

SYNTHESIS AND ANTIMICROBIAL ACTIVITY EVALUATION OF HOMODRIMANE SESQUITERPENOIDS WITH BENZIMIDAZOLE UNIT

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SUPPLEMENTARY INFORMATION

Table S1. Bond distances (Å) and angles (°) for 20.

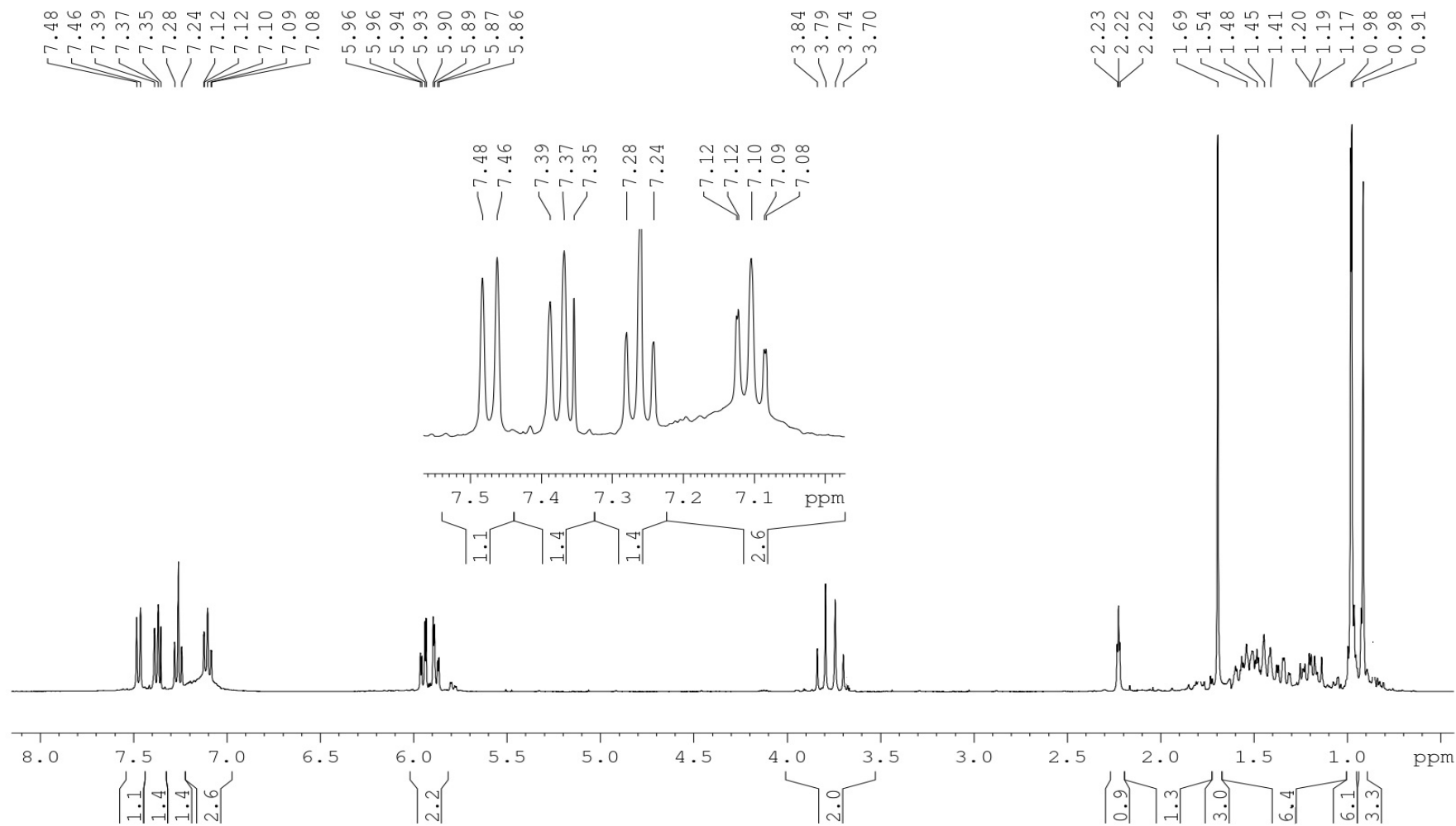
C4-C14	1.528(6)	C5-C6-C7	110.2(3)
C4-C15	1.531(6)	C8-C7-C6	112.5(3)
C5-C6	1.525(4)	O1-C8-C7	108.5(3)
C5-C10	1.559(4)	O1-C8-C9	101.2(2)
C6-C7	1.534(5)	O1-C8-C11	107.7(3)
C7-C8	1.515(5)	C7-C8-C9	109.9(3)
C8-C9	1.562(4)	C7-C8-C11	113.8(3)
C8-C11	1.534(6)	C11-C8-C9	114.8(3)
C9-C10	1.570(5)	C8-C9-C10	114.5(2)
C9-C16	1.544(5)	C16-C9-C8	112.3(3)
C10-C24	1.538(5)	C16-C9-C10	112.4(3)
C12-C13	1.479(7)	C1-C10-C5	107.0(3)
C16-C17	1.513(5)	C1-C10-C9	108.2(2)
C20-C19	1.39	C5-C10-C9	107.4(2)
C20-C21	1.39	C24-C10-C1	107.9(3)
C19-C18	1.39	C24-C10-C5	114.3(3)
C18-C23	1.39	C24-C10-C9	111.8(3)
C23-C22	1.39	O1-C12-C13	110.8(4)
C22-C21	1.39	O2-C12-O1	125.0(4)
C12-O1-C8	122.5(3)	O2-C12-C13	124.2(4)
C17-N1-C18	125.4(8)	C17-C16-C9	116.4(3)

C2-C1-C10	113.4(3)	O3-C17-N1	122.5(3)
C3-C2-C1	111.6(3)	O3-C17-C16	122.9(3)
C2-C3-C4	114.2(3)	C19-C18-N1	114.3(10)
C3-C4-C5	107.2(3)	C23-C18-N1	125.7(10)
C14-C4-C3	110.7(3)	N1-C17-C16	114.4(3)
C14-C4-C5	114.6(3)	C20-C19-N2	112(2)
C14-C4-C15	107.8(3)	C18-C19-N2	127(2)
C15-C4-C3	107.4(3)	C23-C18-C19	120
C15-C4-C5	109.0(3)	C18-C23-C22	120
C6-C5-C4	113.7(2)	C23-C22-C21	120
C6-C5-C10	110.8(3)	C22-C21-C20	120
C10-C5-C4	117.3(3)	C18-C19-C20	120
		C19-C20-C21	120

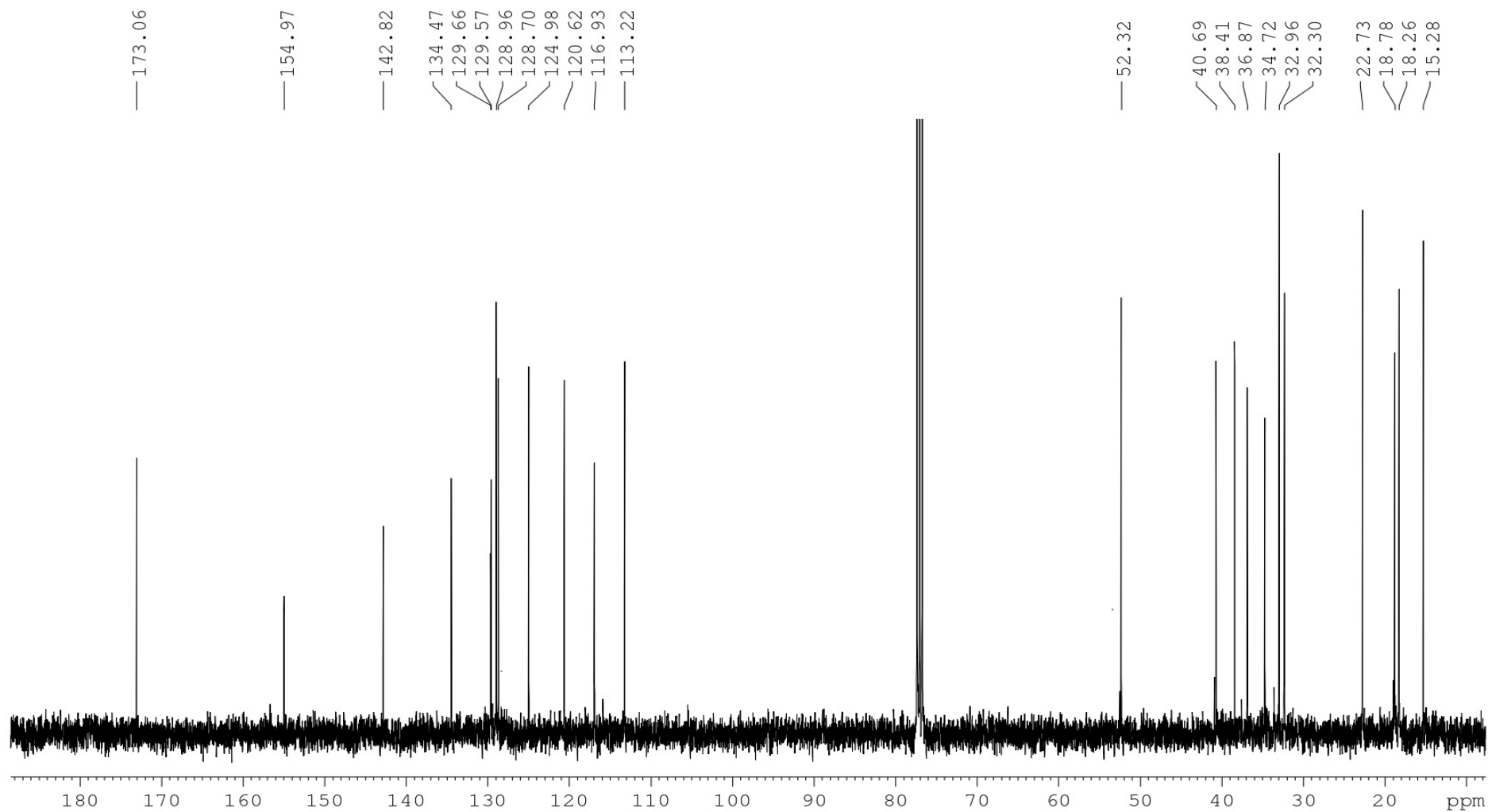
Table S2. Selected crystallographic data refinement parameters for 20.

Formula	$\text{C}_{24}\text{H}_{36}\text{N}_2\text{O}_3$
<i>F</i> _w	400.55
Space group	<i>P</i> 2 ₁
<i>a</i> [Å]	8.2121(3)
<i>b</i> [Å]	9.6498(3)
<i>c</i> [Å]	14.9502(5)
α [°]	90
β [°]	105.745(4)
γ [°]	90
<i>V</i> [Å ³]	1140.28(7)
<i>Z</i>	2
<i>r</i> _{calcd} [g cm ⁻³]	1.167
Crystal size [mm]	0.35×0.15×0.10
<i>T</i> [K]	294
μ [mm ⁻¹]	0.076
2 θ range [°]	5.082 to 52.744
Ref. collected	14240
Indep.refl. <i>R</i> _{int}	4447, 0.0248
Data/restr./param.	4447/2/253
<i>R</i> ₁	0.0578
<i>wR</i> ₂	0.1573
GOF	1.036
CCDC	2225381

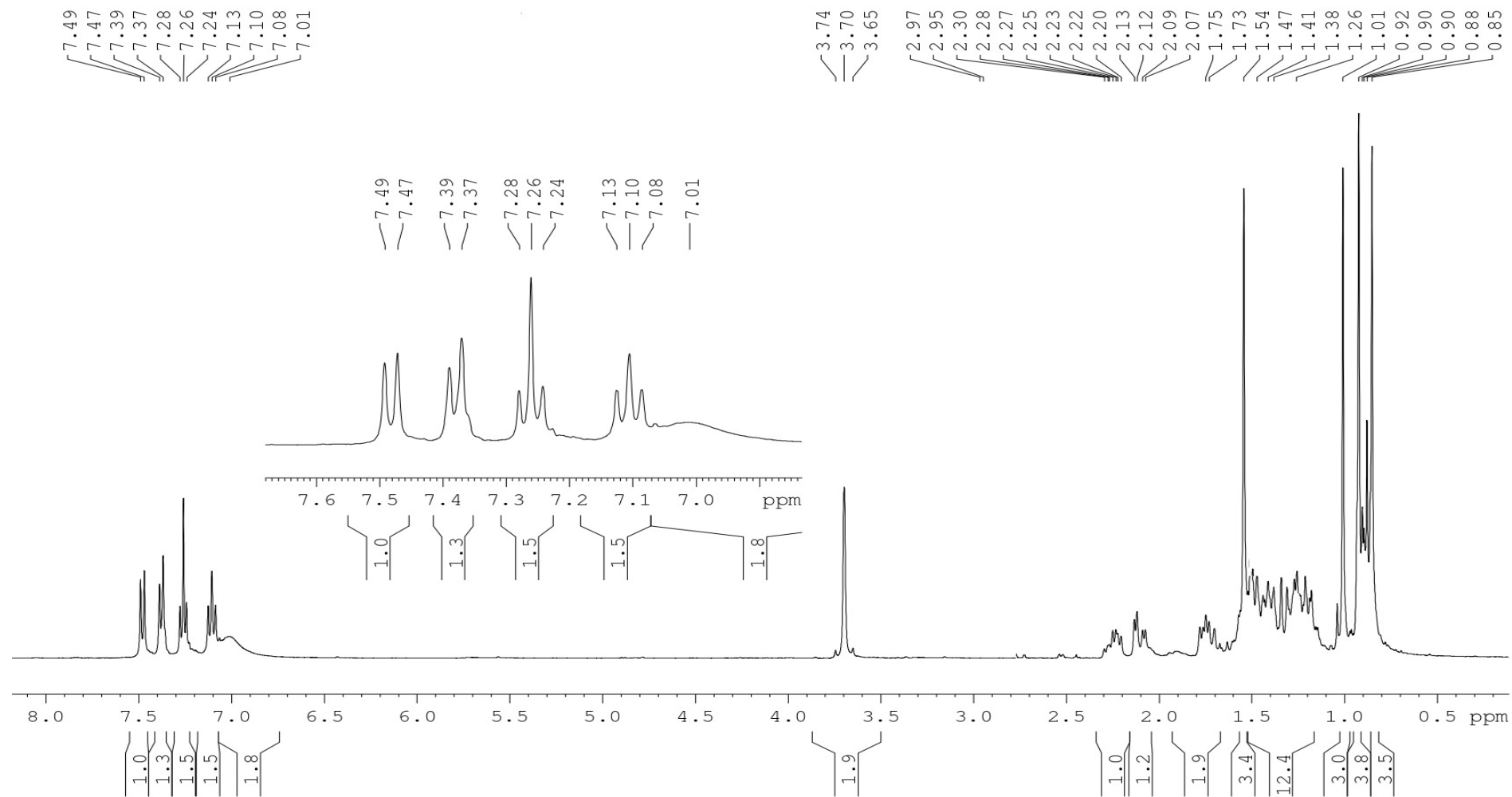
¹H NMR spectrum of compound 4



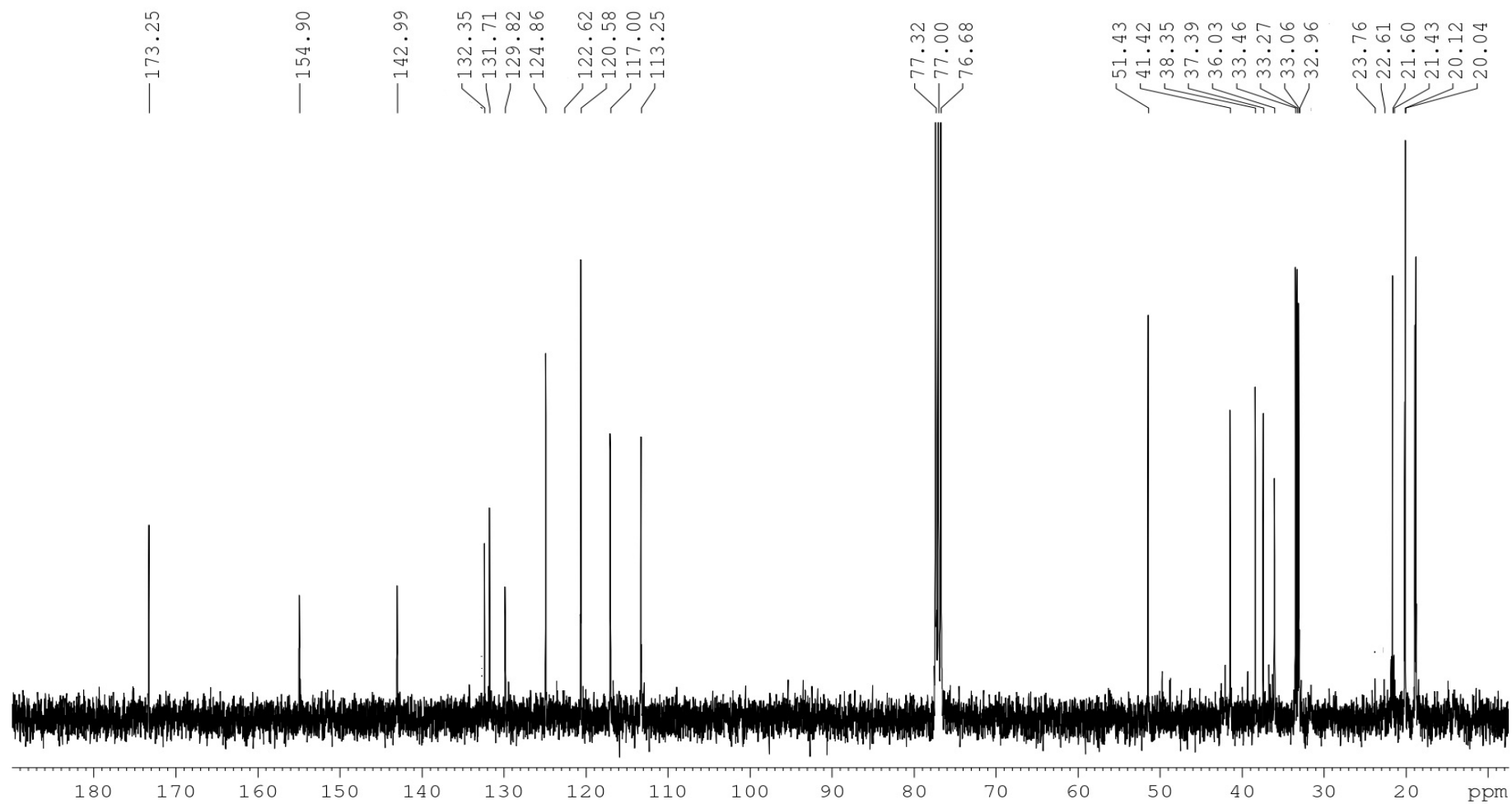
¹³C NMR spectrum of compound 4



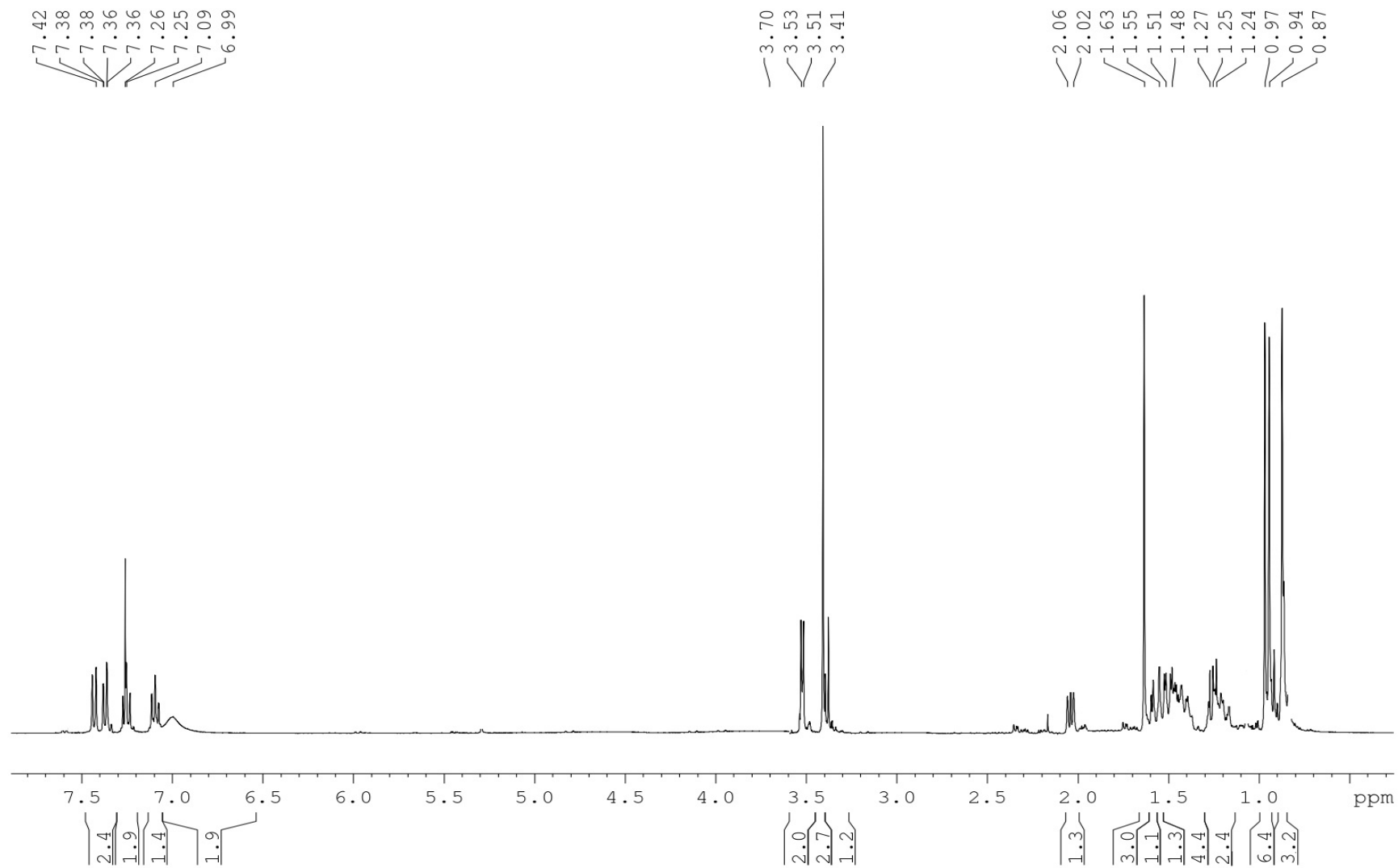
¹H NMR spectrum of compound 7



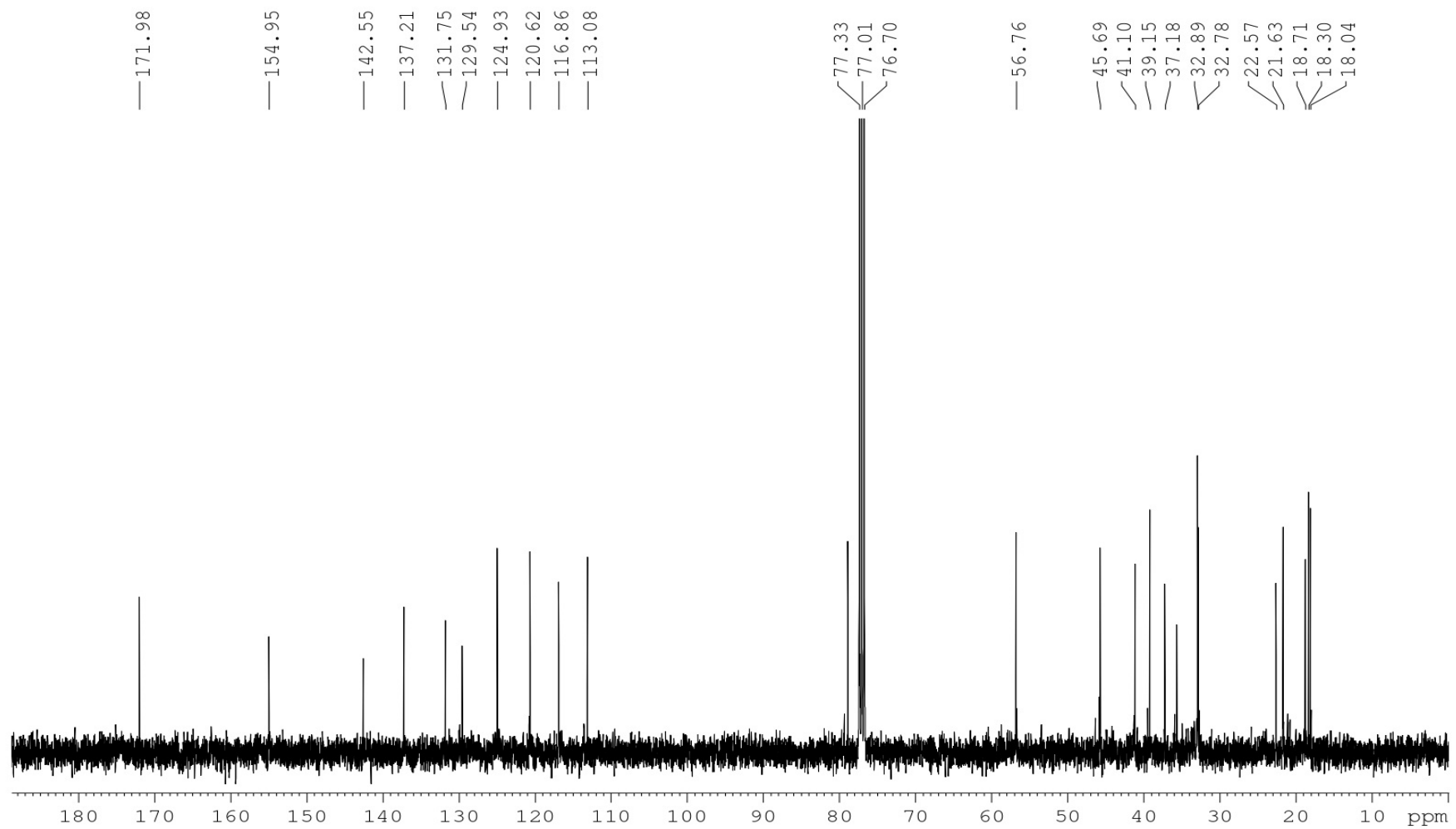
¹³C NMR spectrum of compound 7



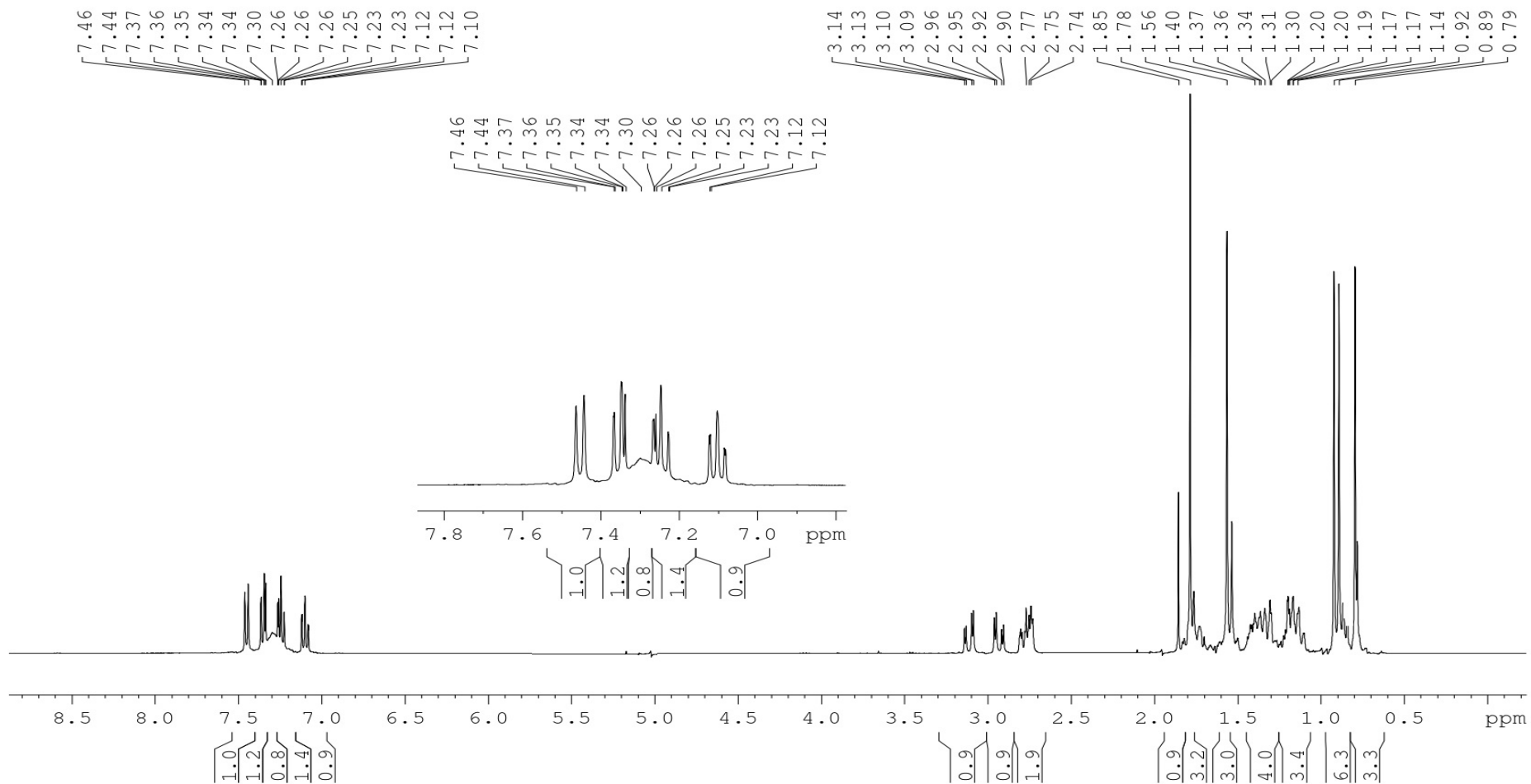
¹H NMR spectrum of compound 10



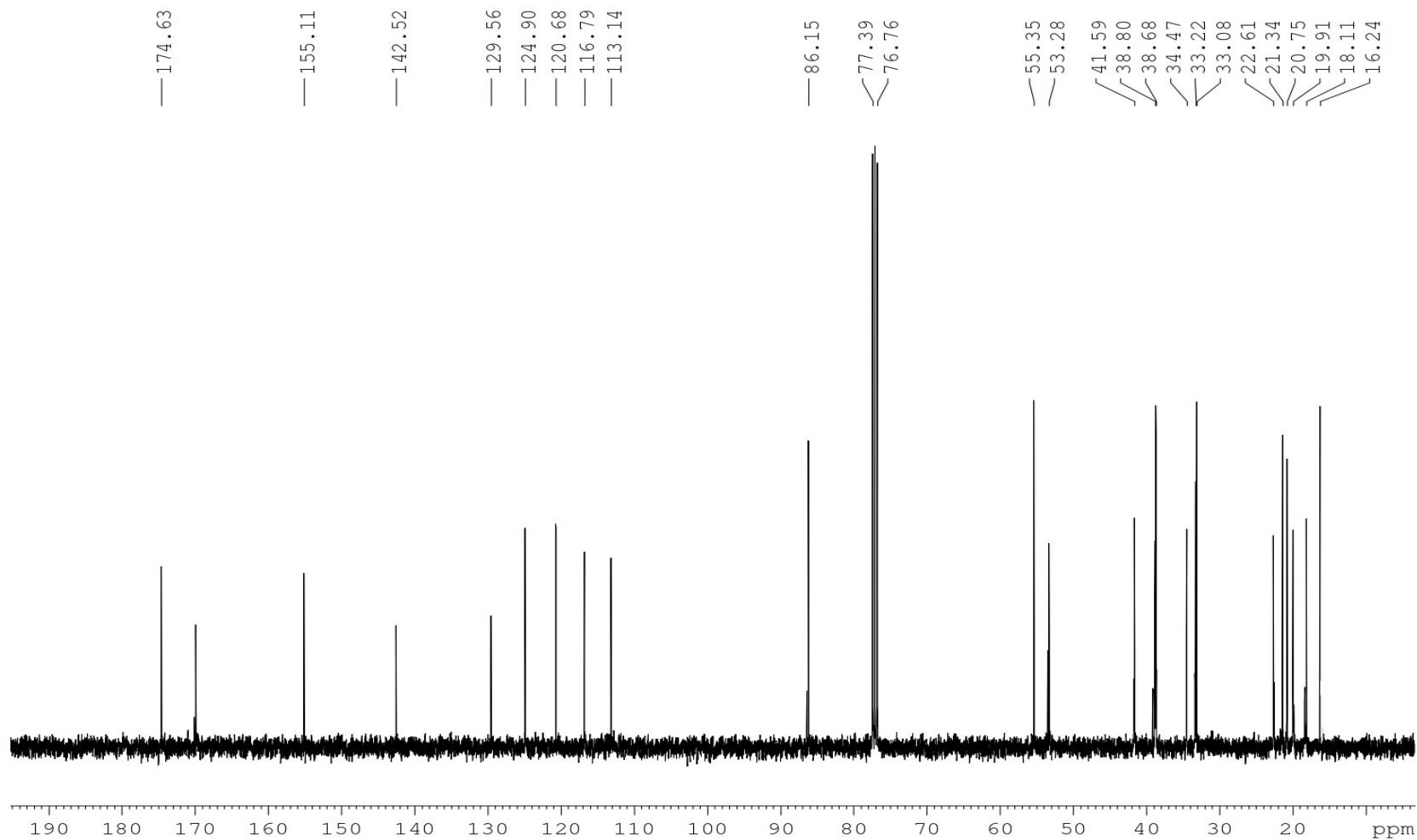
¹³C NMR spectrum of compound 10



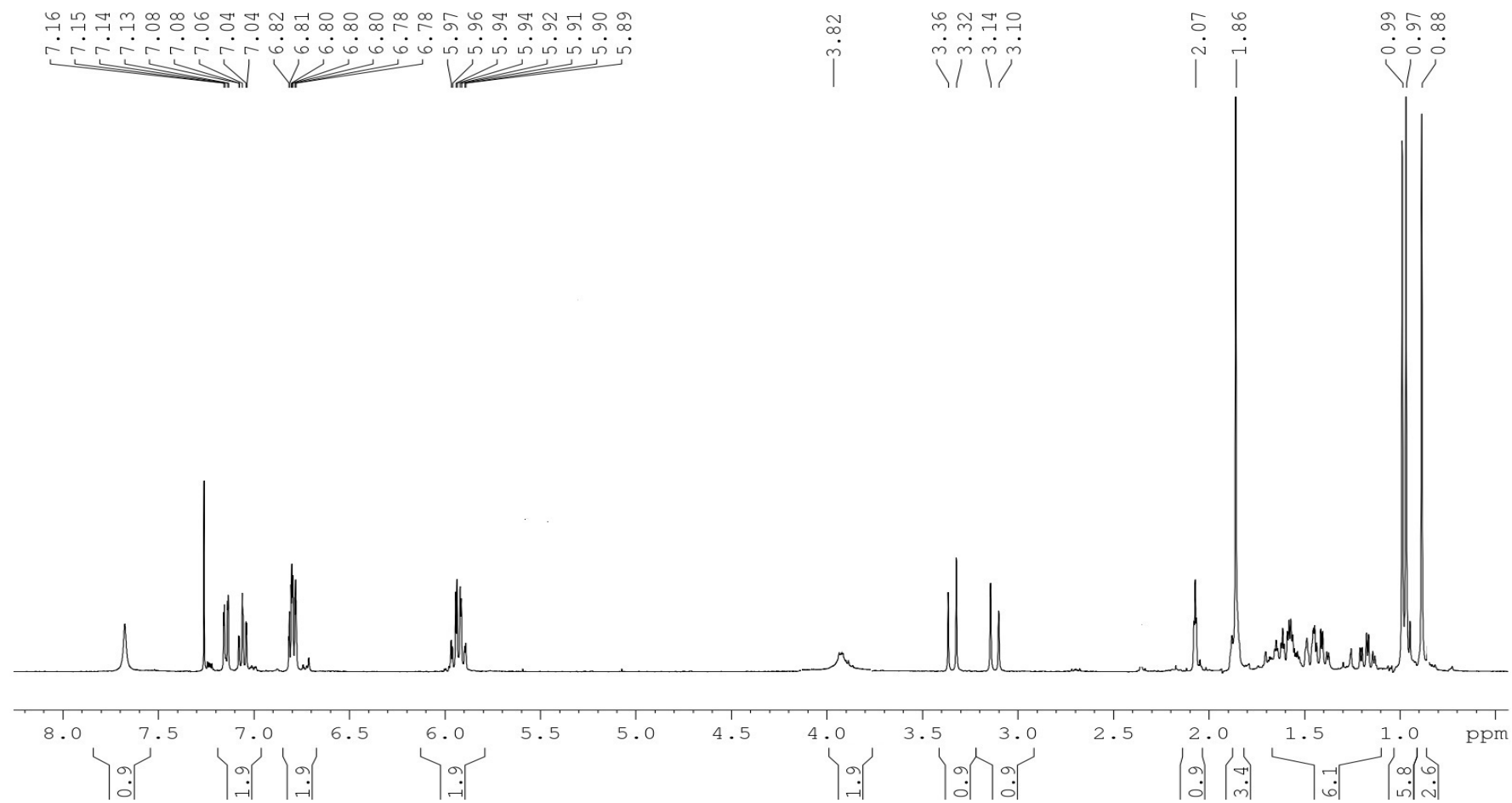
¹H NMR spectrum of compound 14



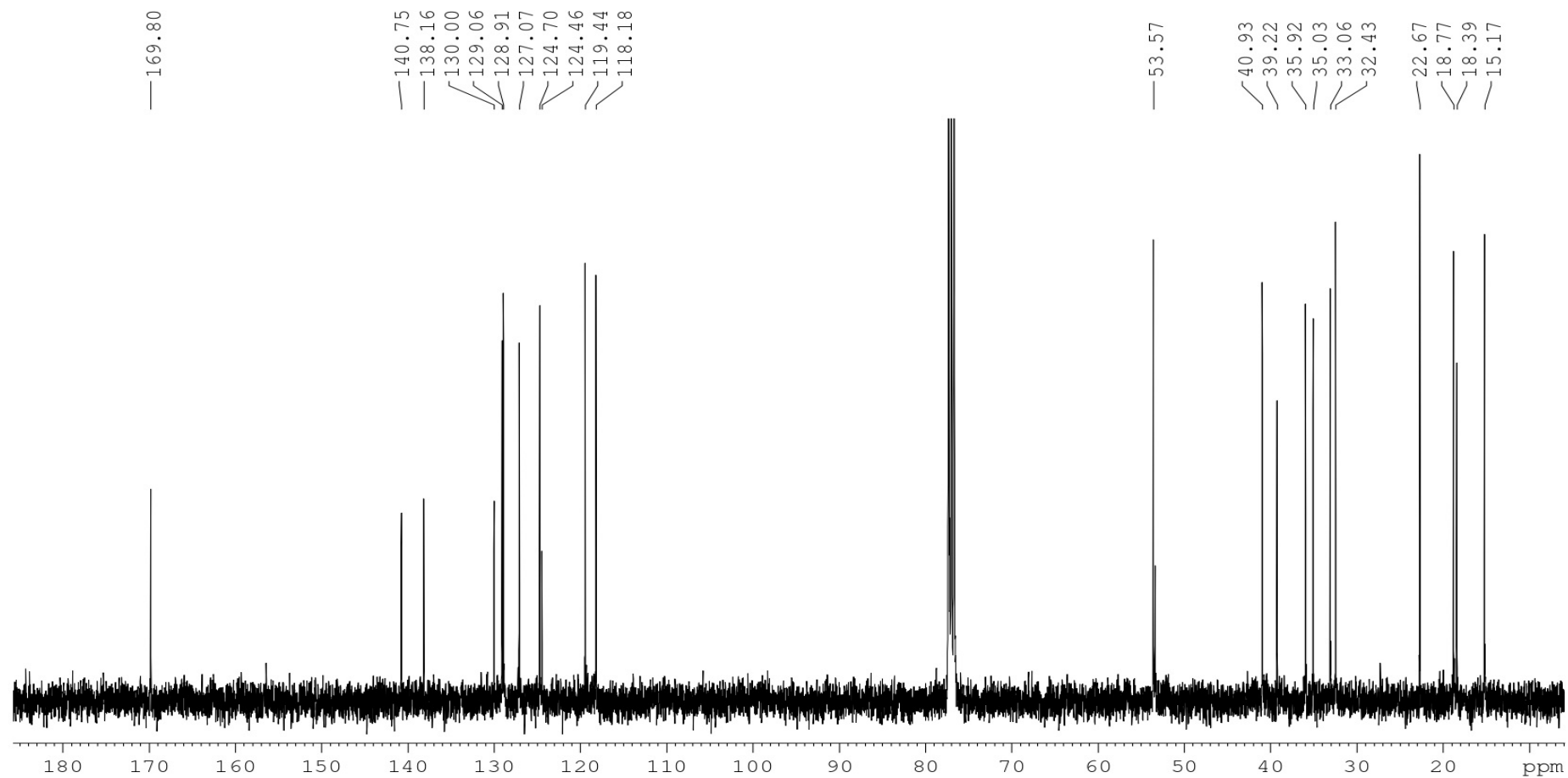
¹³C NMR spectrum of compound 14



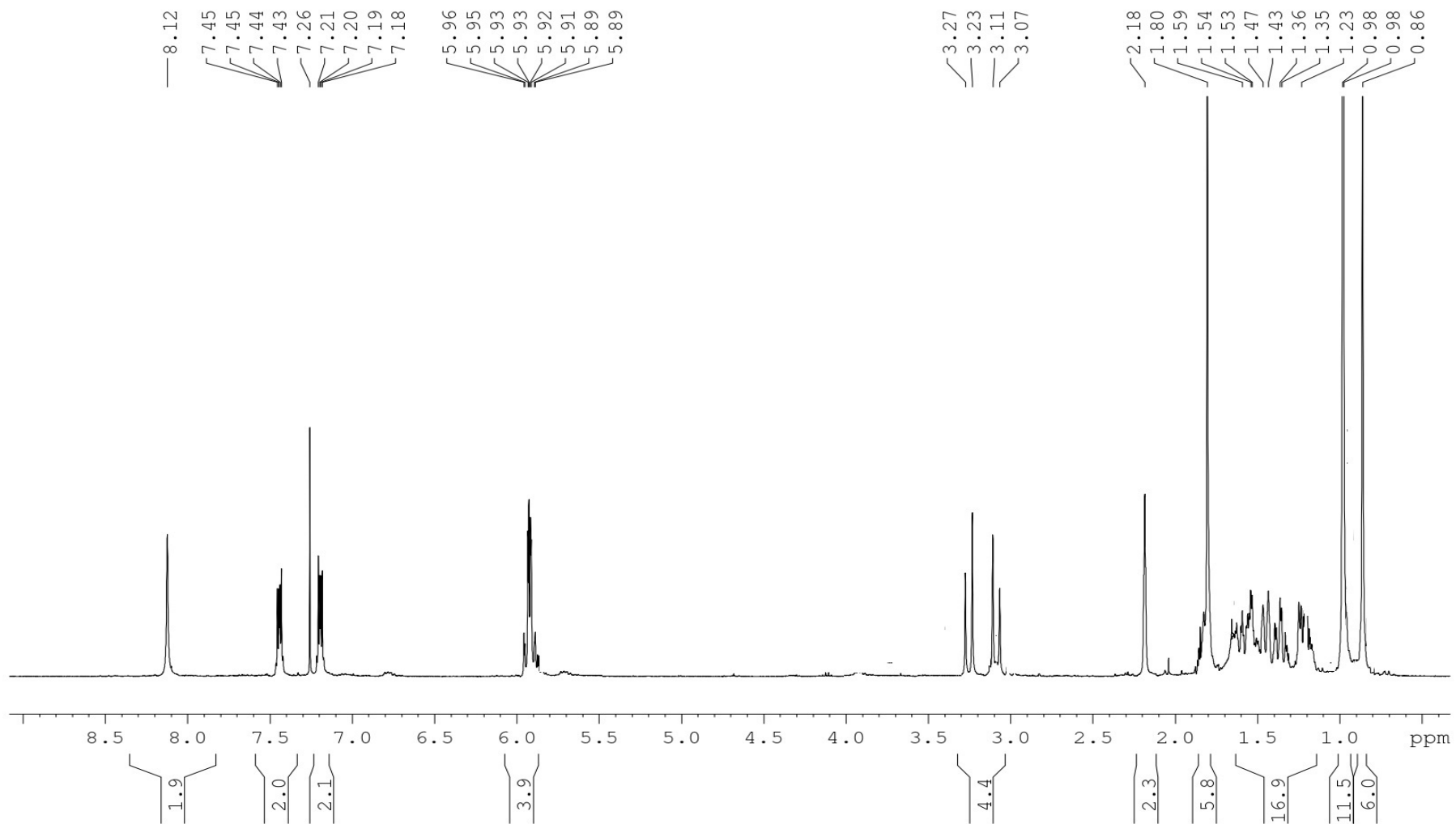
¹H NMR spectrum of compound 15



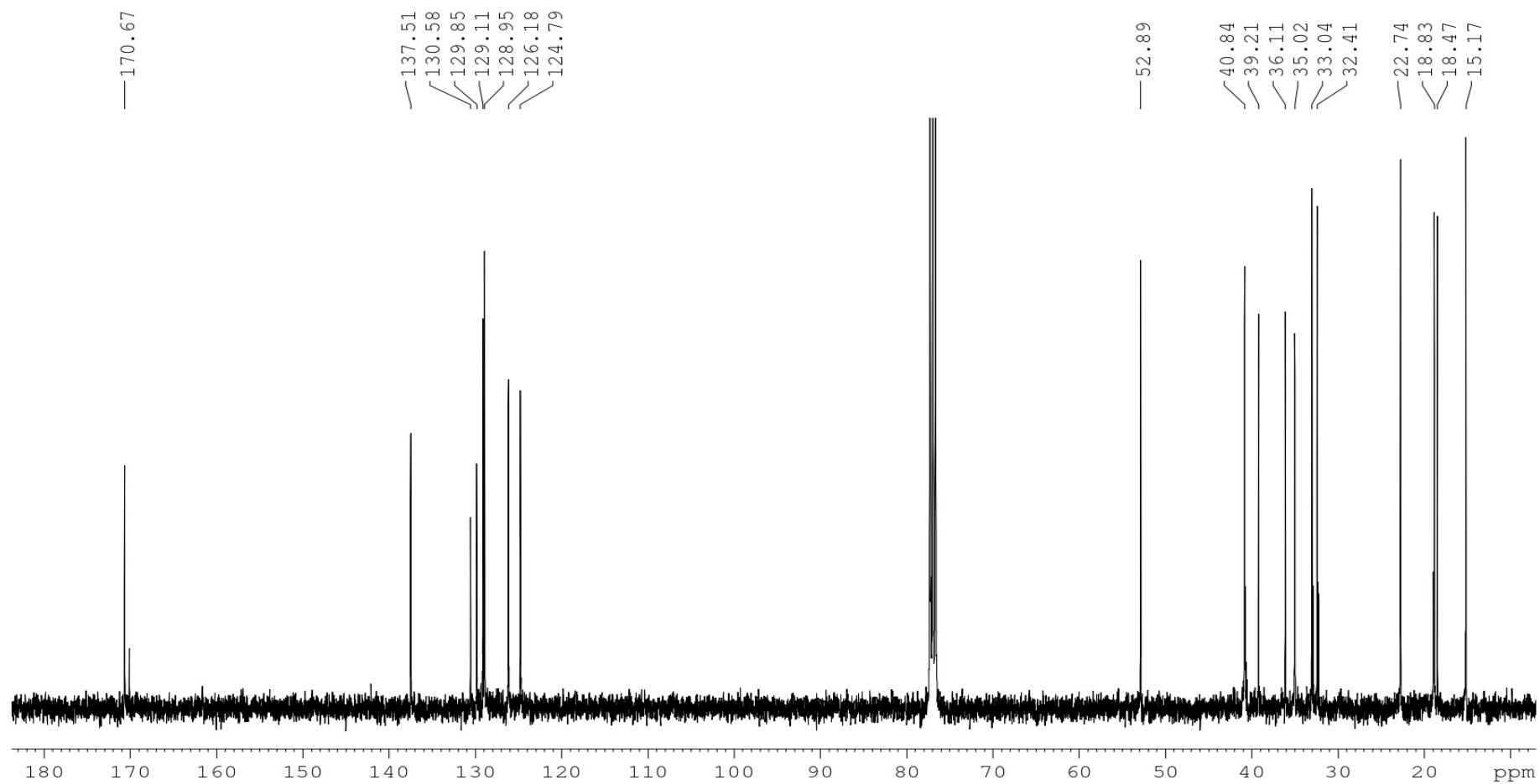
¹³C NMR spectrum of compound 15



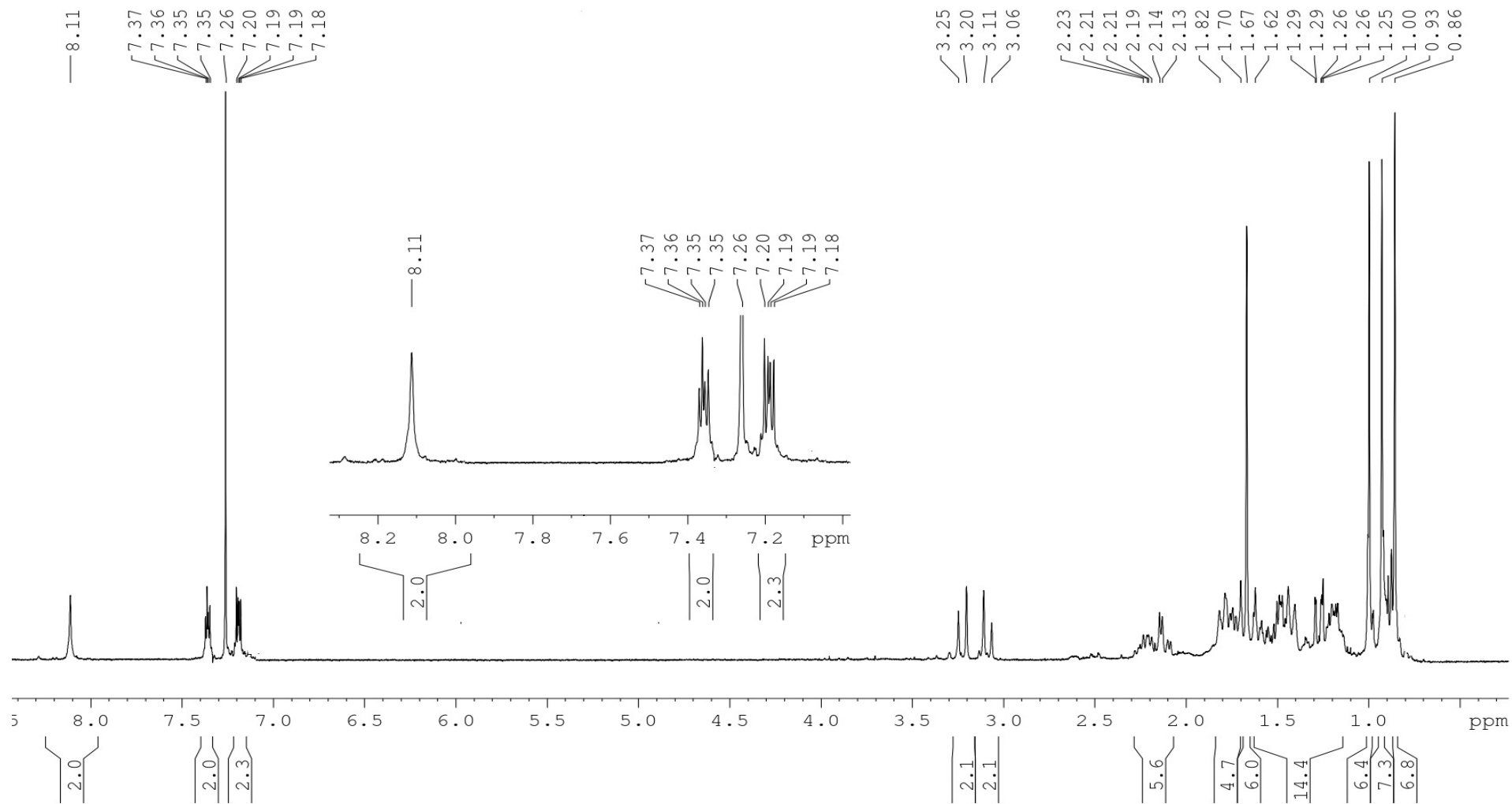
¹H NMR spectrum of compound 16



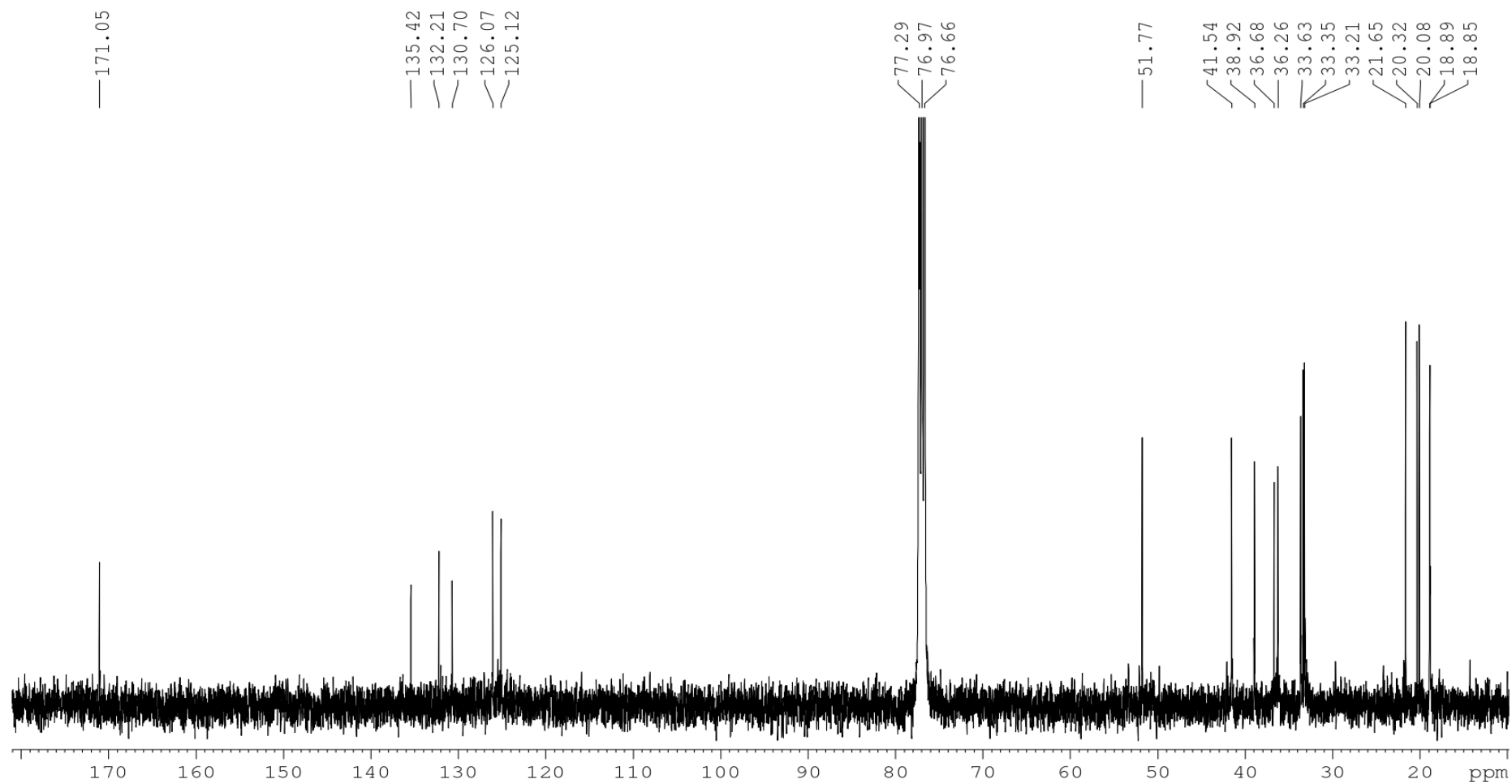
^{13}C NMR spectrum of compound 16



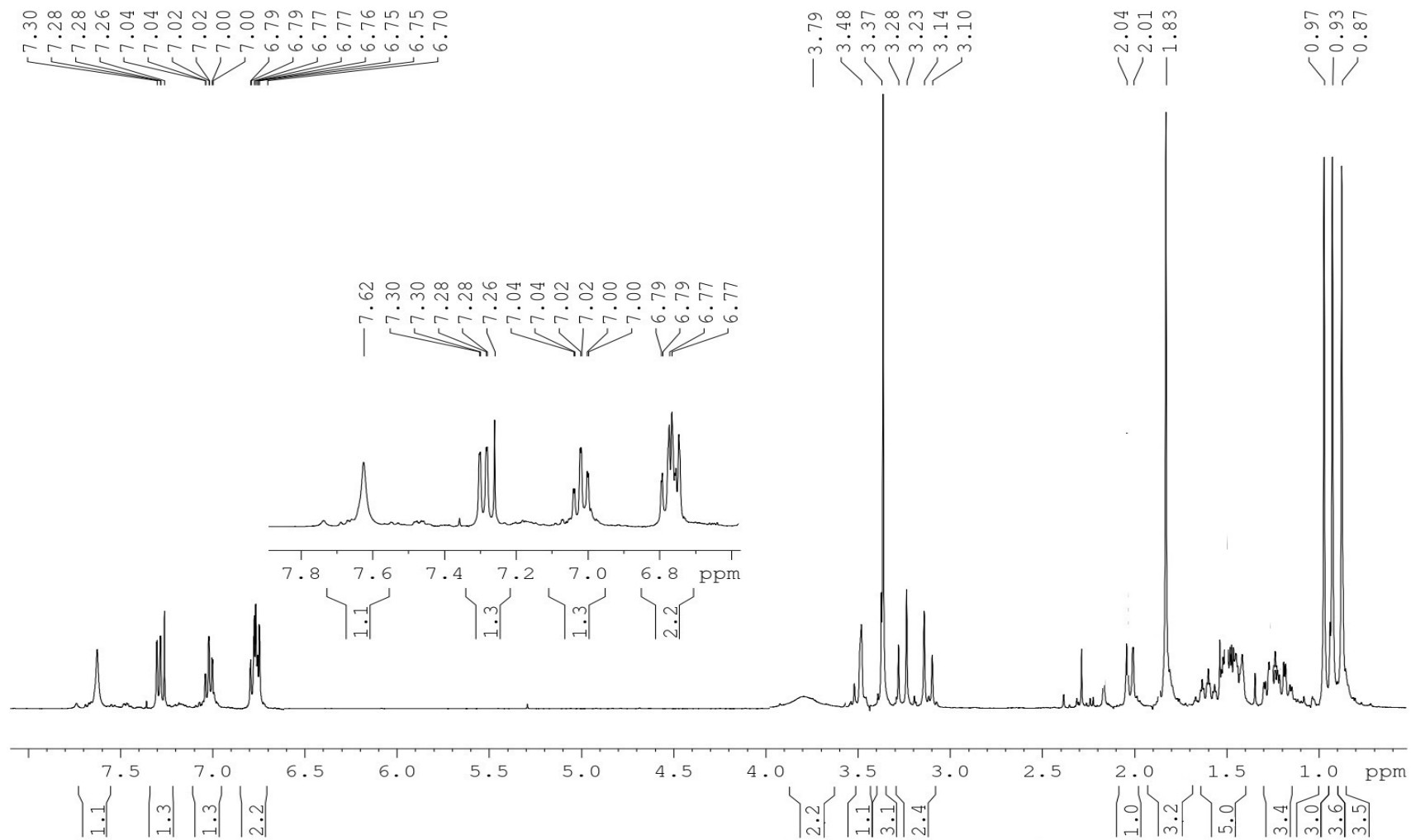
¹H NMR spectrum of compound 18



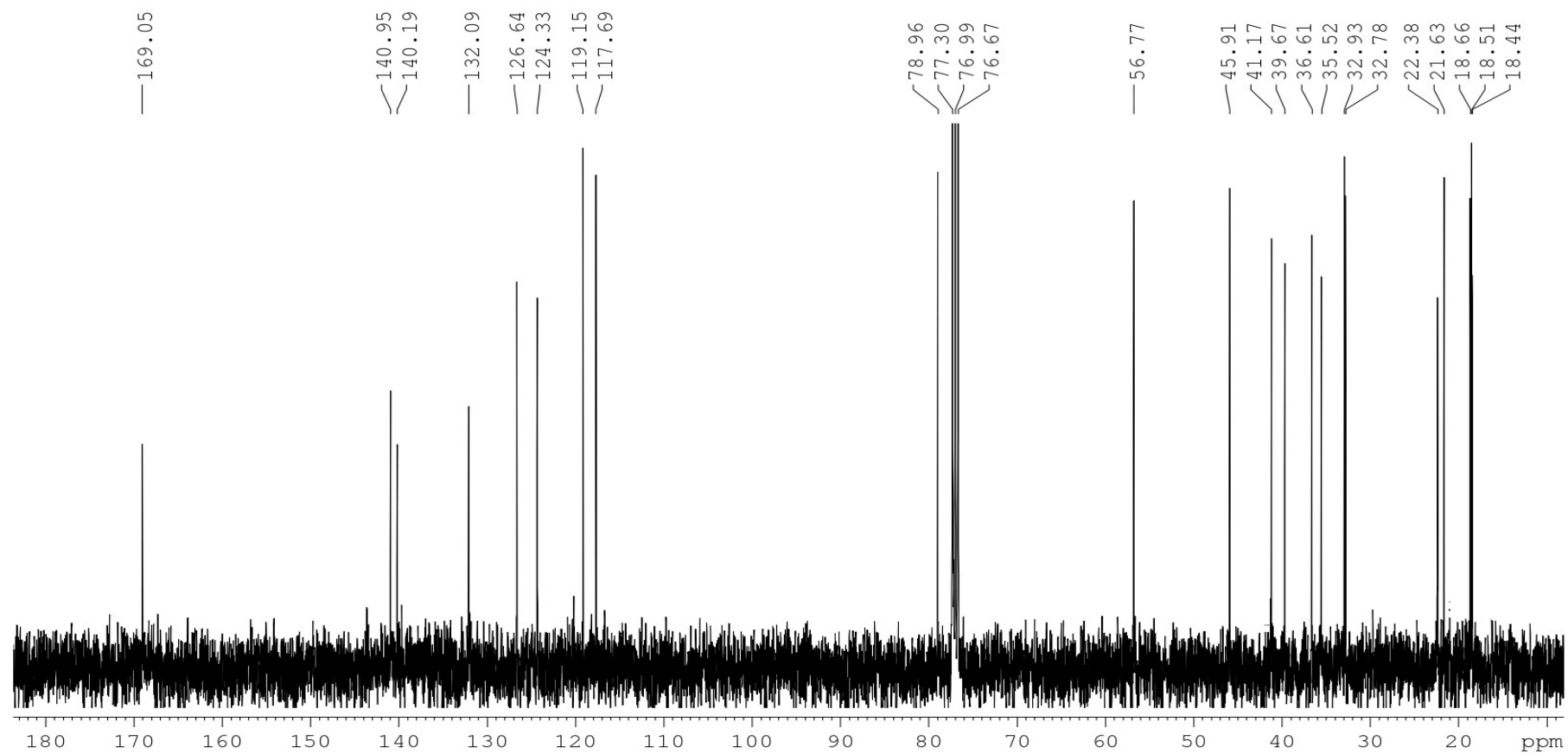
¹³C NMR spectrum of compound 18



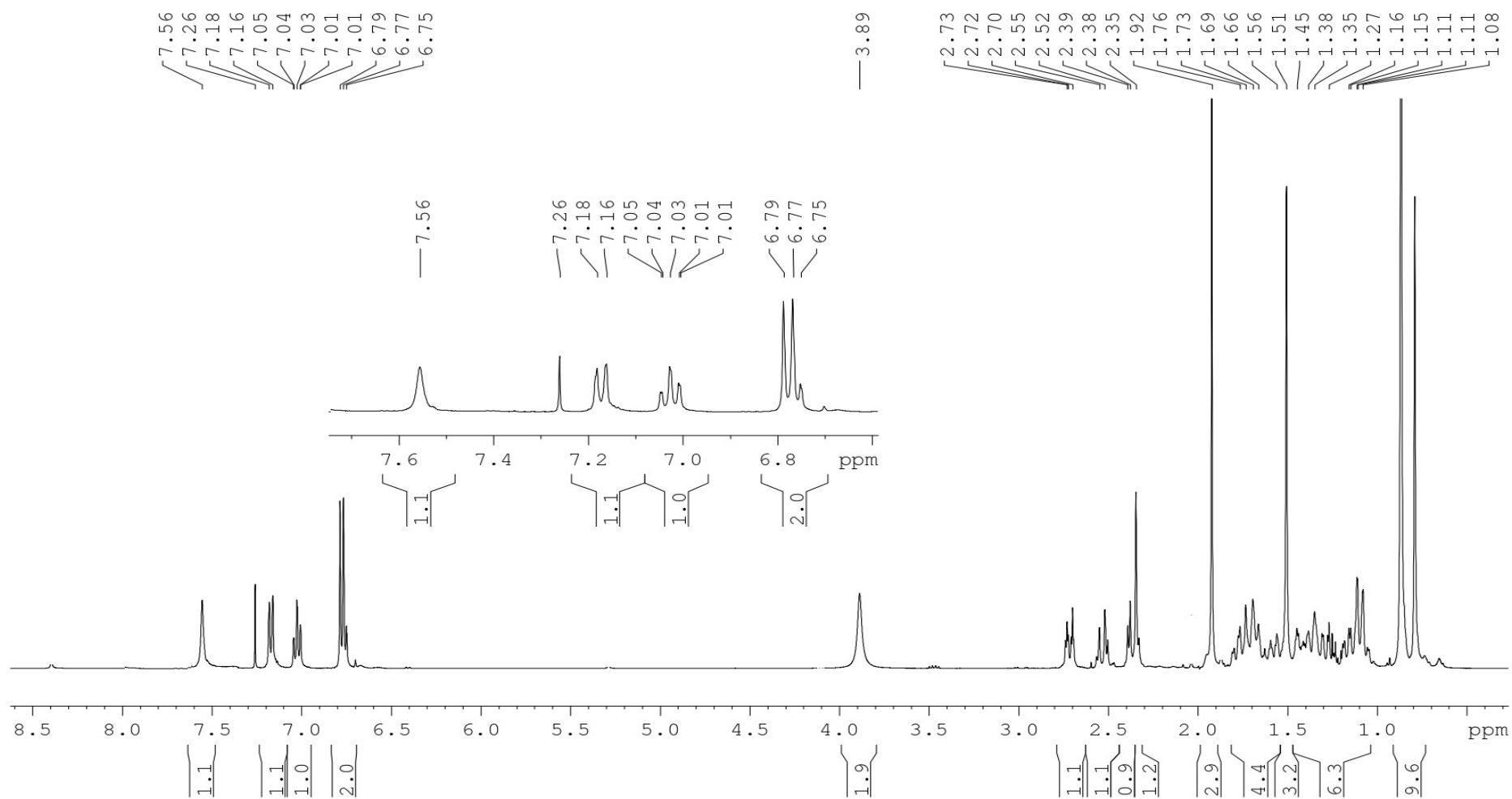
¹H NMR spectrum of compound 19



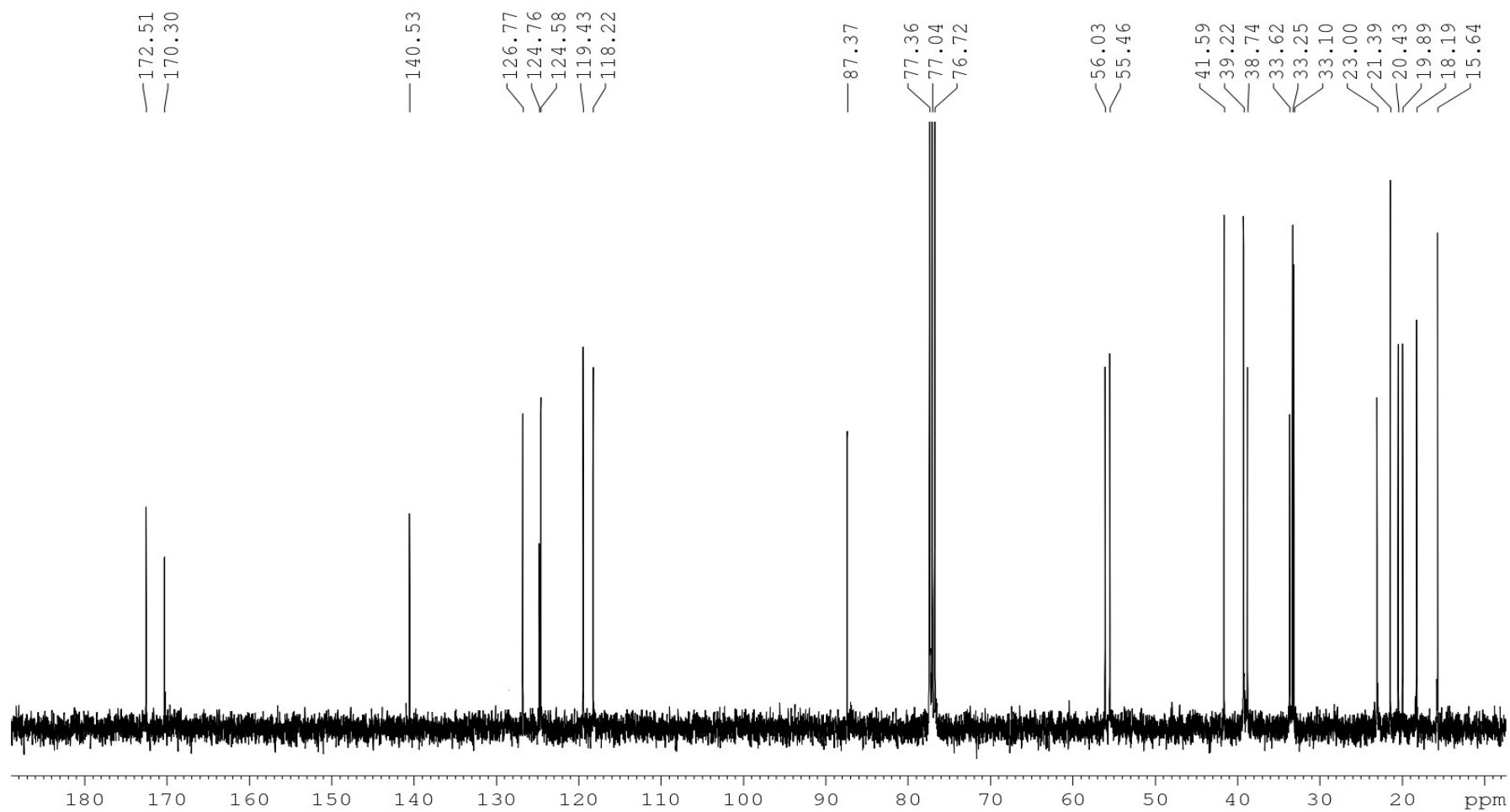
¹³C NMR spectrum of compound 19



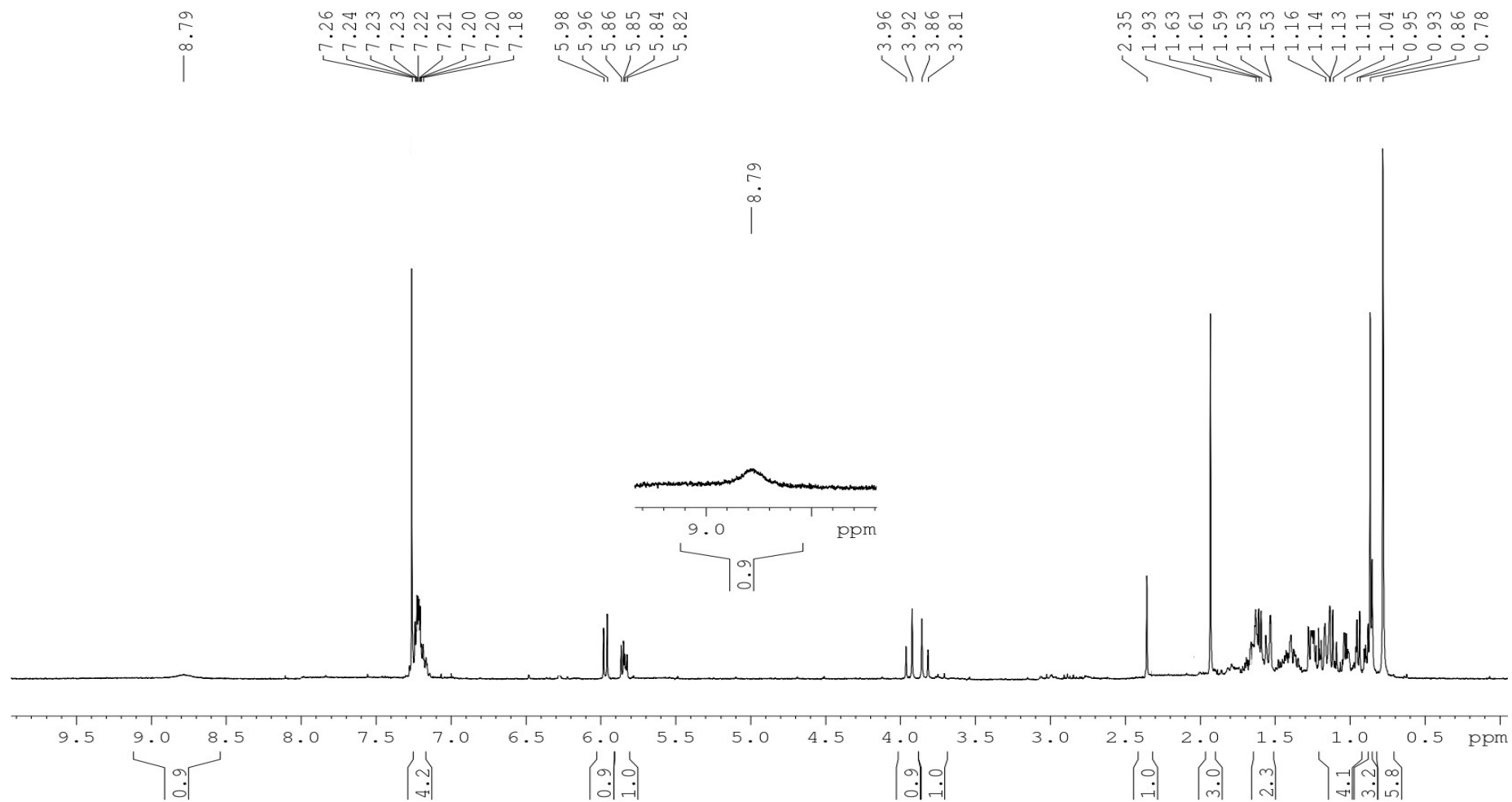
¹H NMR spectrum of compound 20



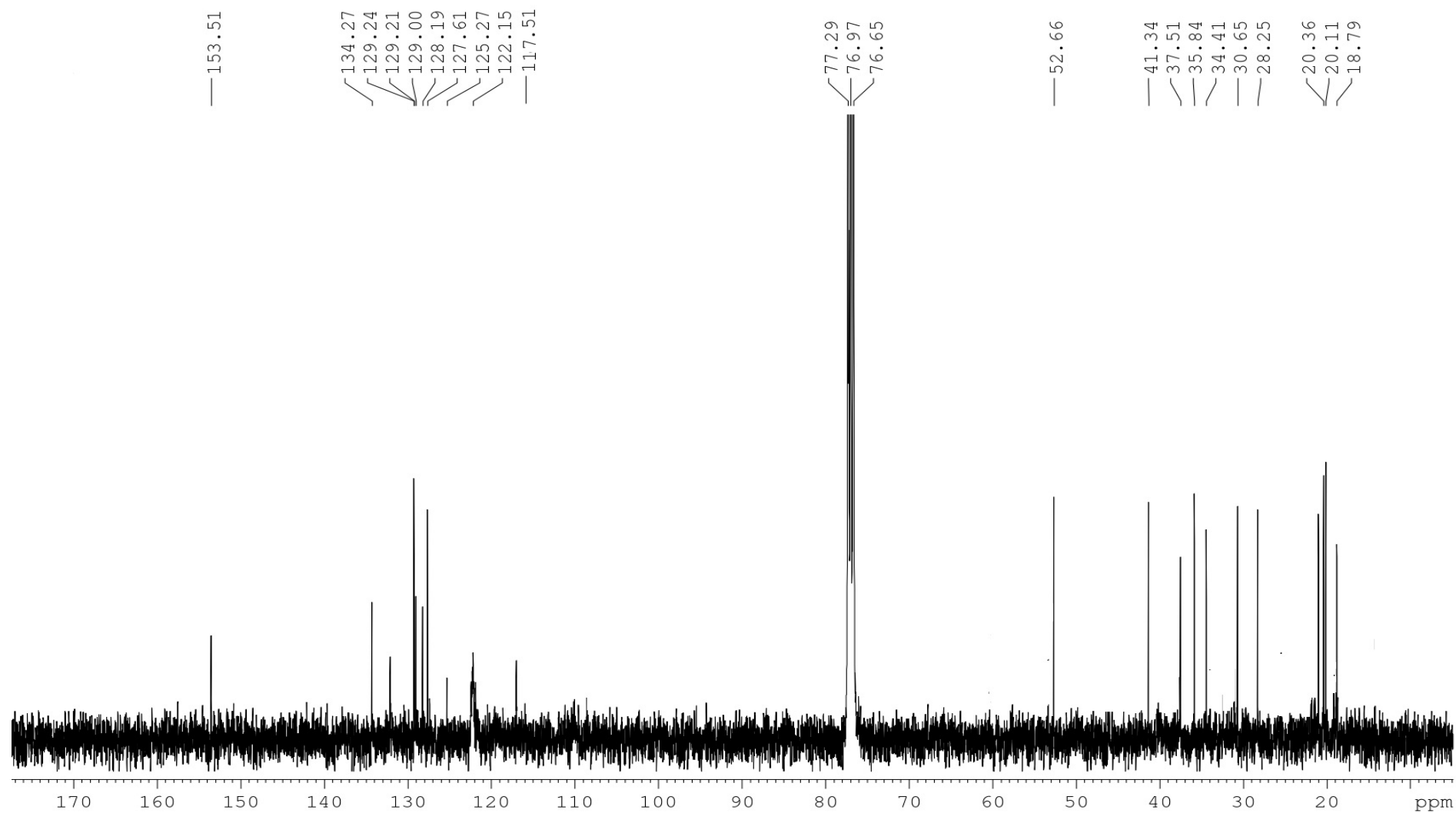
¹³C NMR spectrum of compound 20



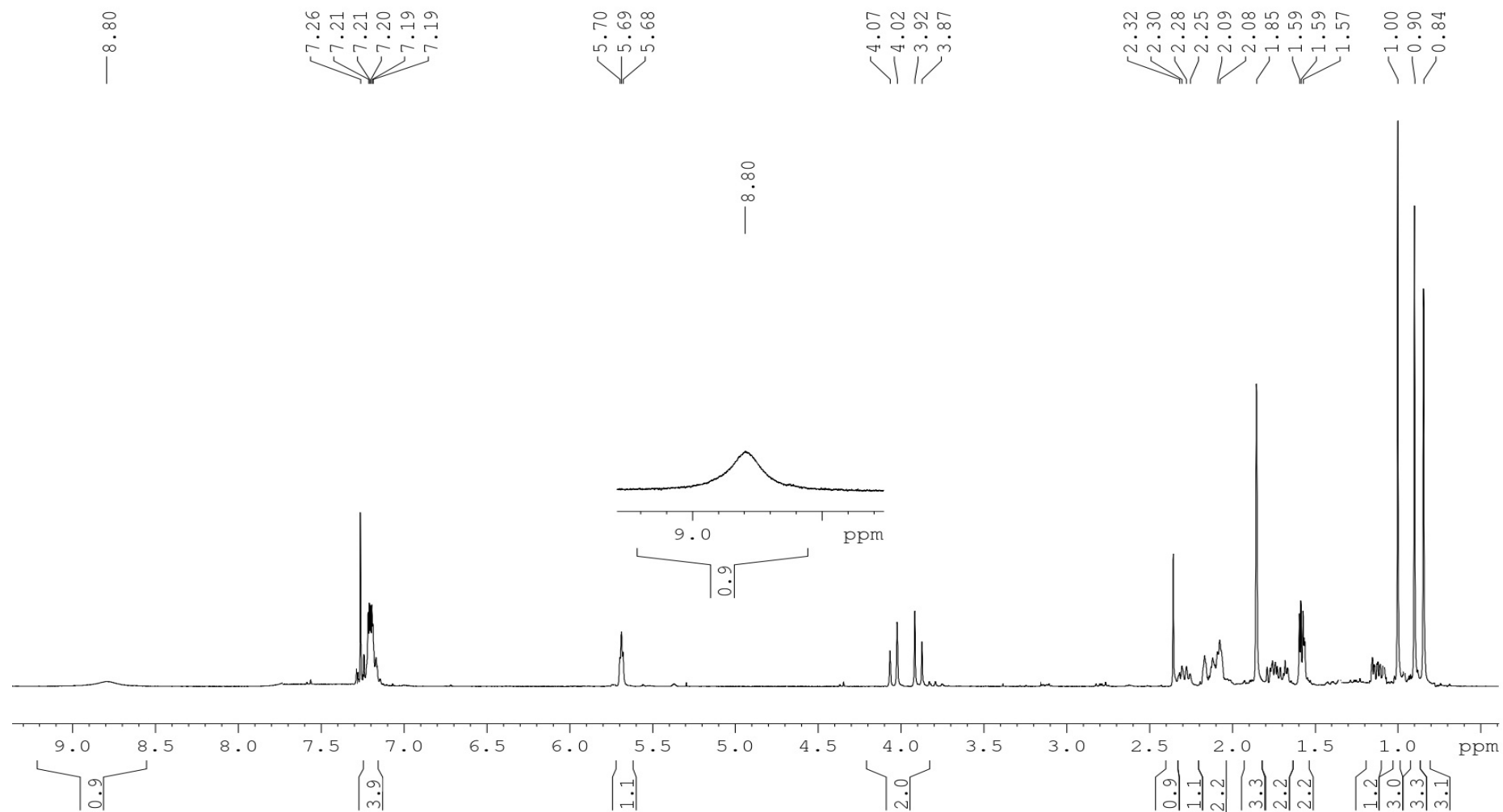
¹H NMR spectrum of compound 21



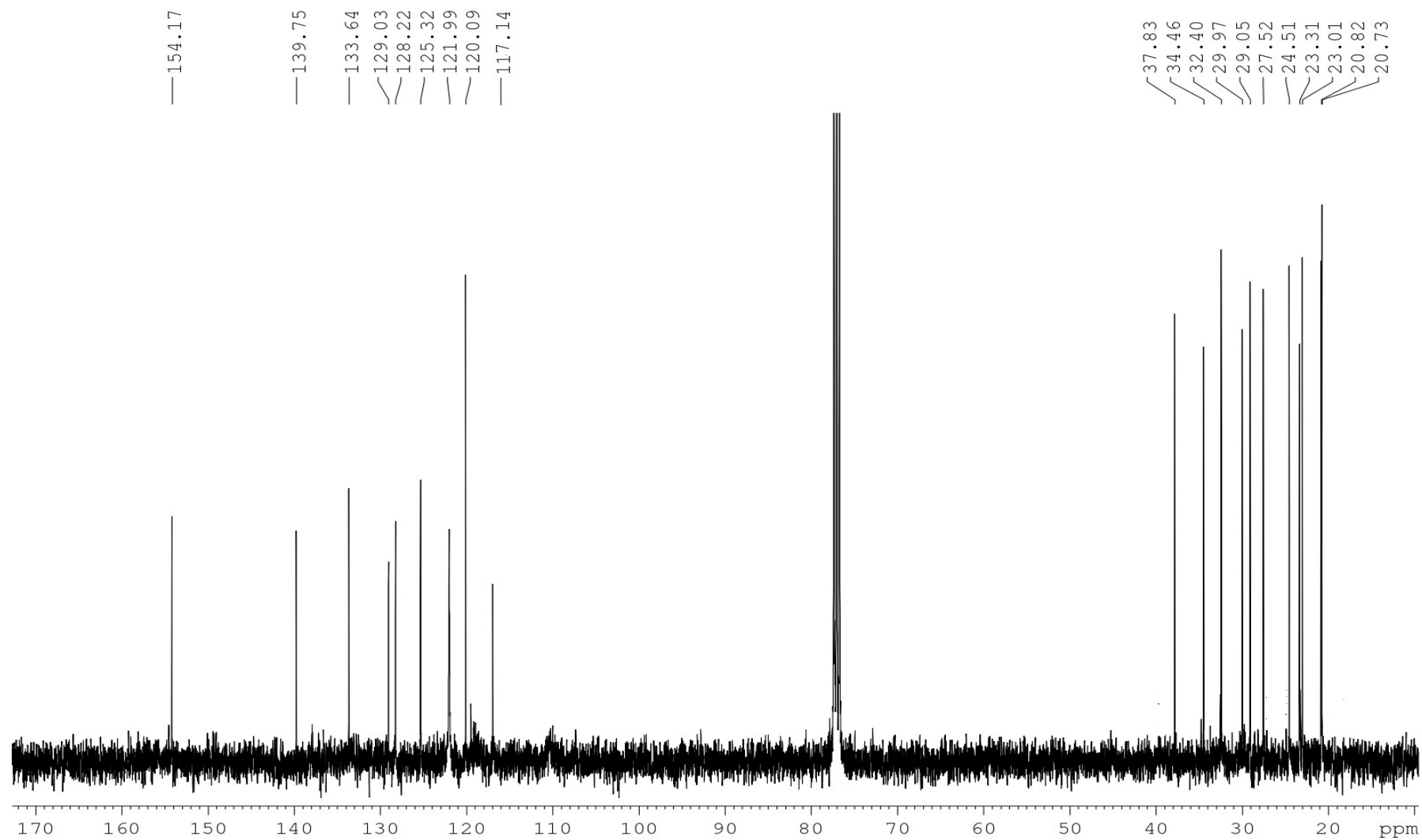
^{13}C NMR spectrum of compound 21



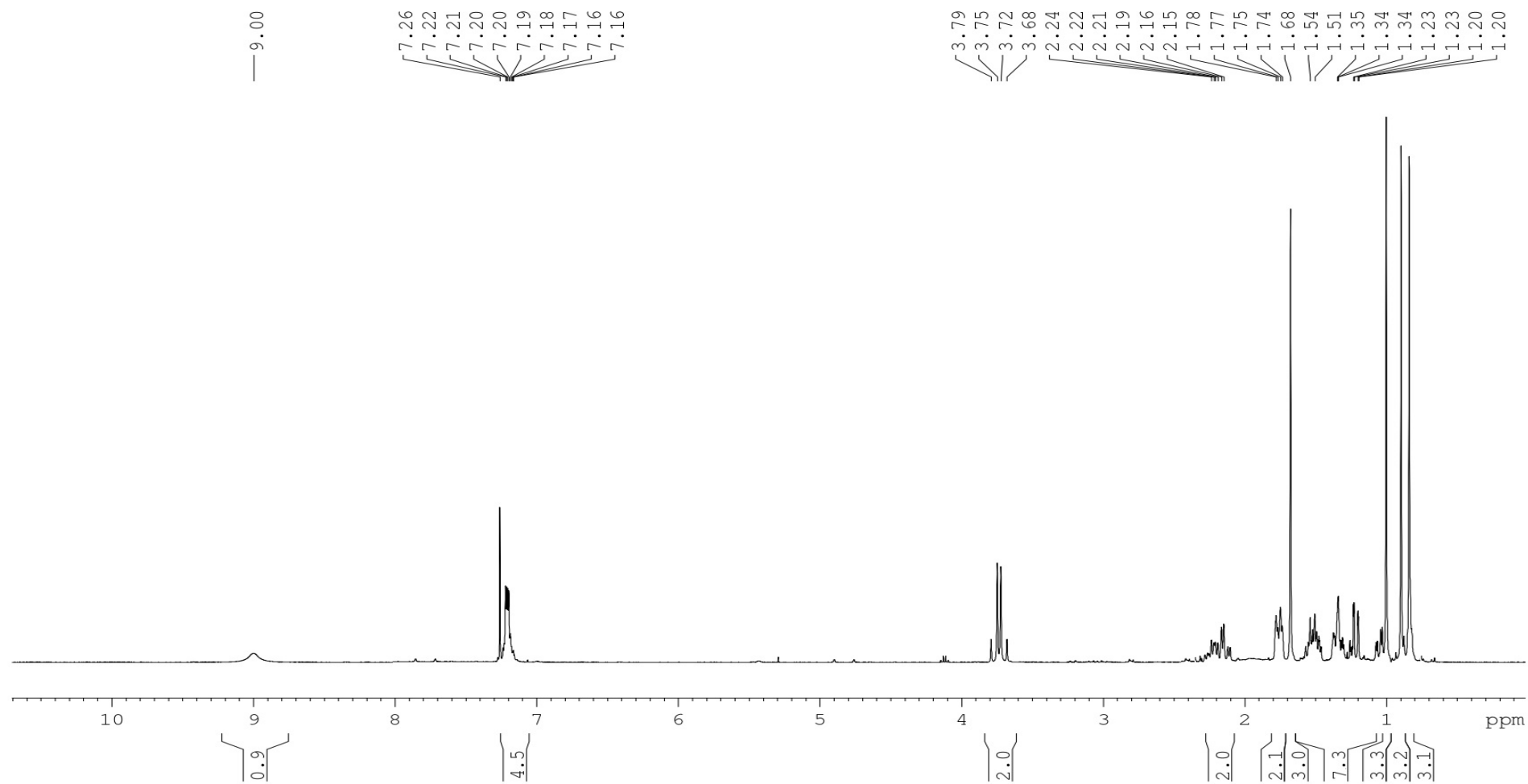
¹H NMR spectrum of compound 22



^{13}C NMR spectrum of compound 22



¹H NMR spectrum of compound 23



¹³C NMR spectrum of compound 23

