

Supplementary data:

Table S1. Designated optimized bond length Å, and bond angle degrees dihedral angle degrees of Compound **11** utilized and B3LYP/6-31G(d):

Bond lengths (Å)			Bond angles (°)		
	X-Ray	<i>DFT/B3LYP</i>		X-Ray	<i>DFT/B3LYP</i>
O1-C5	1.366(2)	1.3689	C5-O1-C10	119.6(1)	119.27
O1-C10	1.428(2)	1.4254	N2-N1-C3	111.8(1)	111.93
N1-N2	1.364(2)	1.3549	N2-N1-C20	117.2(1)	117.99
N1-C3	1.362(2)	1.3791	C3-N1-C20	130.8(1)	129.94
N1-C20	1.435(2)	1.4246	N2-C1-C2	110.7(1)	110.16
C1-N2	1.338(2)	1.3402	N2-C1-C4	118.0(1)	118.78
C1-C2	1.401(2)	1.4187	C2-C1-C4	131.3(1)	131.05
C1-C4	1.483(2)	1.4761	N1-N2-C1	105.1(1)	106.02
C2-H2	0.93	1.0752	C1-C2-H2	126.9	127.53
C2-C3	1.373(2)	1.3837	C1-C2-C3	106.2(1)	106.11
C3-C13	1.474(2)	1.473	H2-C2-C3	126.9	126.27
C4-C5	1.392(2)	1.4163	N1-C3-C2	106.2(1)	105.78
C4-C9	1.381(3)	1.4042	N1-C3-C13	126.1(1)	126.01
C5-C6	1.393(3)	1.4008	C2-C3-C13	127.6(1)	128.08
C10-H10A	0.97	1.0997	C1-C4-C5	123.1(1)	123.56
C10-H10B	0.97	1.0998	C1-C4-C9	119.0(1)	118.81
C10-C11	1.485(3)	1.5227	C5-C4-C9	117.9(2)	117.63
C9-H9	0.93	1.0839	O1-C5-C4	116.8(1)	117.12
C9-C8	1.380(4)	1.3914	O1-C5-C6	123.1(2)	122.59
C8-H8	0.93	1.0856	C4-C5-C6	120.1(2)	120.29
C8-C7	1.362(4)	1.393	O1-C10-H10A	110.1	110.08
C7-H7	0.93	1.0862	O1-C10-H10B	110.1	110.07

C7-C6	1.374(3)	1.3944	O1-C10-C11	108.0(2)	107.99
C6-H6	0.93	1.0827	H10A-C10-H10B	108.4	107.73
C11-H11A	0.97	1.0962	H10A-C10-C11	110.1	110.49
C11-H11B	0.97	1.0961	H10B-C10-C11	110.1	110.49
C11-C12	1.524(3)	1.5316	C4-C9-H9	119	117.49
C12-H12A	0.96	1.0956	C4-C9-C8	122.1(2)	122.15
C12-H12B	0.96	1.0937	H9-C9-C8	118.9	120.37
C12-H12C	0.96	1.0956	C9-C8-H8	120.5	120.01
C15-H15	0.93	1.0872	C9-C8-C7	119.1(3)	119.41
C15-C14	1.378(2)	1.3917	H8-C8-C7	120.4	120.58
C15-C16	1.384(2)	1.4019	C8-C7-H7	119.6	120.6
C14-H14	0.93	1.0849	C8-C7-C6	120.8(2)	120.04
C14-C13	1.391(2)	1.405	H7-C7-C6	119.6	119.36
C13-C18	1.386(2)	1.4036	C5-C6-C7	119.9(2)	120.49
C20-C21	1.377(2)	1.398	C5-C6-H6	120	120.21
C20-C25	1.385(2)	1.3974	C7-C6-H6	120	119.3
C19-H19A	0.96	1.0944	C10-C11-H11A	109.2	108.66
C19-H19B	0.96	1.0939	C10-C11-H11B	109.2	108.64
C19-H19C	0.96	1.0973	C10-C11-C12	111.8(2)	112.1
C19-C16	1.508(2)	1.5101	H11A-C11-H11B	108	106.83
C18-H18	0.93	1.0858	H11A-C11-C12	109.3	110.21
C18-C17	1.380(2)	1.3934	H11B-C11-C12	109.3	110.25
C17-H17	0.93	1.0871	C11-C12-H12A	109.5	111.42
C17-C16	1.384(2)	1.4002	C11-C12-H12B	109.4	110.91
C21-H21	0.93	1.0837	C11-C12-H12C	109.5	111.44
C21-C22	1.377(2)	1.3919	H12A-C12-H12B	109.4	107.6
C22-H22	0.93	1.087	H12A-C12-H12C	109.5	107.68
C22-C23	1.389(2)	1.4016	H12B-C12-H12C	109.5	107.61

C23-C24	1.378(2)	1.4005	H15-C15-C14	119.1	119.2
C23-C26	1.509(2)	1.5101	H15-C15-C16	119.1	119.4
C24-H24	0.93	1.0869	C14-C15-C16	121.7(1)	121.39
C24-C25	1.383(2)	1.3936	C15-C14-H14	119.7	119.64
C25-H25	0.93	1.0837	C15-C14-C13	120.5(1)	120.67
C26-H26A	0.96	1.094	H14-C14-C13	119.8	119.69
C26-H26B	0.96	1.0974	C3-C13-C14	122.3(1)	122.3
C26-H26C	0.96	1.0941	C3-C13-C18	119.7(1)	119.55
			C14-C13-C18	117.9(1)	118.08
			N1-C20-C21	119.1(1)	119.04
			N1-C20-C25	121.0(1)	121.1
			C21-C20-C25	119.8(1)	119.83
			H19A-C19-H19B	109.5	108.05
			H19A-C19-H19C	109.5	107.14
			H19A-C19-C16	109.5	111.48
			H19B-C19-H19C	109.5	107.29
			H19B-C19-C16	109.5	111.47
			H19C-C19-C16	109.5	111.21
			C13-C18-H18	119.5	119.18
			C13-C18-C17	121.1(1)	120.87
			H18-C18-C17	119.5	119.95
			C18-C17-H17	119.4	119.33
			C18-C17-C16	121.2(1)	121.19
			H17-C17-C16	119.4	119.47
			C15-C16-C19	121.3(1)	120.99
			C15-C16-C17	117.6(1)	117.79
			C19-C16-C17	121.2(1)	121.2
			C20-C21-H21	120.1	119.05

			C20-C21-C22	119.8(1)	119.74
			H21-C21-C22	120.1	121.2
			C21-C22-H22	119.2	119.1
			C21-C22-C23	121.6(1)	121.43
			H22-C22-C23	119.2	119.47
			C22-C23-C24	117.5(1)	117.85
			C22-C23-C26	121.1(1)	121.03
			C24-C23-C26	121.4(1)	121.11
			C23-C24-H24	119	119.5
			C23-C24-C25	121.9(1)	121.49
			H24-C24-C25	119	119
			C20-C25-C24	119.3(1)	119.64
			C20-C25-H25	120.4	120.04
			C24-C25-H25	120.4	120.32
			C23-C26-H26A	109.5	111.47
			C23-C26-H26B	109.4	111.27
			C23-C26-H26C	109.5	111.45
			H26A-C26-H26B	109.4	107.24
			H26A-C26-H26C	109.5	108
			H26B-C26-H26C	109.5	107.19

Table S2. Insecticidal activity of compounds **5**, **7**, **9**, **10**, **11**, **14** and **17** against *P. interpunctella* and *Nilaparvata lugens*.

Compd.	<i>Insecticidal activity (%) at different concentrations ($\mu\text{g ml}^{-1}$)</i>									
	<i>P. interpunctella</i>					<i>Nilaparvata lugens</i>				
	25	50	100	200	400	25	50	100	200	400
5	42.4 $\pm$ 3.3	53.2 $\pm$ 3.3	73.5 $\pm$ 3.3	97.6 $\pm$ 3.3	100 $\pm$ 0	40.3 $\pm$ 3.3	48.5 $\pm$ 3.3	65.3 $\pm$ 3.3	77.6 $\pm$ 3.3	82 $\pm$ 5.7
7	31.3 $\pm$ 3.3	46.6 $\pm$ 3.3	66.6 $\pm$ 3.3	78.6 $\pm$ 3.3	83.6 $\pm$ 3.3	26.6 $\pm$ 3.3	33.3 $\pm$ 3.3	51 $\pm$ 5.7	63.3 $\pm$ 3.3	71 $\pm$ 0
9	43.3 $\pm$ 3.3	60.0 $\pm$ 5.7	86.6 $\pm$ 3.3	98.6 $\pm$ 3.3	100 $\pm$ 3.3	32.6 $\pm$ 3.3	46.6 $\pm$ 3.3	66.6 $\pm$ 3.3	78.6 $\pm$ 3.3	86.6 $\pm$ 3.3
10	46.6 $\pm$ 3.3	56.6 $\pm$ 3.3	76.6 $\pm$ 3.3	93.3 $\pm$ 3.3	96.6 $\pm$ 3.3	26.6 $\pm$ 3.3	46.6 $\pm$ 3.3	66.6 $\pm$ 3.3	73.4 $\pm$ 0	83.3 $\pm$ 3.3
11	16.3 $\pm$ 3.3	27.6 $\pm$ 3.3	39.3 $\pm$ 3.3	55.3 $\pm$ 3.3	61.3 $\pm$ 0	14.6 $\pm$ 3.3	22.4 $\pm$ 5.7	35.2 $\pm$ 5.7	46.3 $\pm$ 3.3	53.3 $\pm$ 3.3
14	33.3 $\pm$ 3.3	36.6 $\pm$ 3.3	53.3 $\pm$ 3.3	63.3 $\pm$ 3.3	80 $\pm$ 0	26.6 $\pm$ 3.3	30 $\pm$ 5.7	50 $\pm$ 5.7	63.3 $\pm$ 3.3	73.3 $\pm$ 3.3
17	43.3 $\pm$ 3.3	63.3 $\pm$ 3.3	78.6 $\pm$ 3.3	100 $\pm$ 0	100 $\pm$ 0	33.3 $\pm$ 3.3	48.3 $\pm$ 5.7	69.3 $\pm$ 3.3	80 $\pm$ 0	85.3 $\pm$ 3.3
Thiameth oxam	53.3 $\pm$ 3.3	60 $\pm$ 5.7	86.6 $\pm$ 3.3	100 $\pm$ 0	100 $\pm$ 0	33.3 $\pm$ 3.3	50 $\pm$ 3.3	70 $\pm$ 0	80 $\pm$ 0	86.6 $\pm$ 3.3

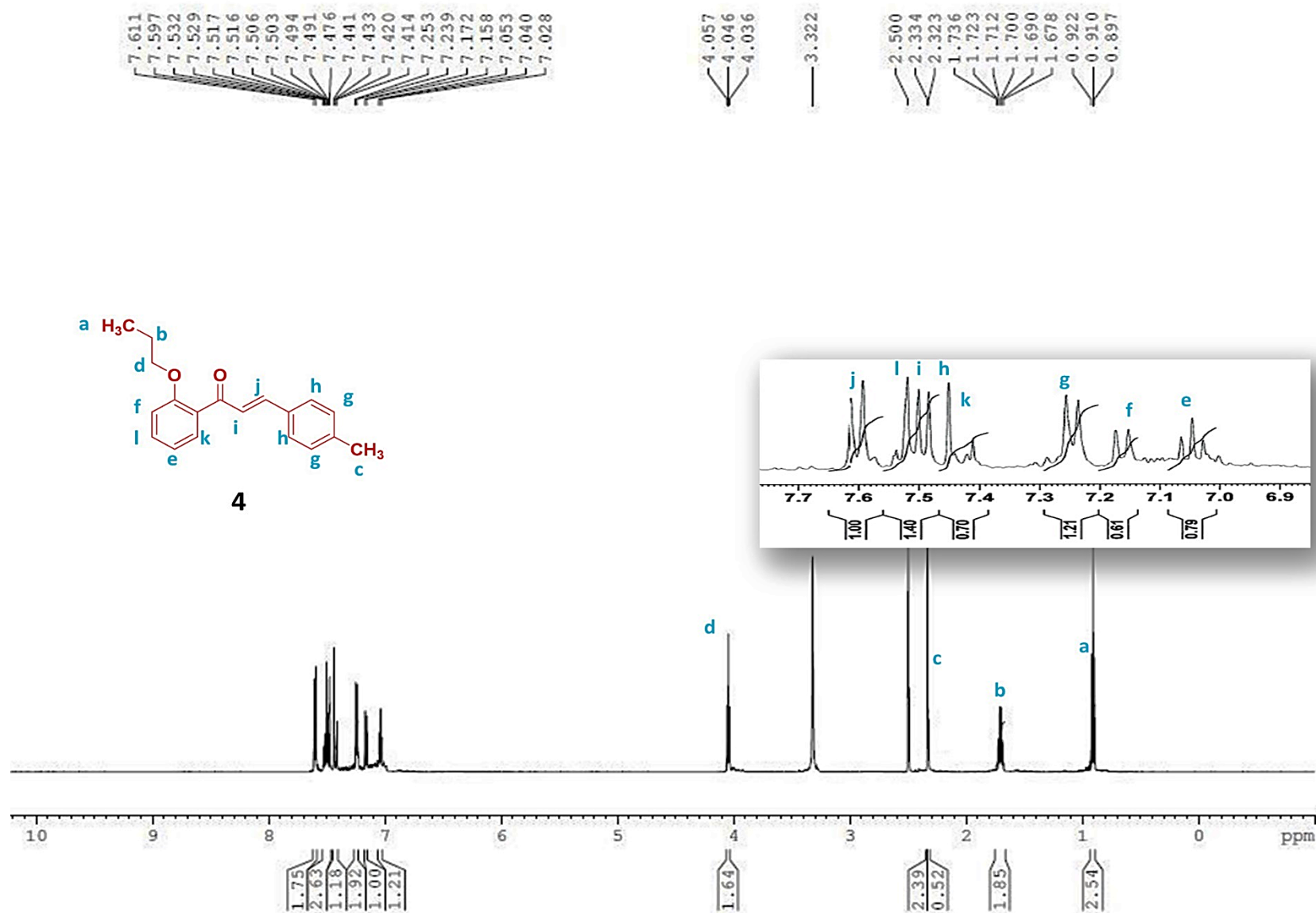


Figure S1. The ¹H NMR spectrum of compound **4** (400 MHz, solvent DMSO- *d*₆)

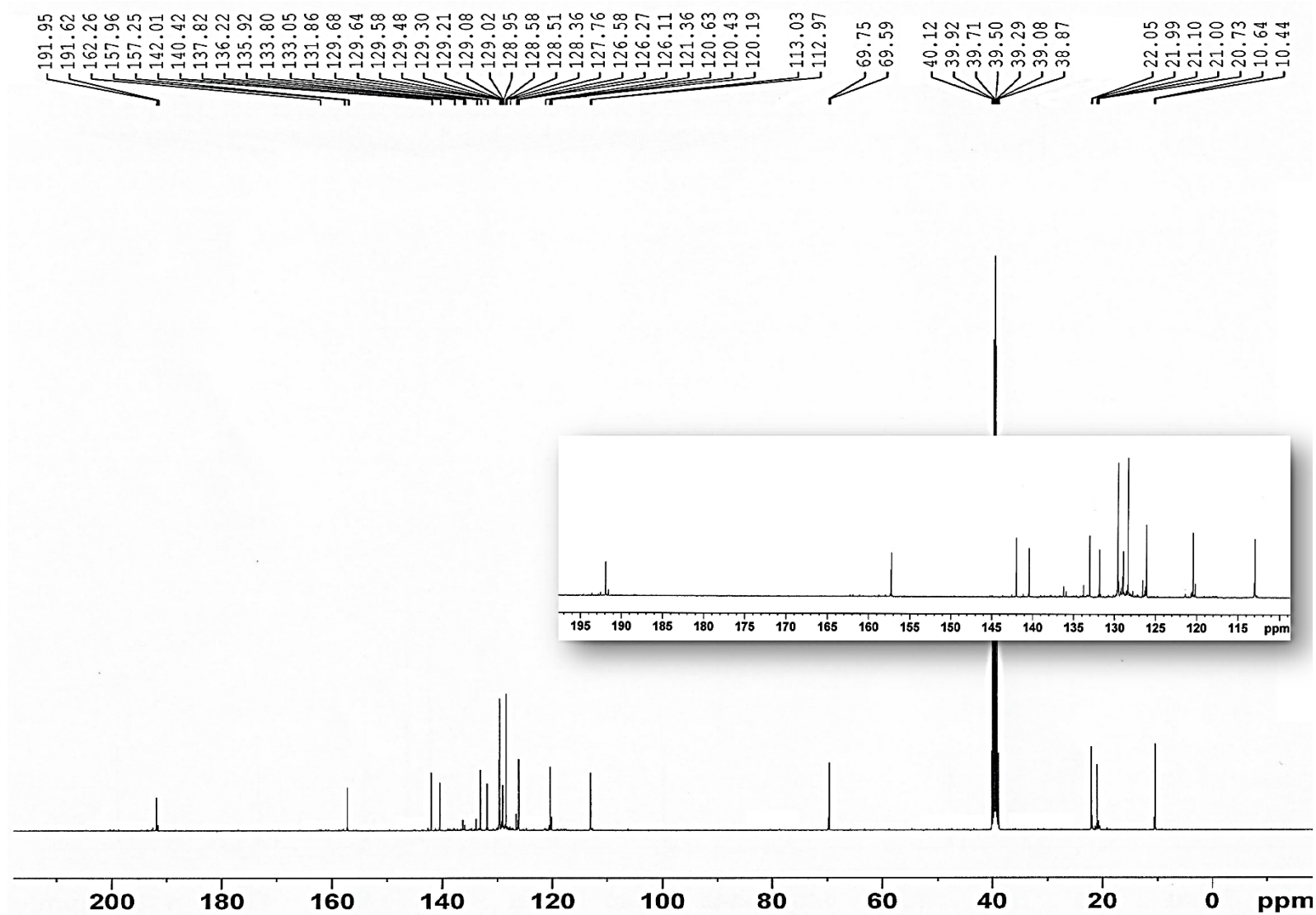


Figure S2. The ¹³C NMR spectrum of compound **4** (100 MHz, solvent DMSO-*d*₆)

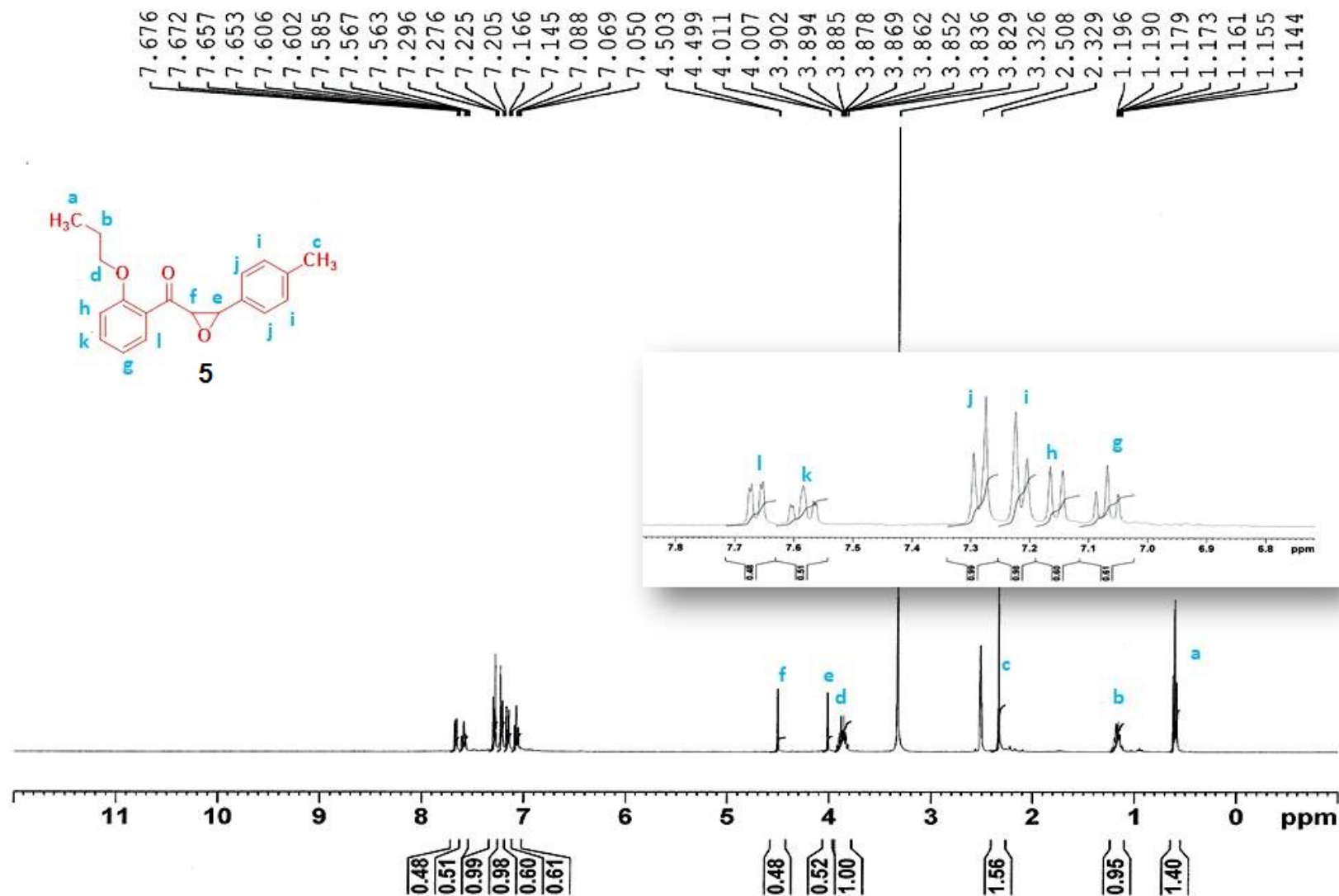


Figure S3. The ¹H NMR spectrum of compound **5** (400 MHz, solvent DMSO- *d*₆)

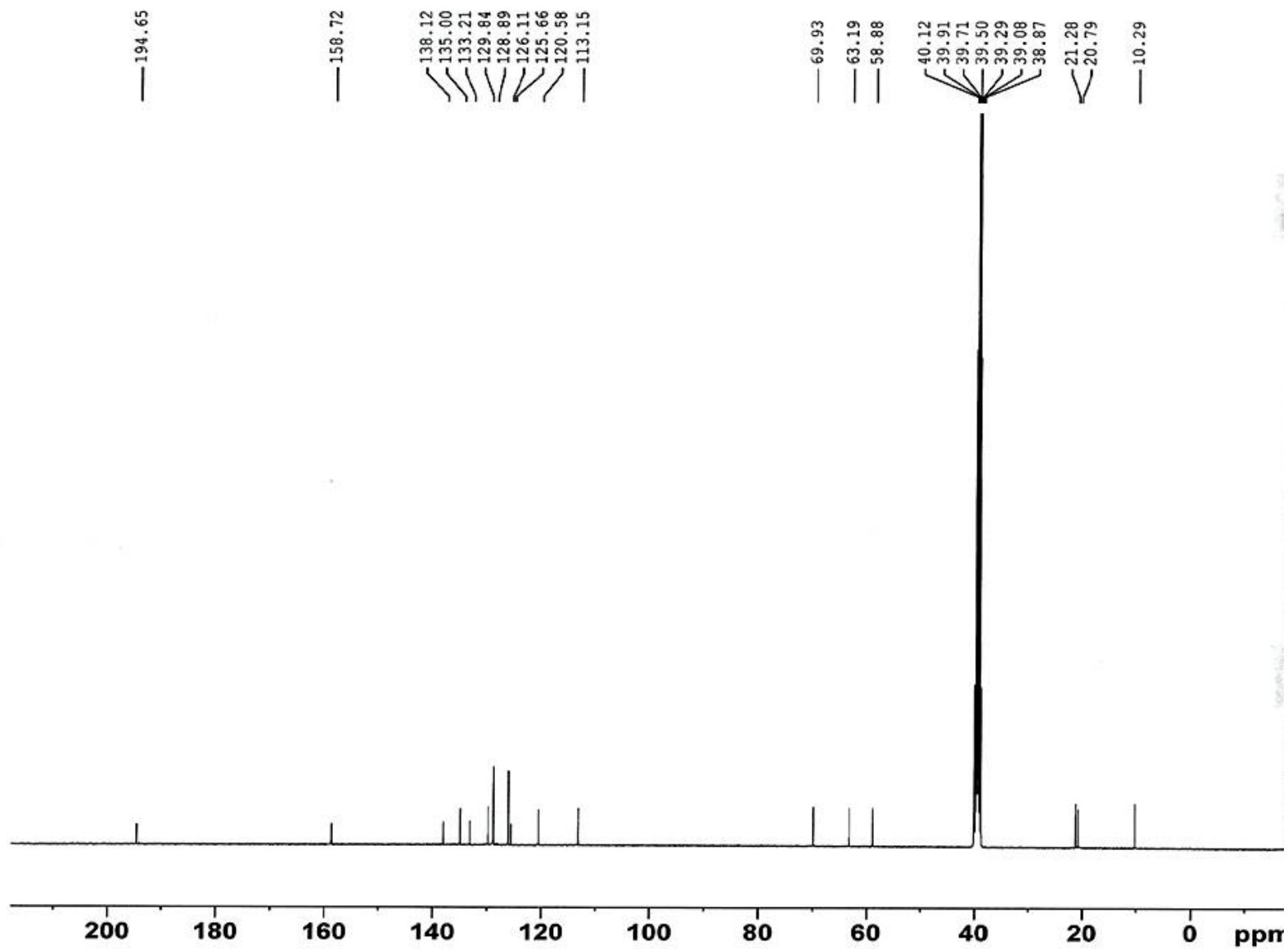


Figure S4. The ^{13}C NMR spectrum of compound **5** (100 MHz, solvent $\text{DMSO-}d_6$)

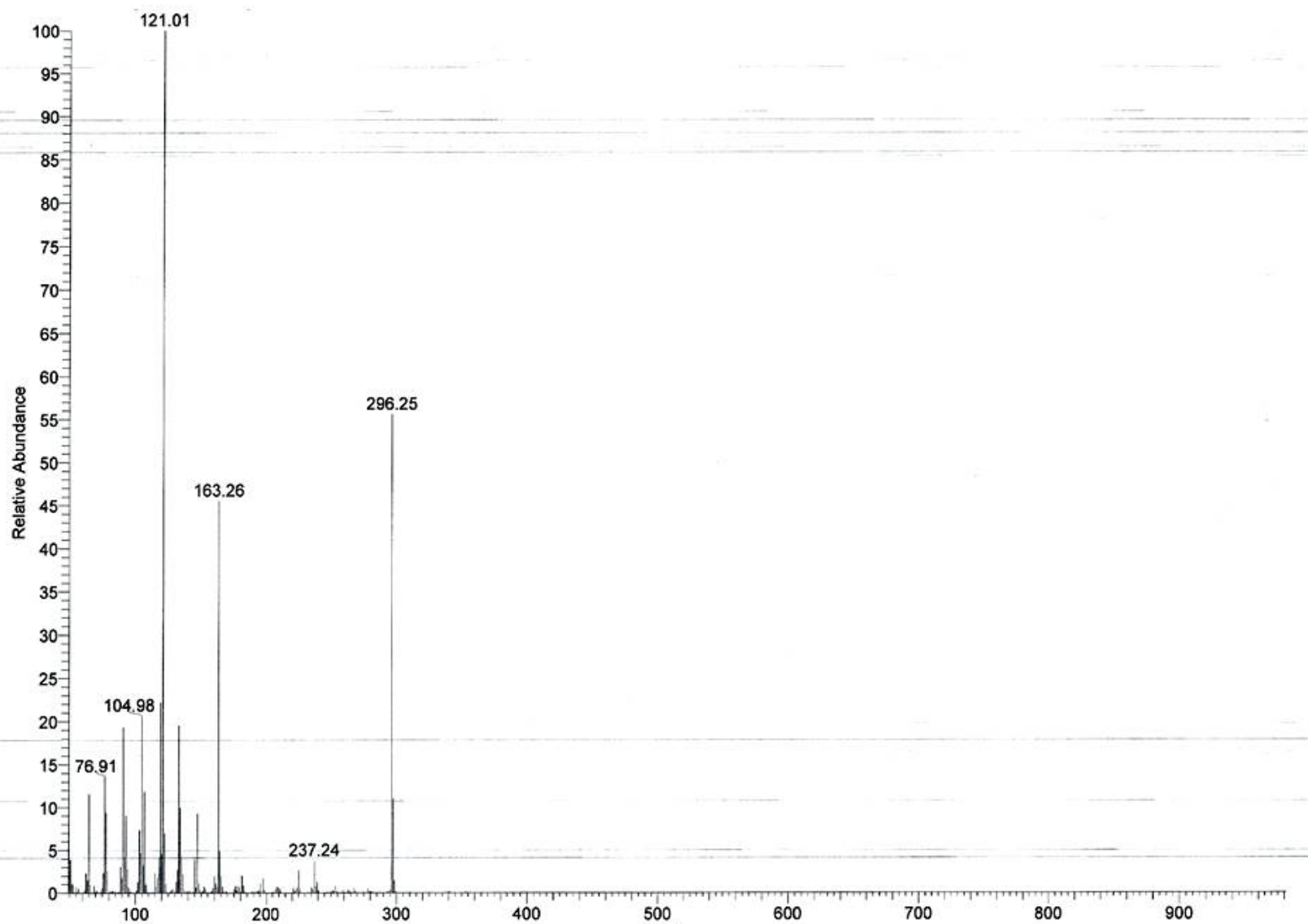


Figure S5. Chemical Ionization Mass Spectrum of compound **5**.

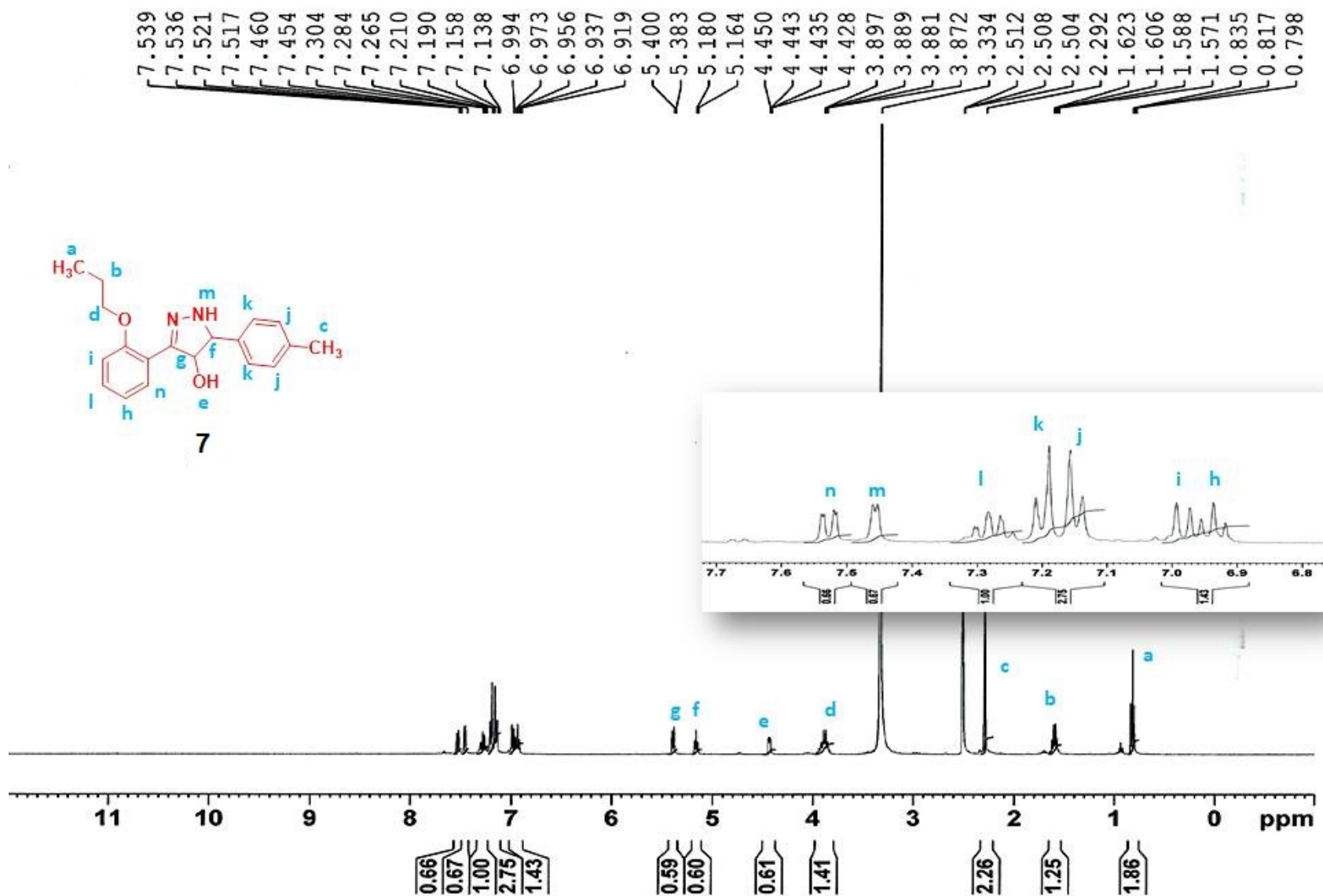


Figure S6. The ¹H NMR spectrum of compound 7 (400 MHz, solvent DMSO-*d*₆)

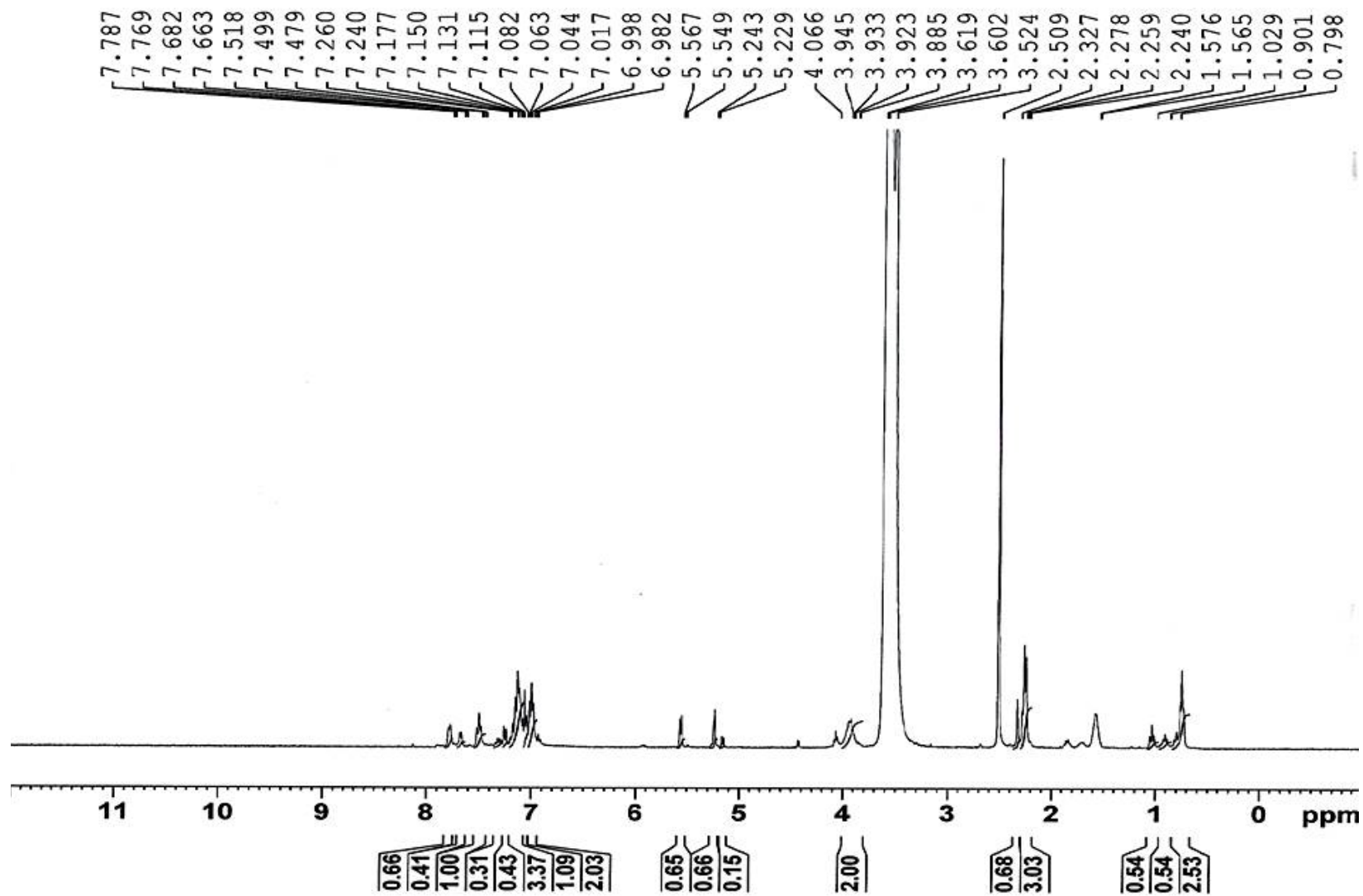


Figure S7. The D_2O 1H NMR spectrum of compound **7** (400 MHz, solvent $DMSO-d_6$)

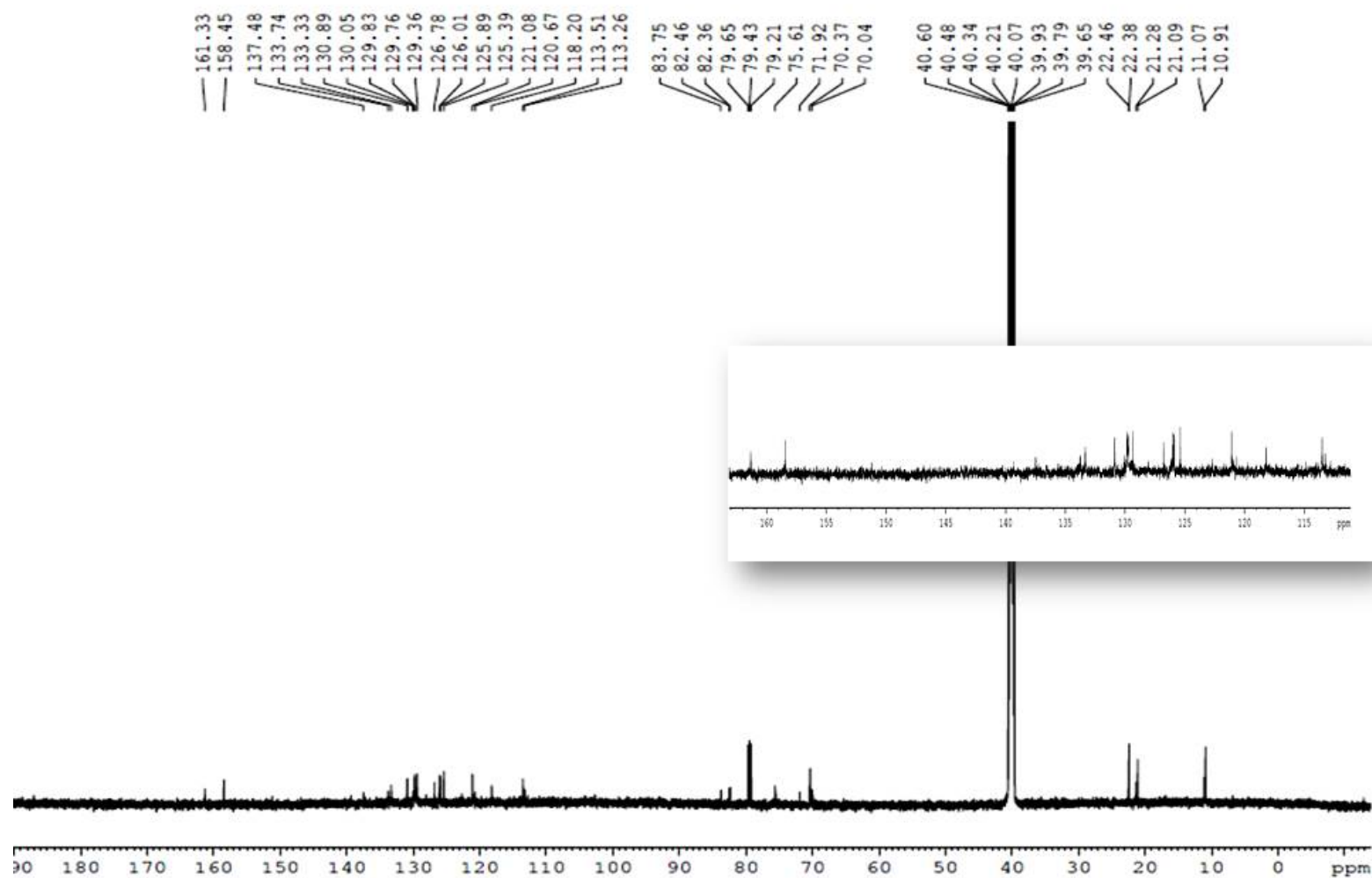


Figure S8. The ¹³C NMR spectrum of compound 7 (100 MHz, solvent DMSO-*d*₆)

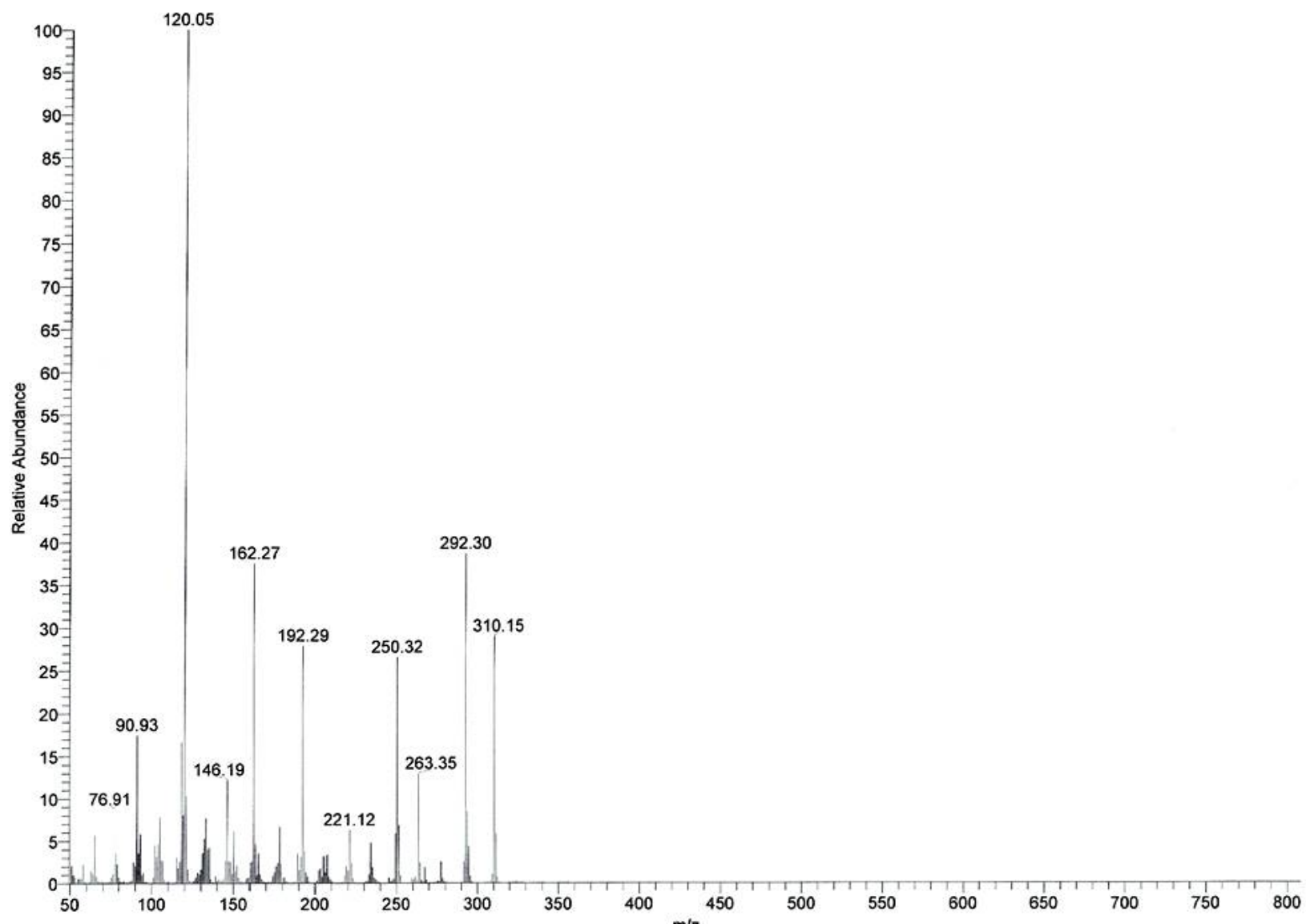


Figure S9. Chemical Ionization Mass Spectrum of compound 7.

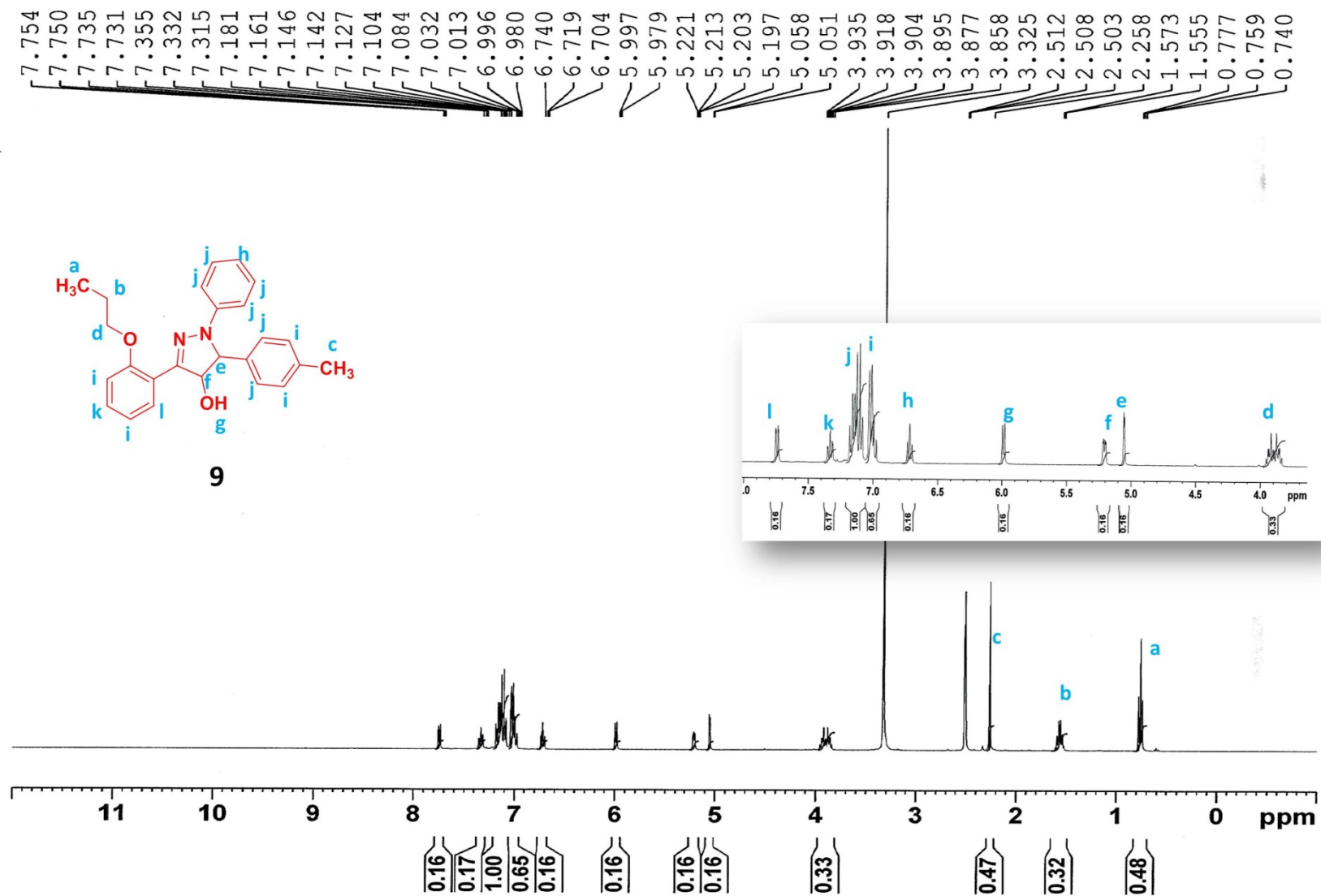


Figure S10. The ¹H NMR spectrum of compound **9** (400 MHz, solvent DMSO-*d*₆)

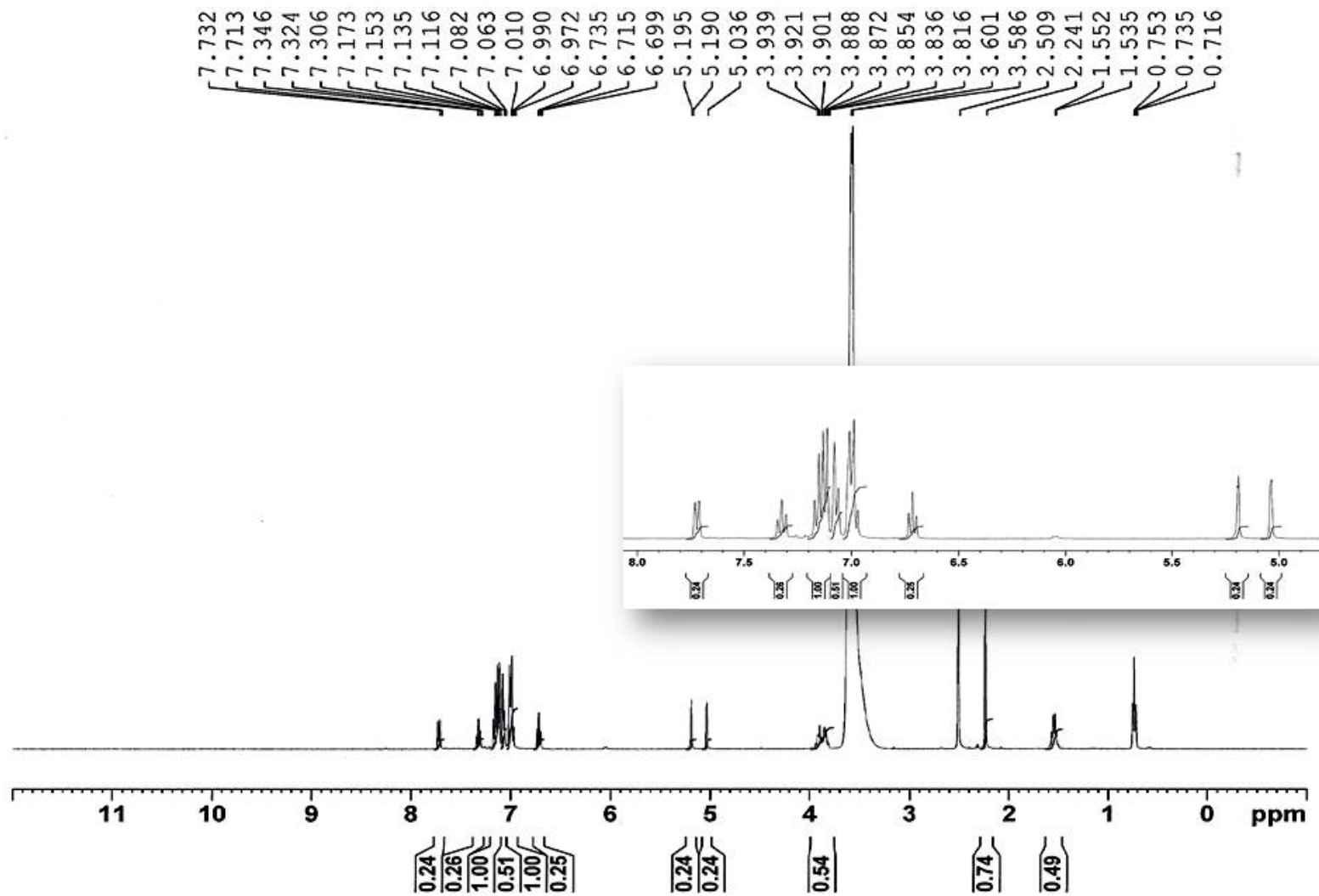


Figure S11. The D_2O ^1H NMR spectrum of compound 9 (400 MHz, solvent $\text{DMSO-}d_6$)

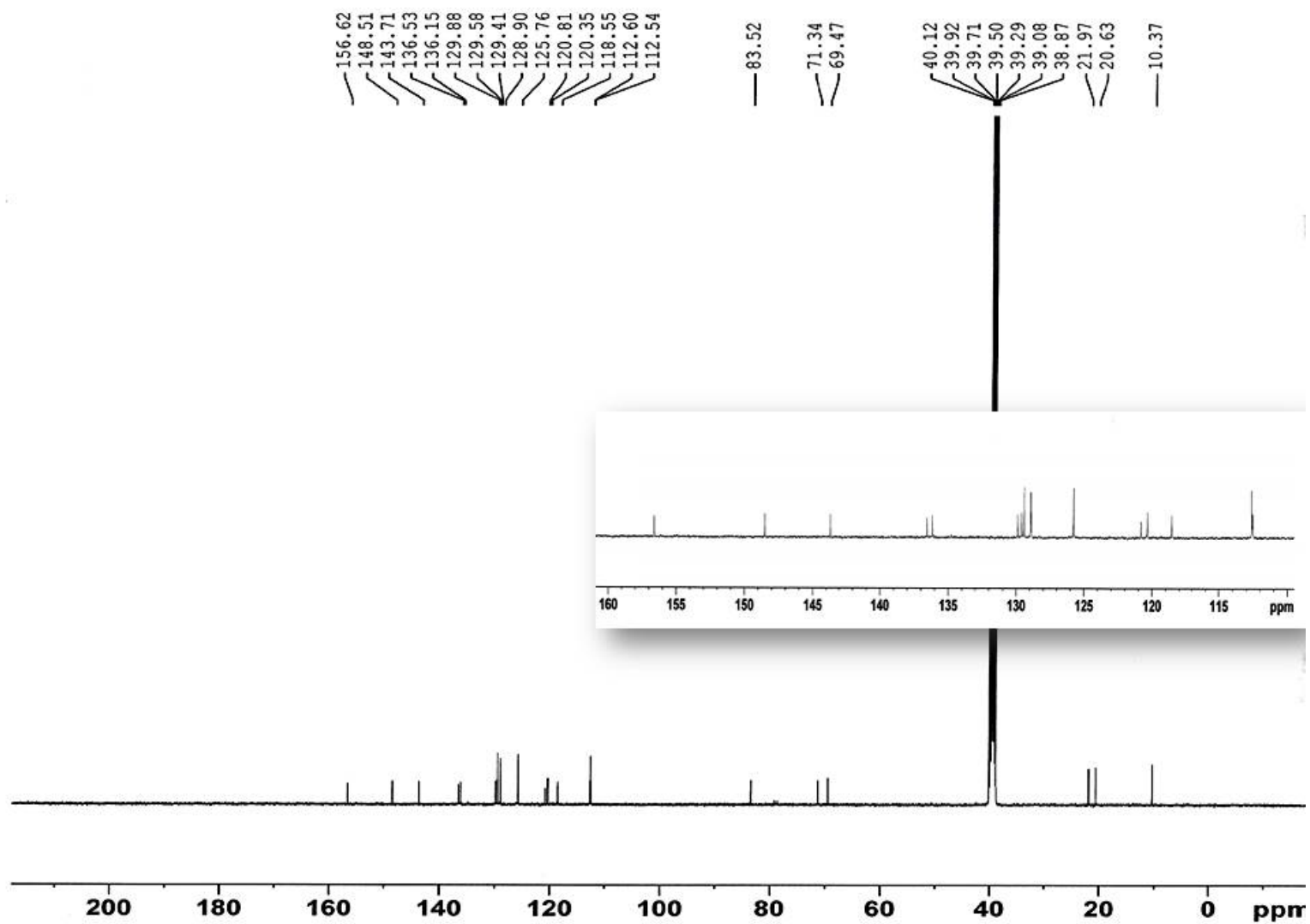


Figure S12. The ¹³C NMR spectrum of compound **9** (100 MHz, solvent DMSO-*d*₆)

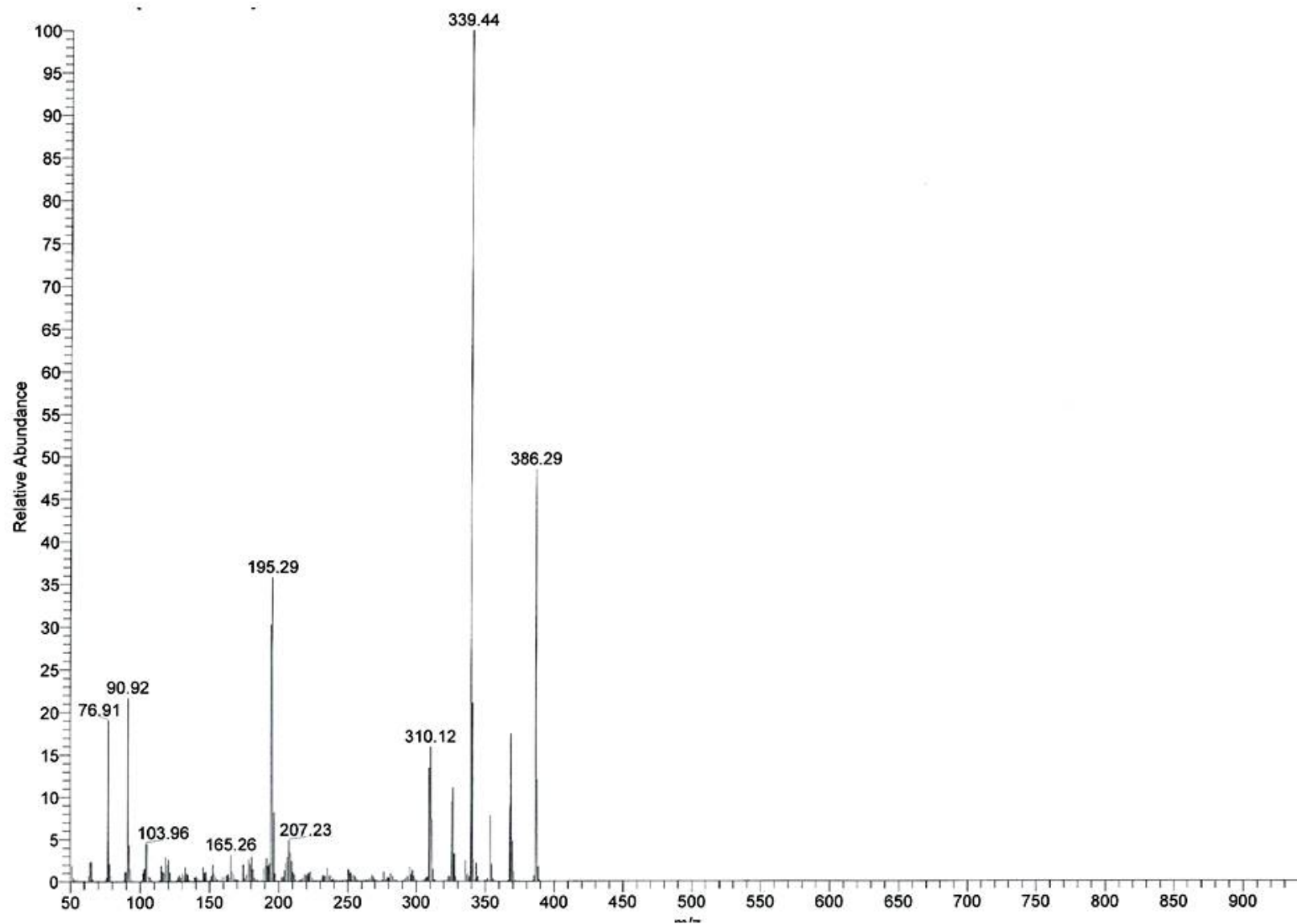


Figure S13. Chemical Ionization Mass Spectrum of compound **9**.

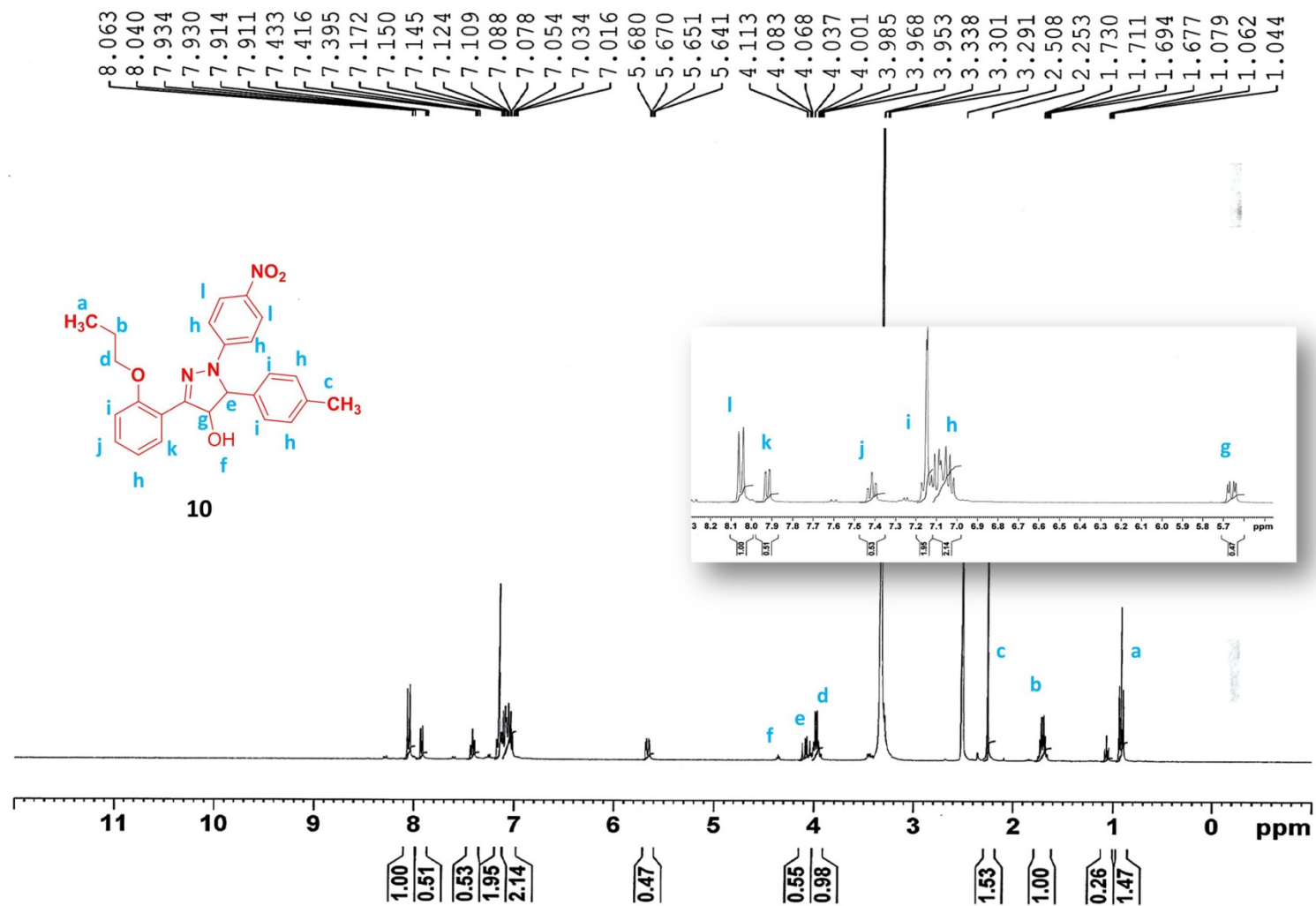


Figure S14. The ¹H NMR spectrum of compound **10** (400 MHz, solvent DMSO-*d*₆)

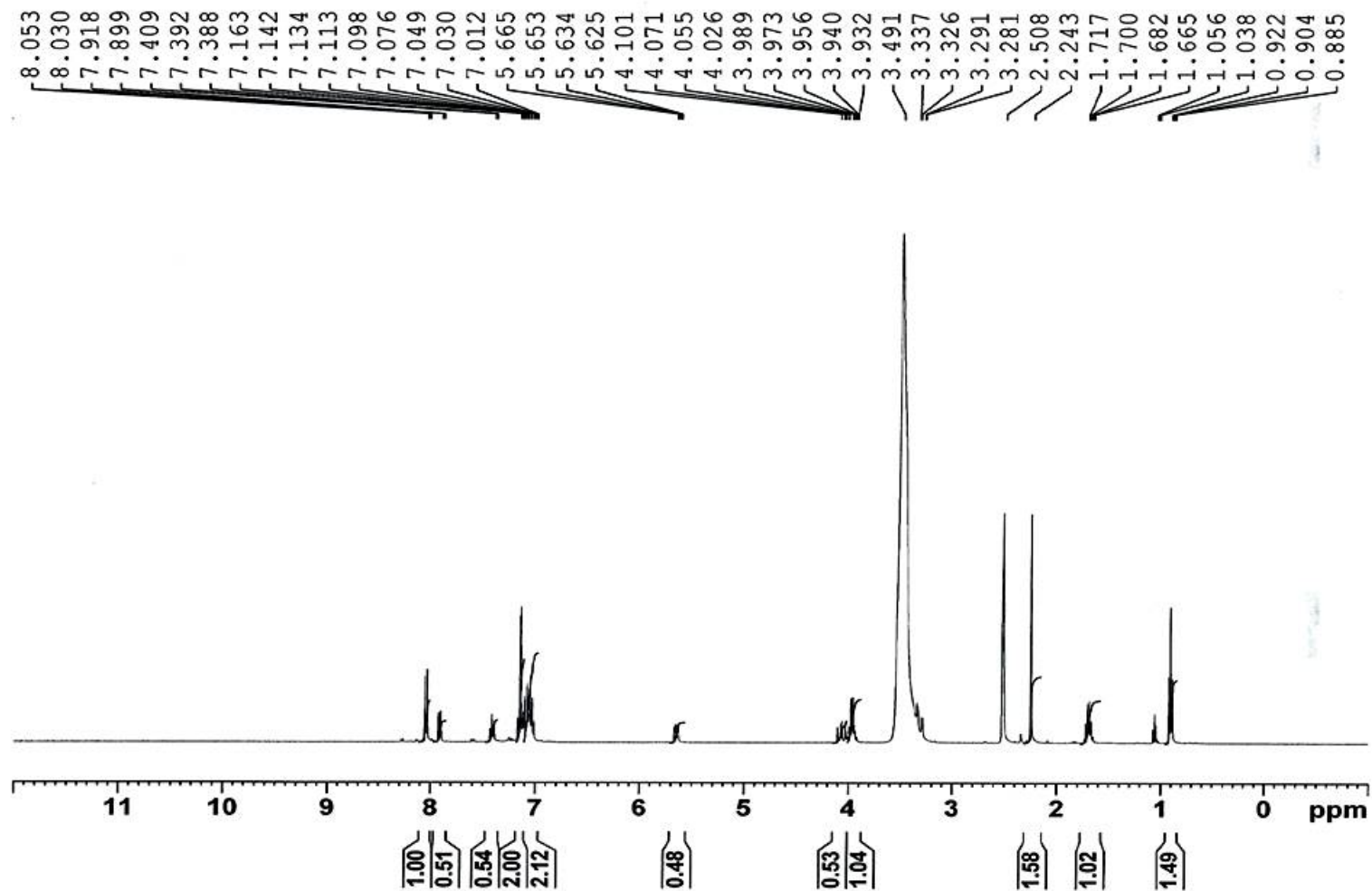


Figure S15. The D₂O ¹H NMR spectrum of compound **10** (400 MHz, solvent DMSO- *d*₆)

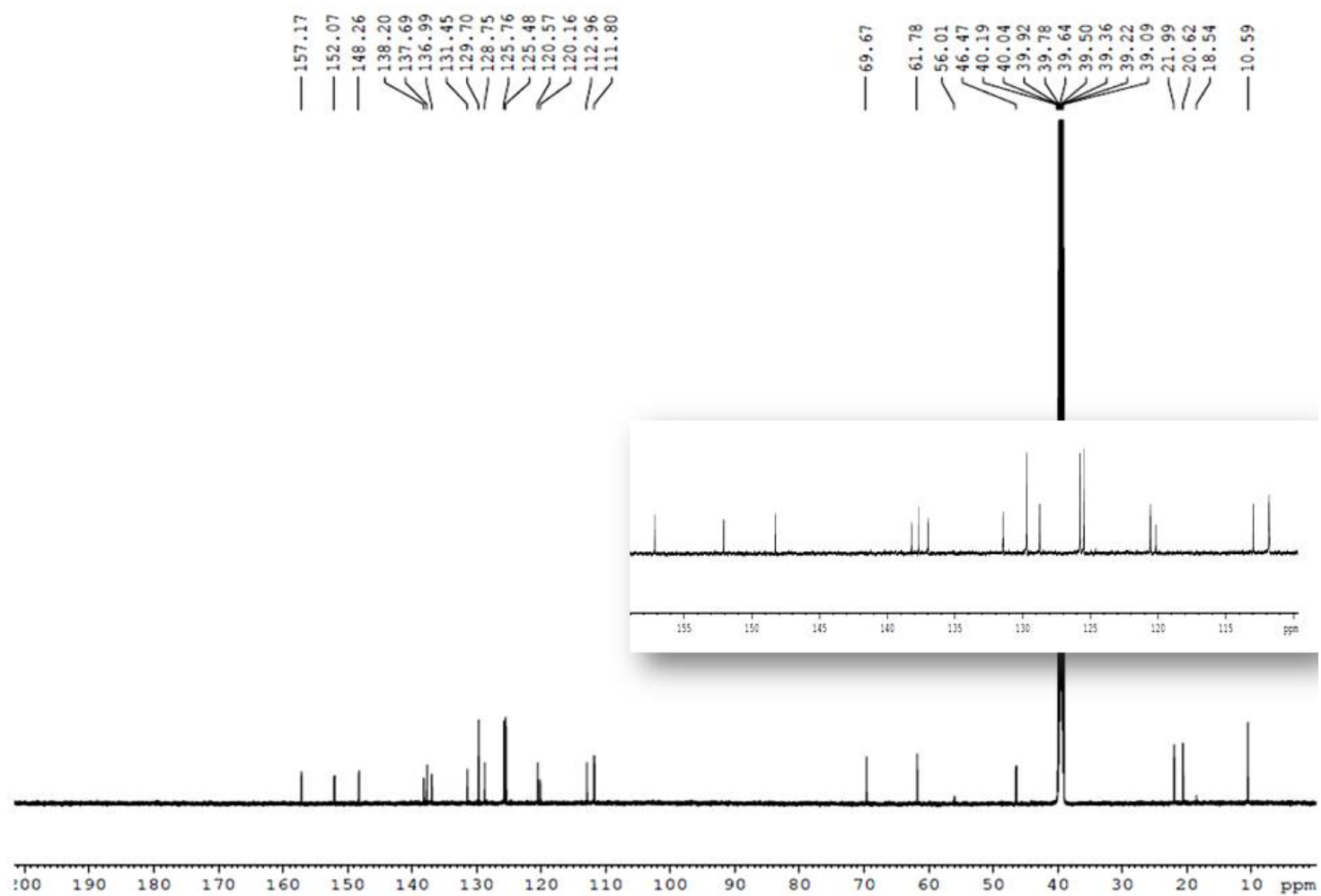


Figure S16. The ¹³C NMR spectrum of compound **10** (100 MHz, solvent DMSO- *d*₆)

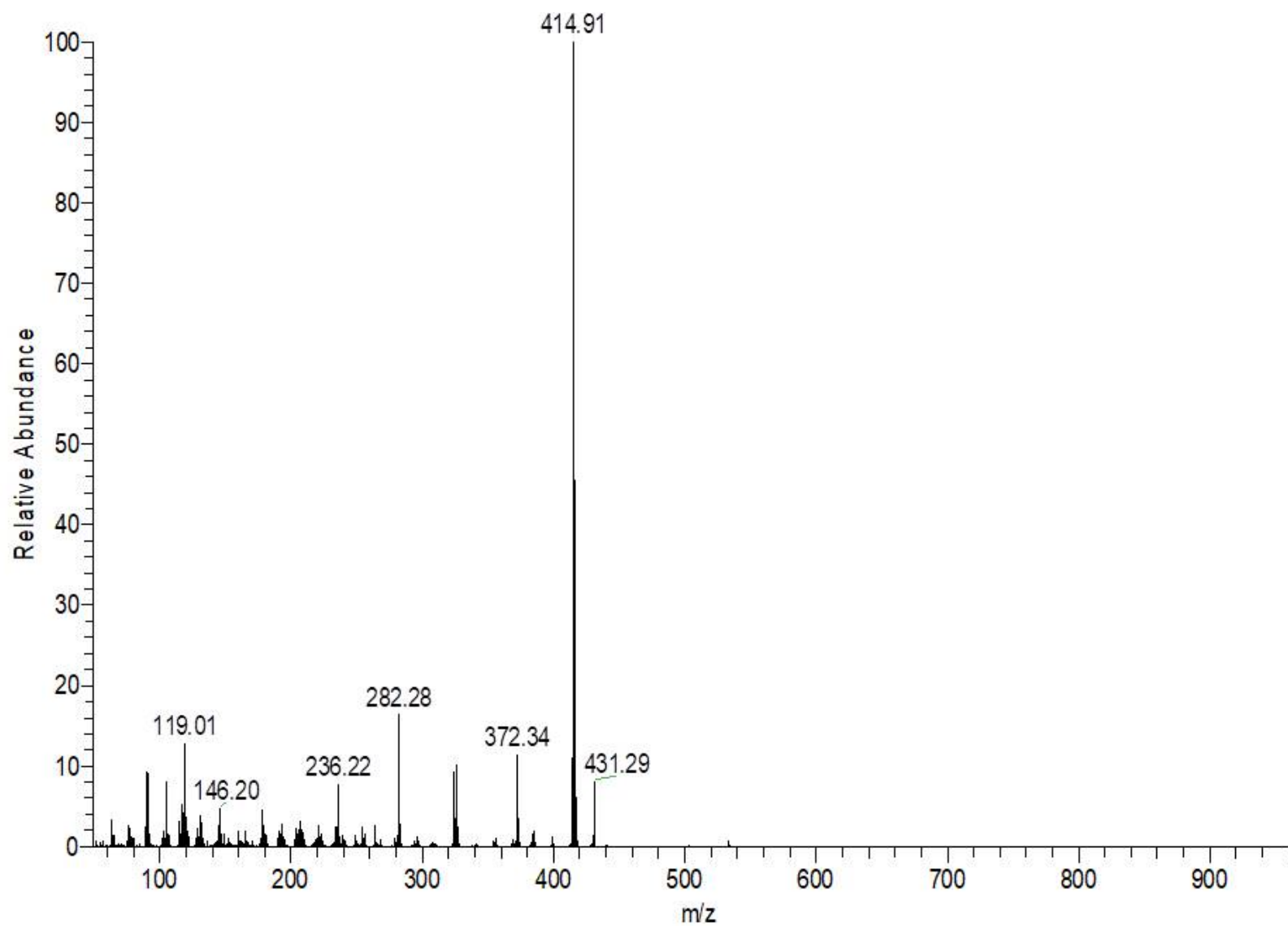


Figure S17. Chemical Ionization Mass Spectrum of compound **10**.

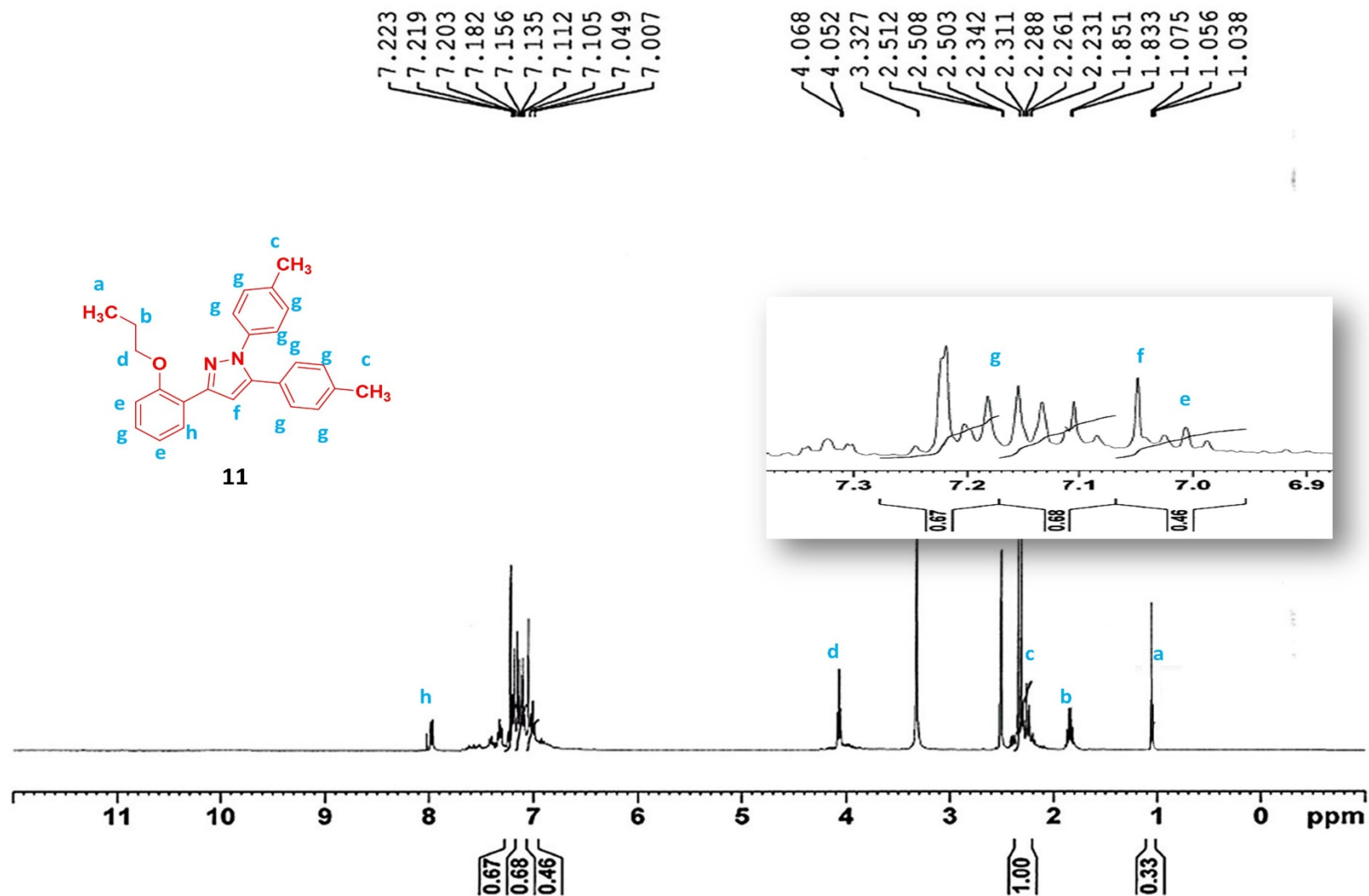


Figure S18. The ¹H NMR spectrum of compound **11** (400 MHz, solvent DMSO-*d*₆)

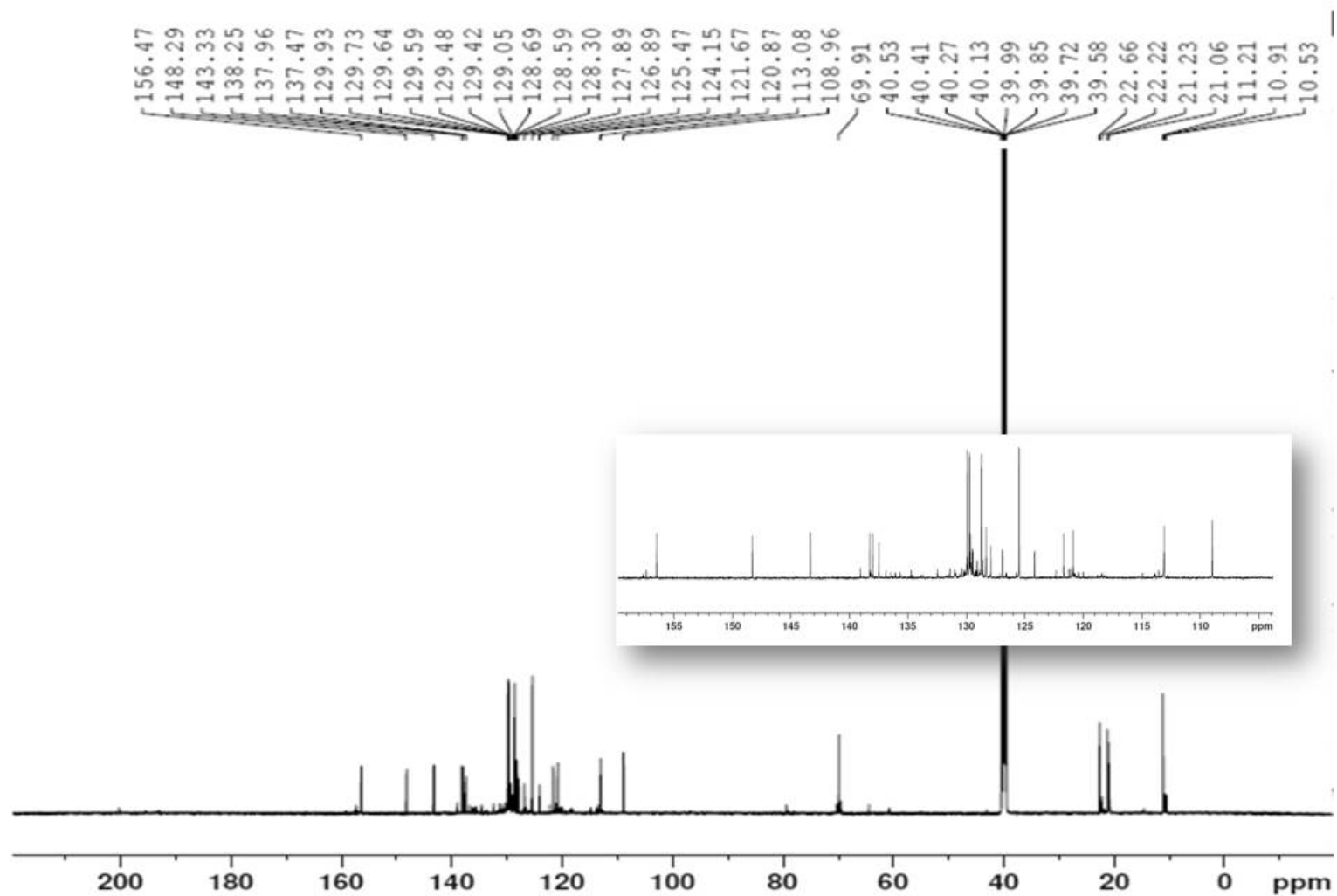


Figure S19. The ^{13}C NMR spectrum of compound **11** (100 MHz, solvent $\text{DMSO}-d_6$)

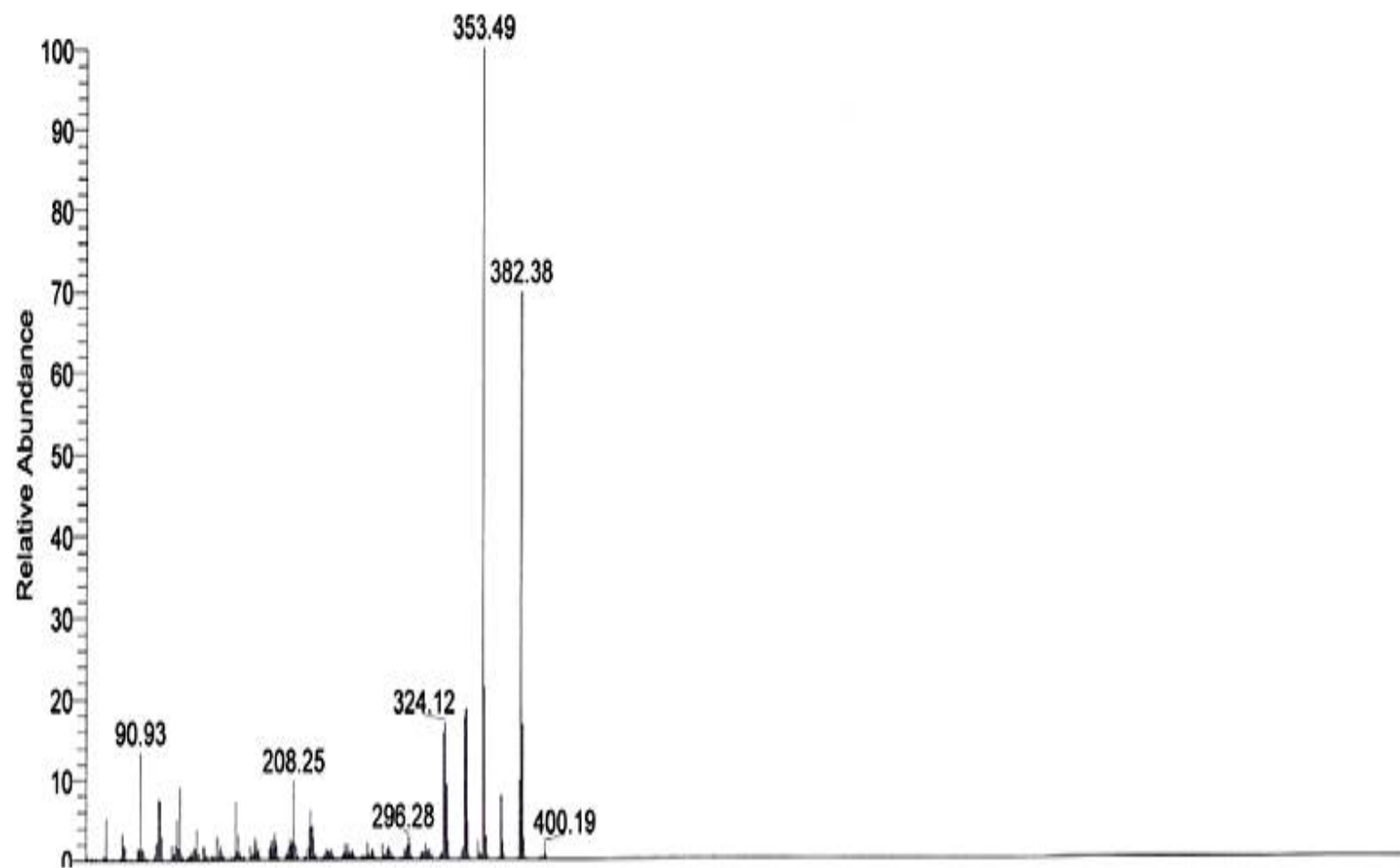


Figure S20. Chemical Ionization Mass Spectrum of compound **11**.

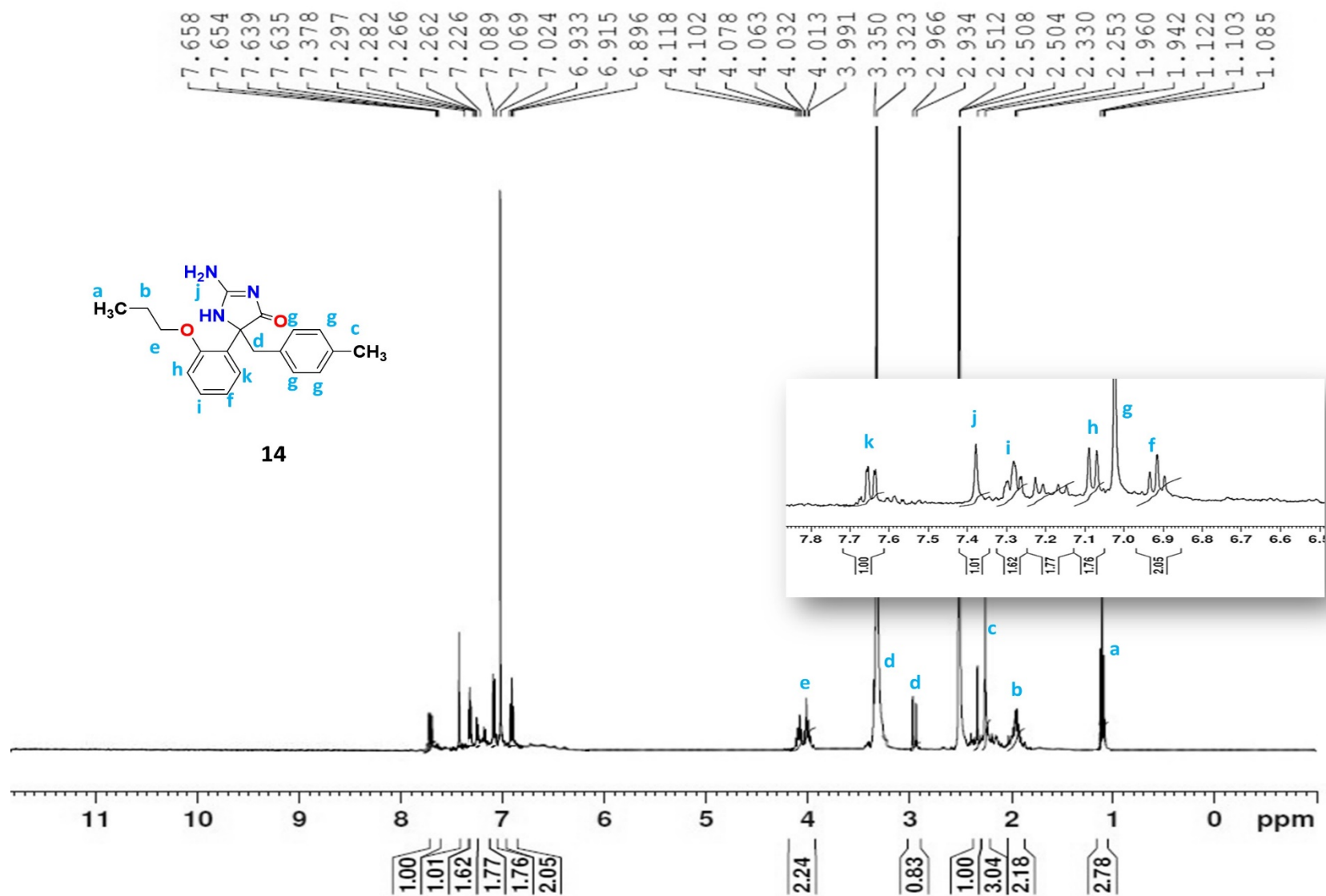


Figure S21. The ¹H NMR spectrum of compound **14** (400 MHz, solvent DMSO-*d*₆)

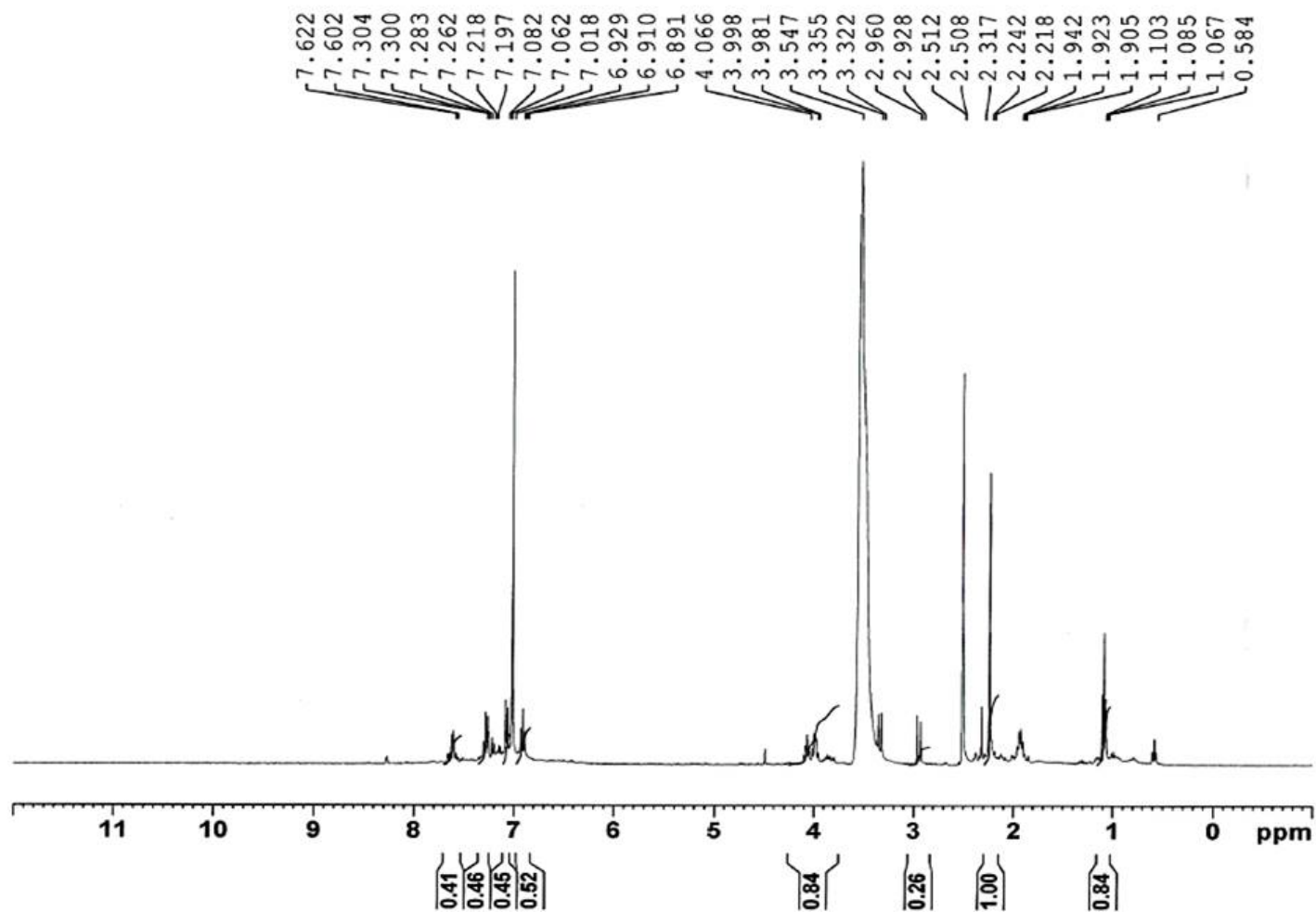


Figure S22. The D_2O ^1H NMR spectrum of compound **14** (400 MHz, solvent $\text{DMSO-}d_6$)

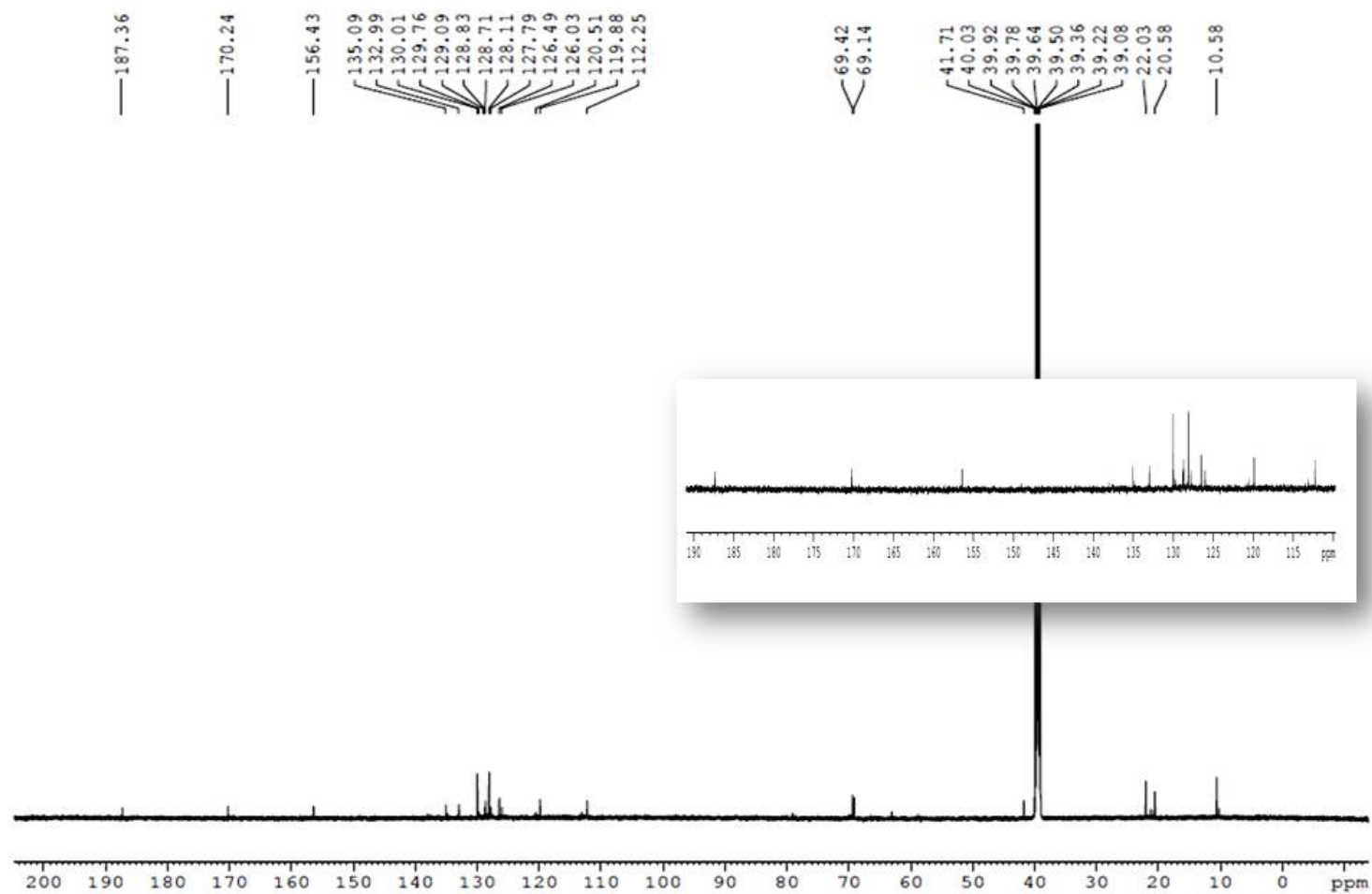


Figure S23. The ¹³C NMR spectrum of compound **14** (100 MHz, solvent DMSO-*d*₆)

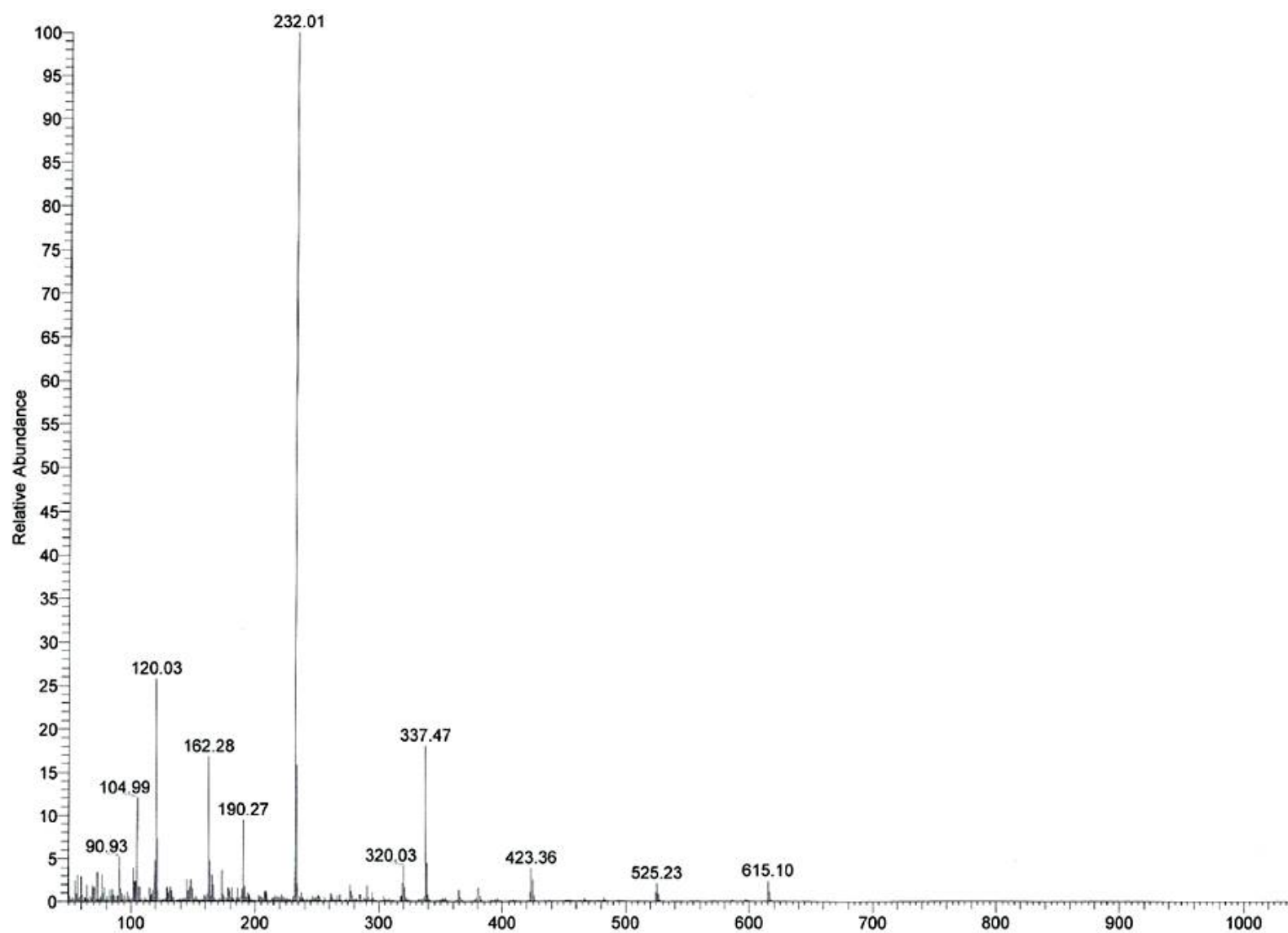


Figure S24. Chemical Ionization Mass Spectrum of compound **14**.

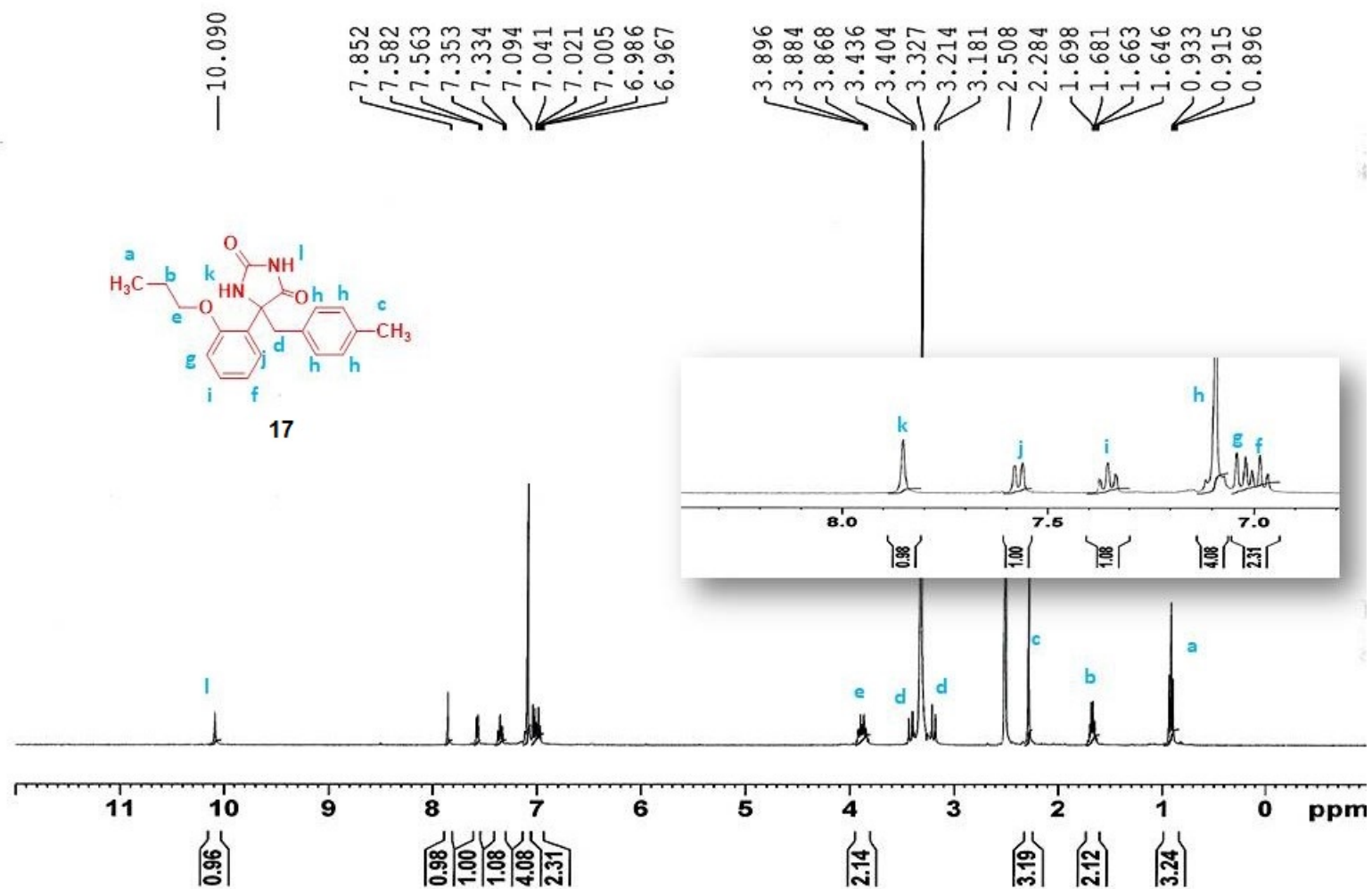


Figure S25. The ¹H NMR spectrum of compound **17** (400 MHz, solvent DMSO- *d*₆)

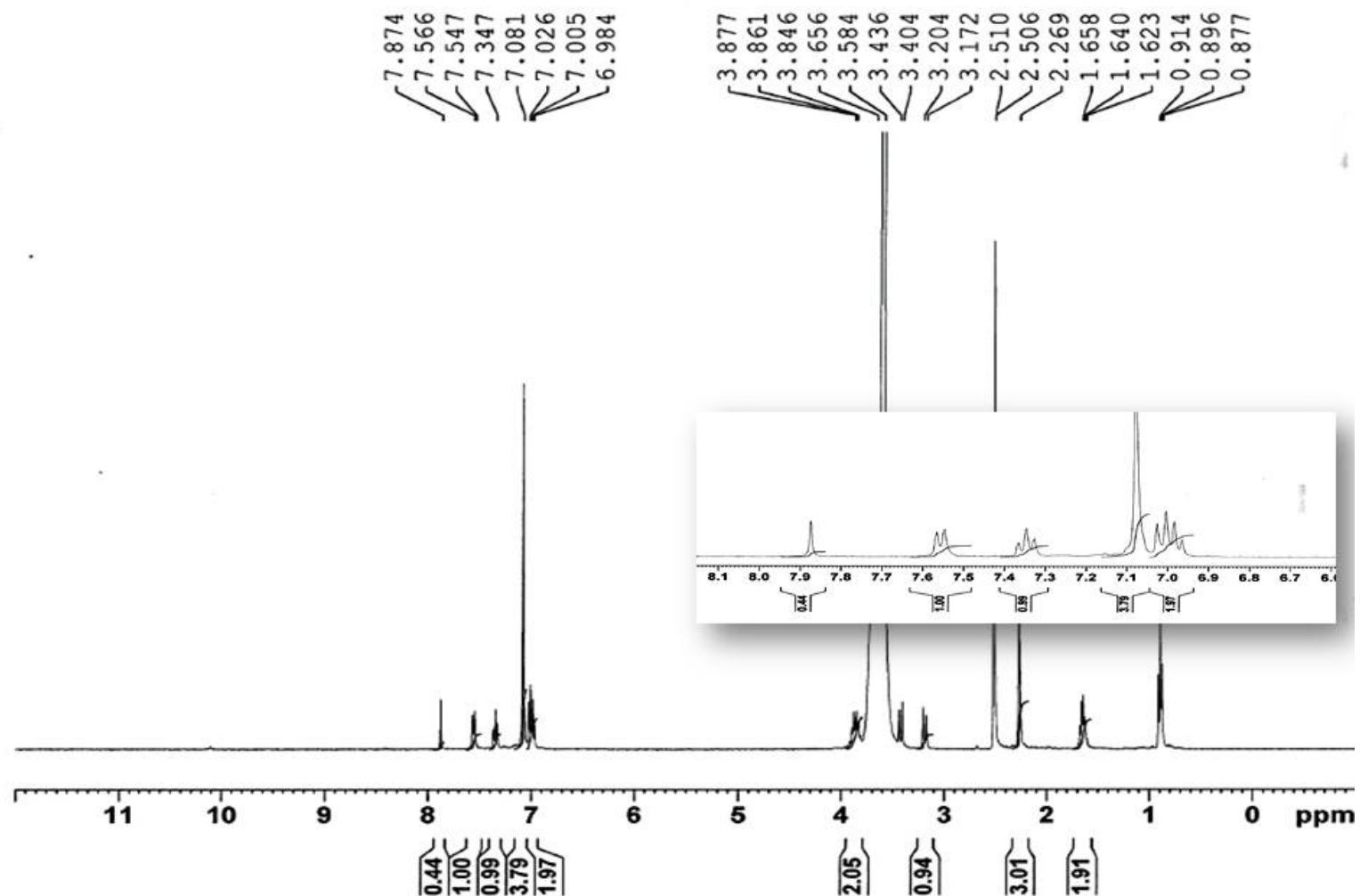


Figure S26. The D_2O ^1H NMR spectrum of compound 17 (400 MHz, solvent $\text{DMSO-}d_6$)

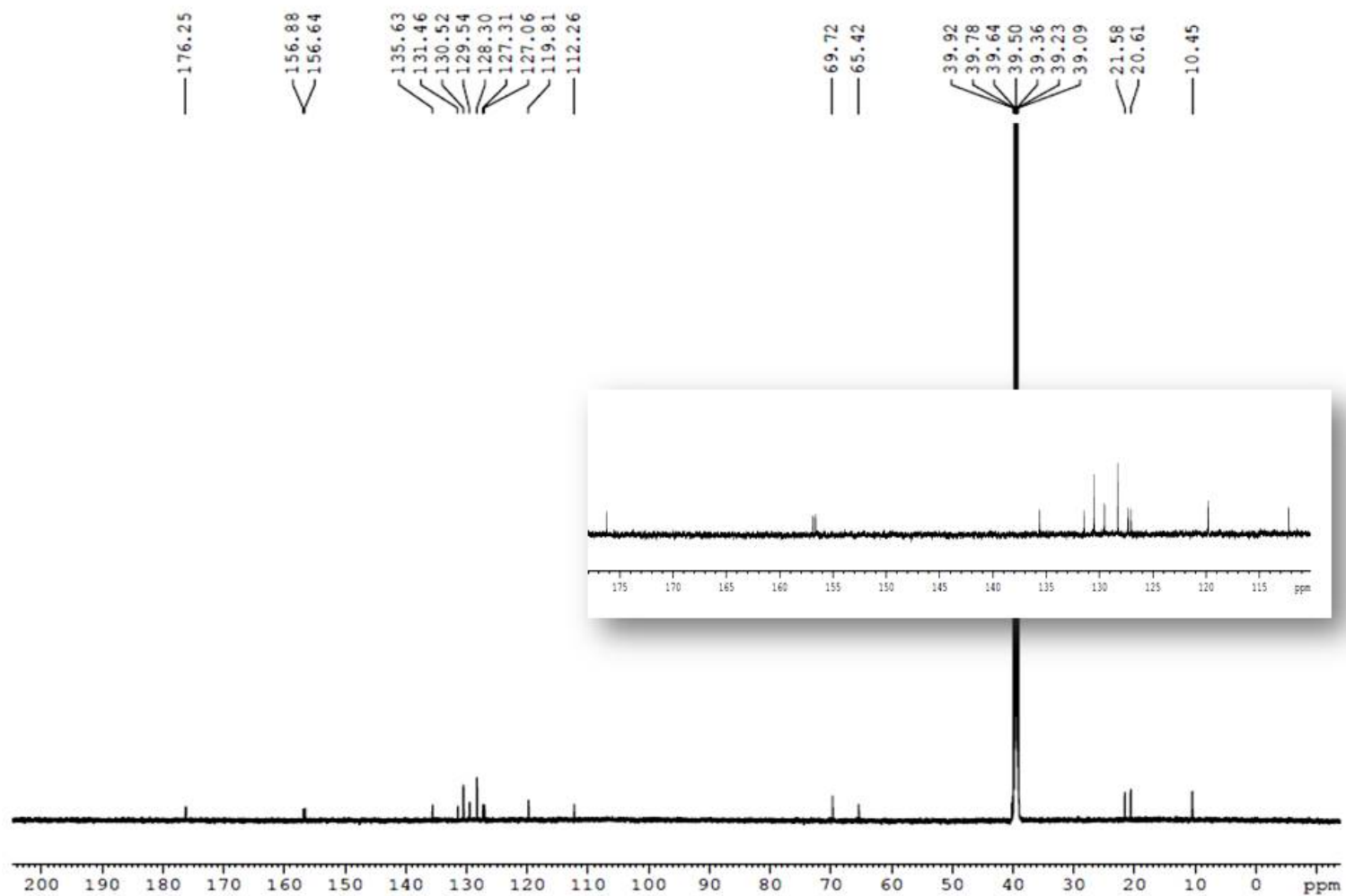


Figure S27. The ¹³C NMR spectrum of compound 17 (100 MHz, solvent DMSO- *d*₆)

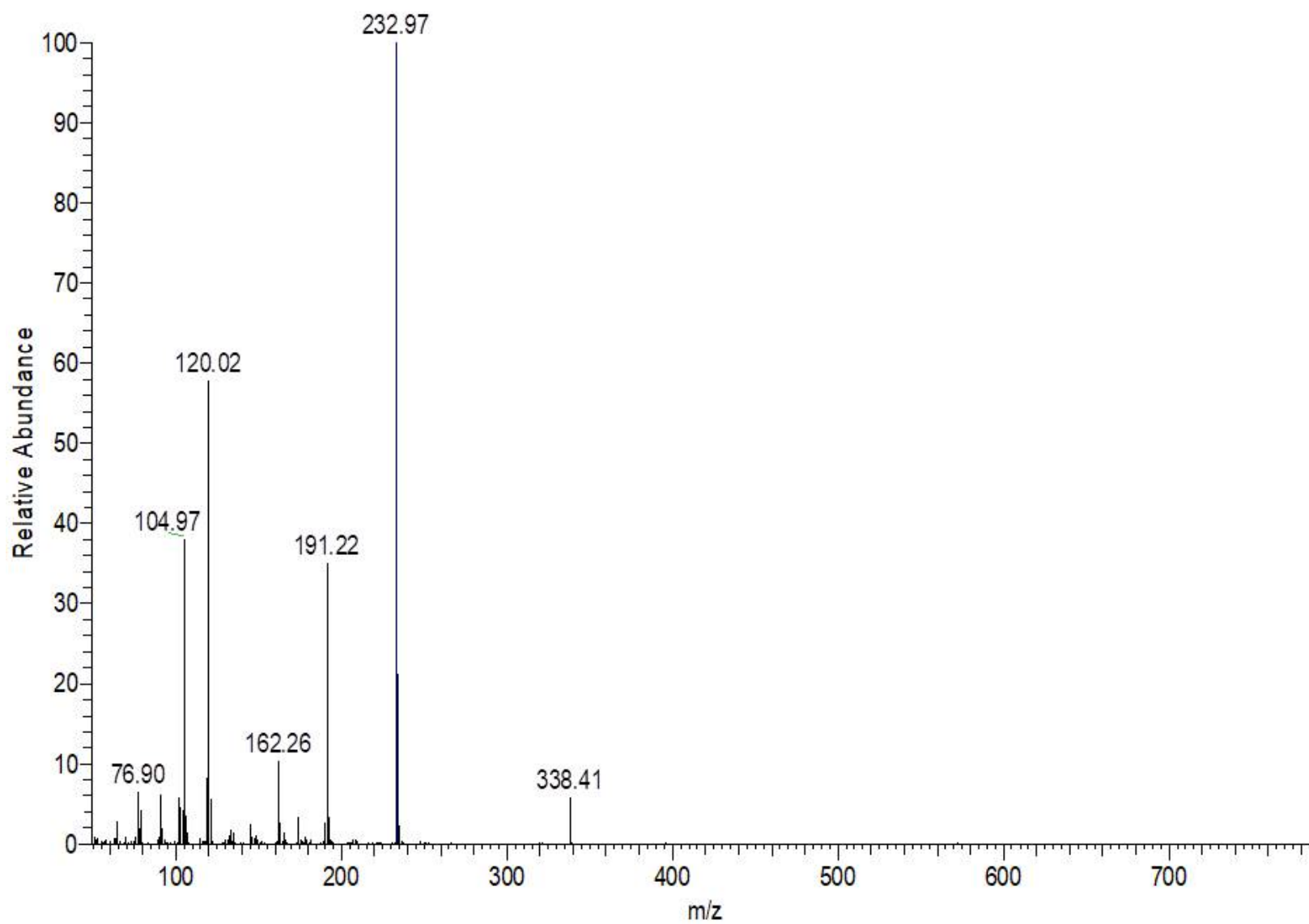


Figure S28. Chemical Ionization Mass Spectrum of compound **17**.