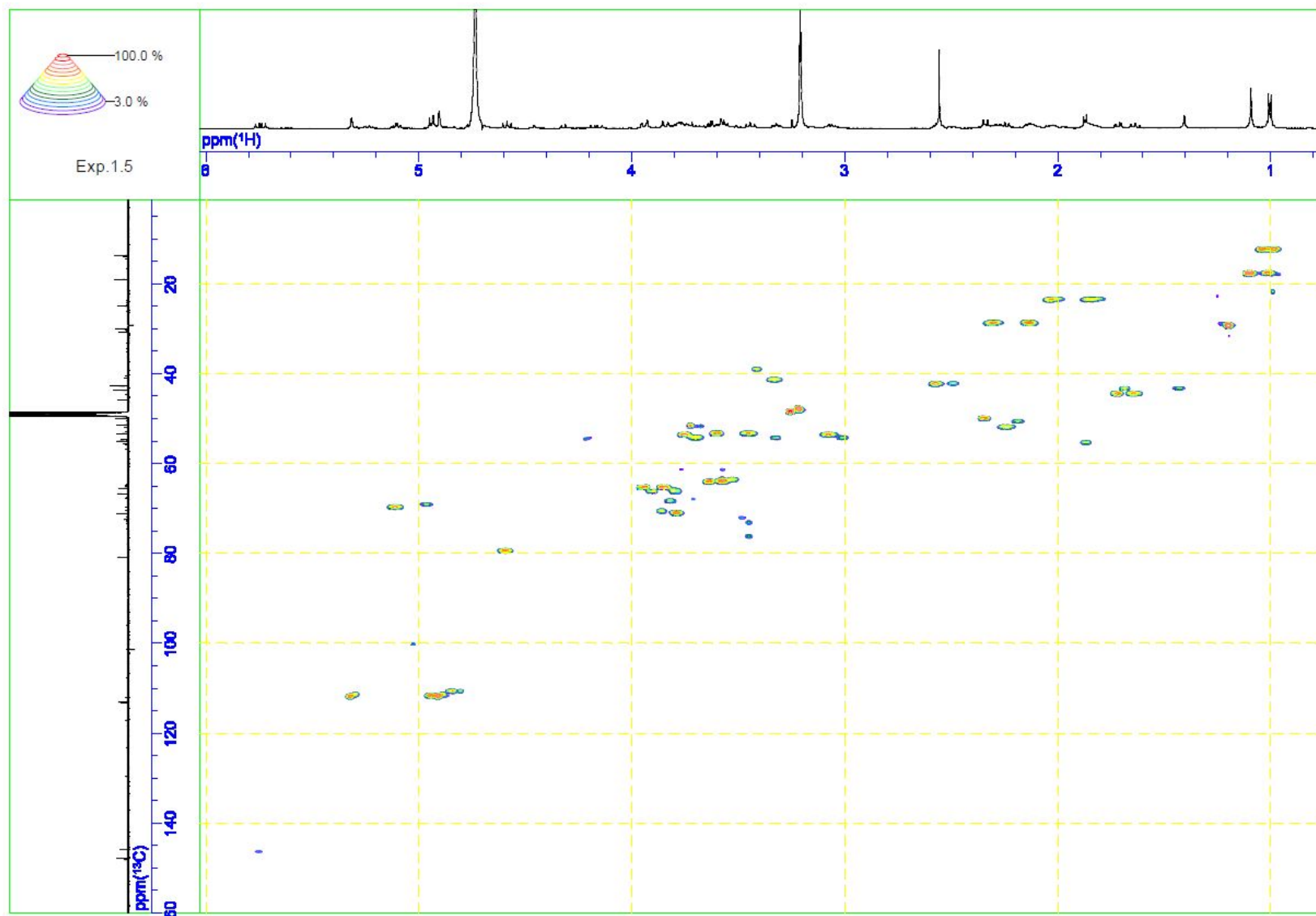


Figure S5. HMBC NMR (600 MHz, CD₃OD) spectrum of the new compound 1

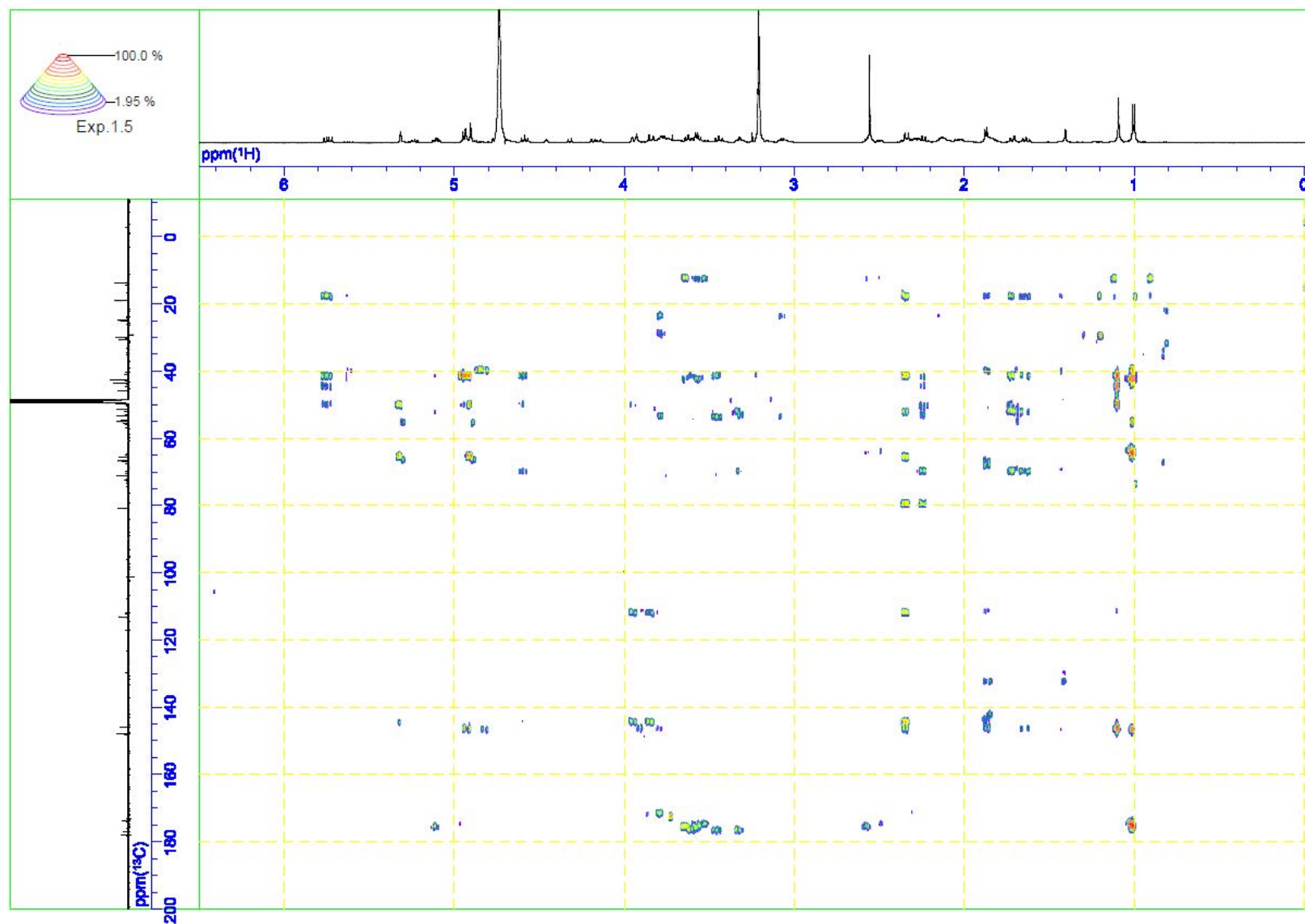


Figure S6. HRESIMS spectrum of the new compound 1

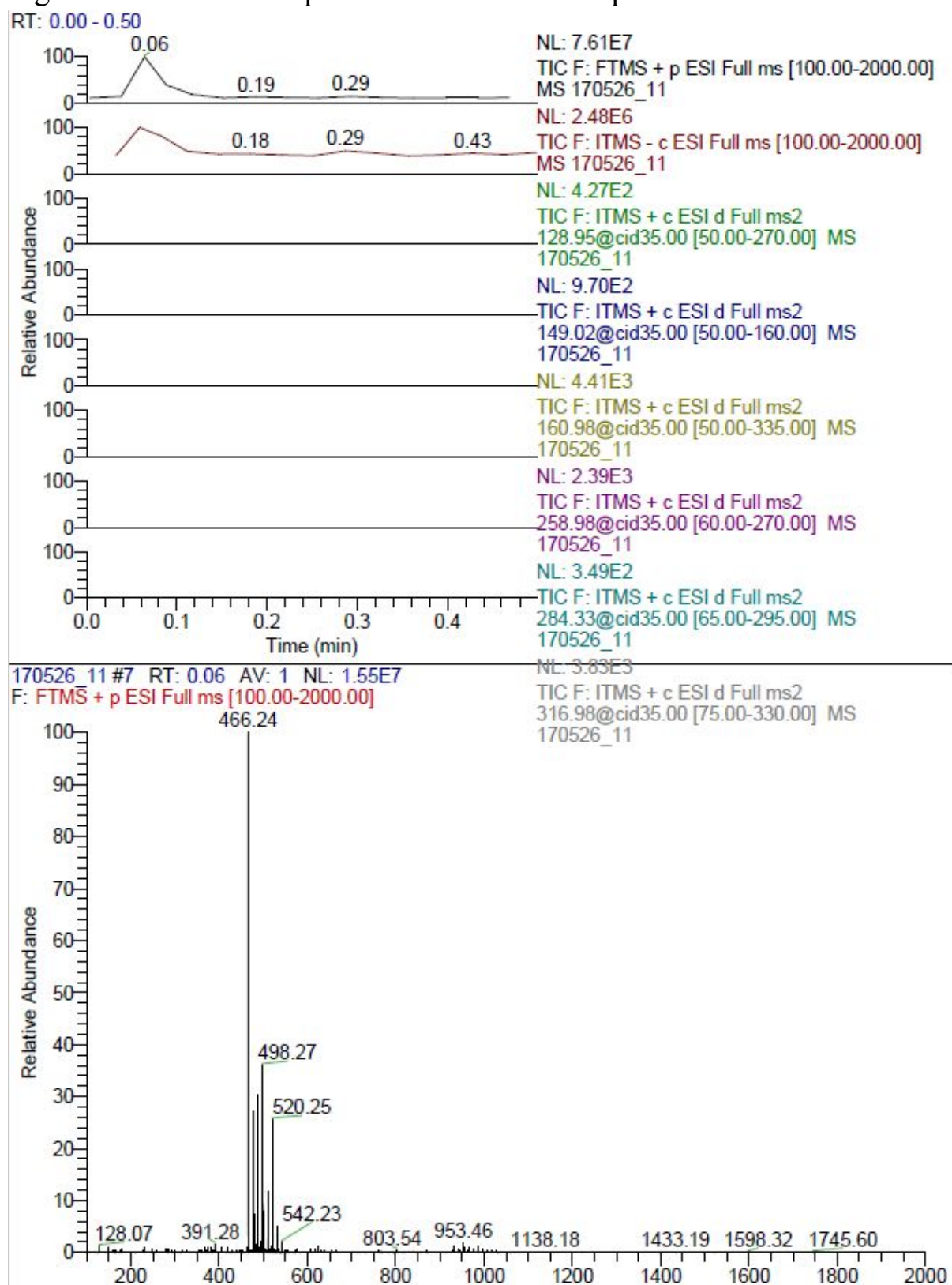


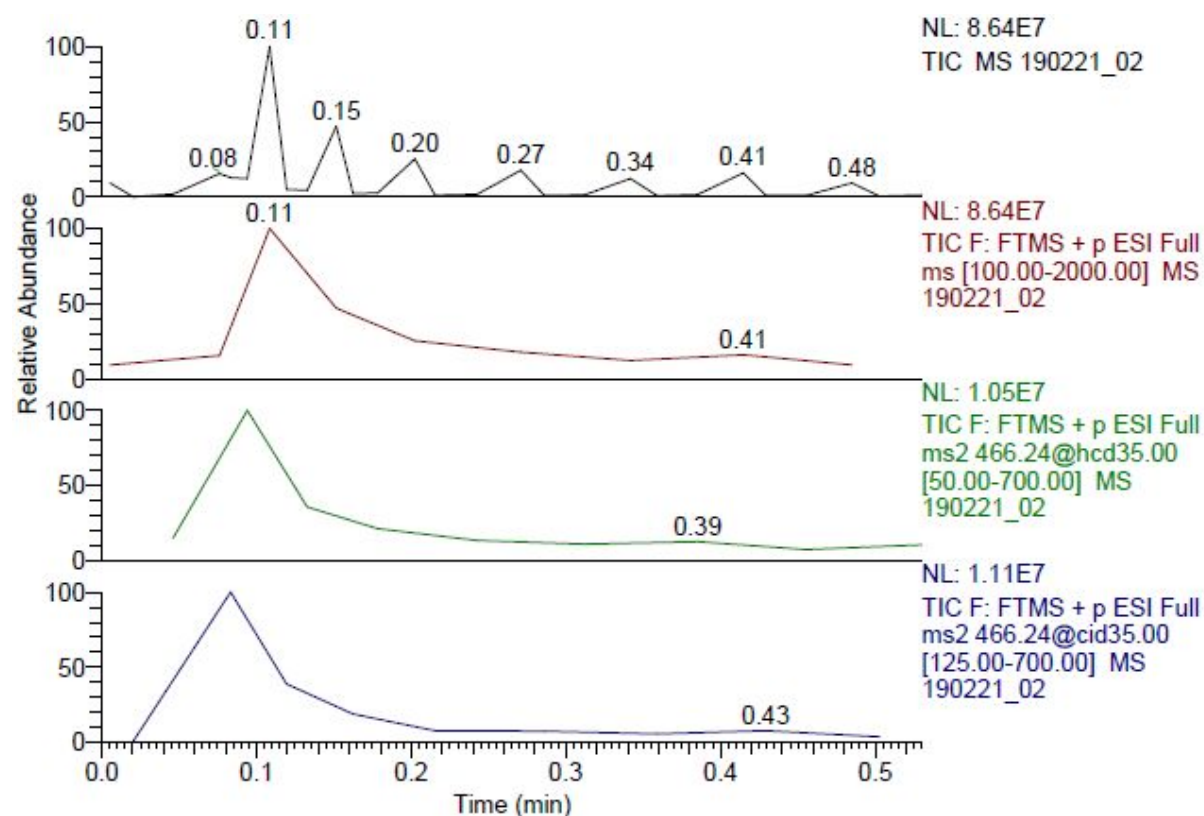
Figure S7. HRESIMS data of the new compound 1

Elemental composition search on mass 466.24

m/z= 461.24-471.24

m/z	Theo. Mass	Delta (ppm)	RDB equiv.	Composition
466.2436	466.2435	0.10	7.5	C ₂₄ H ₃₆ O ₈ N
	466.2411	5.26	4.5	C ₂₂ H ₃₇ O ₈ NNa
	466.2409	5.85	3.0	C ₂₁ H ₃₈ O ₁₁
	466.2478	-9.12	13.0	C ₃₀ H ₃₅ O ₃ Na
	466.2385	11.01	0.0	C ₁₉ H ₃₉ O ₁₁ Na
	466.2353	17.86	13.5	C ₂₉ H ₃₃ O ₃ NNa
	466.2350	18.44	12.0	C ₂₈ H ₃₄ O ₆
	466.2537	-21.71	4.0	C ₂₃ H ₃₉ O ₈ Na
	466.2326	23.60	9.0	C ₂₆ H ₃₅ O ₆ Na
	466.2561	-26.87	7.0	C ₂₅ H ₃₈ O ₈

Figure S8. ESIMS (in-source fragmentation) spectrum of compound 1



190221_02 #3-8 RT: 0.05-0.09 AV: 2 NL: 2.05E6
 ∴ FTMS + p ESI Full ms2 466.24@hcd35.00 [50.00-700.00]

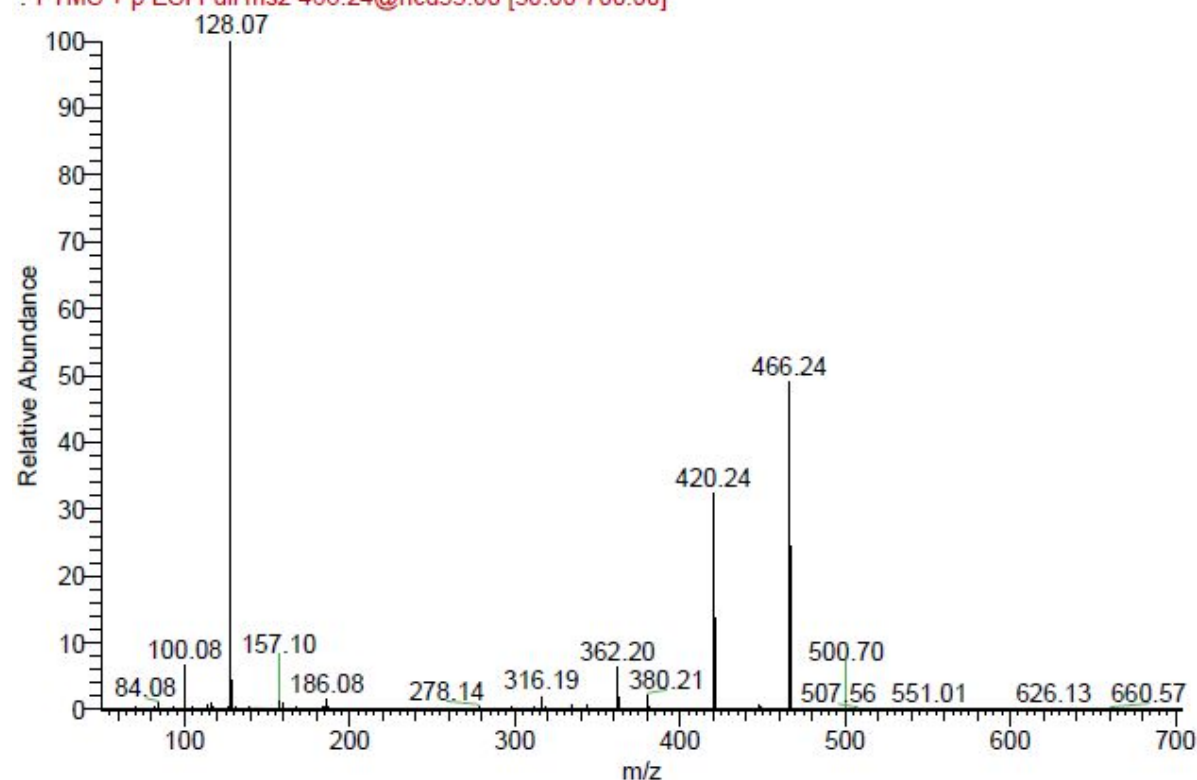


Figure S9. ^1H NMR (600 MHz, CD_3OD) spectrum of the new compound 2

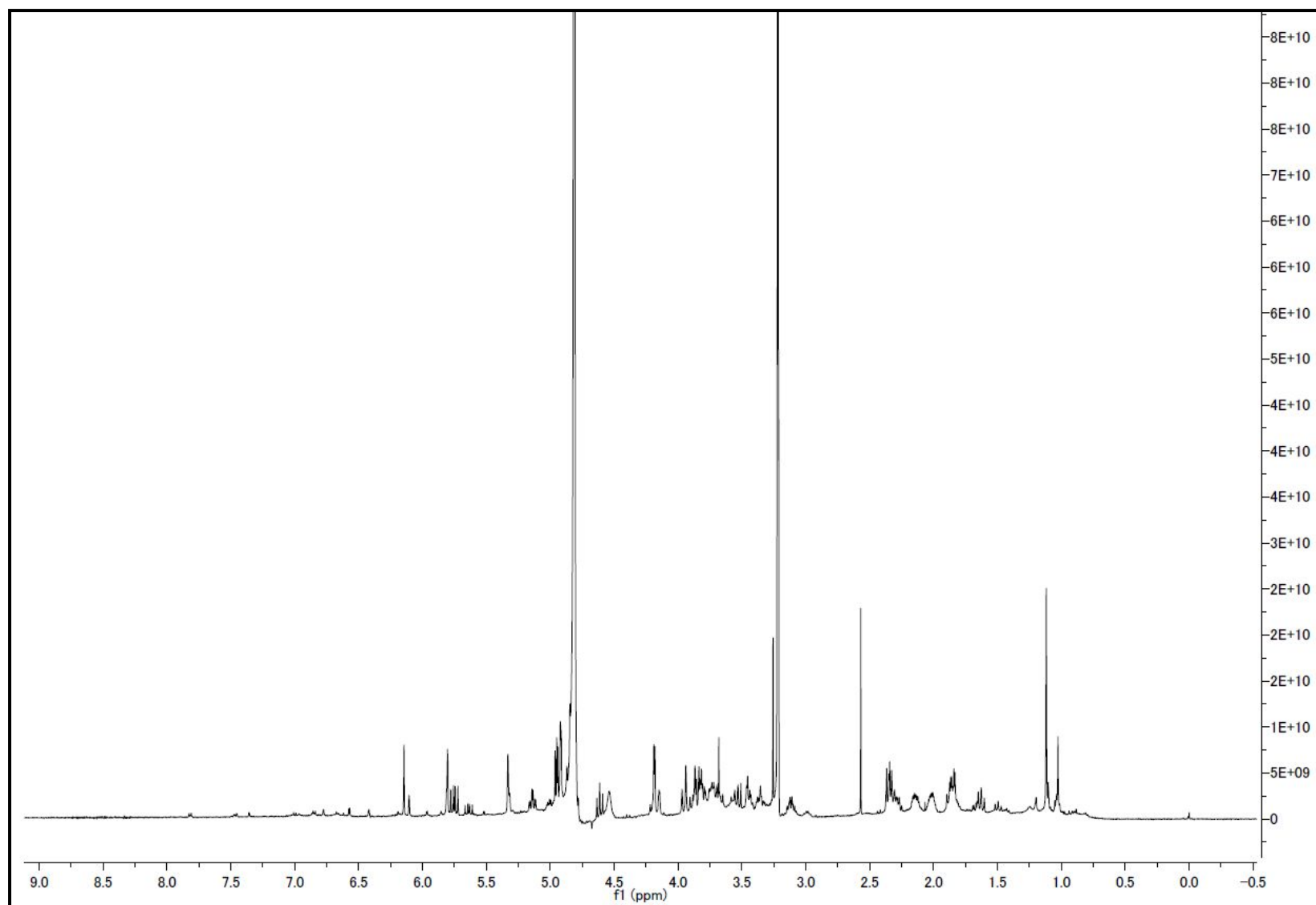


Figure S10. ^{13}C NMR (150 MHz, CD_3OD) spectrum of the new compound 2

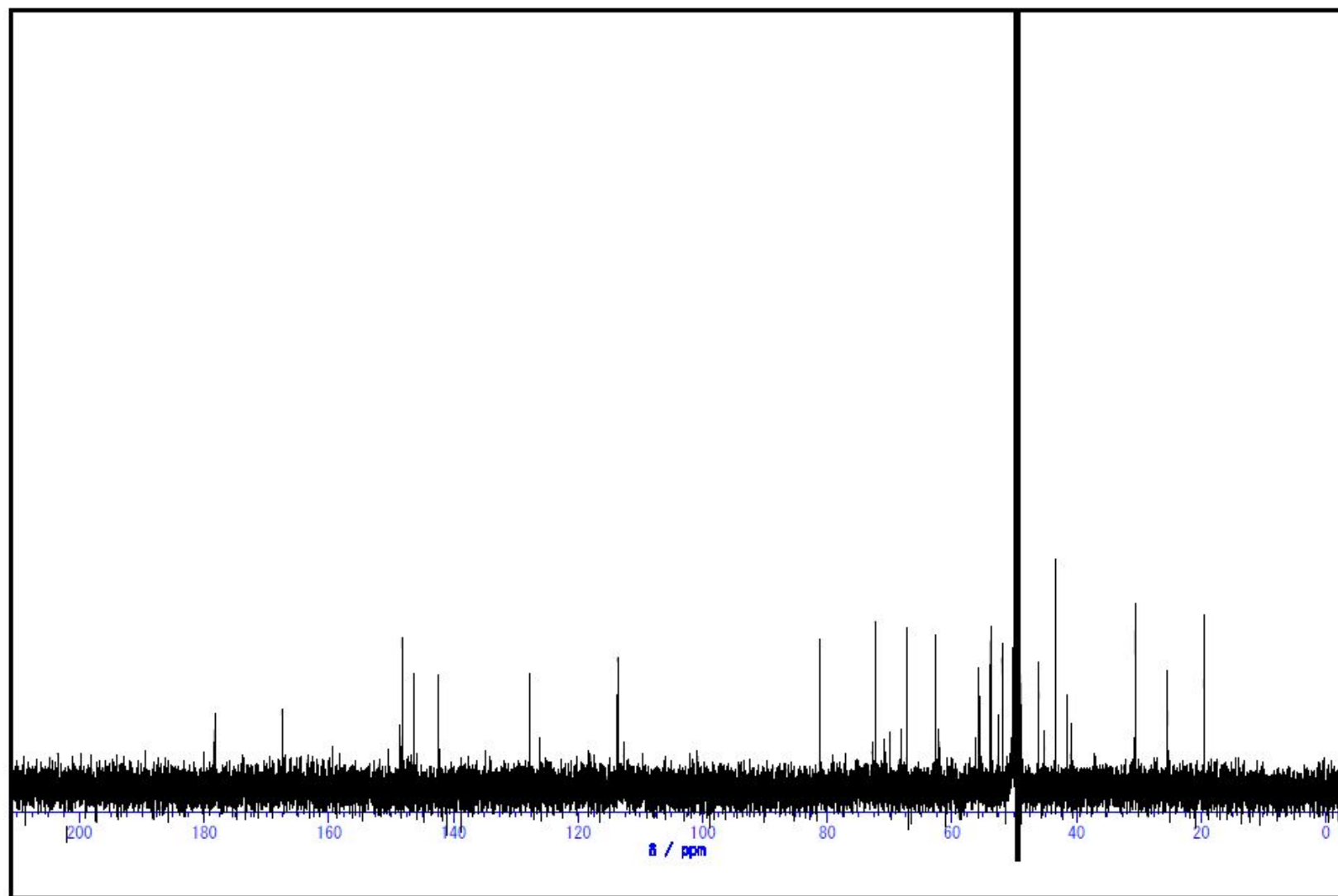


Figure S11. ^1H - ^1H COSY NMR (600 MHz, CD_3OD) spectrum of the new compound 2

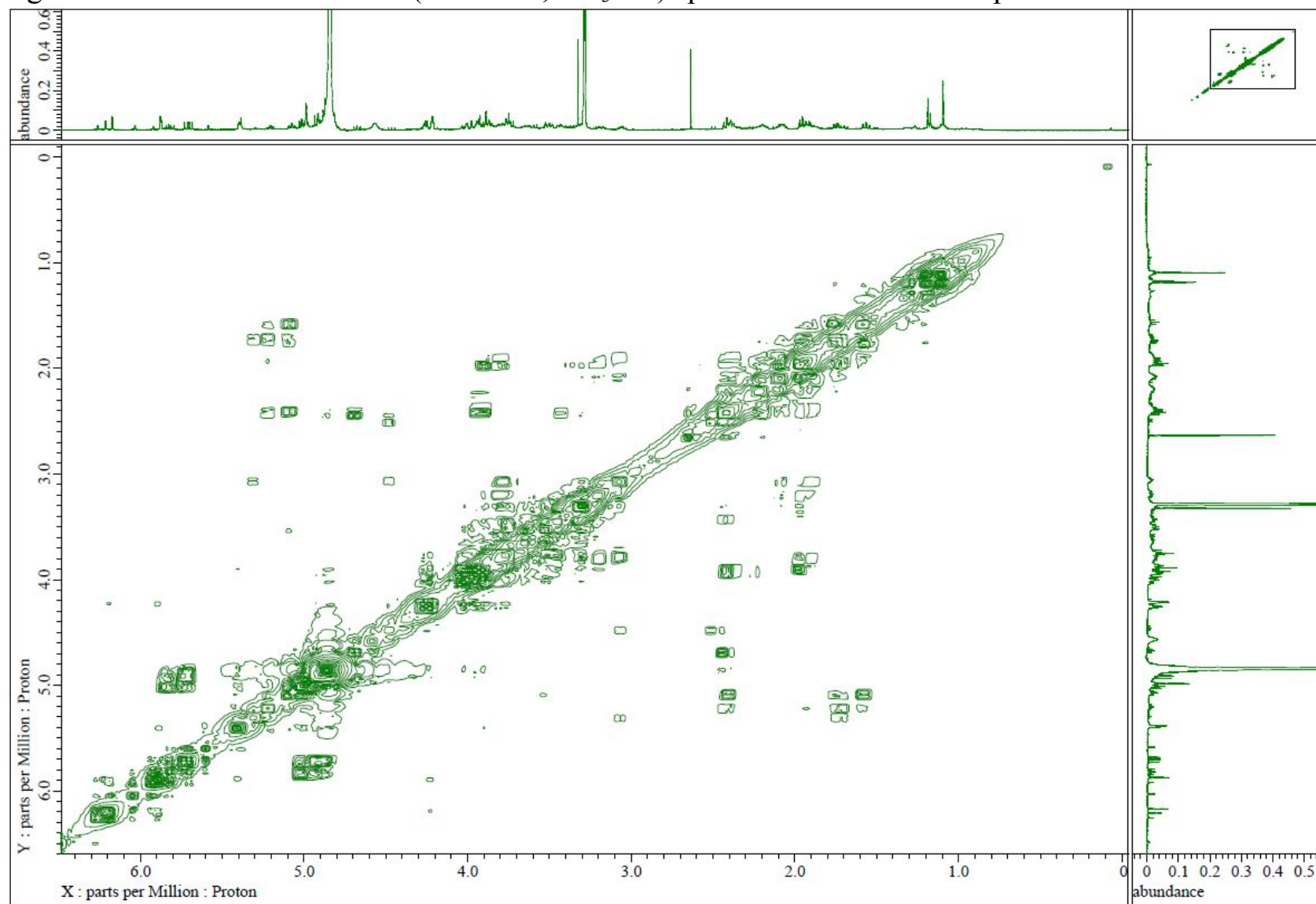


Figure S12. HMQC NMR (600 MHz, CD₃OD) spectrum of the new compound 2

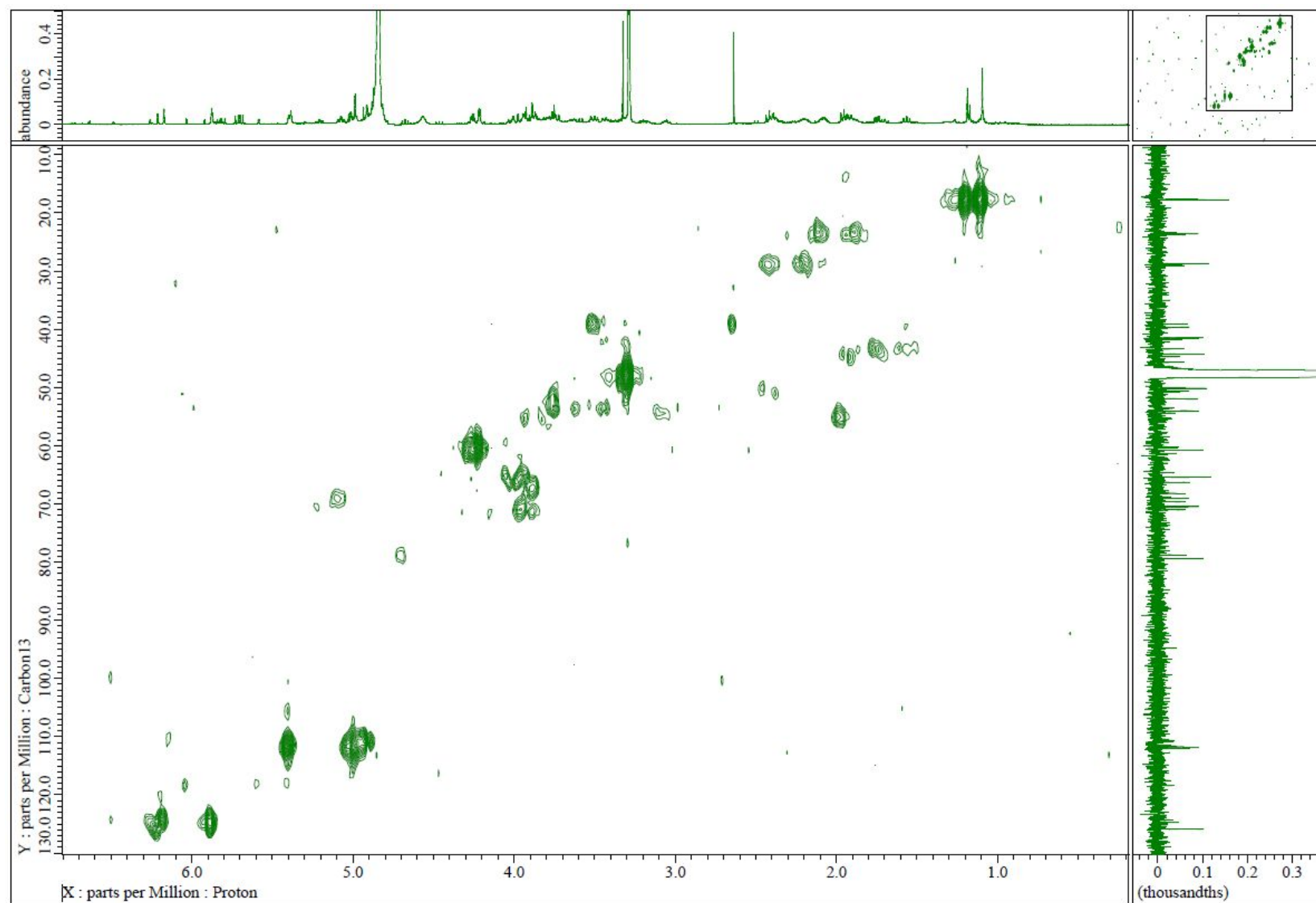


Figure S13. HMBC NMR (600 MHz, CD₃OD) spectrum of the new compound 2

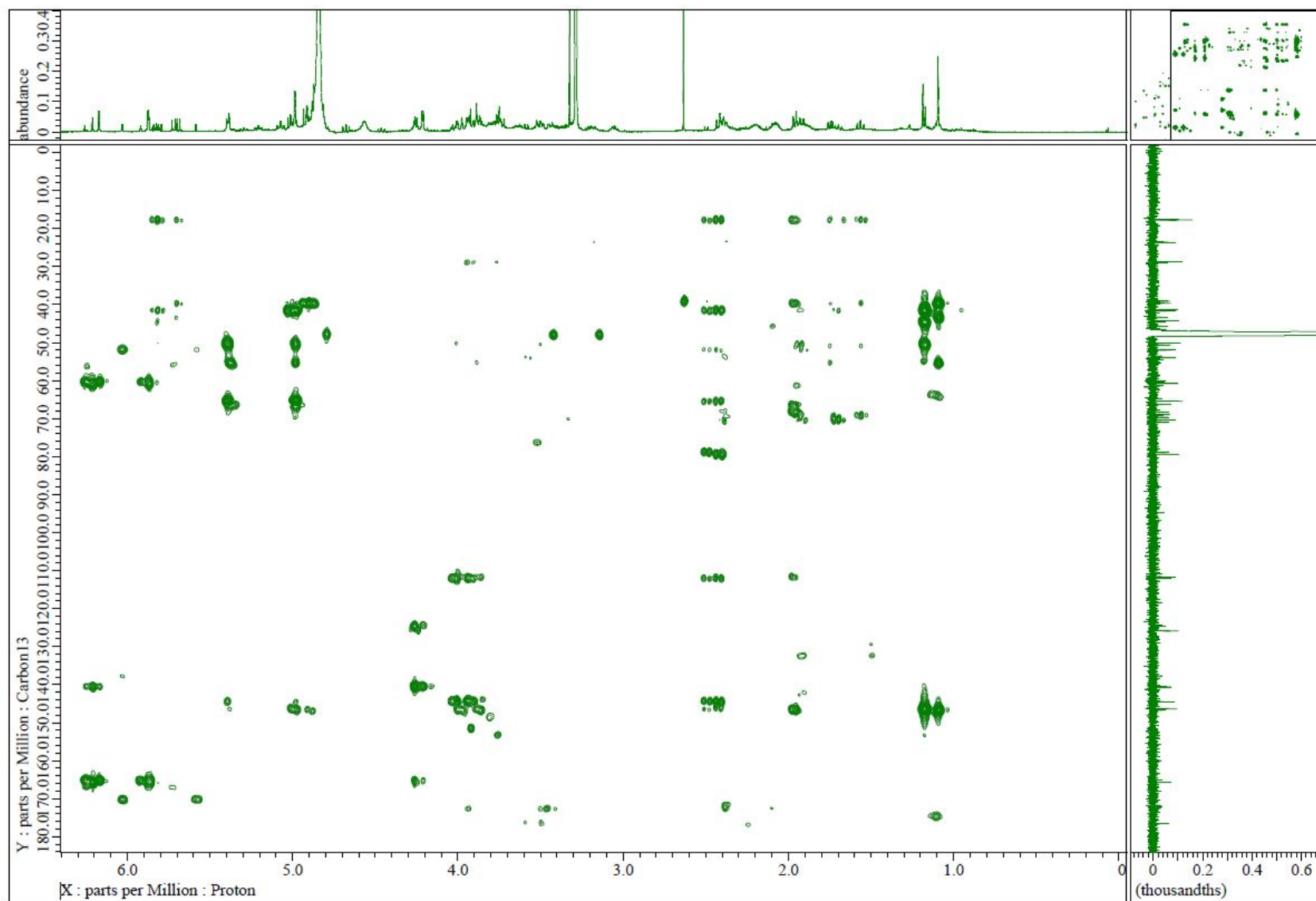


Figure S14. HRESIMS spectrum of the new compound 2

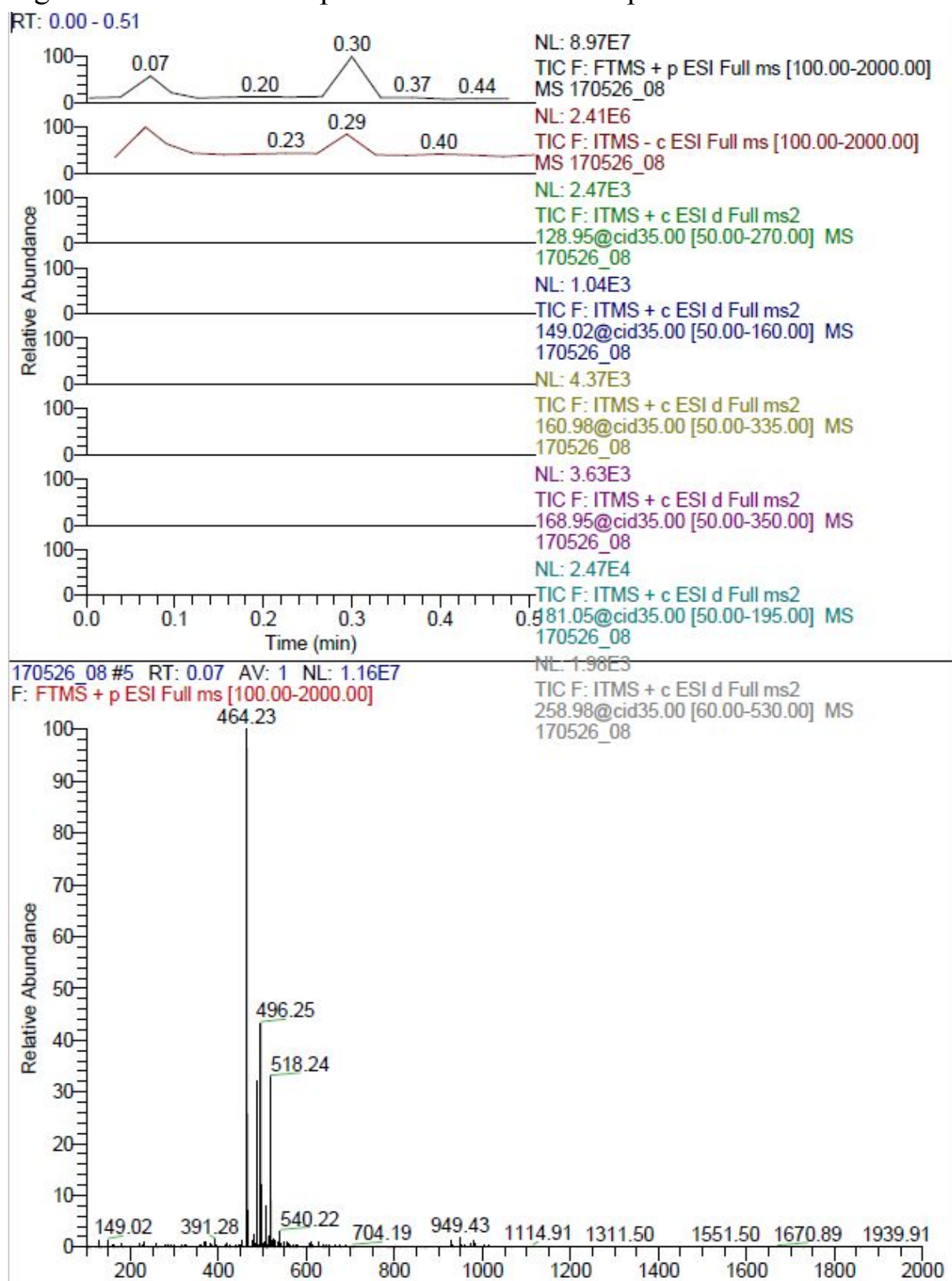


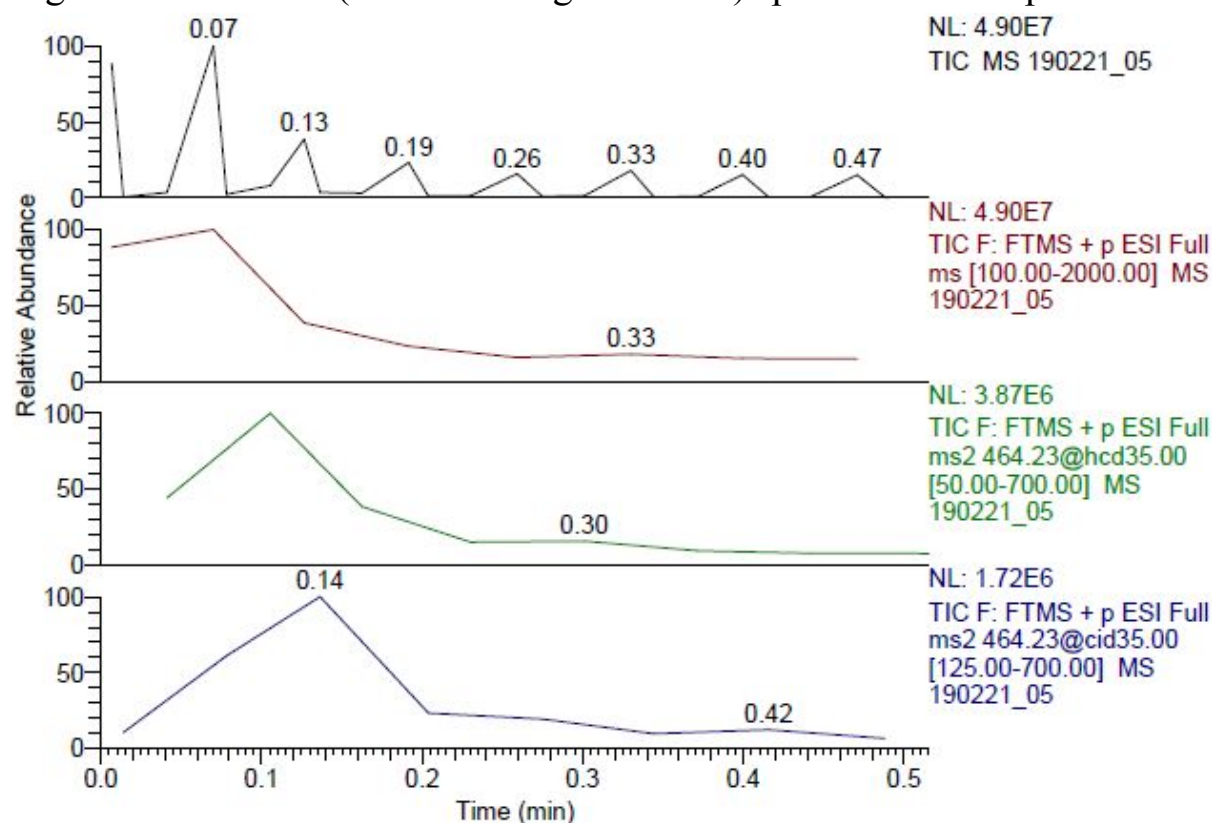
Figure S15. HRESIMS data of the new compound 2

Elemental composition search on mass 464.23

m/z= 459.23-469.23

m/z	Theo. Mass	Delta (ppm)	RDB equiv.	Composition
464.2280	464.2279	0.16	8.5	C ₂₄ H ₃₄ O ₈ N
	464.2255	5.35	5.5	C ₂₂ H ₃₅ O ₈ NNa
	464.2252	5.94	4.0	C ₂₁ H ₃₆ O ₁₁
	464.2322	-9.09	14.0	C ₃₀ H ₃₃ O ₃ Na
	464.2228	11.12	1.0	C ₁₉ H ₃₇ O ₁₁ Na
	464.2338	-12.49	-0.5	C ₁₇ H ₃₈ O ₁₃ N
	464.2196	18.00	14.5	C ₂₉ H ₃₁ O ₃ NNa
	464.2193	18.59	13.0	C ₂₈ H ₃₂ O ₆
	464.2381	-21.74	5.0	C ₂₃ H ₃₇ O ₈ Na
	464.2169	23.77	10.0	C ₂₆ H ₃₃ O ₆ Na

Figure S16. ESIMS (in-source fragmentation) spectrum of compound 2



90221_05 #6 RT: 0.11 AV: 1 NL: 1.55E6
FTMS + p ESI Full ms2 464.23@hcd35.00 [50.00-700.00]

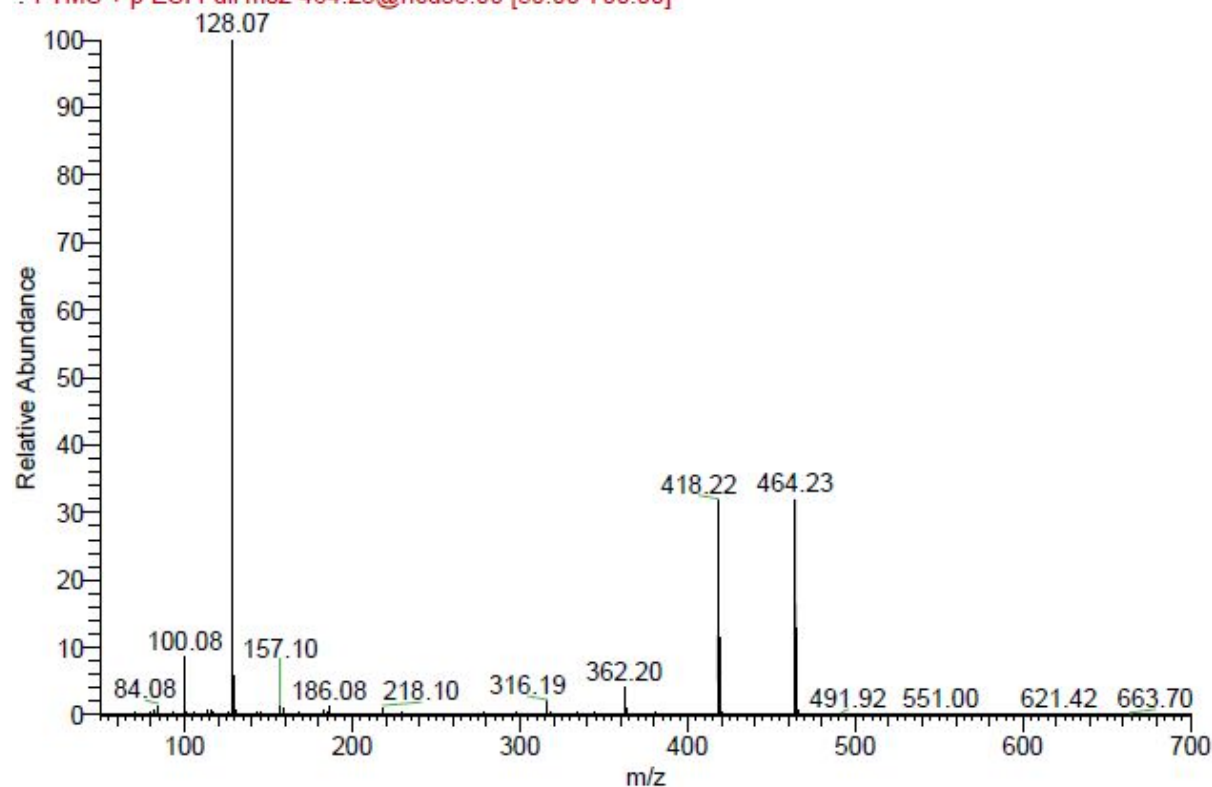


Figure S17. ^1H NMR (600 MHz, CD_3OD) spectrum of the new compound 3

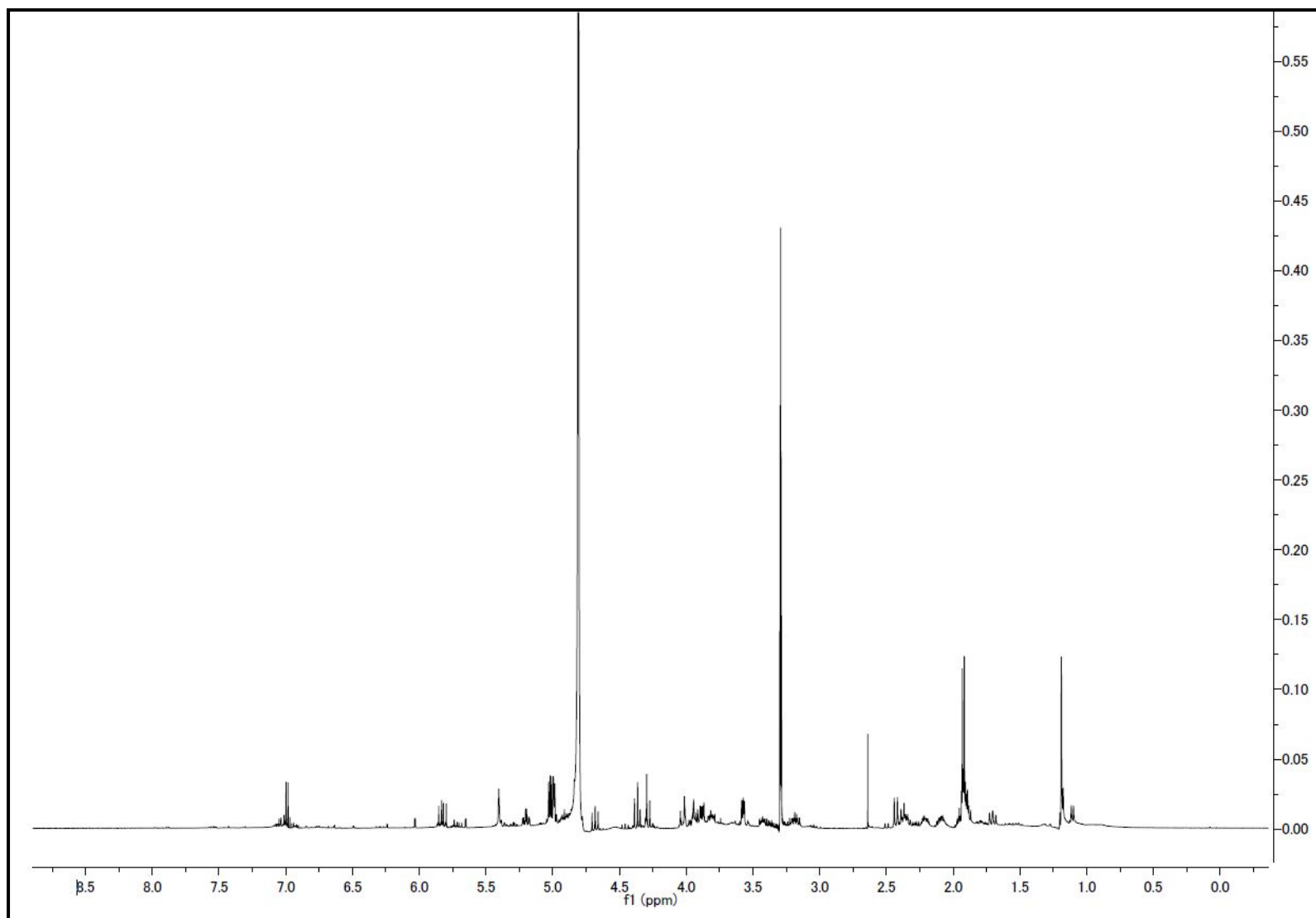


Figure S18. ^{13}C NMR (150 MHz, CD_3OD) spectrum of the new compound 3

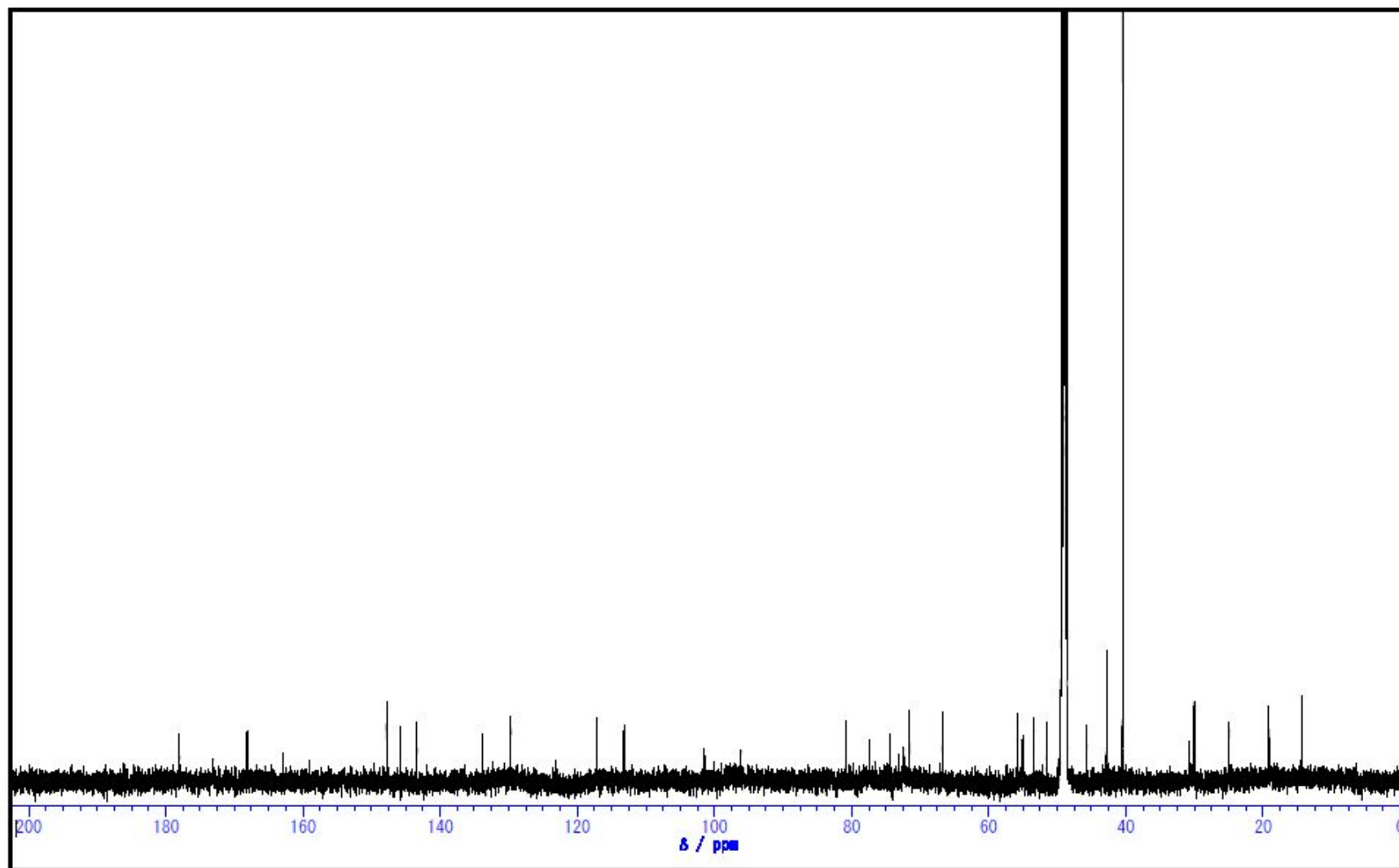


Figure S19. ^1H - ^1H COSY NMR (600 MHz, CD_3OD) spectrum of the new compound 3

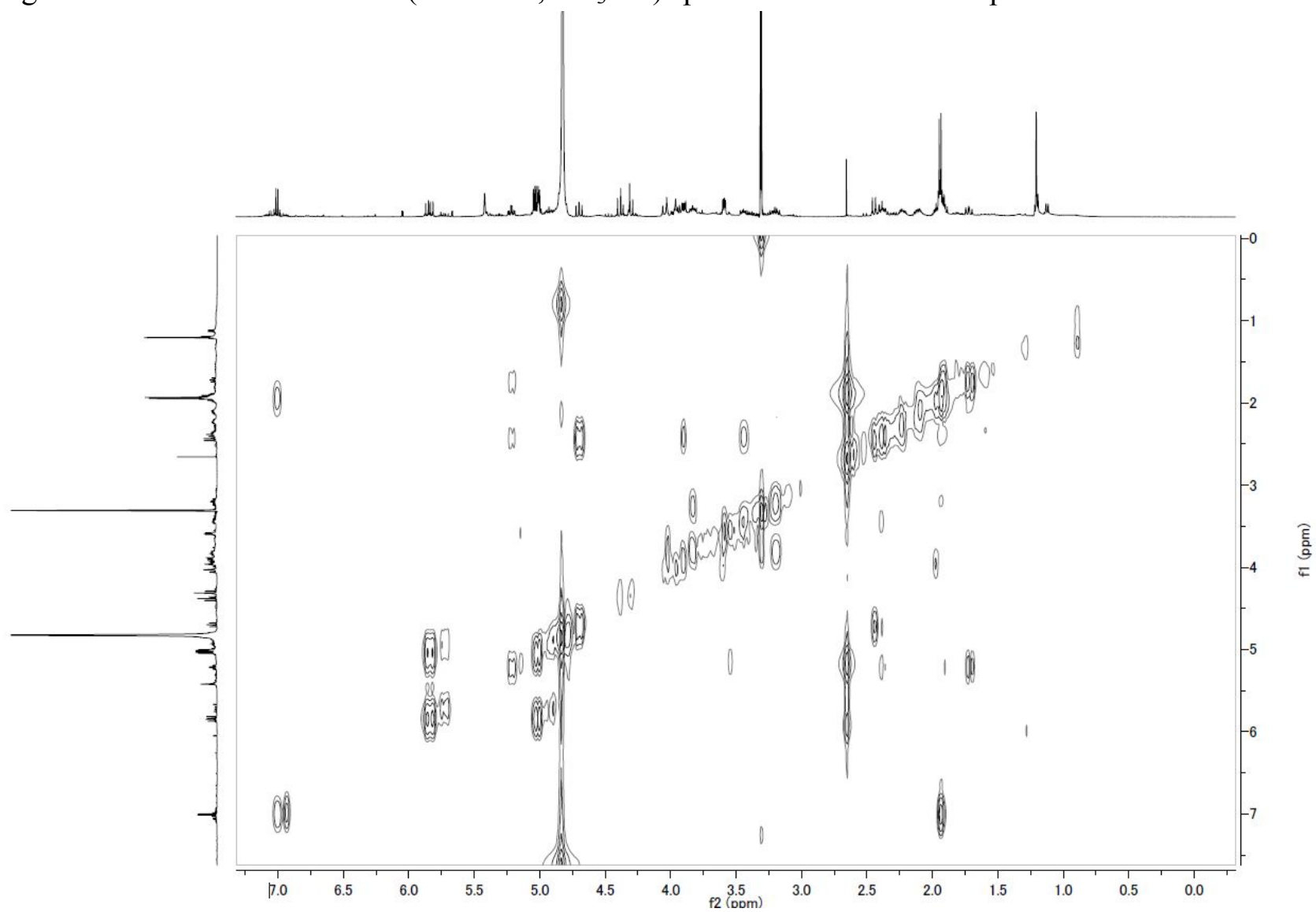


Figure S20. HMQC NMR (600 MHz, CD₃OD) spectrum of the new compound 3

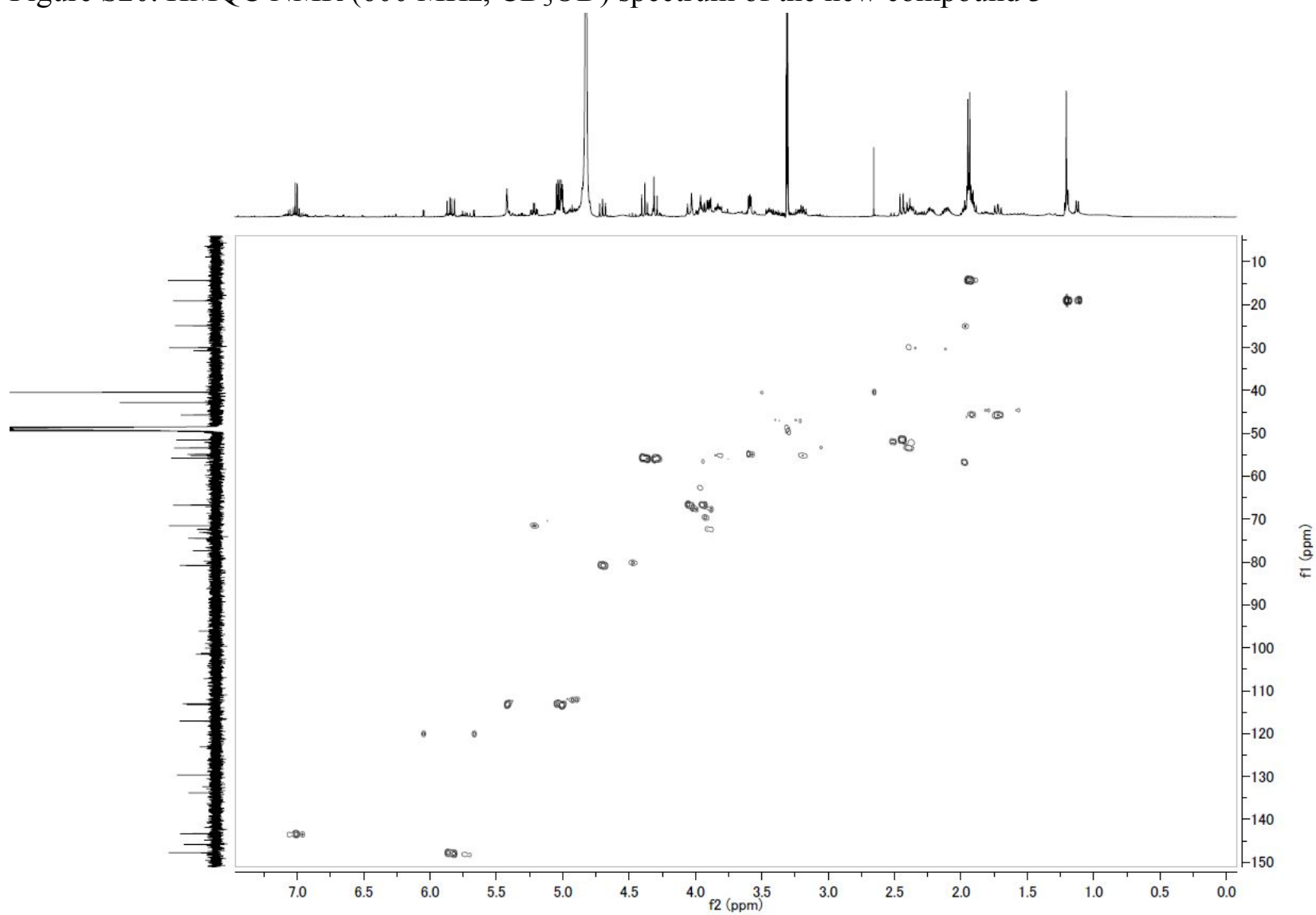


Figure S21. HMBC NMR (600 MHz, CD₃OD) spectrum of the new compound 3

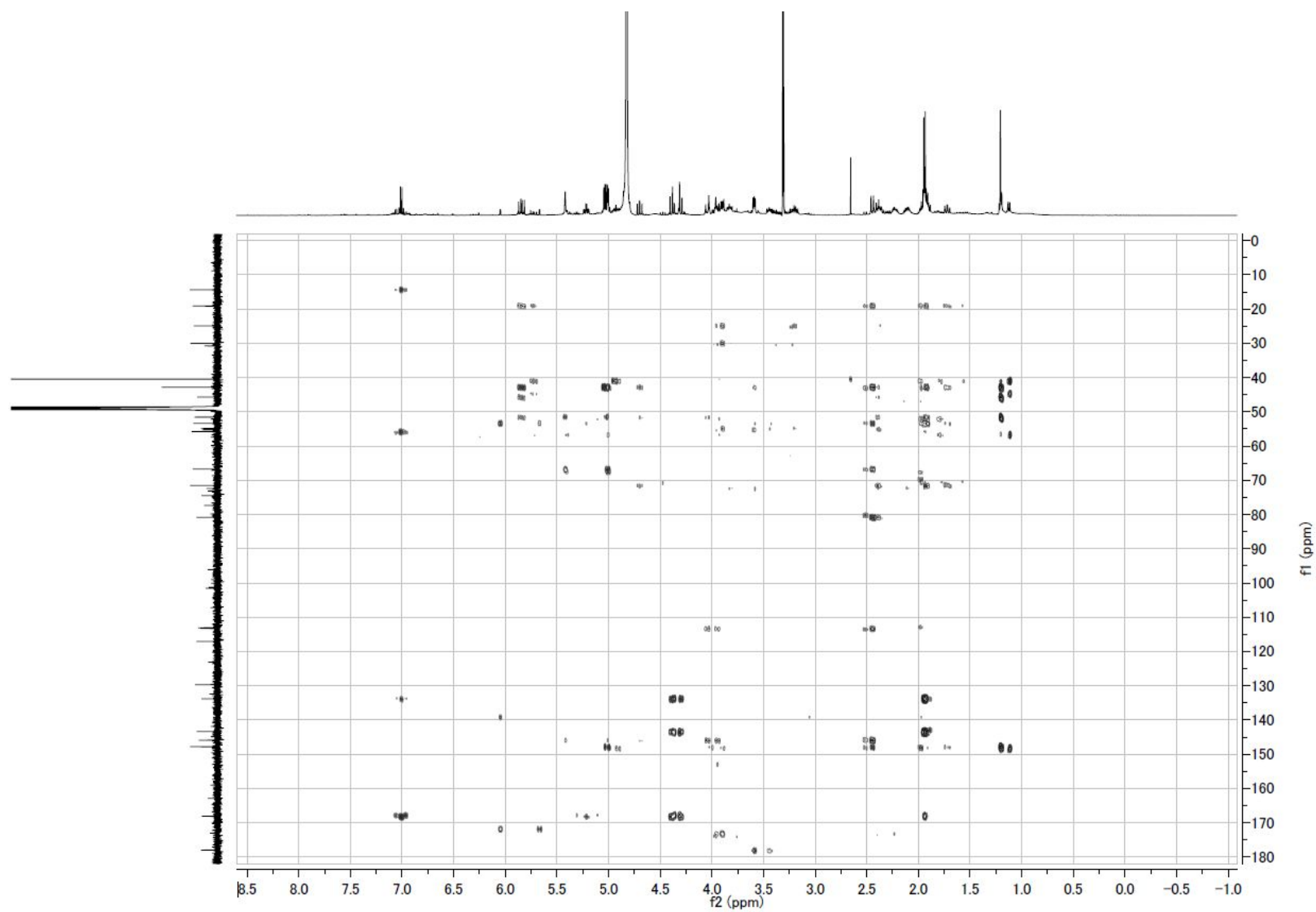


Figure S22. HRESIMS spectrum of the new compound 3

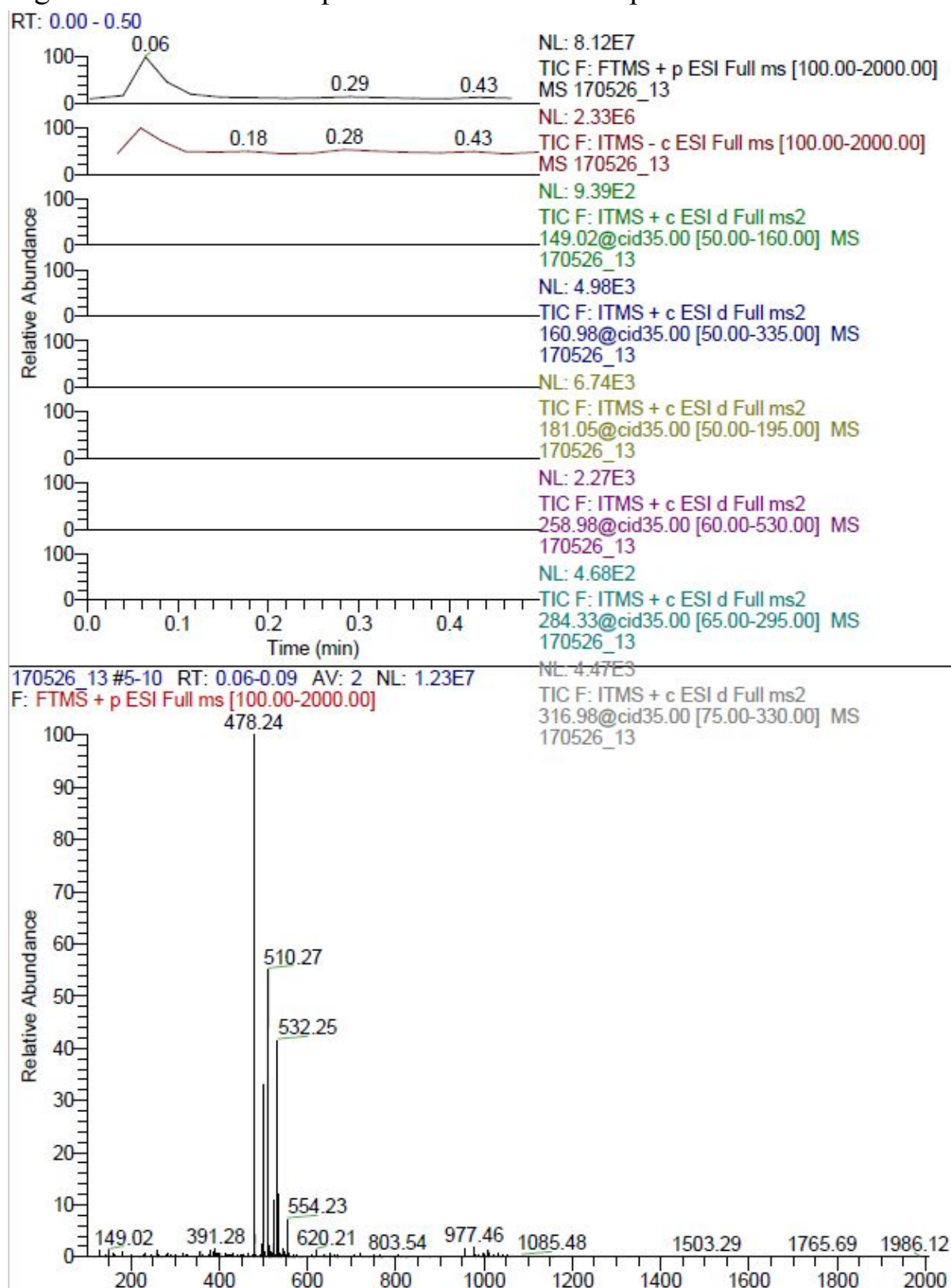


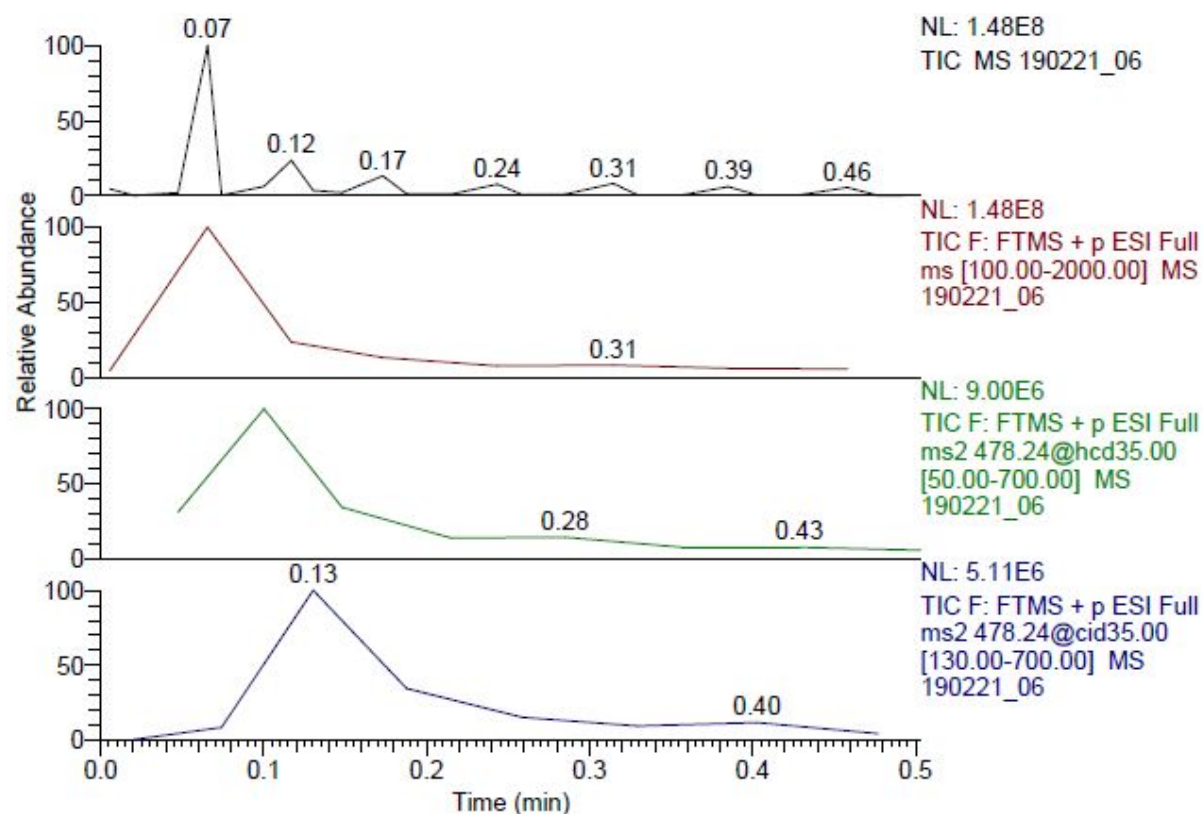
Figure S23. HRESIMS data of the new compound 3

Elemental composition search on mass 478.24

m/z= 473.24-483.24

m/z	Theo. Mass	Delta (ppm)	RDB equiv.	Composition
478.2435	478.2435	-0.07	8.5	C ₂₅ H ₃₆ O ₈ N
	478.2411	4.96	5.5	C ₂₃ H ₃₇ O ₈ NNa
	478.2409	5.53	4.0	C ₂₂ H ₃₈ O ₁₁
	478.2385	10.56	1.0	C ₂₀ H ₃₉ O ₁₁ Na
	478.2494	-12.35	-0.5	C ₁₈ H ₄₀ O ₁₃ N
	478.2353	17.24	14.5	C ₃₀ H ₃₃ O ₃ NNa
	478.2350	17.81	13.0	C ₂₉ H ₃₄ O ₆
	478.2537	-21.34	5.0	C ₂₄ H ₃₉ O ₈ Na
	478.2326	22.84	10.0	C ₂₇ H ₃₅ O ₆ Na
	478.2561	-26.37	8.0	C ₂₆ H ₃₈ O ₈

Figure S24. ESIMS (in-source fragmentation) spectrum of compound 3



190221_06 #6 RT: 0.10 AV: 1 NL: 3.58E6
F: FTMS + p ESI Full ms2 478.24@hcd35.00 [50.00-700.00]

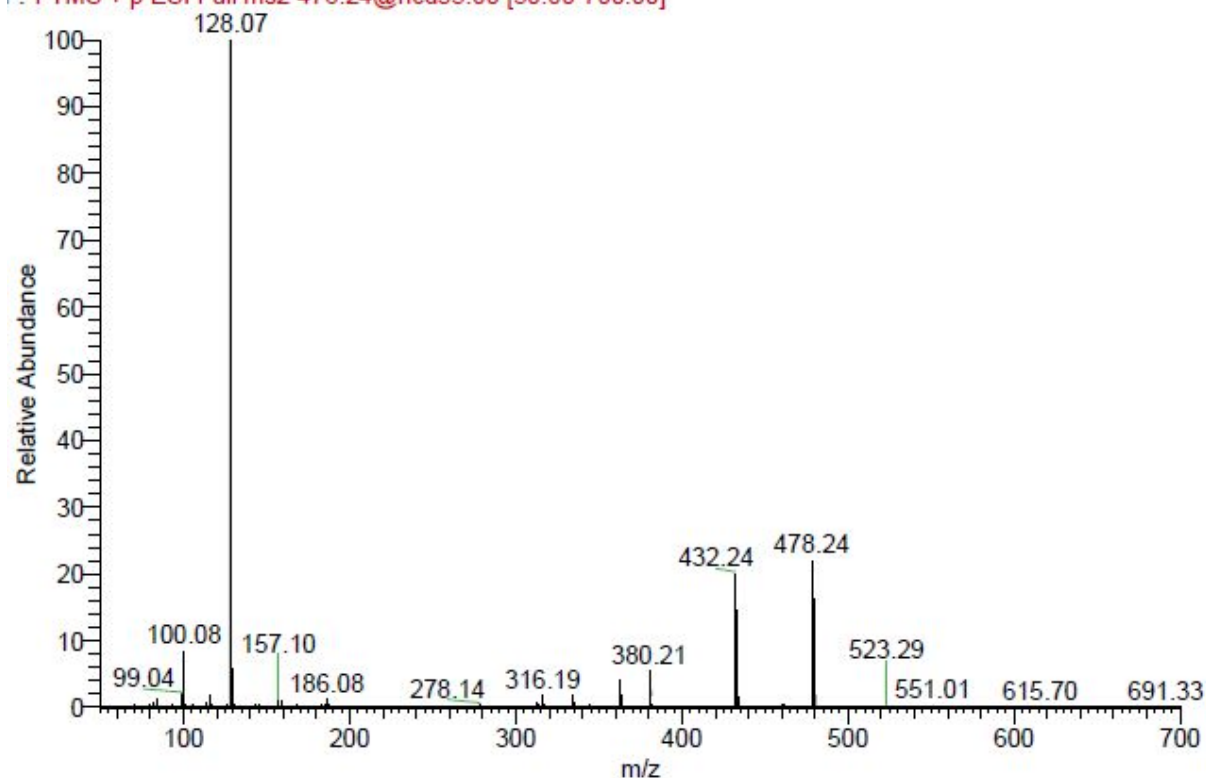


Figure S25. ^1H NMR (600 MHz, CD_3OD) spectrum of the new compound 4

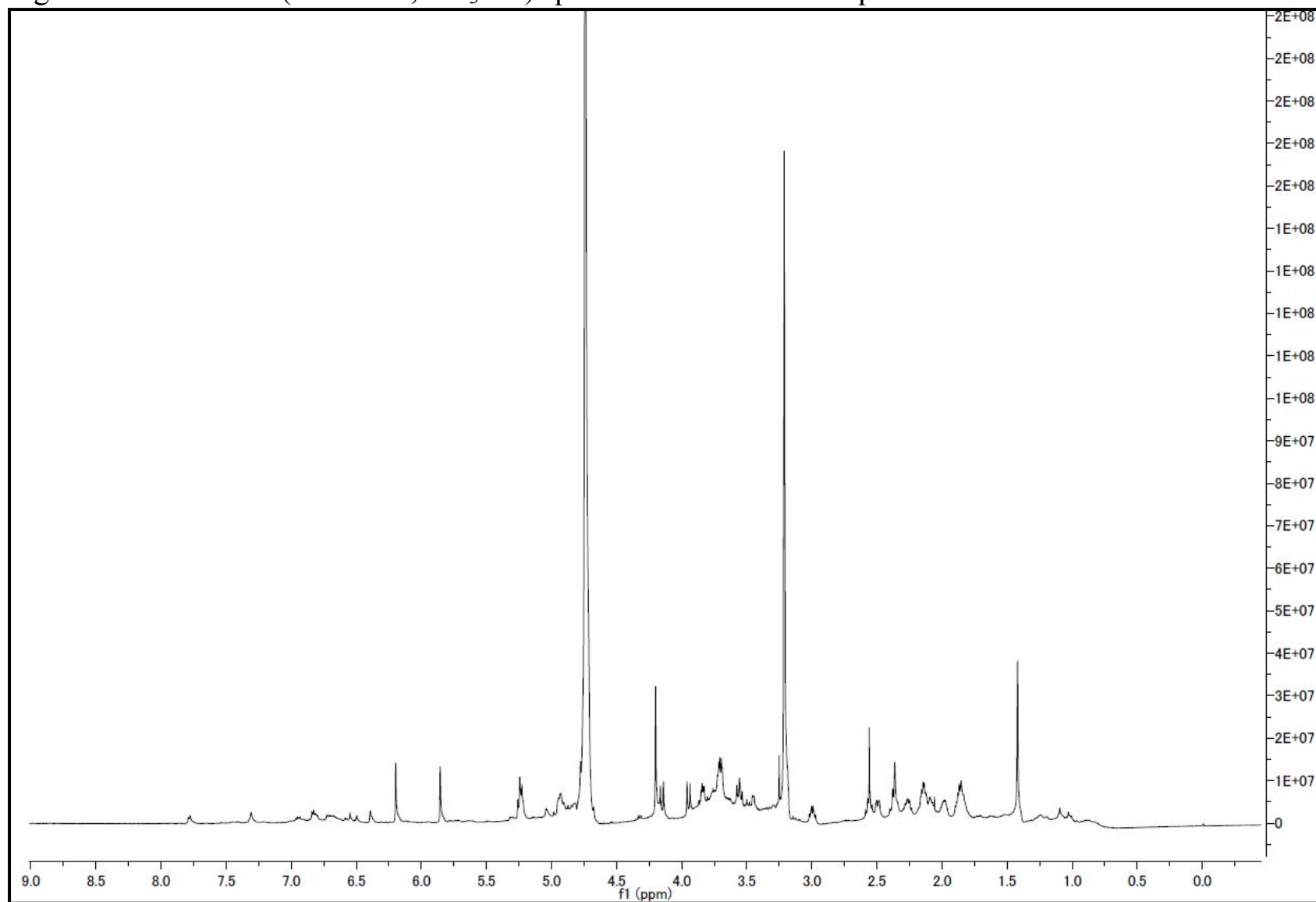


Figure S26. ^{13}C NMR (150 MHz, CD_3OD) spectrum of the new compound 4

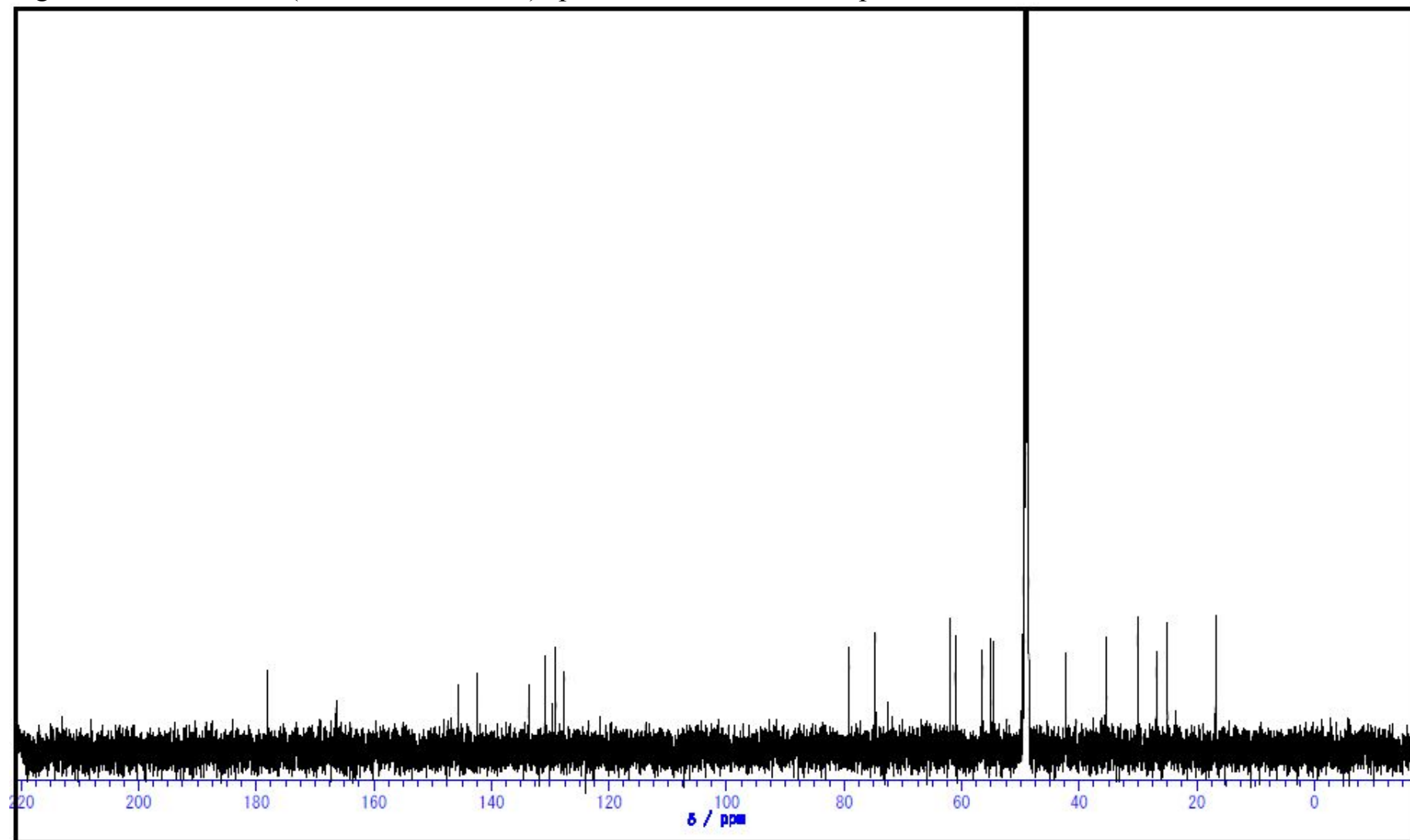


Figure S27. ^1H - ^1H COSY NMR (600 MHz, CD_3OD) spectrum of the new compound 4

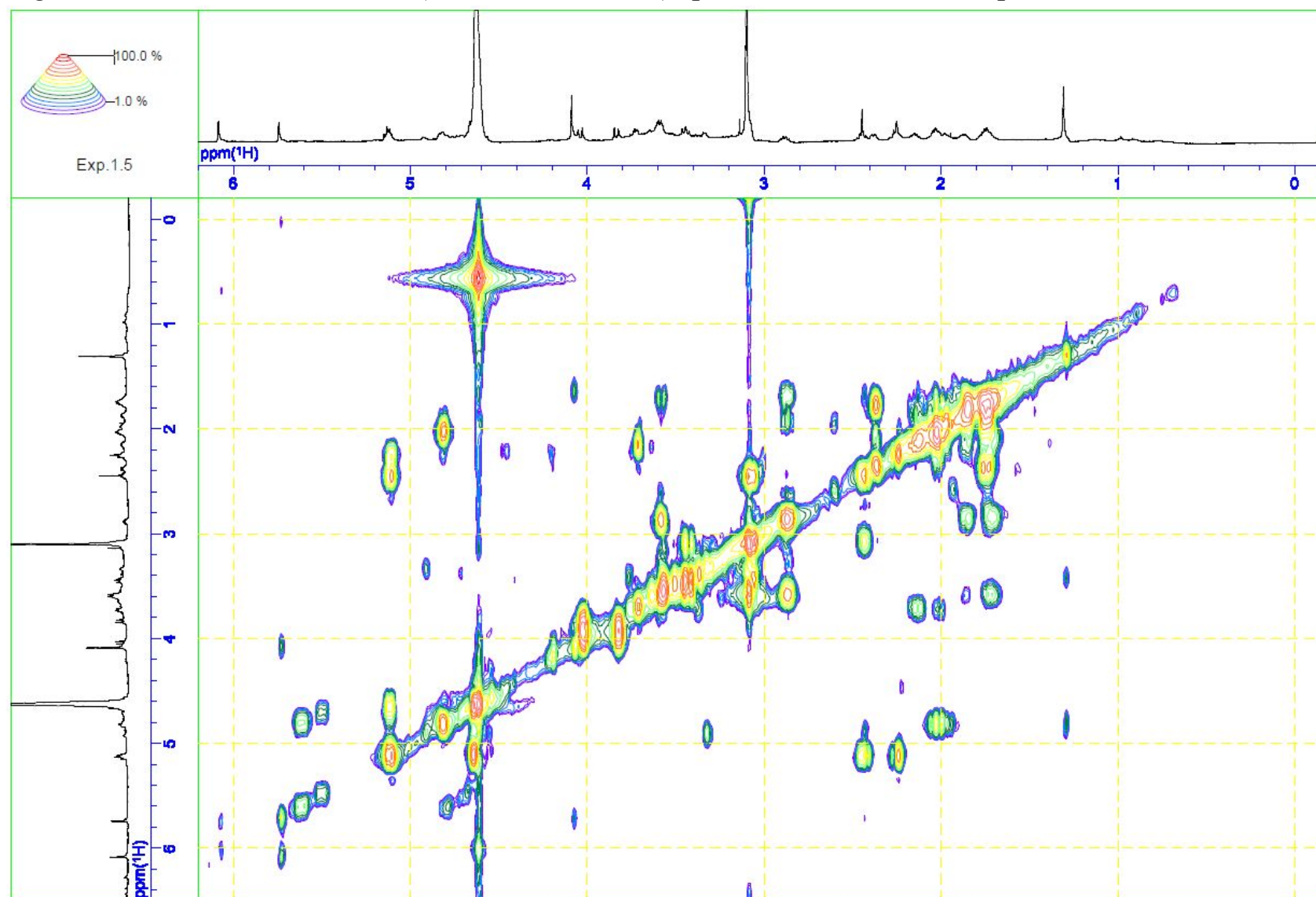


Figure S28. HMQC NMR (600 MHz, CD₃OD) spectrum of the new compound 4

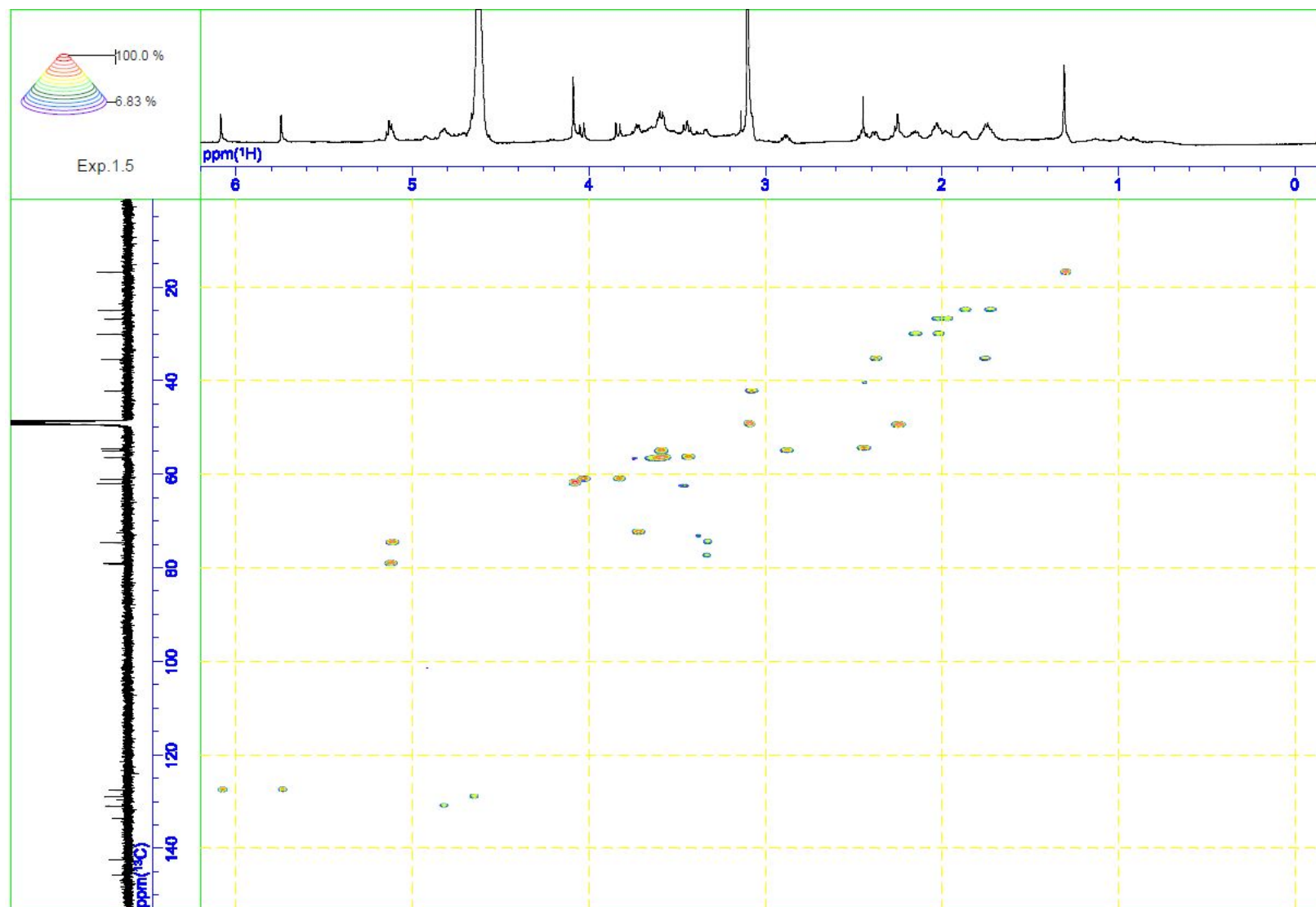


Figure S29. HMBC NMR (600 MHz, CD₃OD) spectrum of the new compound 4

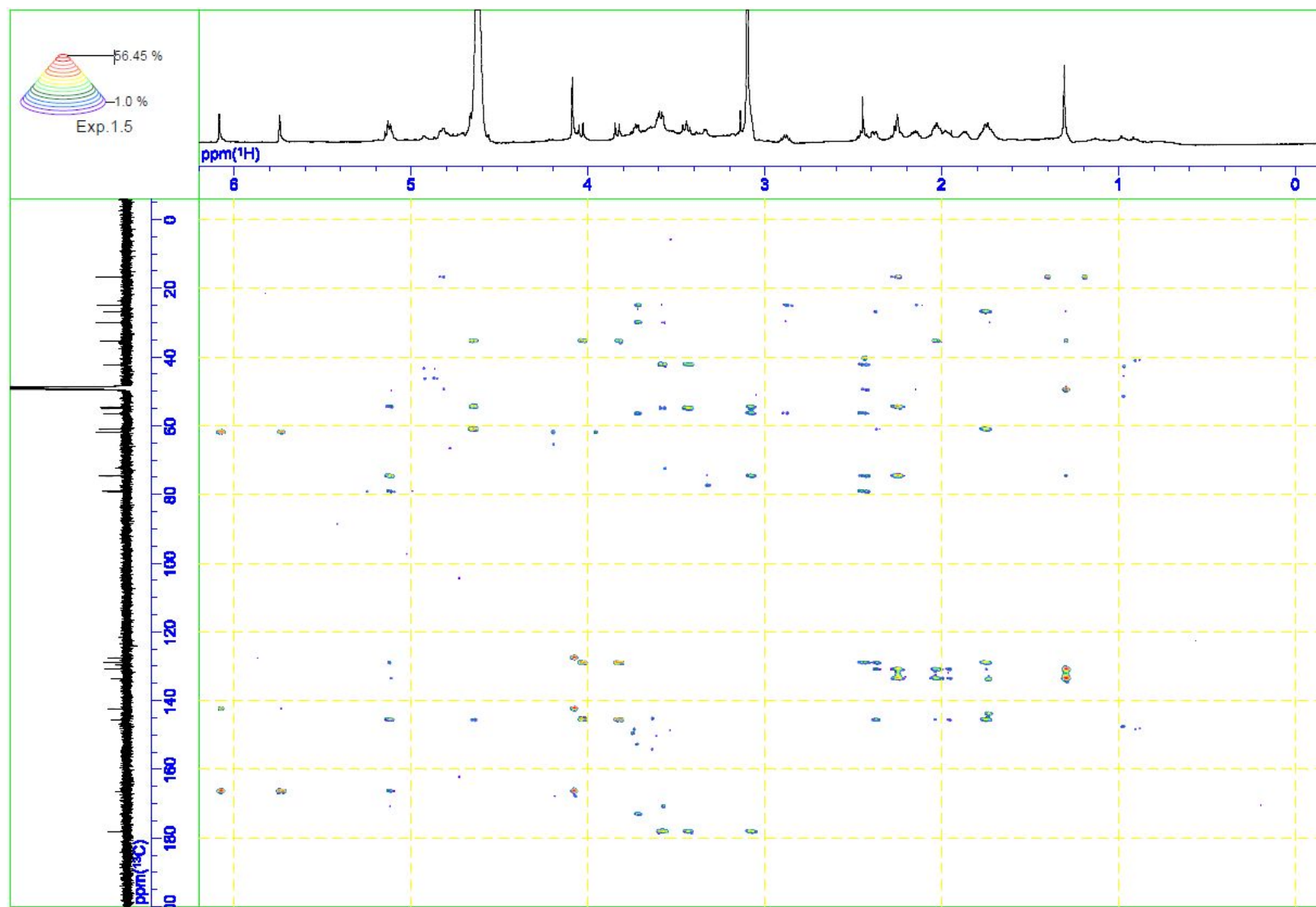


Figure S30. HRESIMS spectrum of the new compound 4

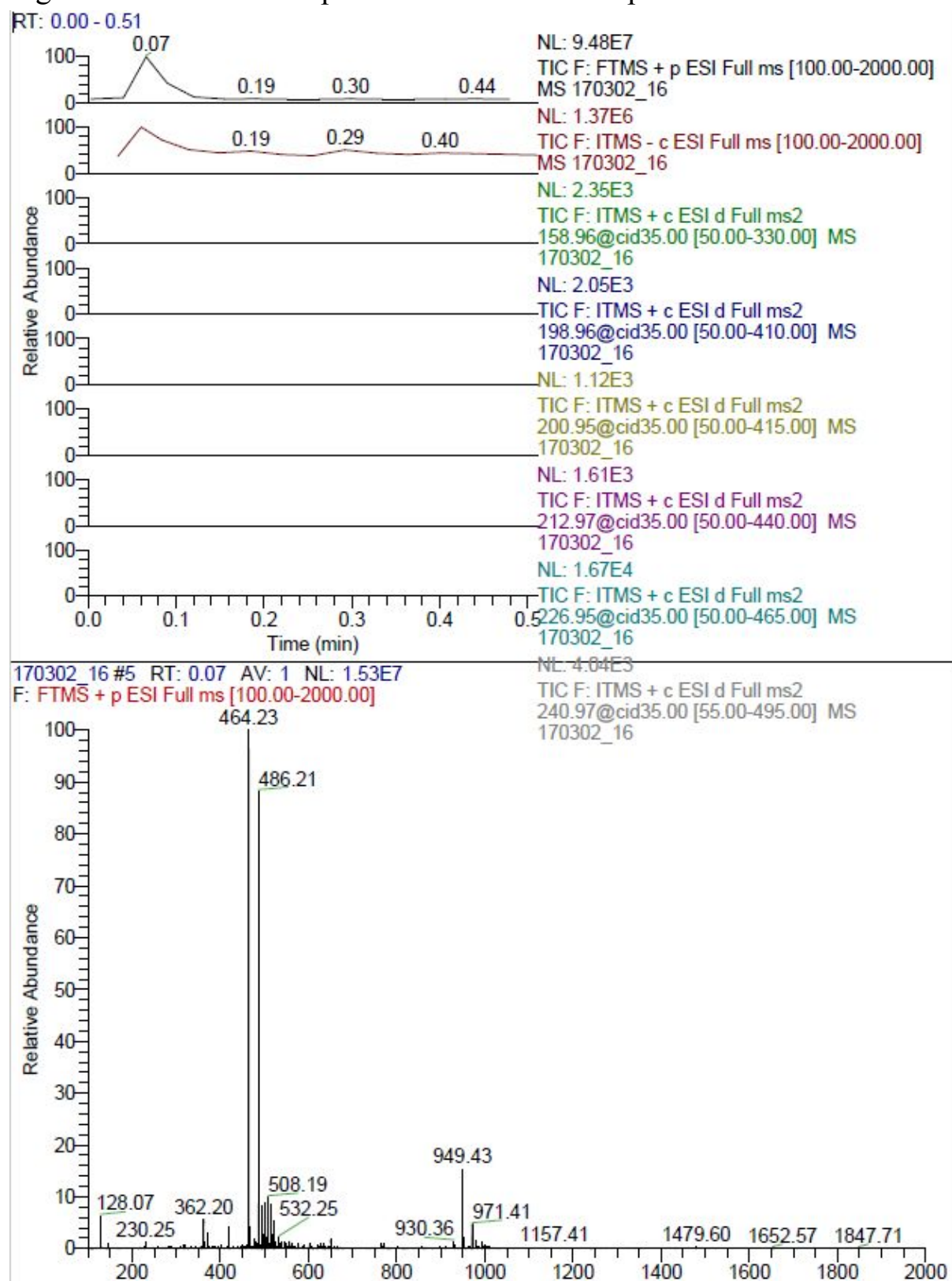
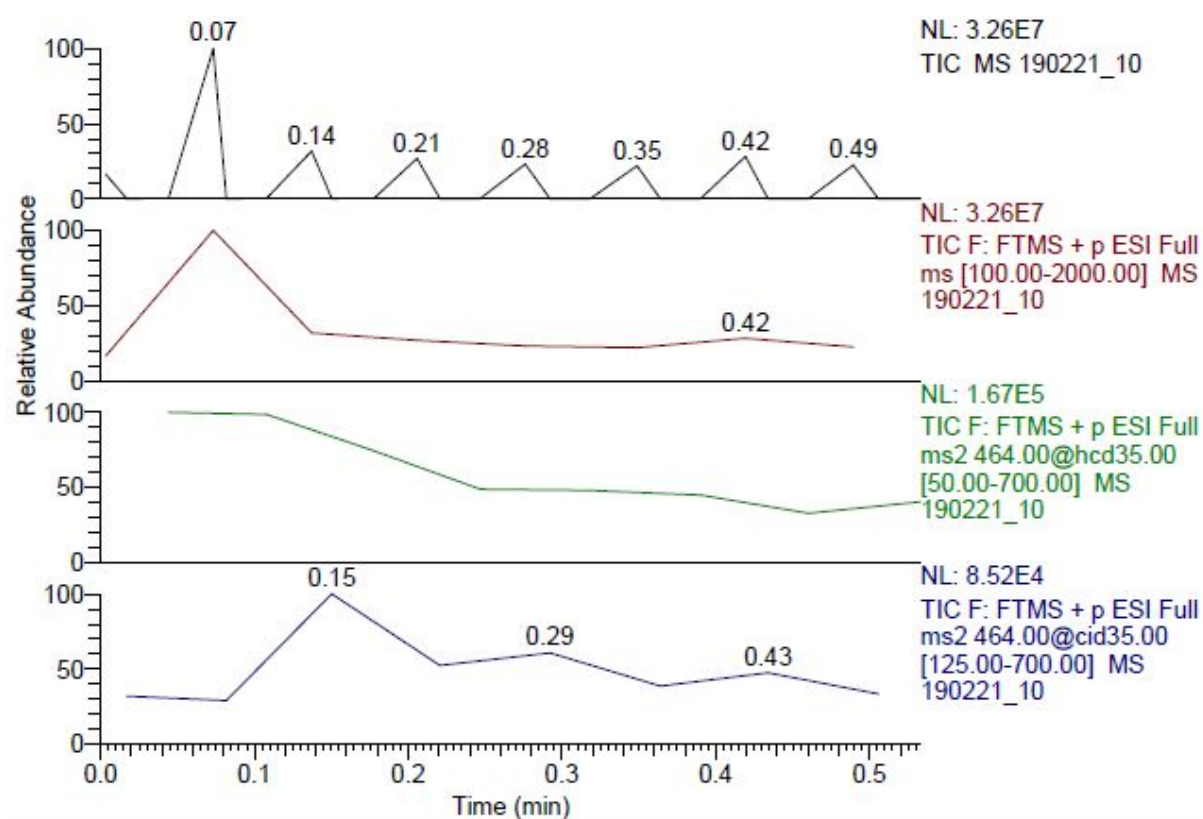


Figure S31. HRESIMS data of the new compound 4

Elemental composition search on mass 464.23				
m/z= 459.23-469.23				
m/z	Theo. Mass	Delta (ppm)	RDB equiv.	Composition
464.2279	464.2279	-0.05	8.5	C ₂₄ H ₃₄ O ₈ N
	464.2255	5.13	5.5	C ₂₂ H ₃₅ O ₈ NNa
	464.2252	5.72	4.0	C ₂₁ H ₃₆ O ₁₁
	464.2322	-9.31	14.0	C ₃₀ H ₃₃ O ₃ Na
	464.2228	10.90	1.0	C ₁₉ H ₃₇ O ₁₁ Na
	464.2338	-12.70	-0.5	C ₁₇ H ₃₈ O ₁₃ N
	464.2196	17.78	14.5	C ₂₉ H ₃₁ O ₃ NNa
	464.2193	18.37	13.0	C ₂₈ H ₃₂ O ₆
	464.2381	-21.96	5.0	C ₂₃ H ₃₇ O ₈ Na
	464.2169	23.56	10.0	C ₂₆ H ₃₃ O ₆ Na

Figure S32. ESIMS (in-source fragmentation) spectrum of compound 4



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F: FTMS + p ESI Full ms2 464.00@hcd35.00 [50.00-700.00]

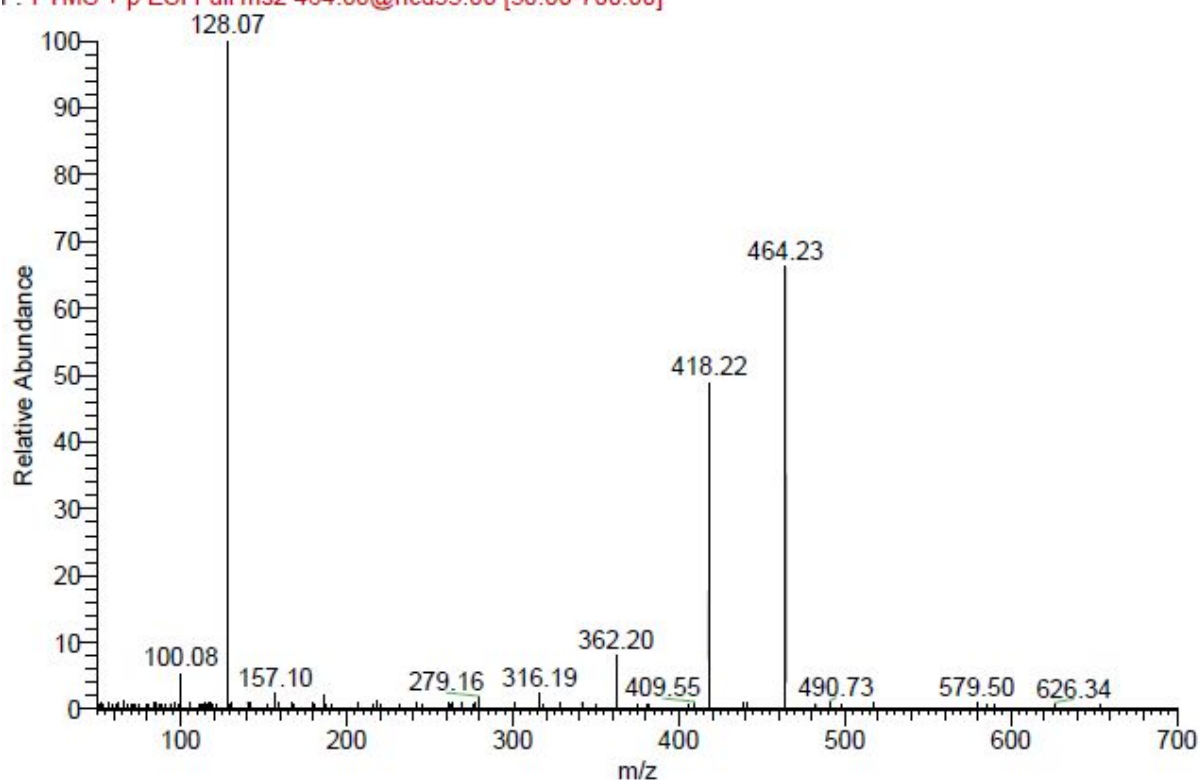


Figure S33. ^1H NMR (600 MHz, DMSO) spectrum of the new compound 5

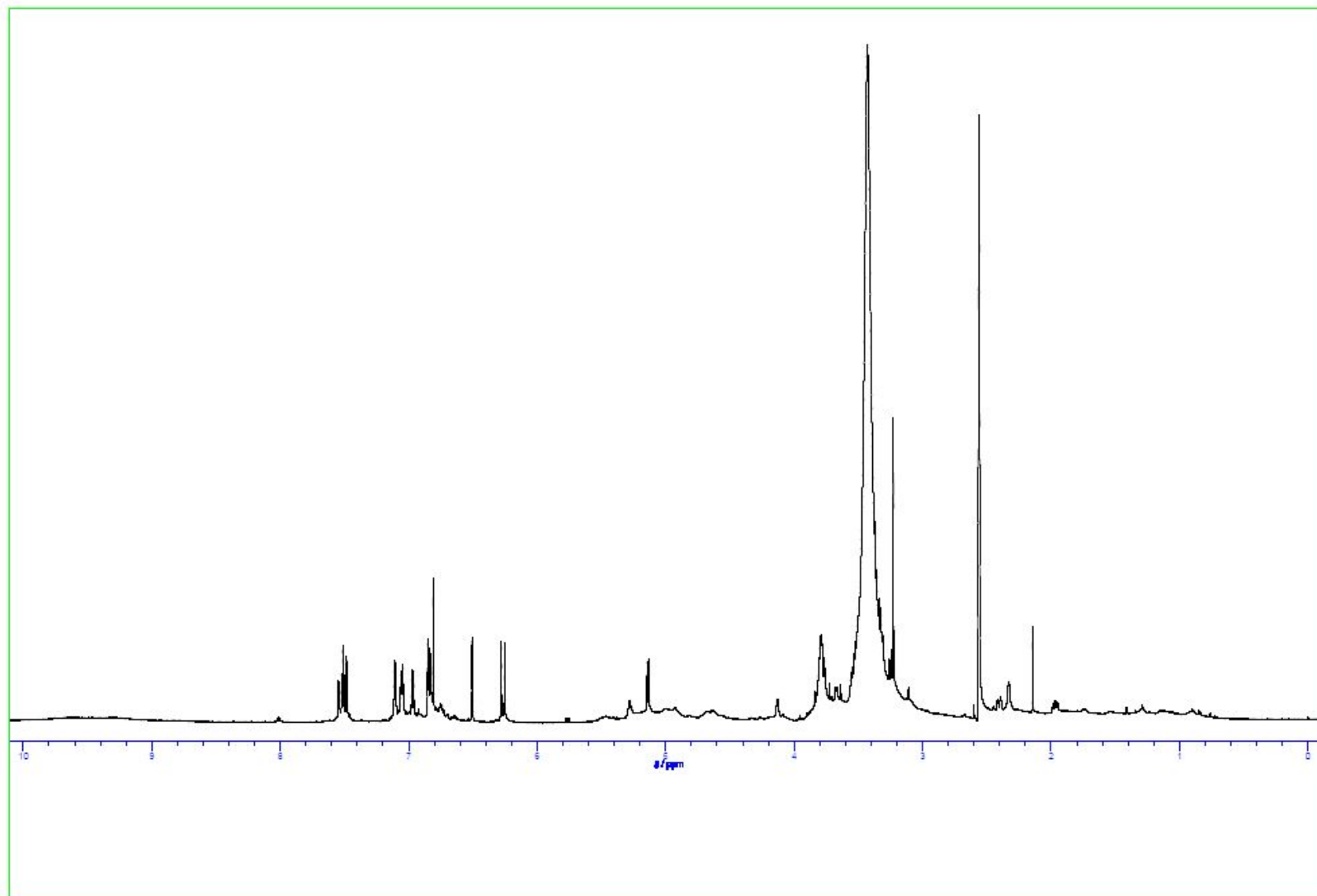
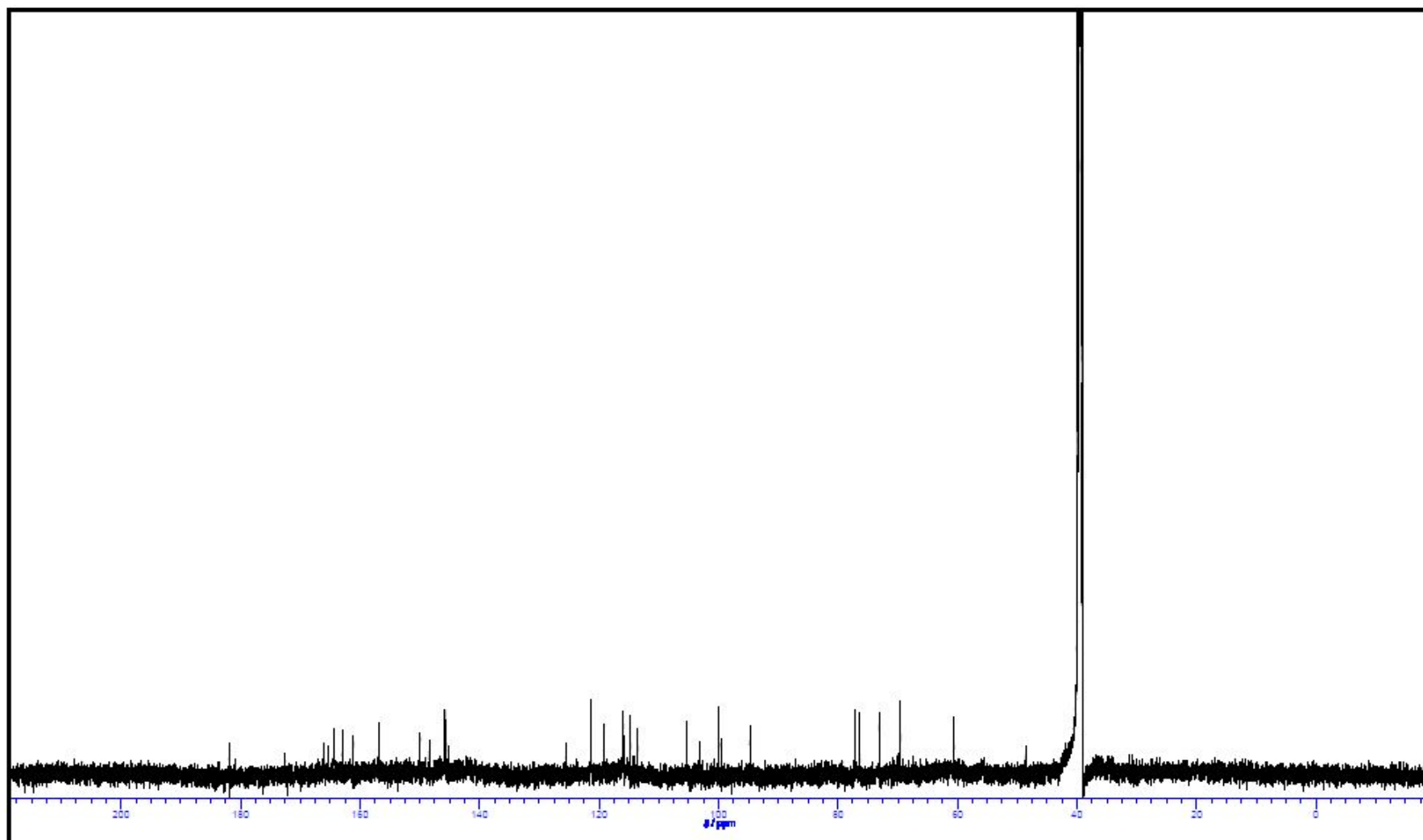


Figure S34. ^{13}C NMR (150 MHz, DMSO) spectrum of the new compound 5



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0.07 0.17 0.31 0.42

NL: 3.21E7
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MS 190121_02

0.16 0.31 0.41

NL: 1.21E6
TIC F: ITMS - c ESI Full ms [100.00-2000.00]
MS 190121_02

NL: 8.26E2
TIC F: ITMS + c ESI d Full ms2
136.06@cid35.00 [50.00-285.00] MS
190121_02

NL: 8.33E2
TIC F: ITMS + c ESI d Full ms2
139.07@cid35.00 [50.00-150.00] MS
190121_02

NL: 4.95E2
TIC F: ITMS + c ESI d Full ms2
143.00@cid35.00 [50.00-300.00] MS
190121_02

NL: 2.32E2
TIC F: ITMS + c ESI d Full ms2
157.08@cid35.00 [50.00-325.00] MS
190121_02

NL: 5.91E3
TIC F: ITMS + c ESI d Full ms2
158.96@cid35.00 [50.00-330.00] MS
190121_02

190121_02 #4-9 RT: 0.04-0.07 AV: 2 NL: 2.12E6
F: FTMS + p ESI Full ms [100.00-2000.00]

633.12

NL: 2.38E3
TIC F: ITMS + c ESI d Full ms2
185.07@cid35.00 [50.00-200.00] MS
190121_02

139.07 313.16 537.19 663.13 701.11 769.10 927.05 1243.25 1303.27 1579.29 1877.37

158.96 341.27 519.20

Relative Abundance

Time (min)

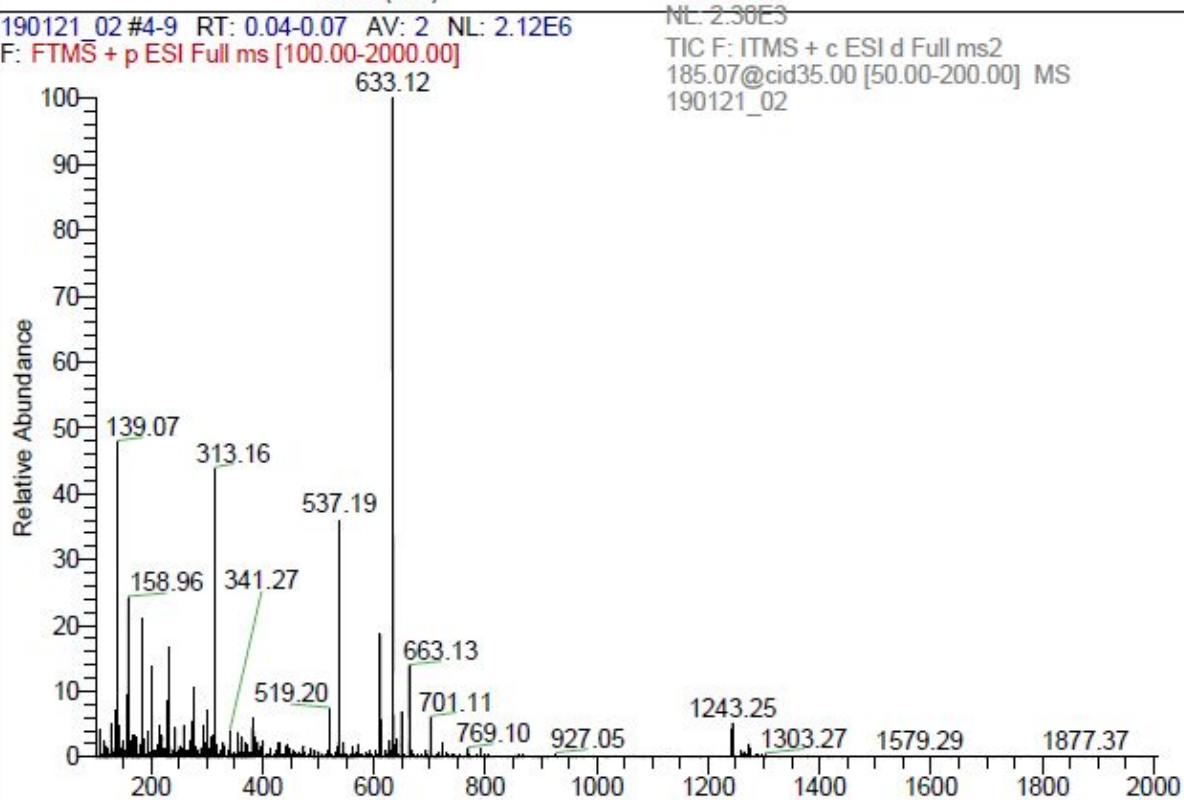


Figure S36. HRESIMS data of the new compound 5

Elemental composition search on mass 633.12

m/z= 628.12-638.12

m/z	Theo. Mass	Delta (ppm)	RDB equiv.	Composition
633.1214	633.1215	-0.19	23.0	C ₂₉ H ₂₀ O ₉ N ₇ Na
	633.1215	-0.20	17.5	C ₃₀ H ₂₆ O ₁₄ Na
	633.1212	0.24	21.5	C ₂₈ H ₂₁ O ₁₂ N ₆
	633.1225	-1.87	26.5	C ₂₉ H ₁₇ O ₈ N ₁₀
	633.1225	-1.88	21.0	C ₃₀ H ₂₃ O ₁₃ N ₃
	633.1201	1.92	18.0	C ₂₈ H ₂₄ O ₁₃ N ₃ Na
	633.1201	1.93	23.5	C ₂₇ H ₁₈ O ₈ N ₁₀ Na
	633.1199	2.36	22.0	C ₂₆ H ₁₉ O ₁₁ N ₉
	633.1188	4.04	18.5	C ₂₆ H ₂₂ O ₁₂ N ₆ Na
	633.1185	4.48	17.0	C ₂₅ H ₂₃ O ₁₅ N ₅