

Supplementary Material

Structural reassignment of a dibenz[*b,f*][1,4]oxazepin- 11(10*H*)-one with potent anti-giardial activity

Andrew G. Riches^{A,}, Christopher J. S. Hart^{B,C}, Matthieu Schmit^A, Emmanuel A. Debele^A, Snigdha Tiash^B, Erin Clapper^B, Tina S. Skinner-Adams^{B,*} and John H. Ryan^A*

^ACSIRO Manufacturing, Ian Wark Laboratory, Bayview Avenue, Clayton, Vic. 3168, Australia

^BGriffith Institute for Drug Discovery, Griffith University, Nathan, Qld 4111, Australia

^CPresent address: Department of Microbiology and Molecular Genetics, University of California Davis, CA 95616, USA

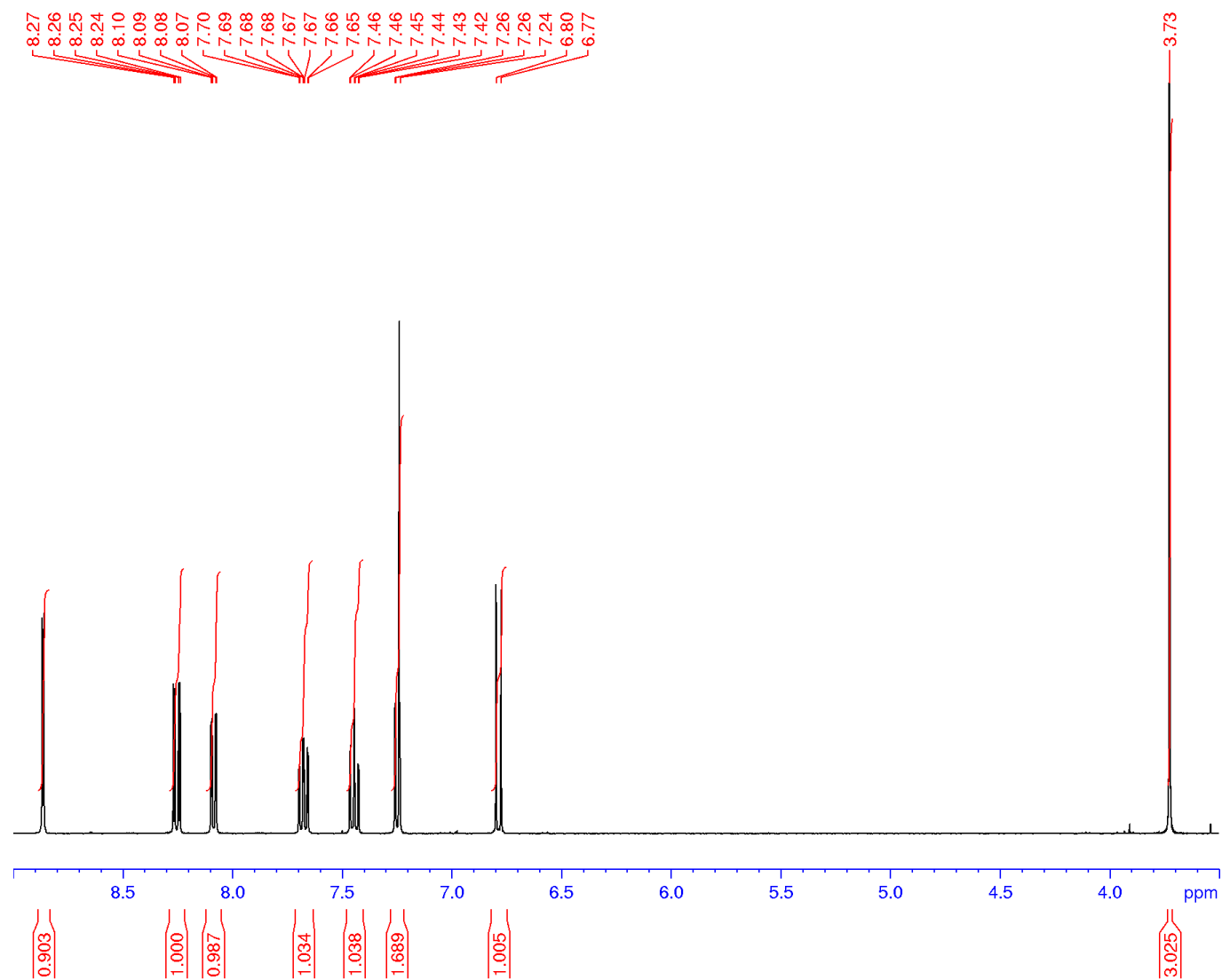
*Correspondence to: Email: andrew.riches@csiro.au, t.skinner-adams@griffith.edu.au

Supplementary Material

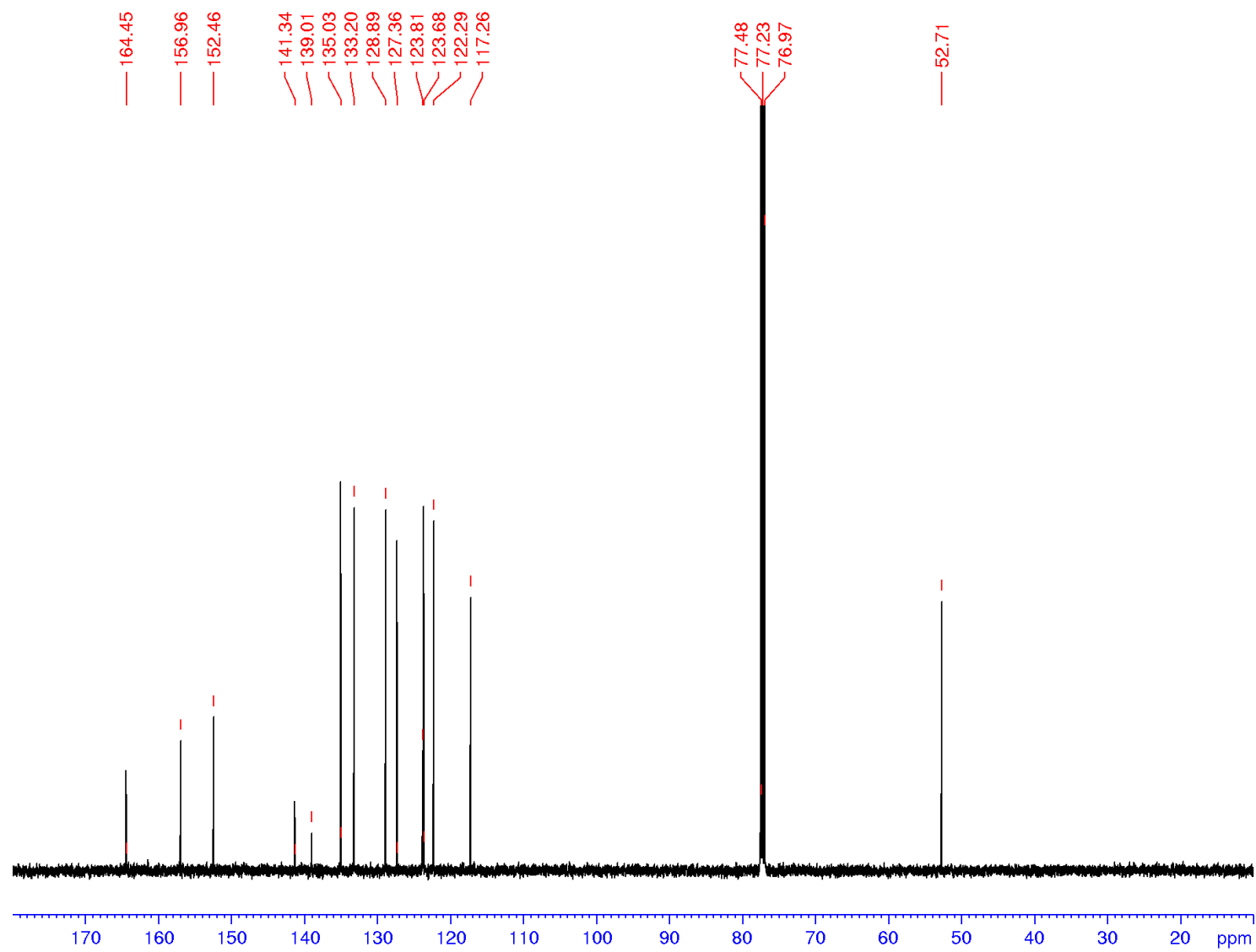
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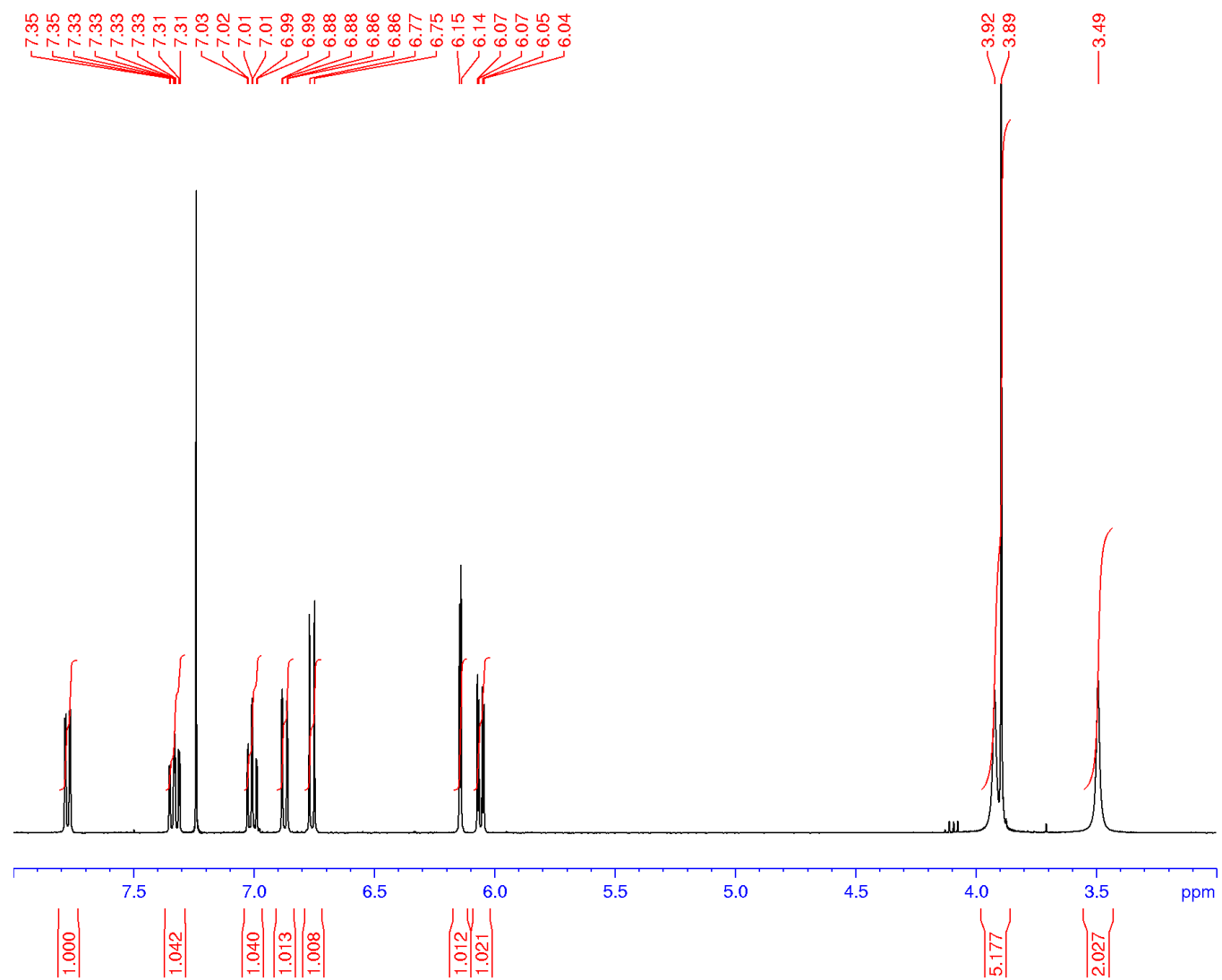
^1H NMR spectrum of **4** (400 MHz, CDCl_3)



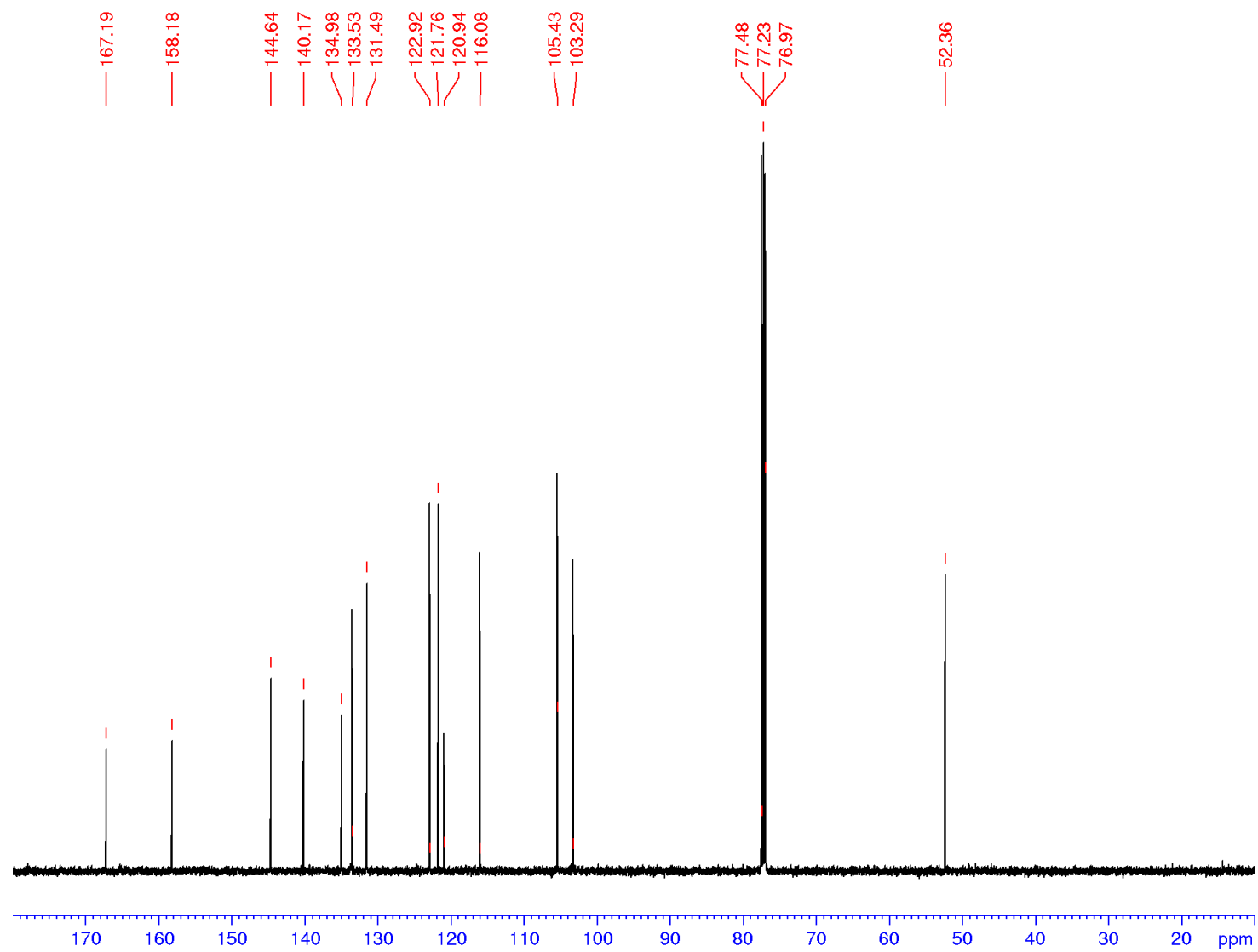
^{13}C NMR spectrum of **4** (125 MHz, CDCl_3)



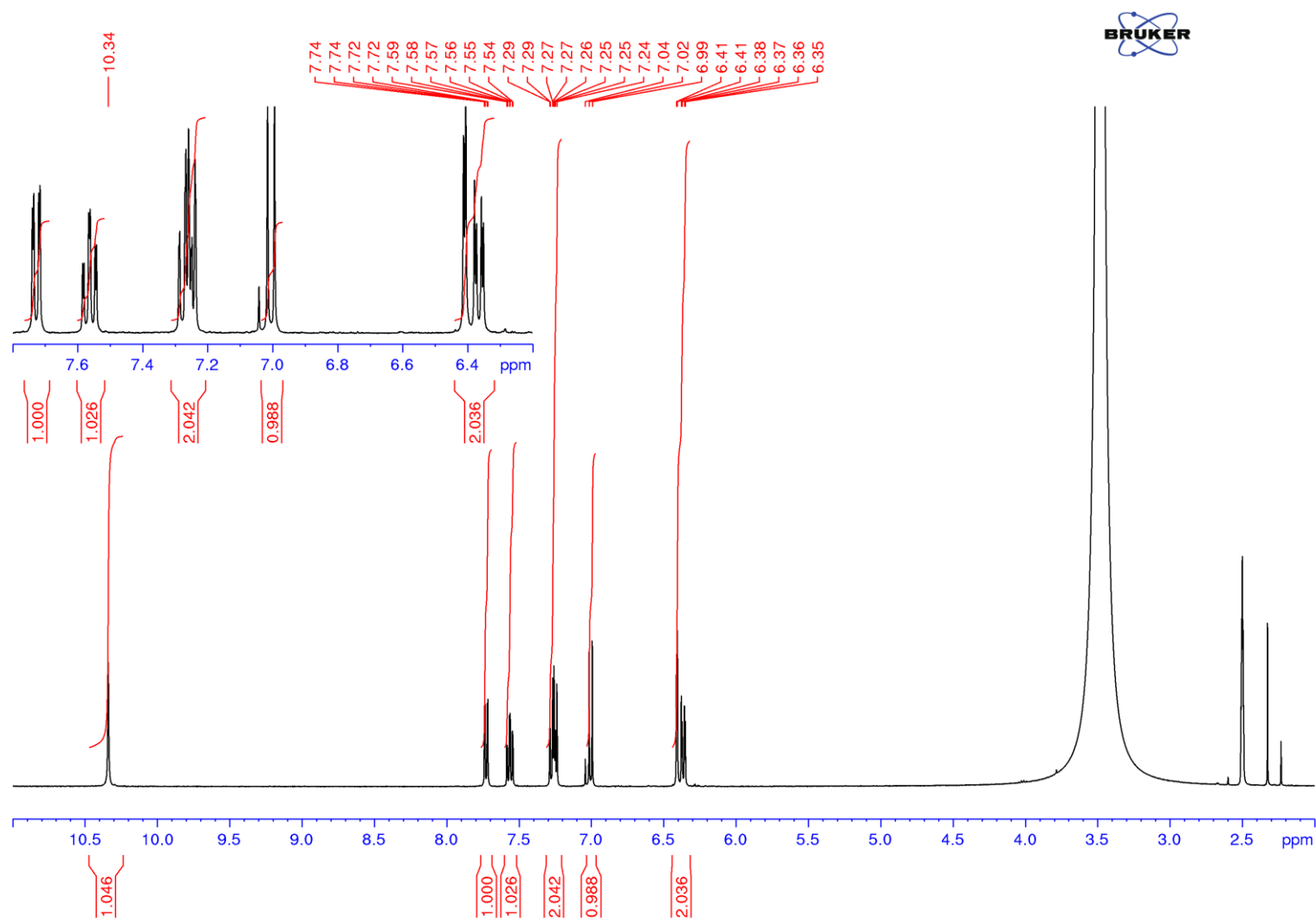
^1H NMR spectrum of **5** (400 MHz, CDCl_3)



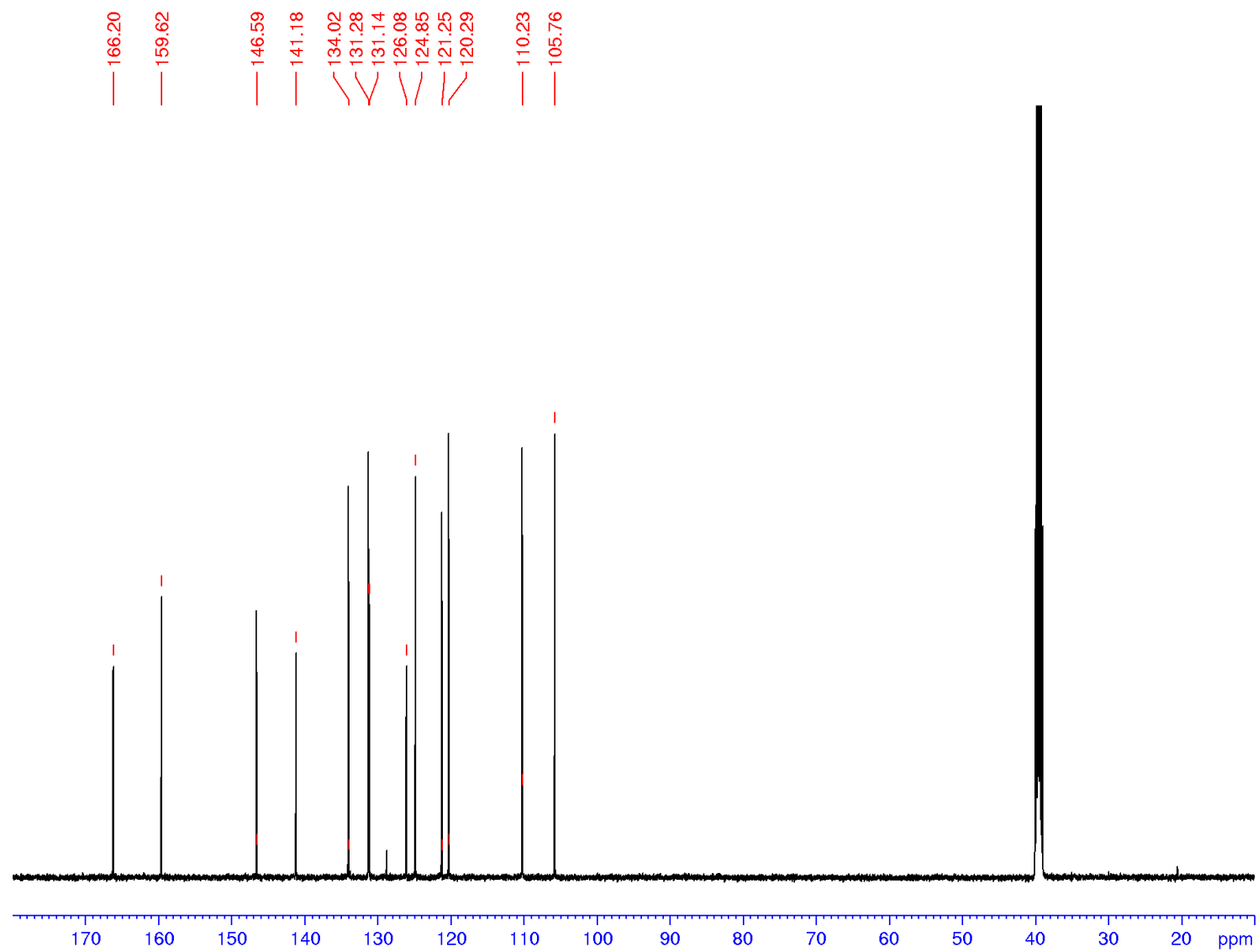
^{13}C NMR spectrum of **5** (125 MHz, CDCl_3)



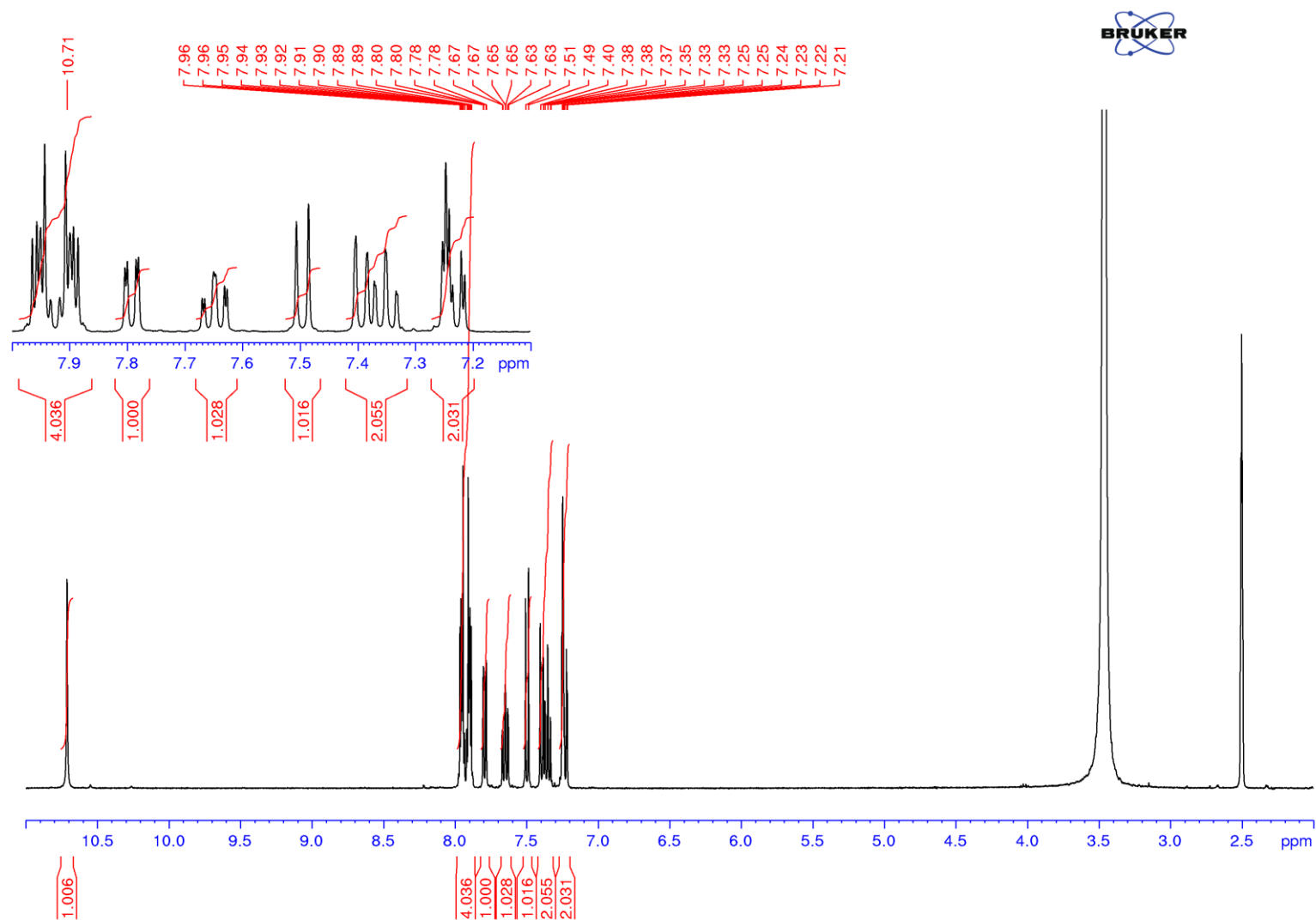
^1H NMR spectrum of **6** (400 MHz, $\text{d}_6\text{-DMSO}$)



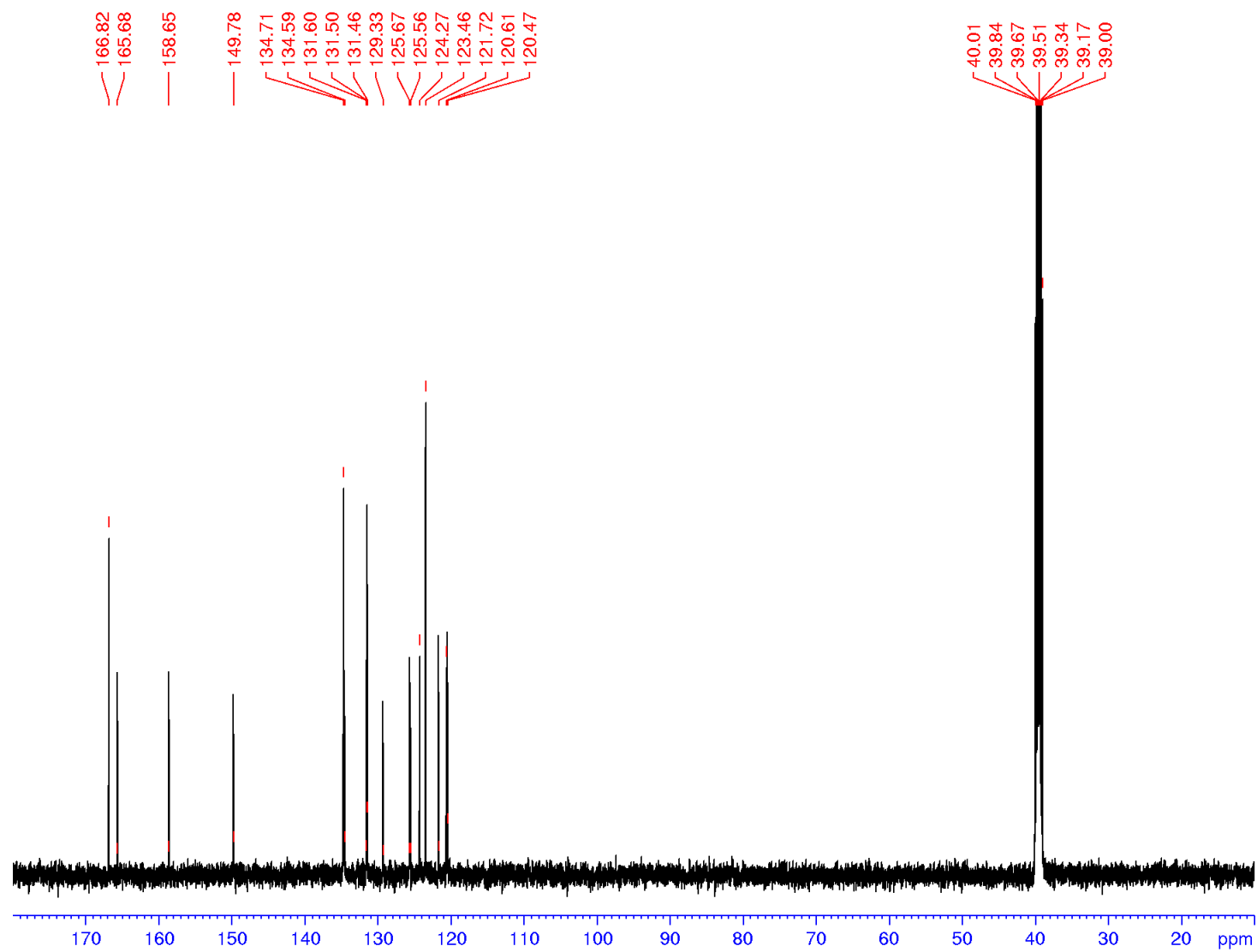
^{13}C NMR spectrum of **6** (125 MHz, $\text{d}_6\text{-DMSO}$)



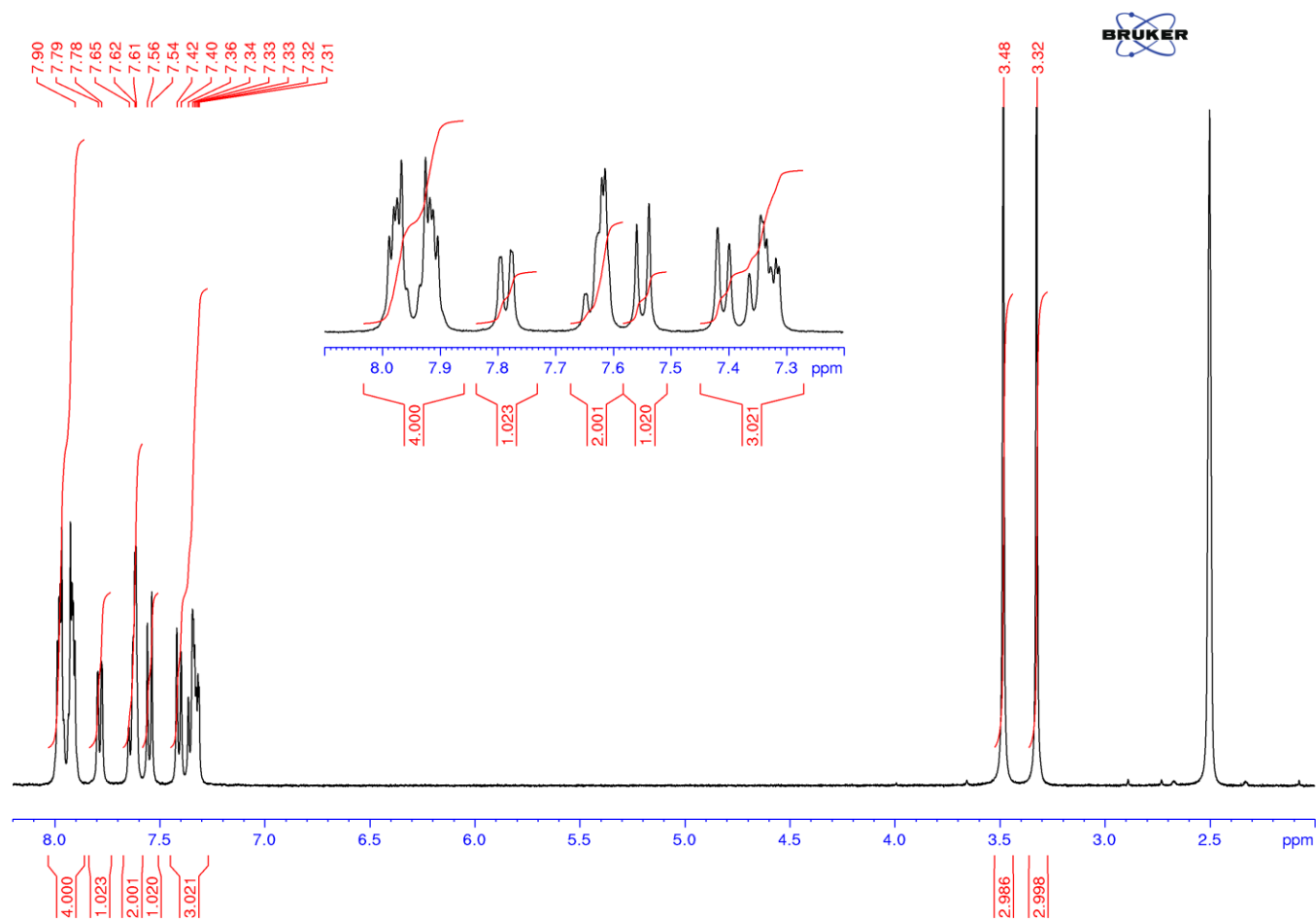
^1H NMR spectrum of **7** (400 MHz, $\text{d}_6\text{-DMSO}$)



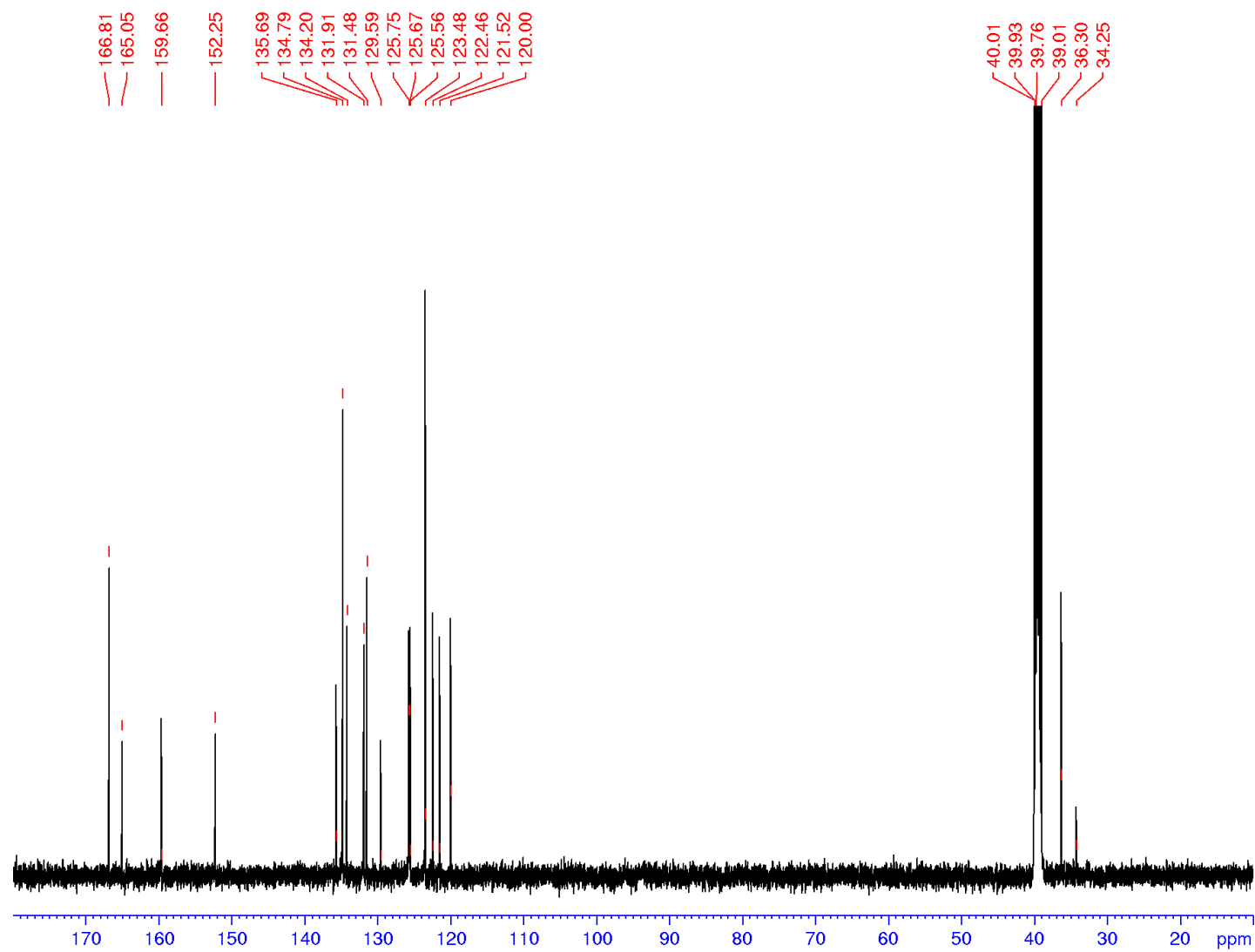
^{13}C NMR spectrum of **7** (125 MHz, $\text{d}_6\text{-DMSO}$)



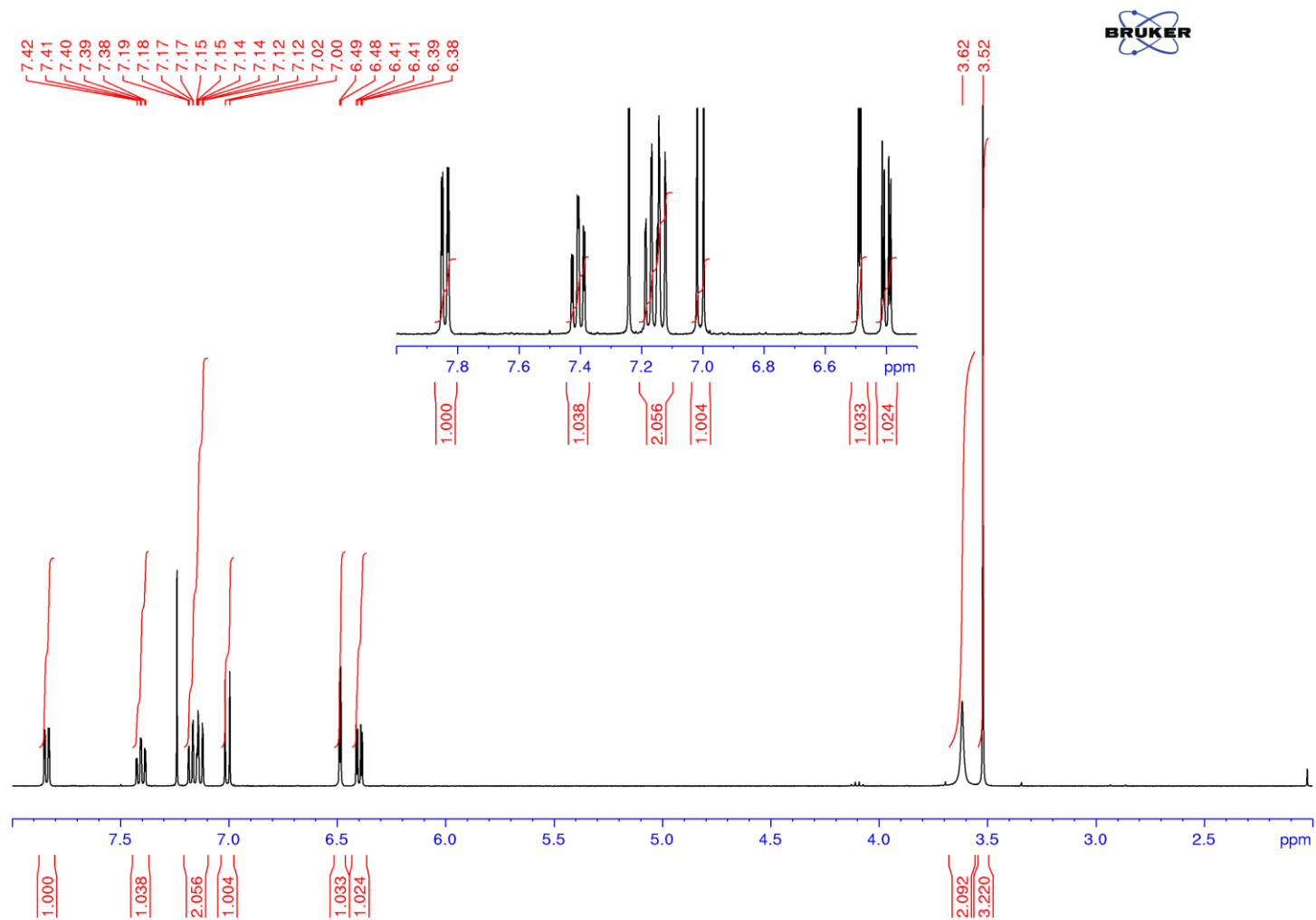
^1H NMR spectrum of **8** (400 MHz, $\text{d}_6\text{-DMSO}$)



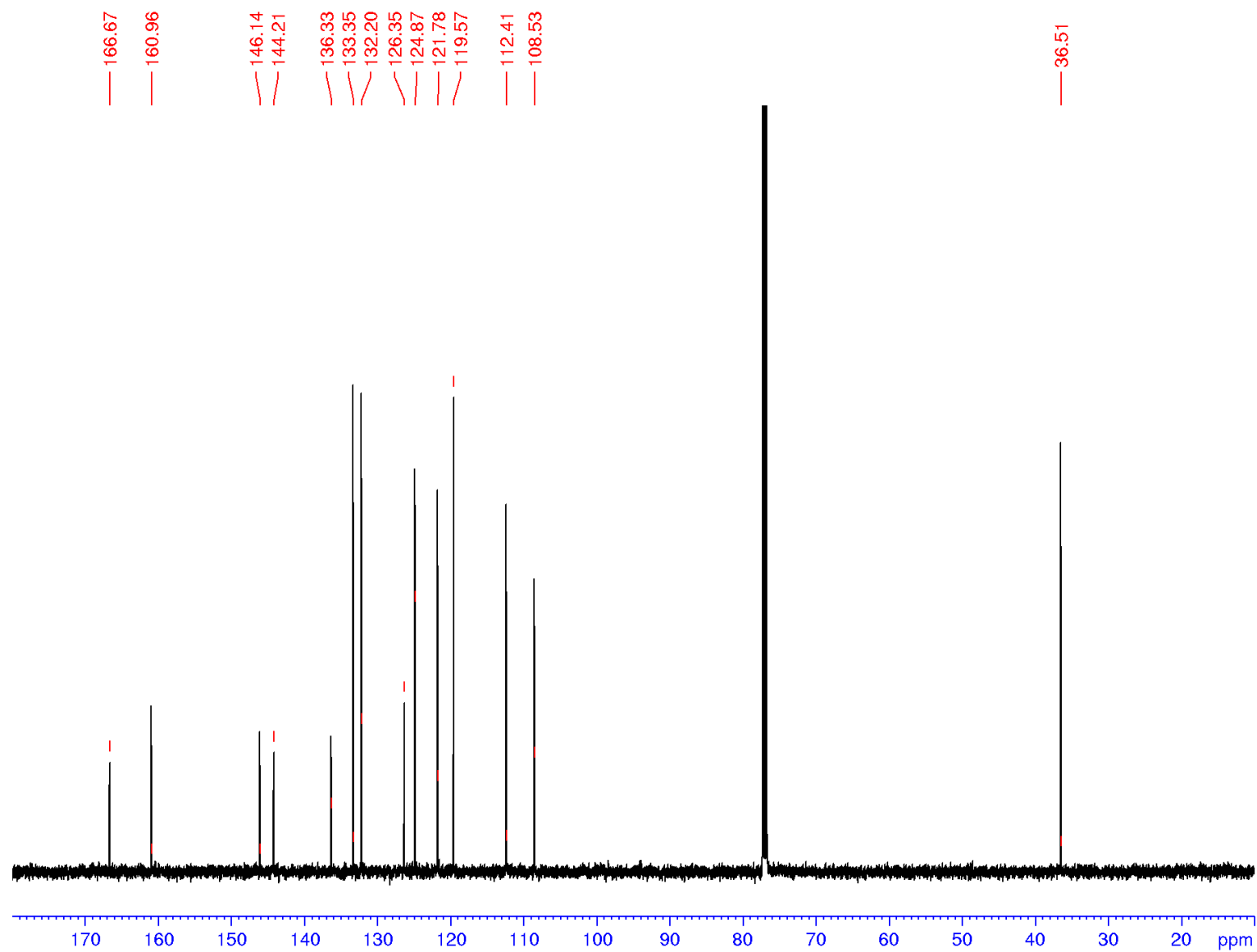
^{13}C NMR spectrum of **8** (125 MHz, $\text{d}_6\text{-DMSO}$)



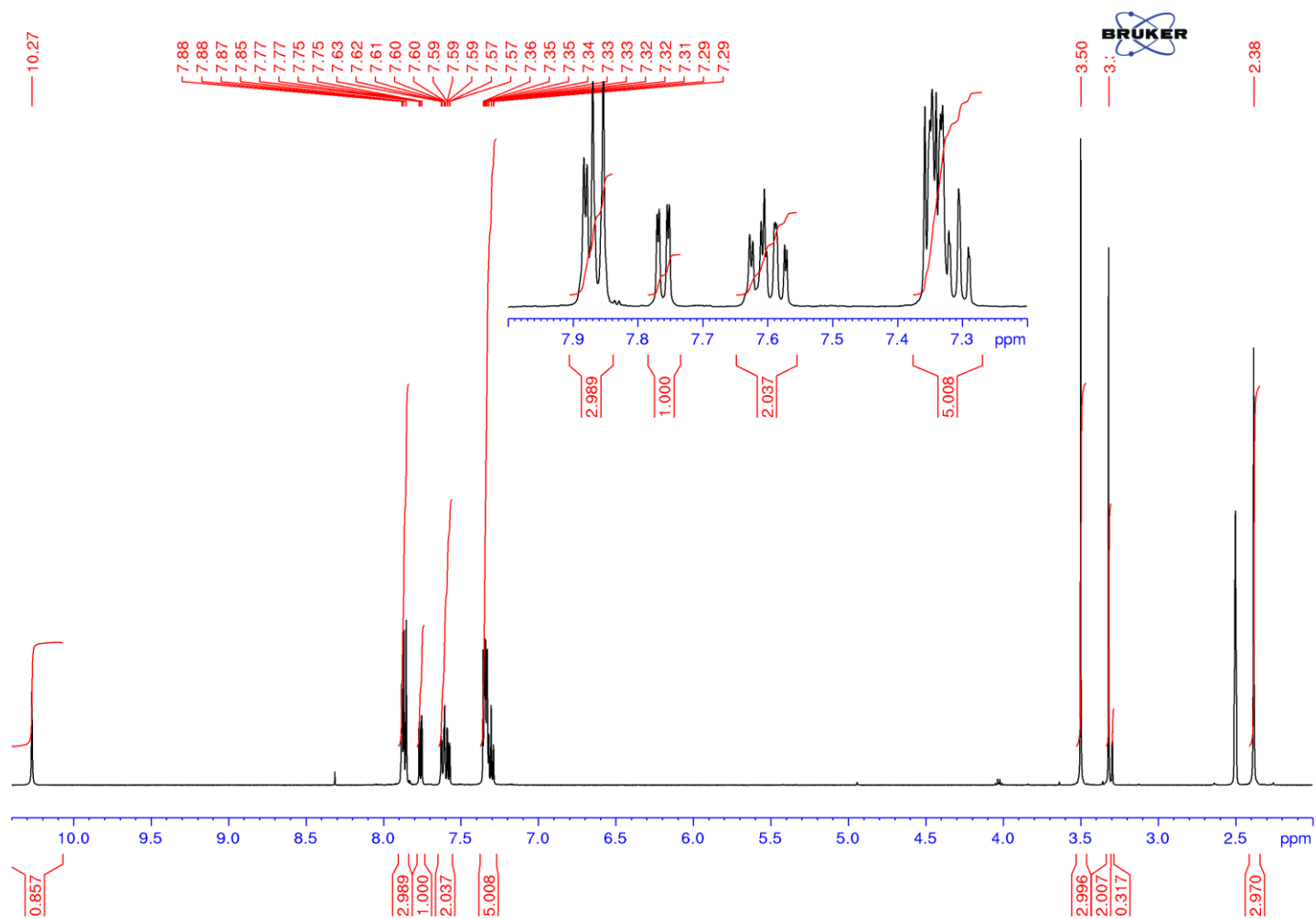
^1H NMR spectrum of **9** (400 MHz, CDCl_3)



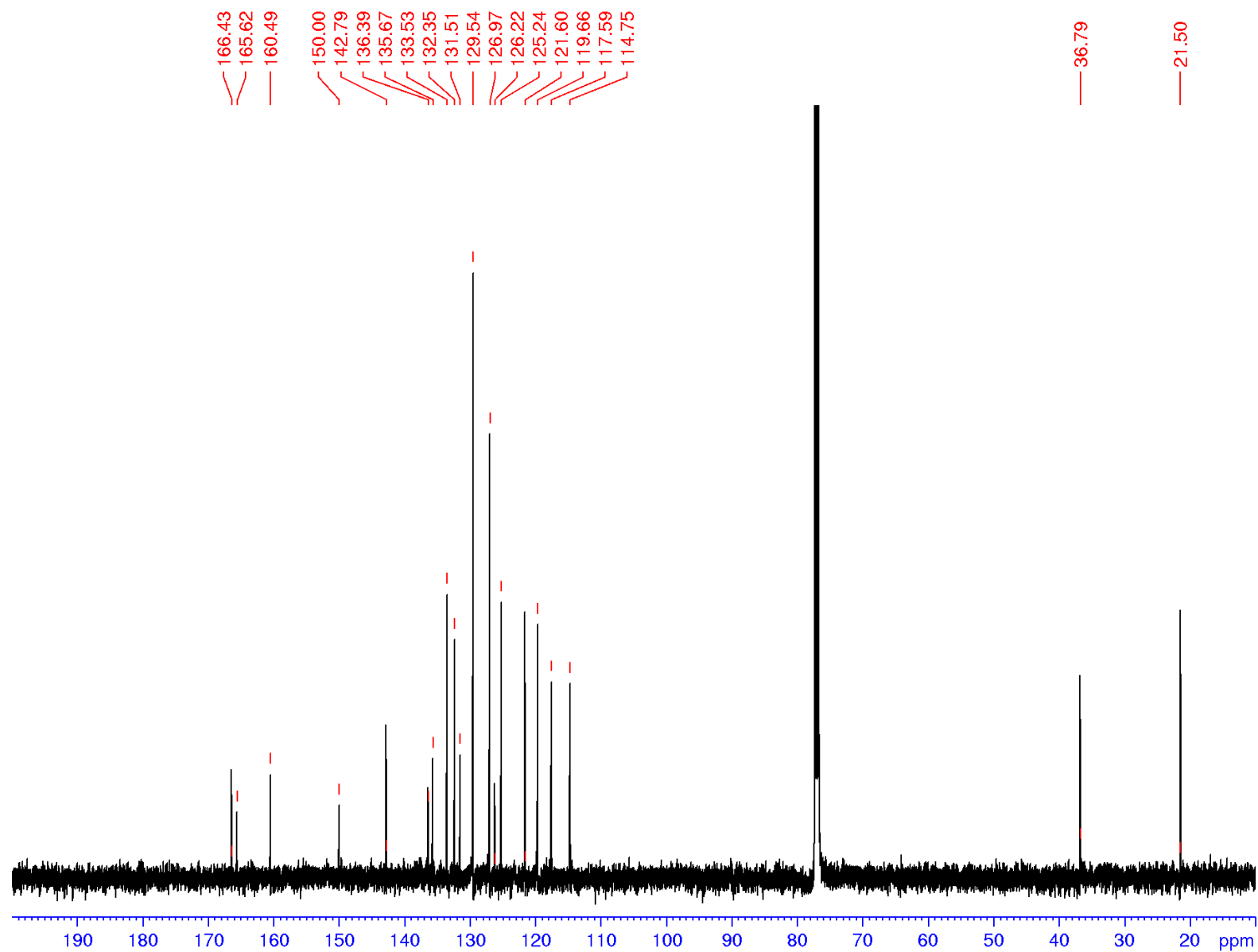
^{13}C NMR spectrum of **9** (125 MHz, CDCl_3)



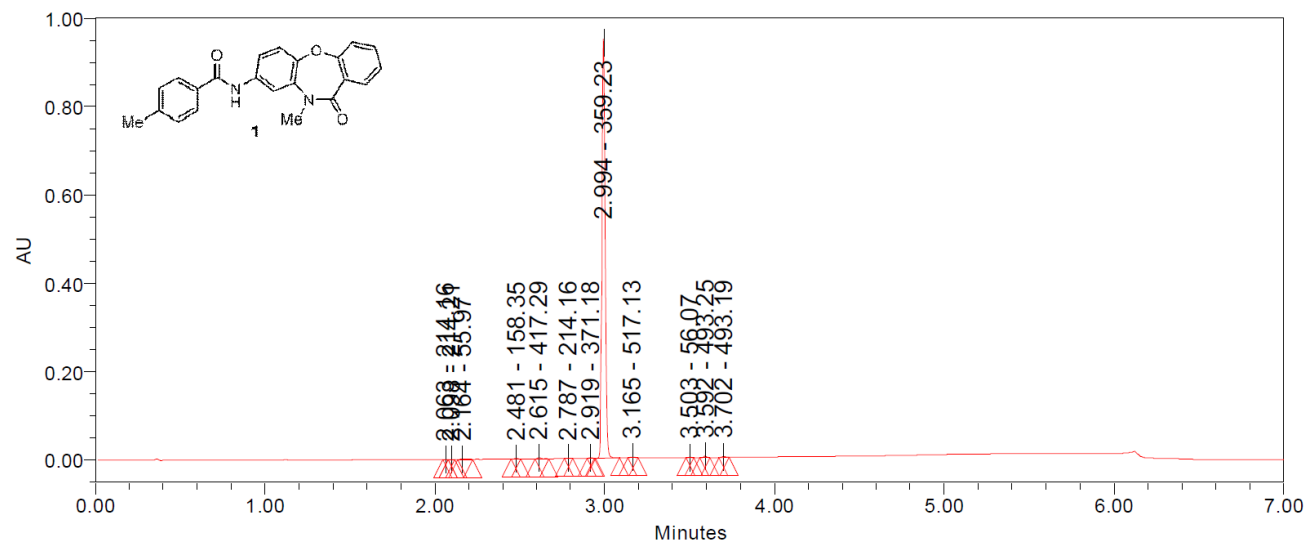
^1H NMR spectrum of **1** (500 MHz, CDCl_3)



^{13}C NMR spectrum of **1** (125 MHz, CDCl_3)



LCMS of 1

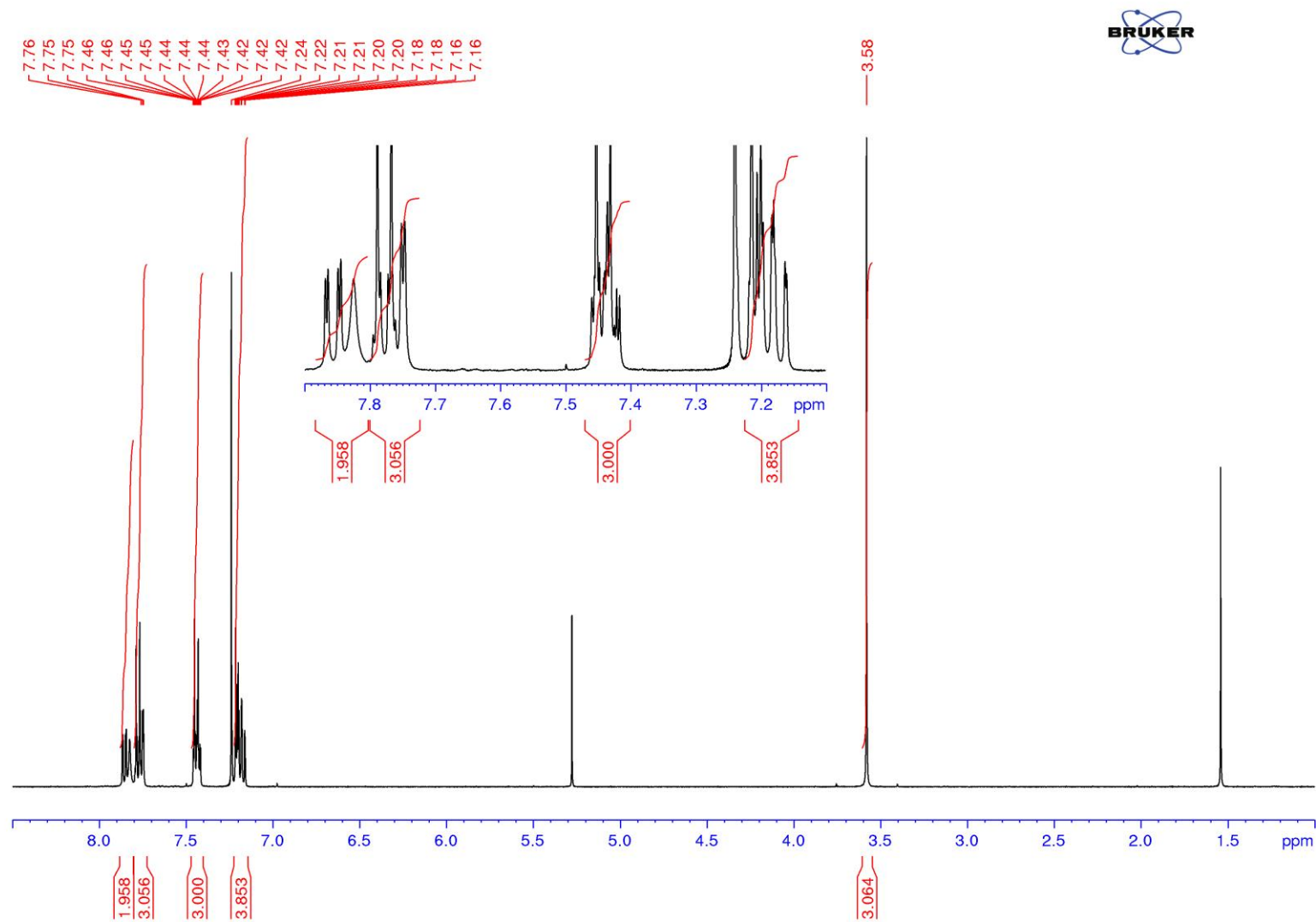


Peak Results

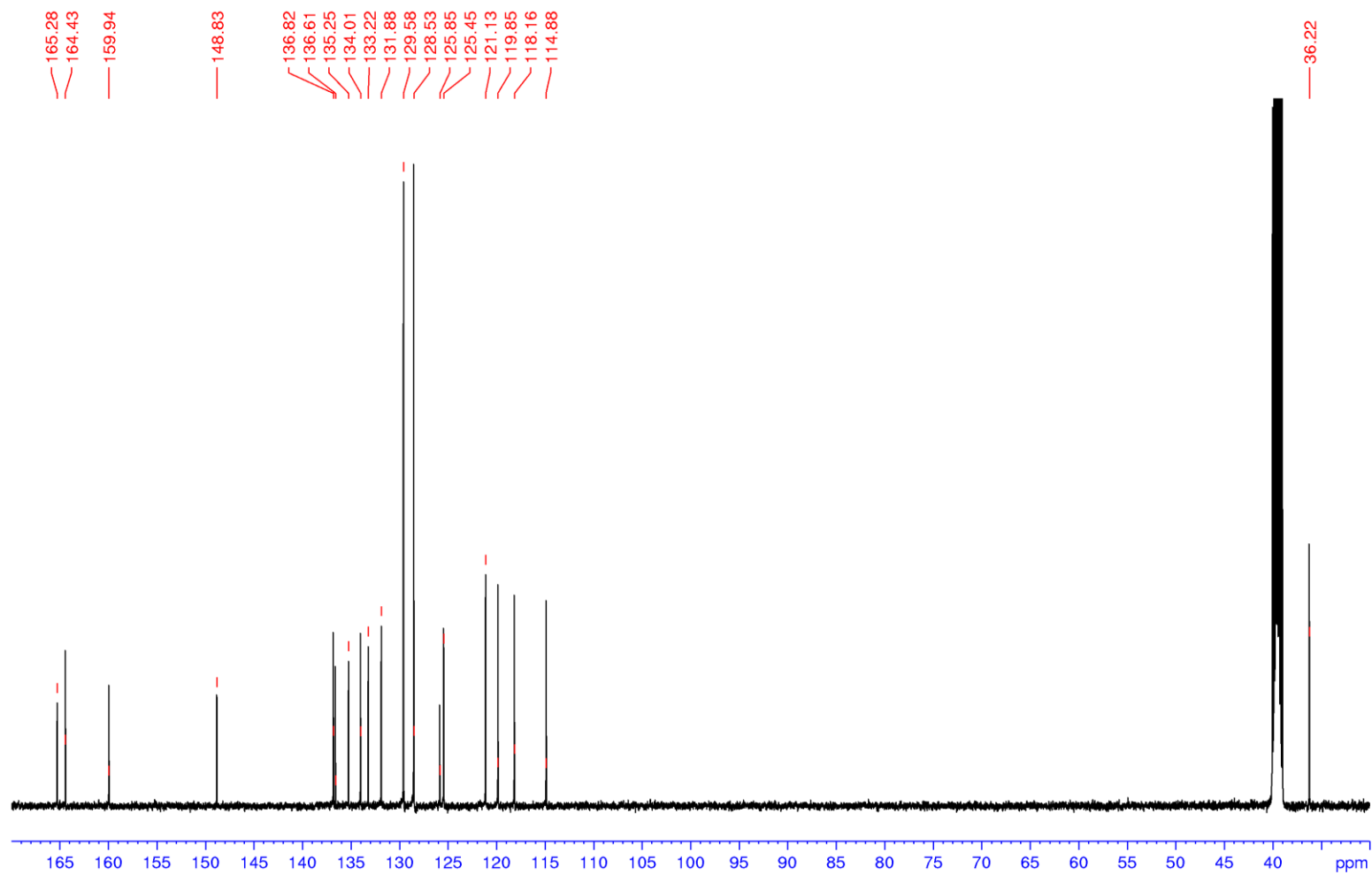
	RT	Area	% Area	Height	Base Peak (m/z)
1	2.063	214	0.02	218	214.16
2	2.098	374	0.03	337	214.21
3	2.164	1387	0.11	536	55.97
4	2.481	1786	0.14	1142	158.35
5	2.615	3417	0.27	2454	417.29
6	2.787	1161	0.09	900	214.16
7	2.919	2195	0.17	1807	371.18
8	2.994	1245743	98.28	946501	359.23
9	3.165	3735	0.29	1832	517.13

	RT	Area	% Area	Height	Base Peak (m/z)
10	3.503	961	0.08	809	56.07
11	3.592	3868	0.31	2980	493.25
12	3.702	2672	0.21	1967	493.19

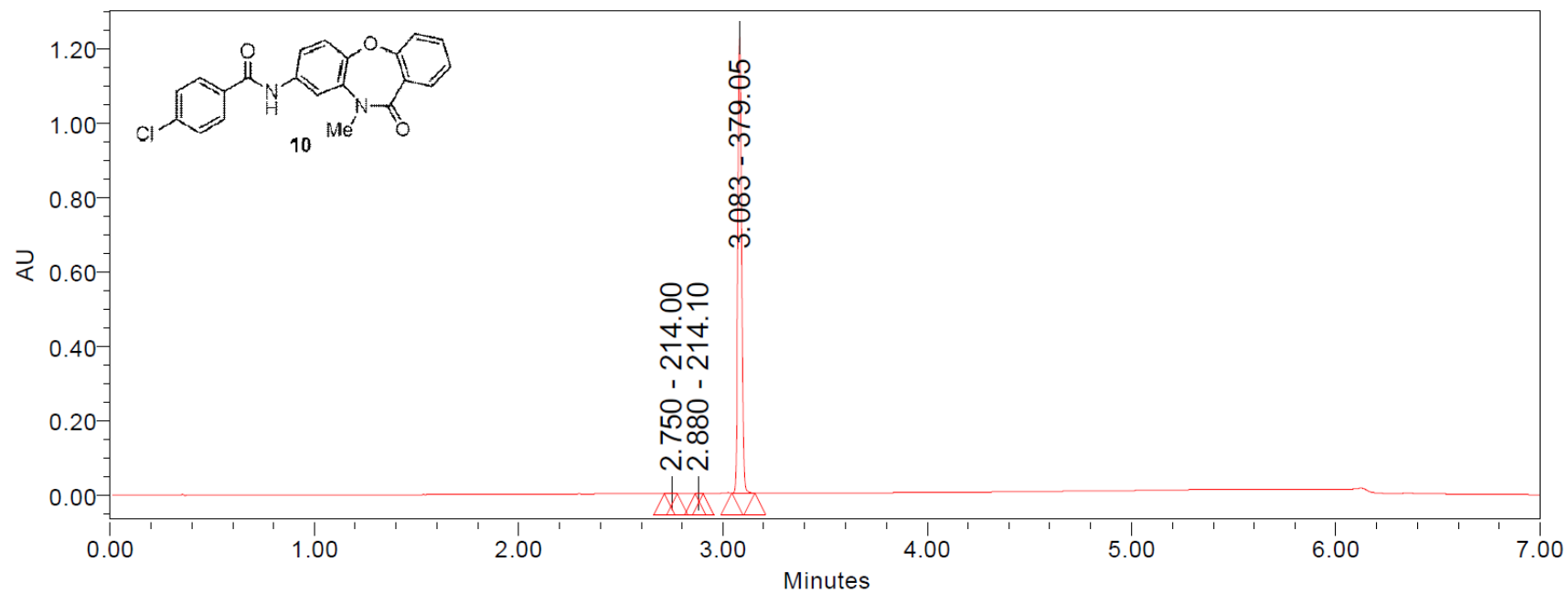
^1H NMR spectrum of **10** (400 MHz, CDCl_3)



^{13}C NMR spectrum of **10** (125 MHz, $\text{d}_6\text{-DMSO}$)



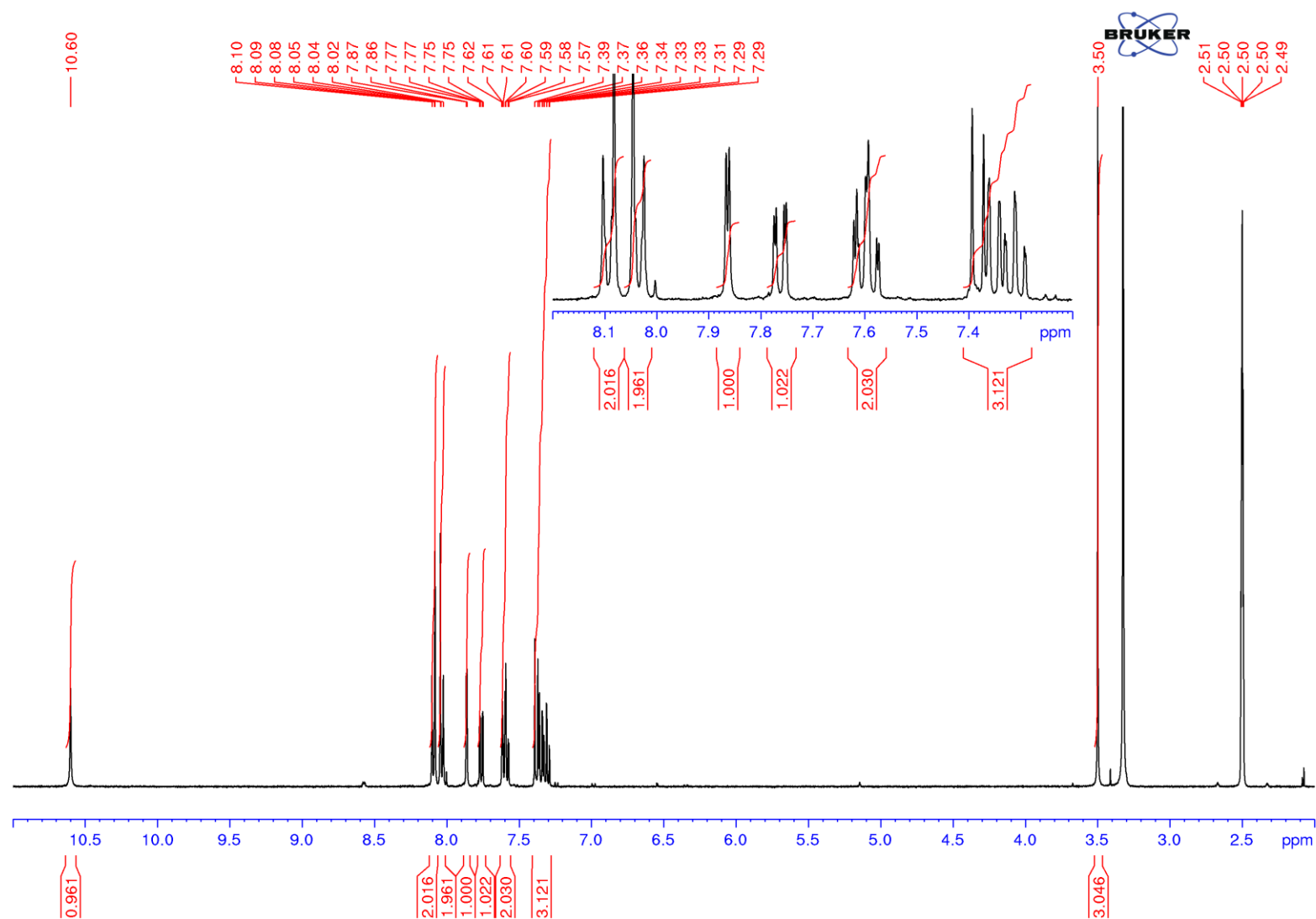
LCMS of **10**



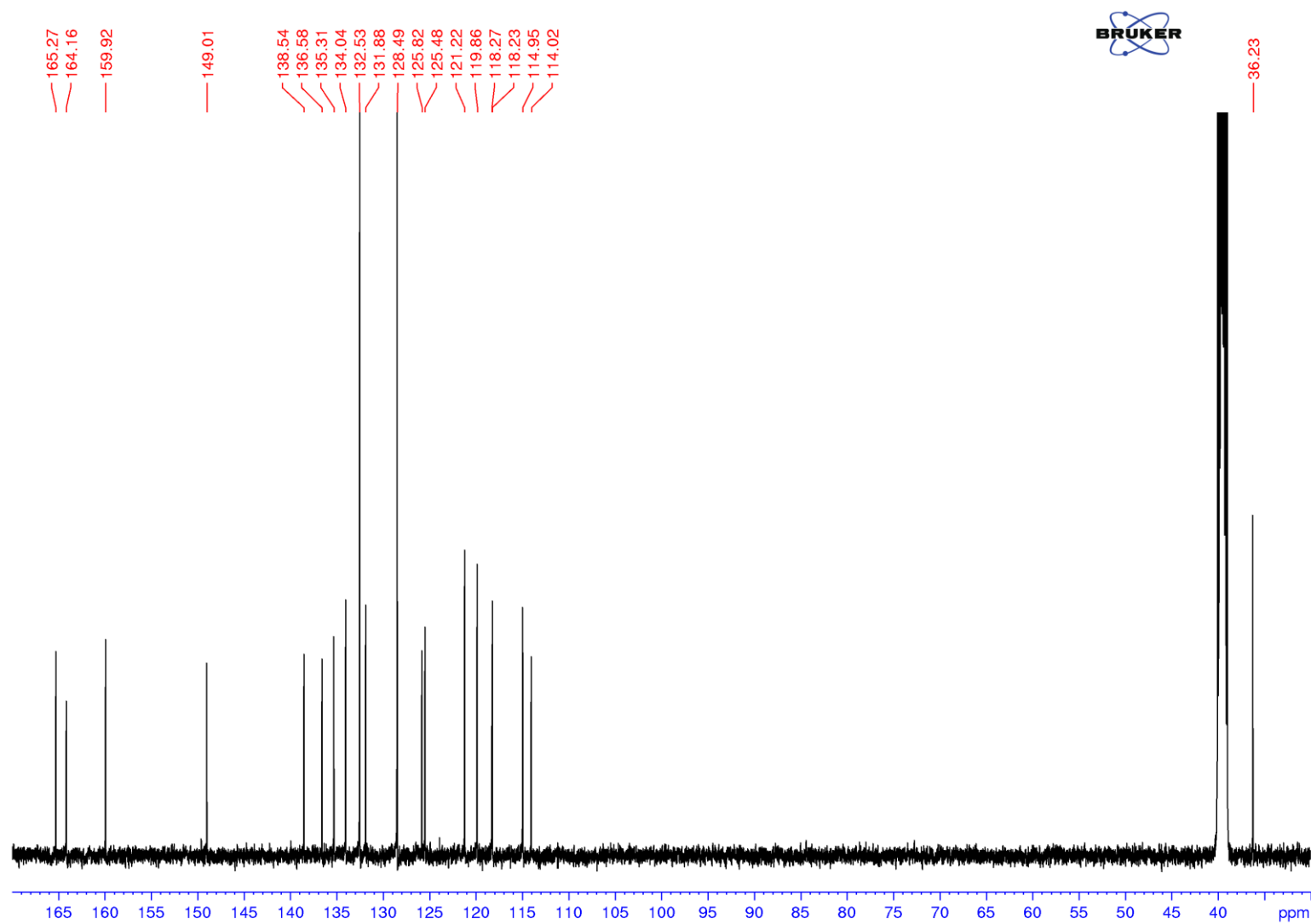
Peak Results

	RT	Area	% Area	Height	Base Peak (m/z)	Base Peak (Combined) (m/z)
1	2.750	1265	0.08	1008	214.00	60.01
2	2.880	456	0.03	428	214.10	56.01
3	3.083	1572979	99.89	1231774	379.05	379.04

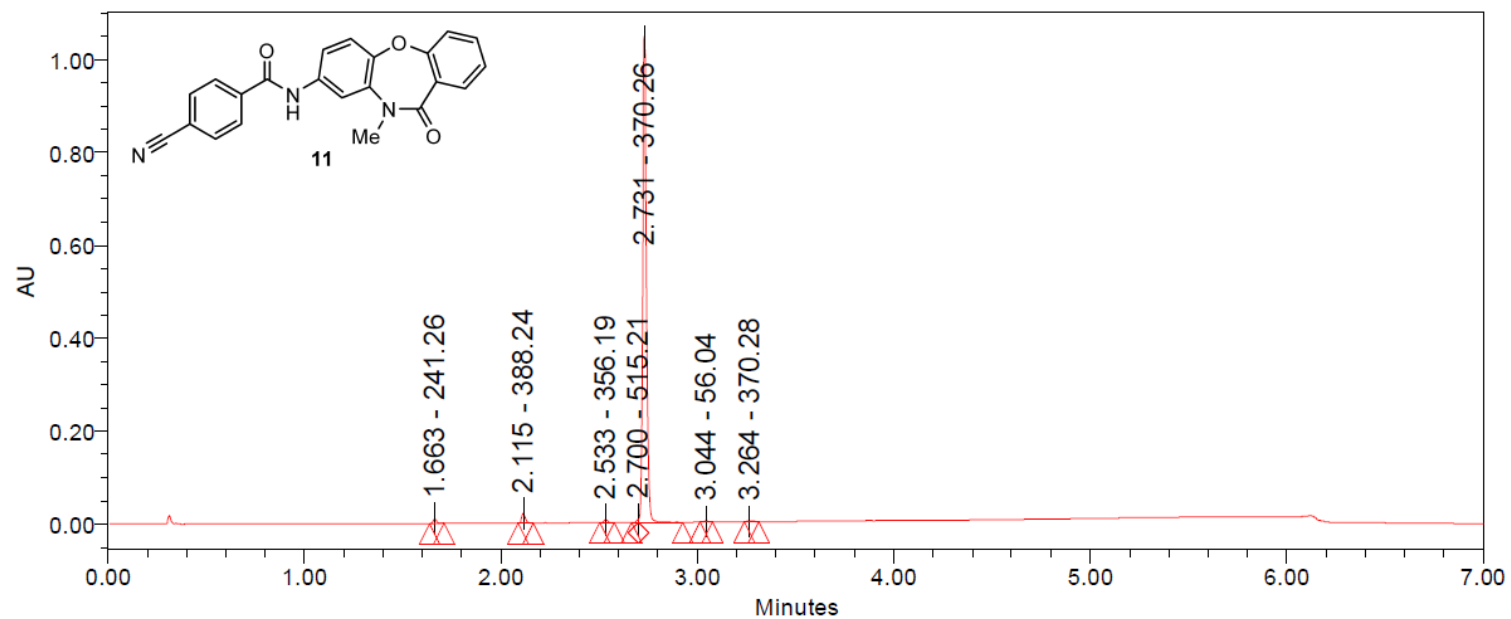
^1H NMR spectrum of **11** (400 MHz, $\text{d}_6\text{-DMSO}$)



^{13}C NMR spectrum of **11** (125 MHz, $\text{d}_6\text{-DMSO}$)



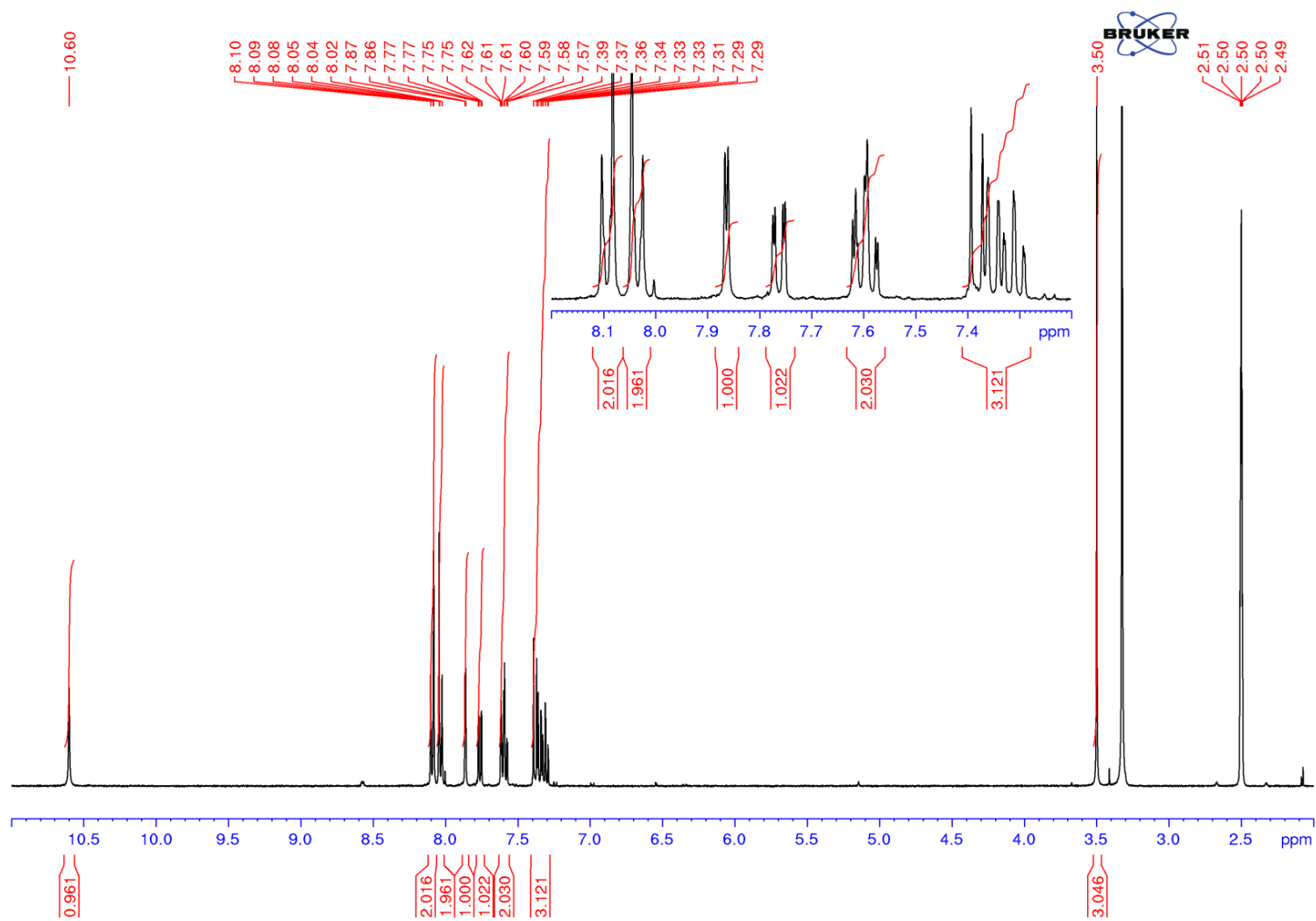
LCMS of 11



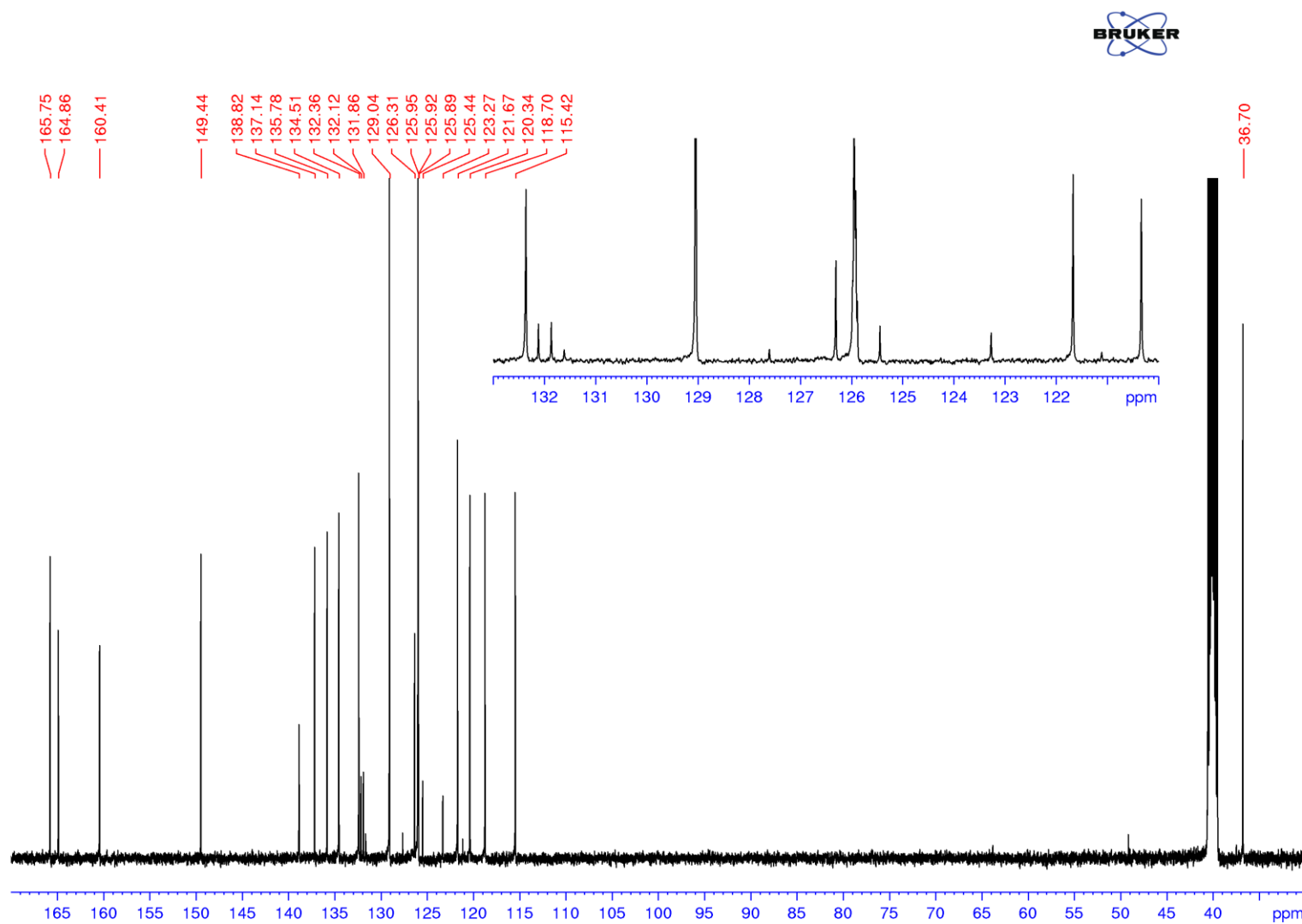
Peak Results

	RT	Area	% Area	Height	Base Peak (m/z)
1	1.663	12358	0.83	9934	241.26
2	2.115	26527	1.78	20580	388.24
3	2.533	8937	0.60	6736	356.19
4	2.700	4109	0.28	6995	515.21
5	2.731	1432494	96.13	1044503	370.26
6	3.044	2741	0.18	2036	56.04
7	3.264	3068	0.21	1435	370.28

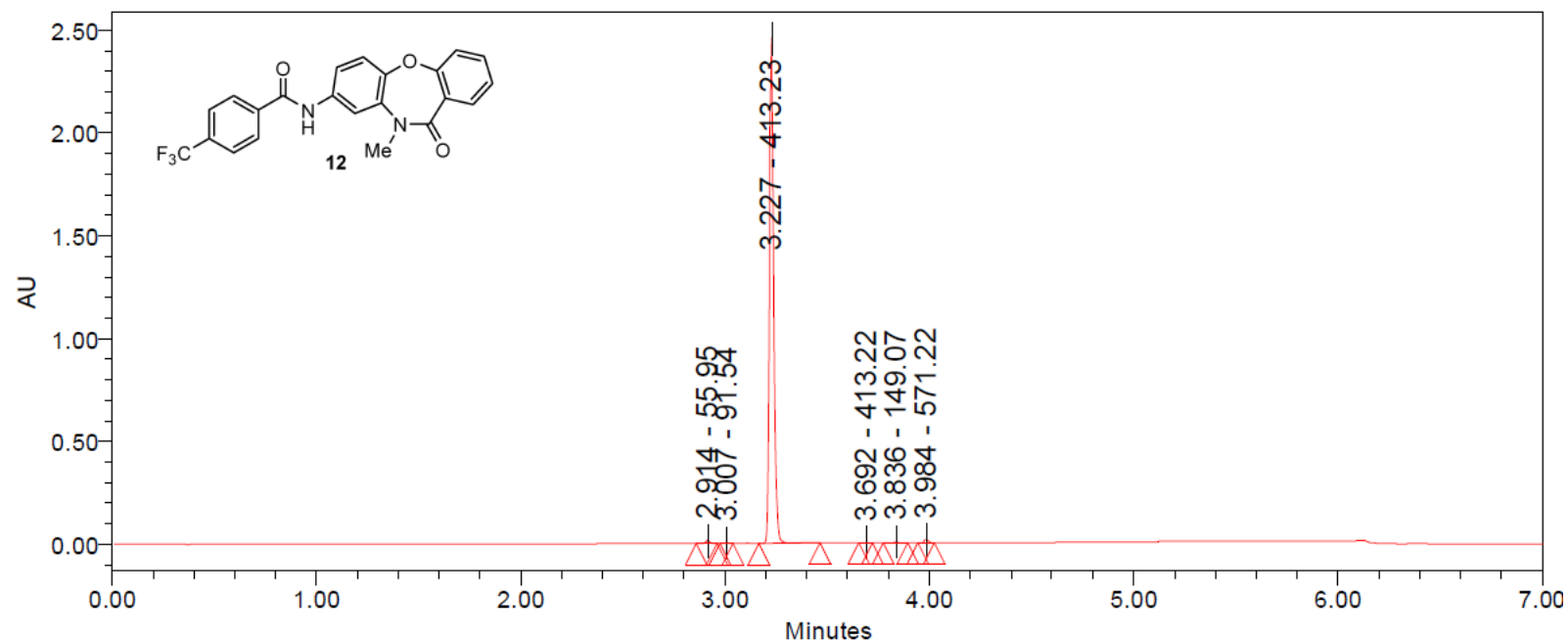
^1H NMR spectrum of **12** (500 MHz, d_6 -DMSO)



^{13}C NMR spectrum of **12** (125 MHz, $\text{d}_6\text{-DMSO}$)



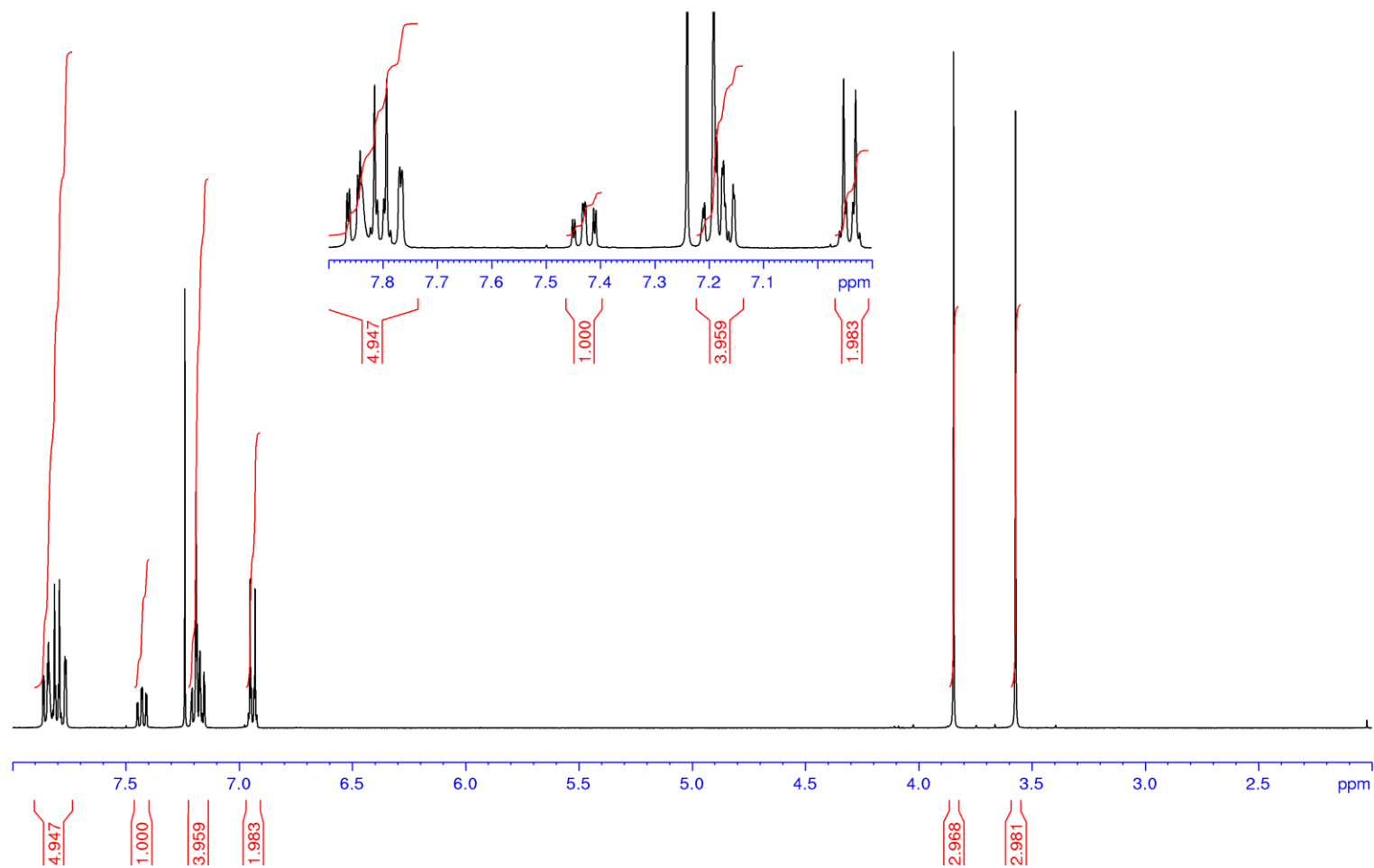
LCMS of 12



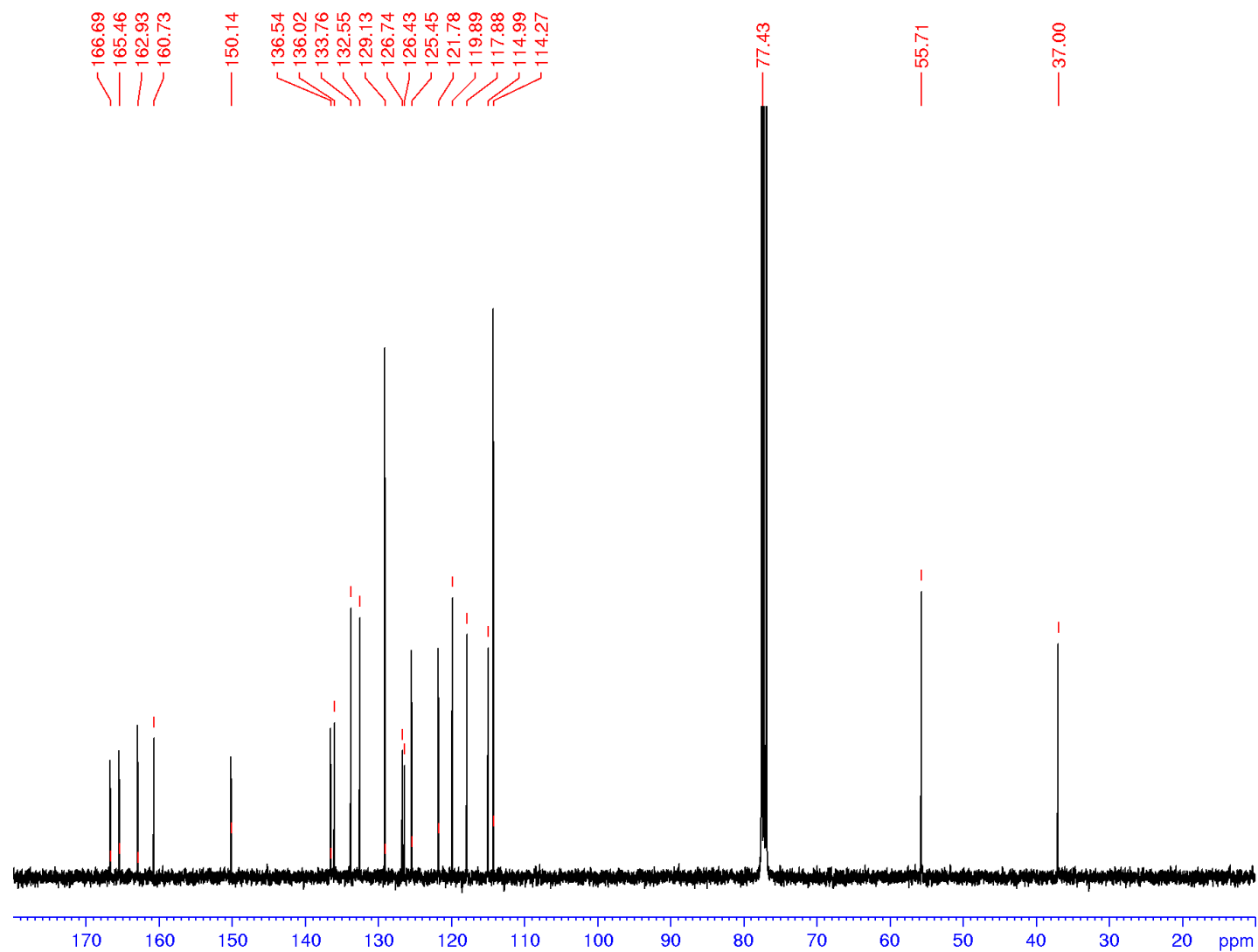
Peak Results

	RT	Area	% Area	Height	Base Peak (m/z)
1	2.914	19258	0.51	12459	55.95
2	3.007	2858	0.08	2069	91.54
3	3.227	3727585	98.53	2453669	413.23
4	3.692	3420	0.09	2498	413.22
5	3.836	8950	0.24	5422	149.07
6	3.984	21030	0.56	15375	571.22

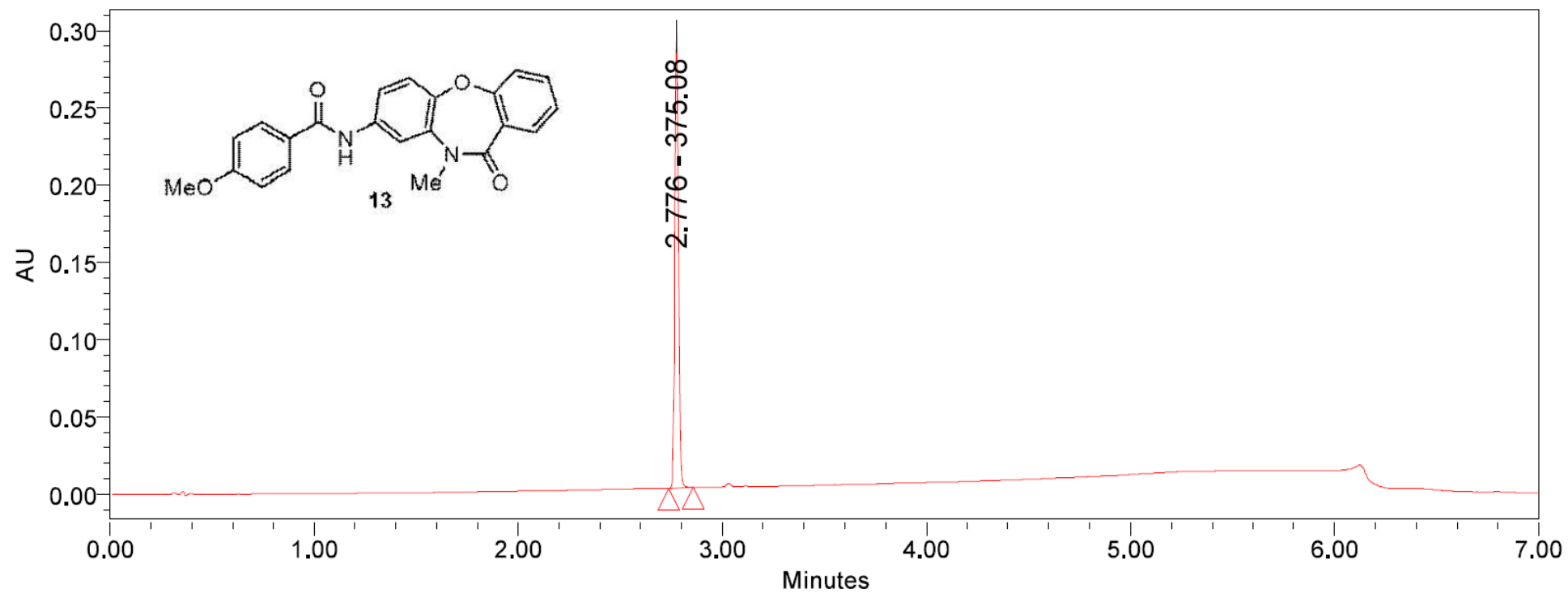
^1H NMR spectrum of **13** (400 MHz, CDCl_3)



^{13}C NMR spectrum of **13** (100 MHz, CDCl_3)



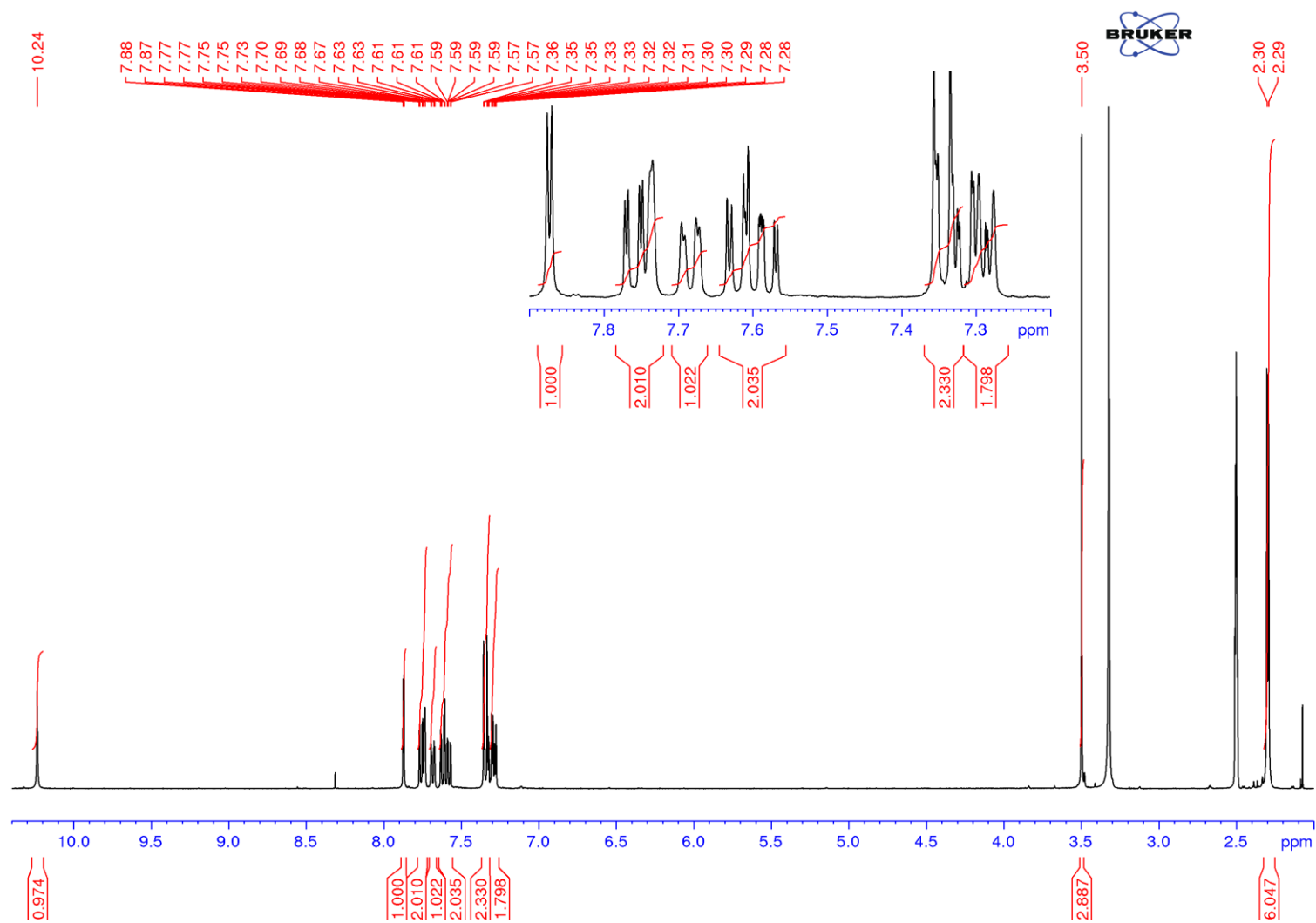
LCMS of **13**



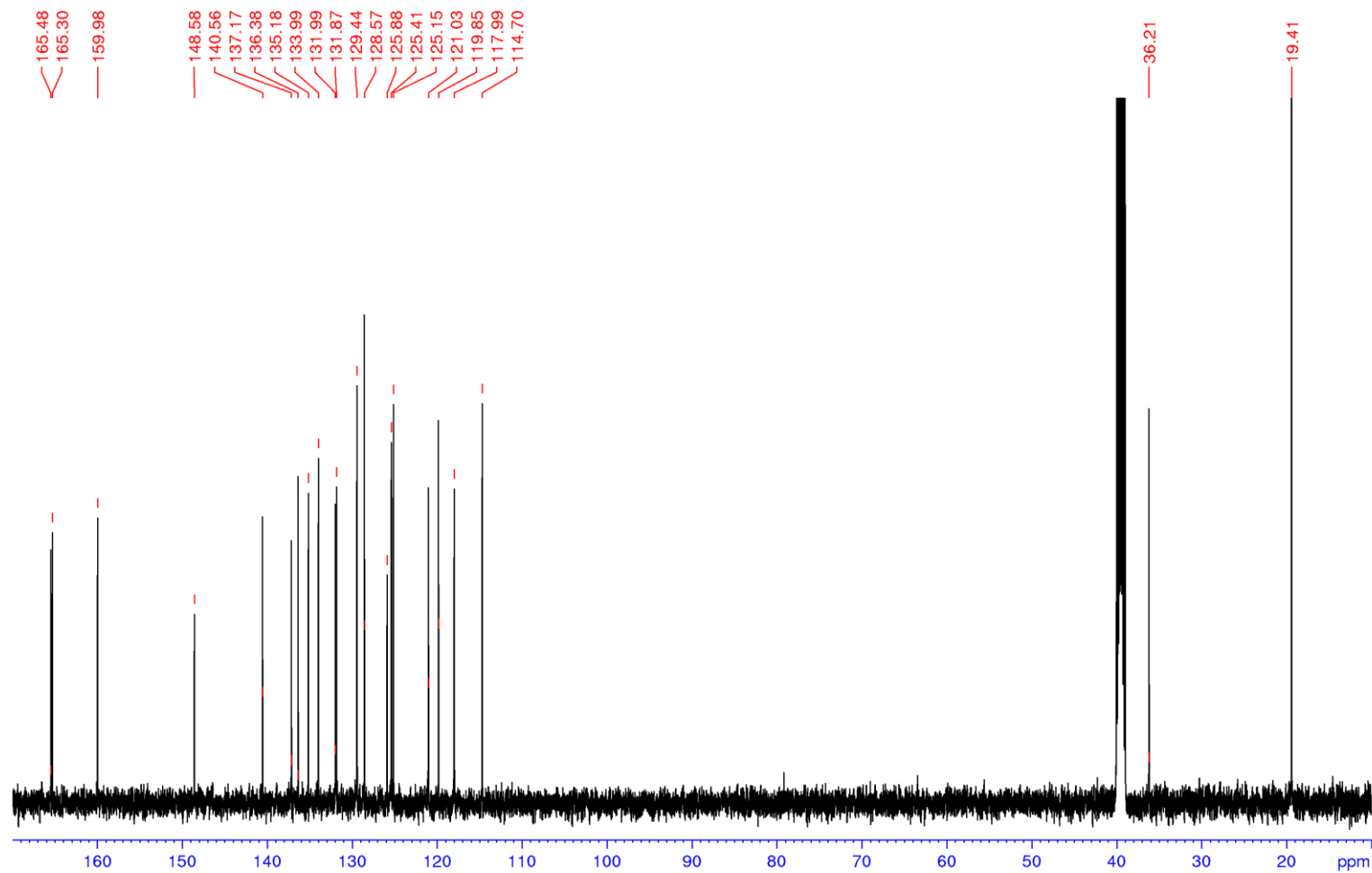
Peak Results

	RT	Area	% Area	Height	Base Peak (m/z)	Base Peak (Combined) (m/z)
1	2.776	367562	100.00	293055	375.08	375.09

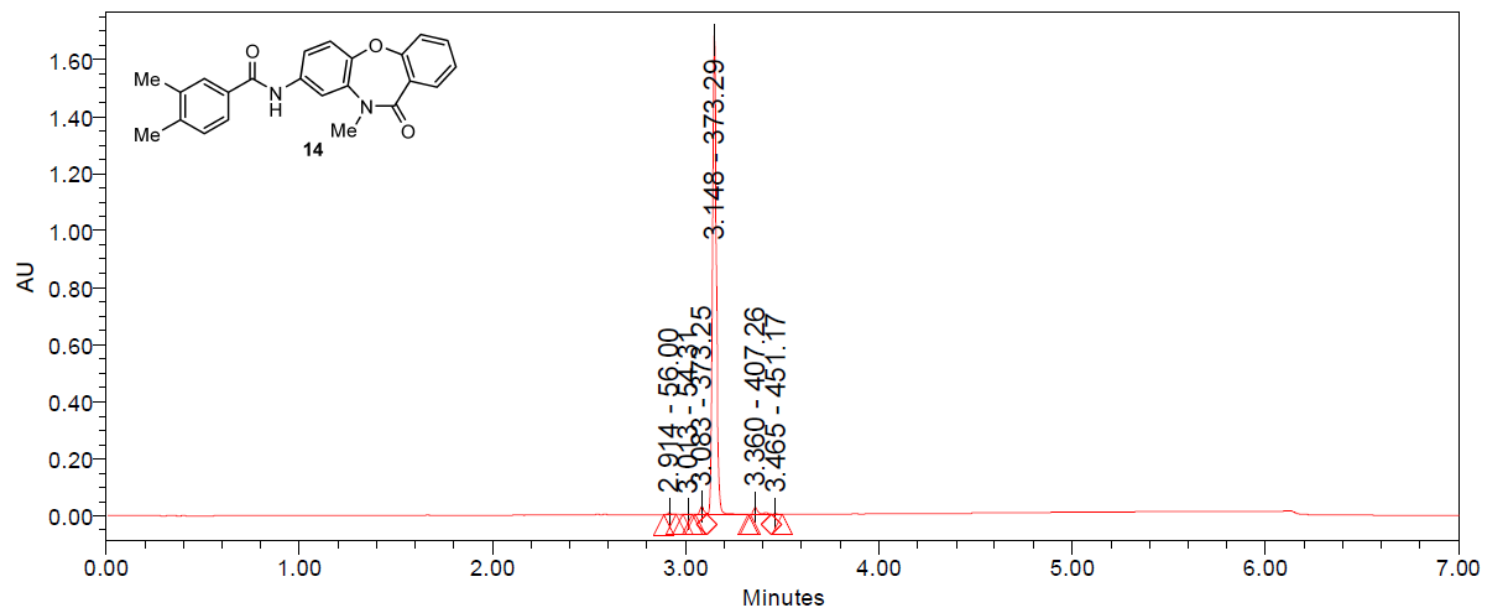
^1H NMR spectrum of **14** (400 MHz, $\text{d}_6\text{-DMSO}$)



^{13}C NMR spectrum of **14** (125 MHz, $\text{d}_6\text{-DMSO}$)



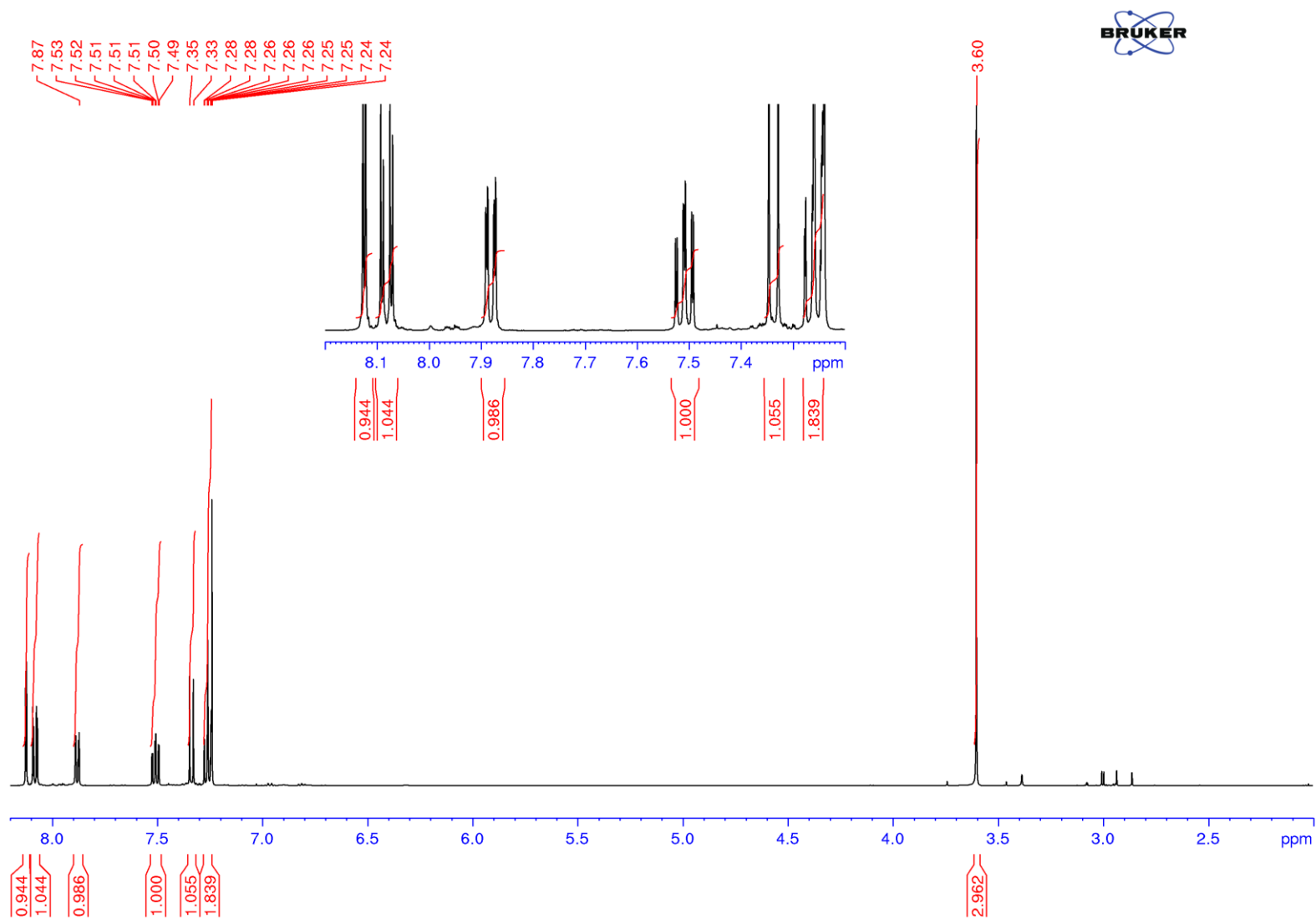
LCMS of **14**



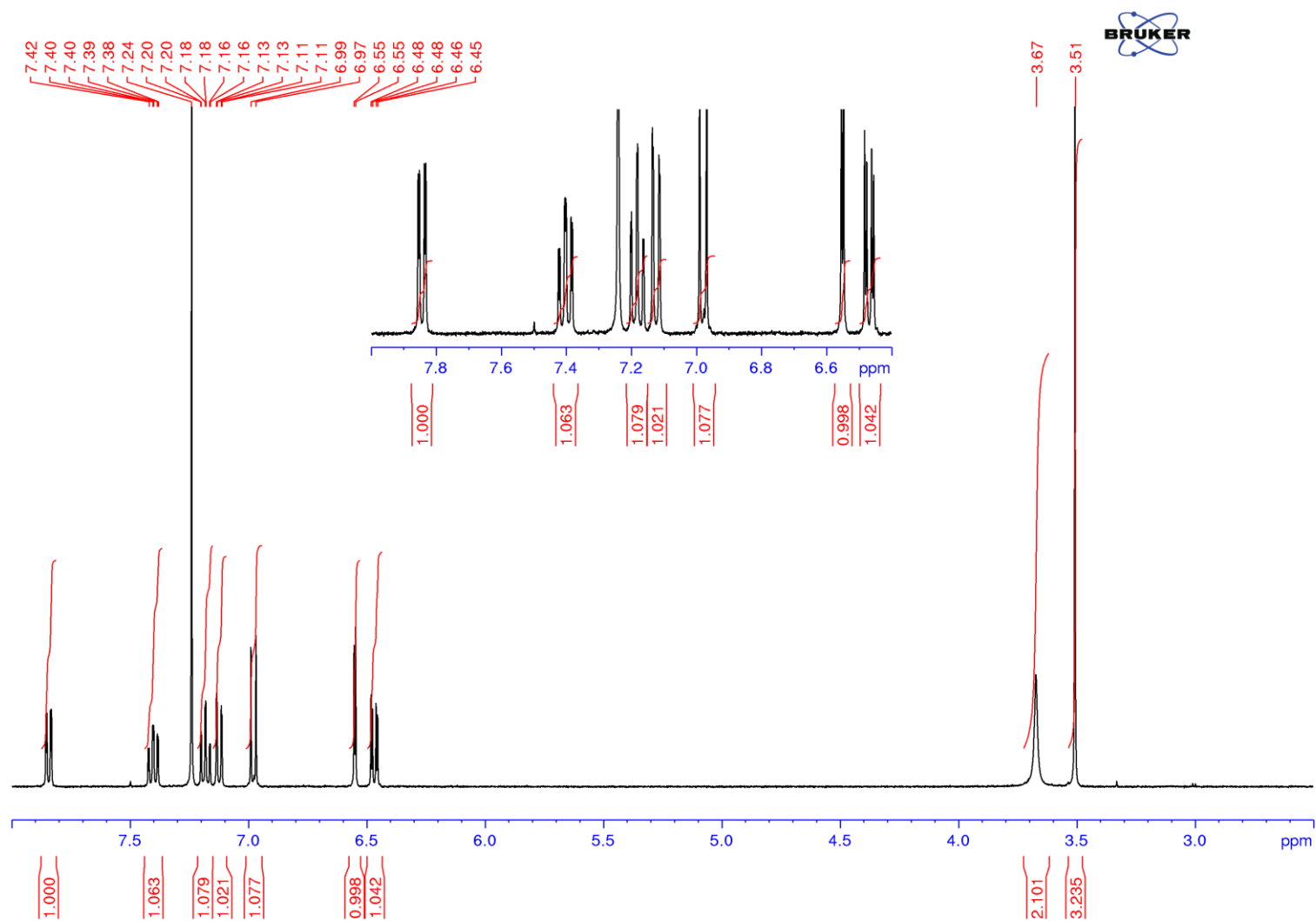
Peak Results

	RT	Area	% Area	Height	Base Peak (m/z)
1	2.914	8701	0.35	6505	56.00
2	3.013	1766	0.07	1365	54.31
3	3.083	39067	1.57	27988	373.25
4	3.148	2390958	96.16	1681987	373.29
5	3.360	42346	1.70	24075	407.26
6	3.465	3684	0.15	2587	451.17

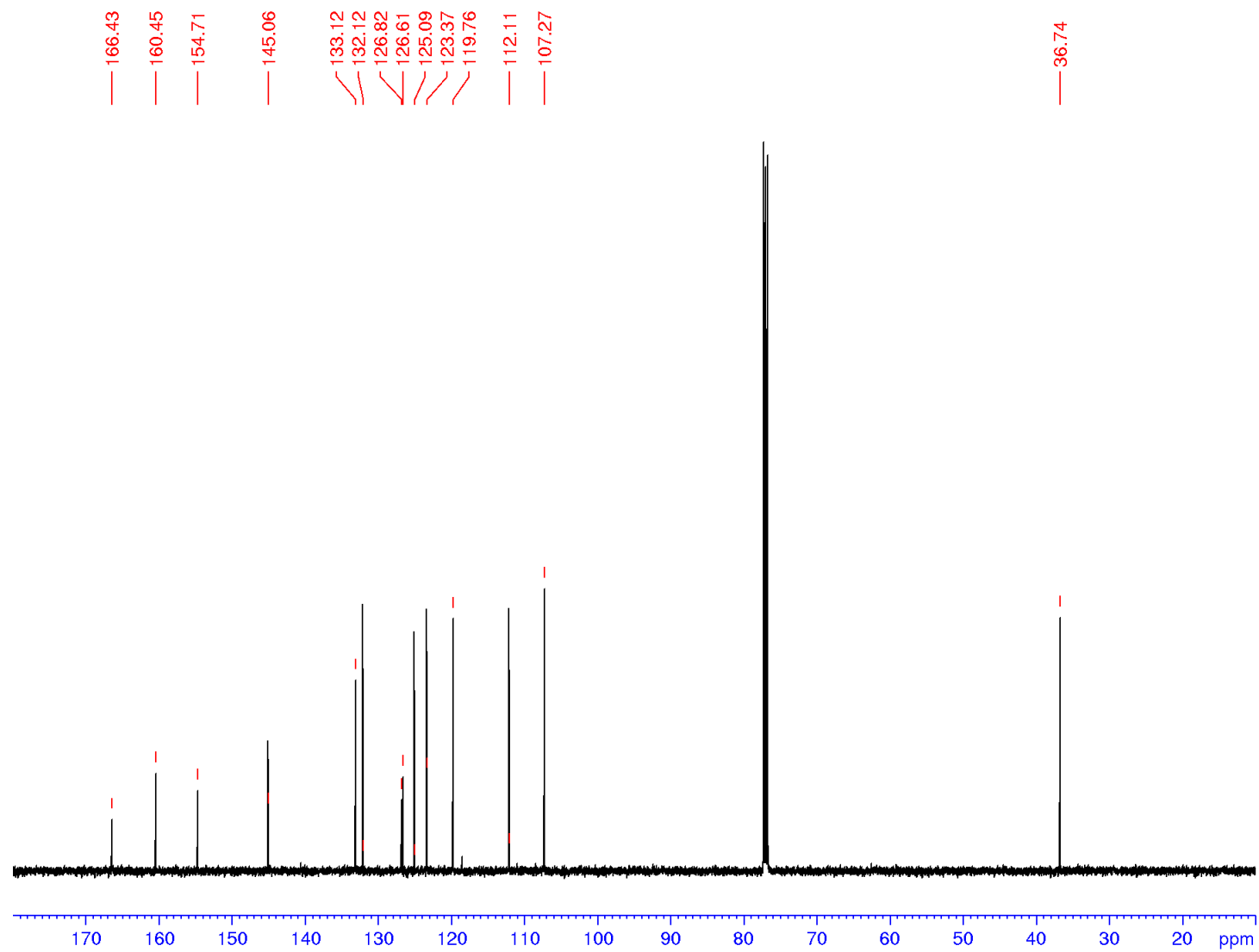
^1H NMR spectrum of **16** (500 MHz, CDCl_3)



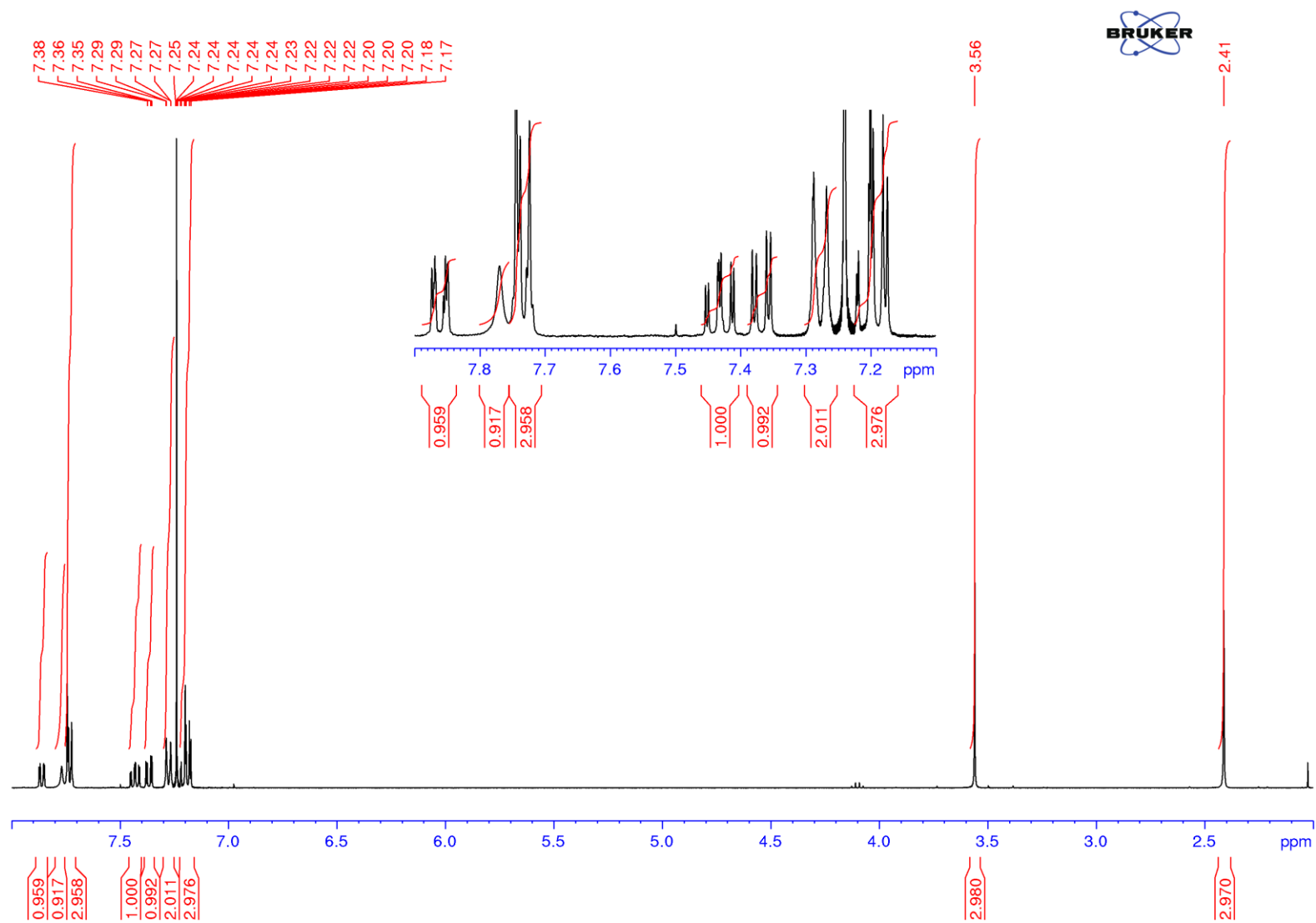
^1H NMR spectrum of **17** (400 MHz, CDCl_3)



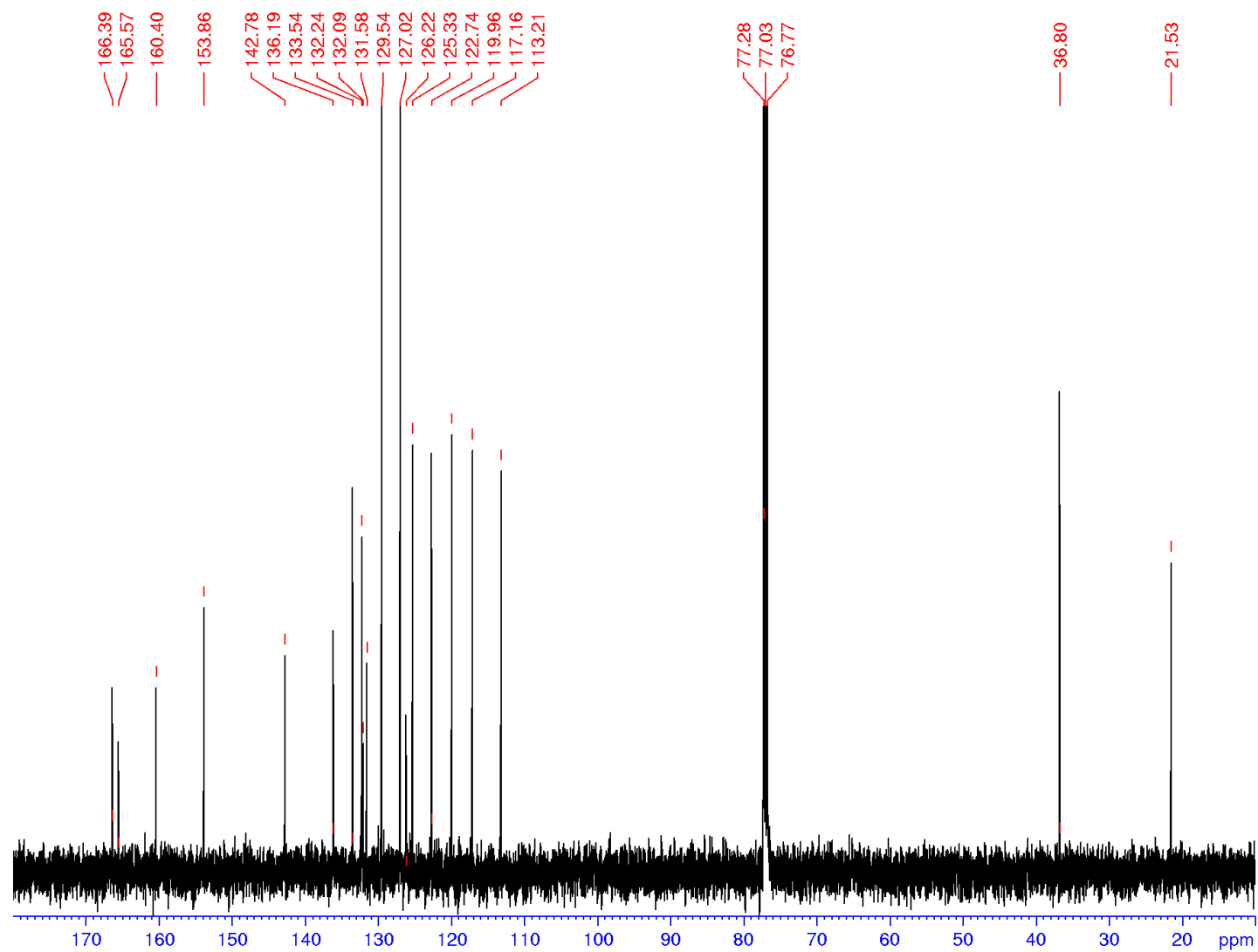
^{13}C NMR spectrum of **17** (125 MHz, CDCl_3)



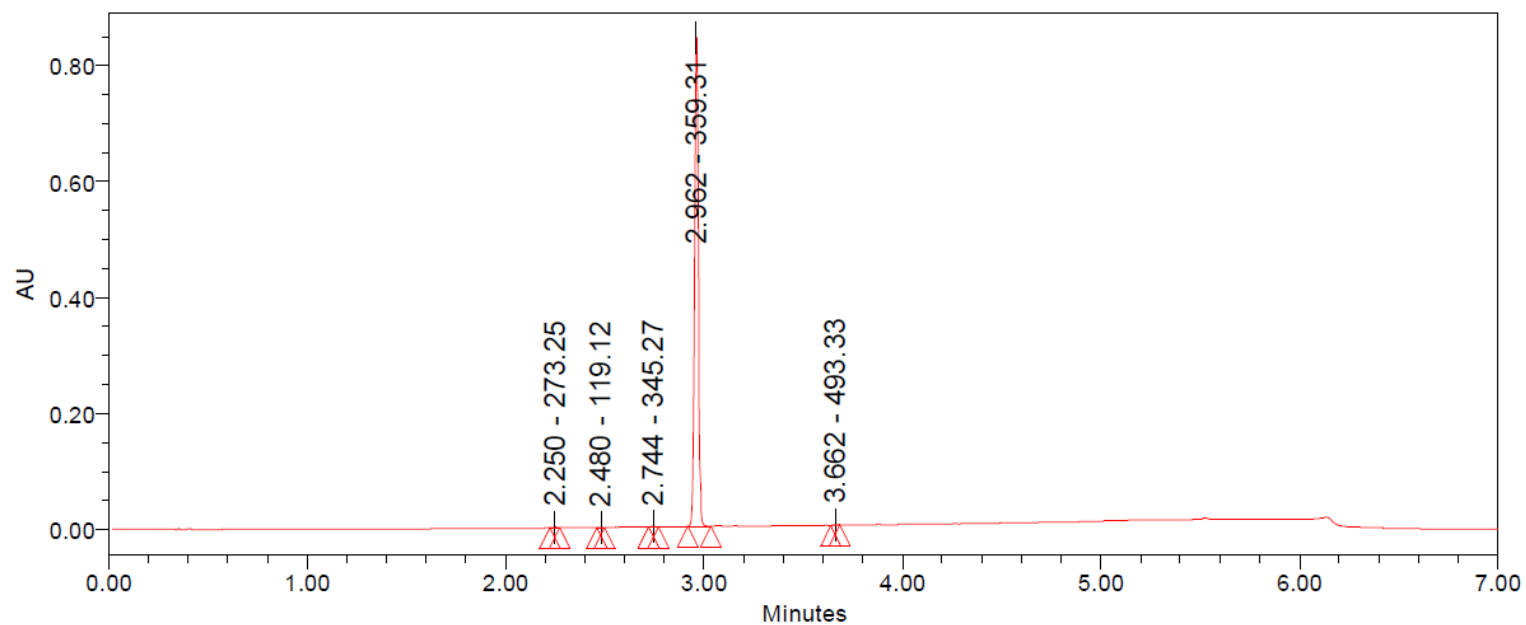
^1H NMR spectrum of **2** (400 MHz, CDCl_3)



^{13}C NMR spectrum of **2** (125 MHz, CDCl_3)



LCMS of 2



Peak Results

	RT	Area	% Area	Height	Base Peak (m/z)
1	2.250	1438	0.13	1098	273.25
2	2.480	288	0.03	249	119.12
3	2.744	1093	0.10	881	345.27
4	2.962	1124753	99.64	851336	359.31
5	3.662	1299	0.12	1059	493.33

^1H NMR spectrum of **SN00797640** (400 MHz, CDCl_3)

