

Supporting Information

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Two New Lignans from *Lycopodium japonicum* Thunb.

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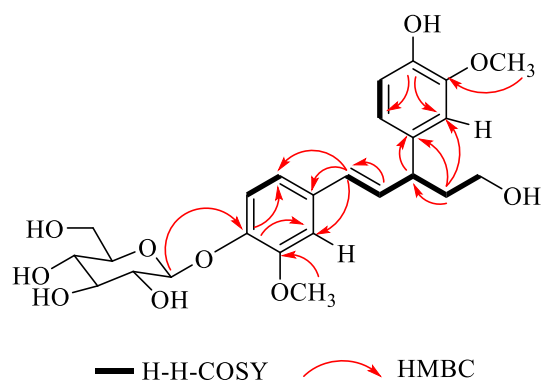


Figure S1: Key ¹H-¹H COSY and HMBC correlations of compound **1**

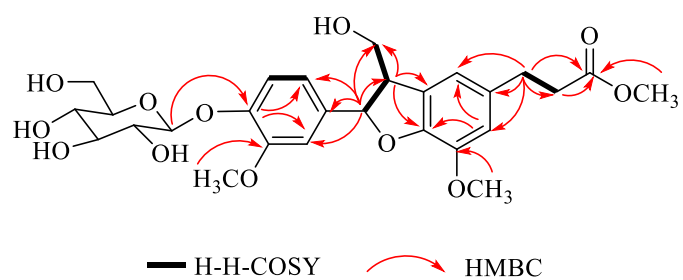
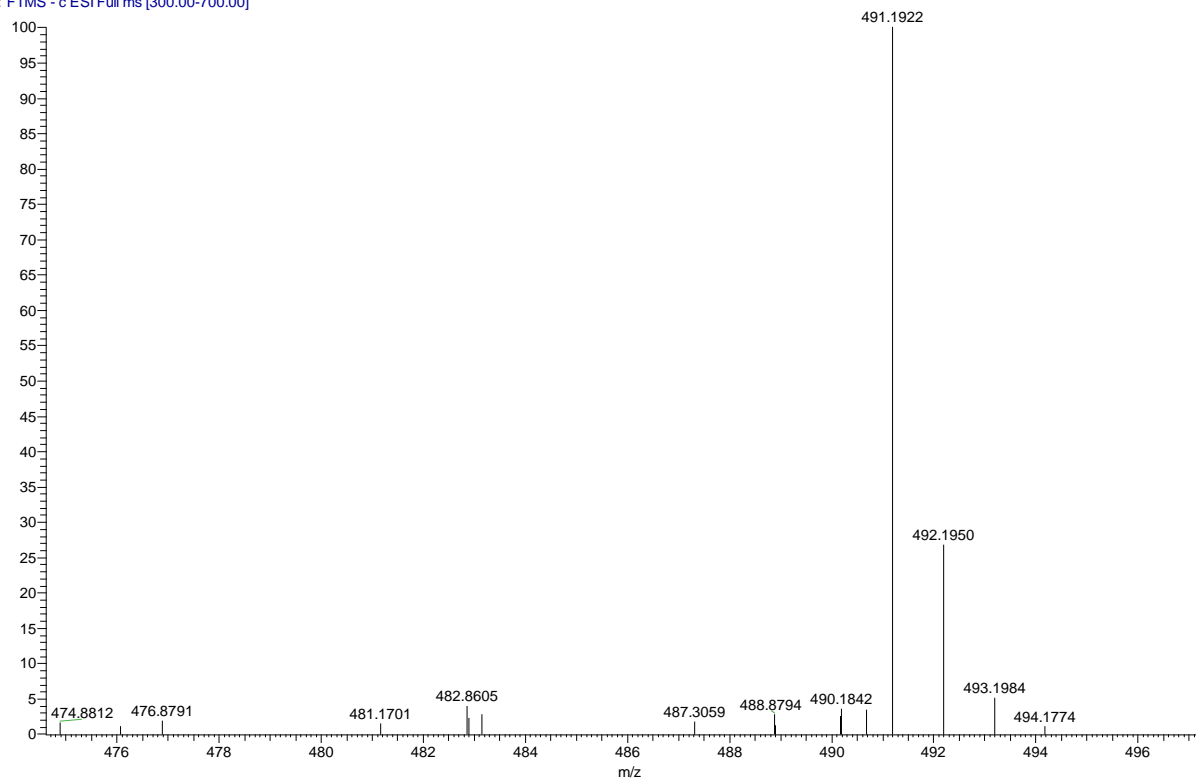


Figure S2: Key ¹H-¹H COSY and HMBC correlations of compound **2**

B320% #102 RT: 0.93 AV: 1 NL: 4.64E4
T: FTMS - c ESI Full ms [300.00-700.00]



Formula (M)	Ion Formula	m/z	Calc m/z
C ₂₅ H ₃₂ O ₁₀	C ₂₅ H ₃₁ O ₁₀	491.1922	491.1917

Figure S3: HRESIMS of compound **1**

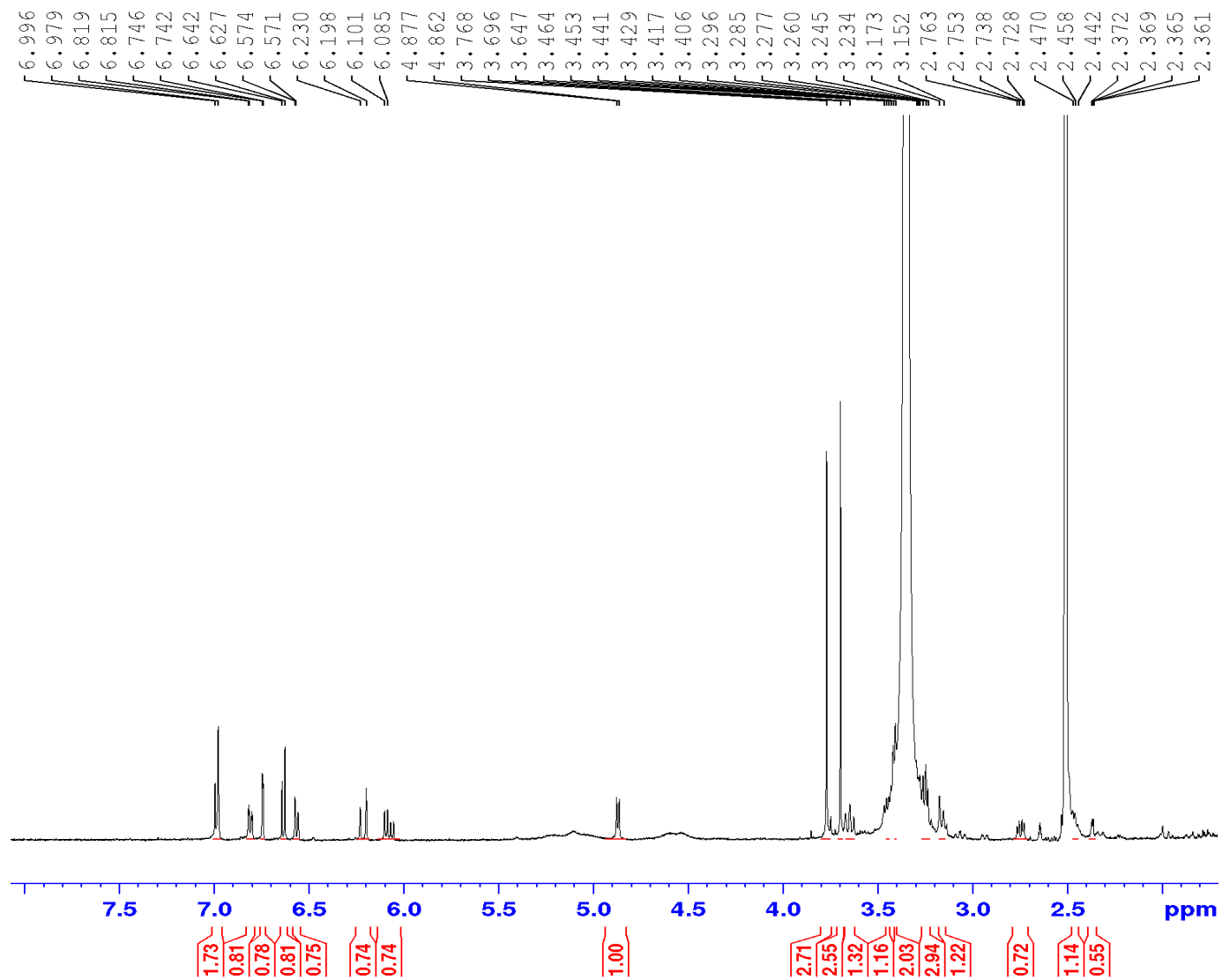


Figure S4: ^1H NMR spectrum of compound **1** (DMSO- d_6 , 500 MHz)

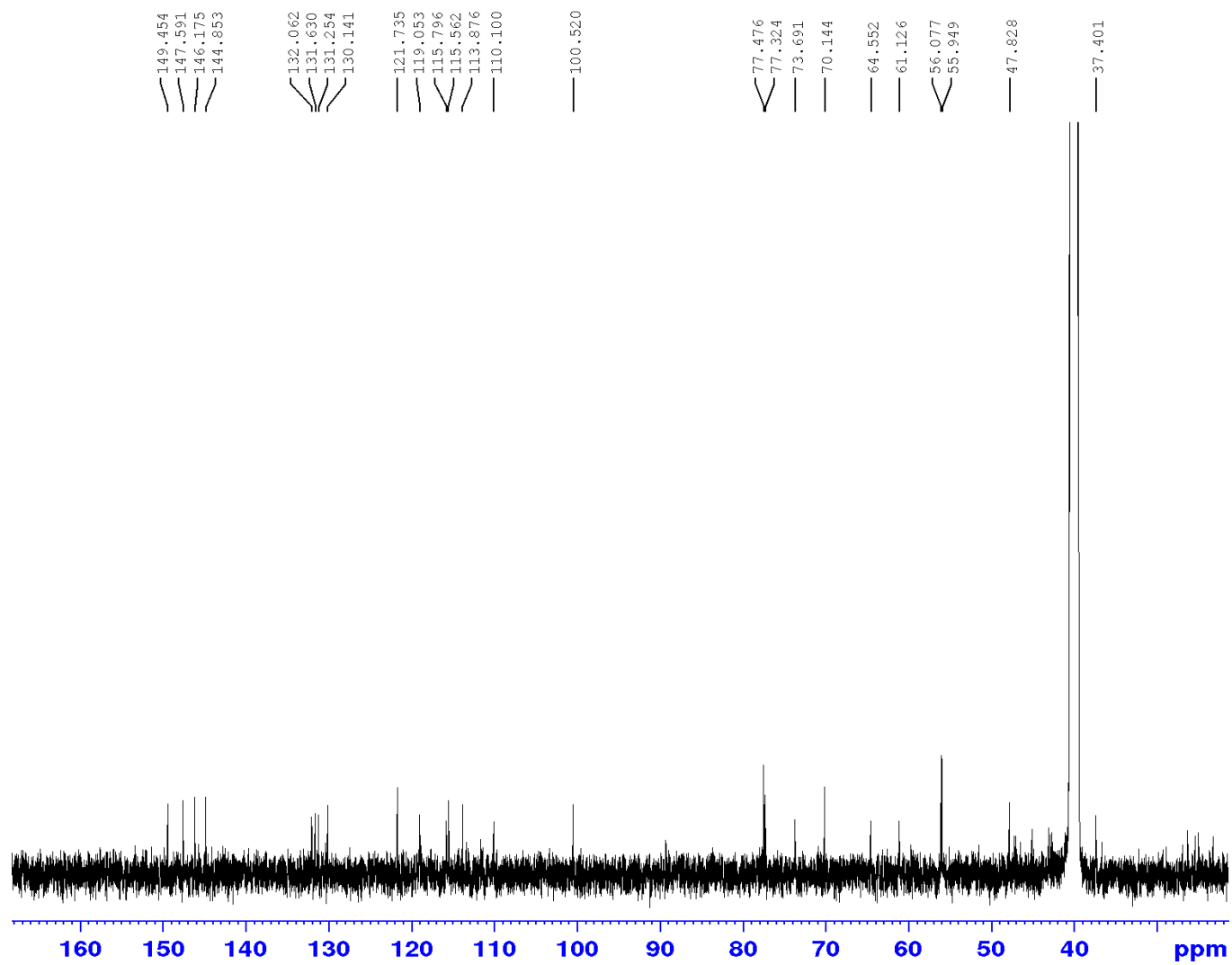


Figure S5: ^{13}C NMR spectrum of compound **1** (DMSO- d_6 , 125 MHz)

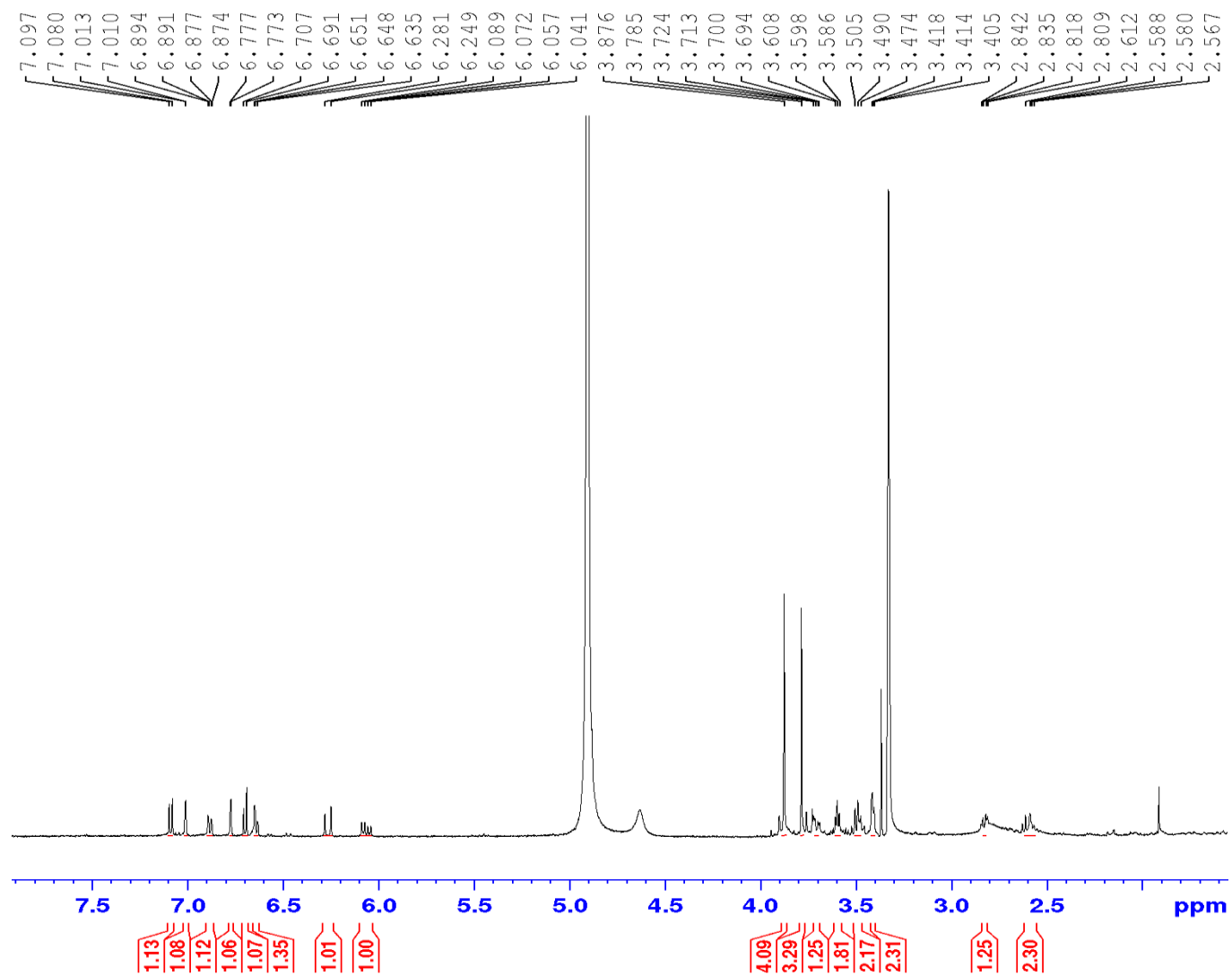


Figure S6: ¹H NMR spectrum of compound 1 (CD₃OD, 500 MHz)

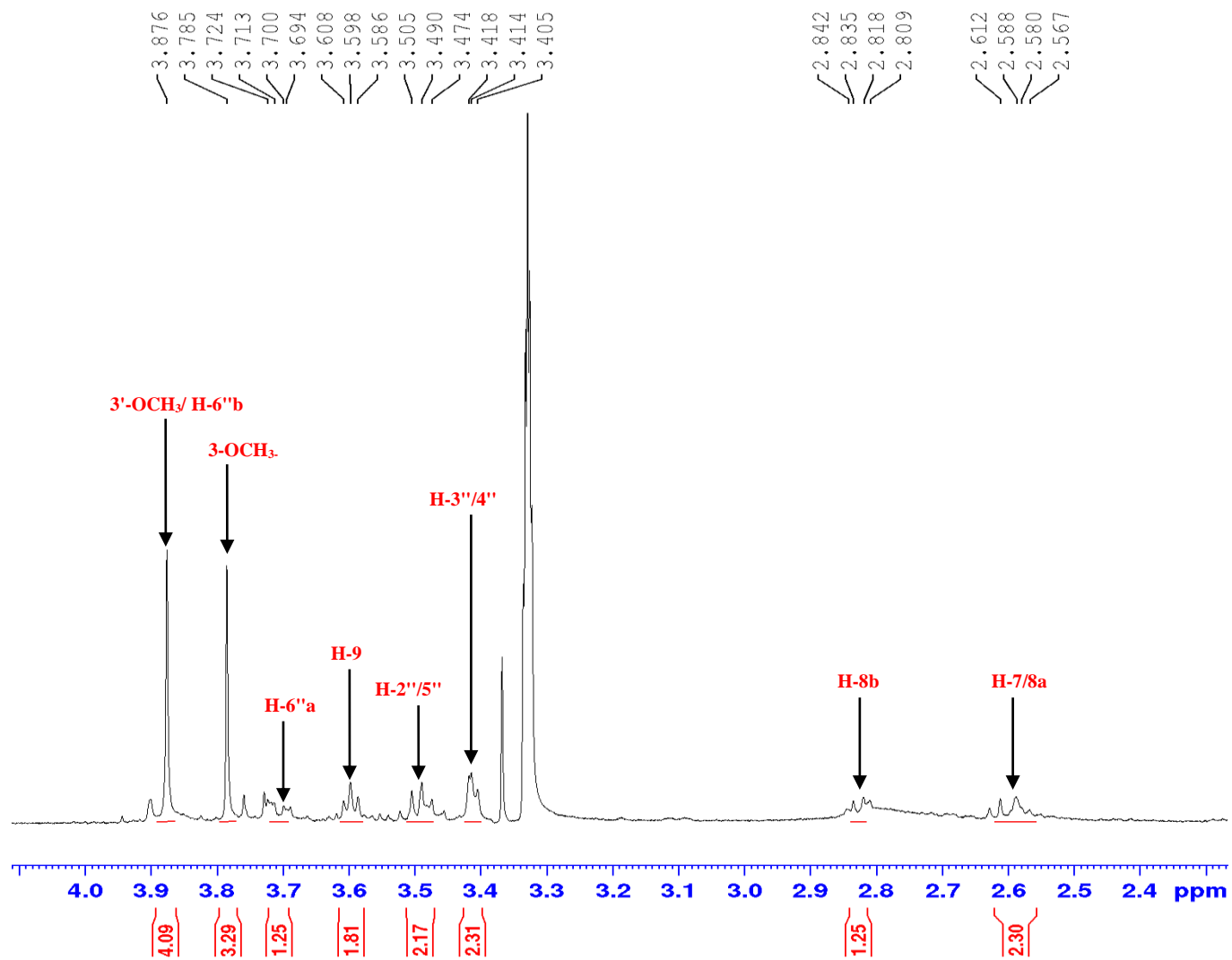


Figure S7: ¹H NMR spectrum of compound **1** (CD₃OD, 500 MHz, from 2.5 to 4.0 ppm)

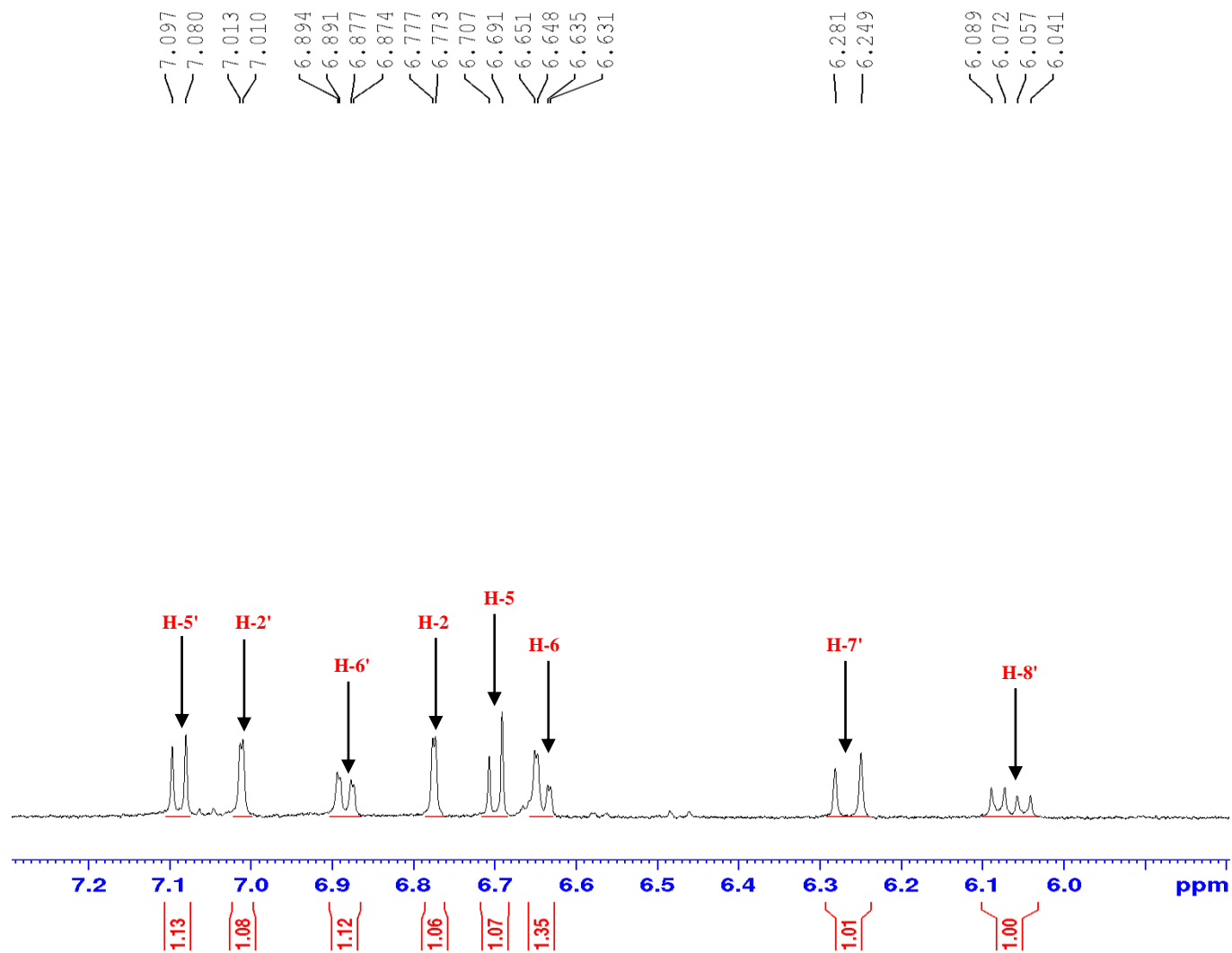


Figure S8: ¹H NMR spectrum of compound **1** (CD₃OD, 500 MHz, from 6.0 to 7.2 ppm)

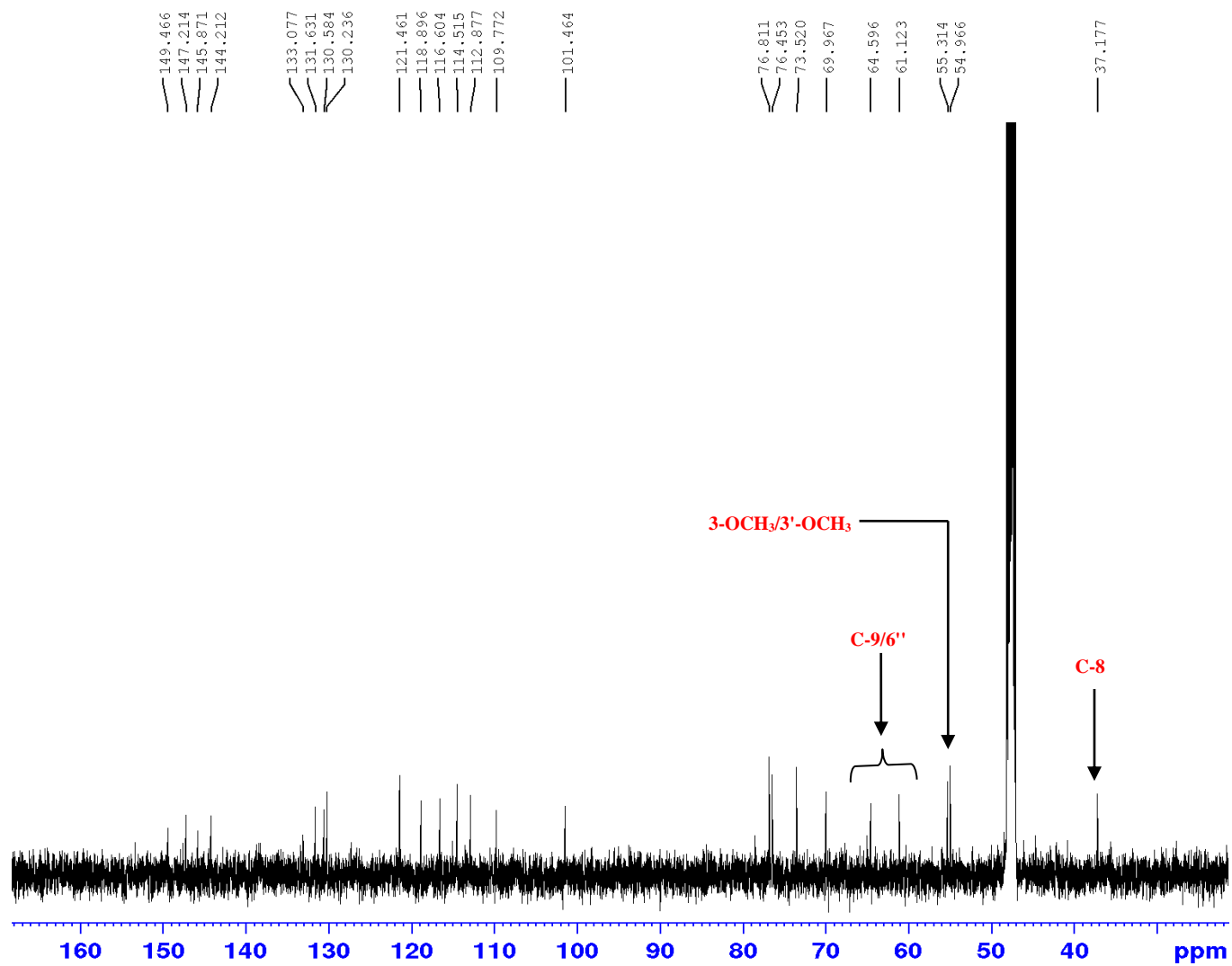


Figure S9: ¹³C NMR spectrum of compound 1 (CD₃OD, 125 MHz)

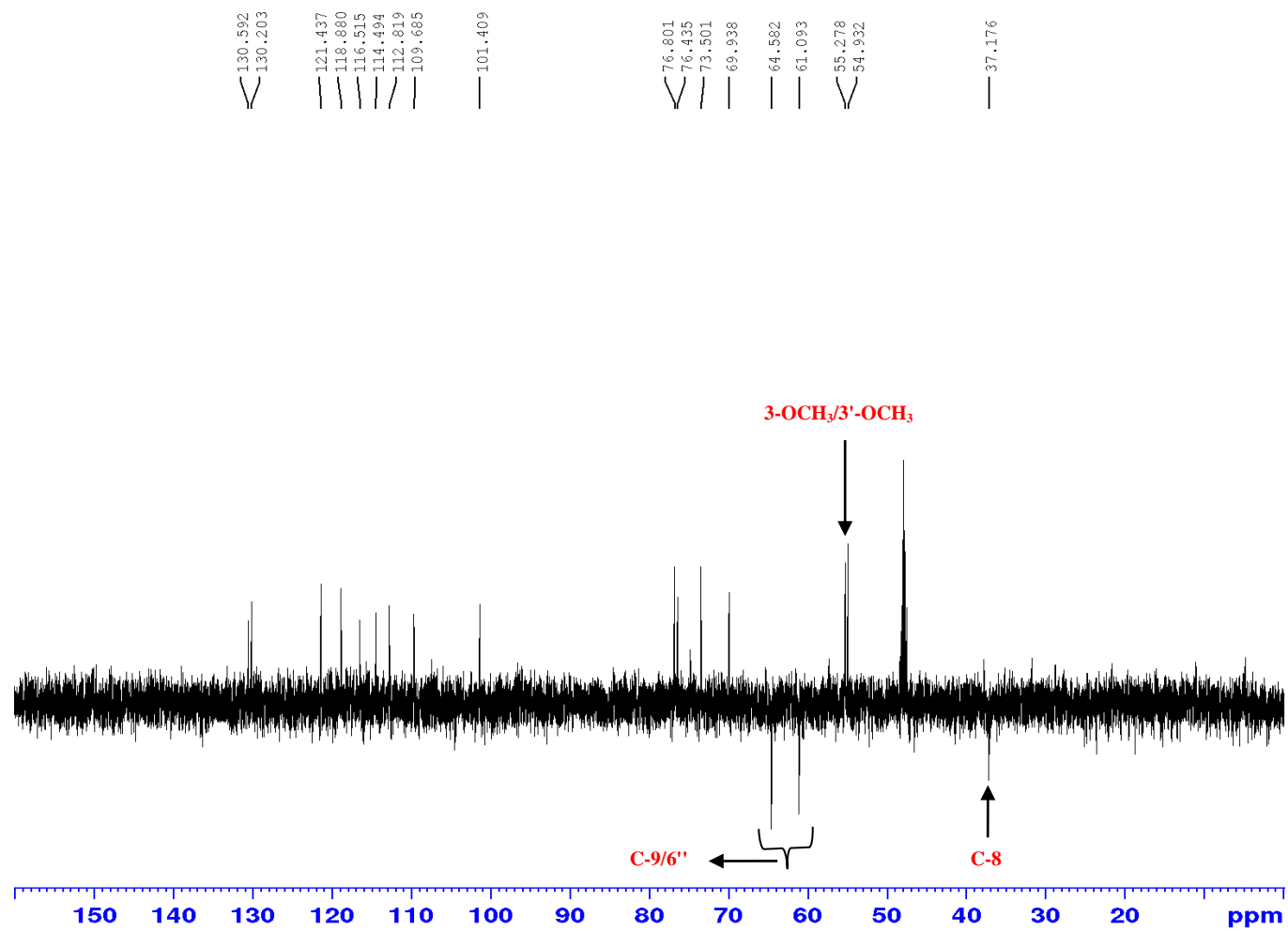


Figure S10: DEPT135 spectrum of compound **1** (CD₃OD, 125 MHz)

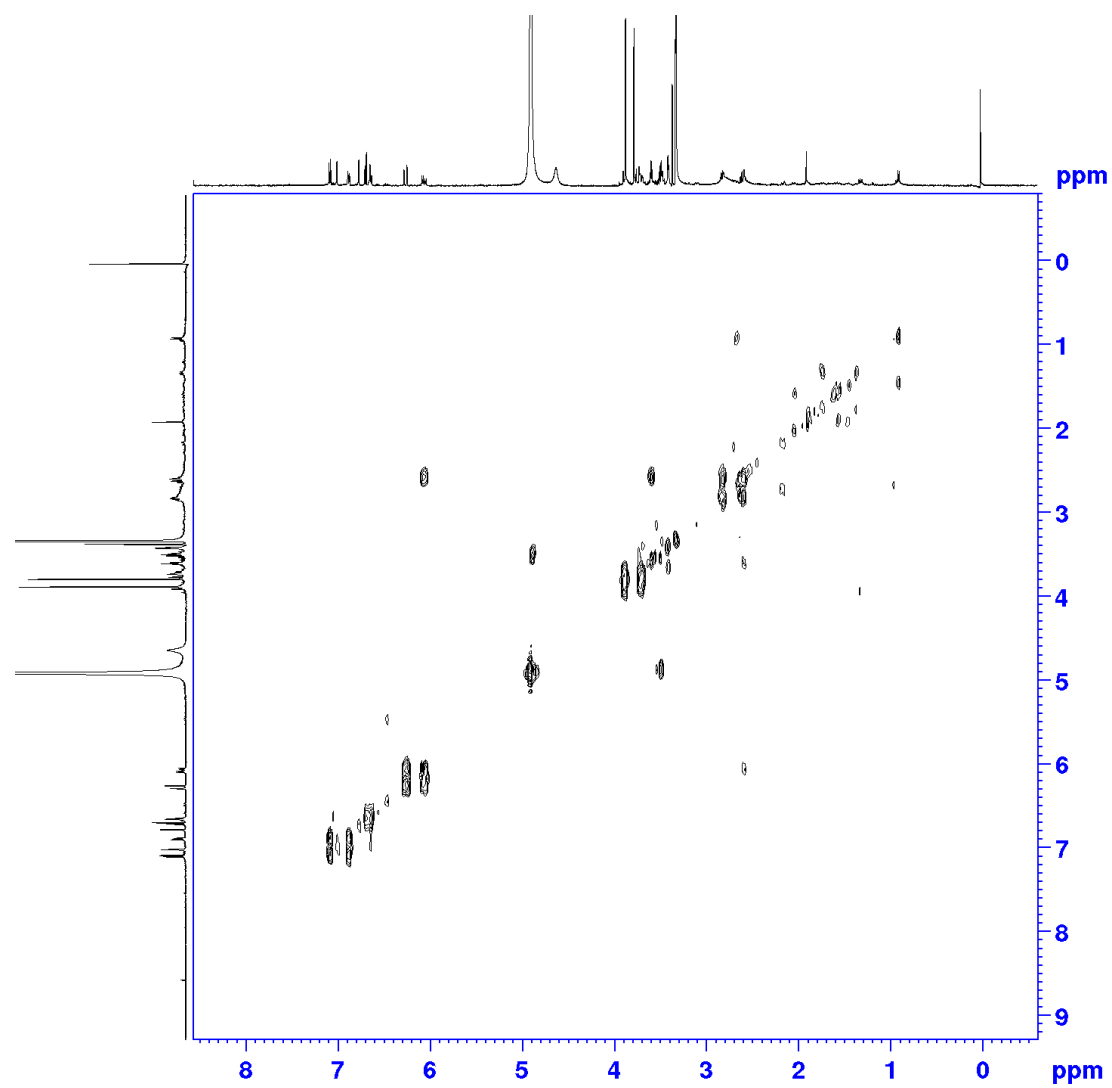


Figure S11: ^1H - ^1H COSY spectrum of compound **1** (CD_3OD , 500 MHz)

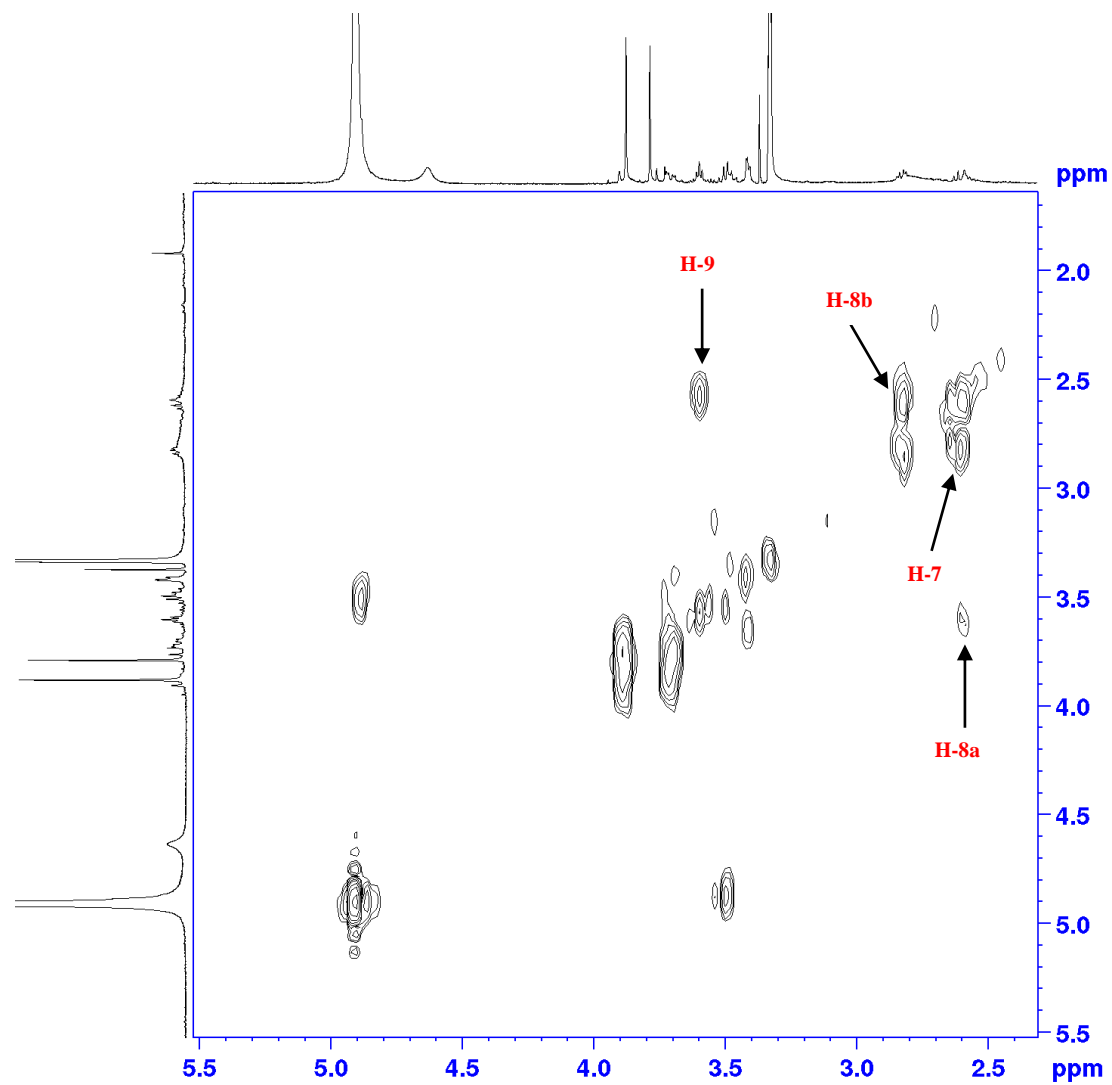


Figure S12: ^1H - ^1H COSY spectrum of compound **1** (CD_3OD , 500 MHz, from 2.5 to 5.5 ppm)

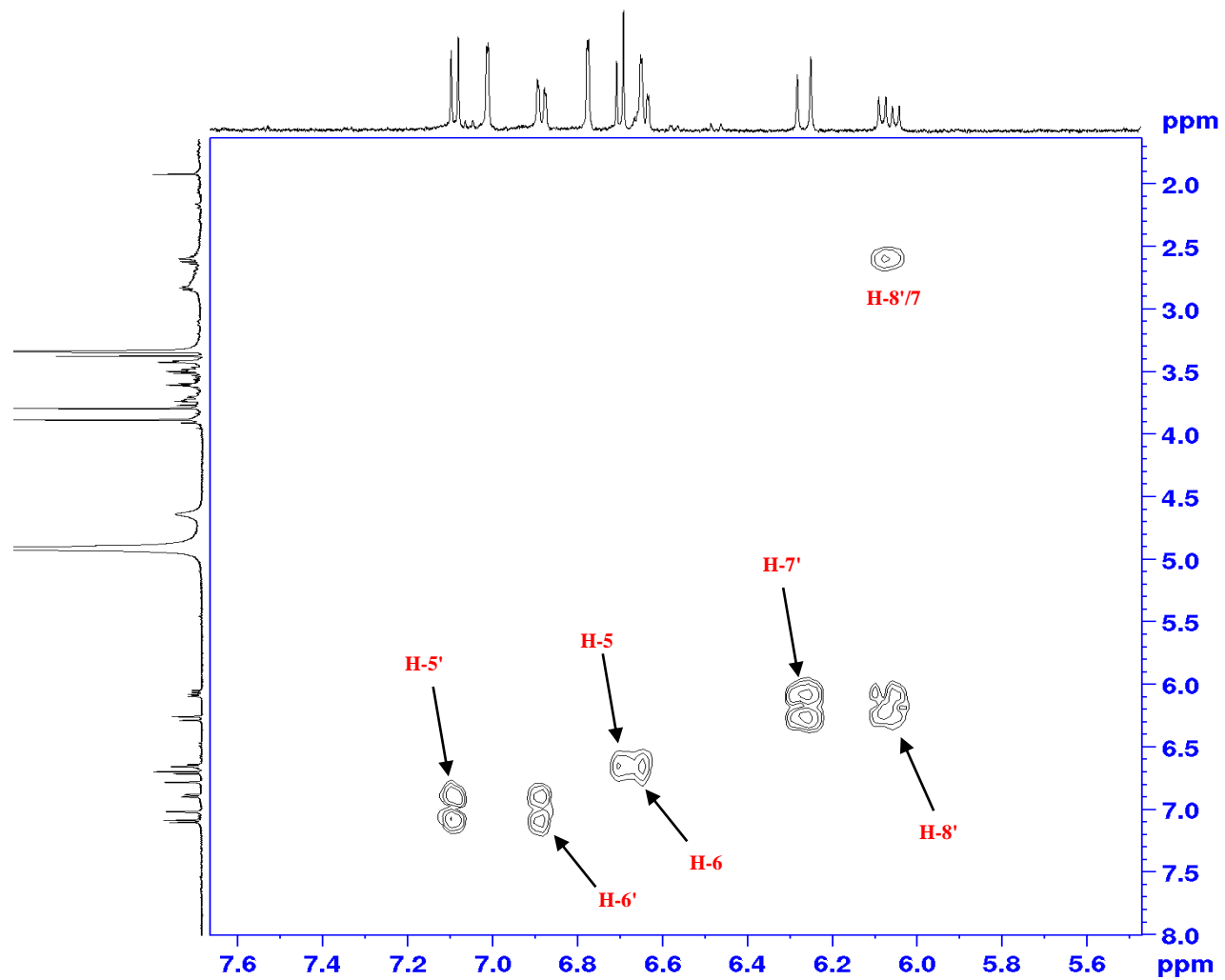


Figure S13: ^1H - ^1H COSY spectrum of compound **1** (CD_3OD , 500 MHz, from 5.6 to 7.6 ppm)

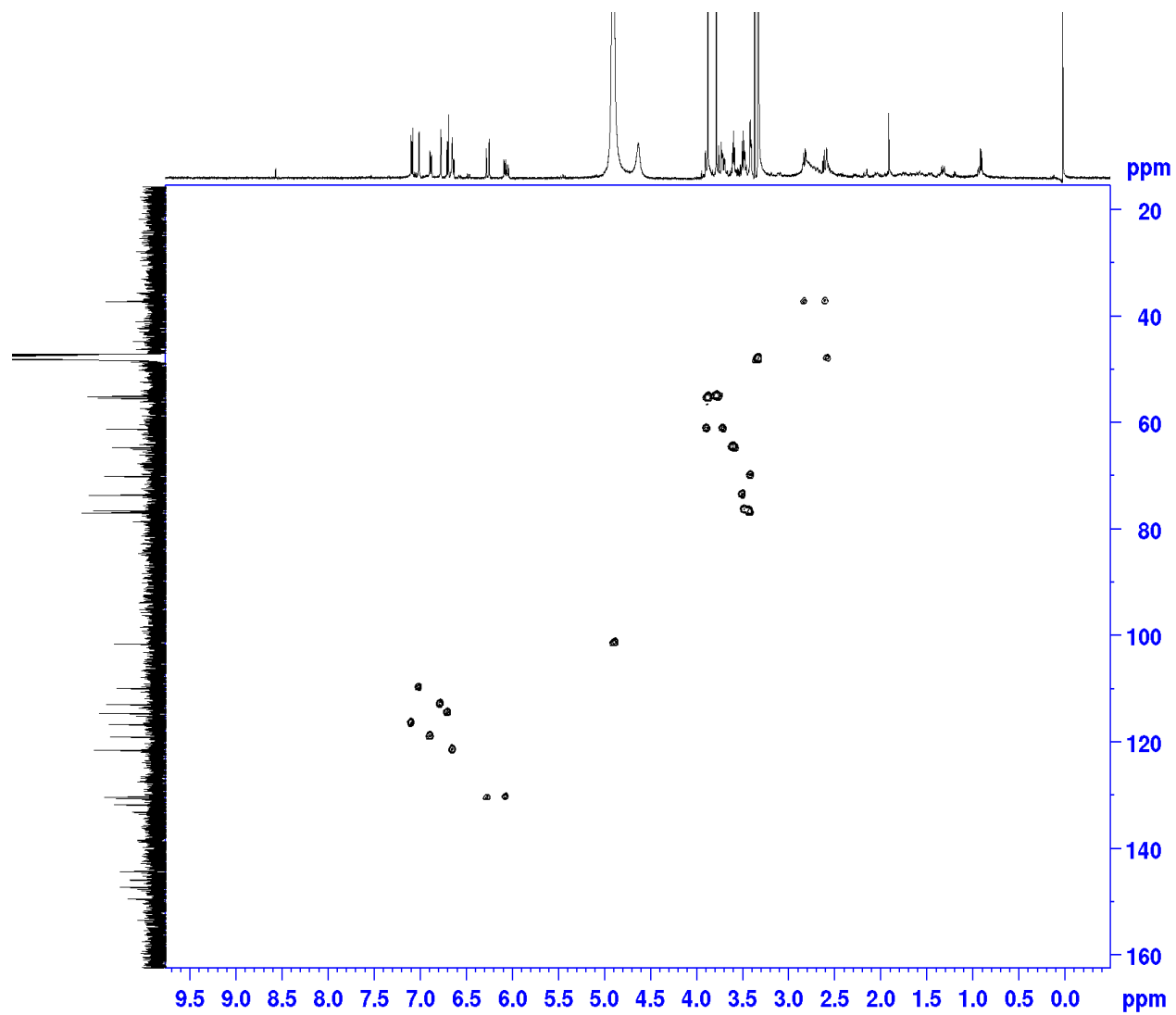


Figure S14: HSQC spectrum of compound **1** (CD_3OD , 500 MHz)

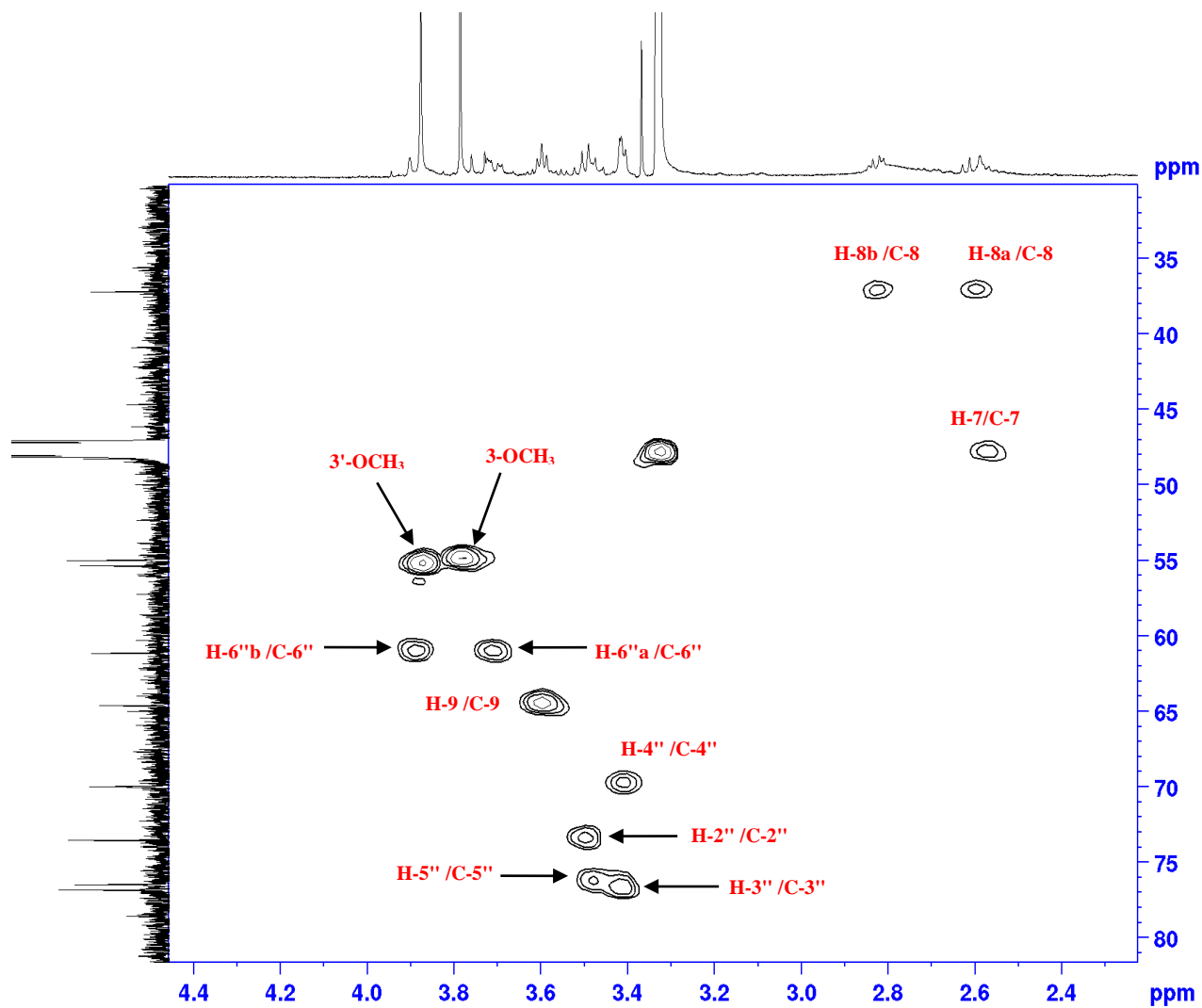


Figure S15: HSQC spectrum of compound 1 (CD_3OD , 500 MHz, from 30 to 80 ppm)

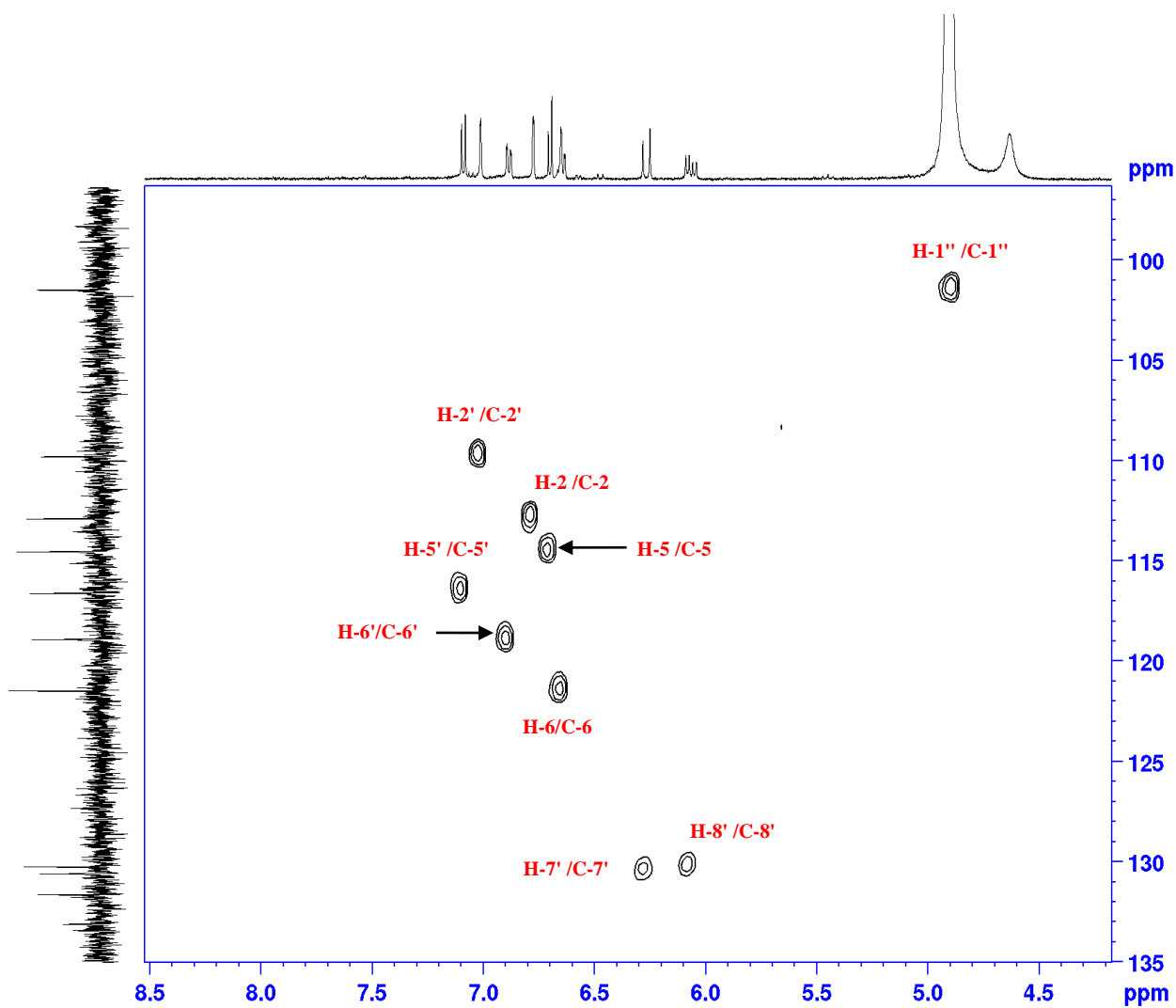


Figure S16: HSQC spectrum of compound **1** (CD₃OD, 500 MHz, from 90 to 135 ppm)

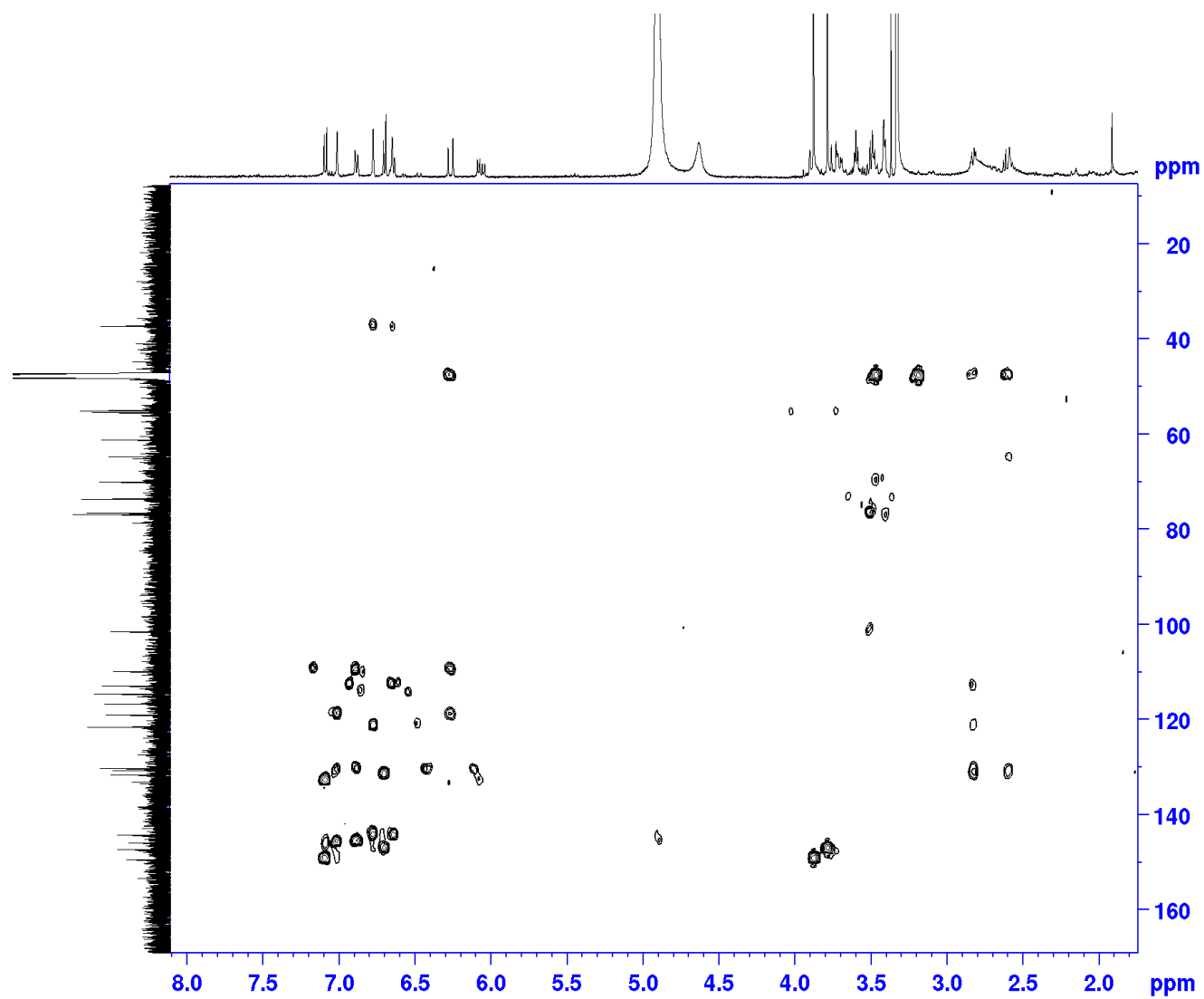


Figure S17: HMBC spectrum of compound **1** (CD₃OD, 500 MHz)

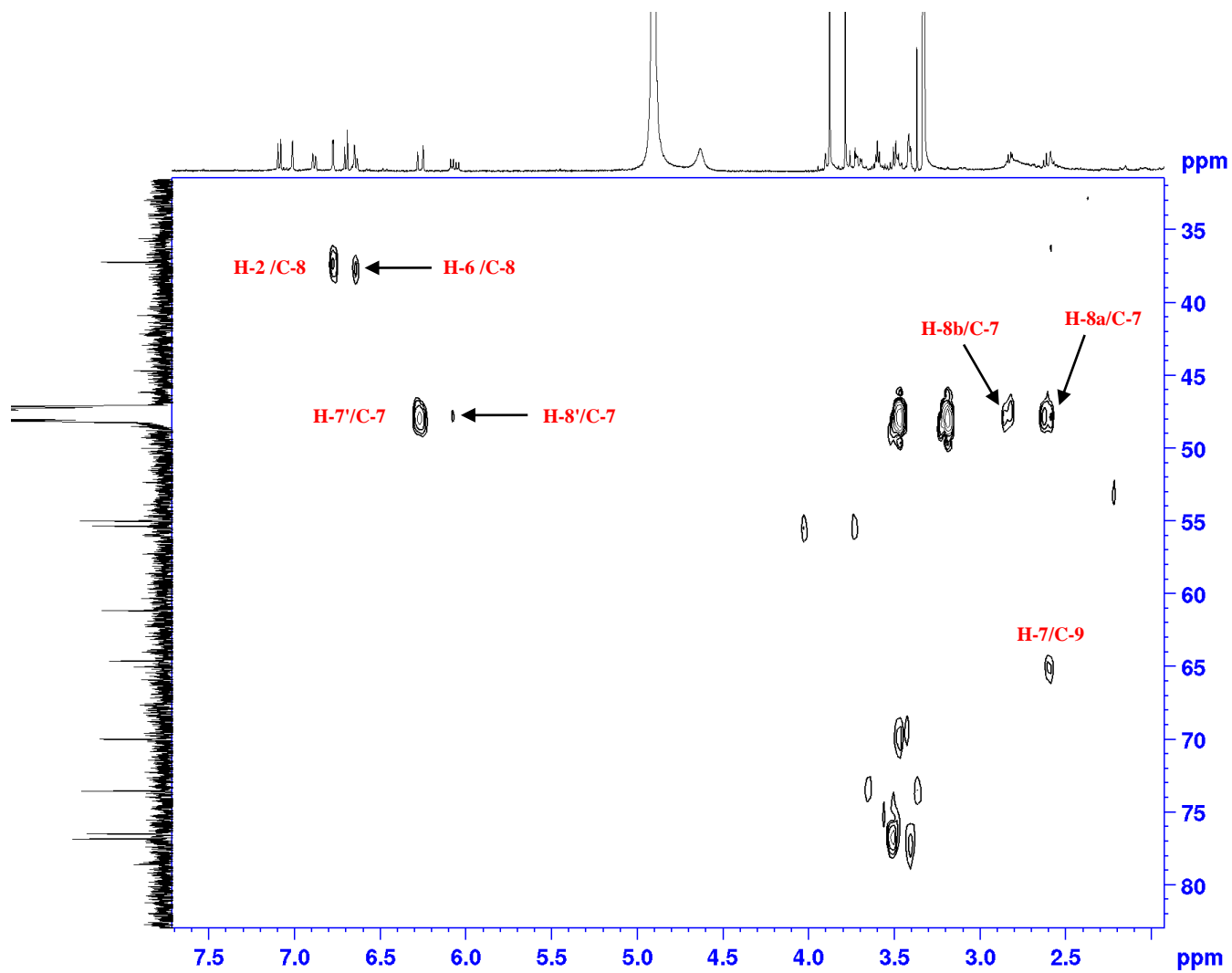


Figure S18: HMBC spectrum of compound **1** (CD₃OD, 500 MHz, from 35 to 80 ppm)

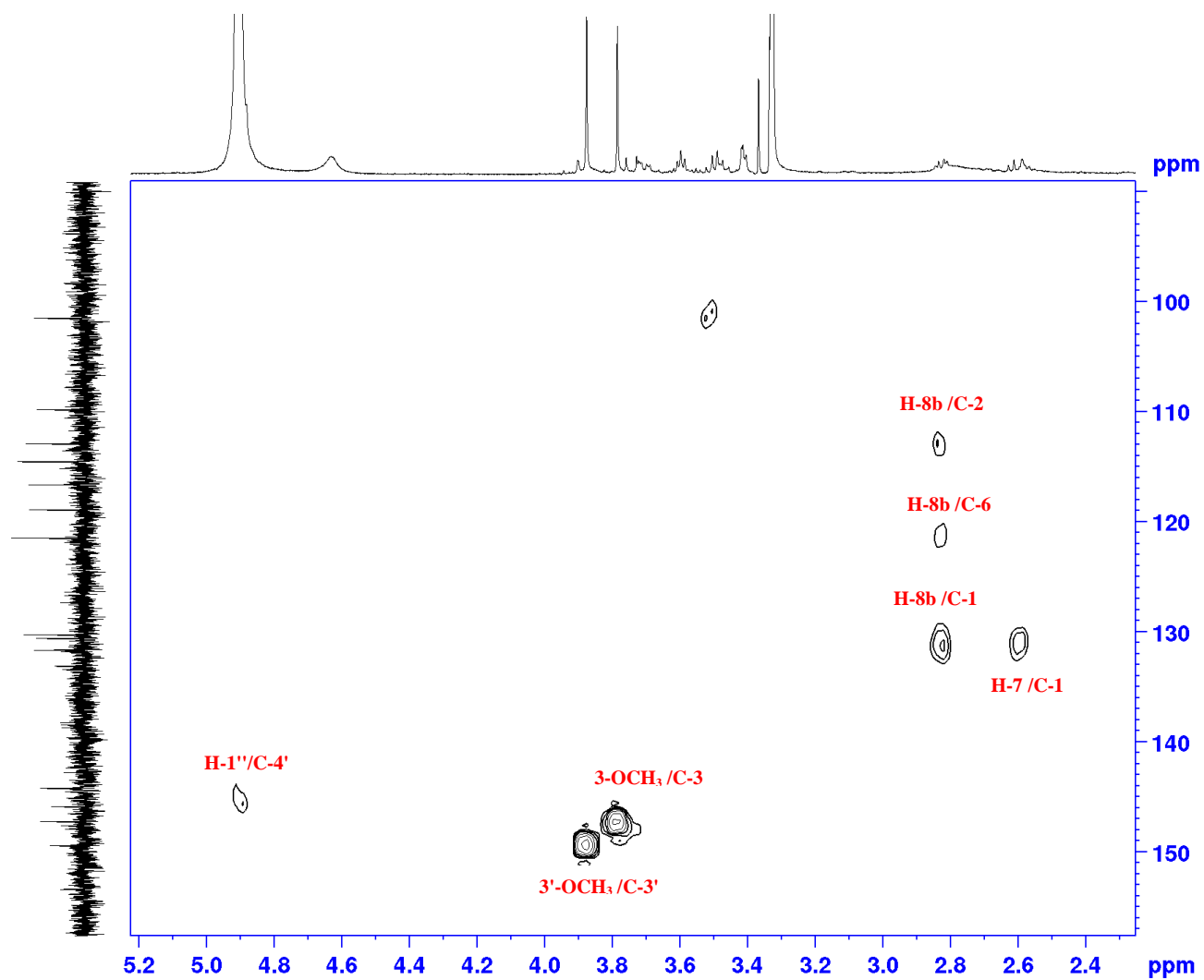


Figure S19: HMBC spectrum of compound 1 (CD₃OD, 500 MHz, from 90 to 160 ppm)

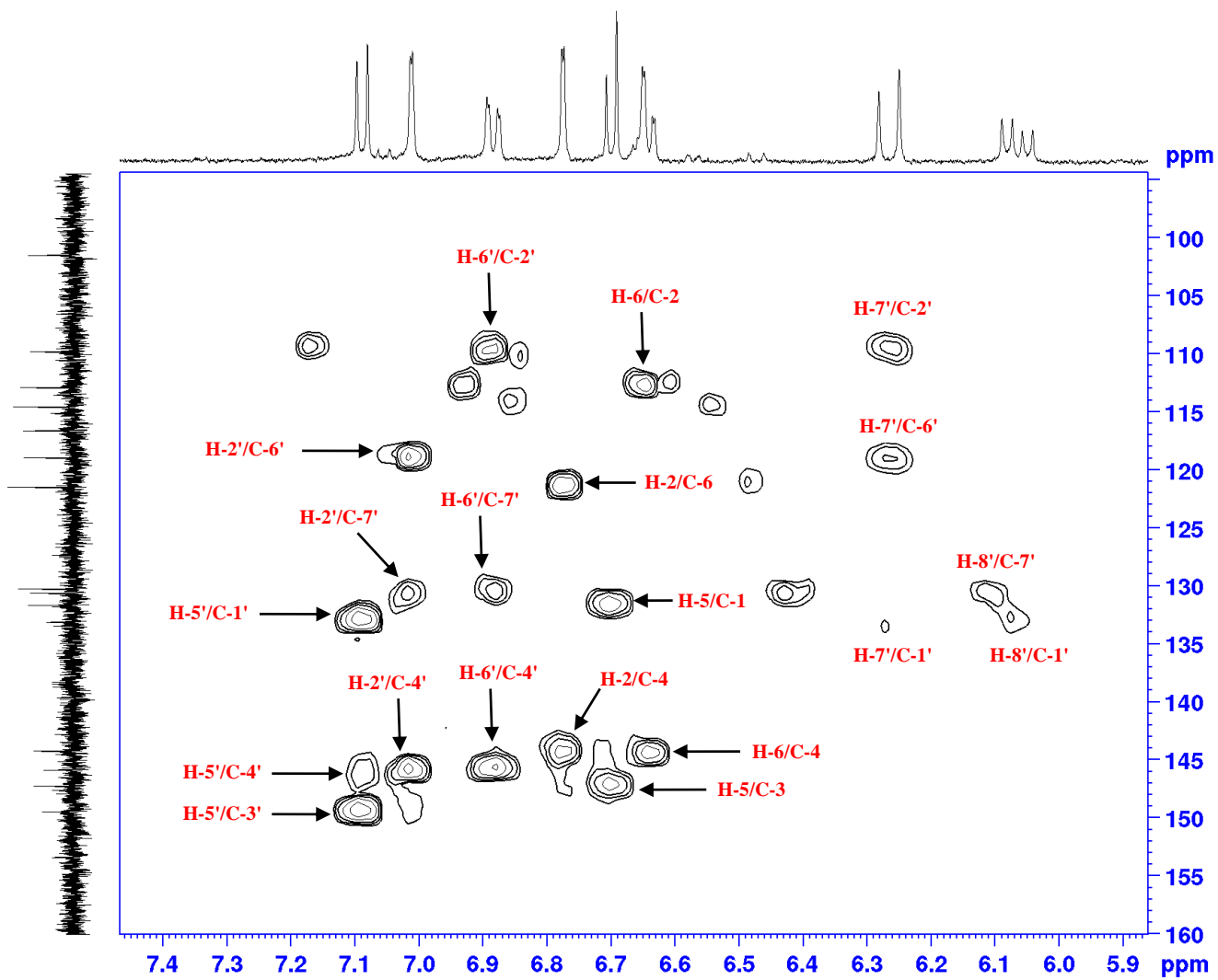


Figure S20: HMBC spectrum of compound 1 (CD₃OD, 500 MHz, from 90 to 160 ppm)

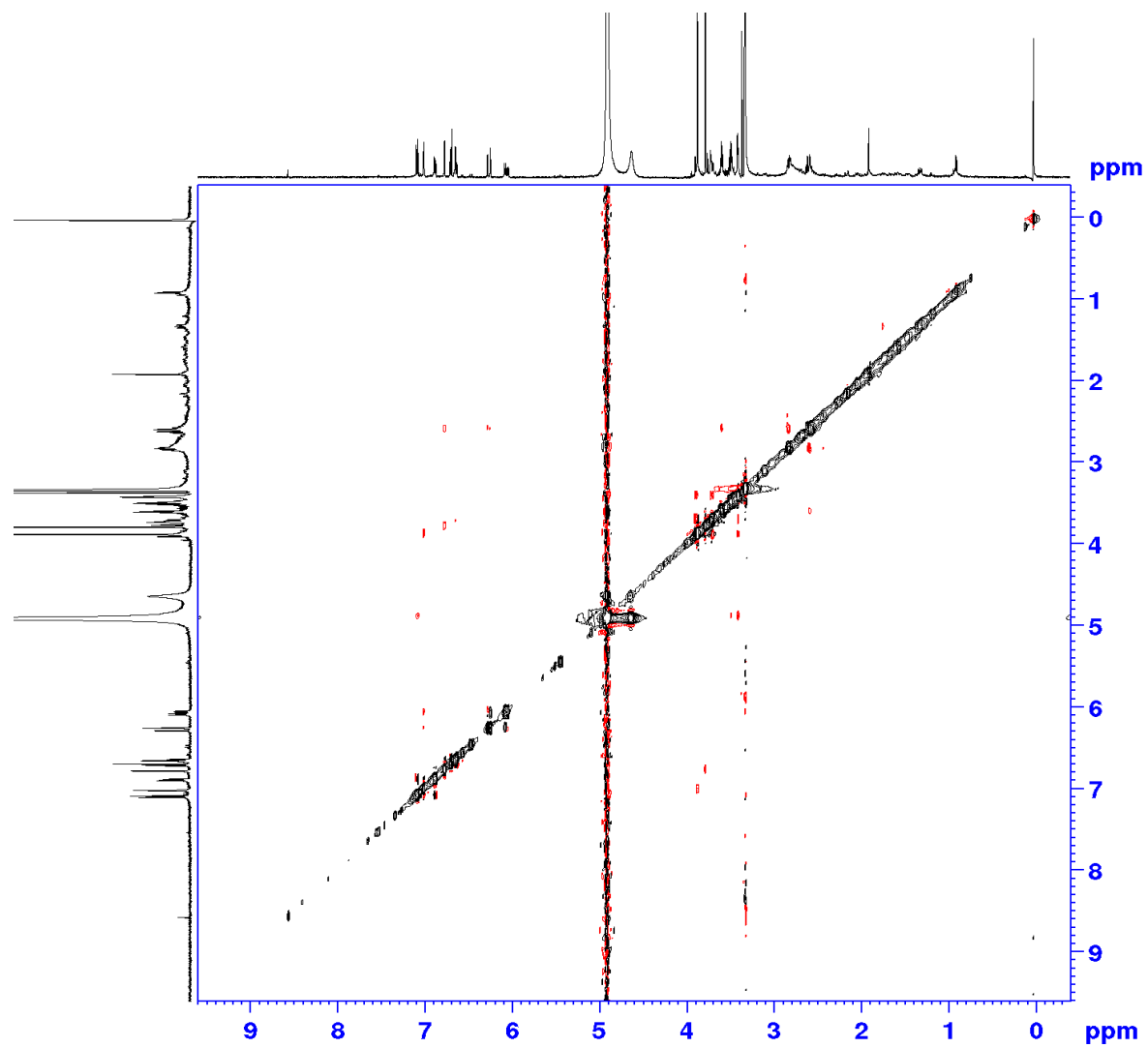


Figure S21: NOESY spectrum of compound **1** (CD₃OD, 500 MHz)

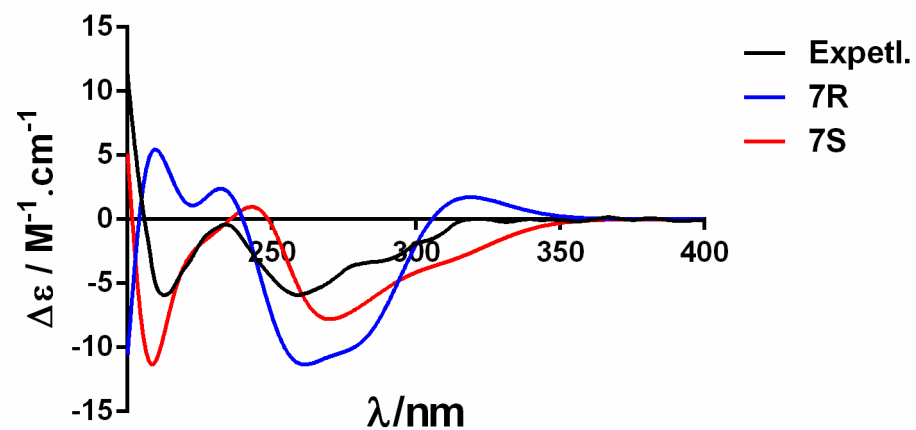


Figure S22: Experimental and calculated ECD spectra of compound **1**

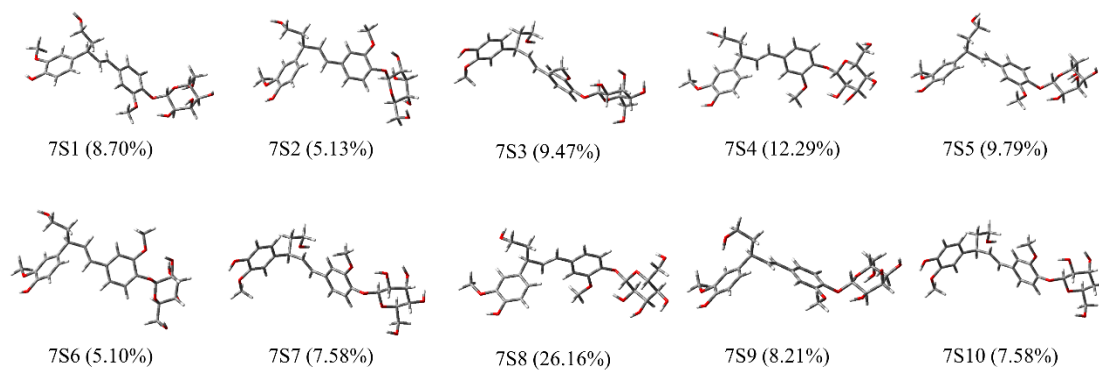


Figure S23: The optimized 10 conformers and equilibrium population of conformers of **7S** for ECD calculation of compound **1**

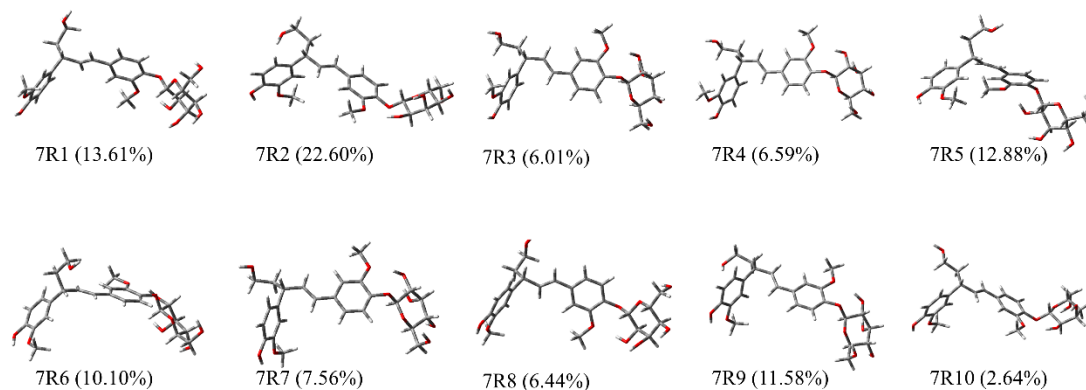


Figure S24: The optimized 10 conformers and equilibrium population of conformers of 7R for ECD calculation of compound **1**

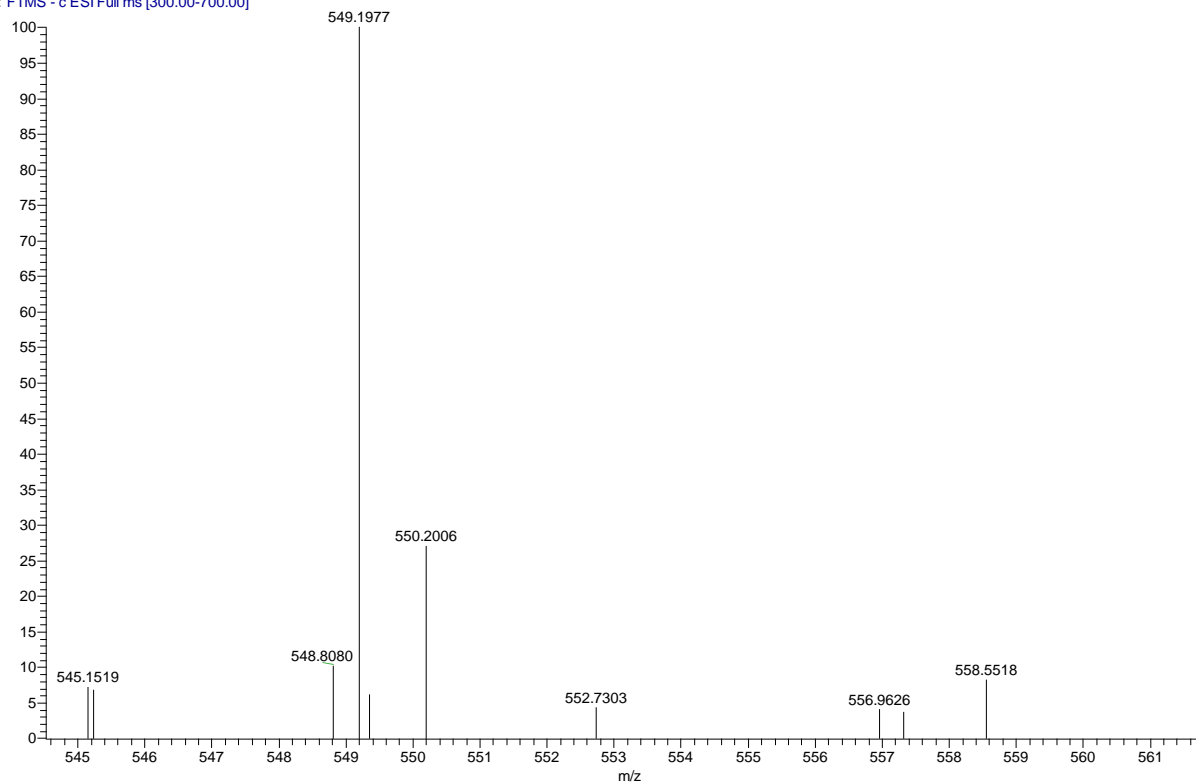
Table S1: Stable conformational energy and Maxwell-Boltzmann distribution population of 7S for ECD calculation of compound **1**

conformer	<i>E</i> (kcal/mol)	<i>P</i> (%)
1	-1081940.00260574	8.70
2	-1081939.68941549	5.13
3	-1081940.05274378	9.47
4	-1081940.20673474	12.29
5	-1081940.07200834	9.79
6	-1081939.68583869	5.10
7	-1081939.92046468	7.58
8	-1081940.65389836	26.16
9	-1081939.96790443	8.21
10	-1081939.92046468	7.58

Table S2: Stable conformational energy and Maxwell-Boltzmann distribution population of 7R for ECD calculation of compound **1**

conformer	<i>E</i> (kcal/mol)	<i>P</i> (%)
1	-1081940.14335623	13.61
2	-1081940.44343151	22.60
3	-1081939.65935776	6.01
4	-1081939.71395114	6.59
5	-1081940.11066296	12.88
6	-1081939.96690042	10.10
7	-1081939.79502543	7.56
8	-1081939.70027142	6.44
9	-1081940.04784921	11.58
10	-1081939.17253551	2.64

C26 #94 RT: 0.83 AV: 1 NL: 1.41E4
T: FTMS - c ESI Full ms [300.00-700.00]



Formula (M)	Ion Formula	m/z	Calc m/z
C27 H34 O12	C27 H33 O12	549.1977	549.1972

Figure S25: HRESIMS of compound 2

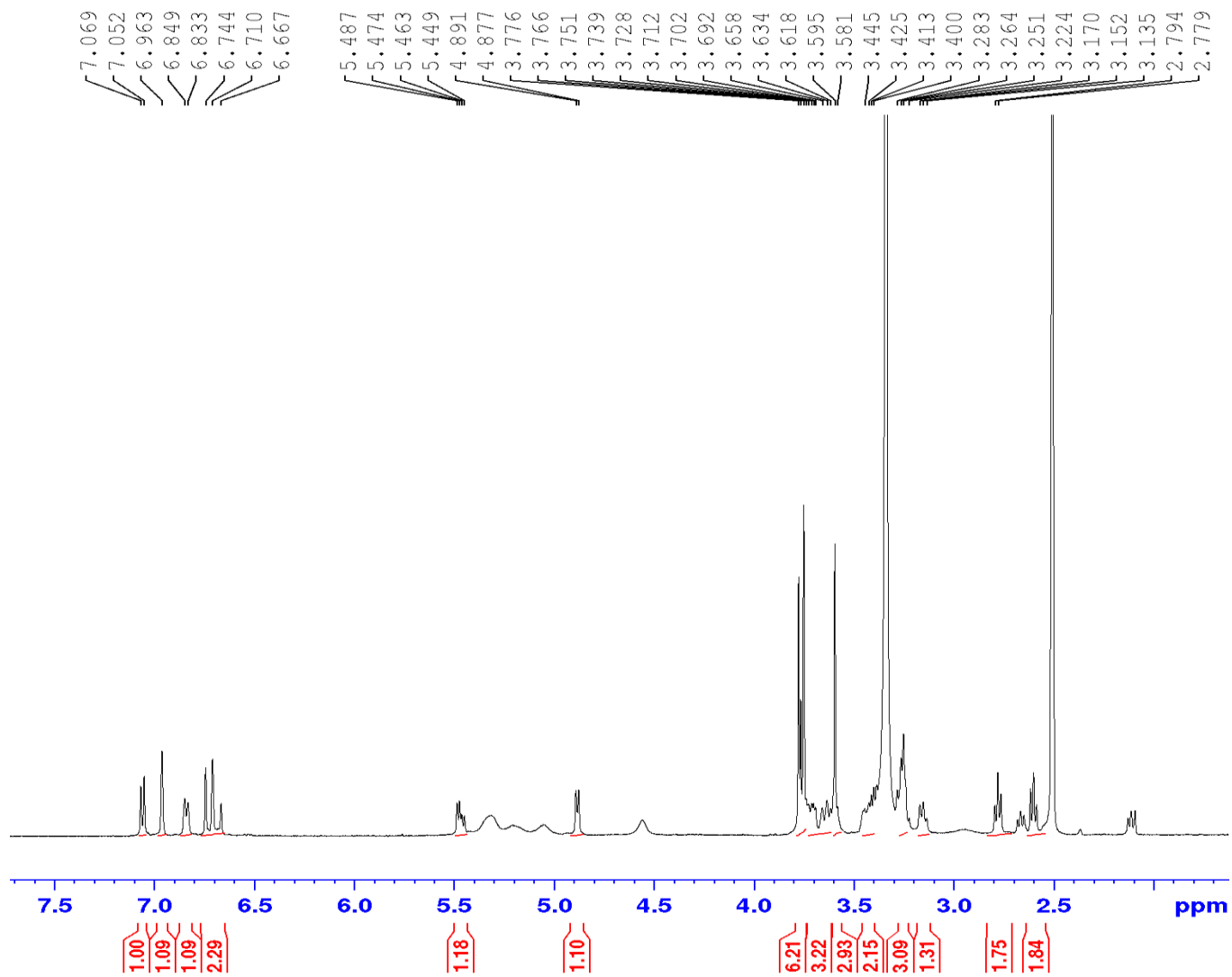


Figure S26: ¹H NMR spectrum of compound **2** (DMSO-*d*₆, 500 MHz)

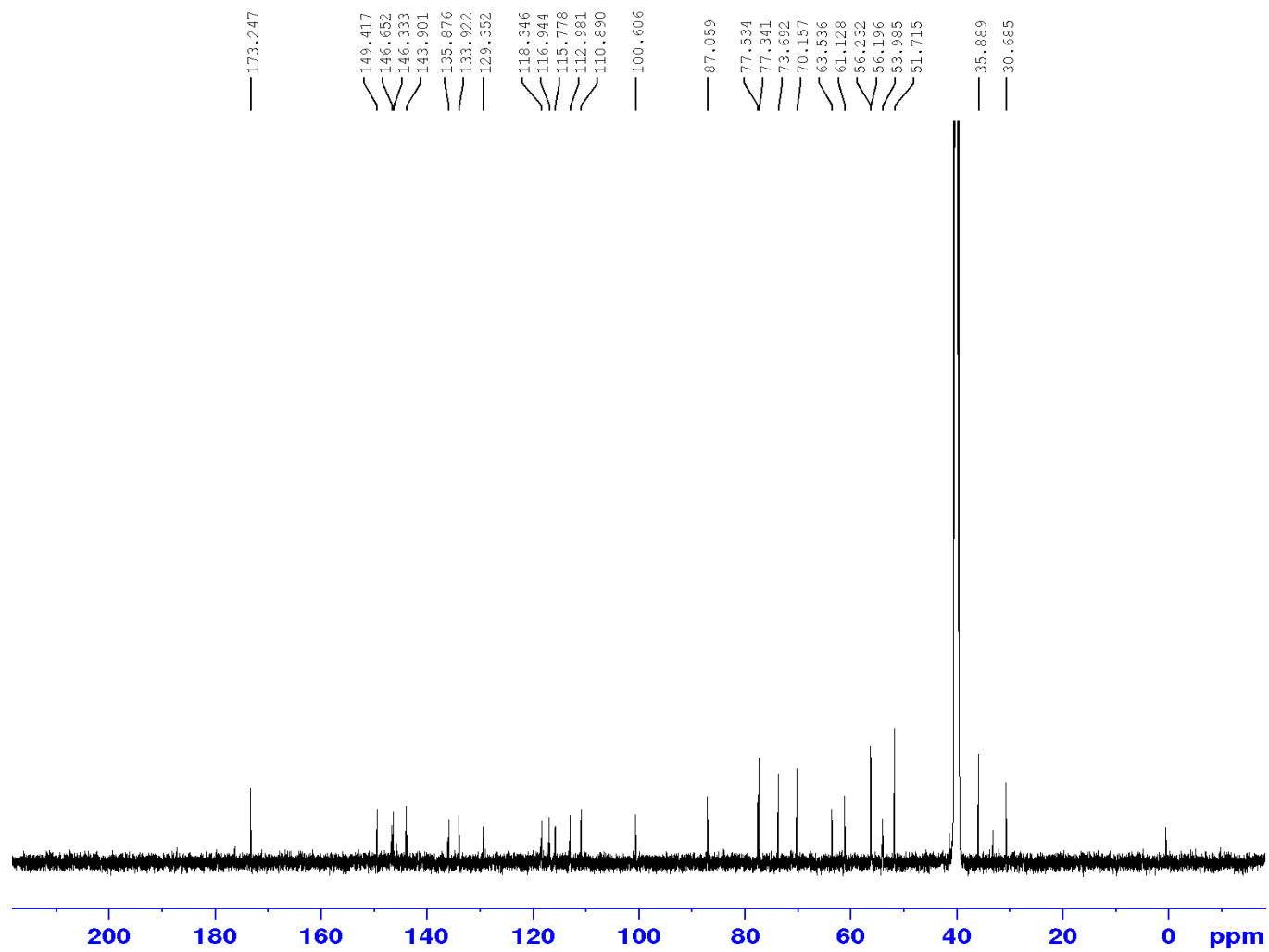


Figure S27: ^{13}C NMR spectrum of compound **2** ($\text{DMSO-}d_6$, 125 MHz)

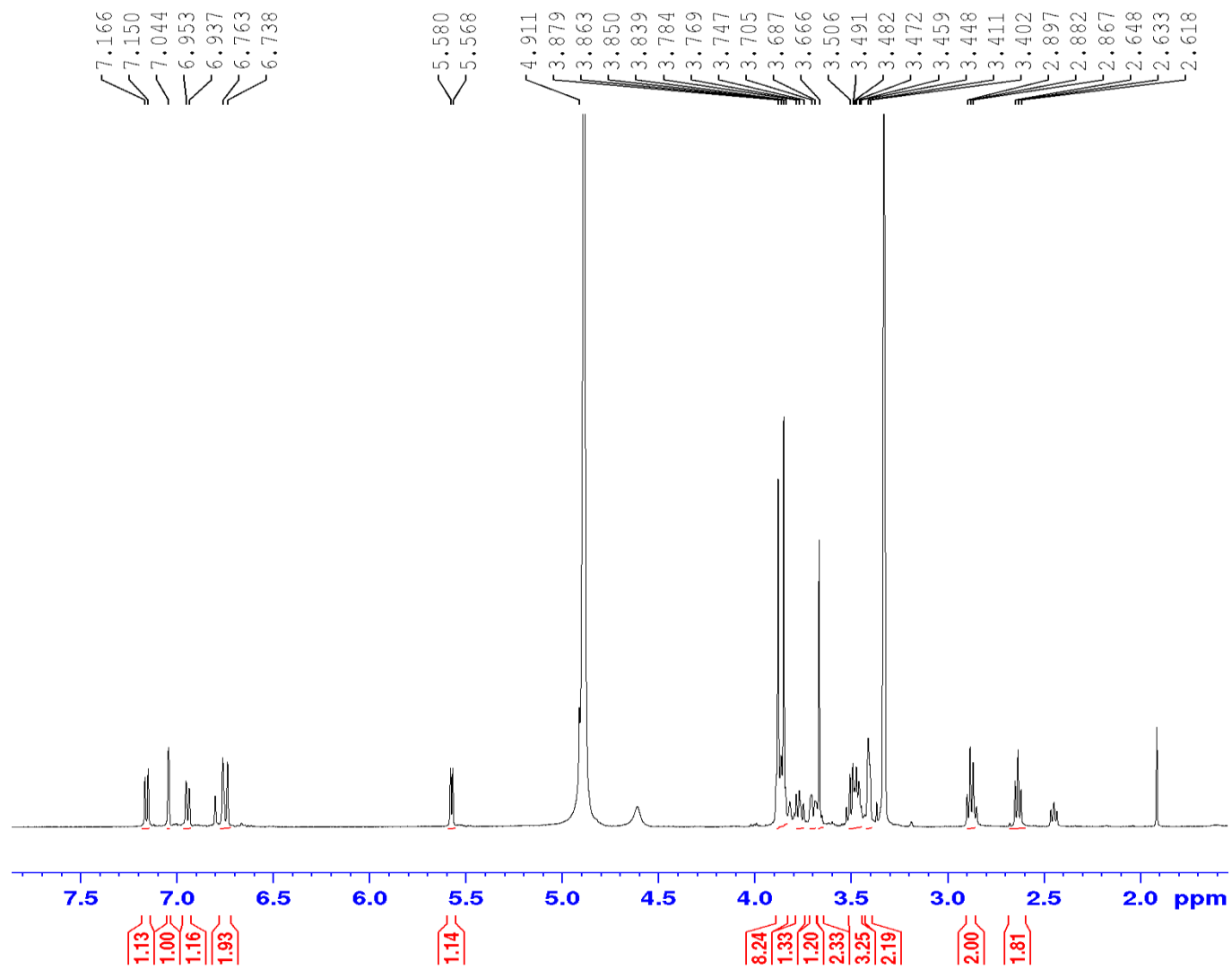


Figure S28: ^1H NMR spectrum of compound **2** (CD_3OD , 500 MHz)

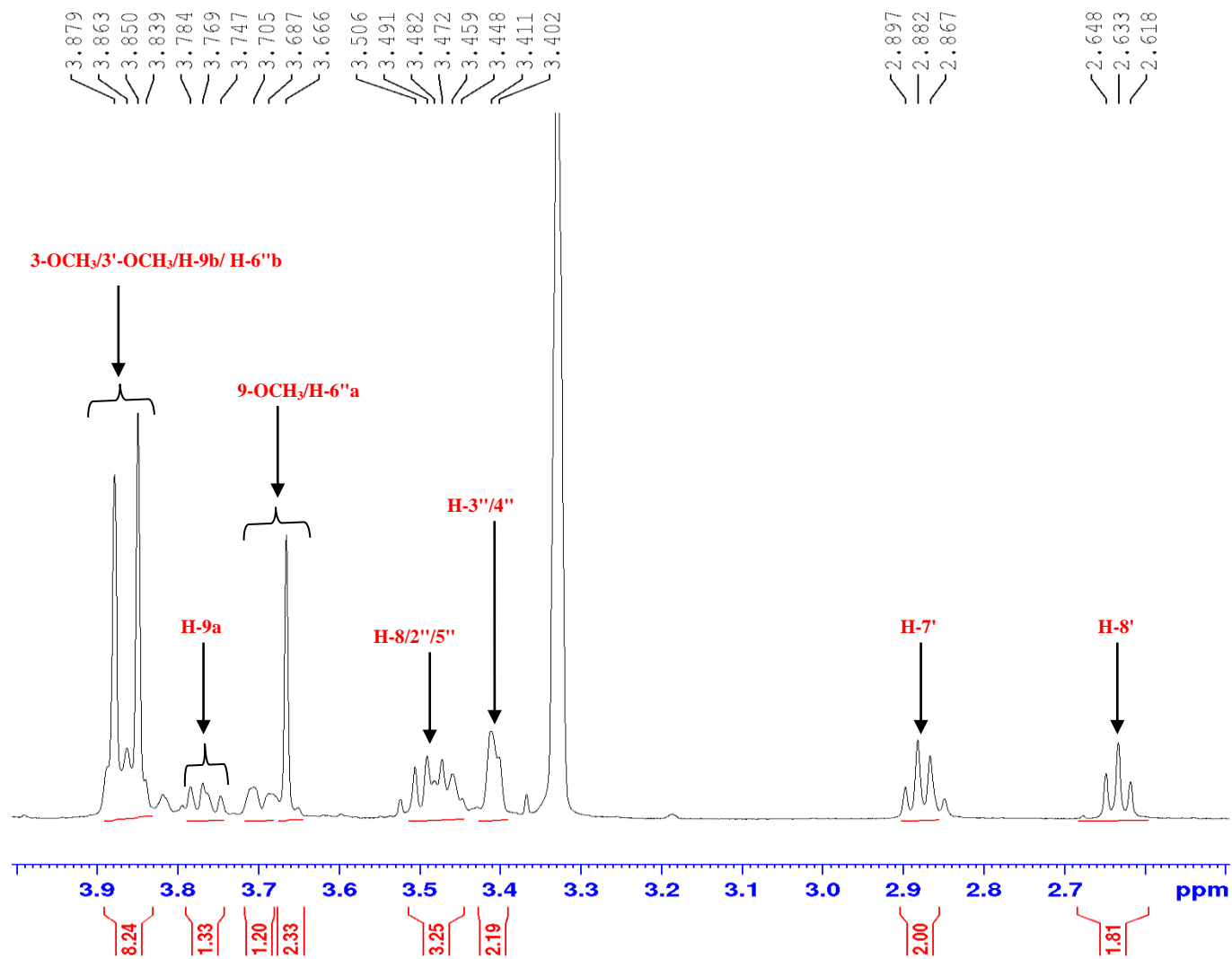


Figure S29: ¹H NMR spectrum of compound **2** (CD₃OD, 500 MHz, from 2.5 to 4.0 ppm)

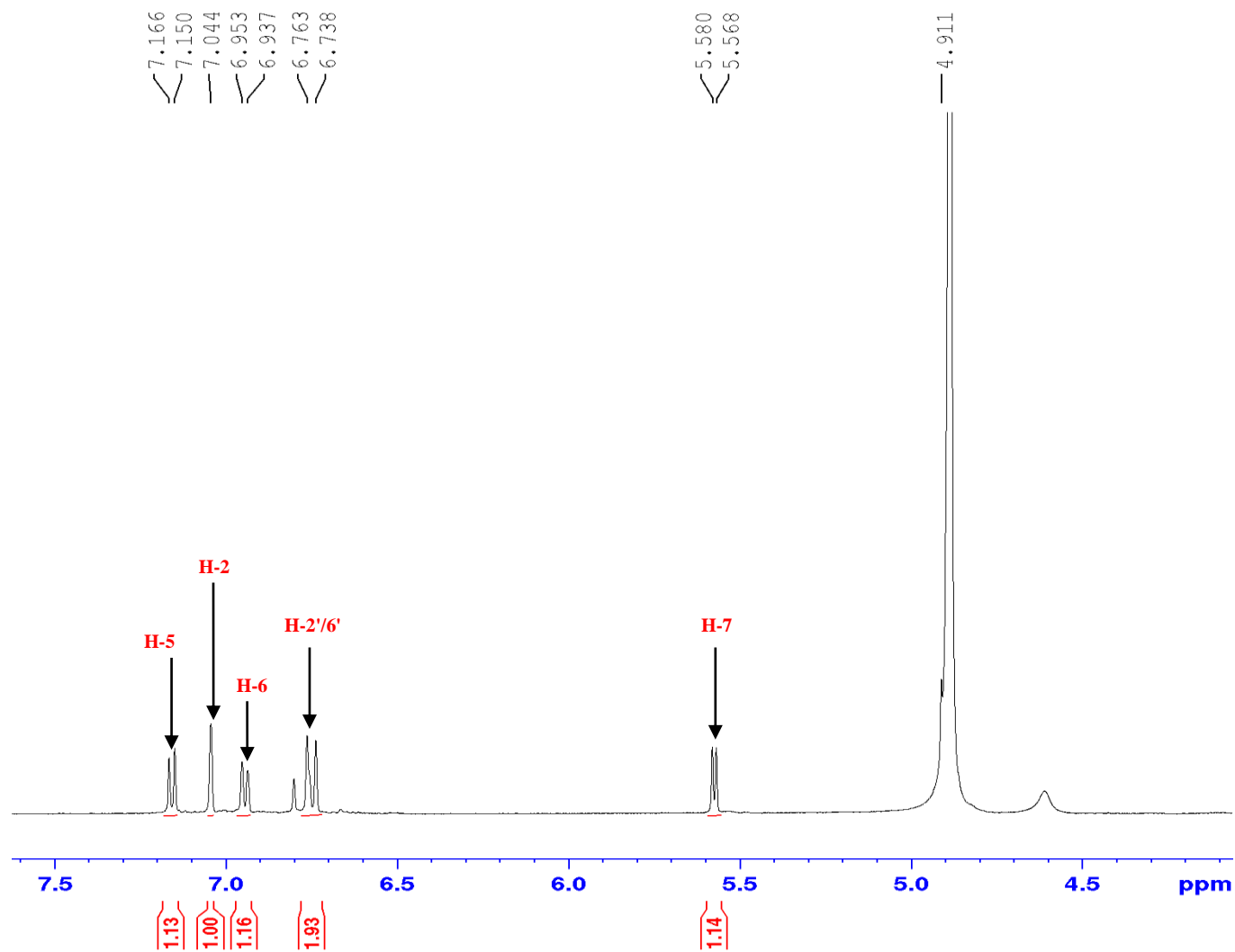


Figure S30: ^1H NMR spectrum of compound **2** (CD_3OD , 500 MHz, from 4.5 to 7.5 ppm)

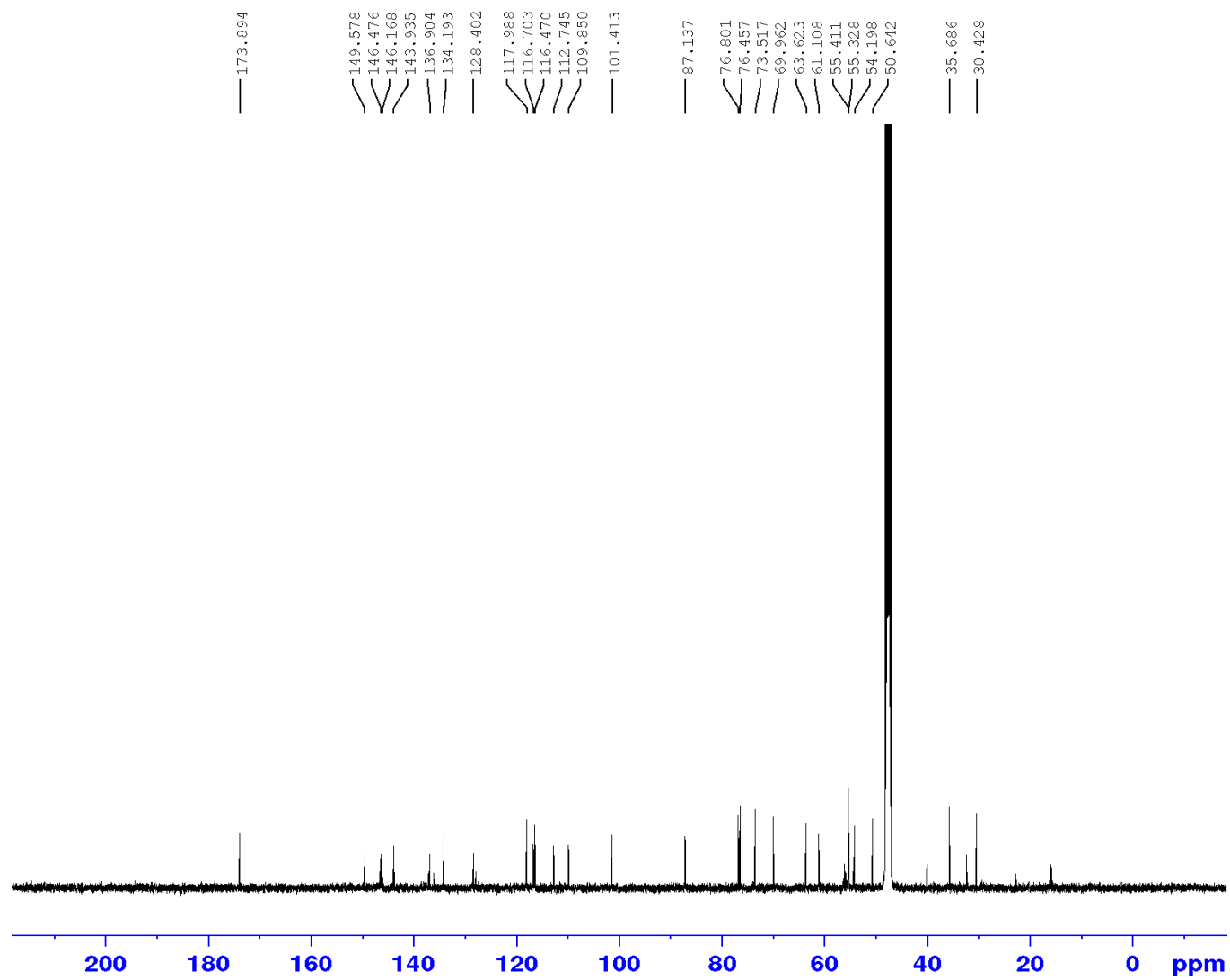


Figure S31: ^{13}C NMR spectrum of compound **2** (CD_3OD , 125 MHz)

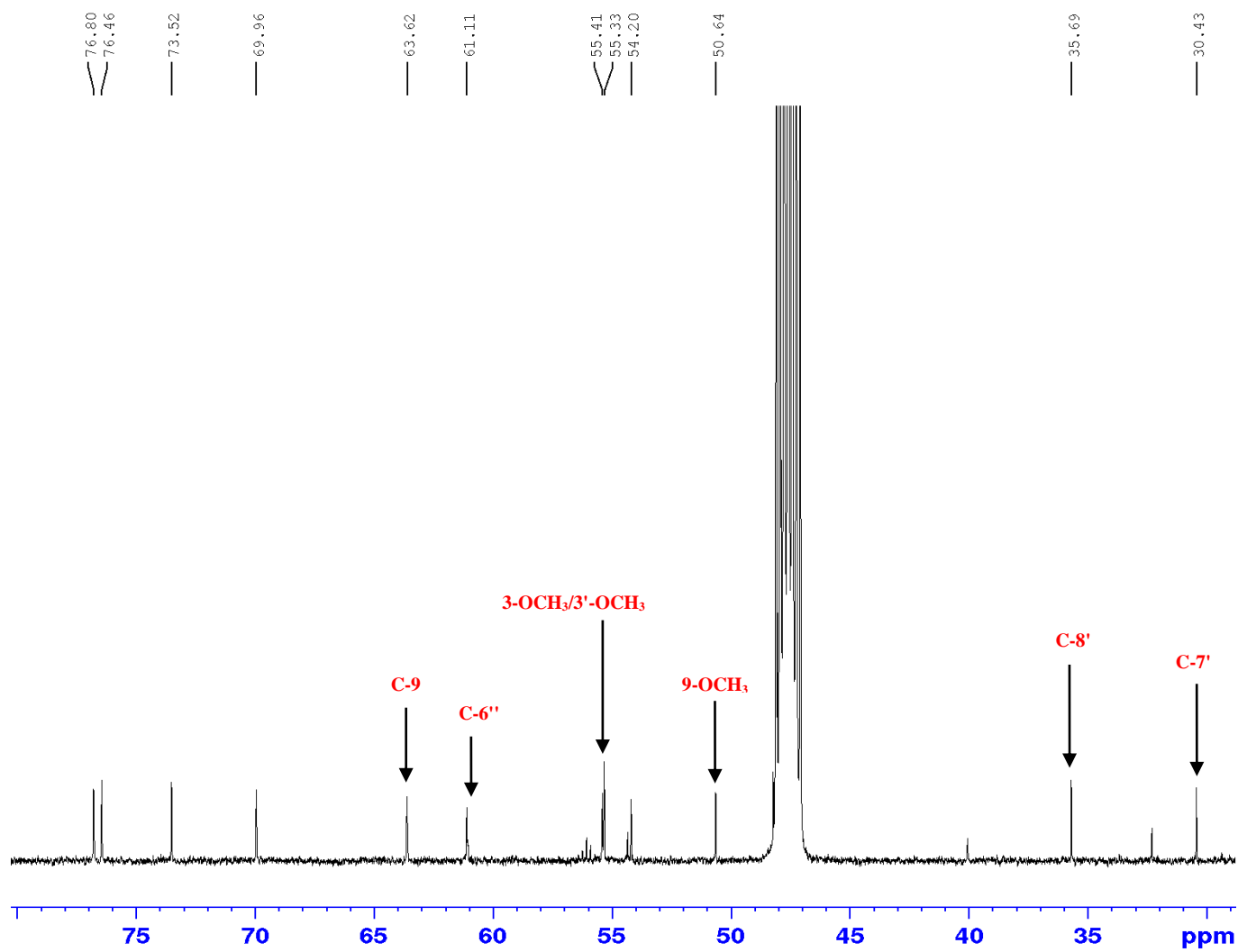


Figure S32: ^{13}C NMR spectrum of compound **2** (CD_3OD , 125 MHz, from 29 to 80 ppm)

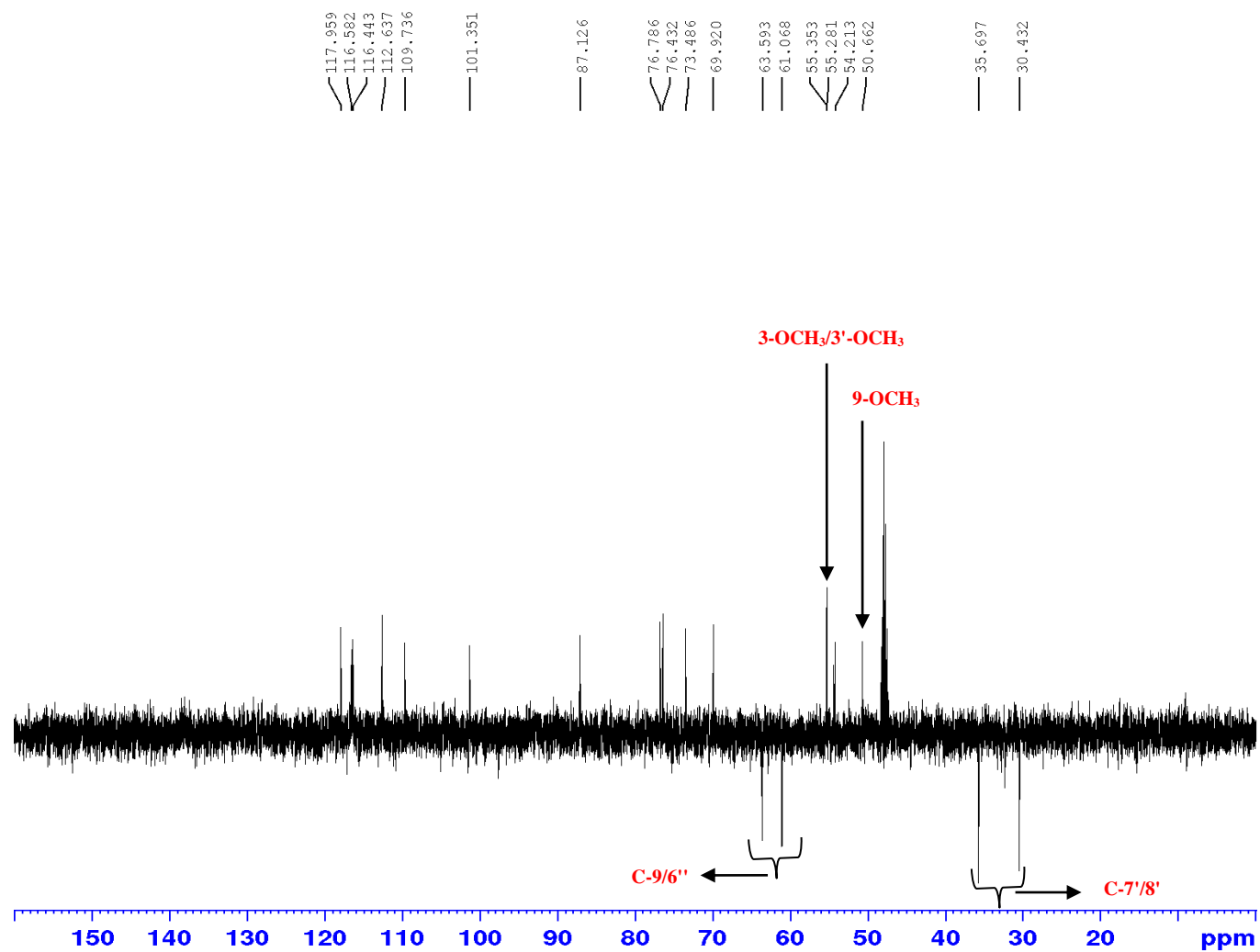


Figure S33: DEPT135 spectrum of compound **2** (CD₃OD, 125 MHz)

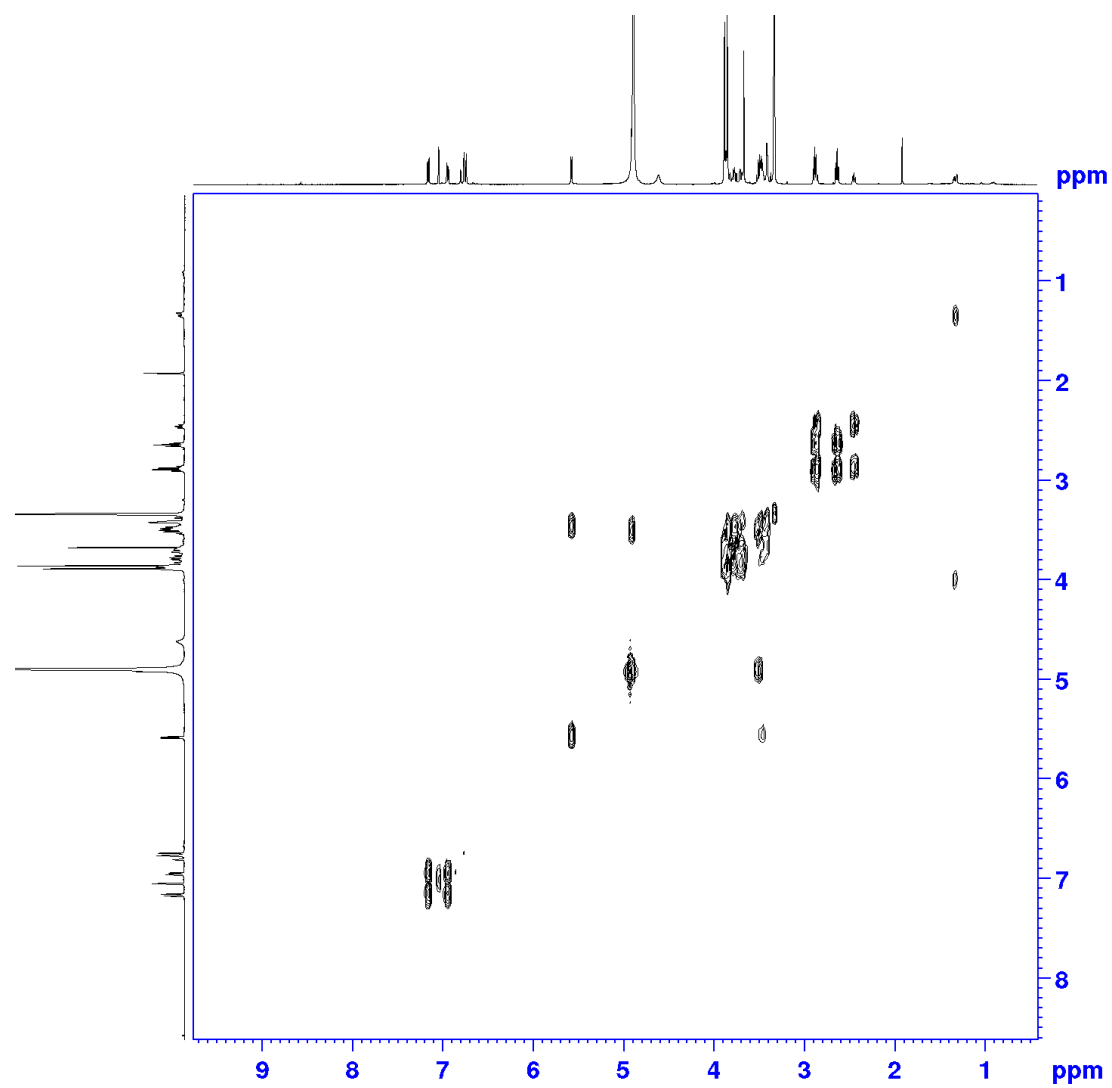


Figure S34: ^1H - ^1H COSY spectrum of compound **2** (CD_3OD , 500 MHz)

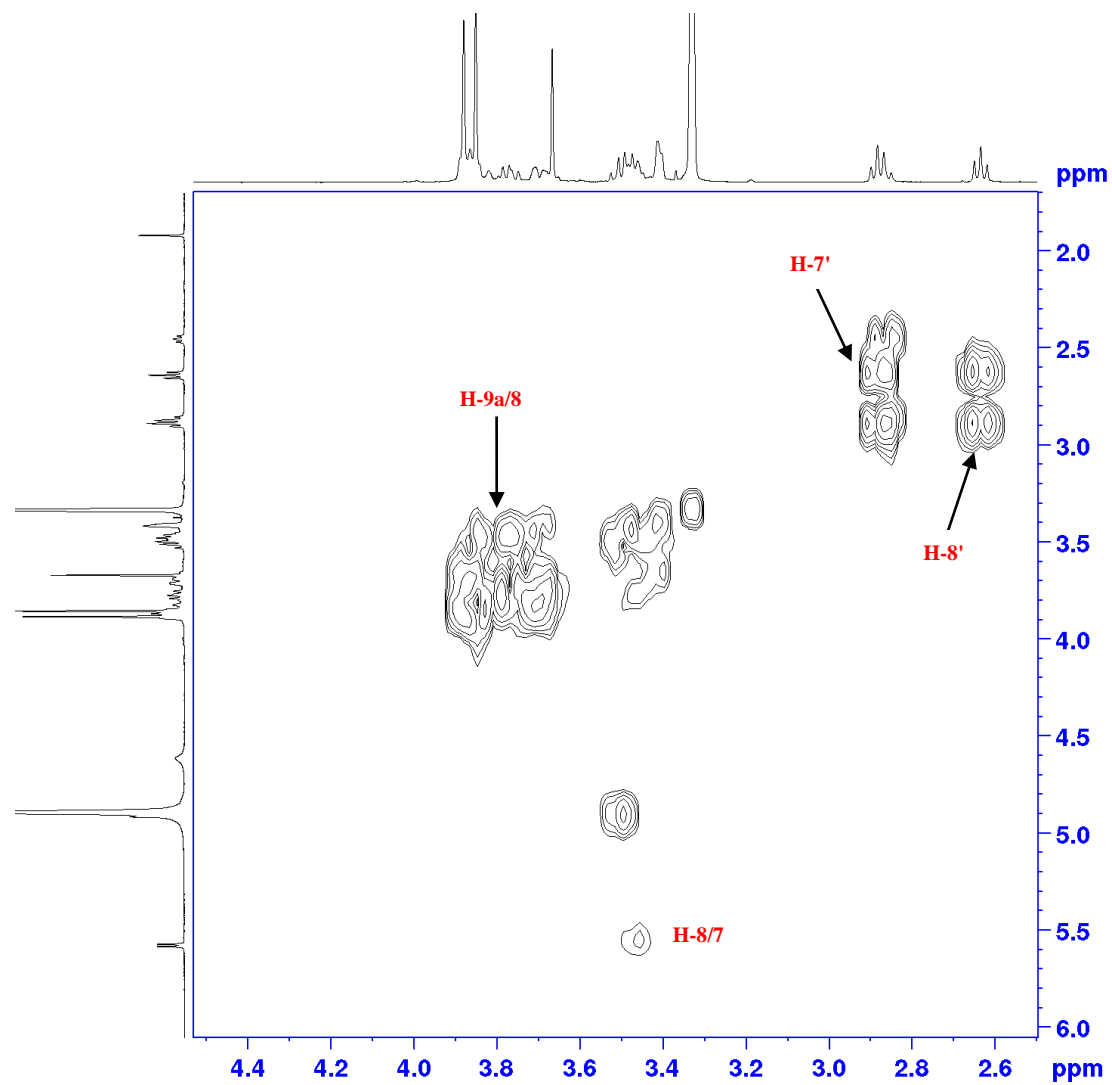


Figure S35: ^1H - ^1H COSY spectrum of compound **2** (CD_3OD , 500 MHz, from 2.5 to 4.4 ppm)

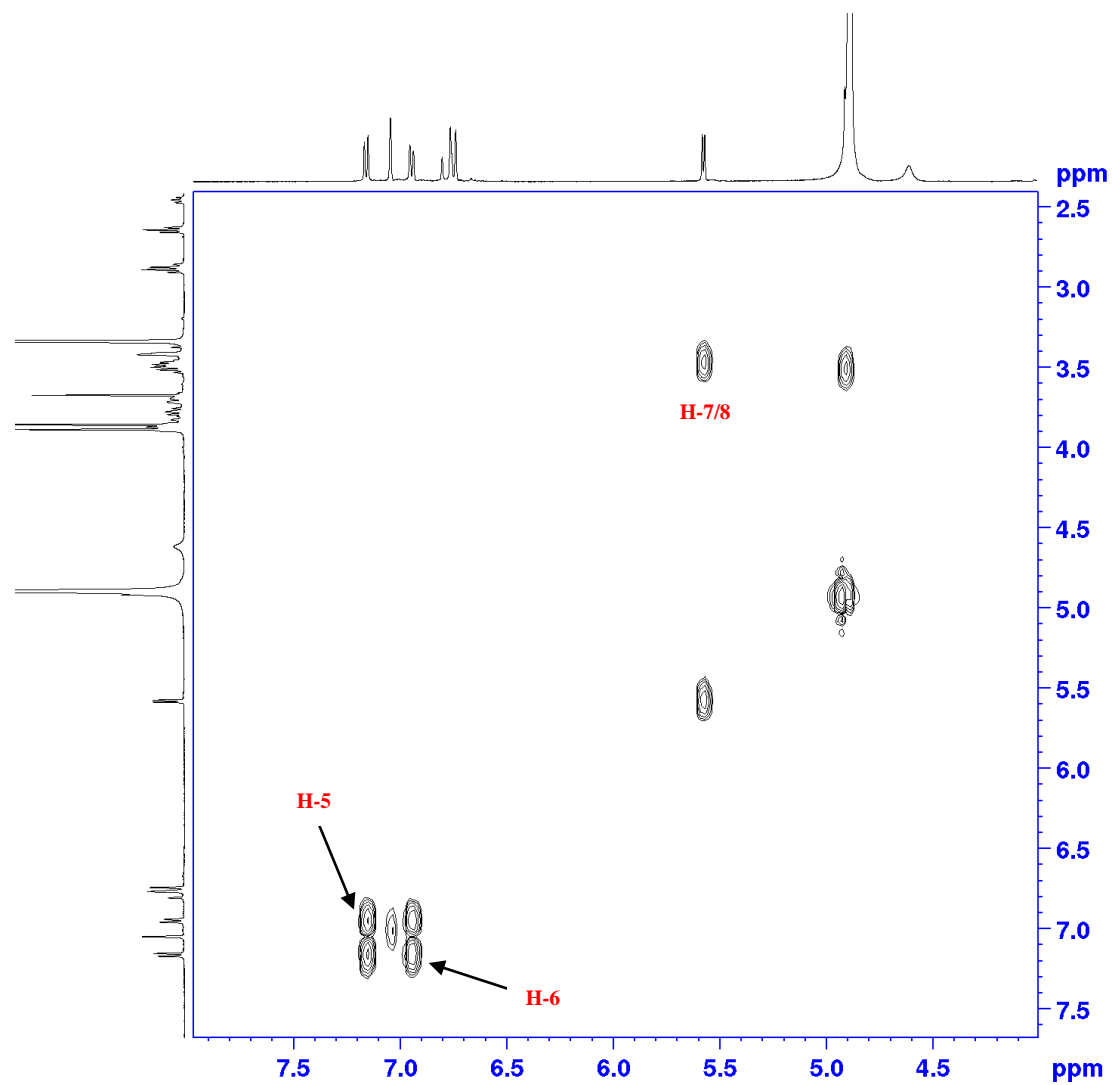


Figure S36: ^1H - ^1H COSY spectrum of compound **2** (CD_3OD , 500 MHz, from 4.5 to 7.5 ppm)

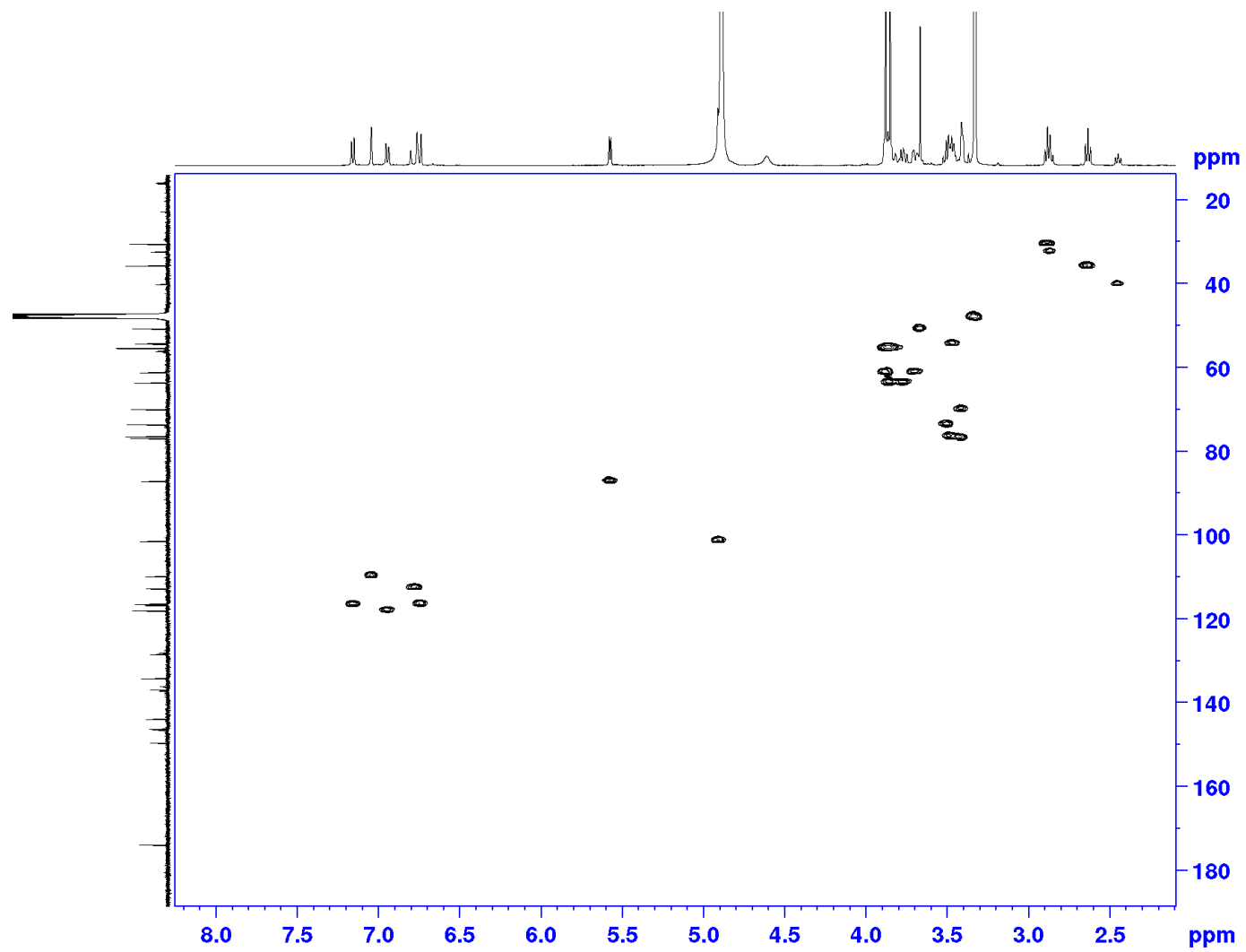


Figure S37: HSQC spectrum of compound **2** (CD₃OD, 500 MHz)



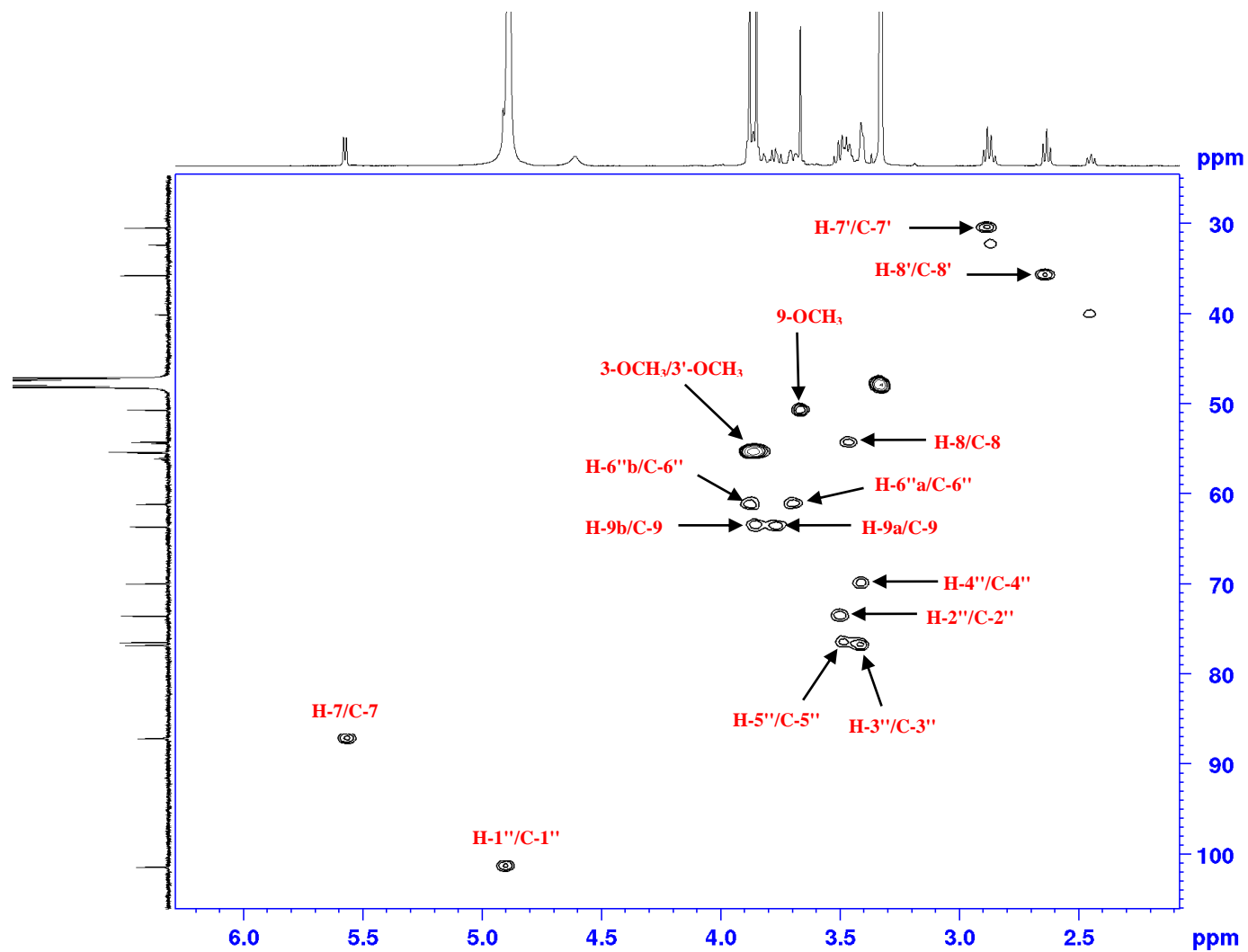


Figure S38: HSQC spectrum of compound 2 (CD₃OD, 500 MHz, from 25 to 105 ppm)

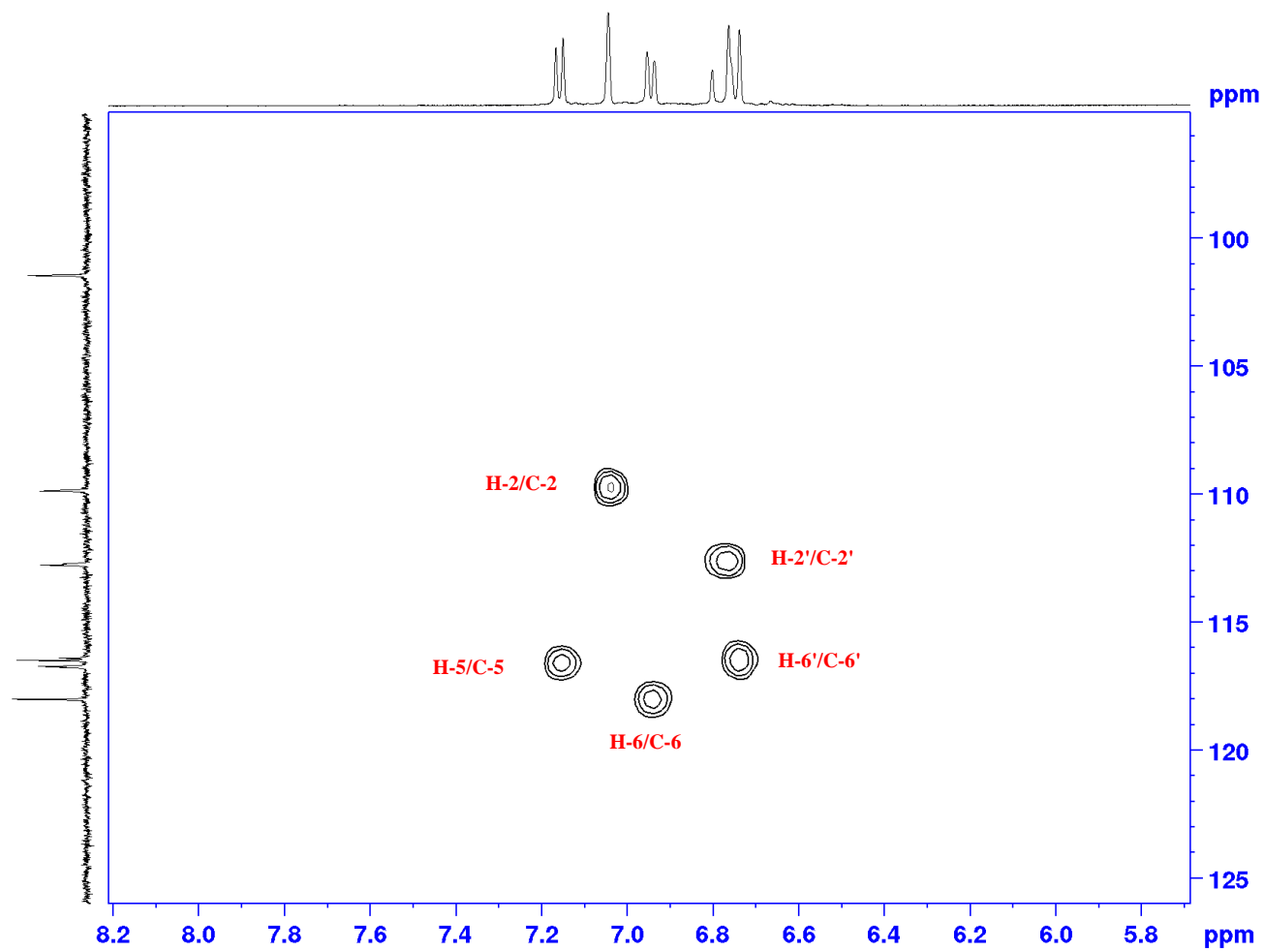


Figure S39: HSQC spectrum of compound 2 (CD₃OD, 500 MHz, from 105 to 125 ppm)

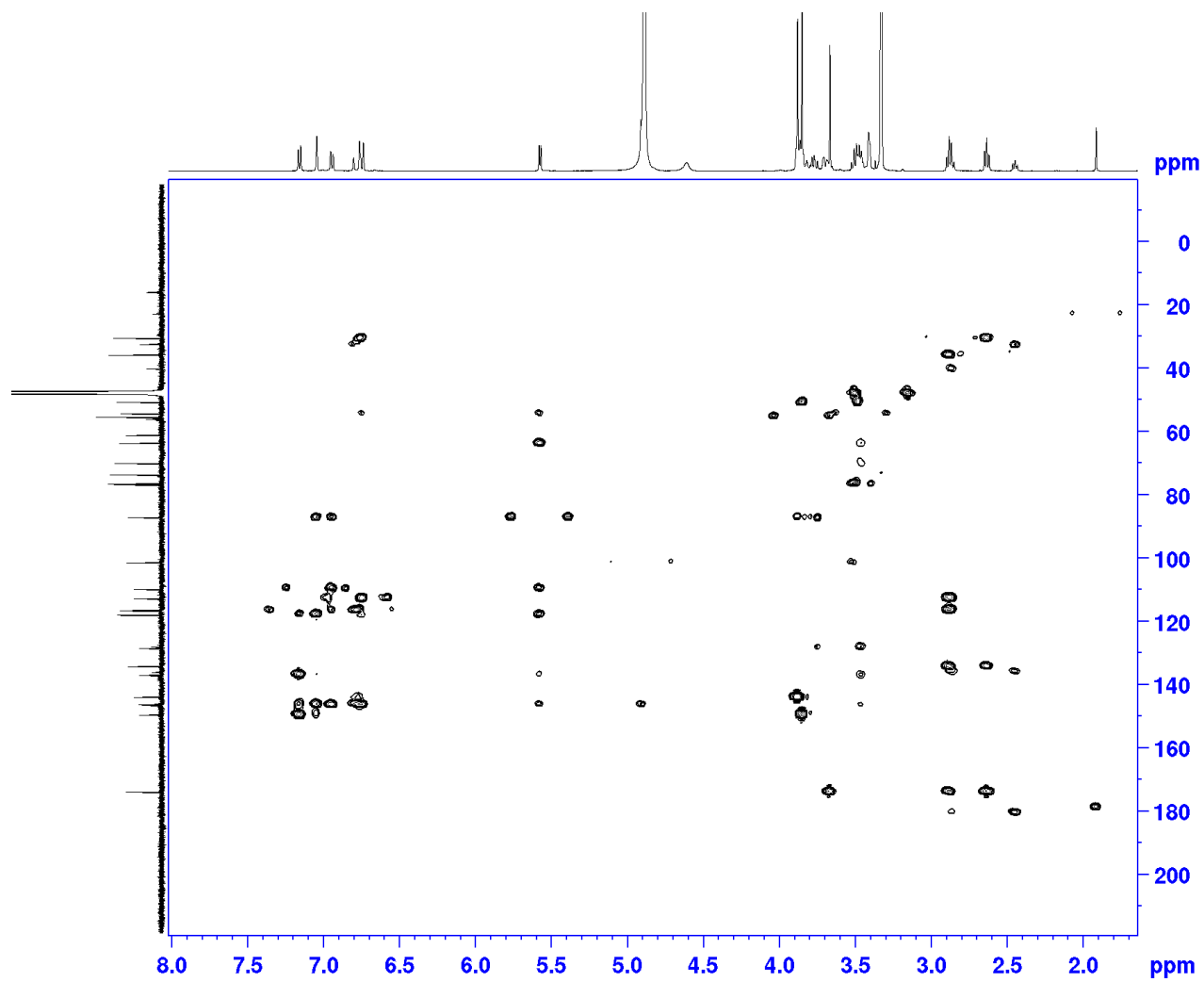


Figure S40: HMBC spectrum of compound **2** (CD₃OD, 500 MHz)

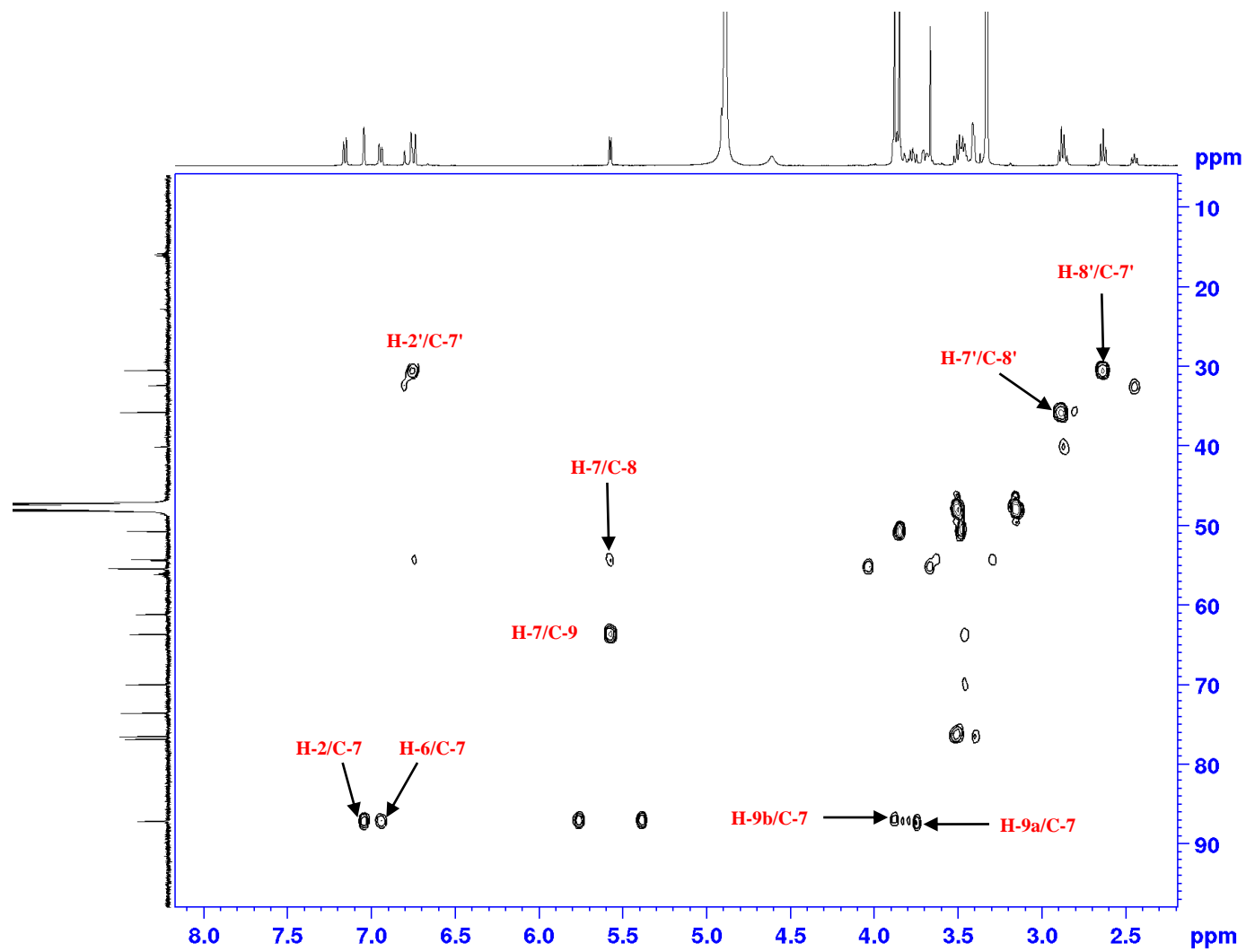


Figure S41: HMBC spectrum of compound **2** (CD_3OD , 500 MHz, from 20 to 95 ppm)

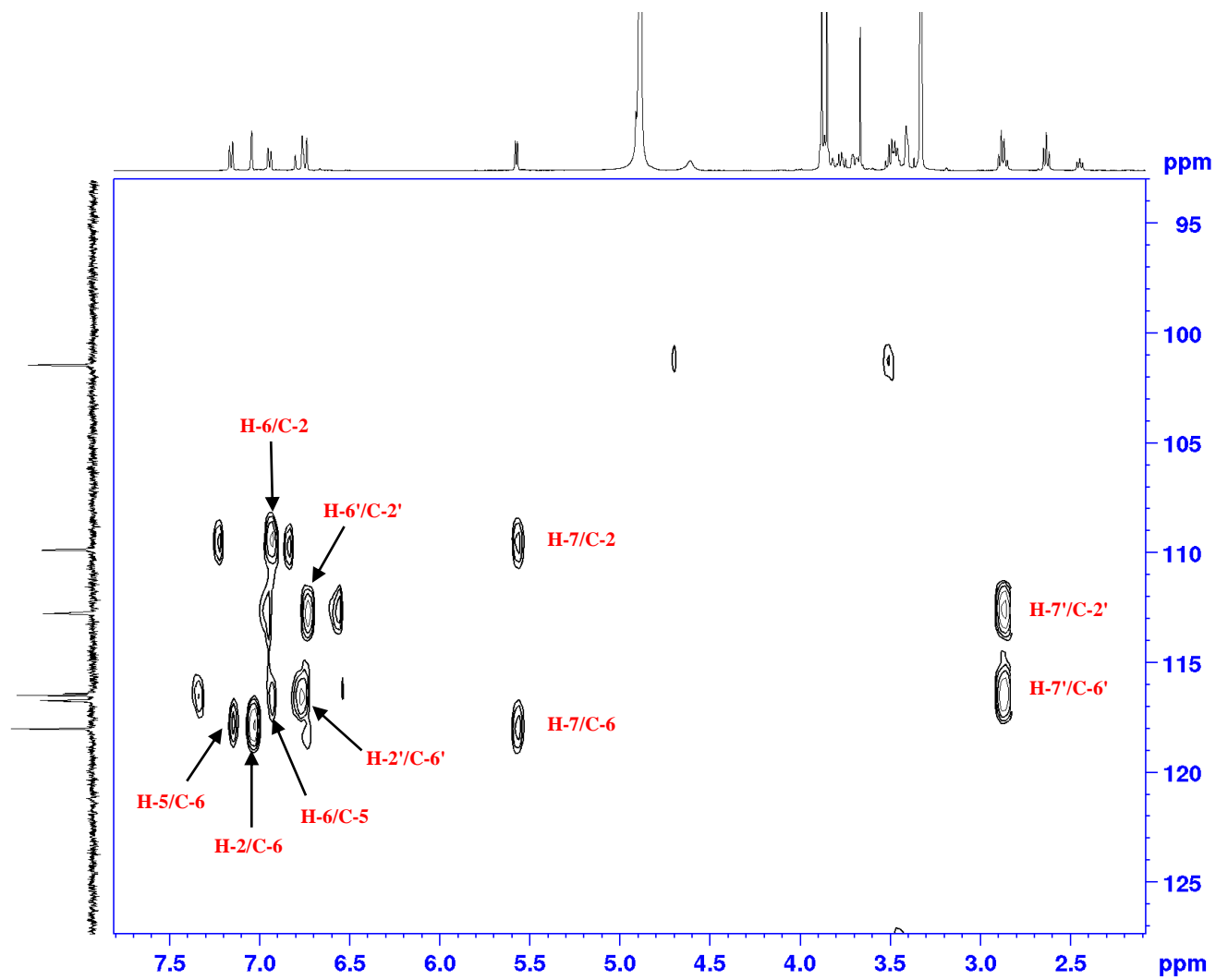


Figure S42: HMBC spectrum of compound 2 (CD₃OD, 500 MHz, from 95 to 125 ppm)

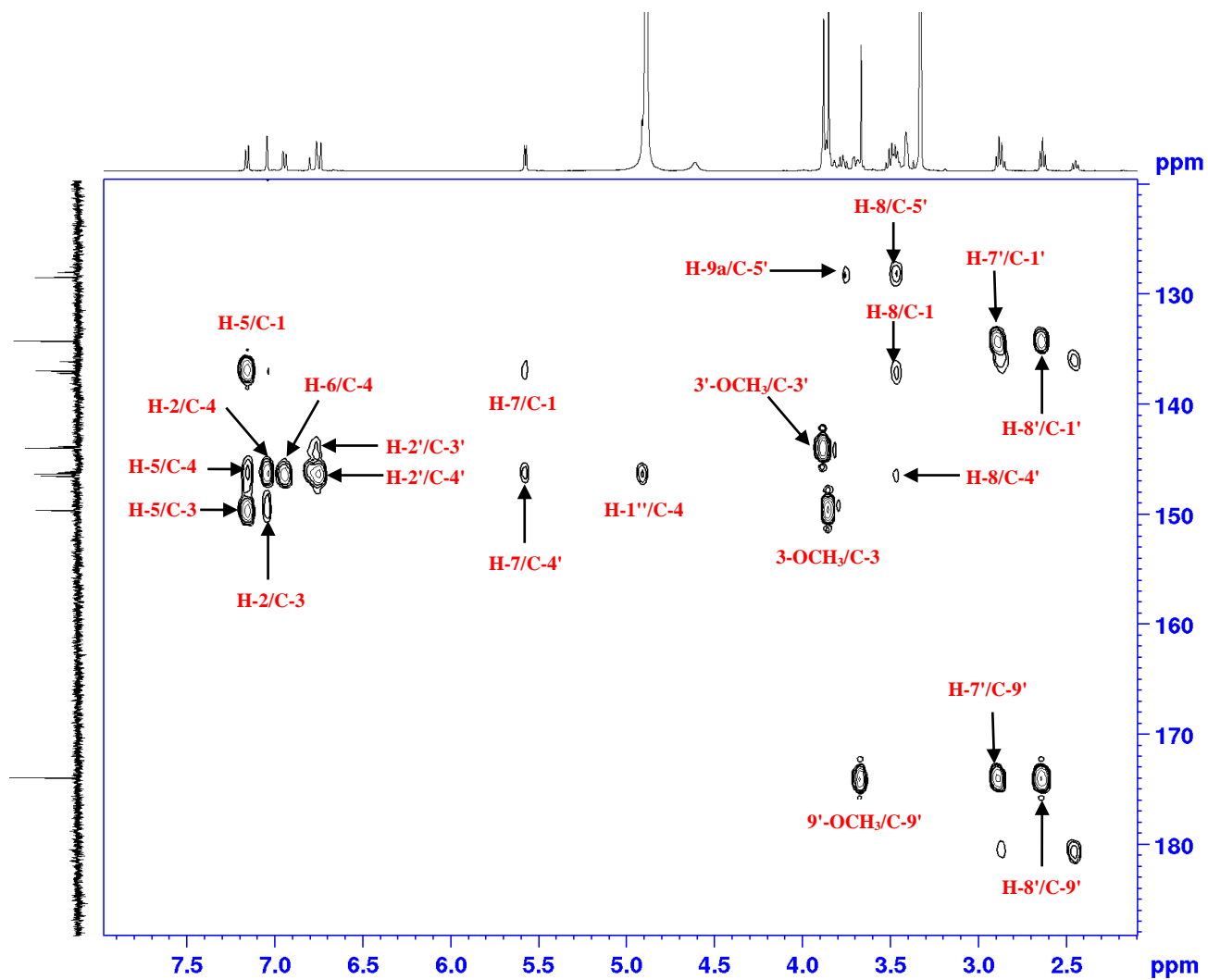


Figure S43: HMBC spectrum of compound **2** (CD_3OD , 500 MHz, from 125 to 175 ppm)

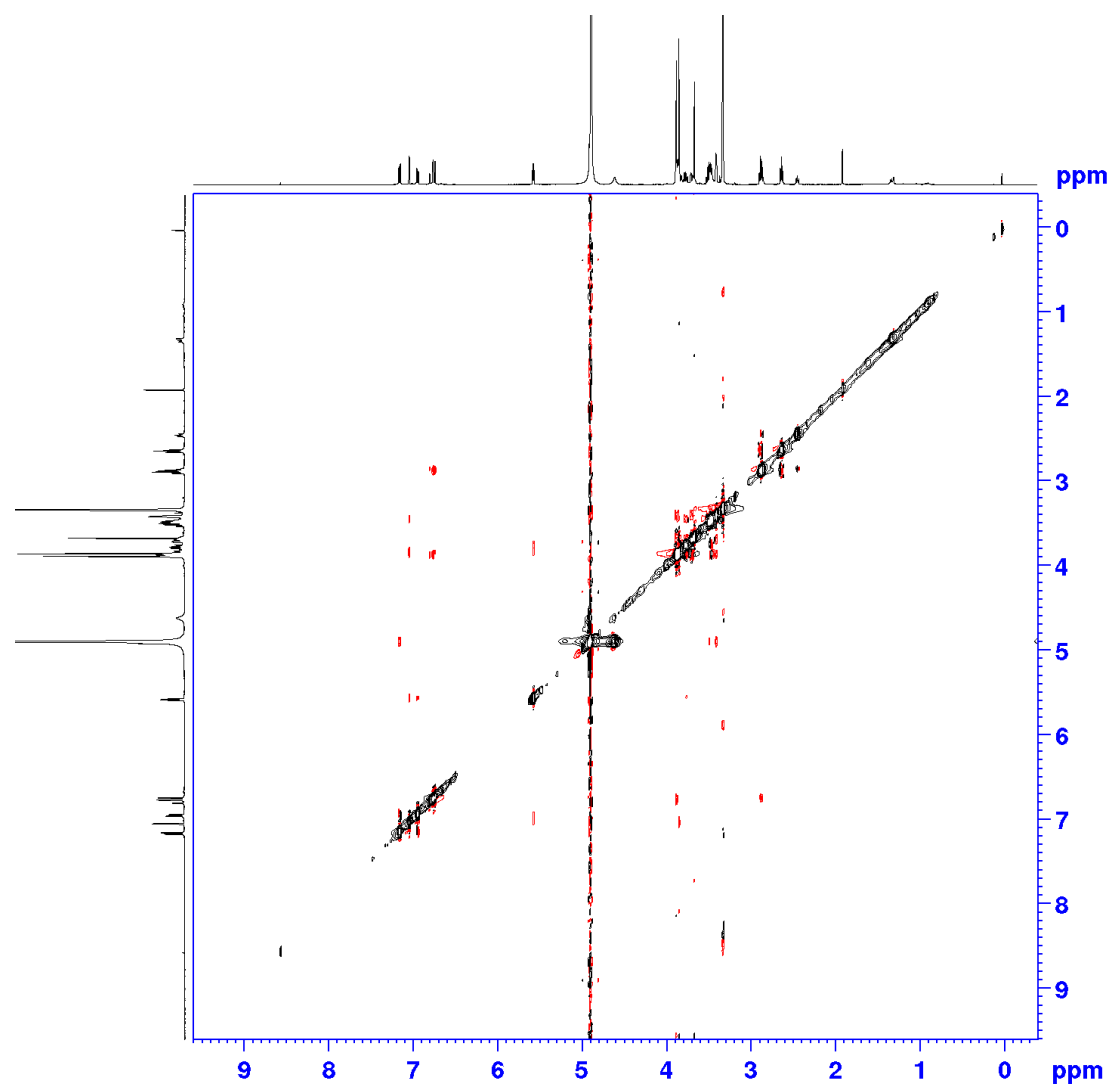


Figure S44: NOESY spectrum of compound **2** (CD₃OD, 500 MHz)

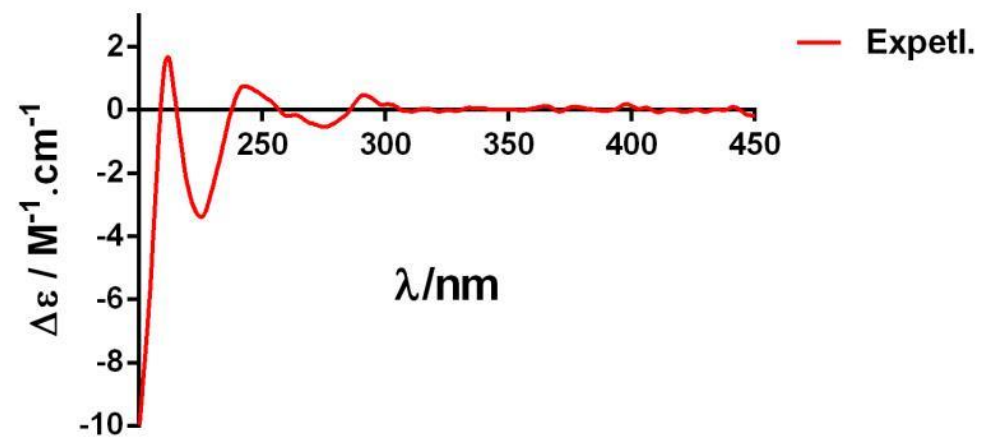


Figure S45: CD spectra of compound 2