Combined *in silico* and *in vitro* analyses to assess the anti-cancer potential of thiazolidinedione-thiosemicarbazone hybrid molecules

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Supplementary Materials

Table S1. DPPH free radical scavenging activity and Ferric-reducing antioxidant power (FRAP) of TZD-TSCs **2**-**5**.

Samples	Concentration [μg/mL]			
	25	**75**	**150**	**200**
DPPH assay (reduction values corresponding to the appropriate concentration of Trolox, μg/mL)				
2	2.942±1.587	6.670±0.205	11.412±0.358	15.068±0.307
3	2.616±0.102	9.168±0.358	17.167±0.410	21.439±0.410
4	2.834±0.717	6.381±0.410	13.982±0.717	17.638±0.256
5	0.768±0.191	2.689±0.307	9.964±0.358	15.177±0.051
FRAP assay (reduction values corresponding to the appropriate concentration of ascorbic acid, μg/mL)				
TZD-TSC **2**	2.43±0.54	4.32±1.62	3.51±0.24	7.84±2.43
TZD-TSC **3**	0.81±0.72	0.27±0.21	1.08±0.72	1.89±0.72
TZD-TSC **4**	1.62±0.81	5.95±2.30	4.05±0.54	5.41±0.90
TZD-TSC **5**	2.70±0.90	2.43±0.81	4.59±0.54	9.19±4.32

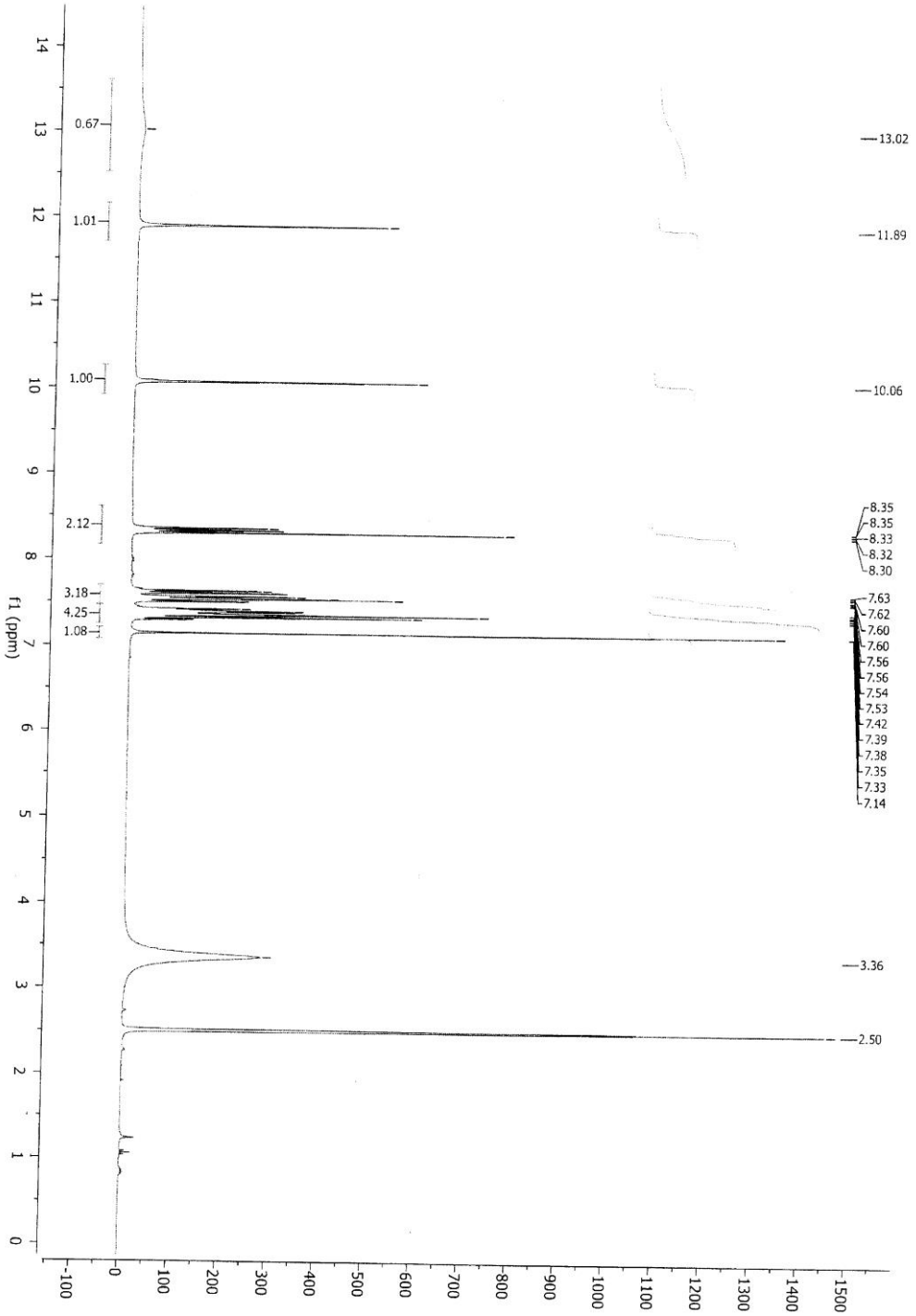

Figure S1. ^{1}H NMR spectra for **2**

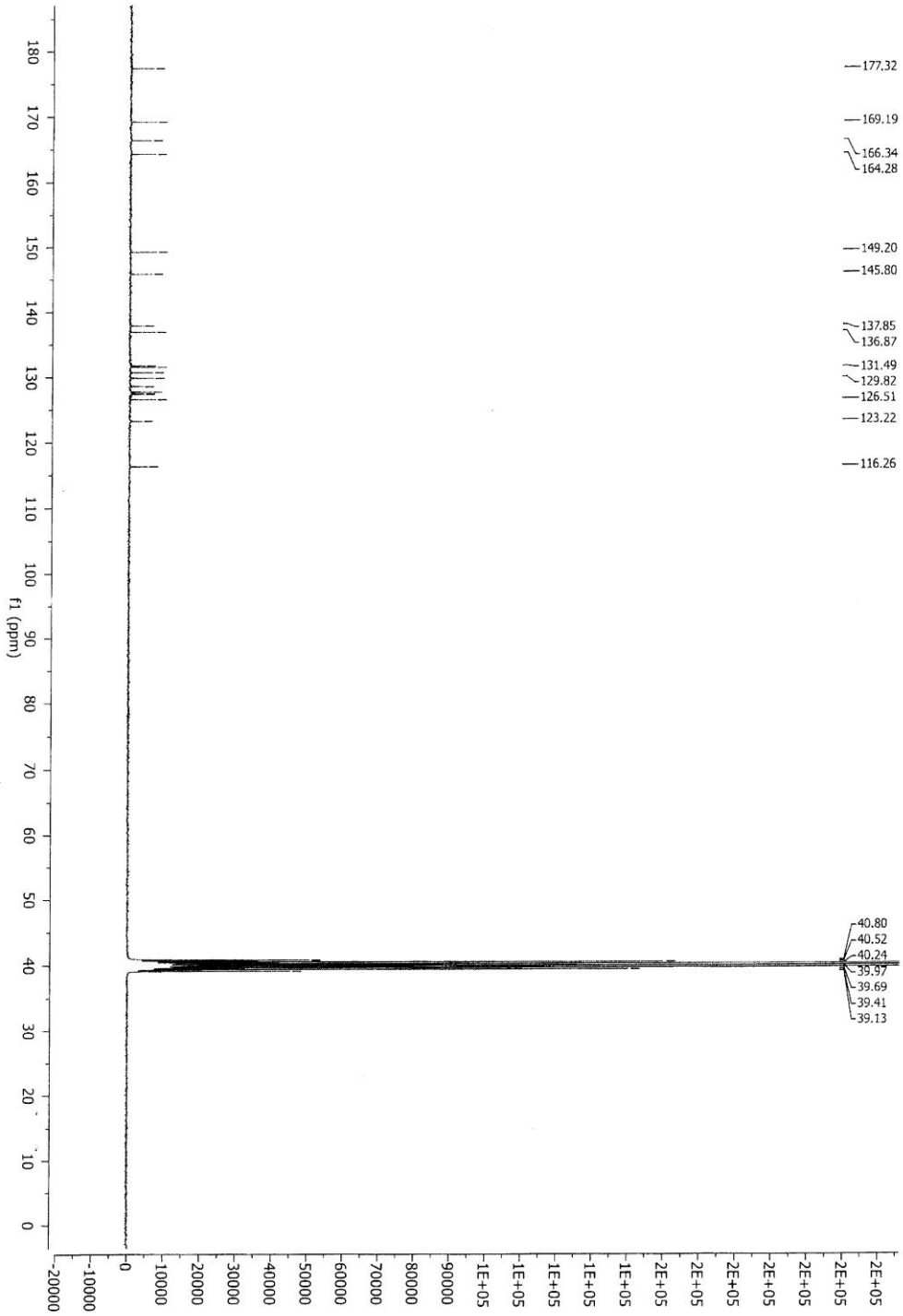

Figure S2. ^{13}C NMR spectra for **2**

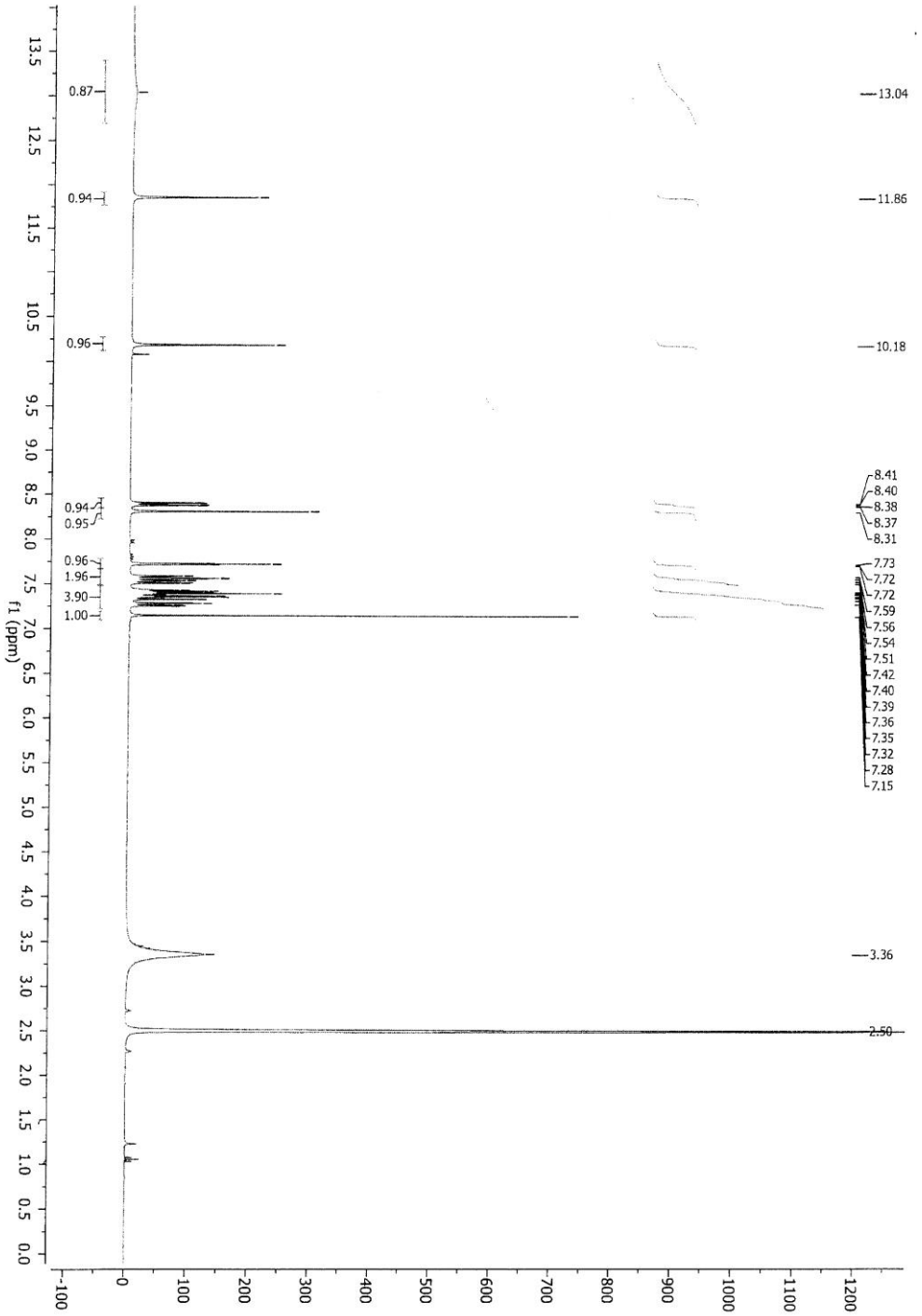

Figure S3. ^{1}H NMR spectra for **3**

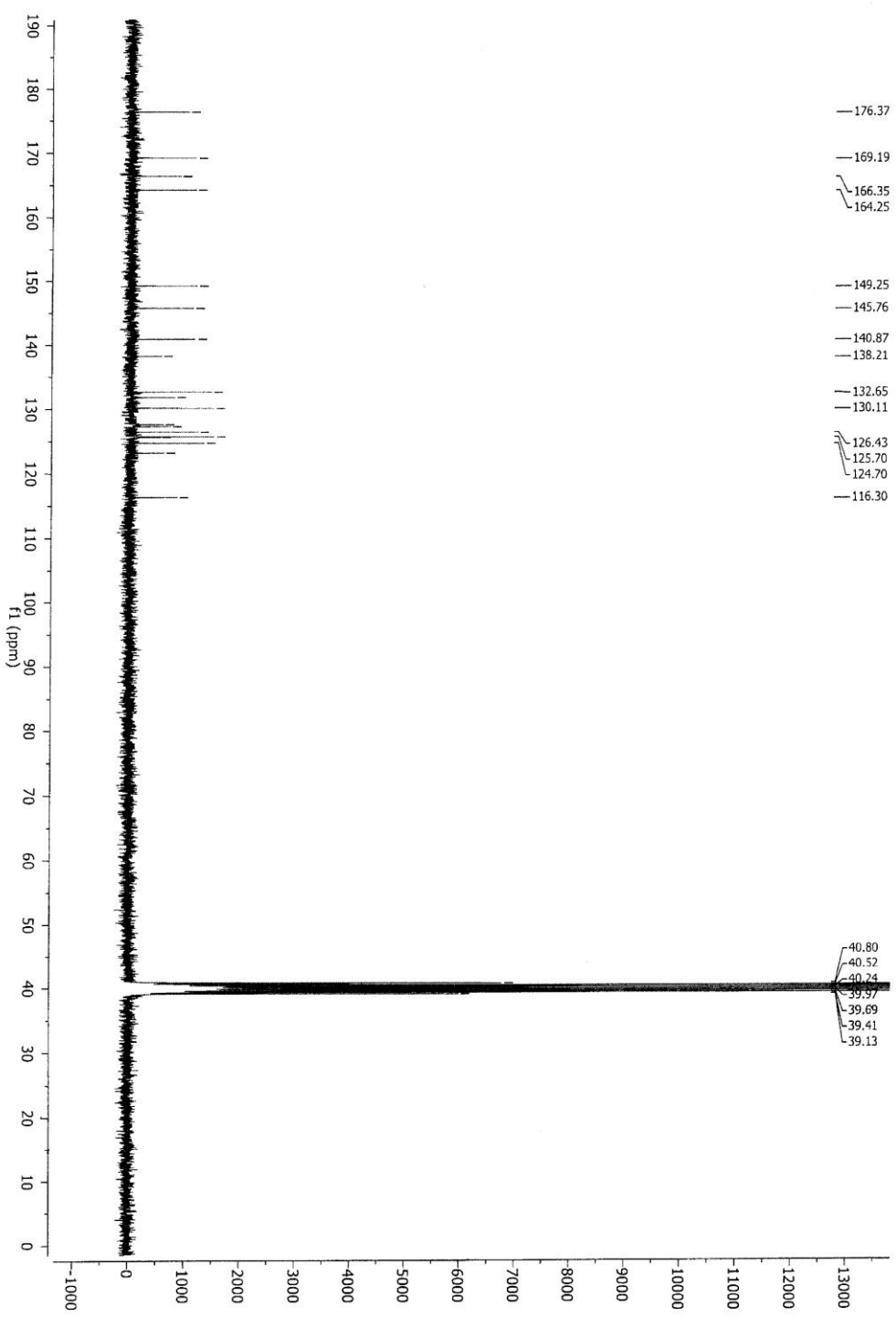

Figure S4. ^{13}C NMR spectra for **3**

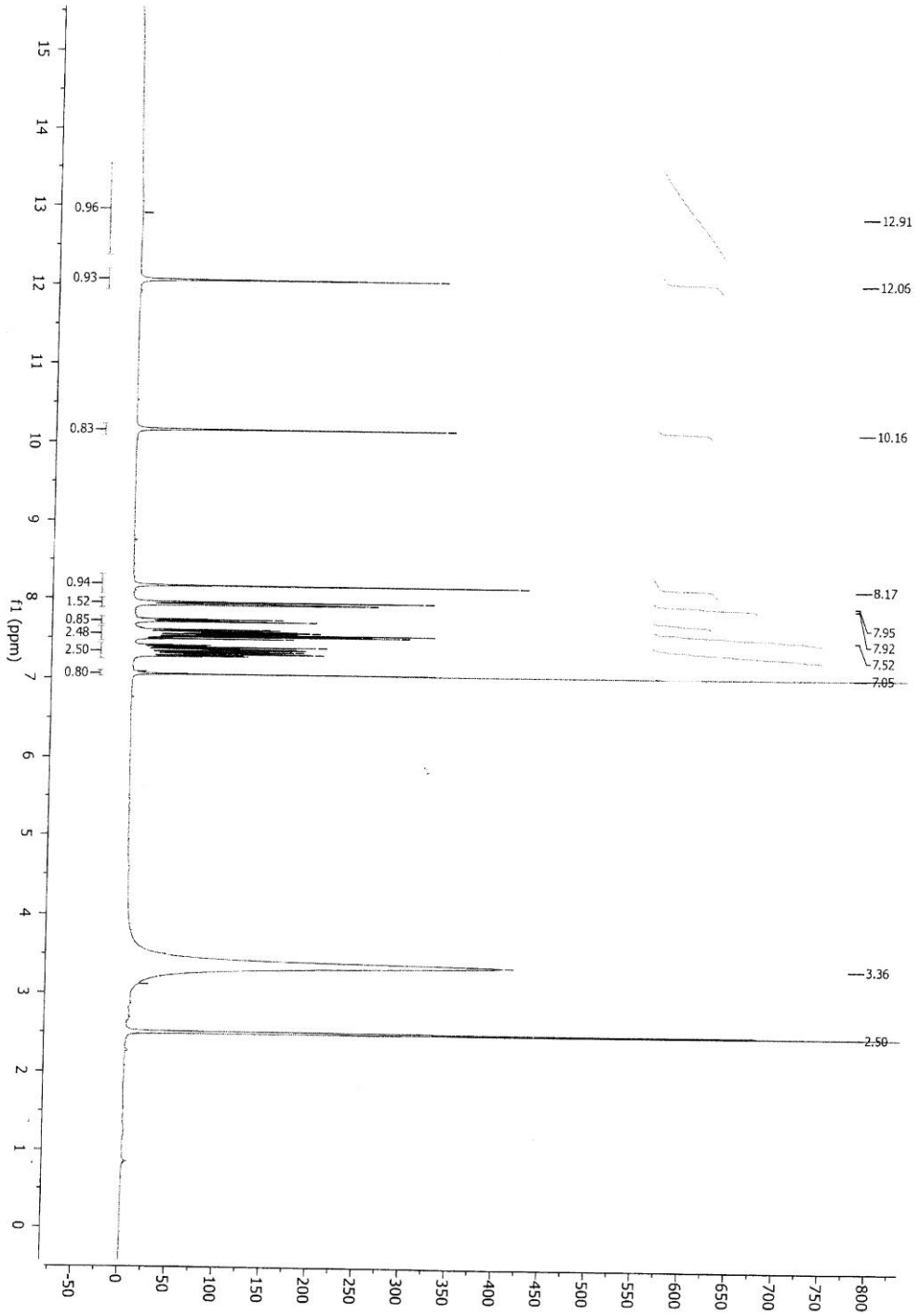

Figure S5. ^{1}H NMR spectra for **4**

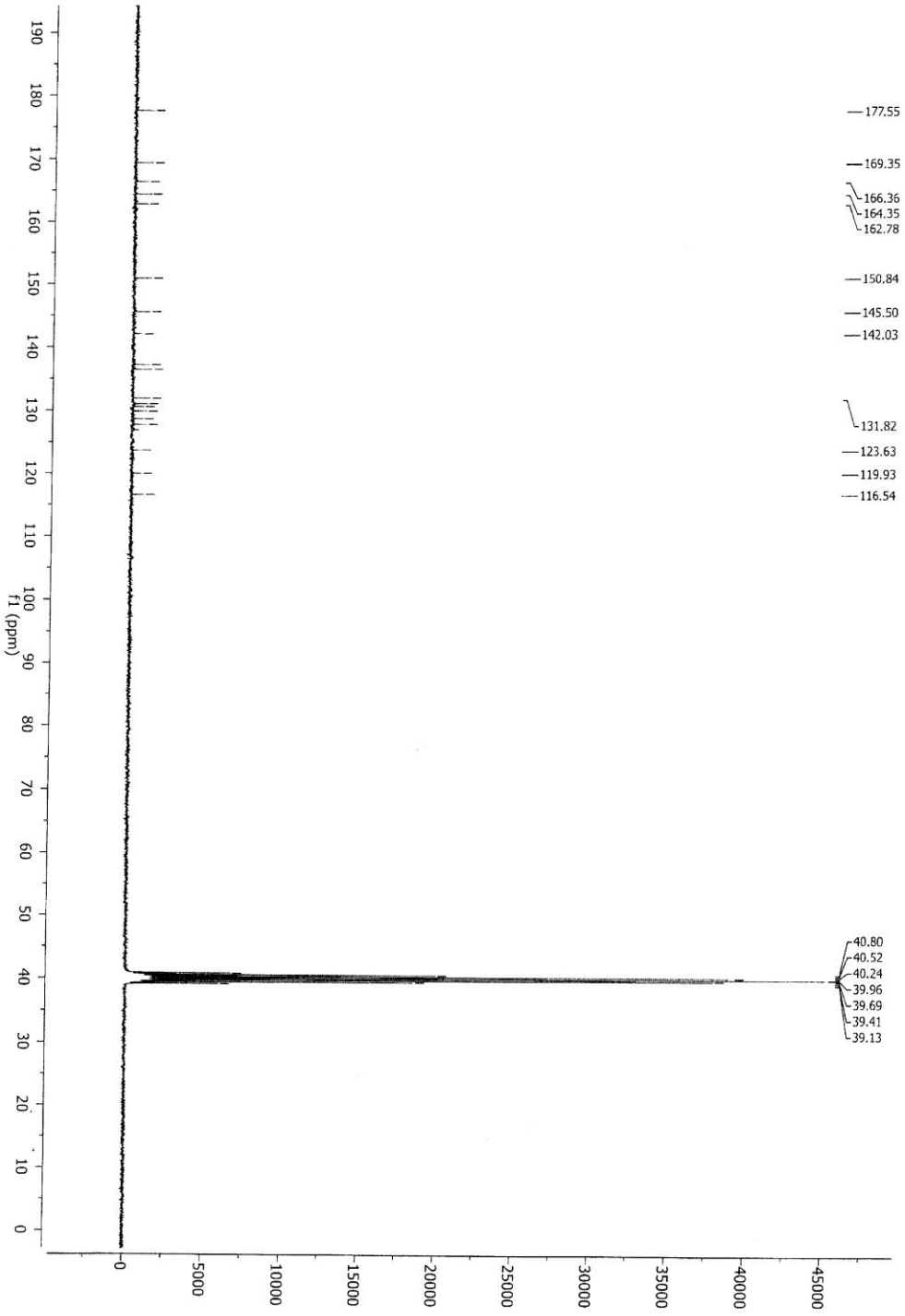

Figure S6. ^{13}C NMR spectra for **4**

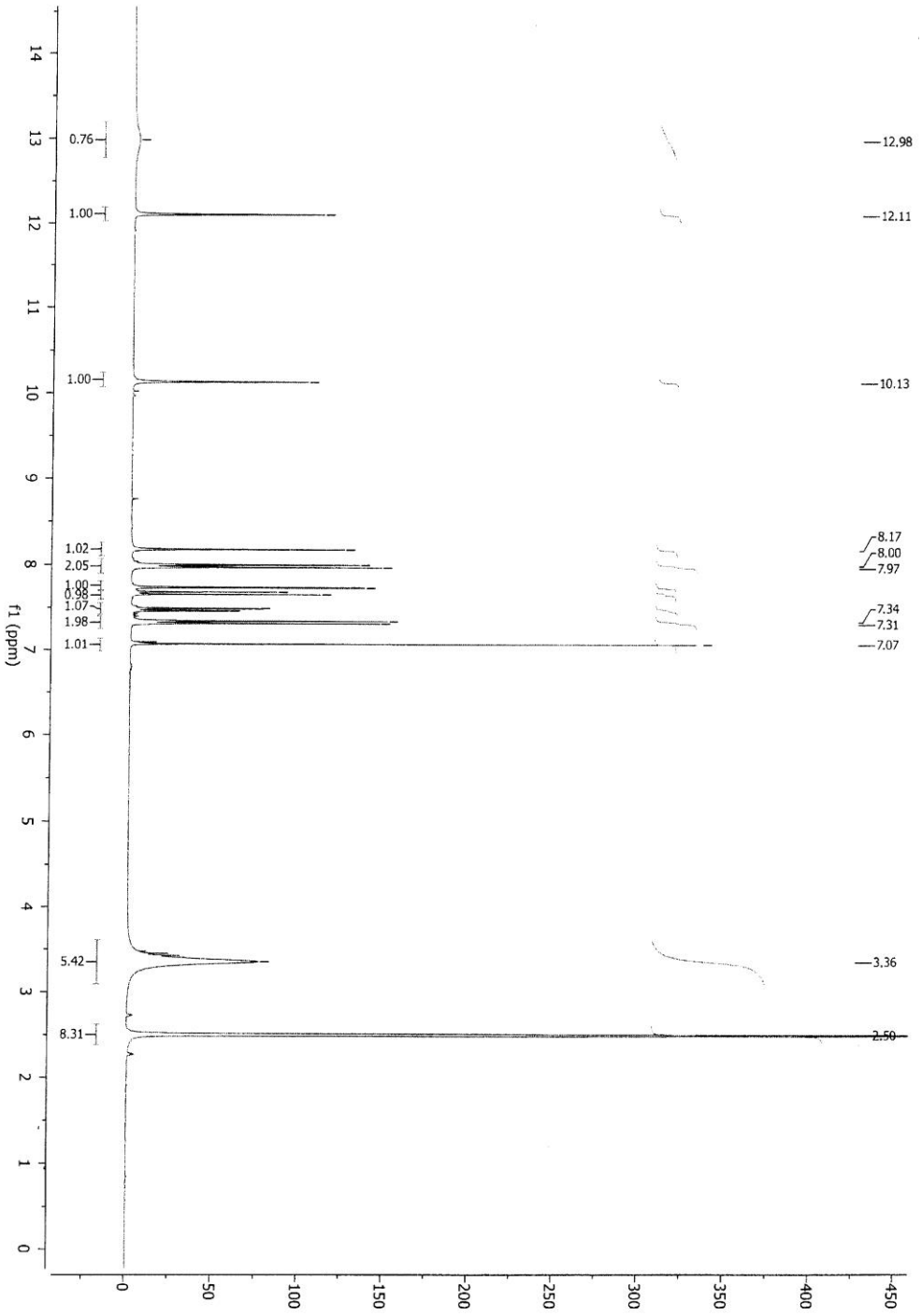

Figure S7. ^{1}H NMR spectra for **5**

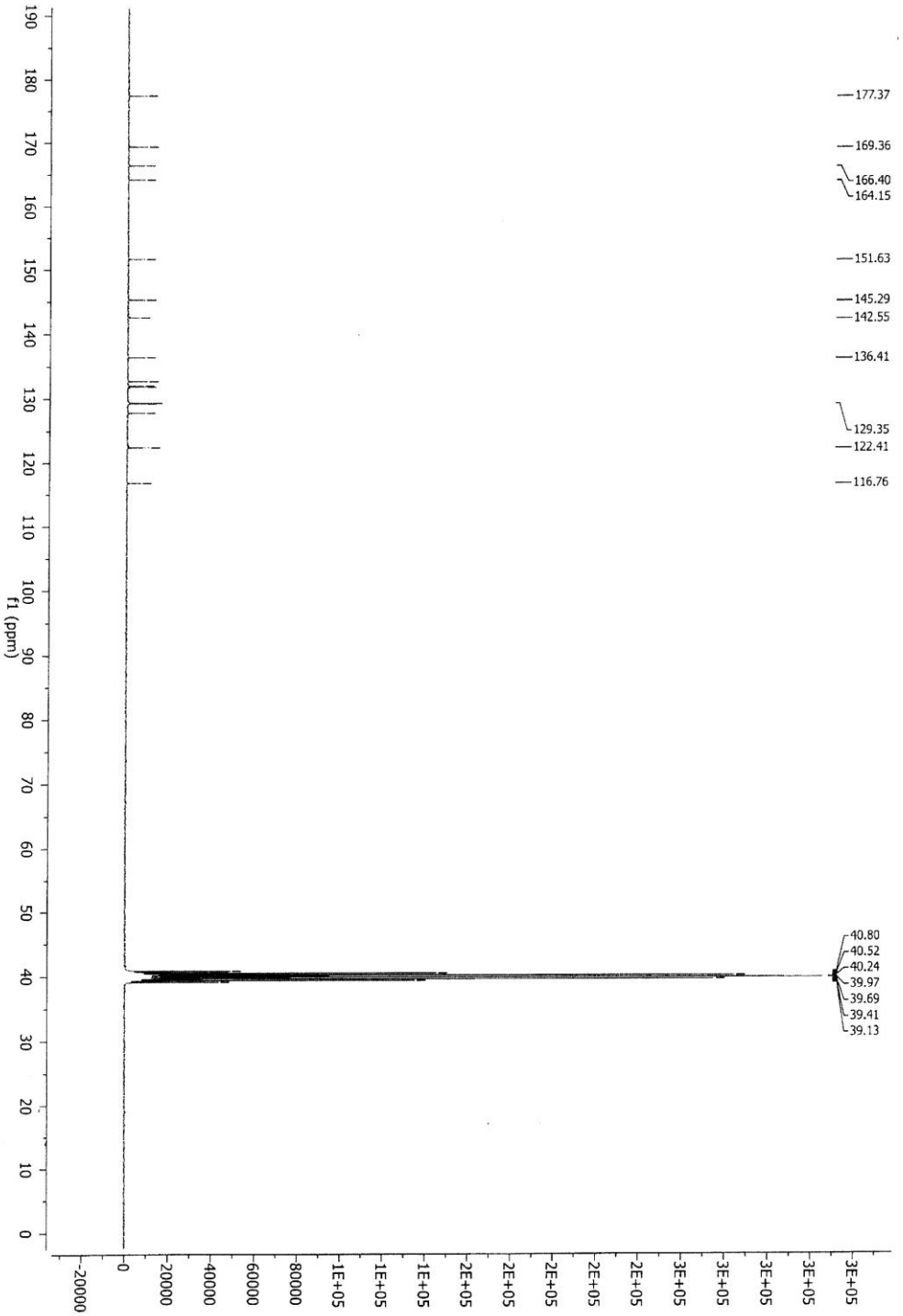

Figure S8. ^{13}C NMR spectra for **5**