

Supporting Information for

Update of spectroscopic data for 4-hydroxydictyolactone and dictyol E isolated from a *Halimeda stuposa* - *Dictyota* sp. Assemblage

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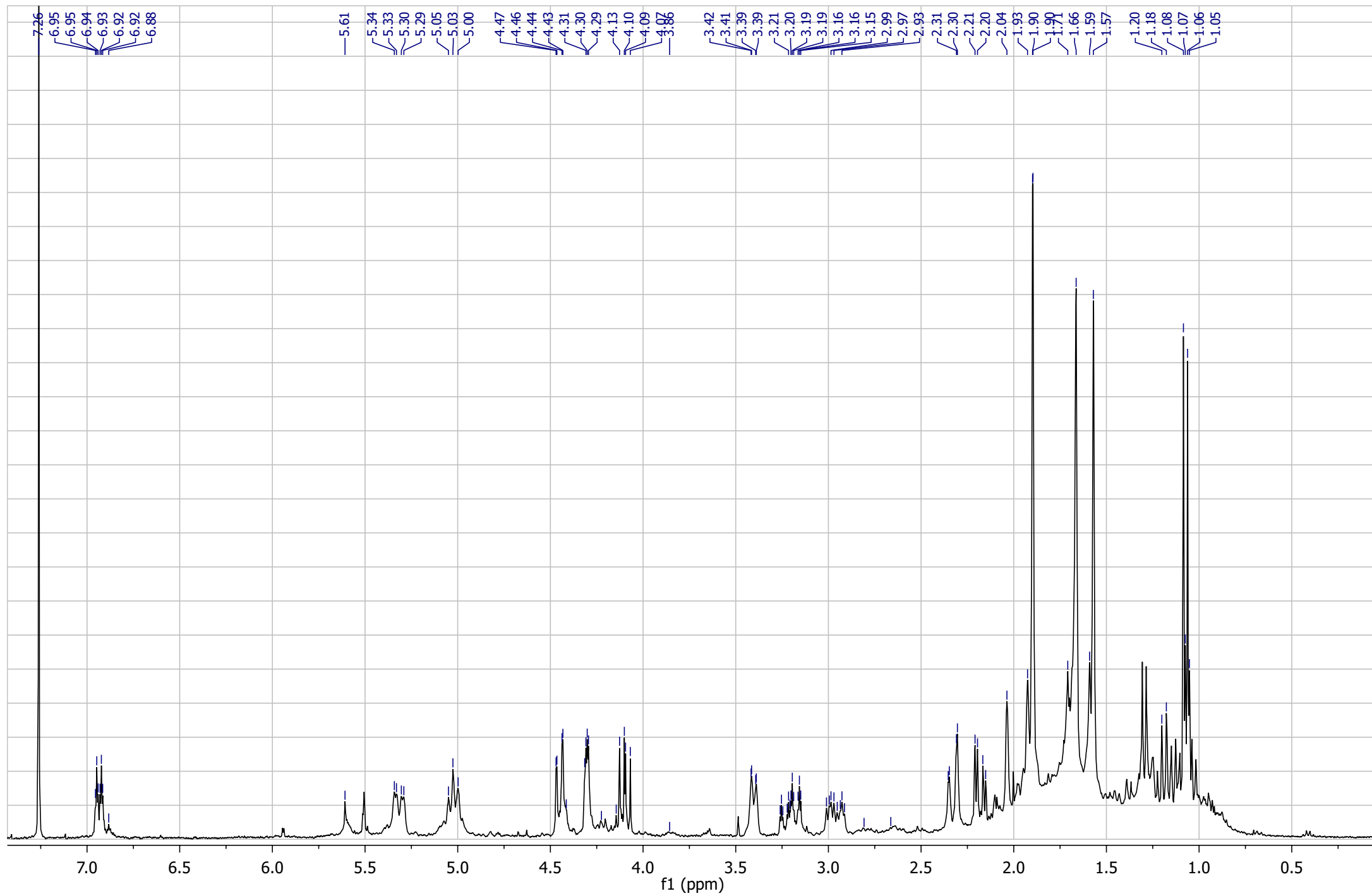
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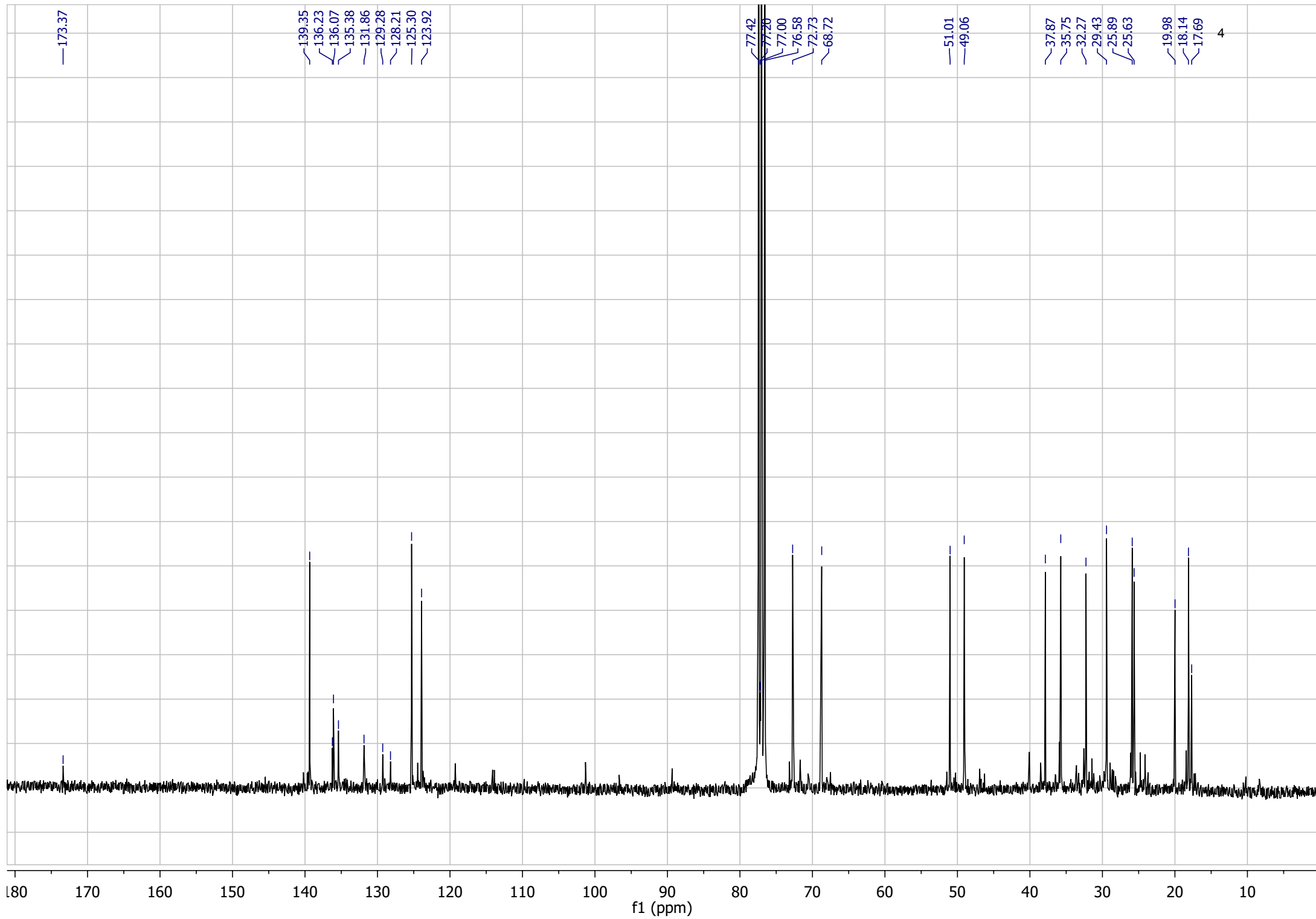
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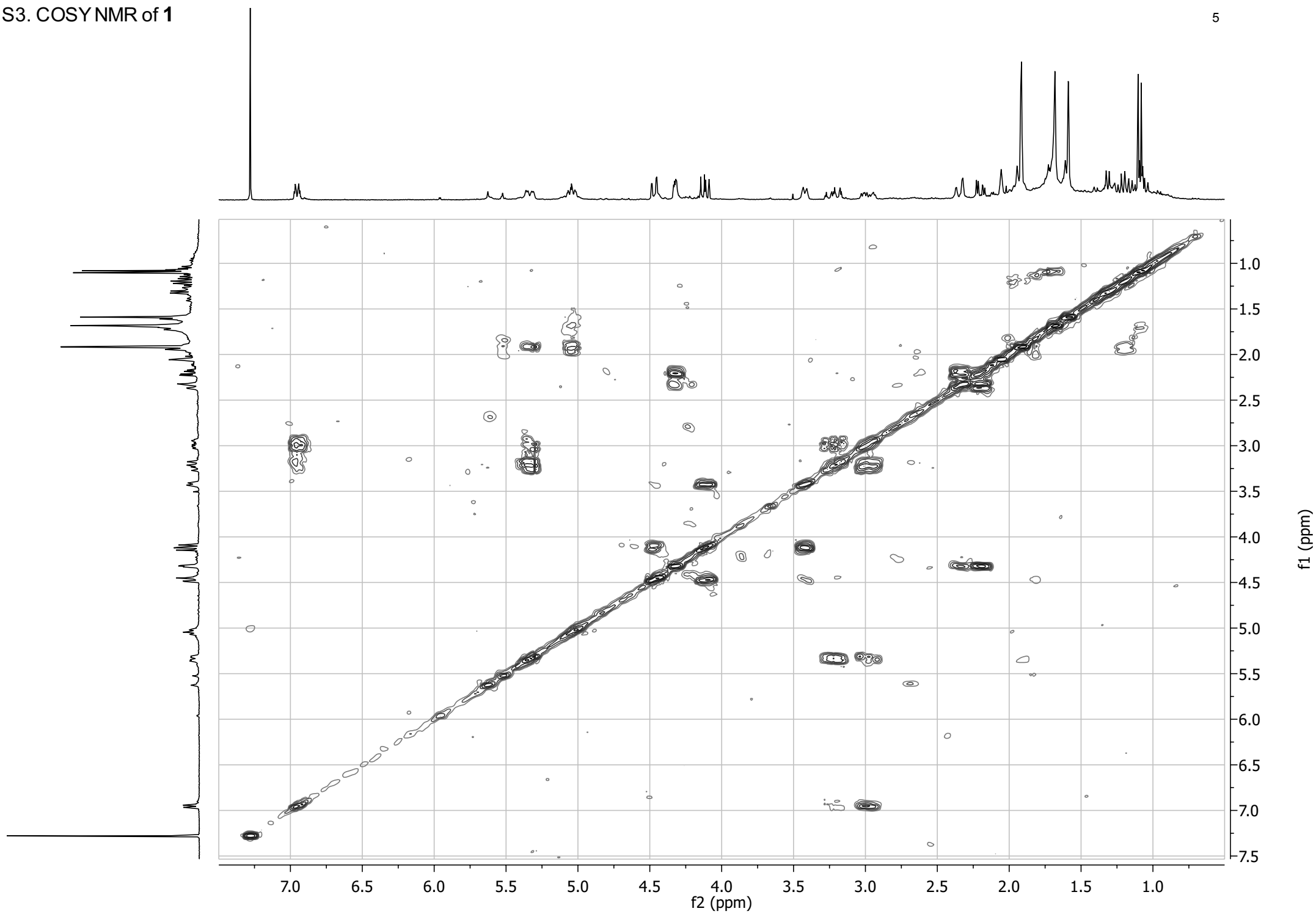
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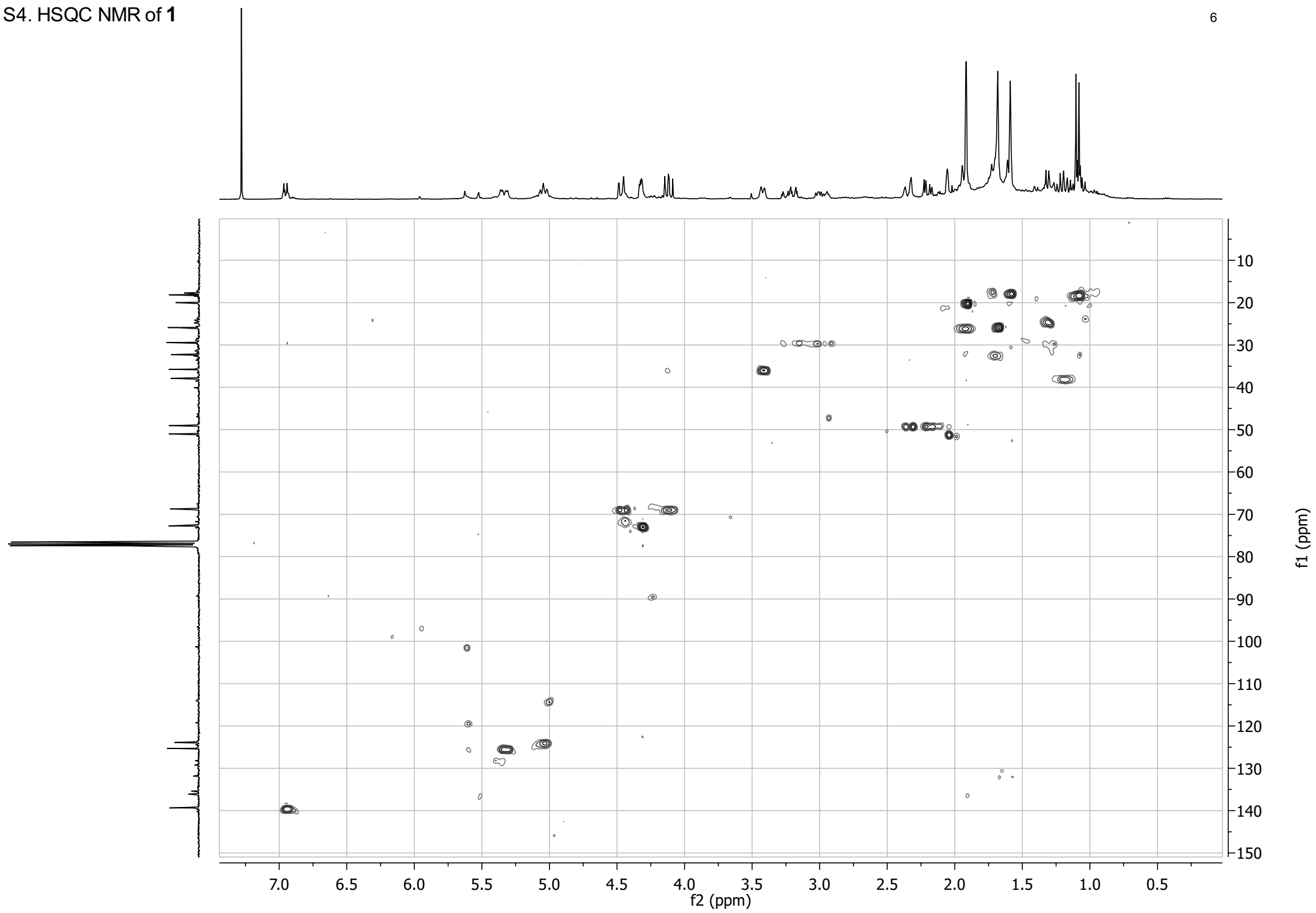
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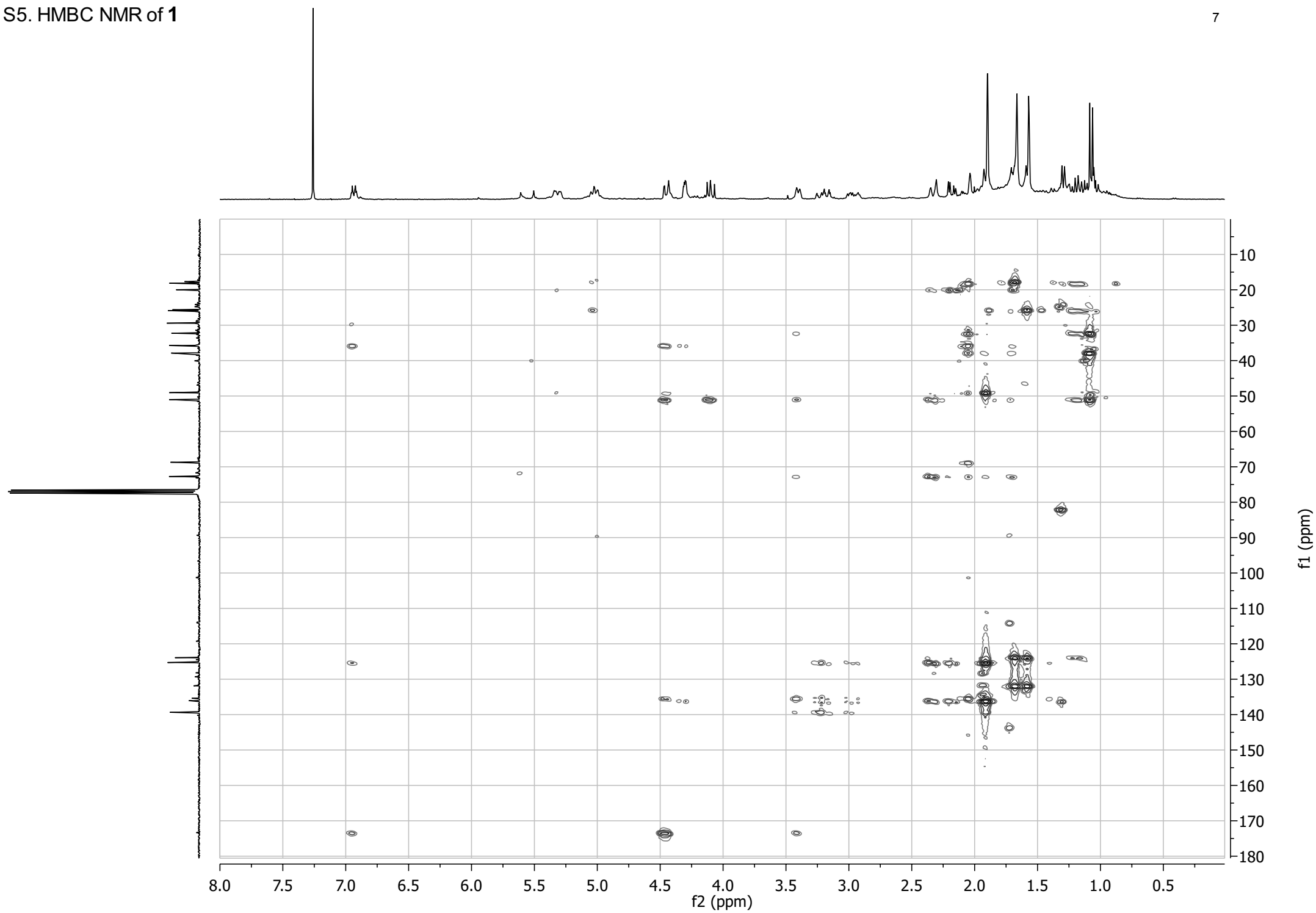
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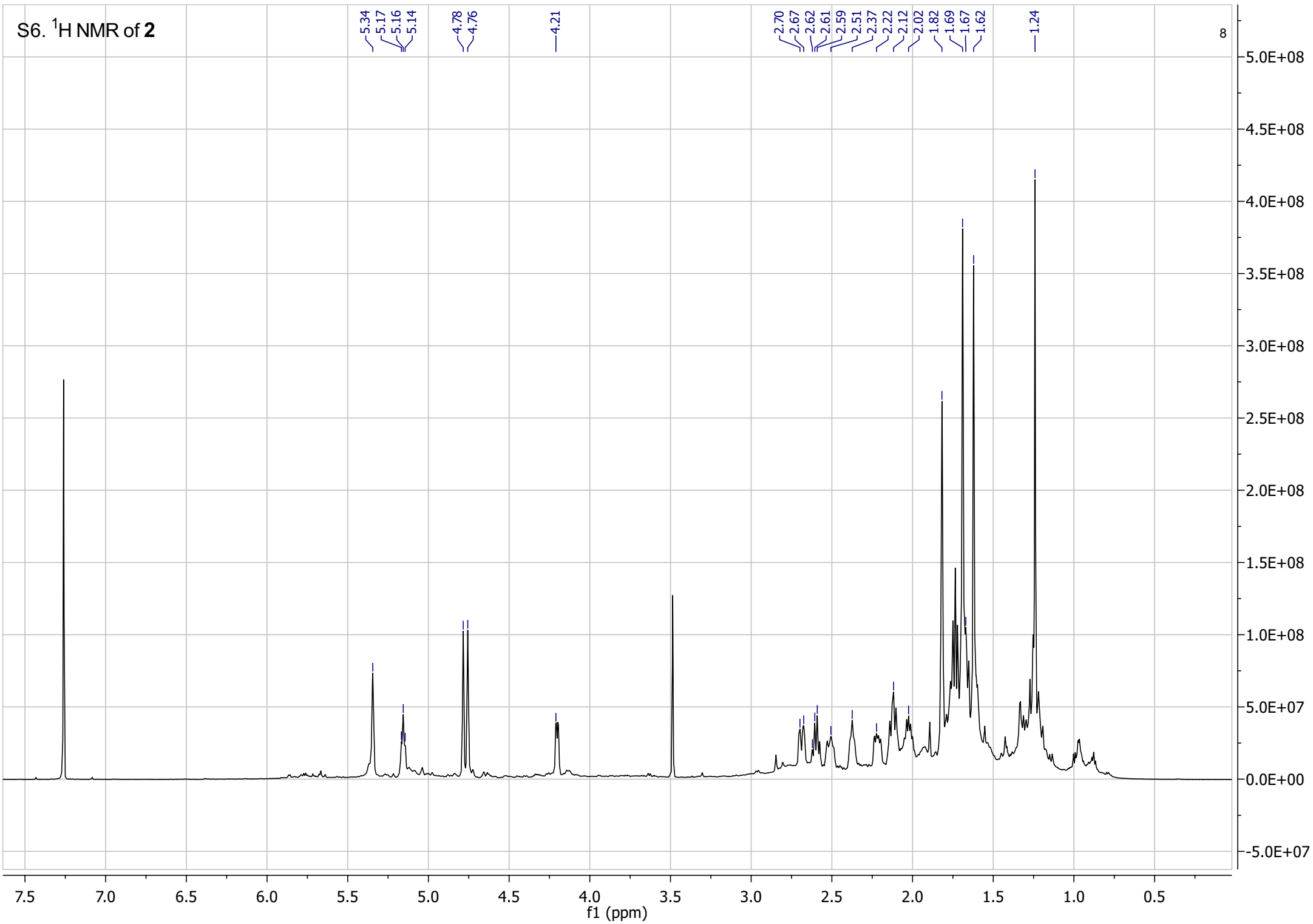


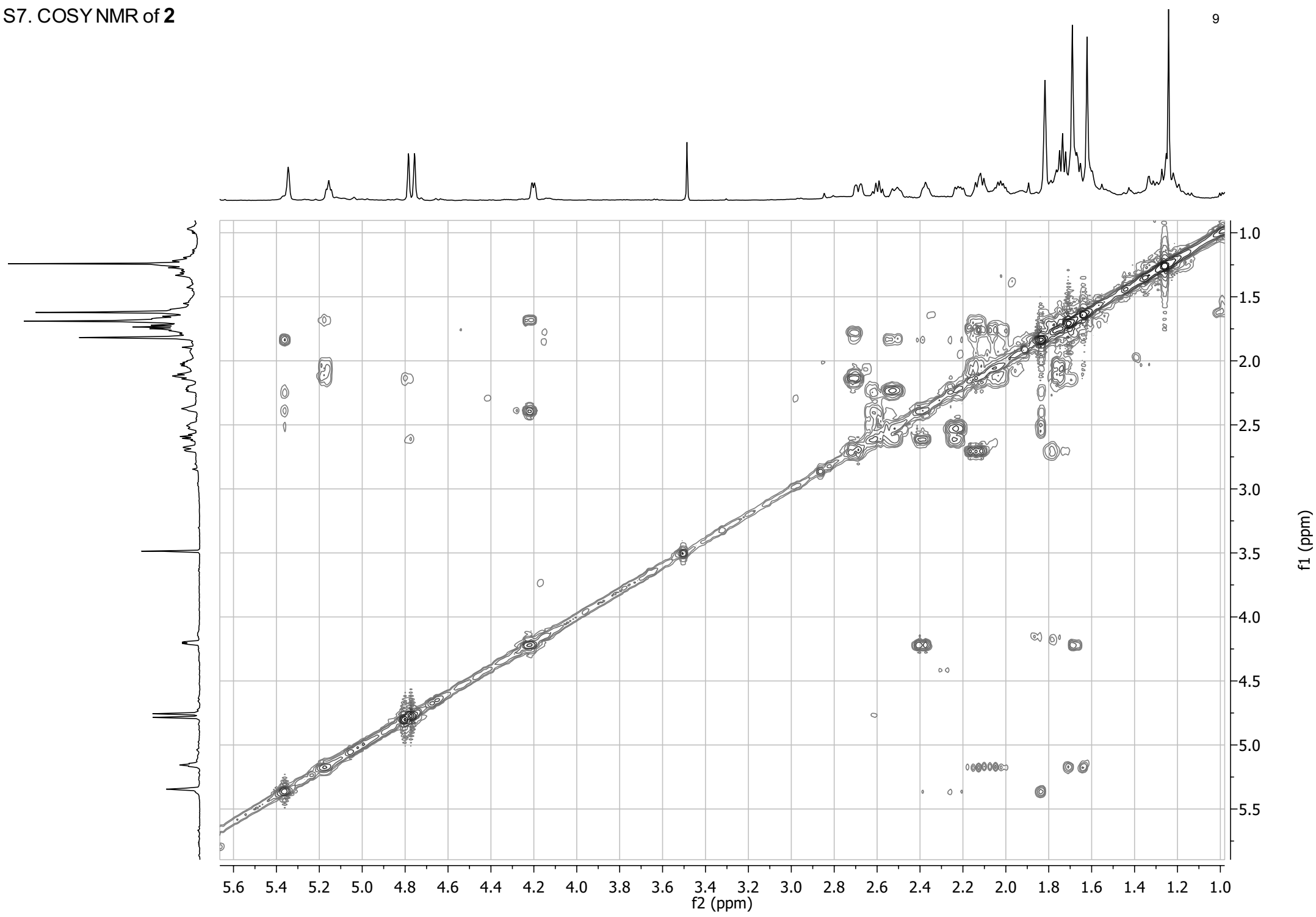




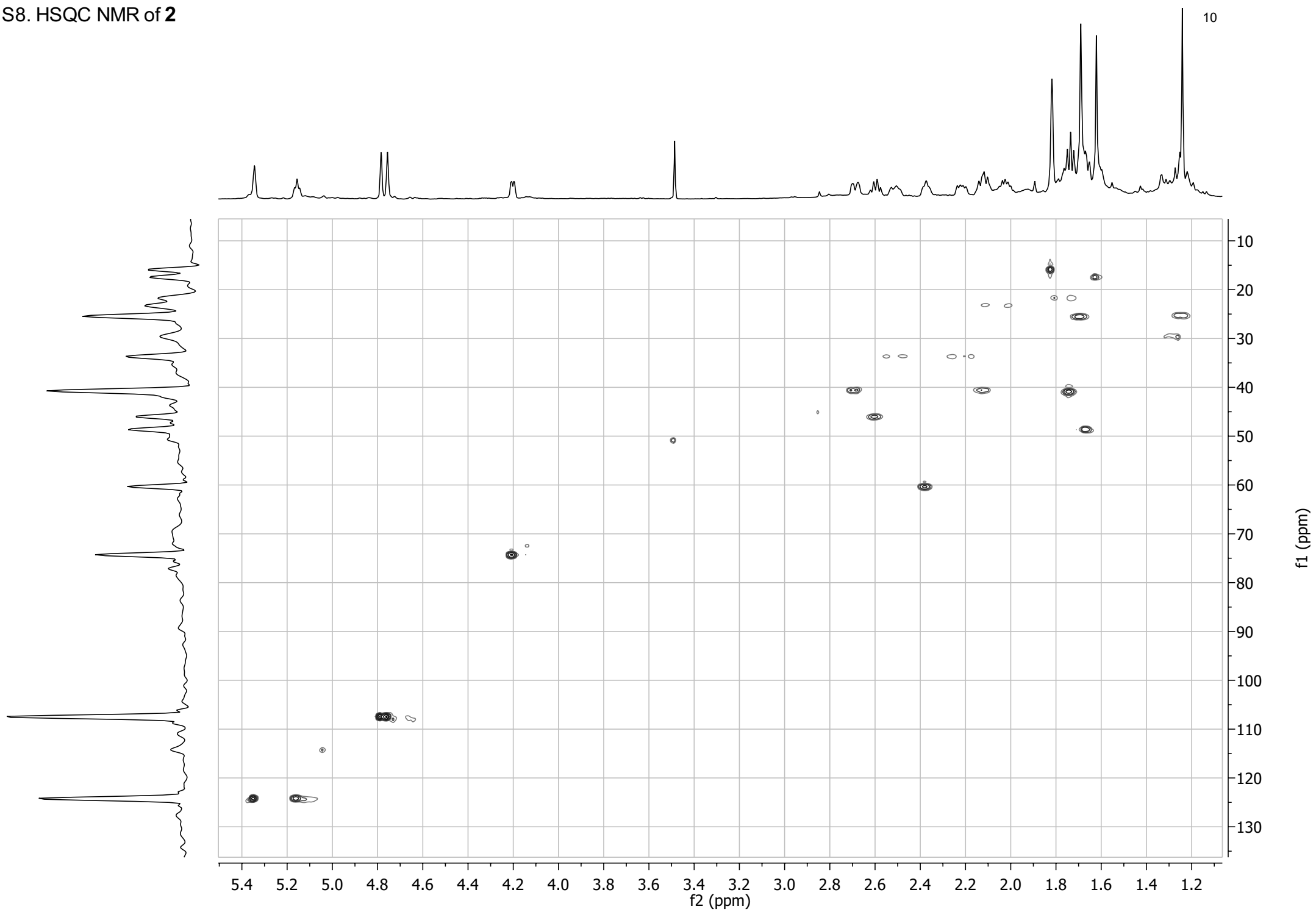


S6. ¹H NMR of 2





S8. HSQC NMR of 2



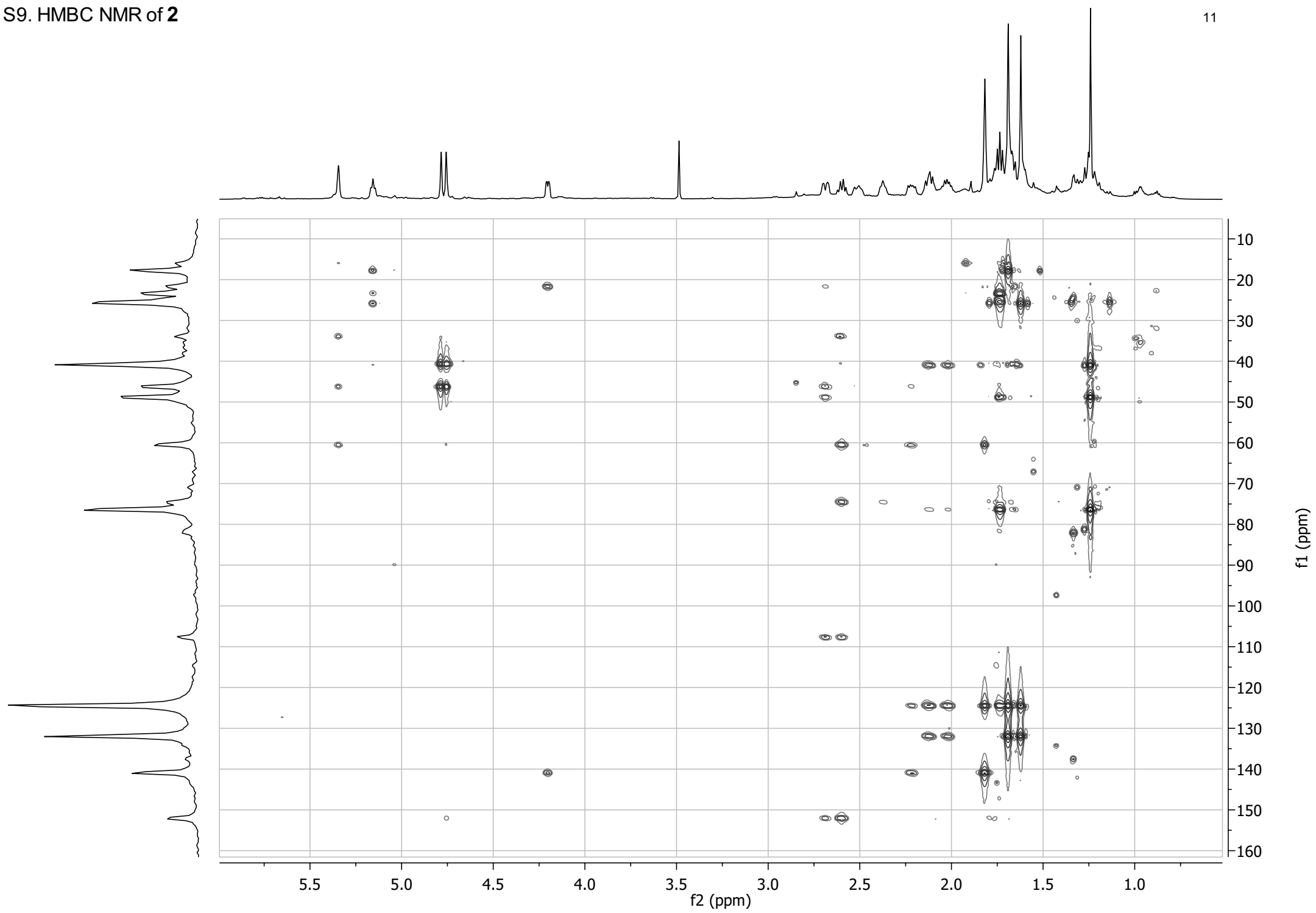


Table S1. ^1H and ^{13}C NMR data (300 MHz and 75 MHz, CDCl_3) for the *trans*- and *cis*-conformers of 4-hydroxydictyolactone (1).

No.	<i>Trans</i> -conformer (major compound)				<i>Cis</i> -conformer (minor compound)	
	^{13}C δ (m)	^1H δ (m, J Hz)	COSY	gHMBC	^{13}C δ (m)	^1H δ (m, J Hz)
1	135.4 (s)					
2	35.8 (d)	3.40 (1H, dd, 7.8, 1.2)	H ₂ -18	C-1, C-3, C-4, C-9, C-10, C-19	35.5 (d)	3.86 (m)
3	51.0 (d)	2.04 (1H, br s)		C-1, C-2, C-4, C-5, C-10, C-11, C-17, C-18	50.9	1.71 (br s)
4	72.7 (d)	4.30 (1H, dd, 4.2, 2.2)	H _a -5, H _b -5	C-2, C-6	68.1 (d)	4.22 (m)
5	49.1 (t)	2.33 (1H, dd, 13.0, 2.2)	H-4, H _b -5	C-3, C-4, C-6, C-7, C-20	ND	2.81 (m)
		2.18 (1H, dd, 13.0, 4.2)	H-4, H _a -5	C-3, C-4, C-6, C-7, C-20		2.32 (m)
6	136.1 (s)					
7	125.3 (d)	5.32 (1H, ddq, 11.4, 4.2, 0.7)	H _a -8, H _b -8, H ₃ -20	C-5, C-20	125.4 (d)	5.61 (m)
8	29.4 (t)	3.20 (1H, dddd, 17.5, 11.4, 2.2, 2.2)	H-7, H _b -8, H-9	C-1, C-6, C-7, C-9	ND	3.21 (m)
		2.98 (1H, ddd, 17.5, 7.4, 4.2)	H-7, H _a -8, H-9	C-1, C-6, C-7, C-9		2.66 (m)
9	139.5 (d)	6.94 (1H, dt, 7.4, 2.2)	H _a -8, H _b -8	C-2, C-7, C-8, C-19	139.8 (d)	6.88 (dt, 8.0, 3.3)
10	32.3 (d)	1.71 (1H, m)	H ₃ -17	C-2, C-3, C-4, C-11, C-12, C-17	32.6 (d)	1.72 (m)
11	37.9 (t)	1.19 (2H, m)	H ₂ -12		ND	
12	25.9 (t)	1.93 (2H, m)	H ₂ -11, H-13	C-14	ND	
13	123.9 (d)	5.02 (1H, t hept, 7.2, 1.4)	H ₂ -12, H ₃ -15, H ₃ -16	C-15, C-16	124.3 (d)	5.07 (1H, t hept, 7.2, 1.4)
14	131.9 (s)					
15	17.7 (q)	1.57 (3H, s)	H-13	C-13, C-14, C-16	25.7 (q)	1.59 (3H, s)
16	25.6 (q)	1.66 (3H, s)	H-13	C-13, C-14, C-15	17.4 (q)	1.74 (3H, s)
17	18.1 (q)	1.07 (3H, d, 6.7)	H-10	C-3, C-10, C-11	18.1 (q)	1.06 (d, 6.7)
18	68.7 (t)	4.45 (1H, dd, 9.7, 1.2)	H-2, H _b -18	C-1, C-2, C-3, C-19	68.9 (t)	4.41 (dd, 9.6, 1.6)
		4.10 (1H, dd, 9.7, 7.8)	H-2, H _a -18	C-3		4.14 (dd, 9.6, 7.3)
19	173.3 (s)				ND	
20	20.0 (q)	1.90 (3H, br d, 0.7)	H-7	C-5, C-6, C-7	25.7 (q)	1.59 (br s)

ND = Not detected

Table S2. Comparison of calculated dihedral angles from the 16 possible stereoisomers of the H-3 – C-20 *trans*-conformers and the corresponding *cis*-conformers of **1** with observed ^1H - ^1H couplings from the ^1H NMR. * indicates those stereoisomers/conformers that match the ^1H NMR data.

C-2, C-3, C-4, C-10 configuration	^1H - ^1H correlation	Calculated dihedral angle Φ	Calculated J (Hz)	Relevant observed ^1H - ^1H couplings
<i>SSSS trans</i>	H2-C2-C3-H3	-94	0.91	No observed coupling: H-2 couples to H ₂ -18 only
	H3-C3-C4-H4	154	8.94	NA
	H3-C3-C10-H10	60	2.72	No observed coupling: H-3 (br s), H-10 couples to H ₃ -17 only.
<i>SSSS cis</i>	H2-C2-C3-H3	138	6.71	NA
	H3-C3-C4-H4	-47	4.94	NA
	H3-C3-C10-H10	166	10.61	NA
<i>SSSR trans</i>	H2-C2-C3-H3	-99	1.18	No observed coupling: H-2 couples to H ₂ -18 only
	H3-C3-C4-H4	158	9.30	NA
	H3-C3-C10-H10	-90	0.80	No observed coupling: H-3 (br s), H-10 couples to H ₃ -17 only.
<i>SSSR cis</i>	H2-C2-C3-H3	139	6.89	NA
	H3-C3-C4-H4	-48	4.81	NA
	H3-C3-C10-H10	-176	11.14	NA
* <i>SSRR trans</i>	H2-C2-C3-H3	-102	1.40	No observed coupling: H-2 couples to H ₂ -18 only
	H3-C3-C4-H4	-87	0.80	No observed coupling: H-3 (br s)
	H3-C3-C10-H10	-85	0.80	No observed coupling: H-3 (br s), H-10 couples to H ₃ -17 only.
<i>SSRR cis</i>	H2-C2-C3-H3	134	6.01	NA
	H3-C3-C4-H4	80	1.31	No observed coupling: H-3 (br s)
	H3-C3-C10-H10	-175	11.11	NA
<i>SRRR trans</i>	H2-C2-C3-H3	-59	2.85	No observed coupling: H-2 couples to H ₂ -18 only
	H3-C3-C4-H4	-127	5.25	NA
	H3-C3-C10-H10	70	1.60	No observed coupling: H-3 (br s), H-10 couples to H ₃ -17 only.
<i>SRRR cis</i>	H2-C2-C3-H3	104	1.58	No observed coupling: H-2 couples to H ₂ -18 only
	H3-C3-C4-H4	62	3.02	NA
	H3-C3-C10-H10	-126	4.61	NA
* <i>SSRS trans</i>	H2-C2-C3-H3	-94	0.91	No observed coupling: H-2 couples to H ₂ -18 only
	H3-C3-C4-H4	-89	0.87	No observed coupling: H-3 (br s)

	H3-C3-C10-H10	70	1.60	No observed coupling: H-3 (br s), H-10 couples to H ₃ -17 only.
<i>SSRS cis</i>	H2-C2-C3-H3	137	6.54	NA
	H3-C3-C4-H4	74	1.76	No observed coupling: H-3 (br s)
	H3-C3-C10-H10	-174	11.08	NA
<i>SRRS trans</i>	H2-C2-C3-H3	-68	1.79	No observed coupling: H-2 couples to H ₂ -18 only
	H3-C3-C4-H4	-125	4.94	NA
	H3-C3-C10-H10	-79	0.97	No observed coupling: H-3 (br s), H-10 couples to H ₃ -17 only.
<i>SRRS cis</i>	H2-C2-C3-H3	68	1.79	No observed coupling: H-2 couples to H ₂ -18 only
	H3-C3-C4-H4	155	7.64	NA
	H3-C3-C10-H10	88	0.78	No observed coupling: H-3 (br s), H-10 couples to H ₃ -17 only.
<i>SRSR-trans</i>	H2-C2-C3-H3	114	2.74	No observed coupling: H-2 couples to H ₂ -18 only
	H3-C3-C4-H4	-48	4.44	NA
	H3-C3-C10-H10	68	1.79	No observed coupling: H-3 (br s), H-10 couples to H ₃ -17 only.
<i>SRSR-cis</i>	H2-C2-C3-H3	71	1.51	
	H3-C3-C4-H4	34		NA
	H3-C3-C10-H10	-82	0.86	No observed coupling: H-3 (br s), H-10 couples to H ₃ -17 only.
<i>SRSS trans</i>	H2-C2-C3-H3	-47	4.59	NA
	H3-C3-C4-H4	110	2.75	No observed coupling: H-3 (br s)
	H3-C3-C10-H10	-60	2.72	No observed coupling: H-3 (br s), H-10 couples to H ₃ -17 only.
<i>SRSS cis</i>	H2-C2-C3-H3	70	1.60	No observed coupling: H-2 couples to H ₂ -18 only
	H3-C3-C4-H4	35	4.70	NA
	H3-C3-C10-H10	67	1.89	No observed coupling: H-3 (br s), H-10 couples to H ₃ -17 only.
<i>RSRS trans</i>	H2-C2-C3-H3	14	8.84	NA
	H3-C3-C4-H4	94	0.89	No observed coupling: H-3 (br s)
	H3-C3-C10-H10	75	1.20	No observed coupling: H-3 (br s), H-10 couples to H ₃ -17 only.
<i>RSRS cis</i>	H2-C2-C3-H3	-109	2.10	No observed coupling: H-2 couples to H ₂ -18 only
	H3-C3-C4-H4	68	2.34	No observed coupling: H-3 (br s)
	H3-C3-C10-H10	-157	9.67	NA
<i>*RRSR trans</i>	H2-C2-C3-H3	102	1.40	No observed coupling: H-2 couples to H ₂ -18 only
	H3-C3-C4-H4	87	0.80	No observed coupling: H-3 (br s)
	H3-C3-C10-H10	84	0.81	No observed coupling: H-3 (br s), H-10 couples to H ₃ -17 only.
<i>RRSR cis</i>	H2-C2-C3-H3	-139	6.89	NA
	H3-C3-C4-H4	-71	2.03	No observed coupling: H-3 (br s)

	H3-C3-C10-H10	-178	11.18	NA
<i>RSSR trans</i>	H2-C2-C3-H3	58	2.98	No observed coupling: H-2 couples to H ₂ -18 only
	H3-C3-C4-H4	121	4.32	NA
	H3-C3-C10-H10	-60	2.72	No observed coupling: H-3 (br s), H-10 couples to H ₃ -17 only.
<i>RSSR cis</i>	H2-C2-C3-H3	-108	1.99	No observed coupling: H-2 couples to H ₂ -18 only
	H3-C3-C4-H4	-51	4.42	NA
	H3-C3-C10-H10	-173	11.04	NA
<i>RSRR trans</i>	H2-C2-C3-H3	48	4.44	NA
	H3-C3-C4-H4	-106	2.26	No observed coupling: H-3 (br s)
	H3-C3-C10-H10	54	3.54	NA
<i>RSRR cis</i>	H2-C2-C3-H3	-104	1.58	No observed coupling: H-2 couples to H ₂ -18 only
	H3-C3-C4-H4	63	2.90	No observed coupling: H-3 (br s)
	H3-C3-C10-H10	-142	7.40	NA
<i>RRRR trans</i>	H2-C2-C3-H3	99	1.18	No observed coupling: H-2 couples to H ₂ -18 only
	H3-C3-C4-H4	-154	8.94	NA
	H3-C3-C10-H10	82	0.86	No observed coupling: H-3 (br s), H-10 couples to H ₃ -17 only.
<i>RRRR cis</i>	H2-C2-C3-H3	-146	8.07	NA
	H3-C3-C4-H4	58	3.51	NA
	H3-C3-C10-H10	-134	6.01	NA
<i>RRRS trans</i>	H2-C2-C3-H3	97	1.05	No observed coupling: H-2 couples to H ₂ -18 only
	H3-C3-C4-H4	-158	9.30	NA
	H3-C3-C10-H10	-54	3.54	NA
<i>RRRS cis</i>	H2-C2-C3-H3	-155	9.41	NA
	H3-C3-C4-H4	71	2.03	No observed coupling: H-3 (br s)
	H3-C3-C10-H10	80	0.93	No observed coupling: H-3 (br s), H-10 couples to H ₃ -17 only.
<i>*RRSS trans</i>	H2-C2-C3-H3	102	1.40	No observed coupling: H-2 couples to H ₂ -18 only
	H3-C3-C4-H4	86	0.77	No observed coupling: H-3 (br s)
	H3-C3-C10-H10	86	0.79	No observed coupling: H-3 (br s), H-10 couples to H ₃ -17 only.
<i>RRSS cis</i>	H2-C2-C3-H3	-135	6.18	NA
	H3-C3-C4-H4	-74	1.76	No observed coupling: H-3 (br s)
	H3-C3-C10-H10	-178	11.18	NA
<i>RSSS trans</i>	H2-C2-C3-H3	49	4.28	NA
	H3-C3-C4-H4	121	4.32	NA

	H3-C3-C10-H10	173	11.04	NA
<i>RSSS cis</i>	H2-C2-C3-H3	-111	2.35	No observed coupling: H-2 couples to H ₂ -18 only
	H3-C3-C4-H4	-51	4.42	NA
	H3-C3-C10-H10	-161	10.13	NA