

Supplementary

Design, synthesis, antitumor, and antiplasmodial evaluation of new 7-chloroquinoline-benzimidazole hybrids

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Table S1. Experimental and calculated log3D7 by model (1), with values of descriptors included in the model.

ID	Name	Status	Exp. endpoint	Pred. by model eq.(1)	<i>GATS7v</i>	<i>G(N..Br)</i>	<i>RDF135</i> <i>v</i>
1	10a	Training	0.427	0.7372	1.375	0	1.477
2	10b	Test	0.544	0.9202	1.313	0	2.189
3	10c	Test	0.831	0.8254	1.334	0	1.695
4	10d	Training	1.767	1.4727	1.222	0	5.418
5	11a	Training	1.567	1.5998	1.26	21.951	4.613
6	11b	Training	1.941	1.7545	1.215	21.845	5.309
7	11c	Training	1.294	1.551	1.218	22.328	3.728
8	11d	Training	2.507	2.5346	1.132	43.852	8.164
9	12a	Training	1.162	1.0478	1.439	0	4.587
10	12b	Training	1.043	1.3329	1.389	0	6.219
11	12c	Training	0.988	0.812	1.374	0	2.042
12	12d	Training	2.28	2.1358	1.284	0	11.217
13	13a	Training	0.407	0.4299	1.851	0	4.462
14	13b	Training	0.387	0.6118	1.766	0	4.907
15	13c	Training	1.107	0.705	1.675	0	4.601
16	13d	Training	1.759	1.7516	1.53	0	11.025
17	14a	Training	0.968	0.9973	1.844	22.921	6.443
18	14b	Test	0.699	0.8416	1.777	25.4	4.242
19	14c	Training	1.057	0.8828	1.664	24.51	3.379
20	14d	Test	2.2	1.9995	1.542	45.921	8.446
21	15a	Test	0.646	0.6549	1.542	0	2.721
22	15b	Training	0.672	0.7674	1.488	0	2.98
23	15c	Training	0.831	0.867	1.457	0	3.398
24	15d	Training	1.457	1.7179	1.358	0	8.833
25	CQ	Training	1.043	0.9548	1.192	0	1.095

Table S2. Experimental and calculated logDd2 by model (2). with values of descriptors included in the model

ID	Name	Status	Exp endpoint	Pred by model eq	RBF	LAI	F10[C- N]
1	10a	Training	0.524	0.7946	0.113	0	6
2	10b	Training	0.69	0.7946	0.113	0	6
3	10c	Training	10.020	12.668	0.123	0	6
4	10d	Training	15.660	18.082	0.125	0	8
5	11a	Training	0.94	0.7946	0.113	0	6
6	11b	Training	19.460	17.290	0.113	1	6
7	11c	Test	14.470	12.668	0.123	0	6
8	11d	Training	29.930	27.426	0.125	1	8
9	12a	Training	19.600	12.668	0.123	0	6
10	12b	Training	13.320	12.668	0.123	0	6
11	12c	Training	11.880	16.445	0.131	0	6
12	12d	Training	20.790	21.387	0.132	0	8
13	13a	Training	0.677	0.4673	0.125	0	2
14	13b	Training	0.585	0.4673	0.125	0	2
15	13c	Training	10.760	0.845	0.133	0	2
16	13d	Training	22.970	22.263	0.133	1	4
17	14a	Training	11.140	14.016	0.125	1	2
18	14b	Training	11.510	14.016	0.125	1	2
19	14c	Test	10.700	0.845	0.133	0	2
20	14d	Test	26.540	22.263	0.133	1	4
21	15a	Test	10.470	0.845	0.133	0	2
22	15b	Training	0.716	0.845	0.133	0	2
23	15c	Training	12.170	12.227	0.141	0	2
24	15d	Test	13.600	15.753	0.139	0	4
25	CQ	Training	25.560	24.850	0.163	0	3

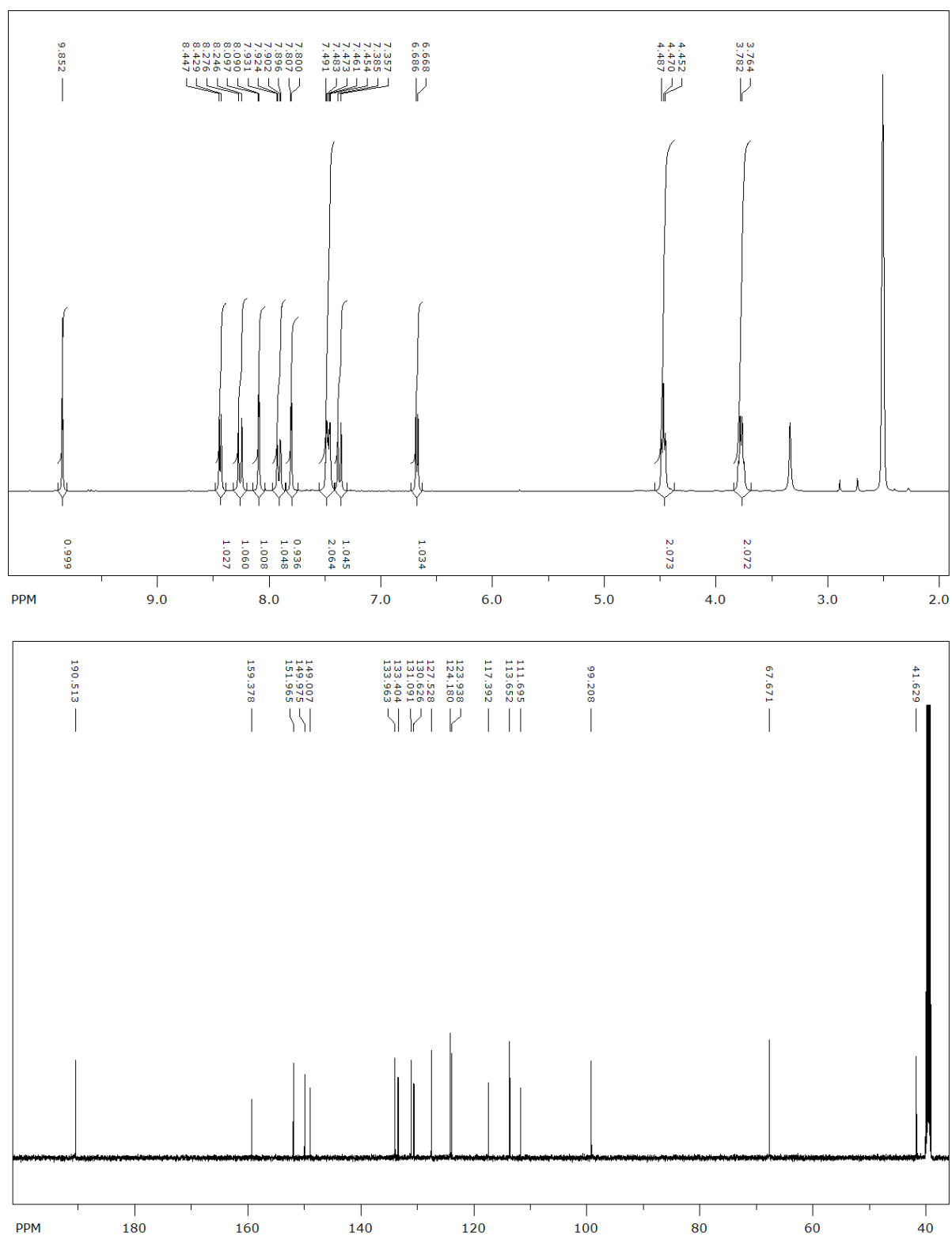


Figure S1 ¹H NMR and ¹³C NMR of compound **4**

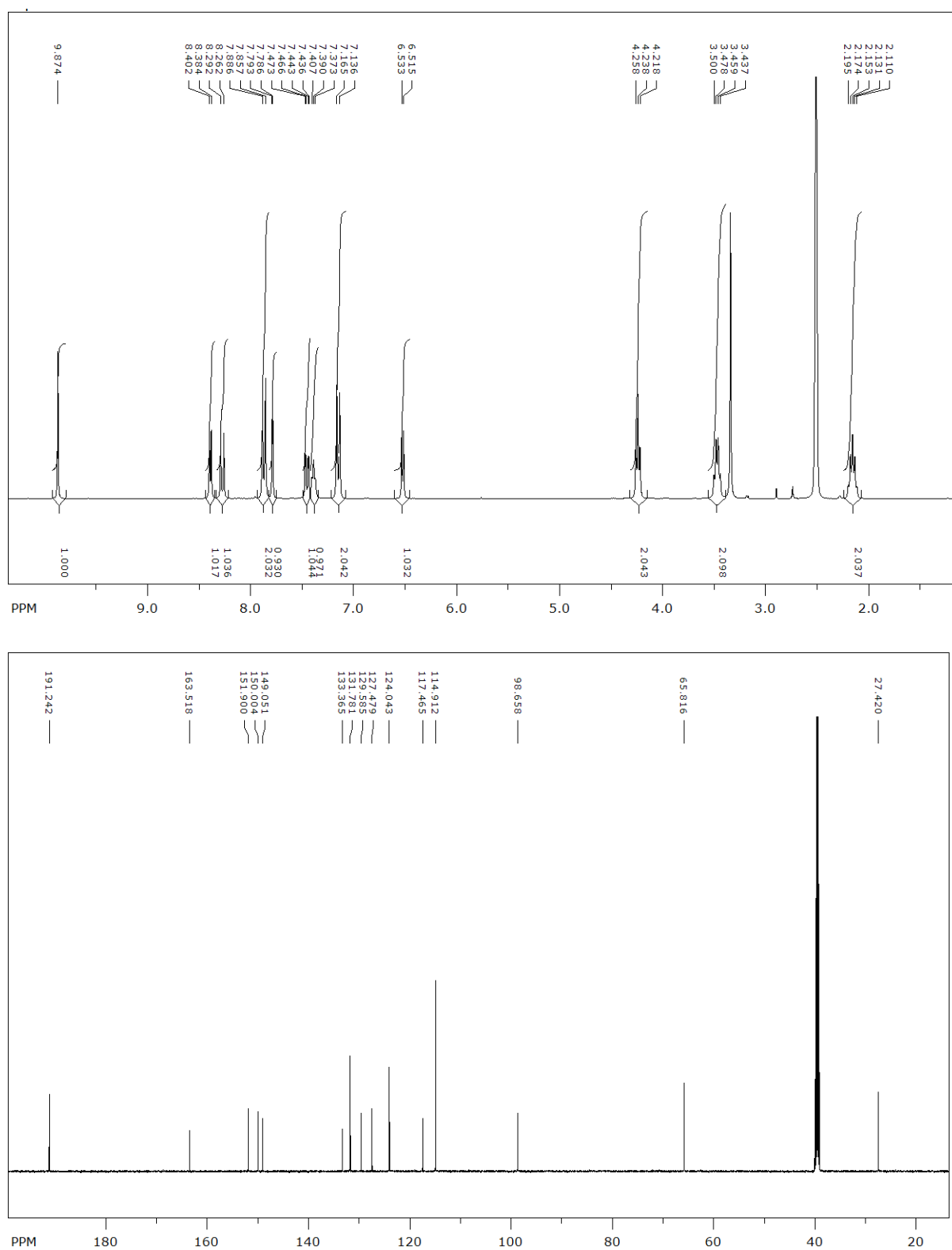


Figure S2 ¹H NMR and ¹³C NMR of compound **6**

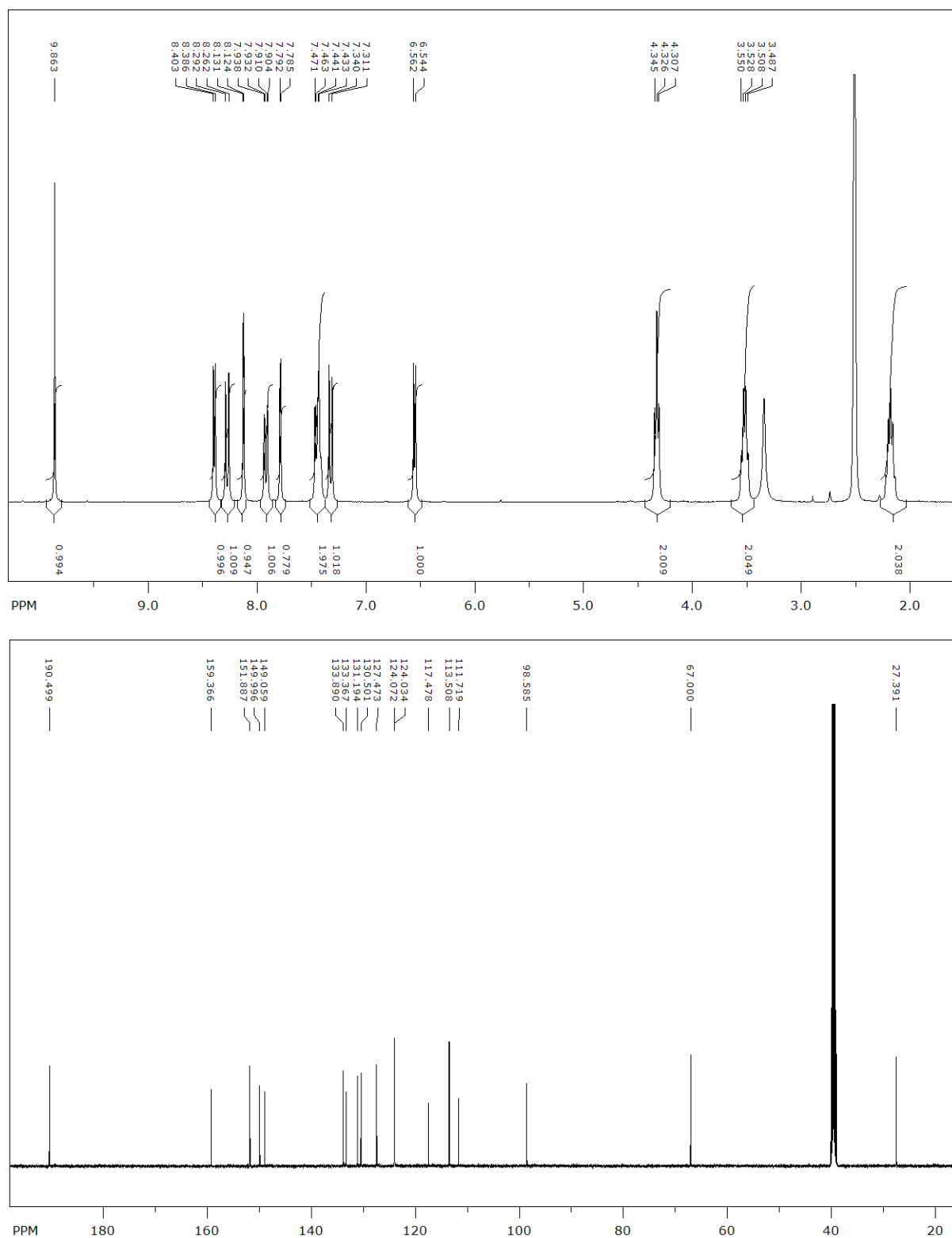


Figure S3 ¹H NMR and ¹³C NMR of compound **7**

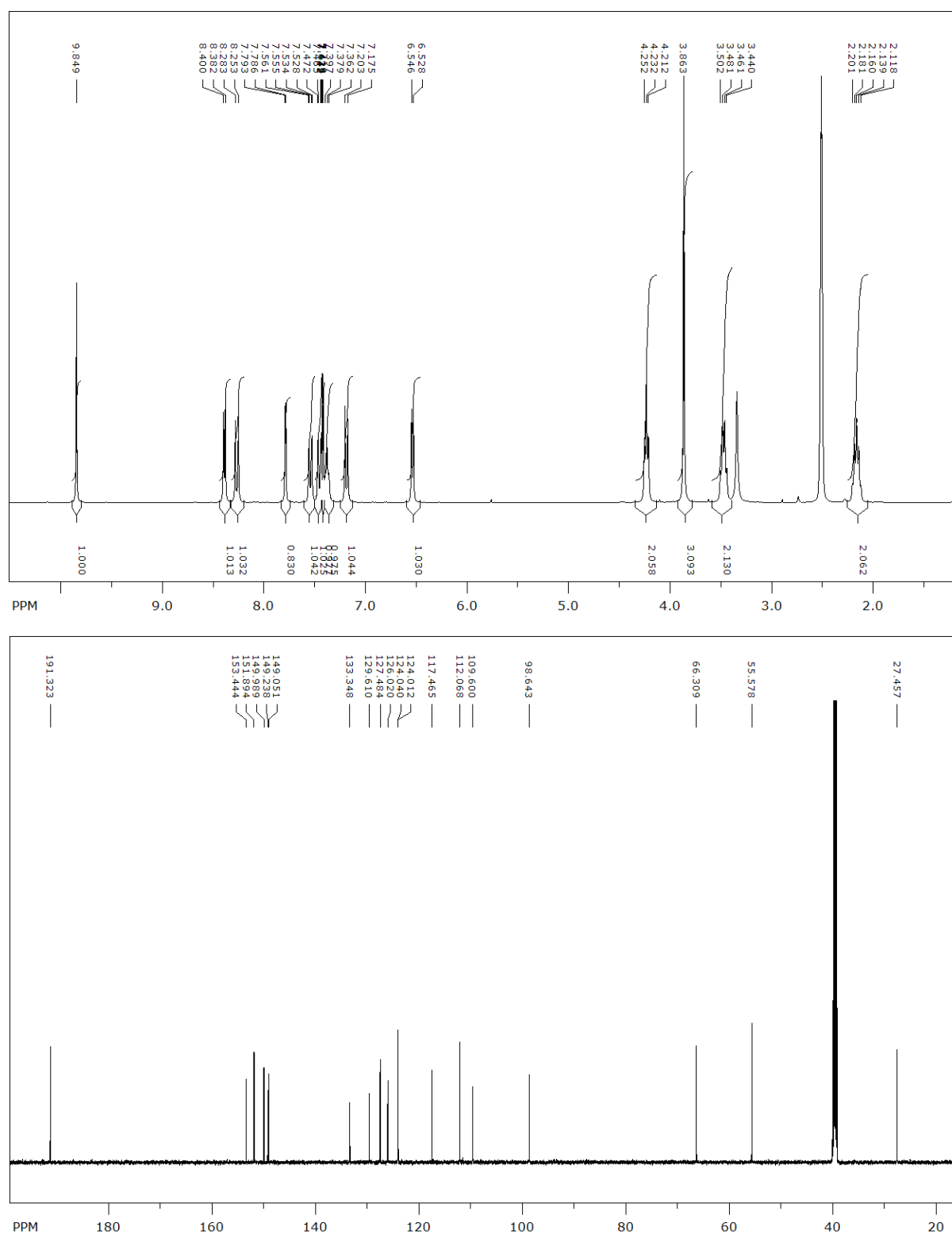


Figure S4 ^1H NMR and ^{13}C NMR of compound **8**

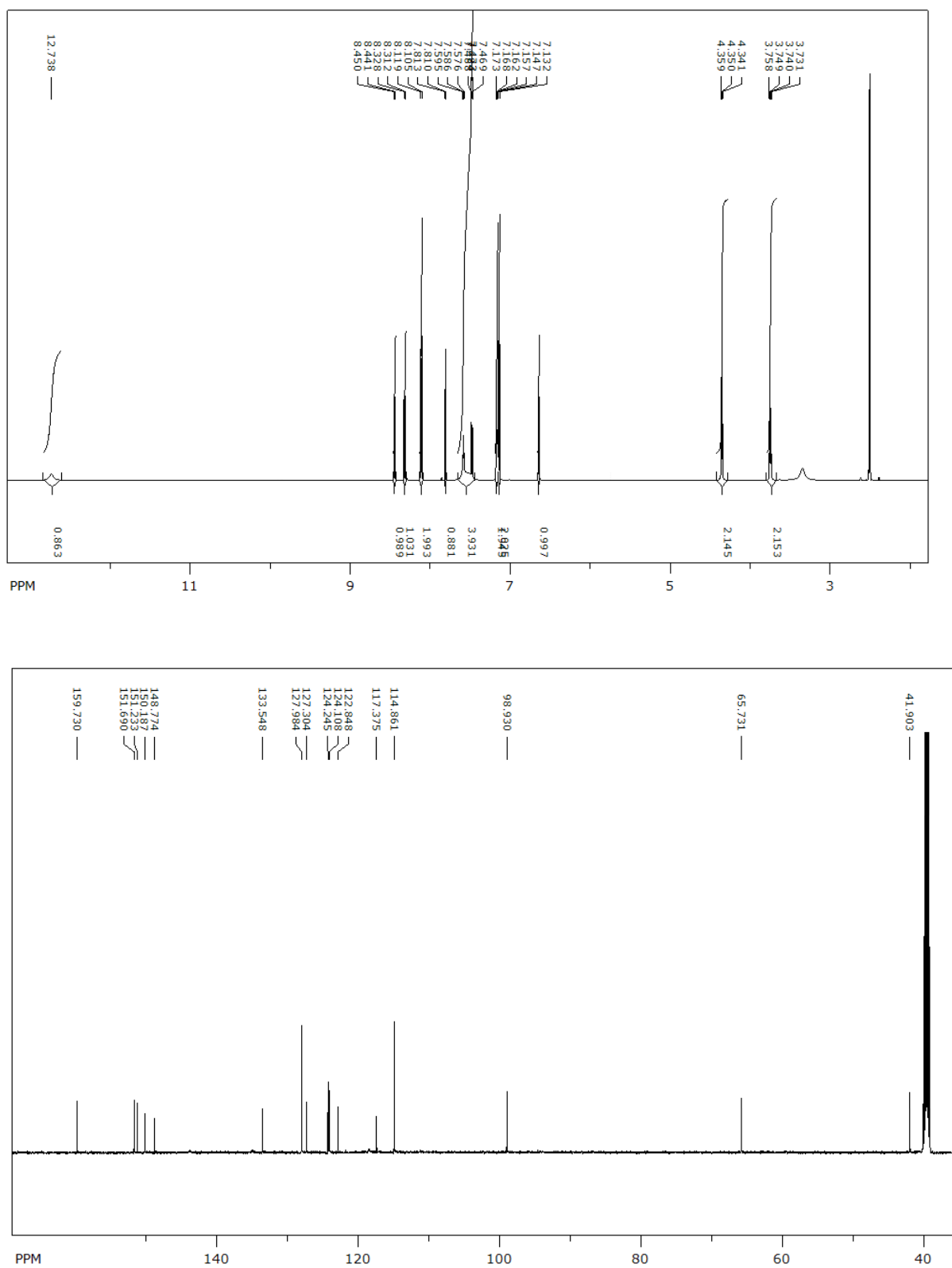


Figure S5 ^1H NMR and ^{13}C NMR of compound 10a

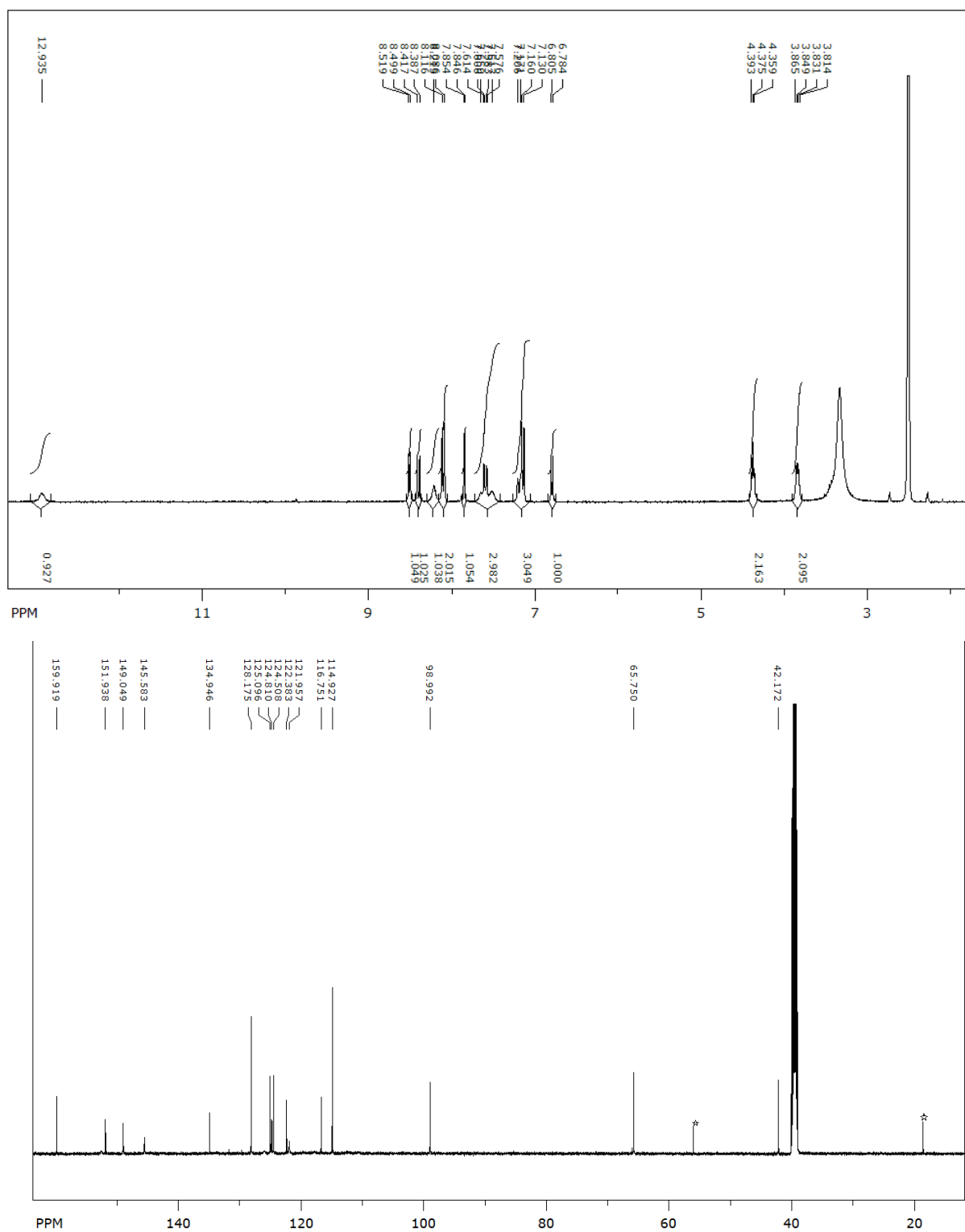


Figure S6 ¹H NMR and ¹³C NMR of compound **10b** (*ethanol; residual solvent signals)

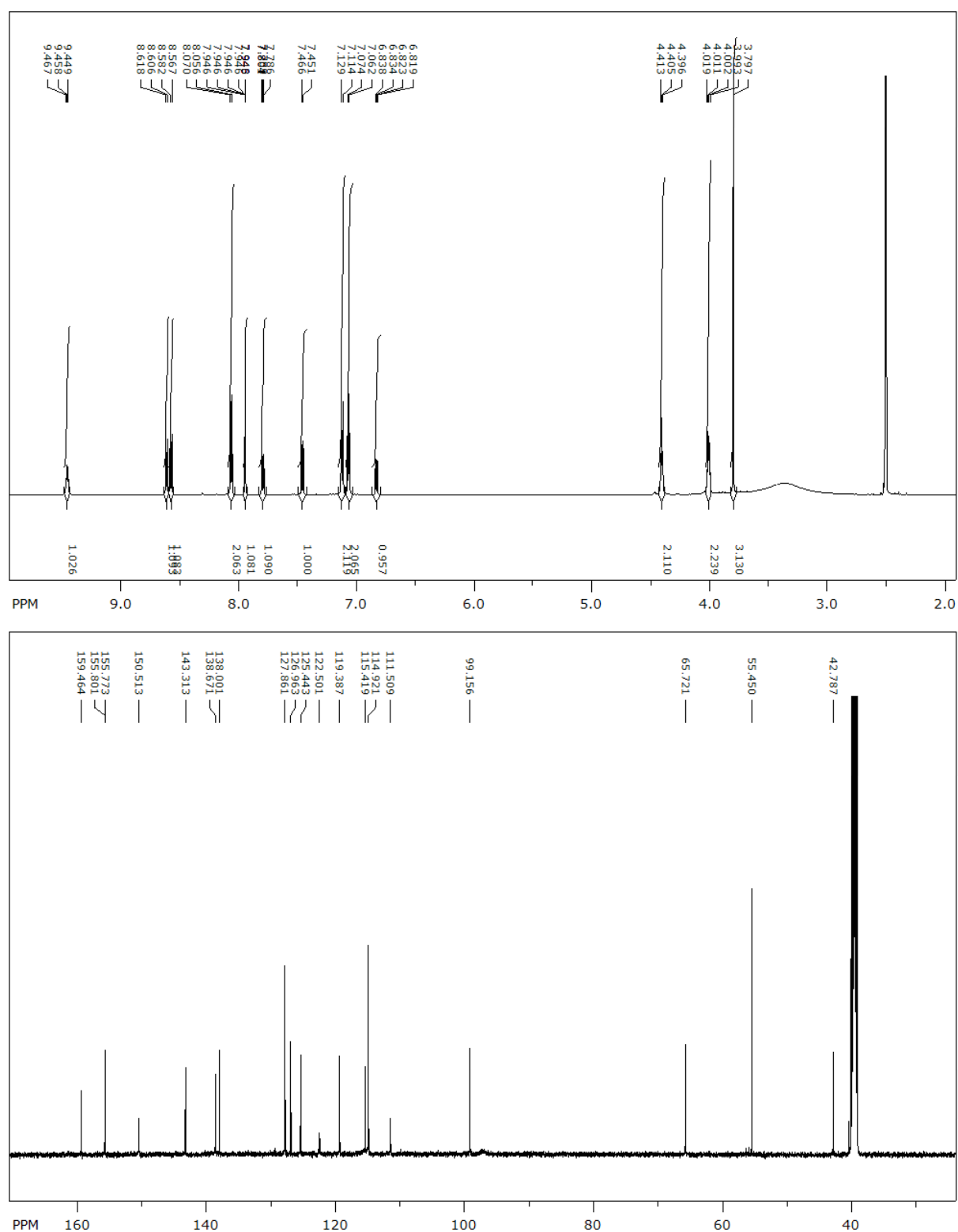


Figure S7 ¹H NMR and ¹³C NMR of compound **10c**

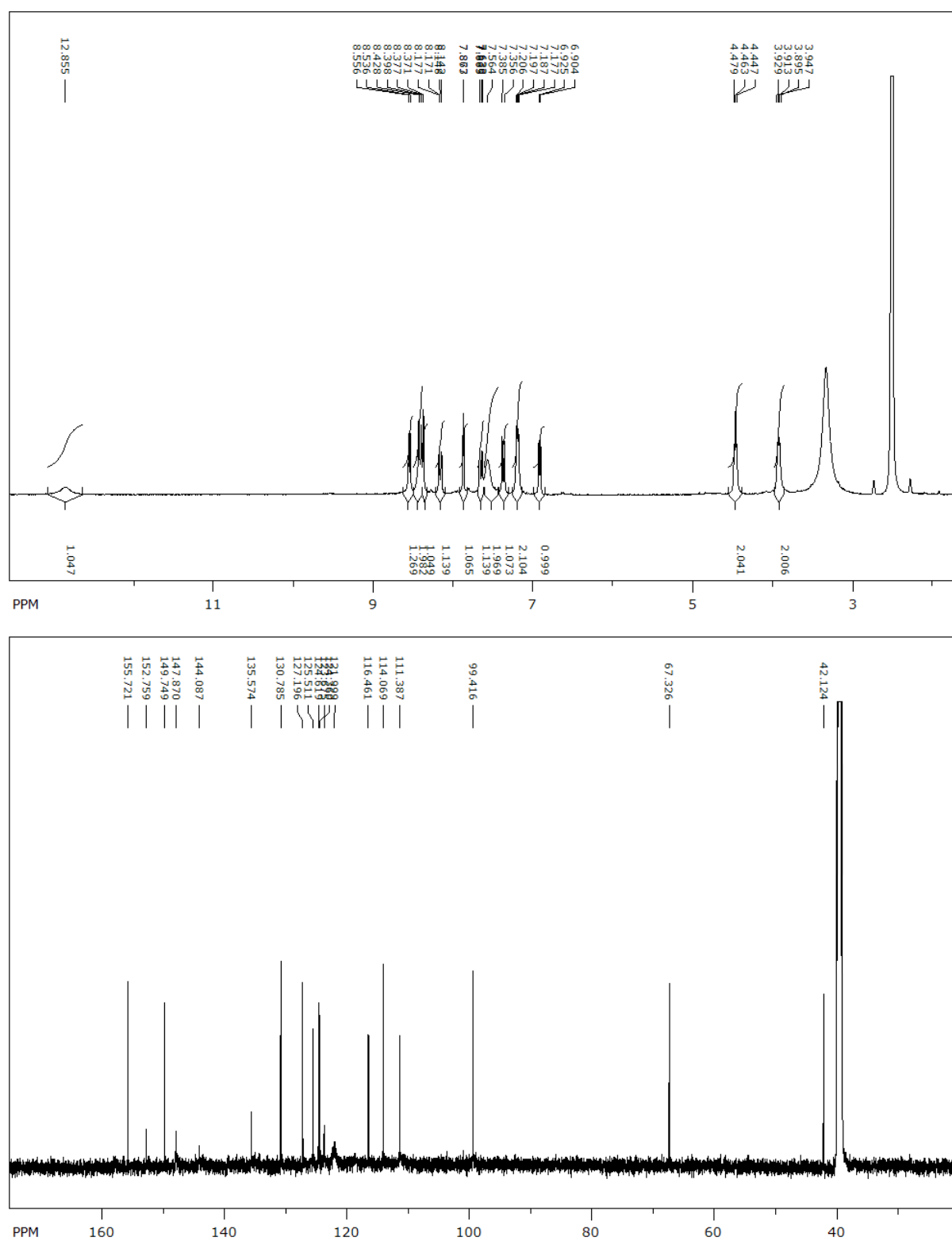


Figure S8 ¹H NMR and ¹³C NMR of compound **11a**

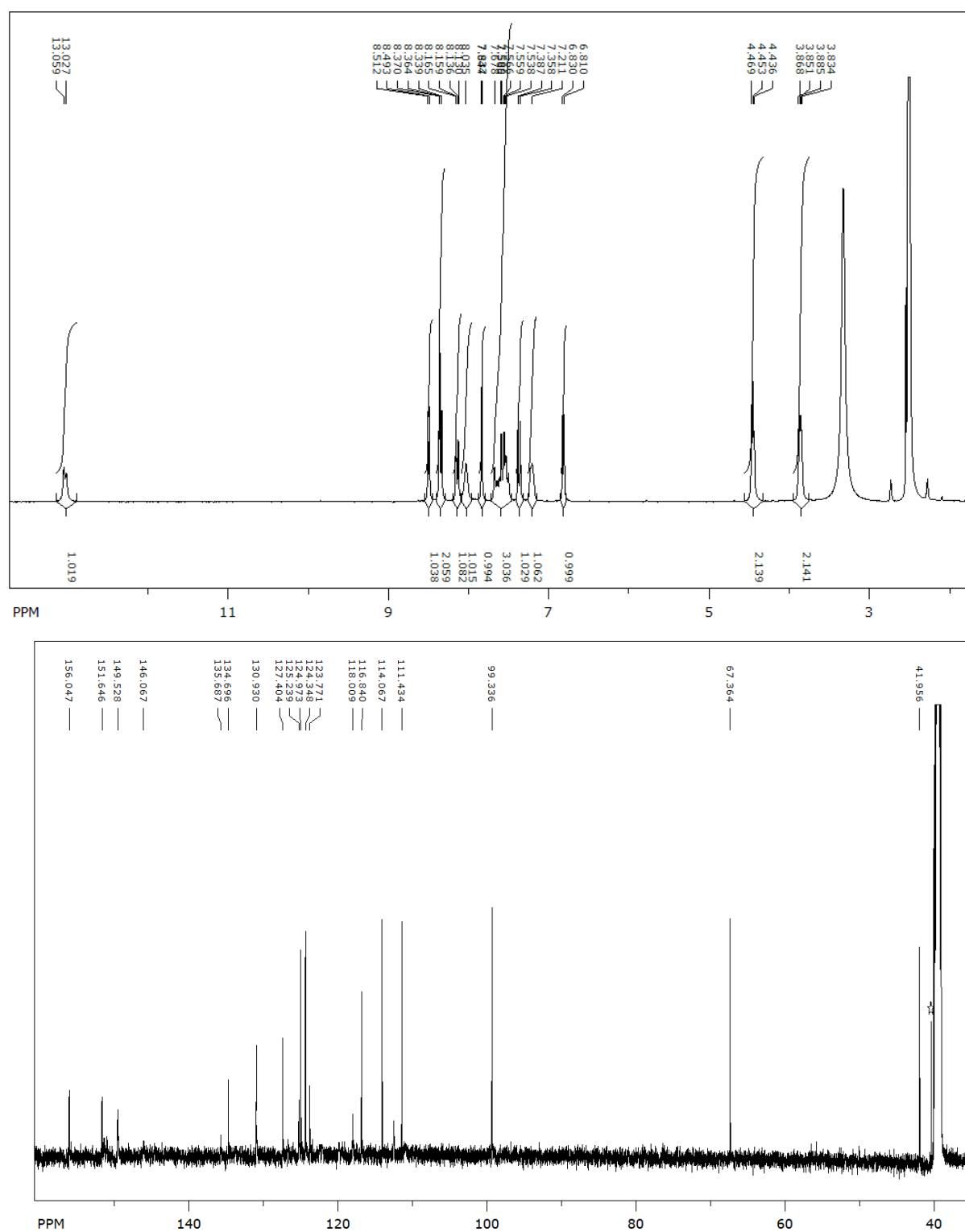


Figure S9 ¹H NMR and ¹³C NMR of compound **11b** (*DMSO; residual solvent signal)

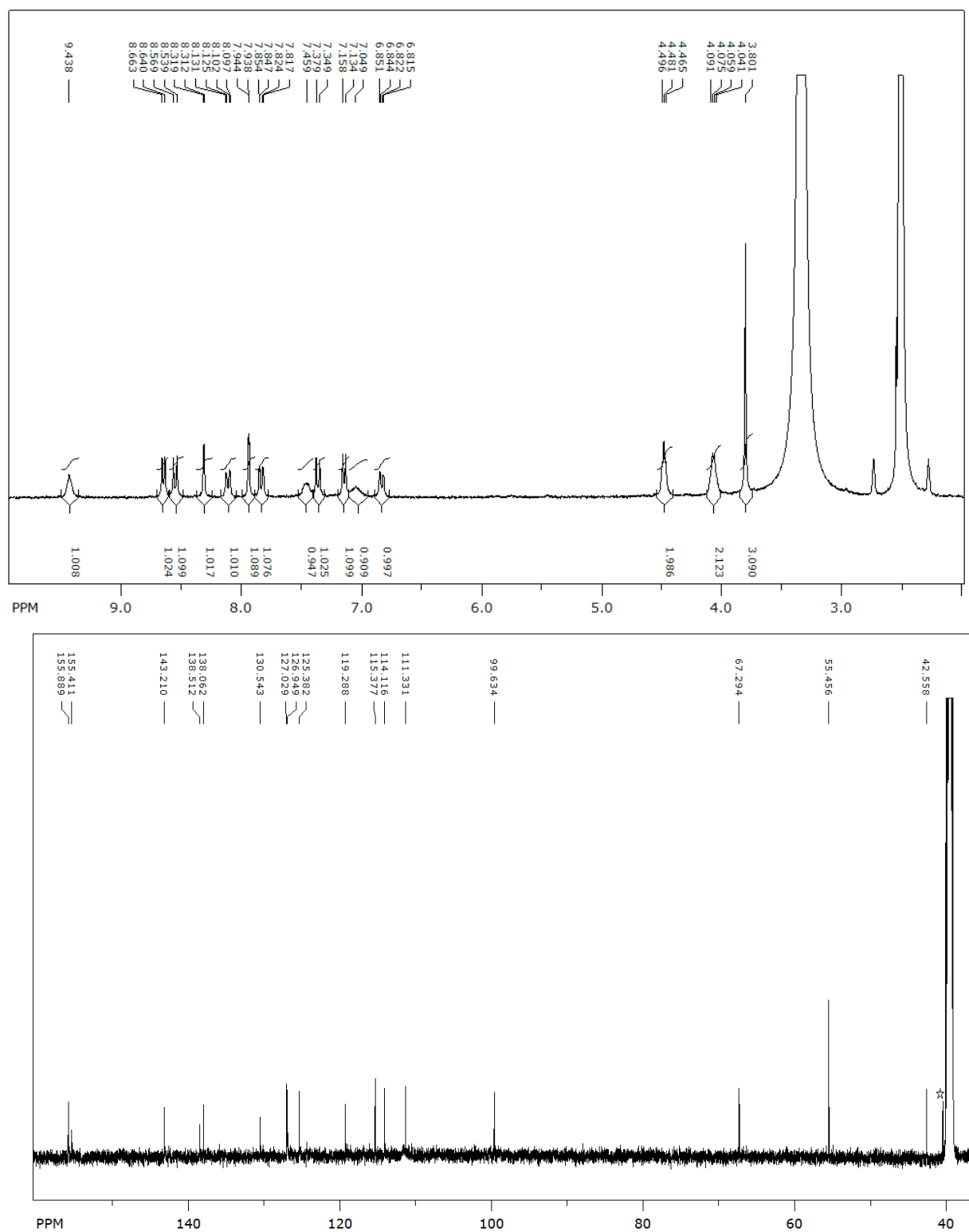


Figure S10 ¹H NMR and ¹³C NMR of compound **11c** (*DMSO; residual solvent signal)

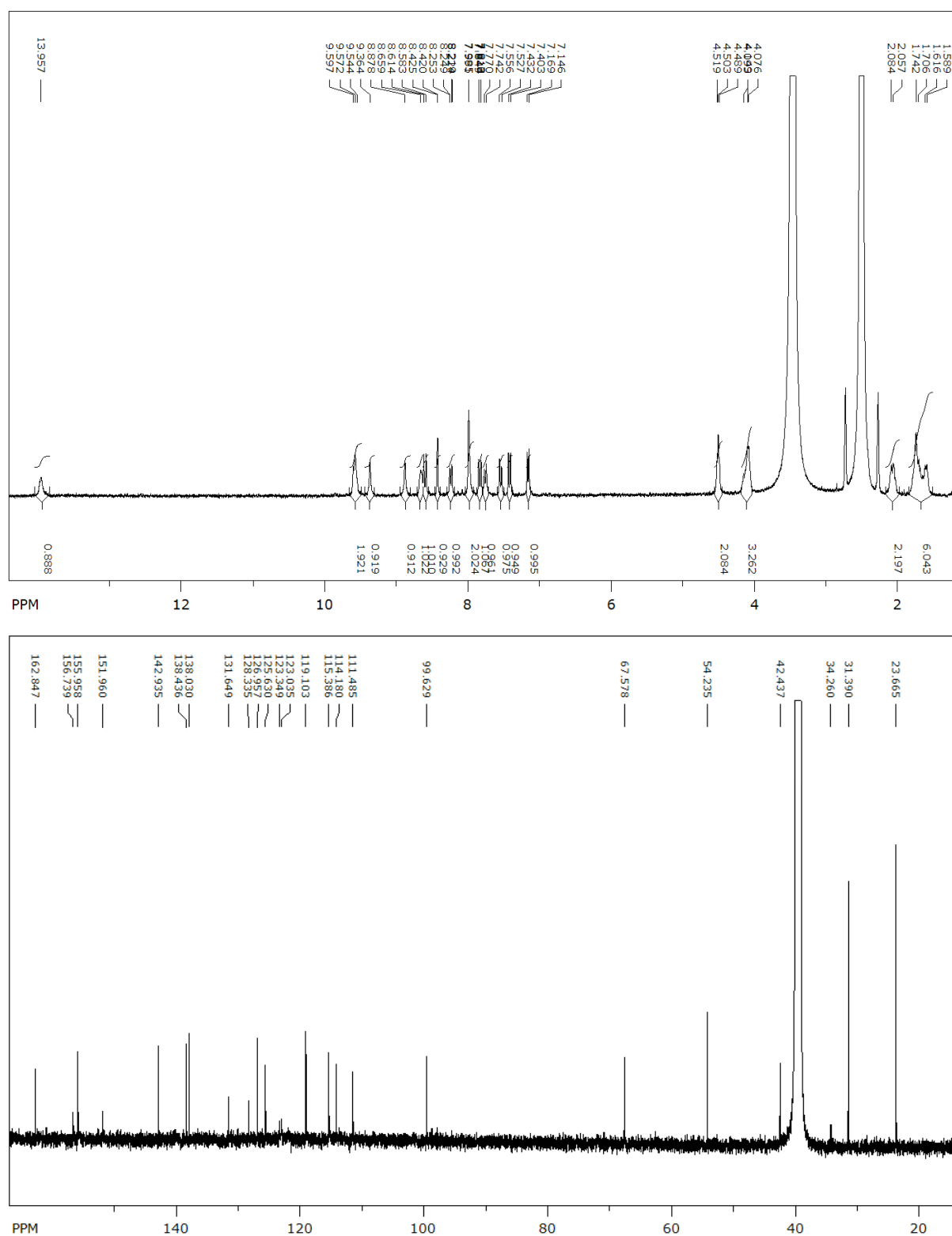


Figure S11 ¹H NMR and ¹³C NMR of compound **11d**

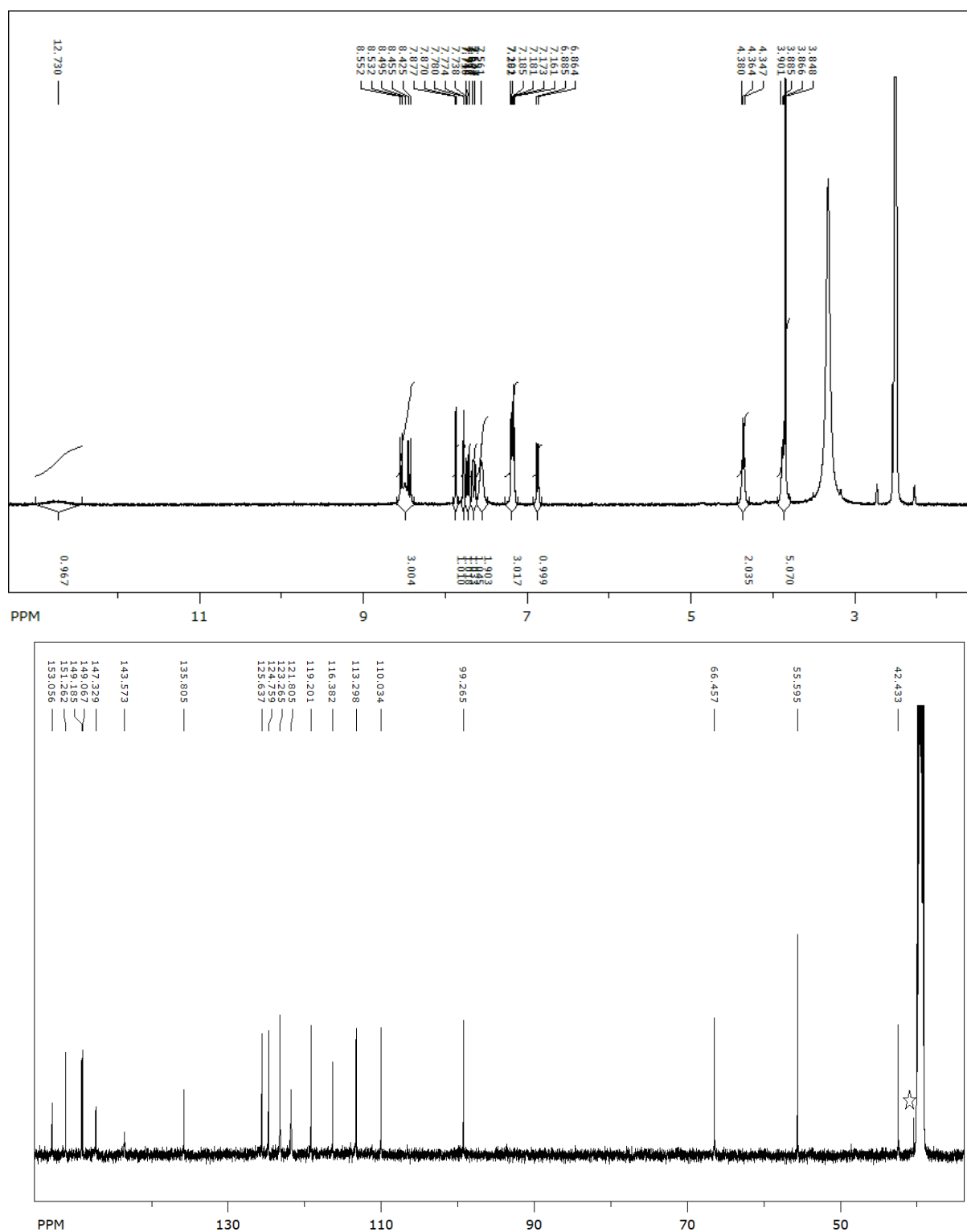


Figure S12 ¹H NMR and ¹³C NMR of compound **12a** (*DMSO; residual solvent signal)

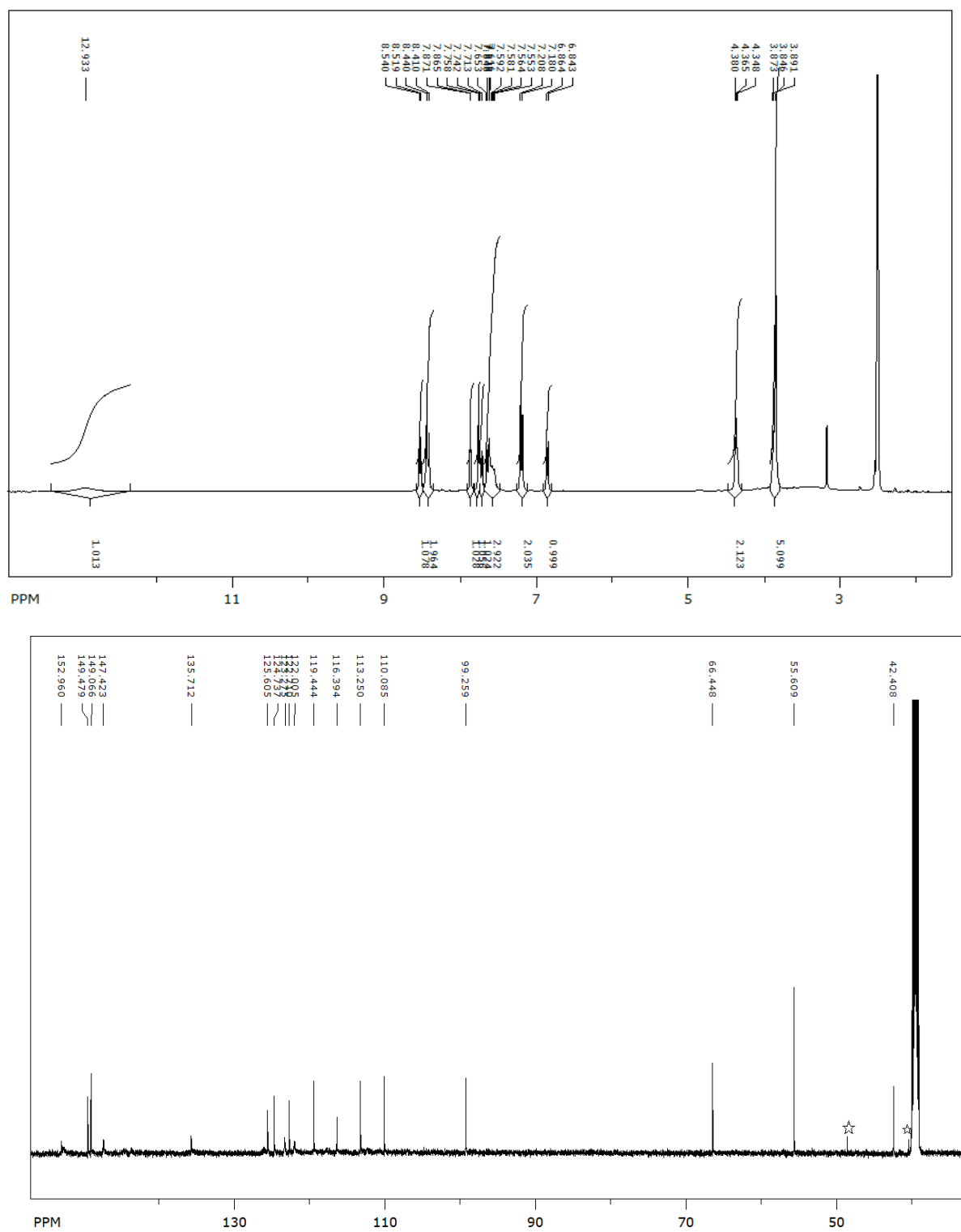


Figure S13 ¹H NMR and ¹³C NMR of compound **12b** (*methanol and DMSO; residual solvent signals)

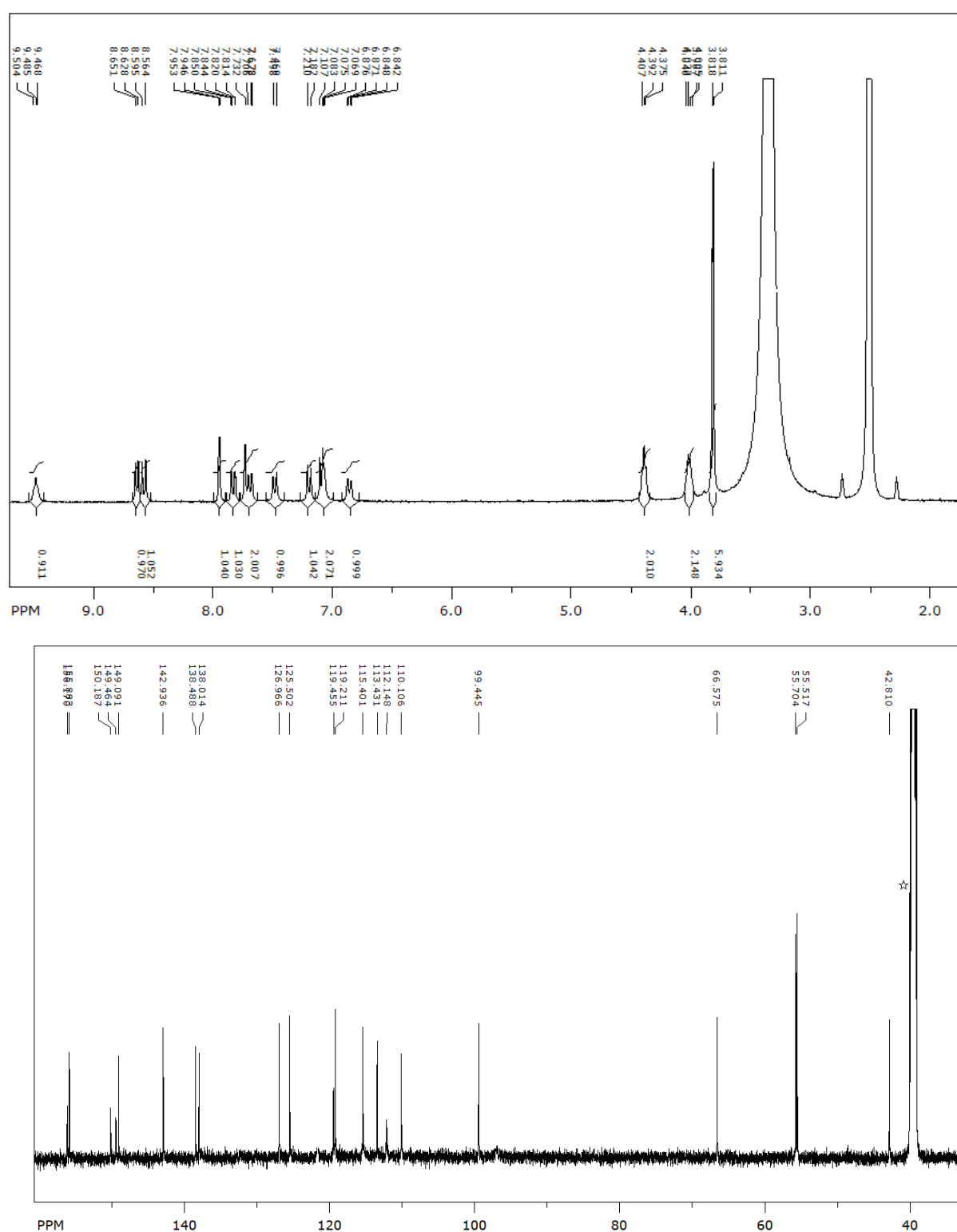


Figure S14 ¹H NMR and ¹³C NMR of compound **12c** (DMSO; residual solvent signals)

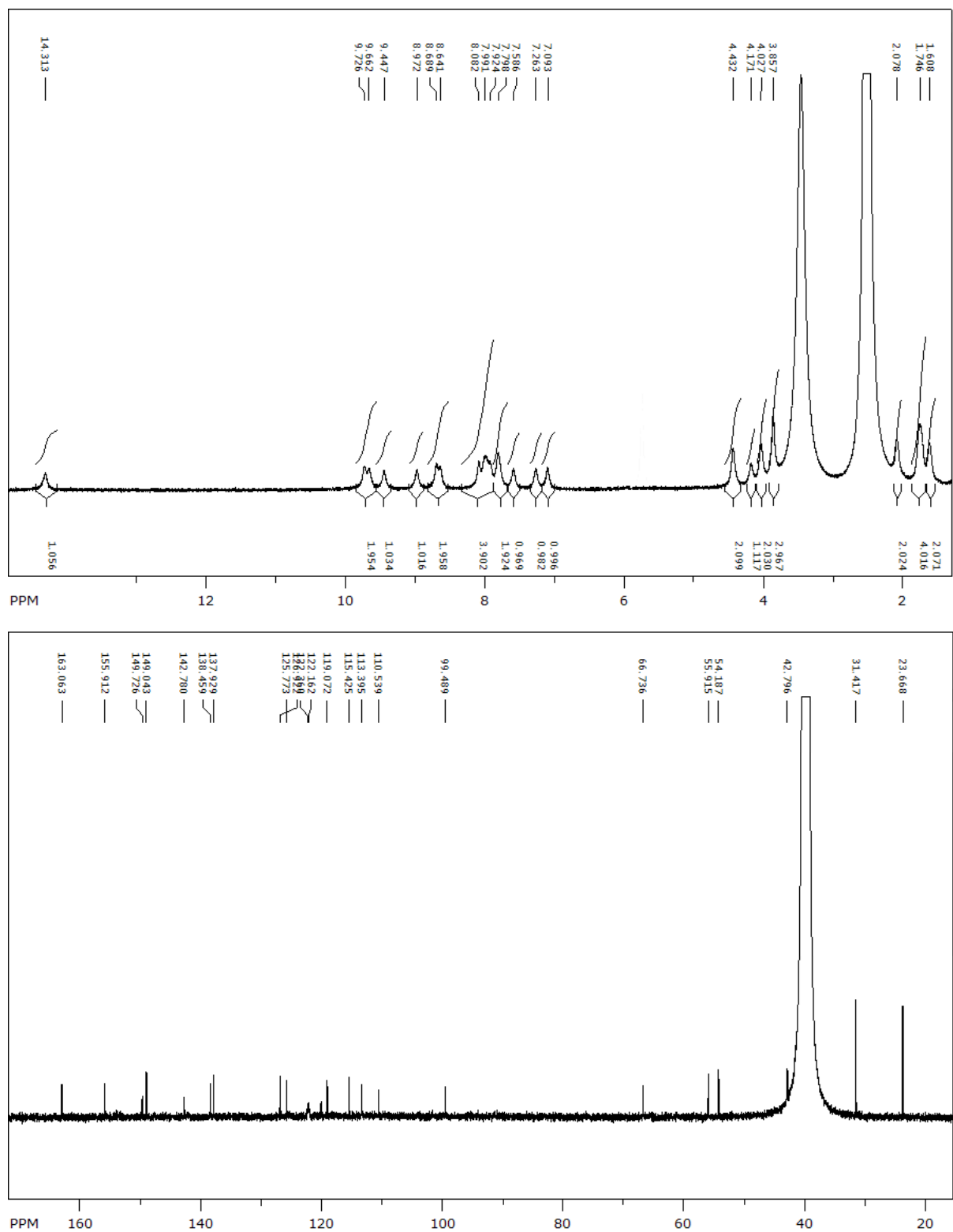


Figure S15 ¹H NMR and ¹³C NMR of compound **12d**

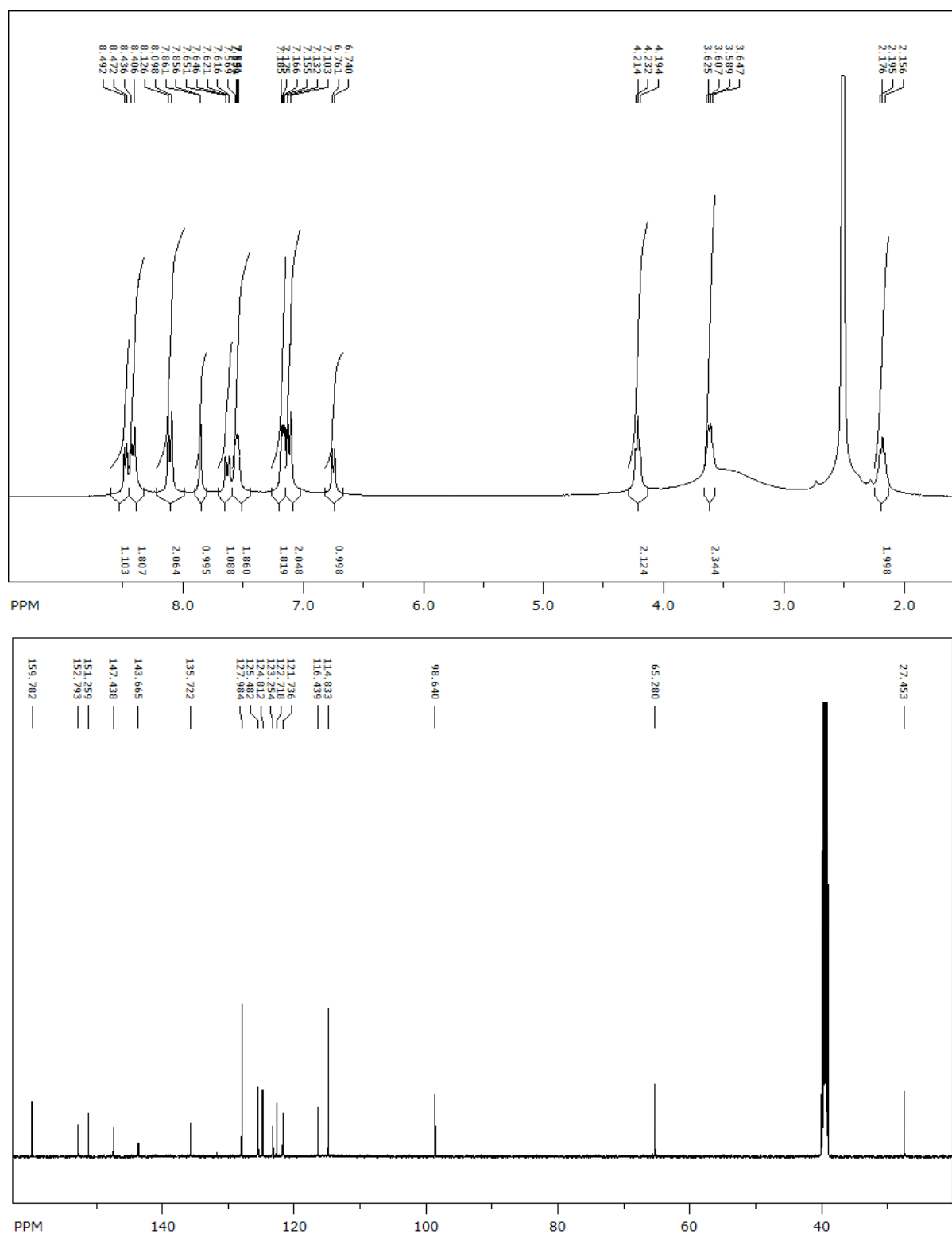


Figure S16 ¹H NMR and ¹³C NMR of compound **13a**

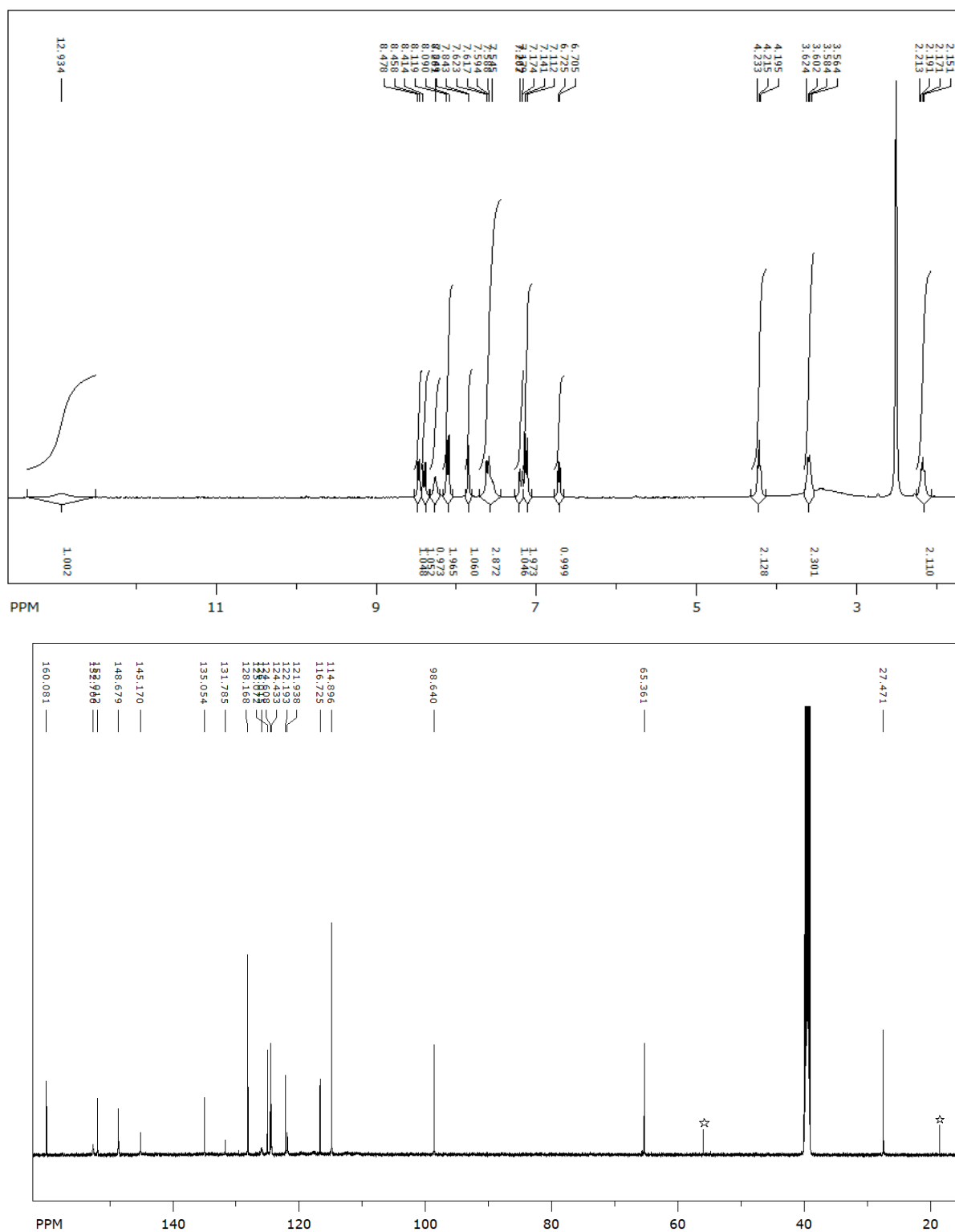


Figure S17 ¹H NMR and ¹³C NMR of compound **13b** (*ethanol; residual solvent signal)

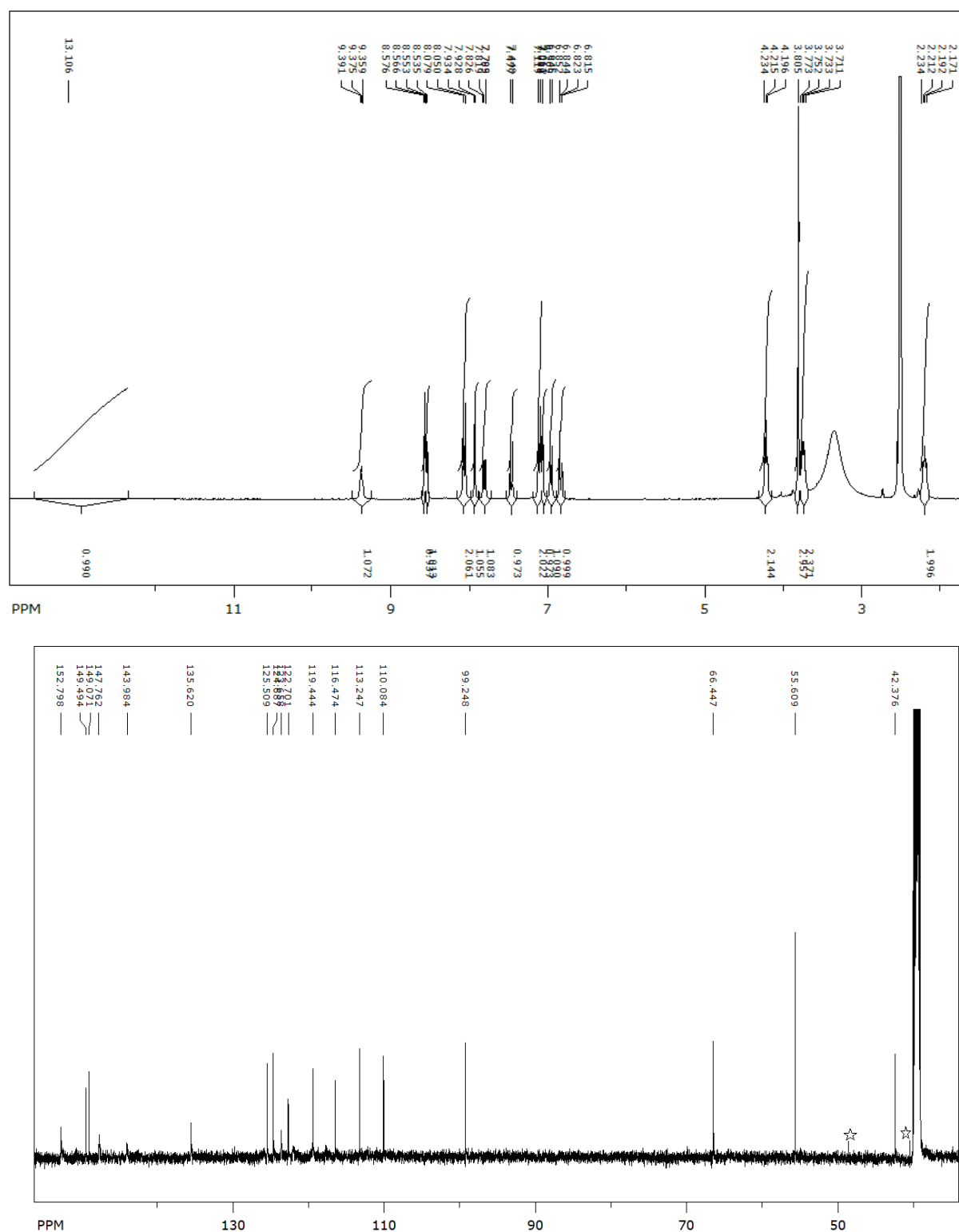


Figure S18 ¹H NMR and ¹³C NMR of compound **13c** (*methanol, *DMSO; residual solvent signals)

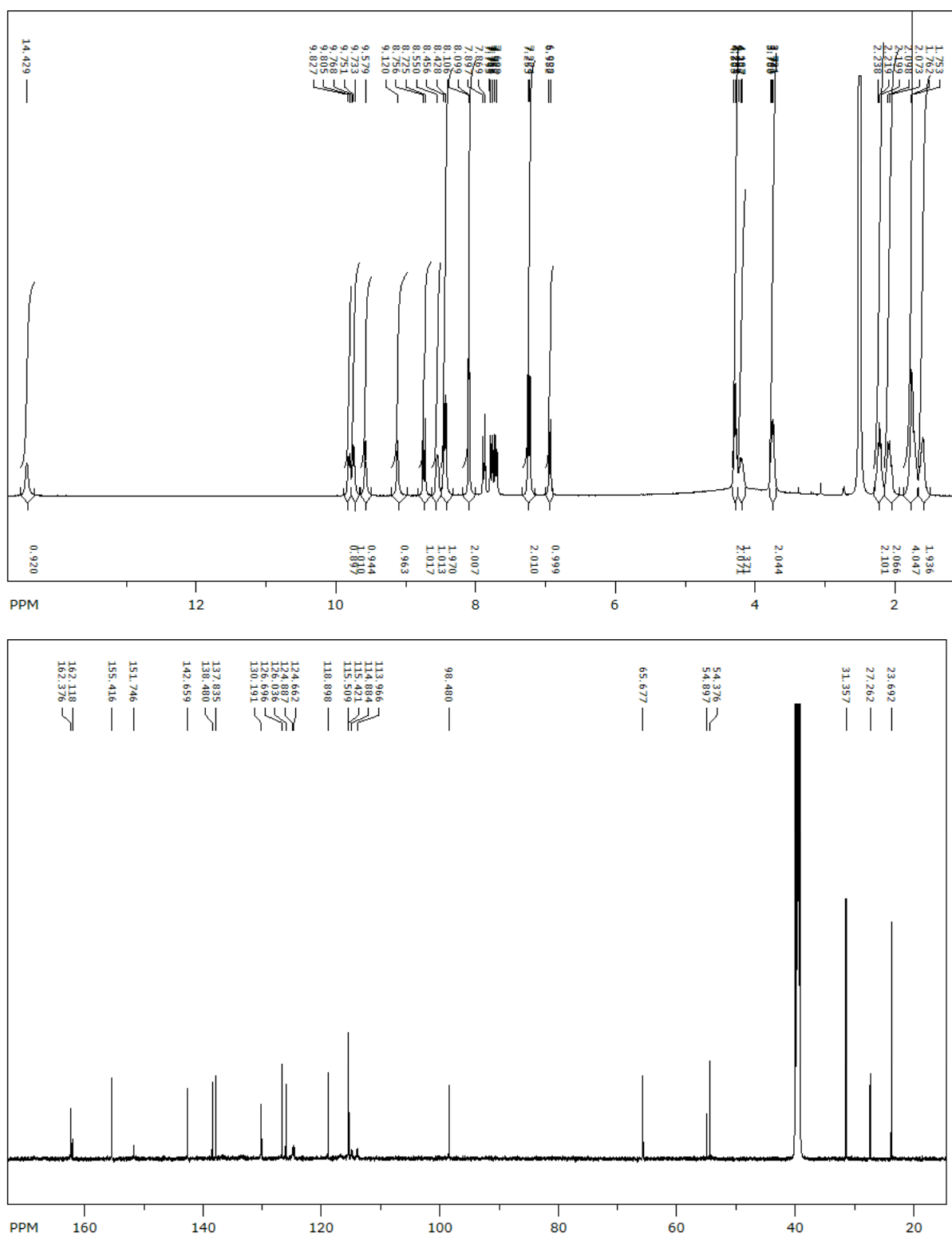


Figure S19 ¹H NMR and ¹³C NMR of compound **13d**

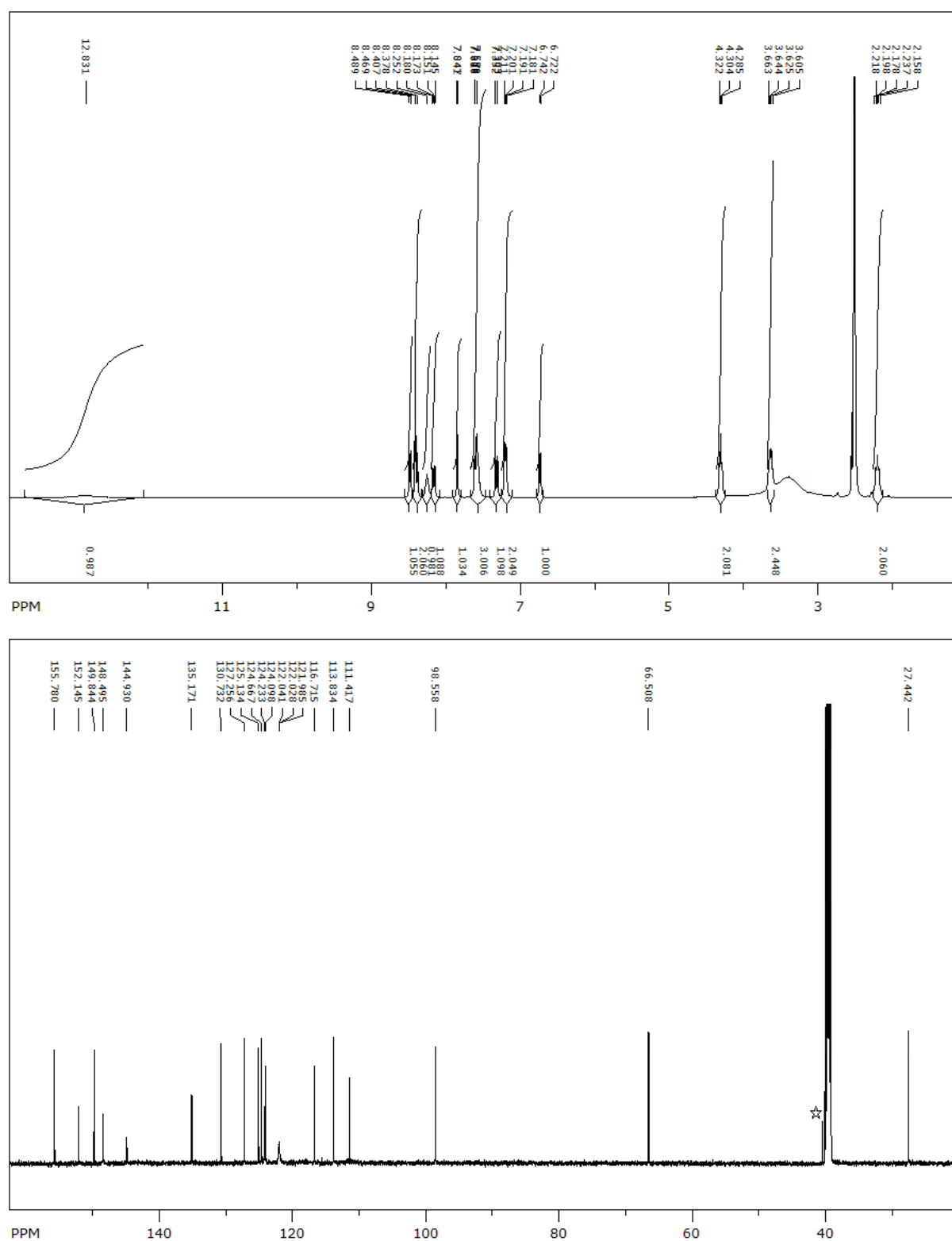


Figure S20 ¹H NMR and ¹³C NMR of compound **14a** (*DMSO; residual solvent signal)

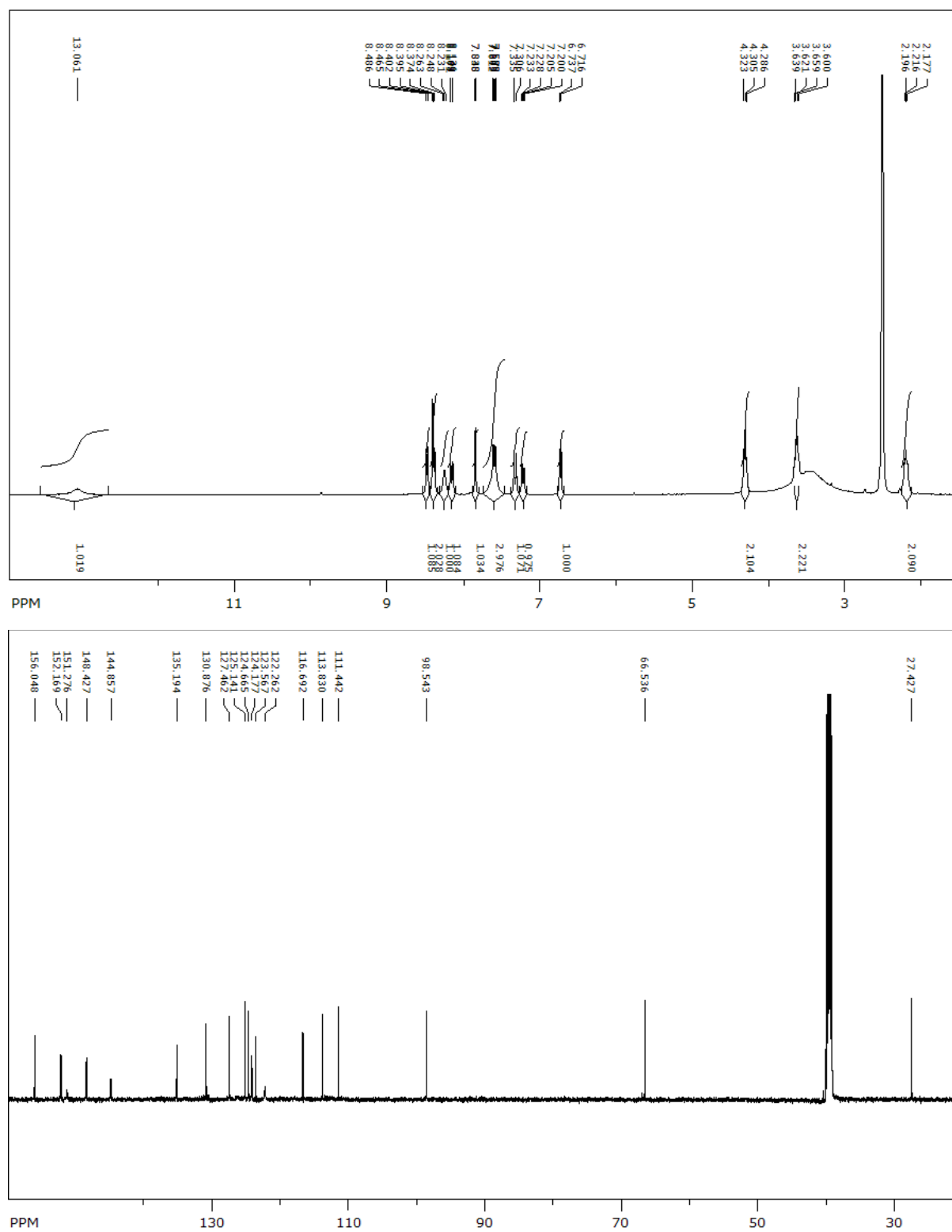


Figure S21 ¹H NMR and ¹³C NMR of compound **14b**

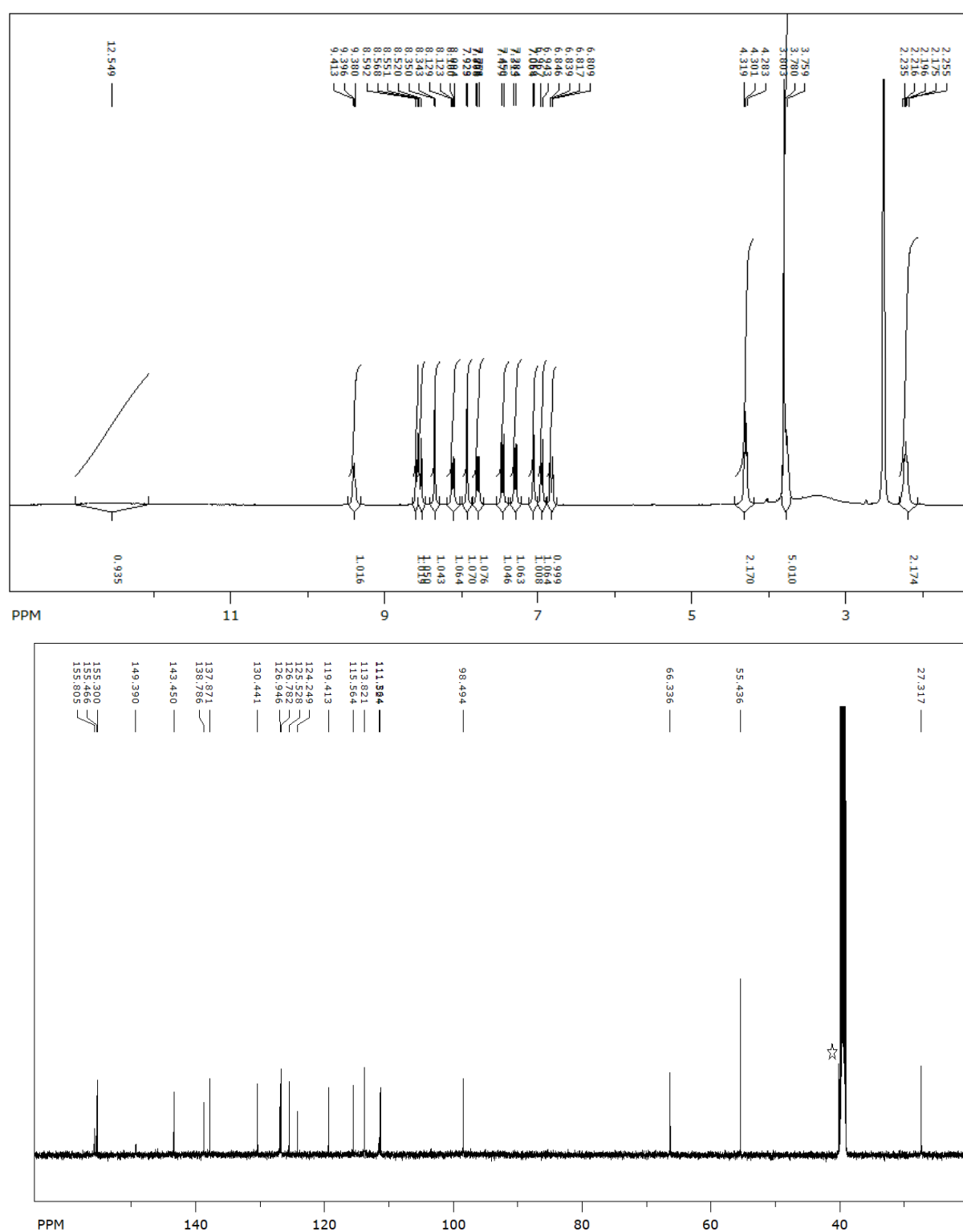


Figure S22 ¹H NMR and ¹³C NMR of compound **14c** (*DMSO; residual solvent signal)

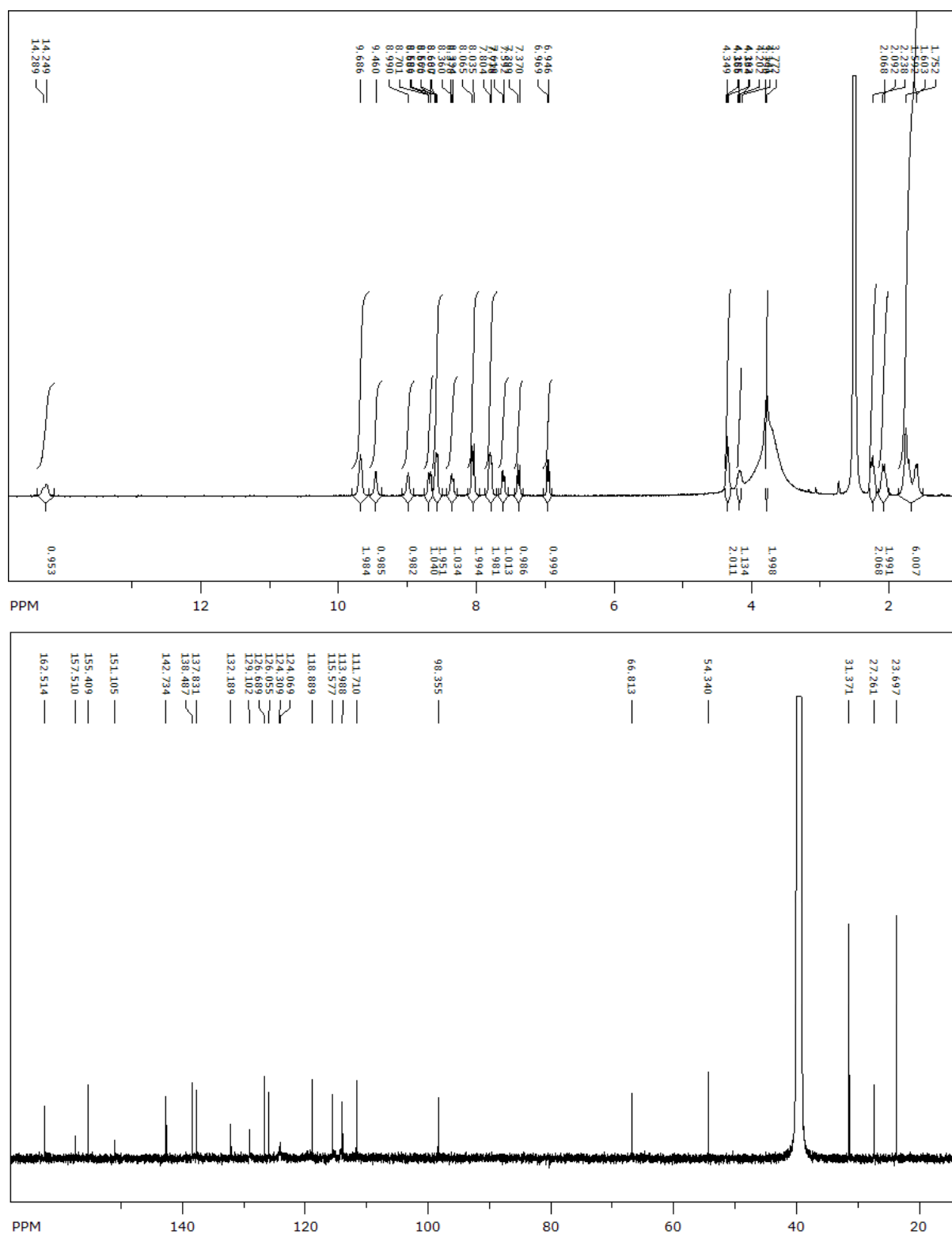


Figure S23 ¹H NMR and ¹³C NMR of compound **14d**

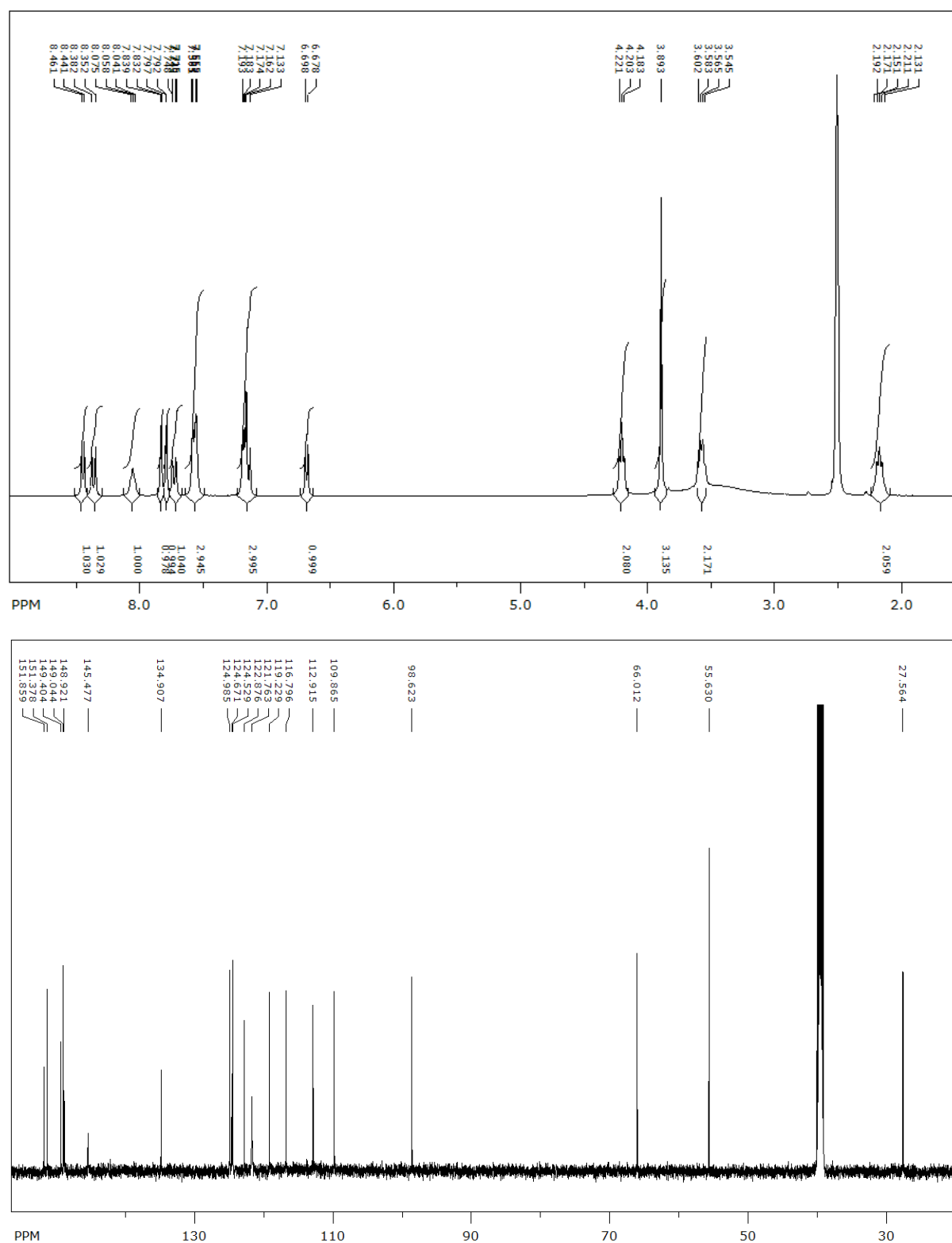


Figure S24 ^1H NMR and ^{13}C NMR of compound **15a**

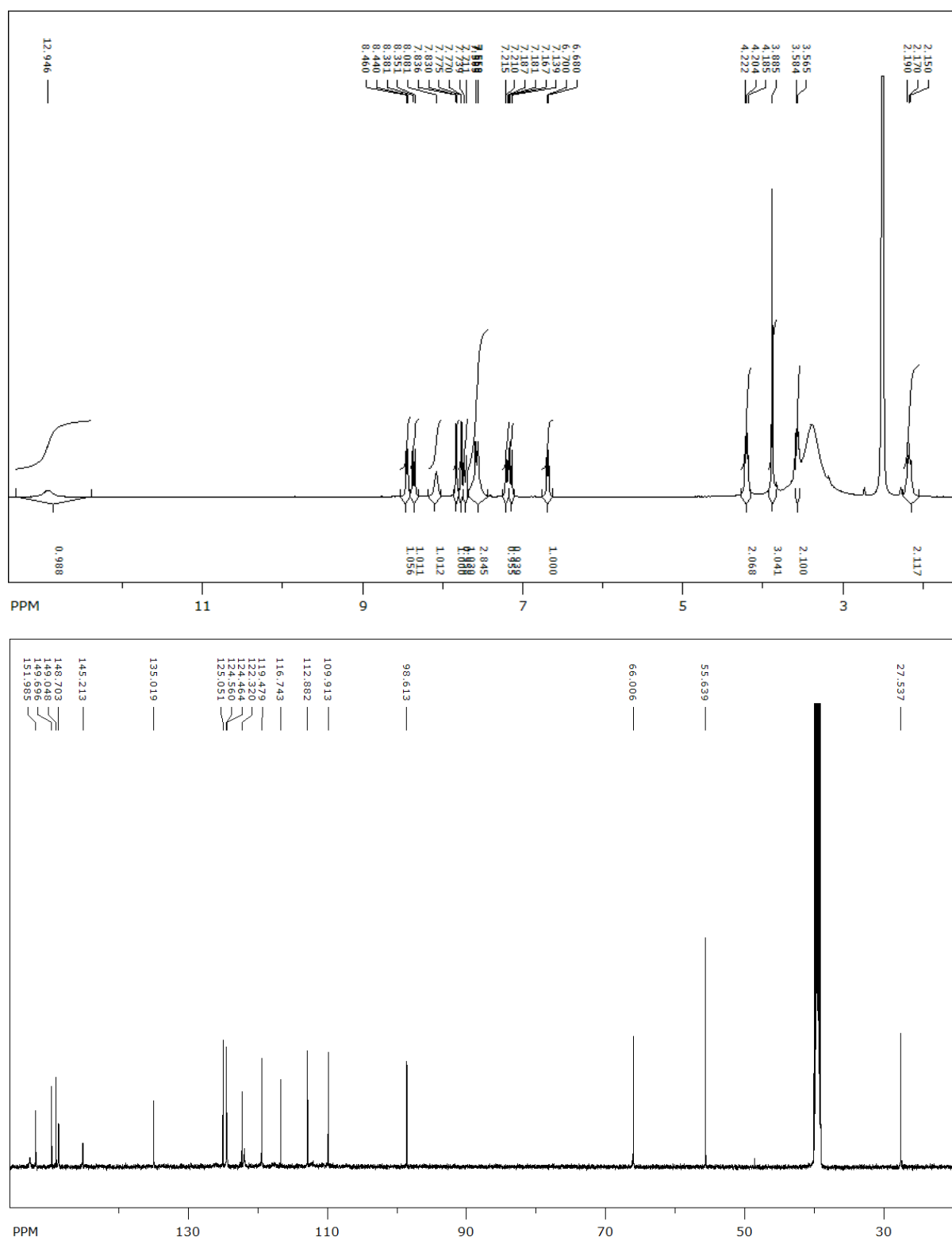


Figure S25 ¹H NMR and ¹³C NMR of compound **15b**

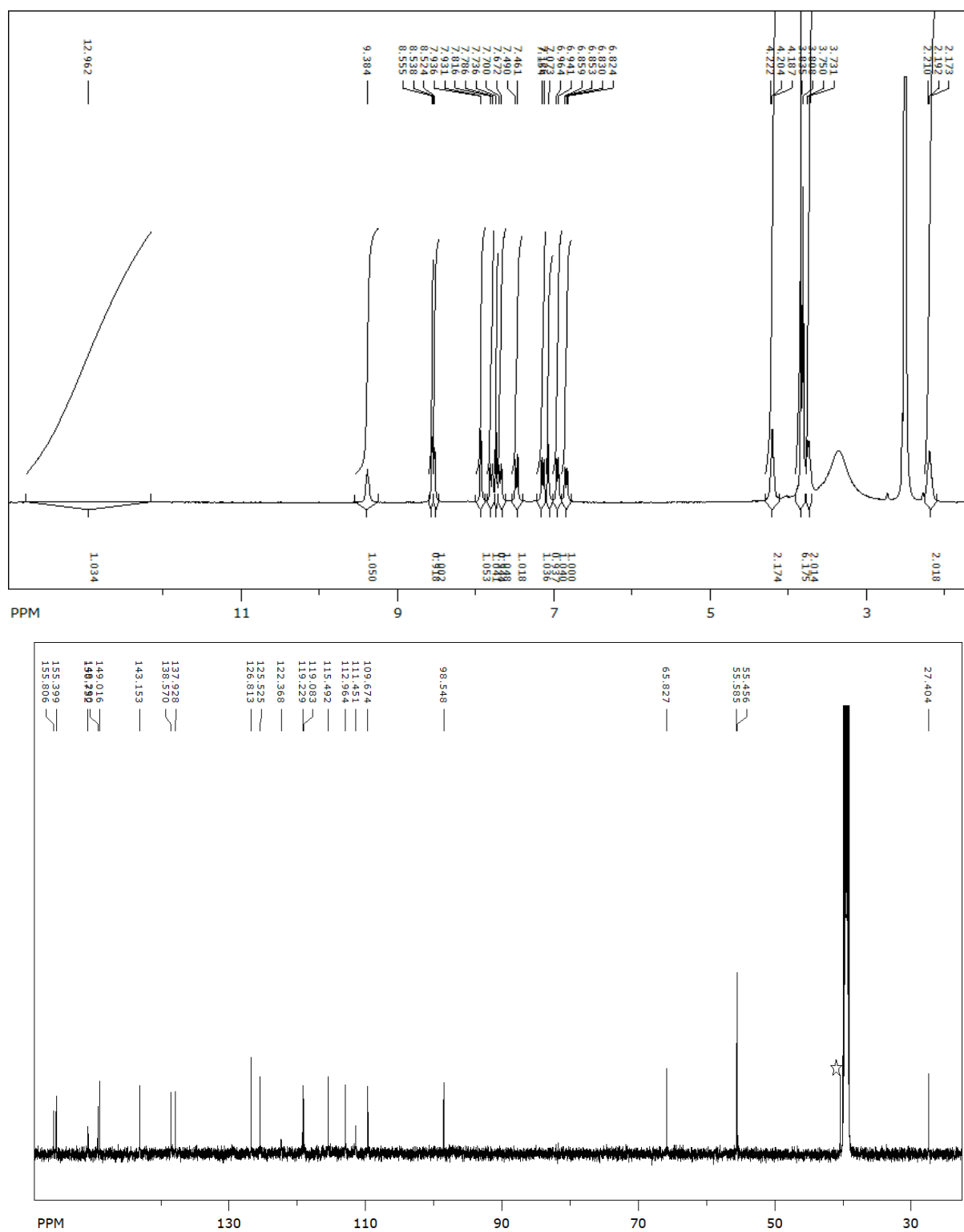


Figure S26 ¹H NMR and ¹³C NMR of compound **15c** (*DMSO; residual solvent signal)

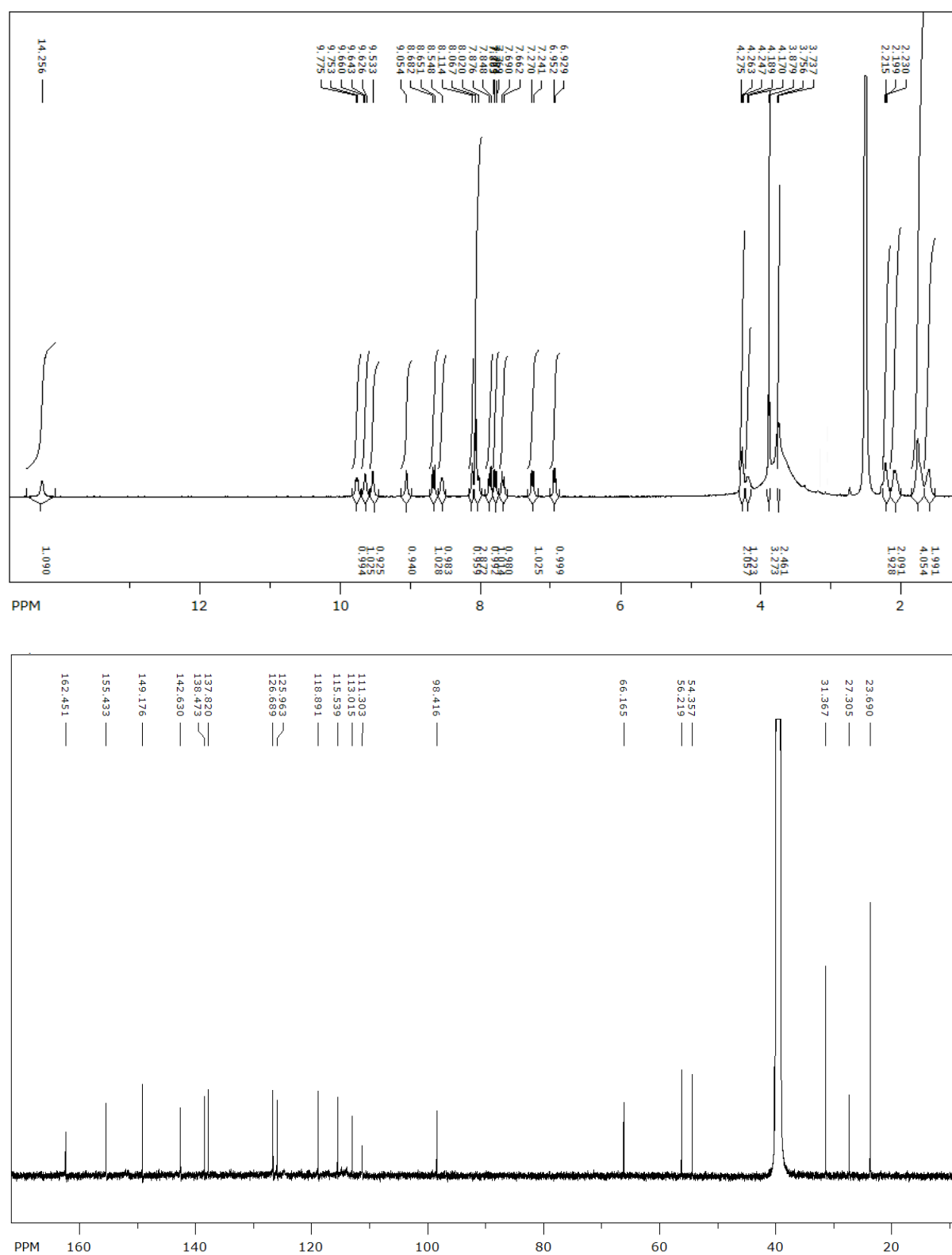


Figure S27 ¹H NMR and ¹³C NMR of compound **15d**