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Supporting Information

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Glycosyl Triazole based Pyridinamide/ CuI Catalyzed Coupling of 2-Halobenzamides with Active Methylene Compounds

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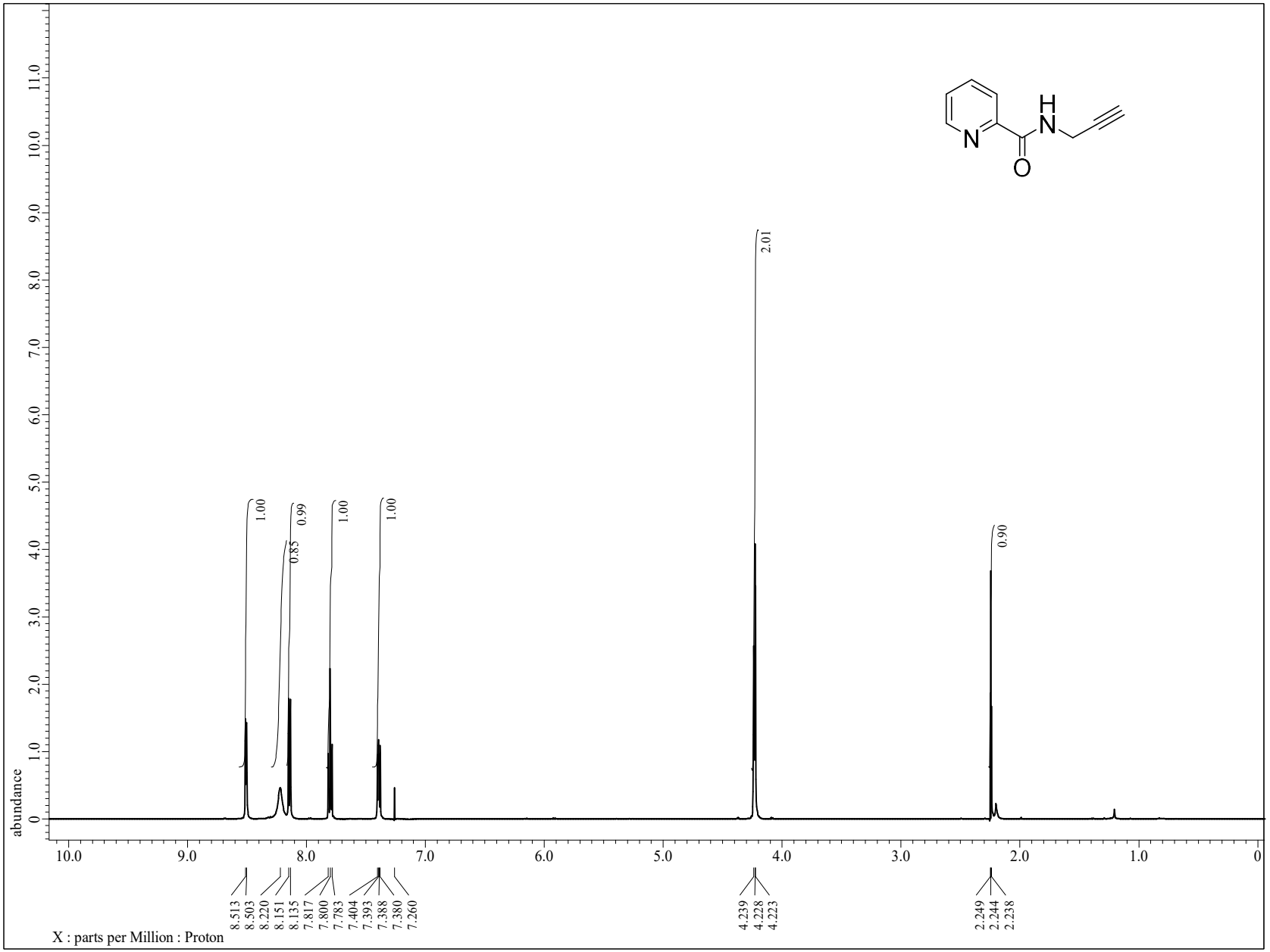

Figure S1: ^{1}H NMR (500 MHz,$CDCl_3$) of compound **1**

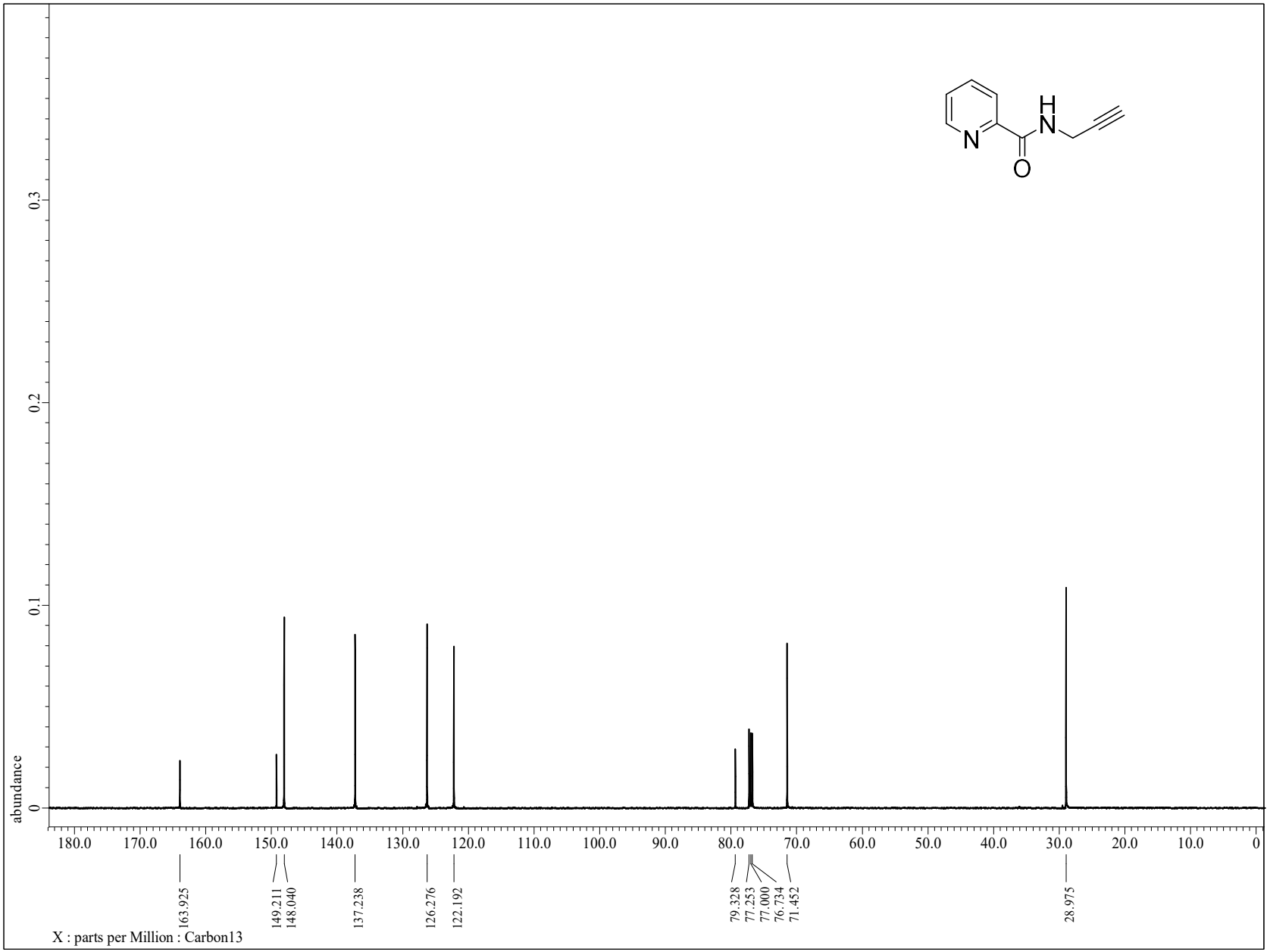

Figure S2: $^{13}C\{^{1}H\}$ NMR (125 MHz, $CDCl_3$) of compound **1**

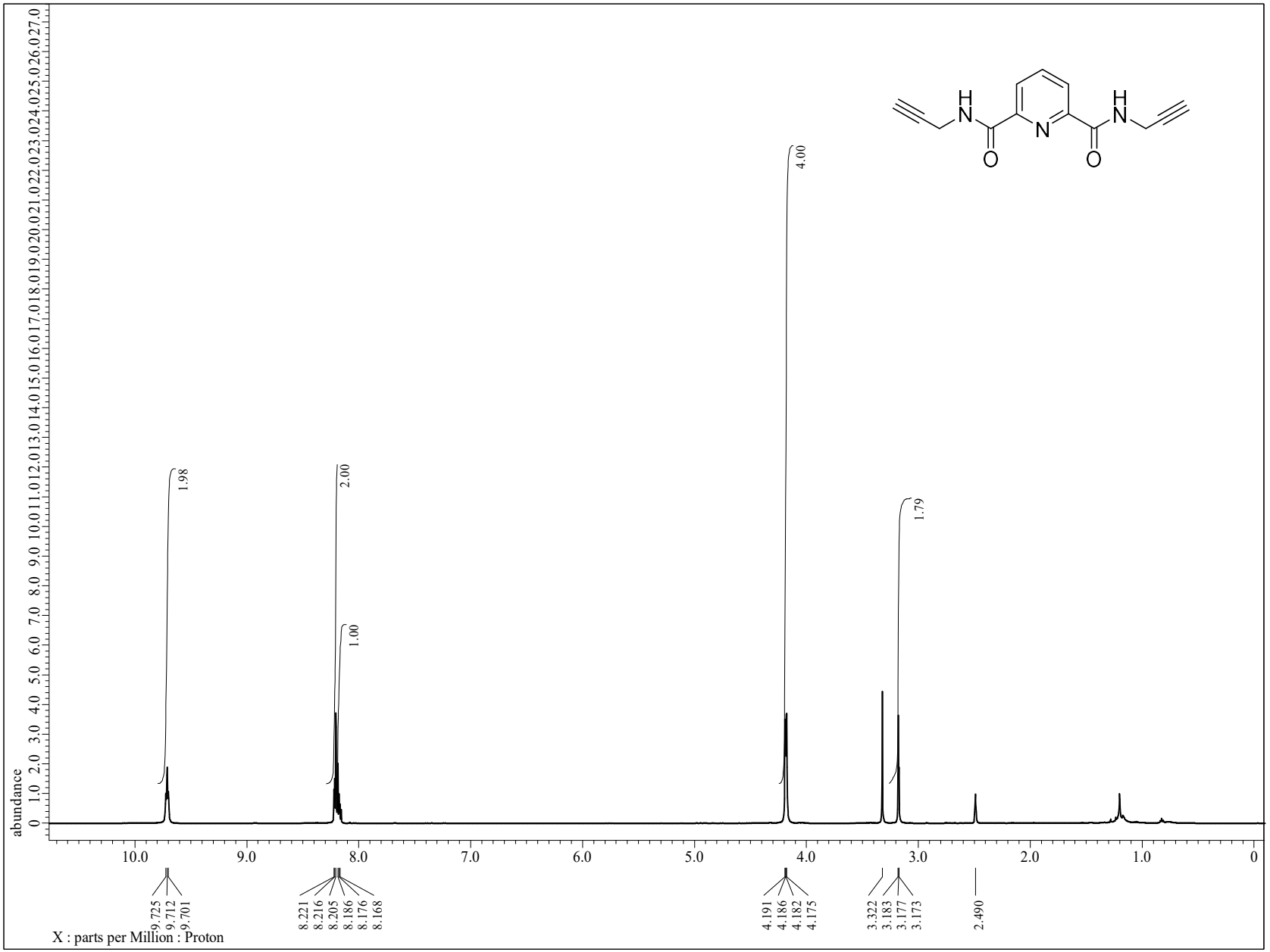

Figure S3: ^{1}H NMR (500 MHz, DMSO-d_6) of compound **2**

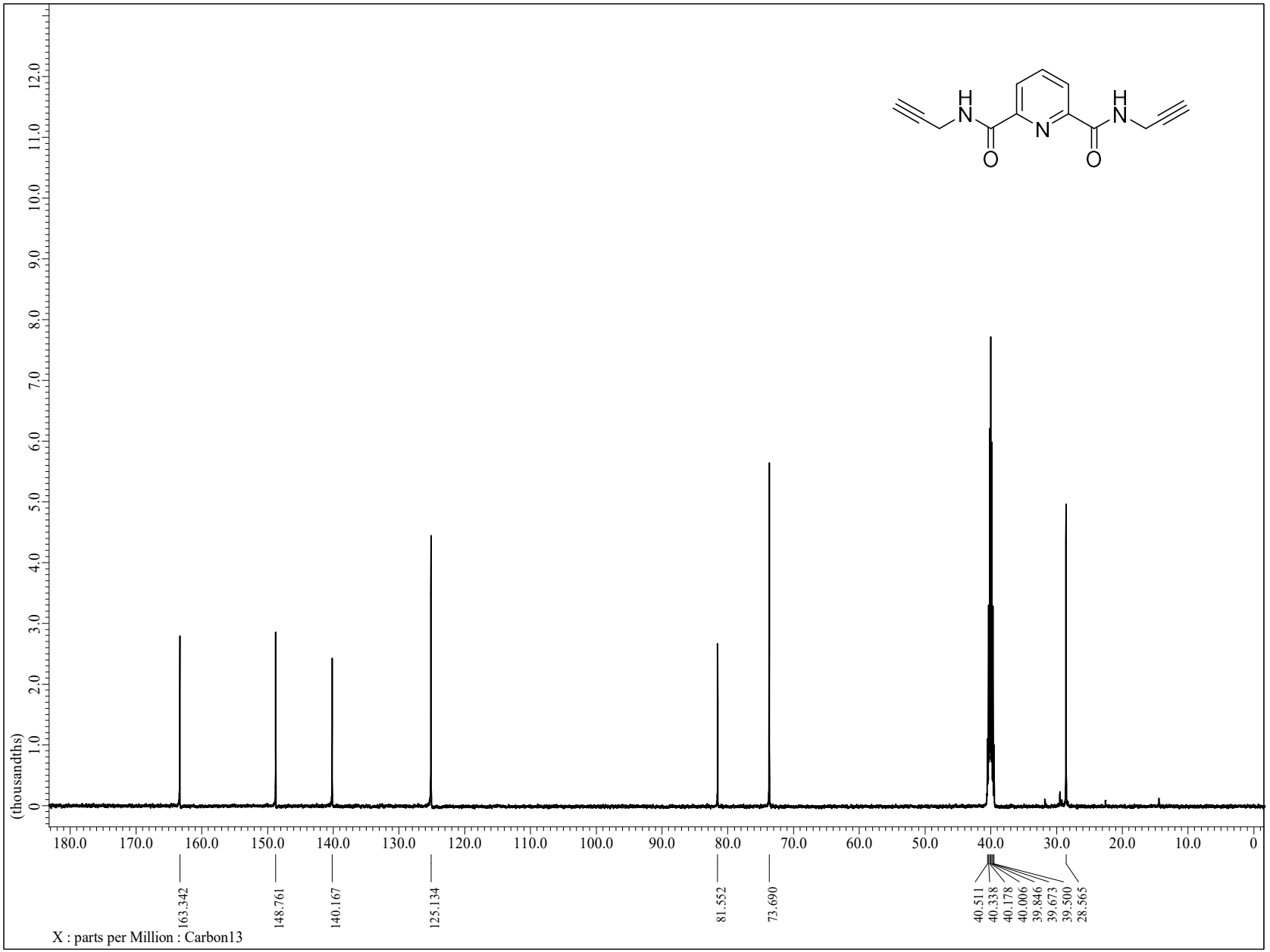

Figure S4: $^{13}C\{^{1}H\}$ NMR (125 MHz, DMSO-d_6) of compound **2**

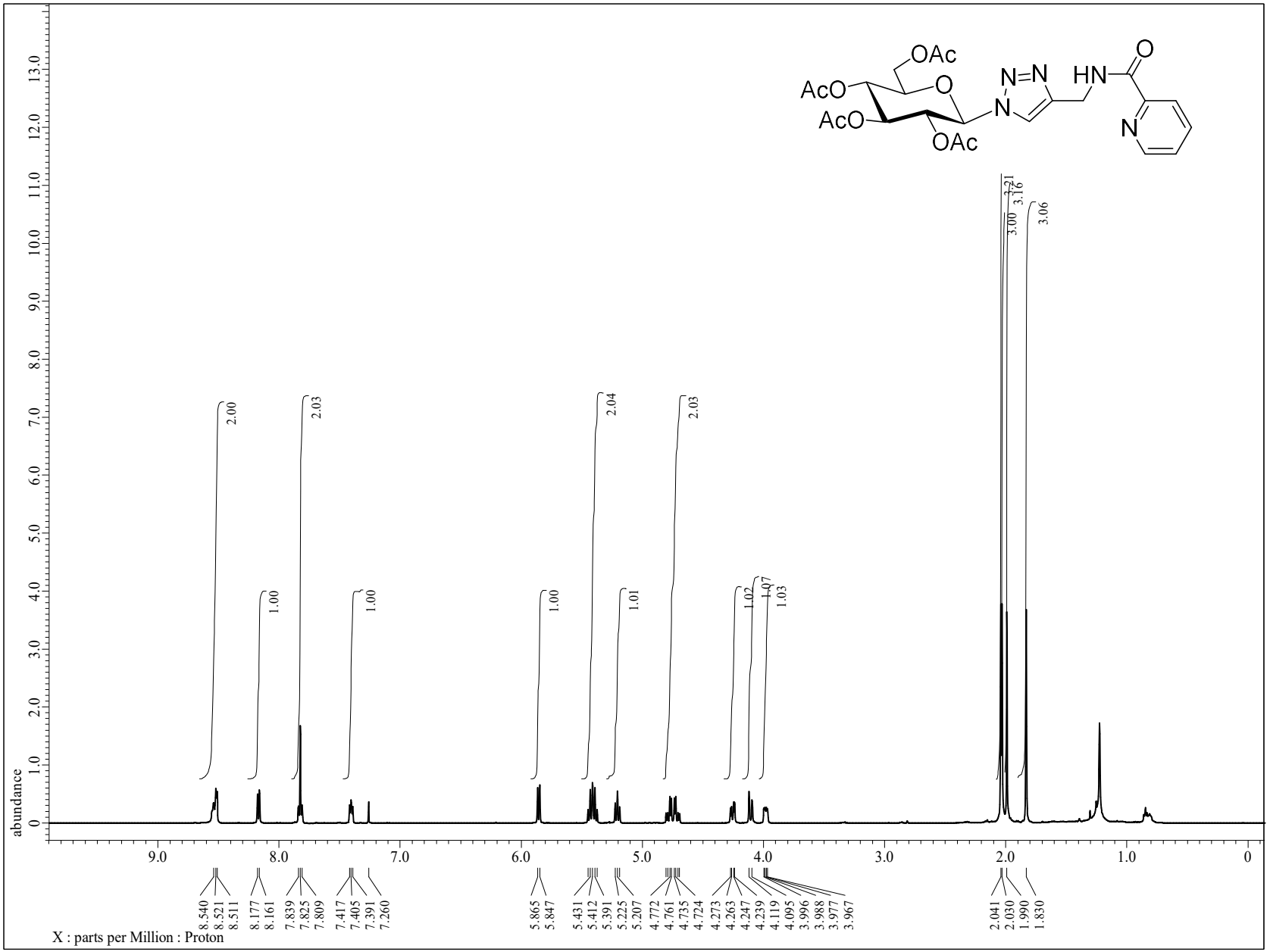

Figure S5: ^{1}H NMR (500 MHz,$CDCl_3$) of compound **L1**

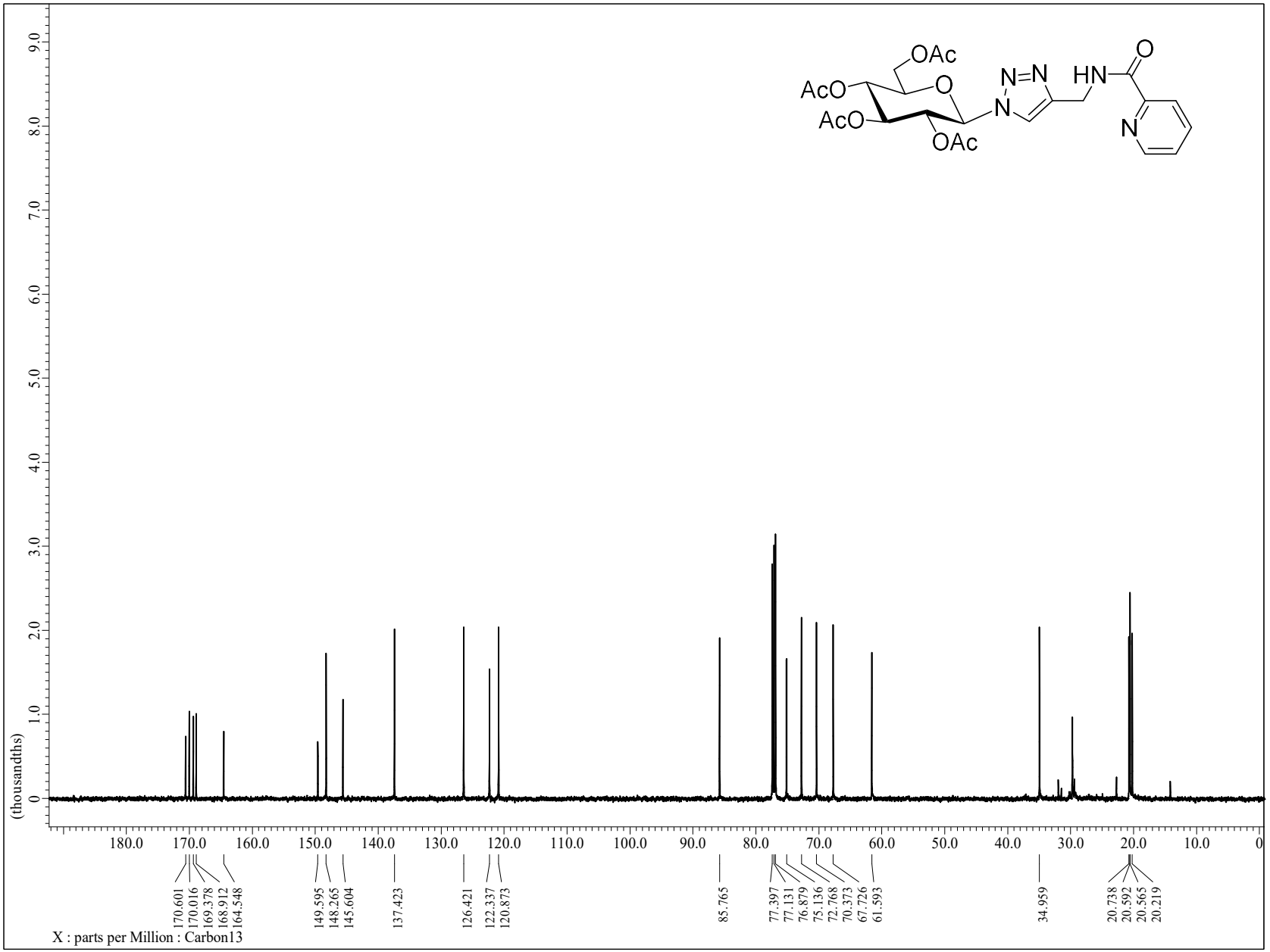

Figure S6: $^{13}C\{^{1}H\}$ NMR (125 MHz, $CDCl_3$) of compound **L1**

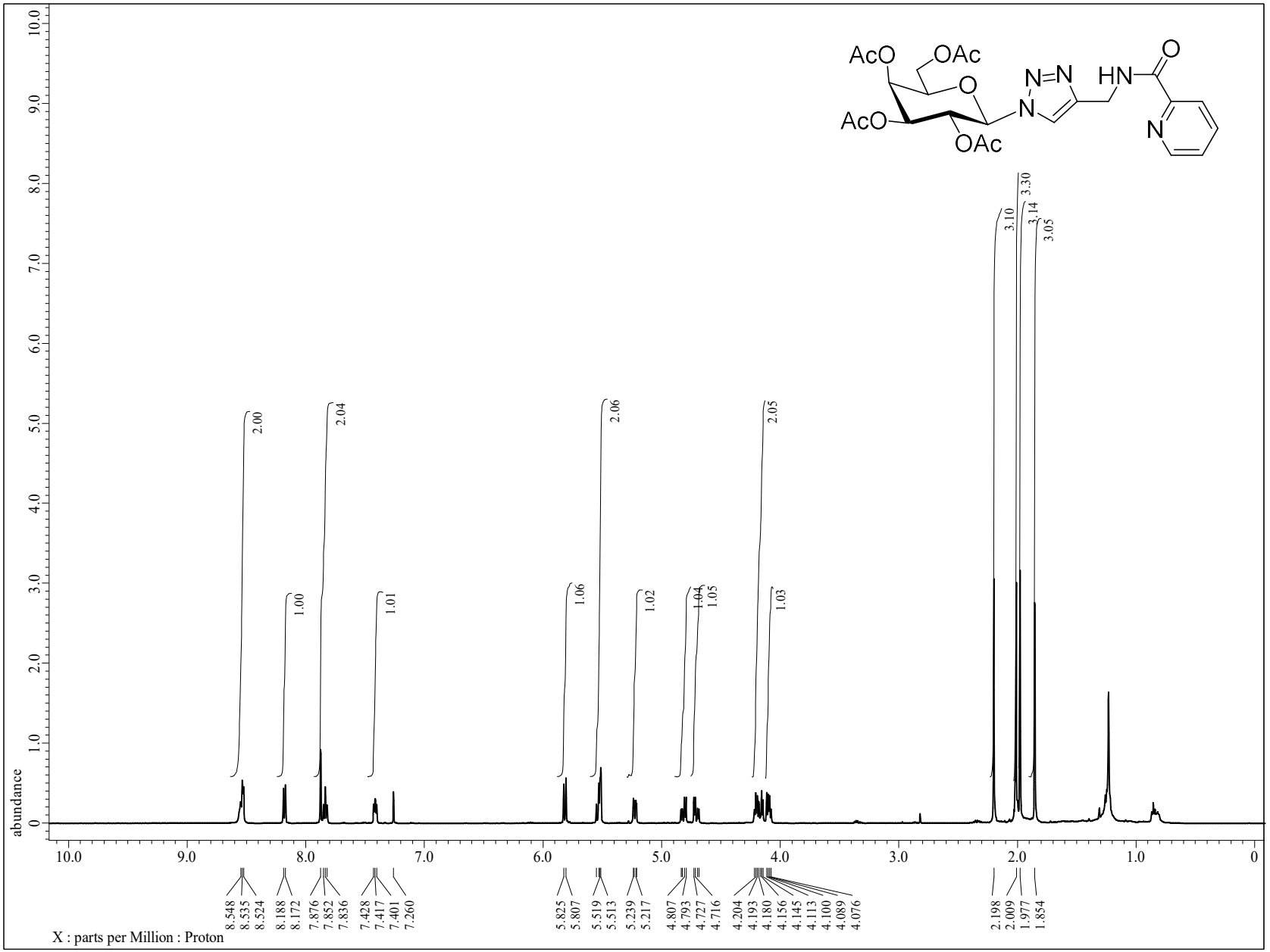

Figure S7: ^{1}H NMR (500 MHz, $CDCl_3$) of compound **L2**

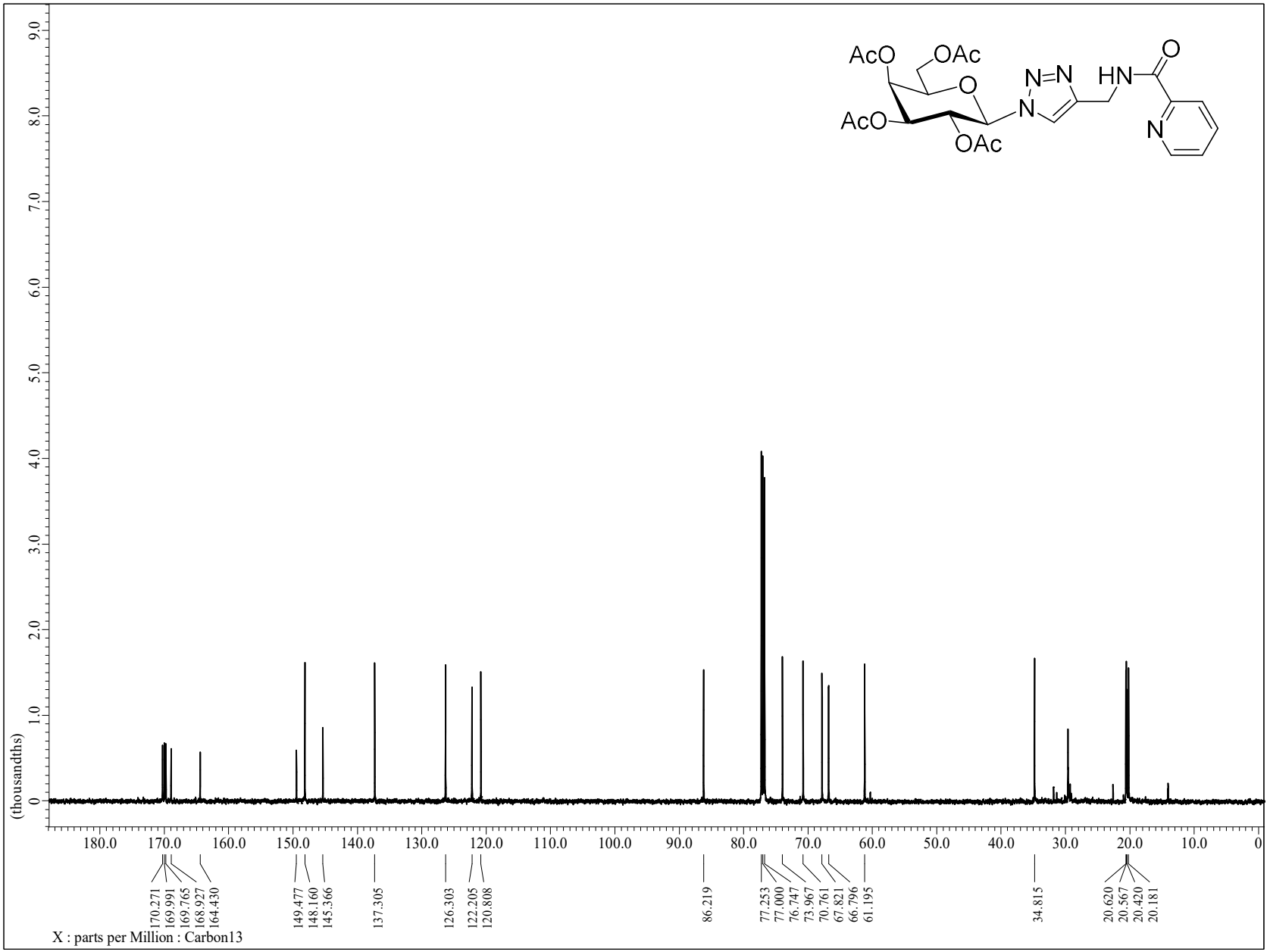

Figure S8: $^{13}C\{^{1}H\}$ NMR (125 MHz, $CDCl_3$) of compound **L2**

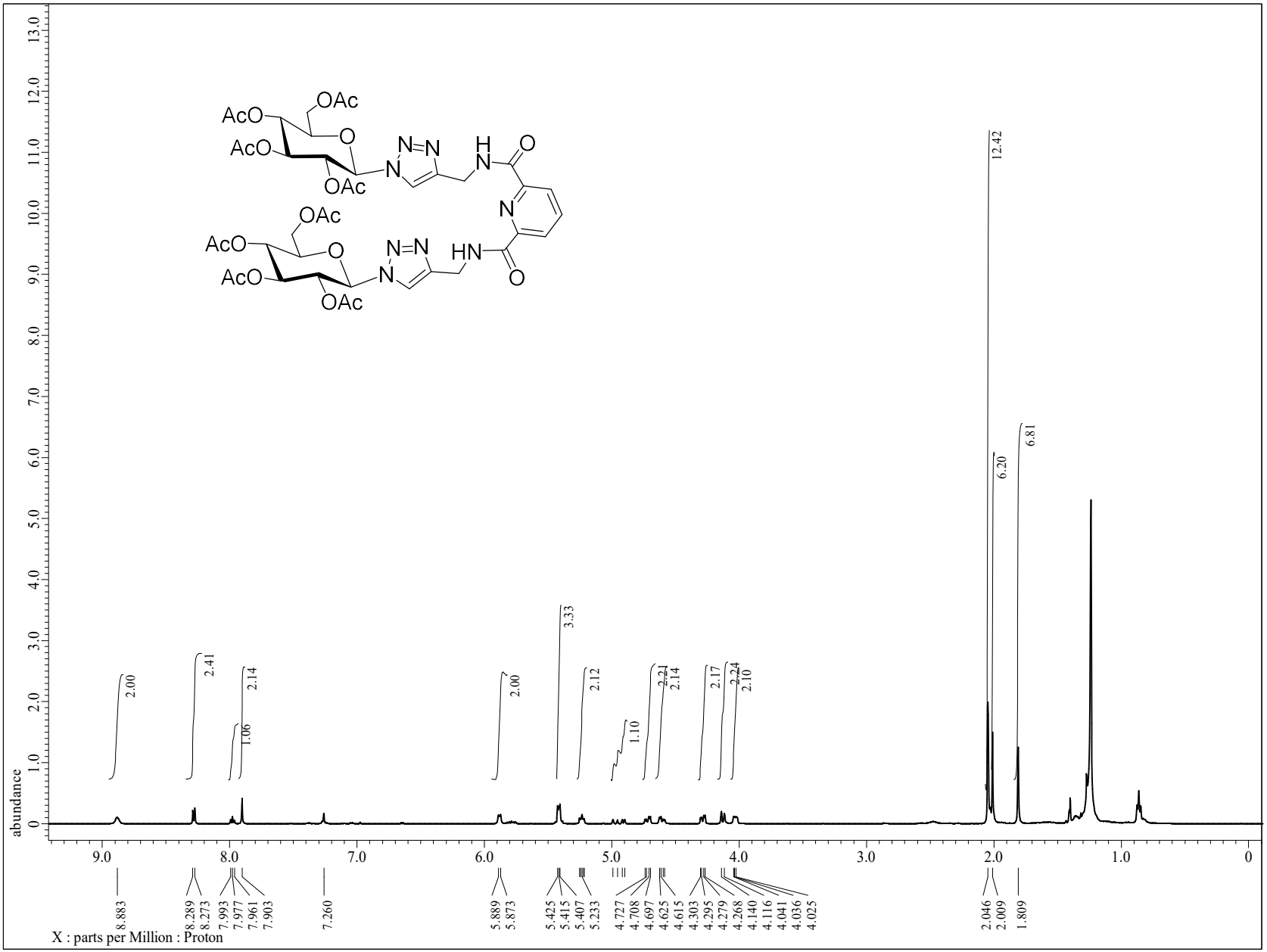

Figure S9: ^{1}H NMR (500 MHz, $CDCl_3$) of compound **L3**

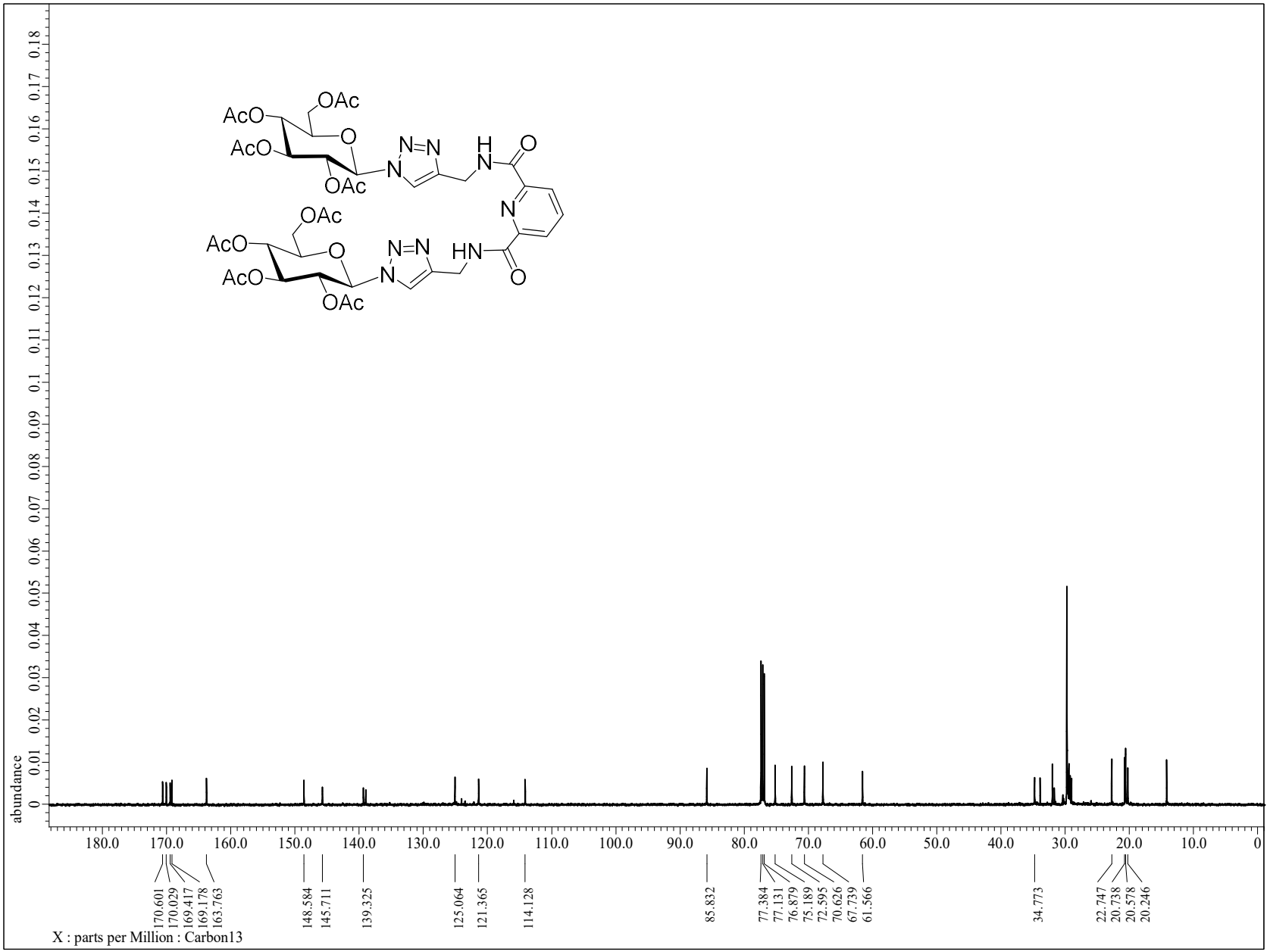

Figure S10: $^{13}C\{^{1}H\}$ NMR (125 MHz, $CDCl_3$) of compound **L3**

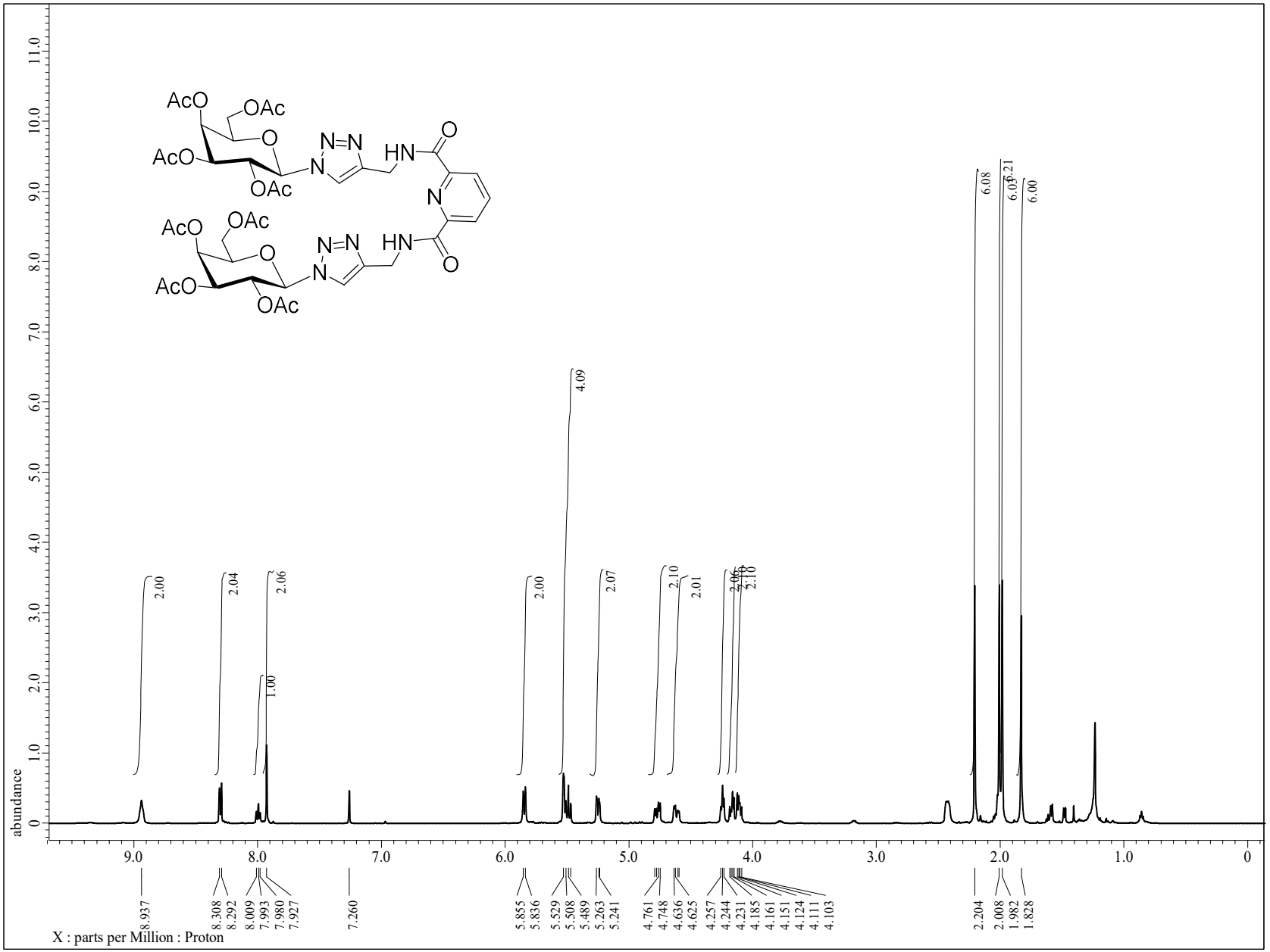

Figure S11: ^{1}H NMR (500 MHz, $CDCl_3$) of compound **L4**

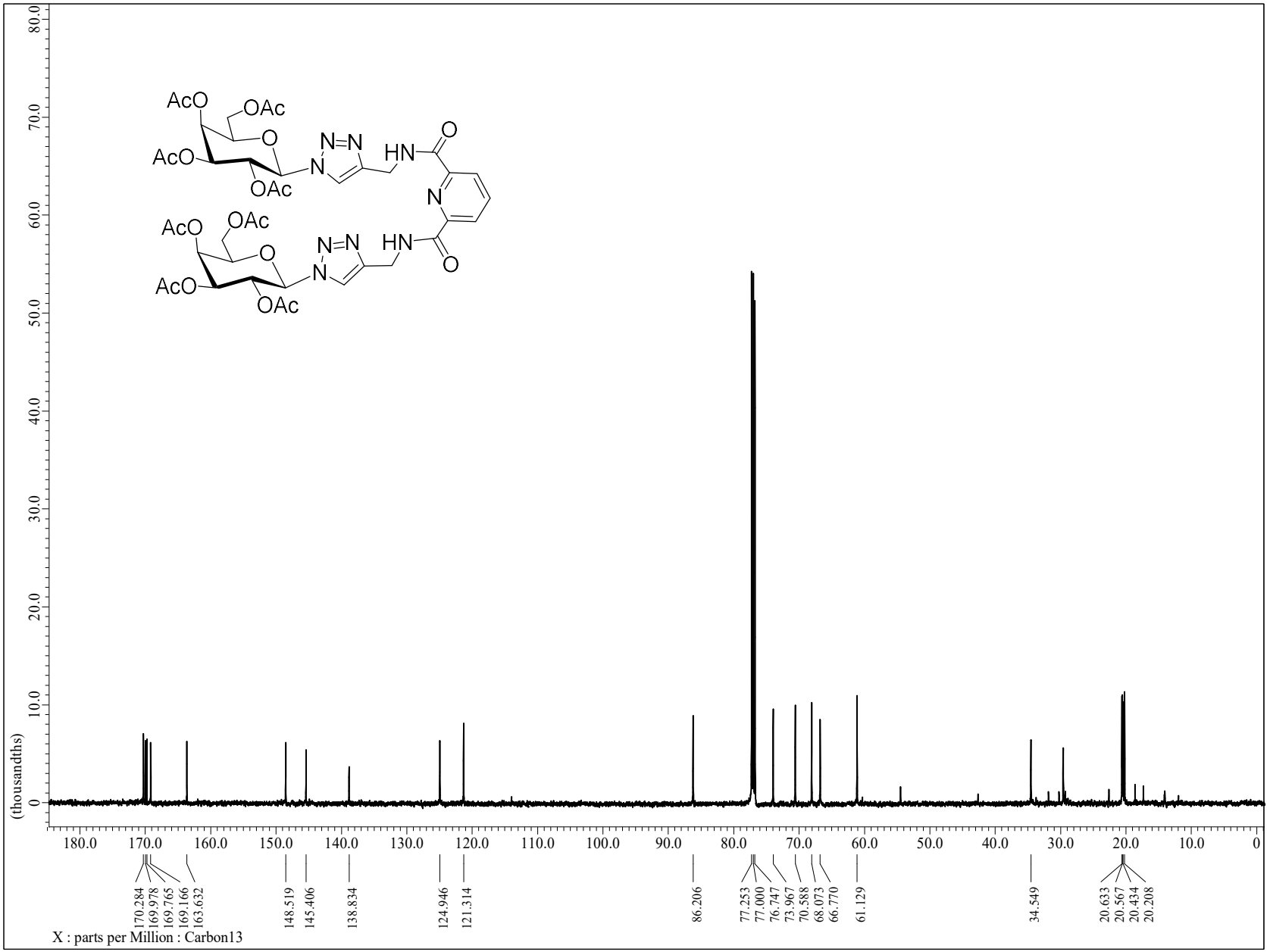

Figure S12: $^{13}C\{^{1}H\}$ NMR (125 MHz, $CDCl_3$) of compound **L4**

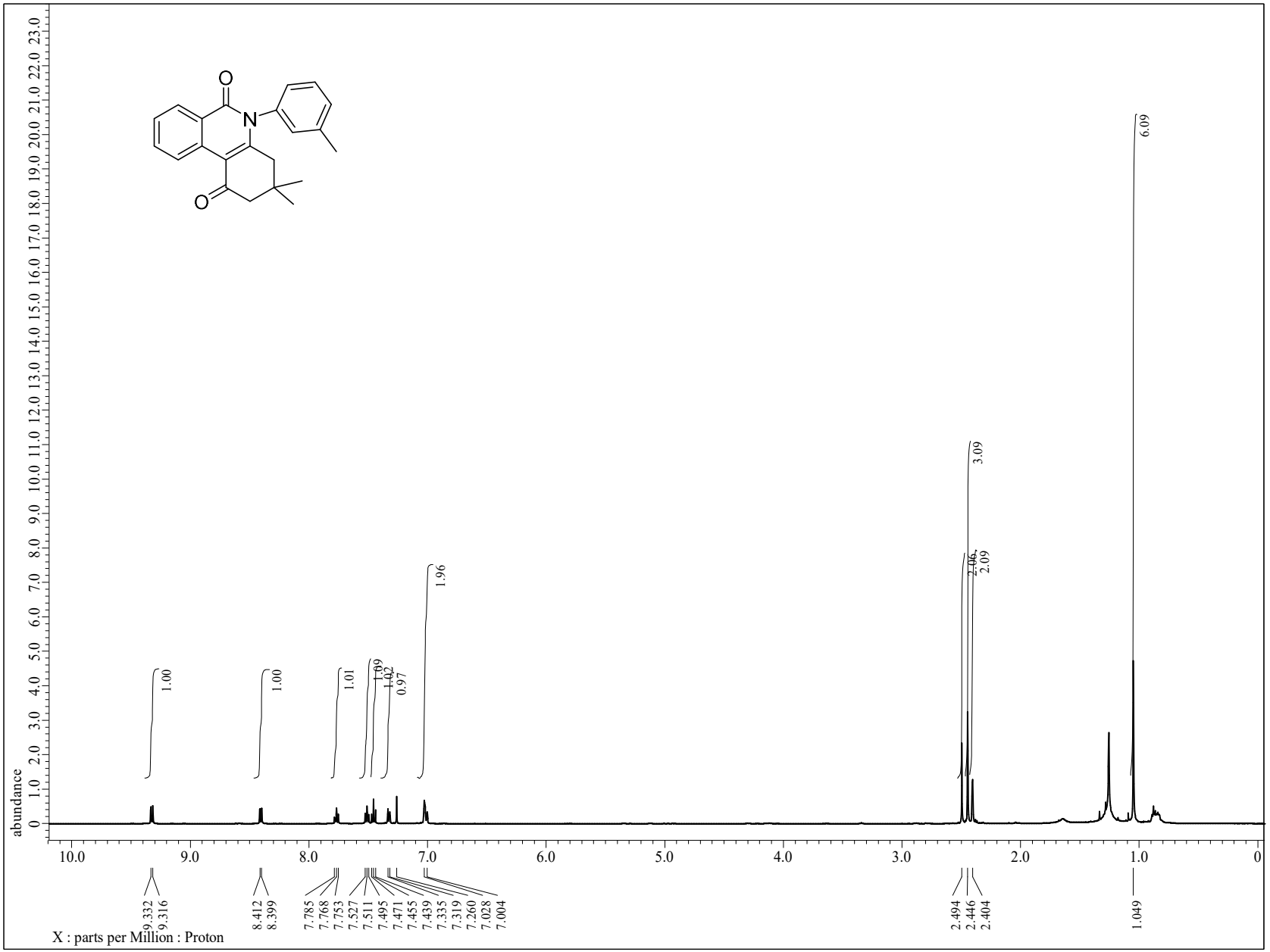

Figure S13: ^{1}H NMR (500 MHz, $CDCl_3$) of compound **6a**

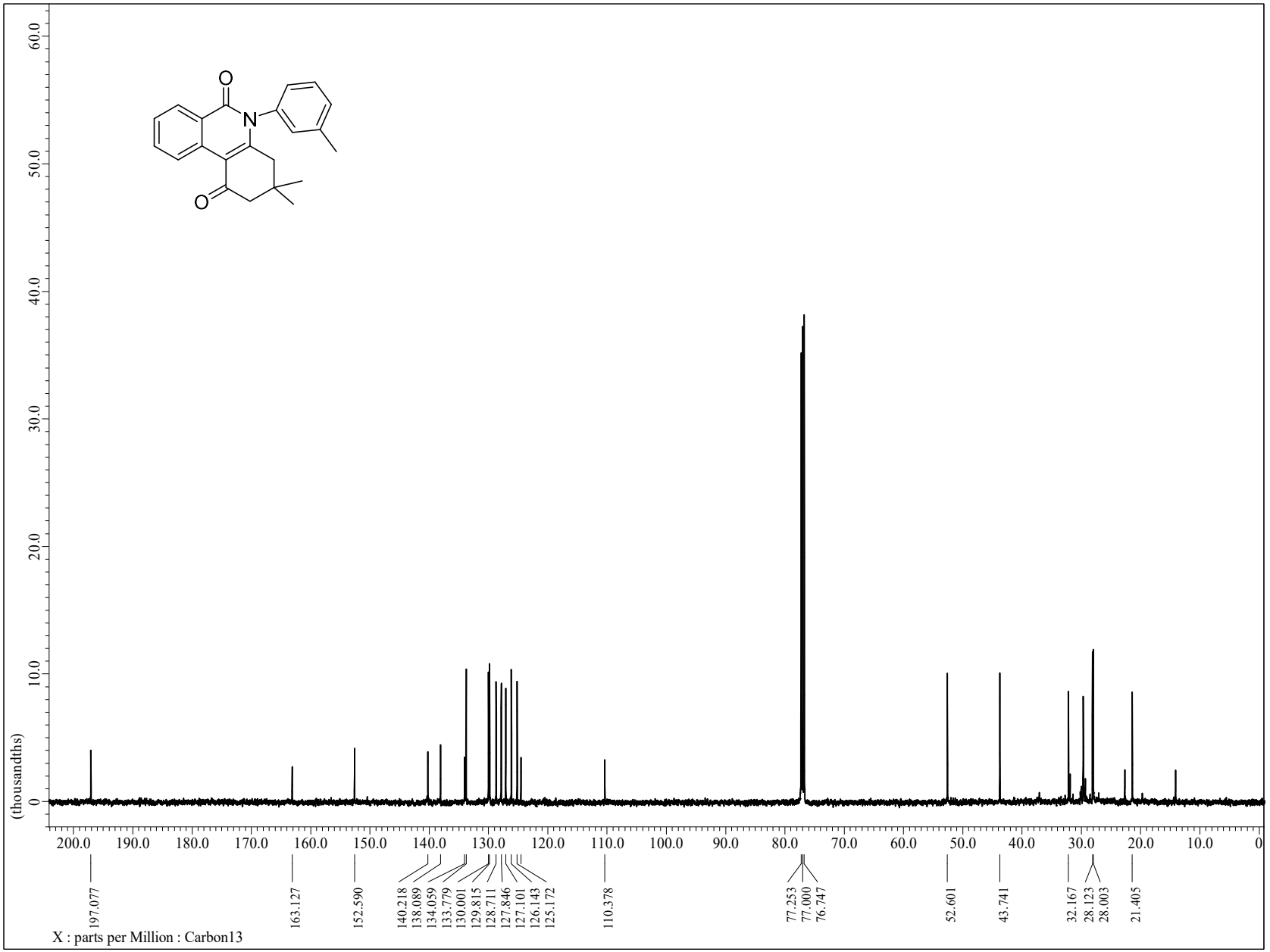

Figure S14: $^{13}C\{^{1}H\}$ NMR (125 MHz, $CDCl_3$) of compound **6a**

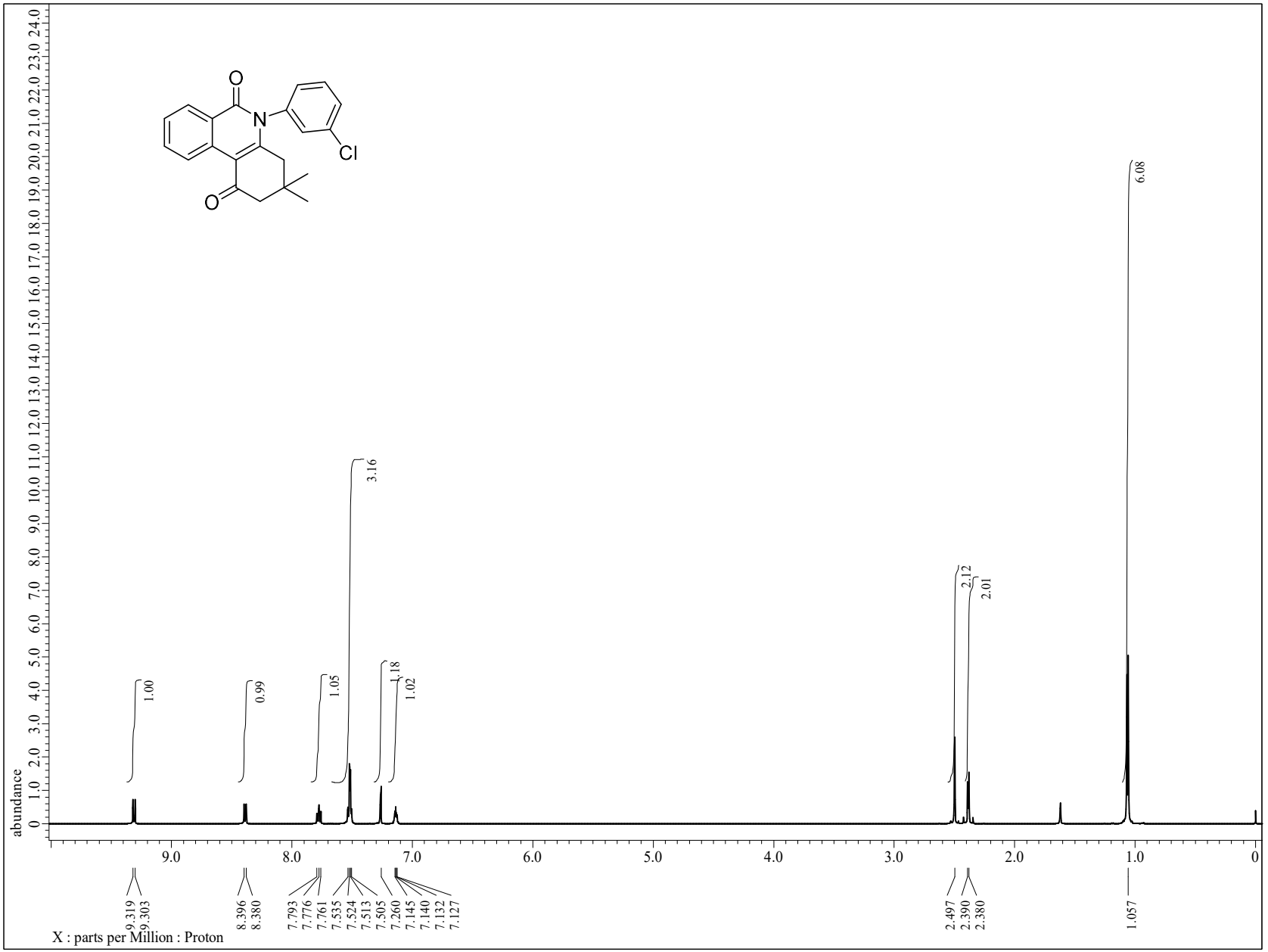

Figure S15: ^{1}H NMR (500 MHz, $CDCl_3$) of compound **6b**

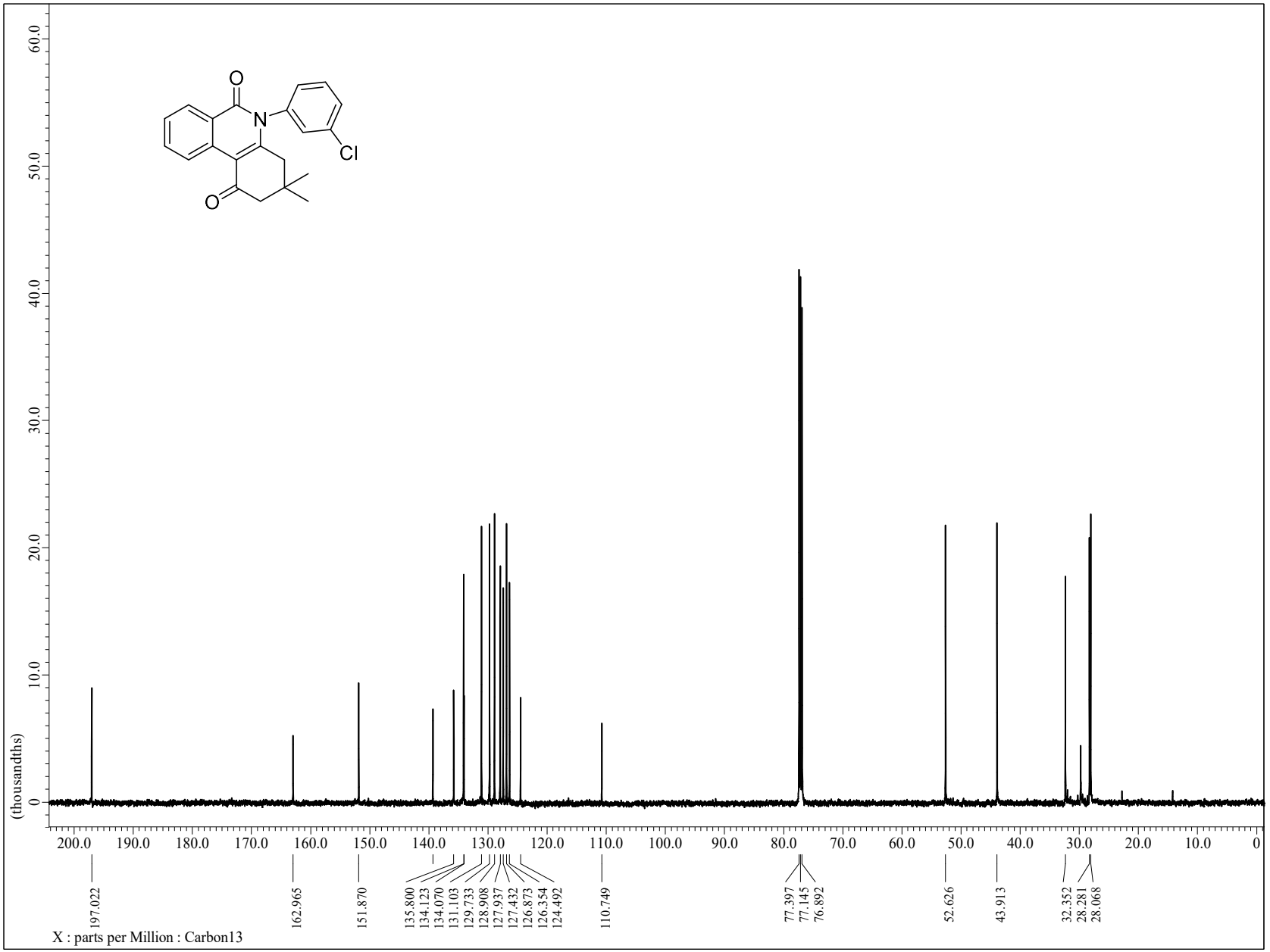

Figure S16: $^{13}C\{^{1}H\}$ NMR (125 MHz, $CDCl_3$) of compound **6b**

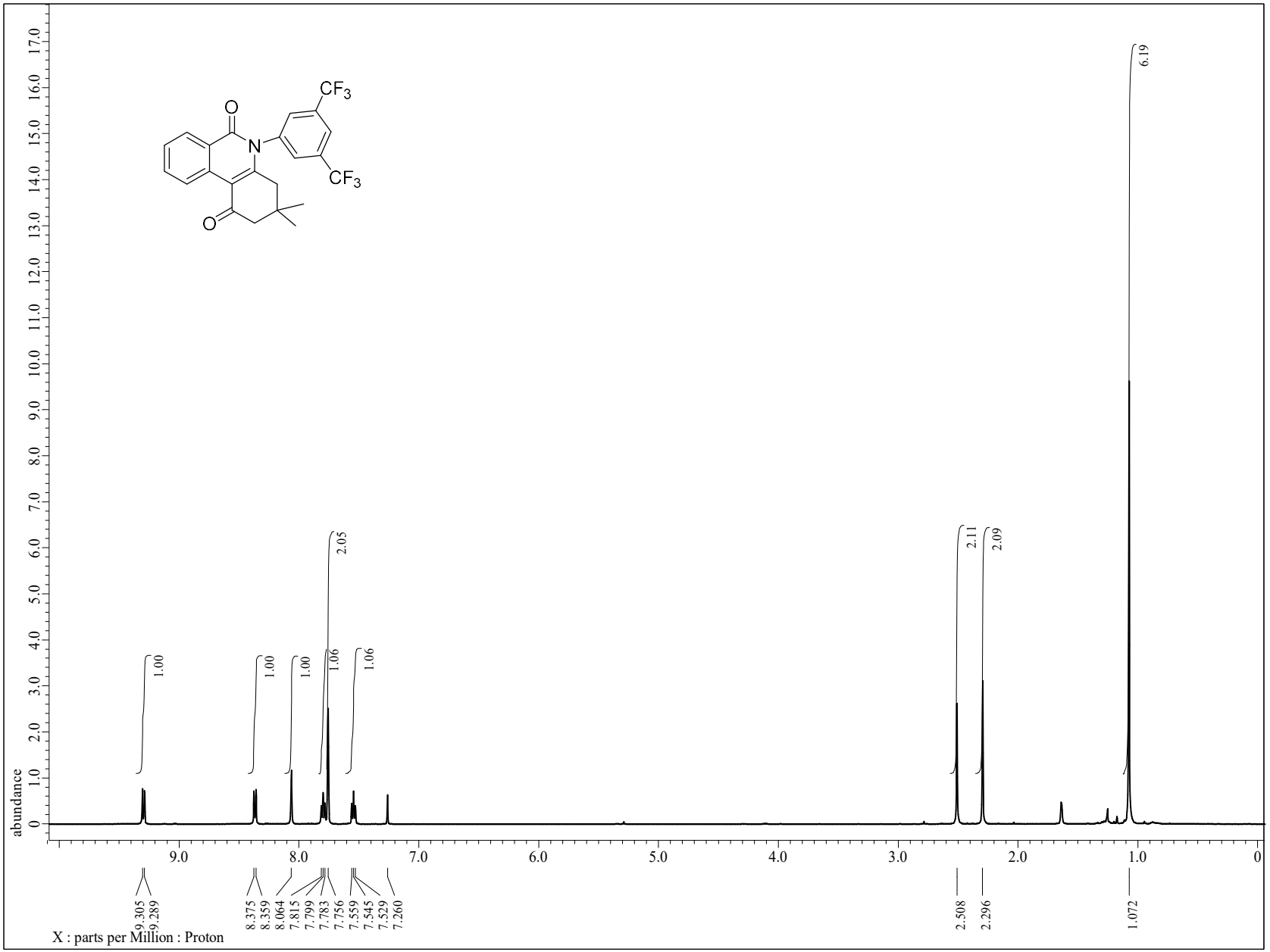

Figure S17: ^{1}H NMR (500 MHz, $CDCl_3$) of compound **6c**

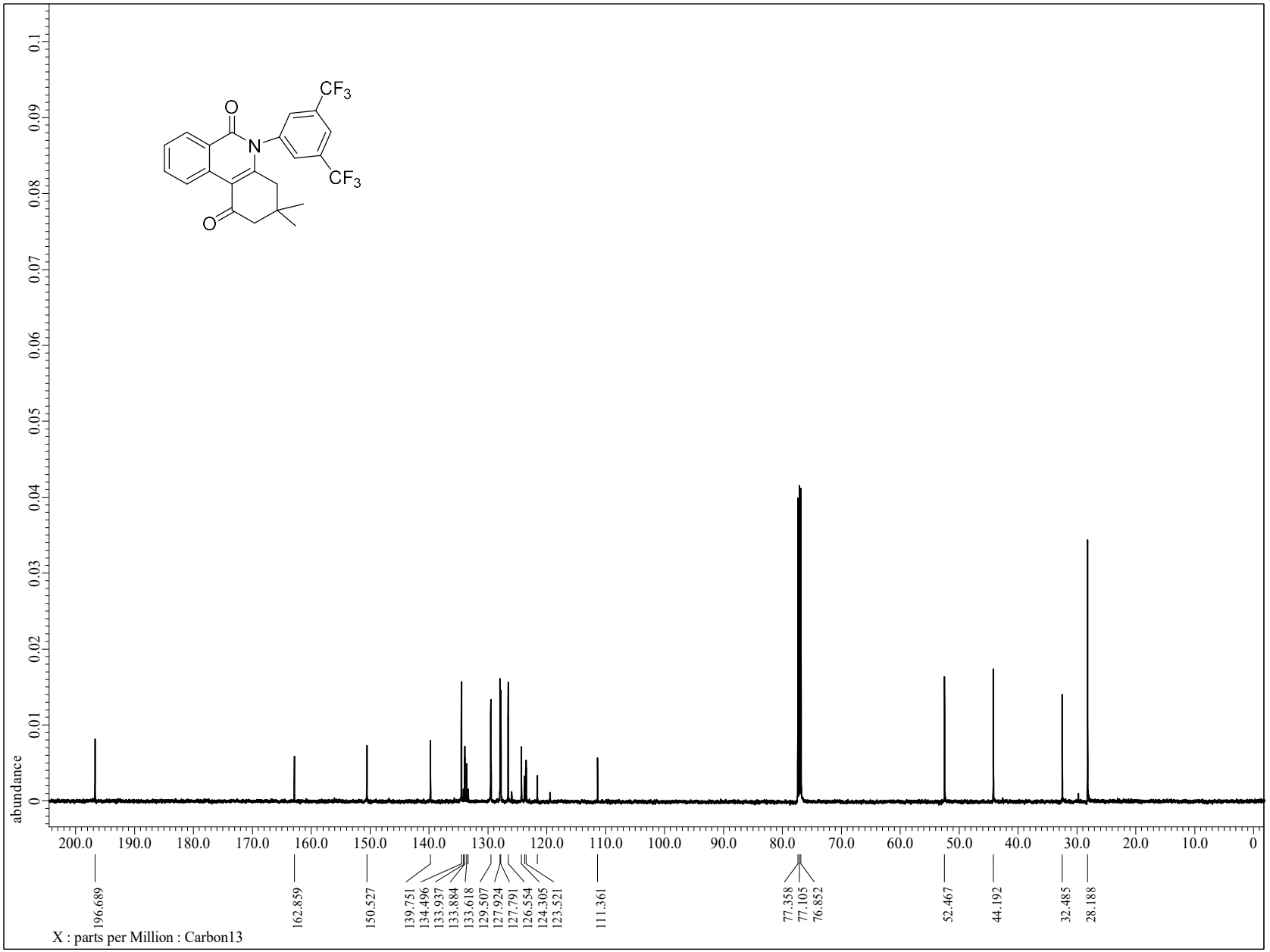

Figure S18: $^{13}C\{^{1}H\}$ NMR (125 MHz, $CDCl_3$) of compound **6c**

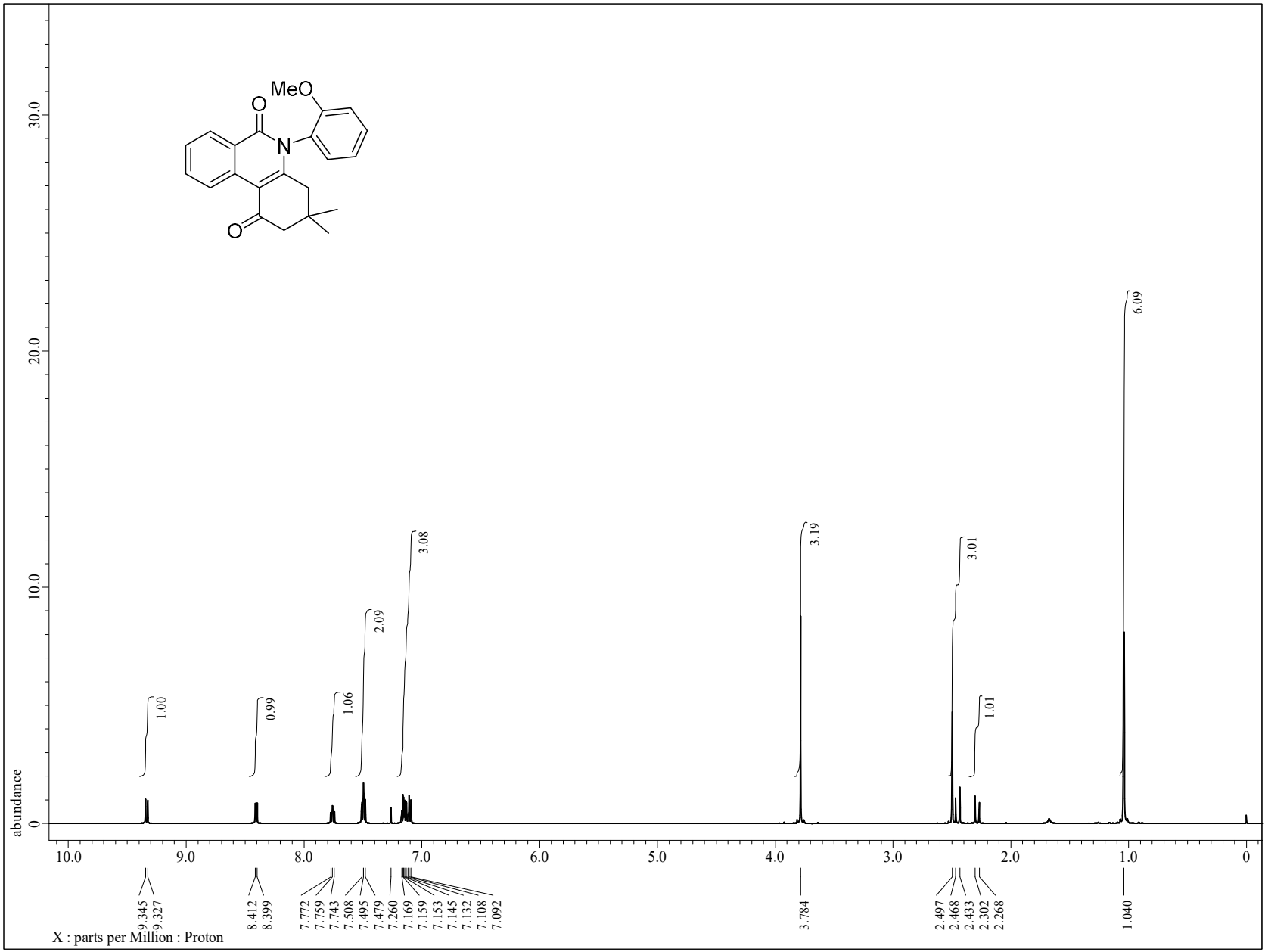

Figure S19: ^{1}H NMR (500 MHz, $CDCl_3$) of compound **6d**

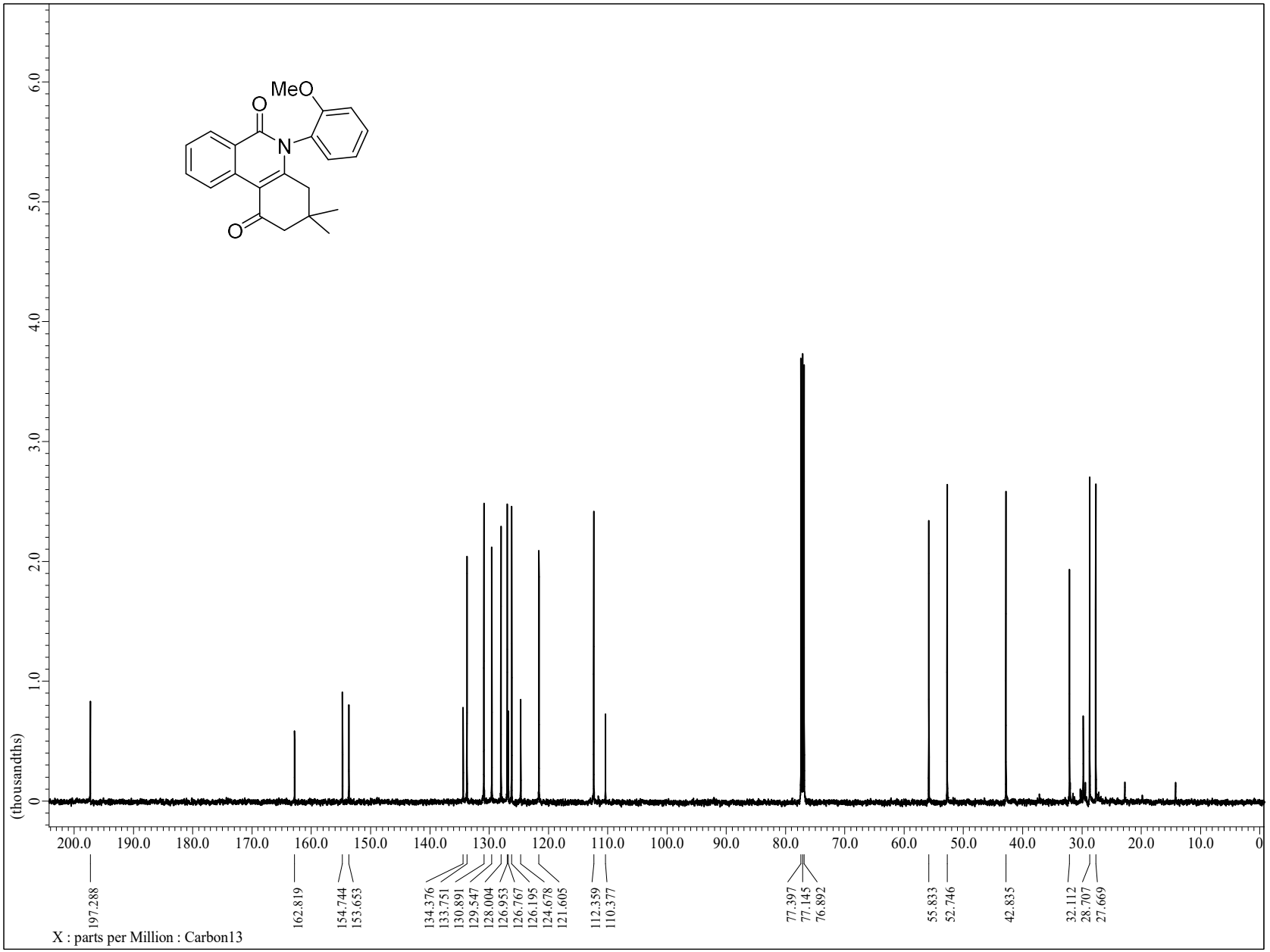

Figure S20: $^{13}C\{^{1}H\}$ NMR (125 MHz, $CDCl_3$) of compound **6d**

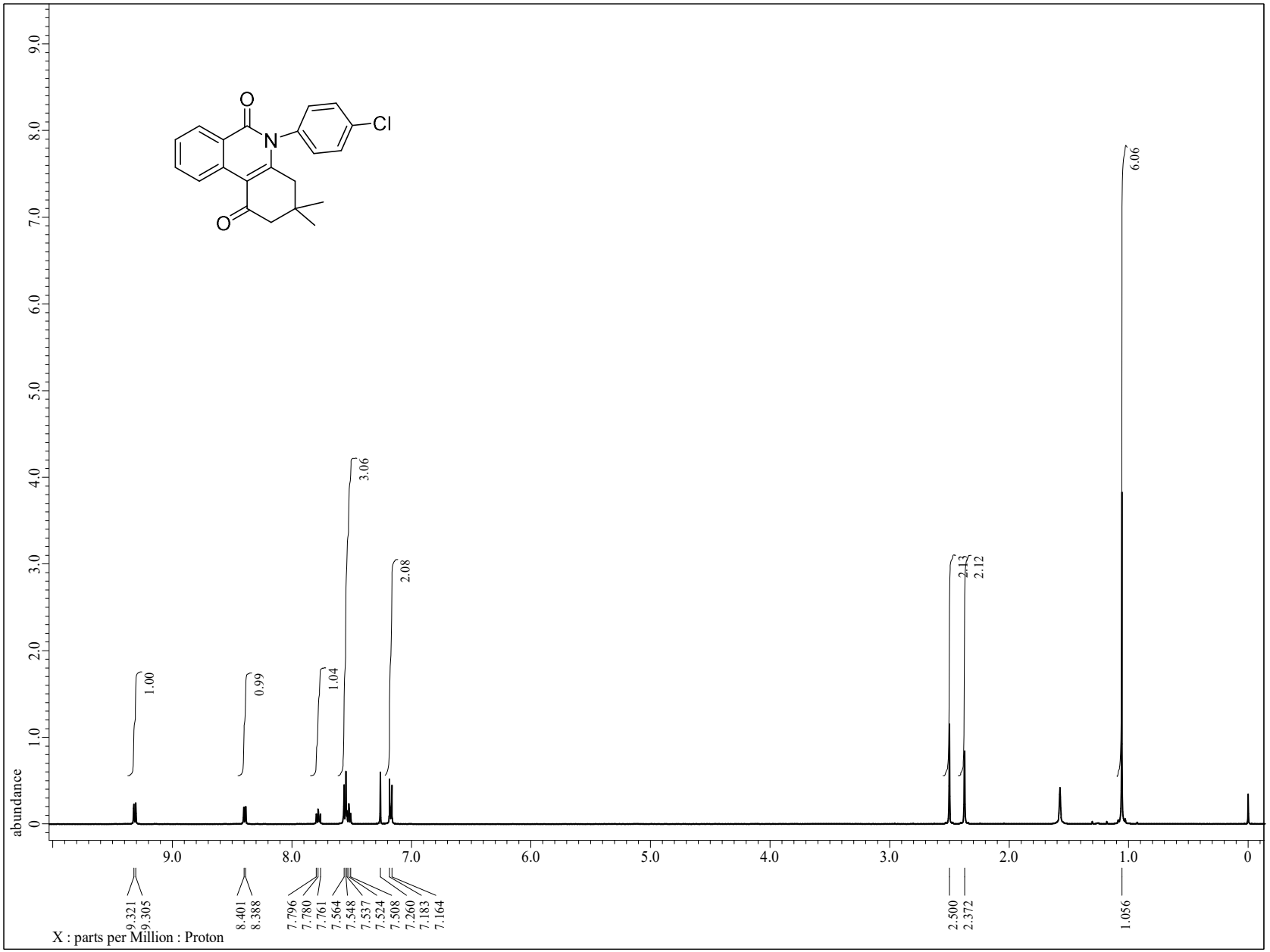

Figure S21: ^{1}H NMR (500 MHz, $CDCl_3$) of compound **6e**

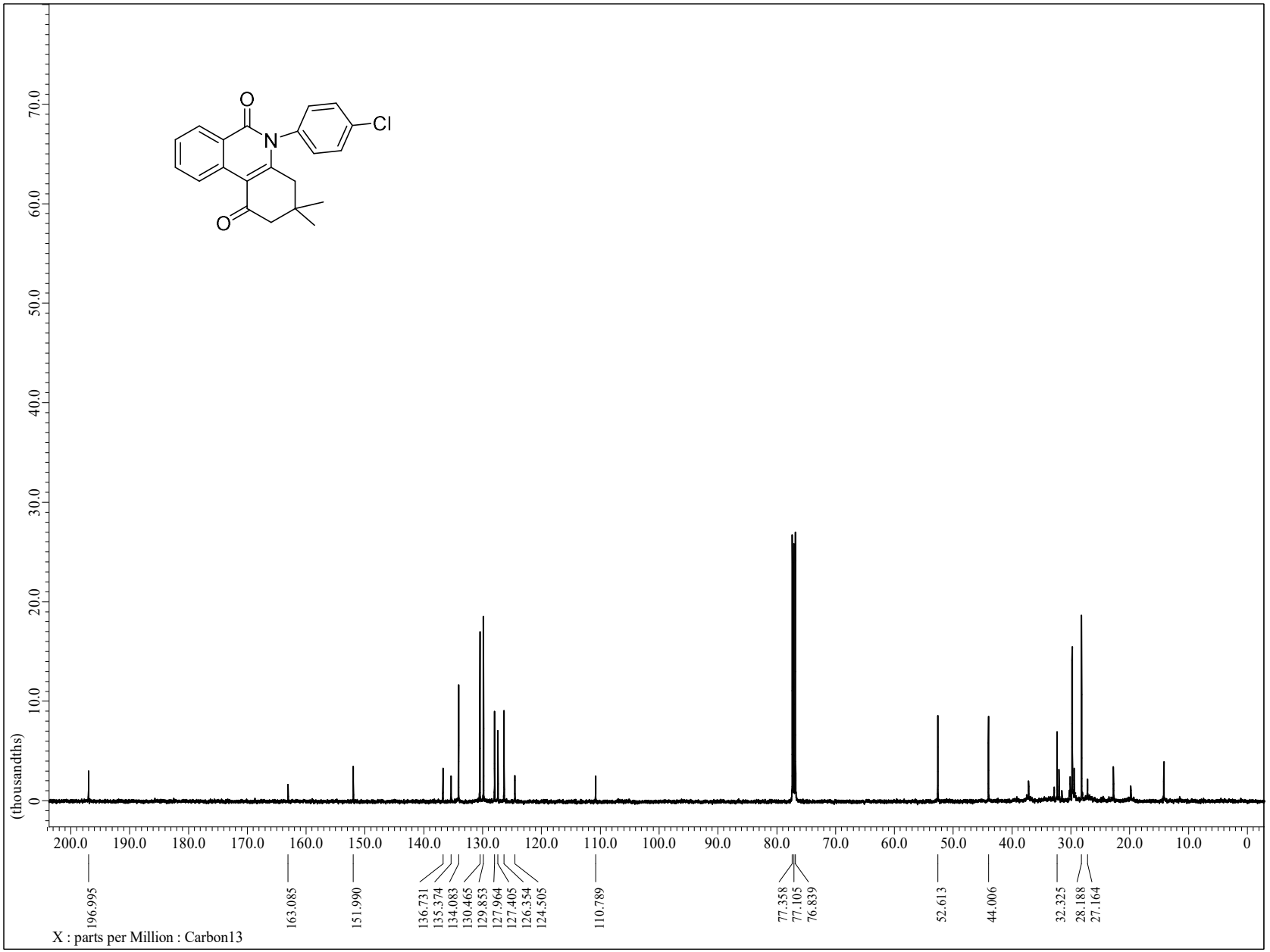

Figure S22: $^{13}C\{^{1}H\}$ NMR (125 MHz, $CDCl_3$) of compound **6e**

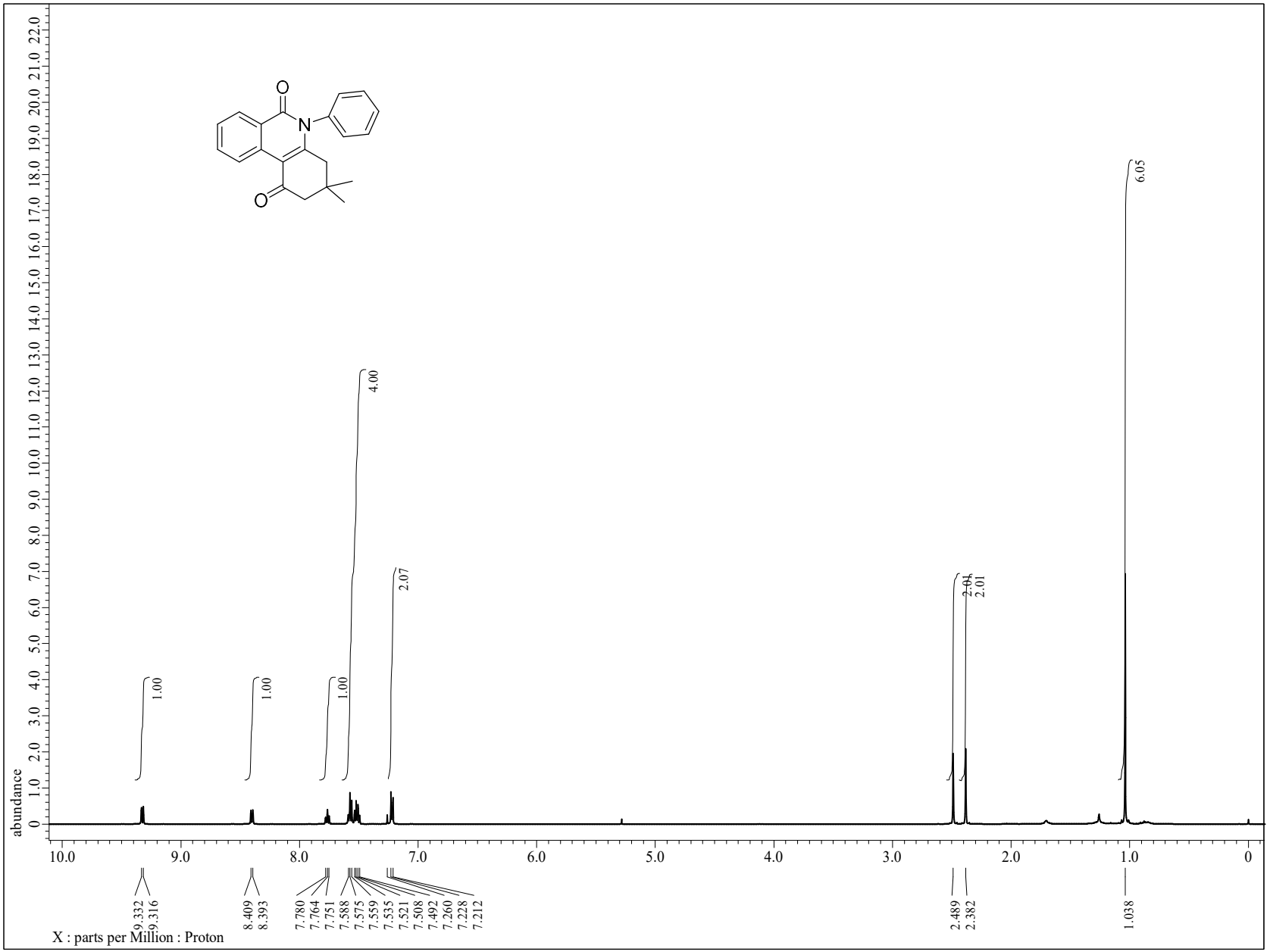

Figure S23: ^{1}H NMR (500 MHz, $CDCl_3$) of compound **6f**

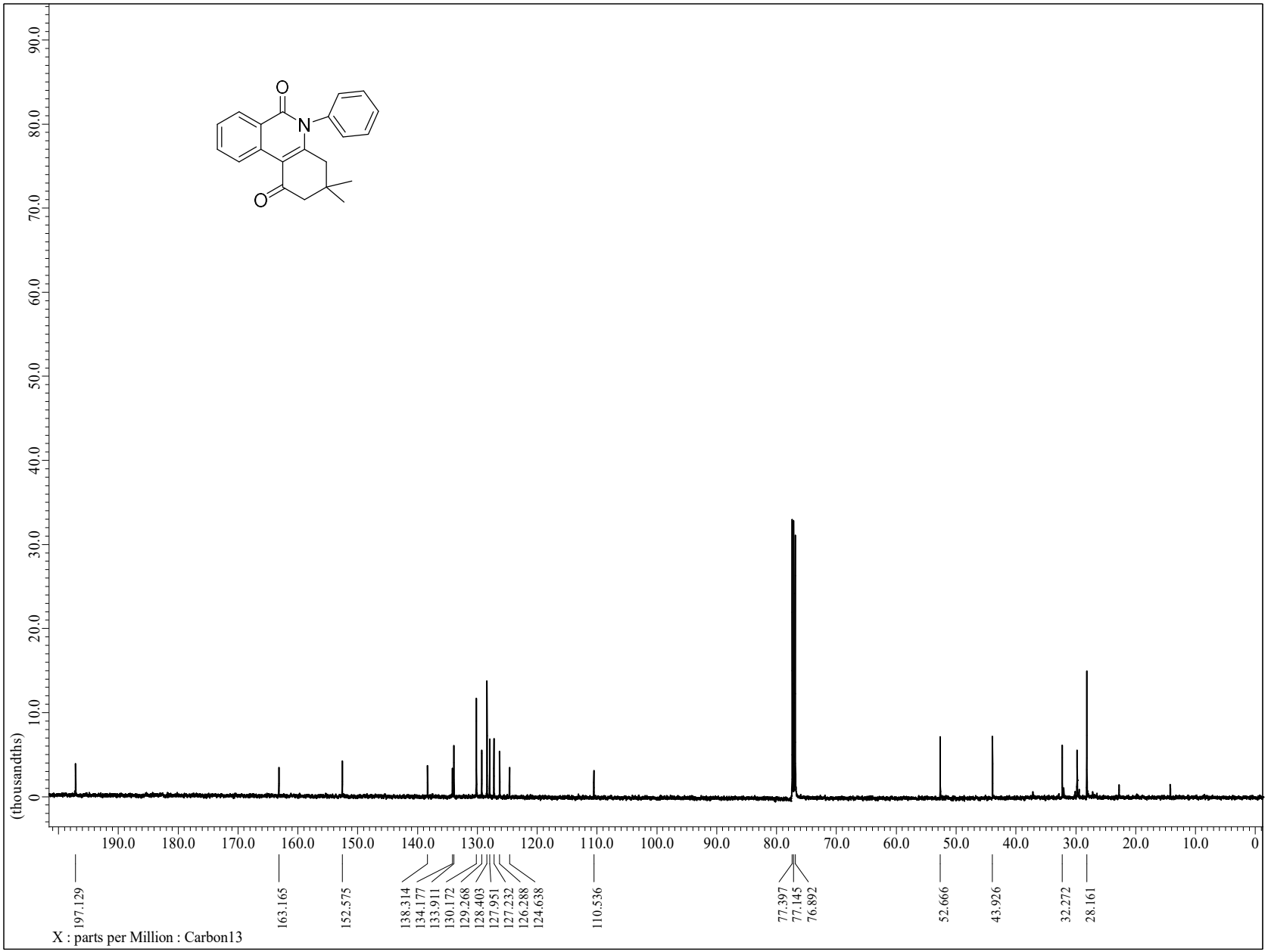

Figure S24: $^{13}C\{^{1}H\}$ NMR (125 MHz, $CDCl_3$) of compound **6f**

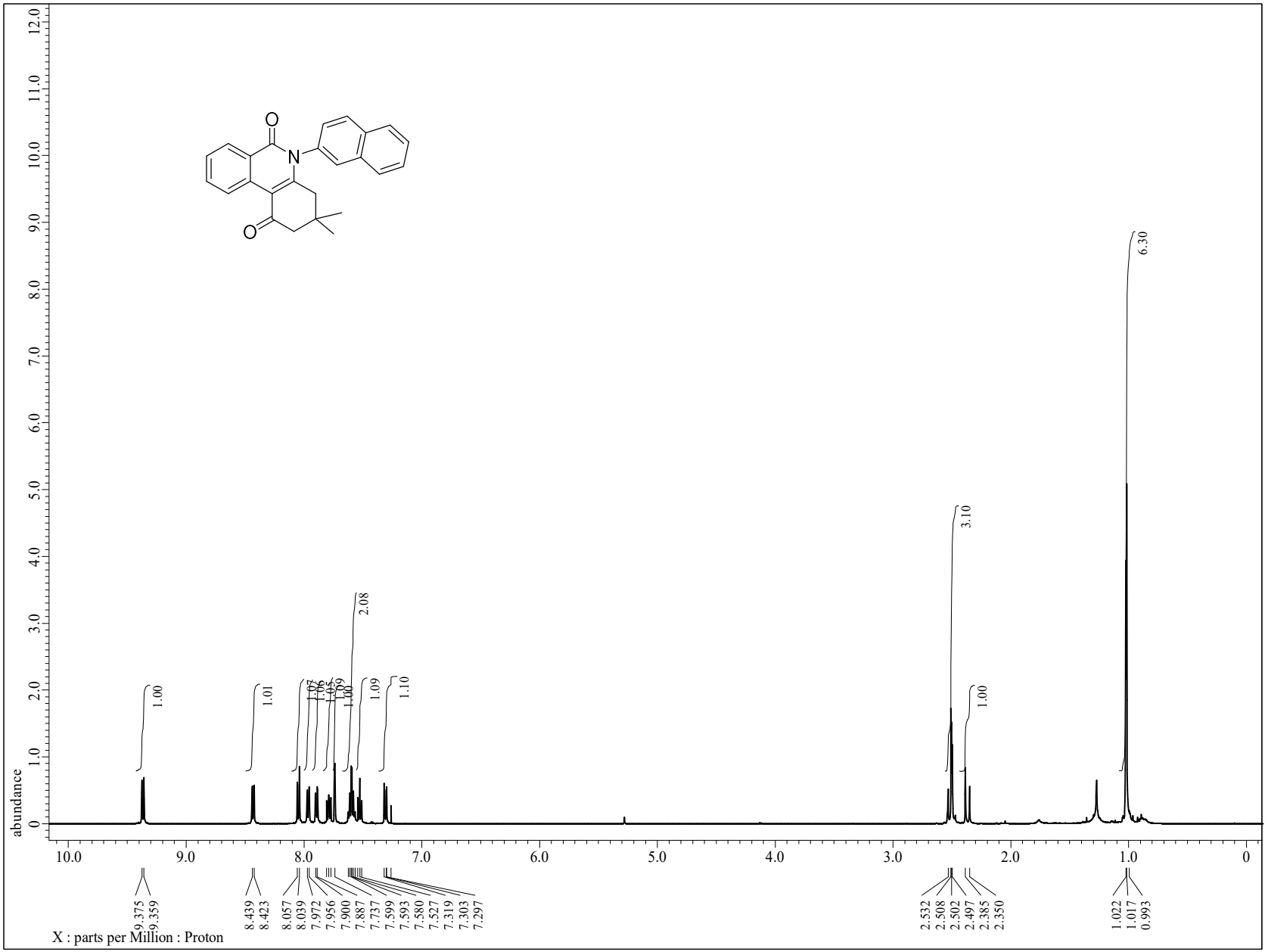

Figure S25: ^{1}H NMR (500 MHz, $CDCl_3$) of compound **6g**

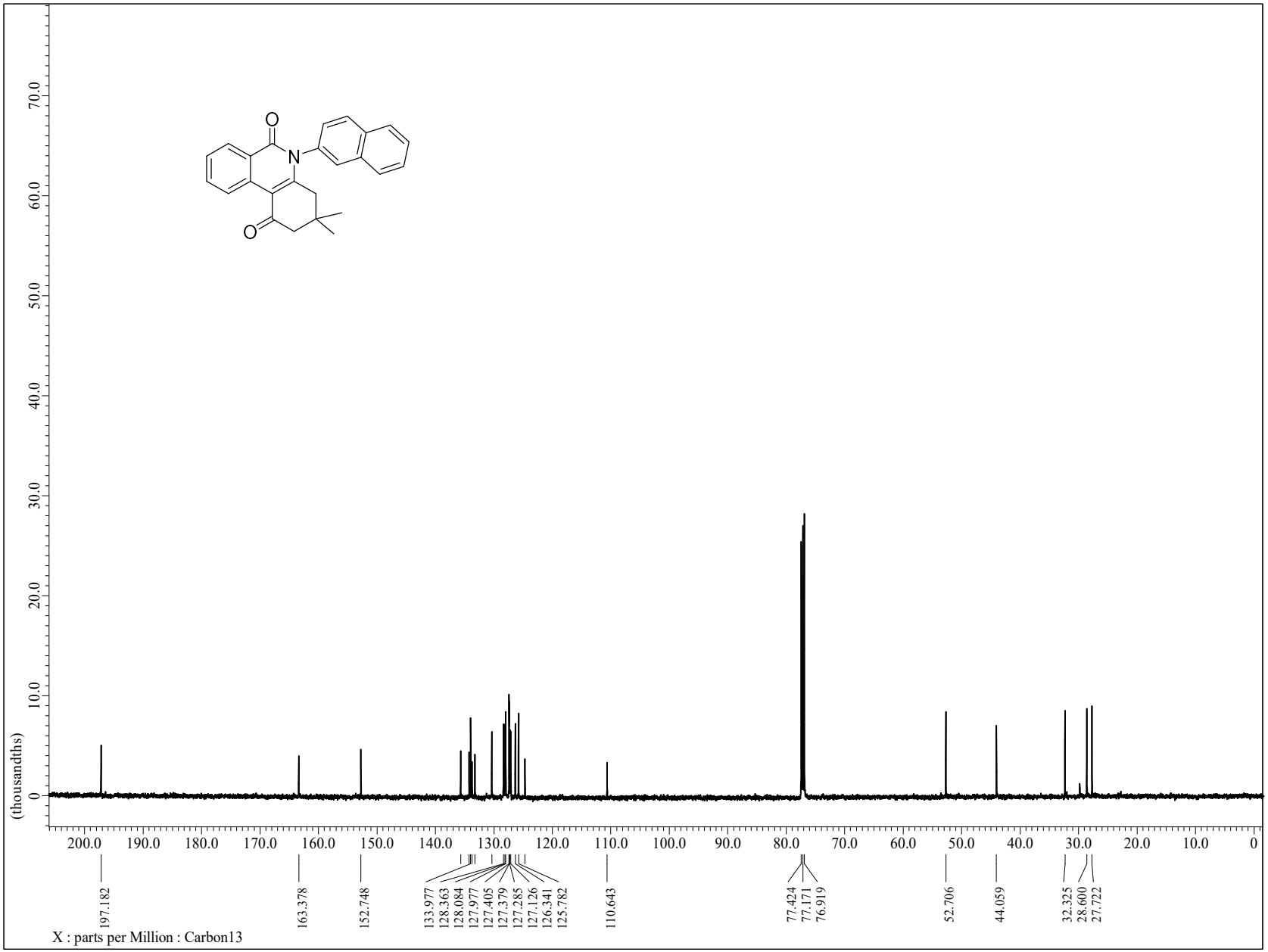

Figure S26: $^{13}C\{^{1}H\}$ NMR (125 MHz, $CDCl_3$) of compound **6g**

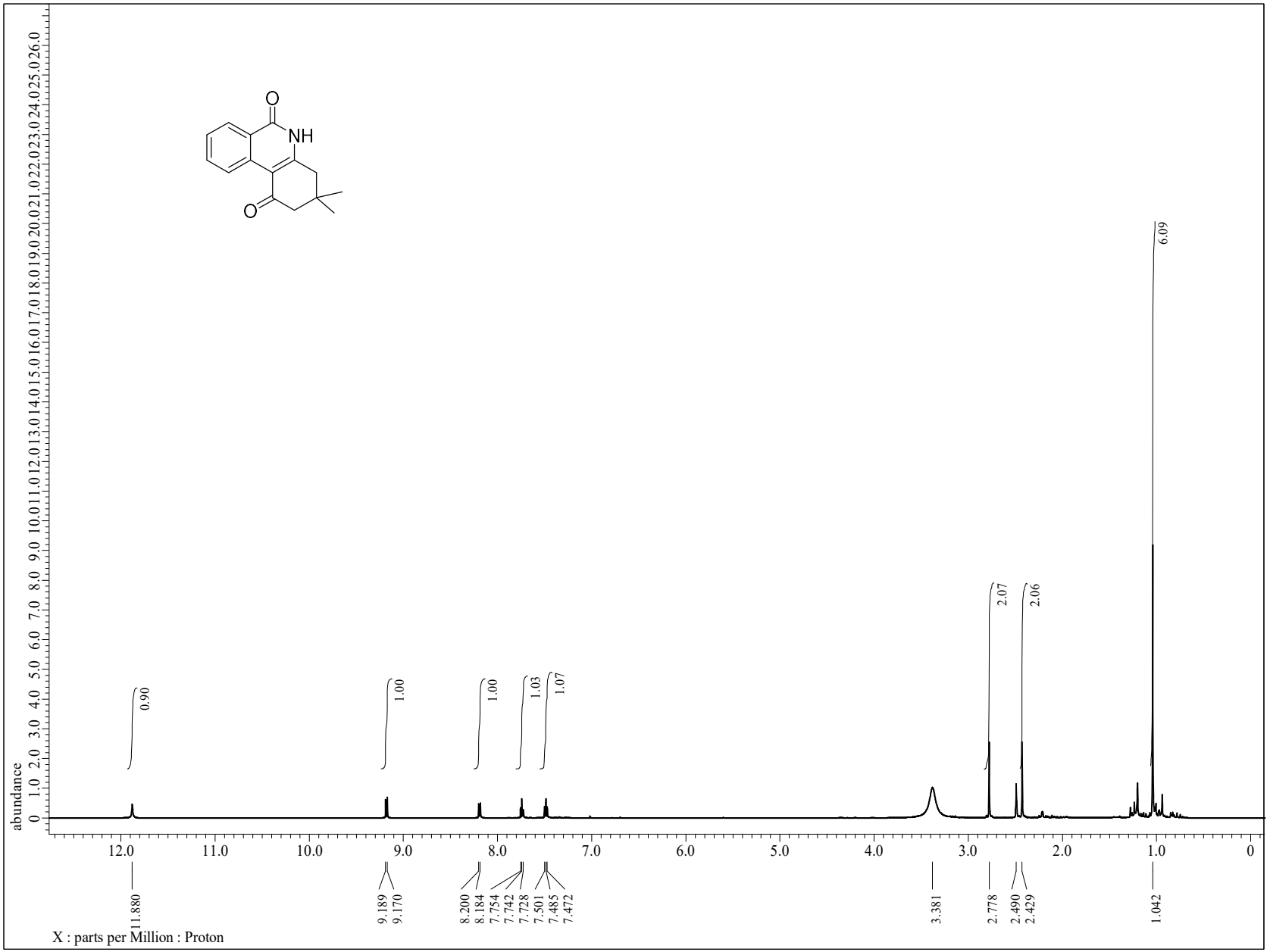

Figure S27: ^{1}H NMR (500 MHz, DMSO-d_6) of compound **6h**

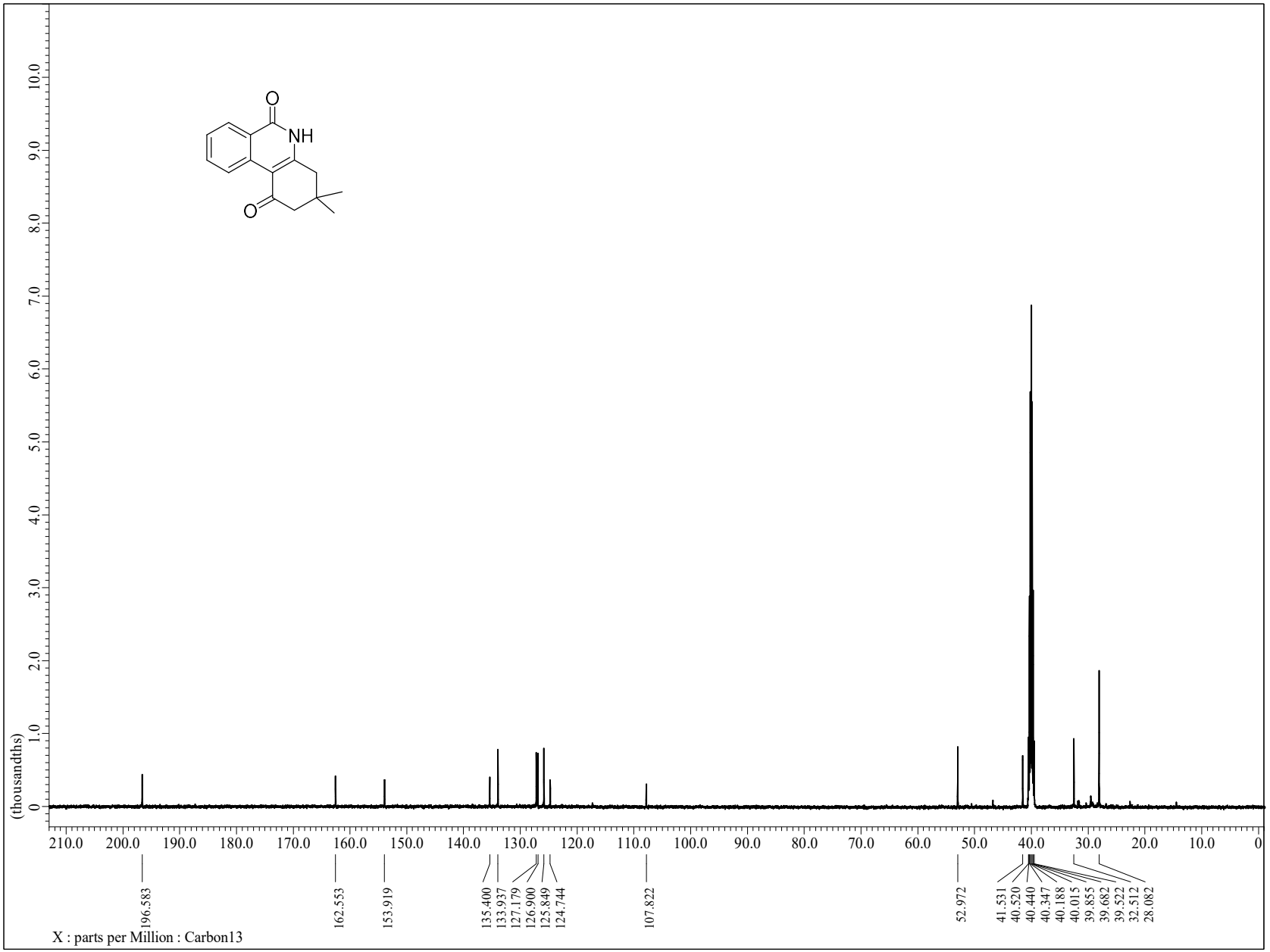

Figure S28: $^{13}C\{^{1}H\}$ NMR (125 MHz, DMSO-d_6) of compound **6h**

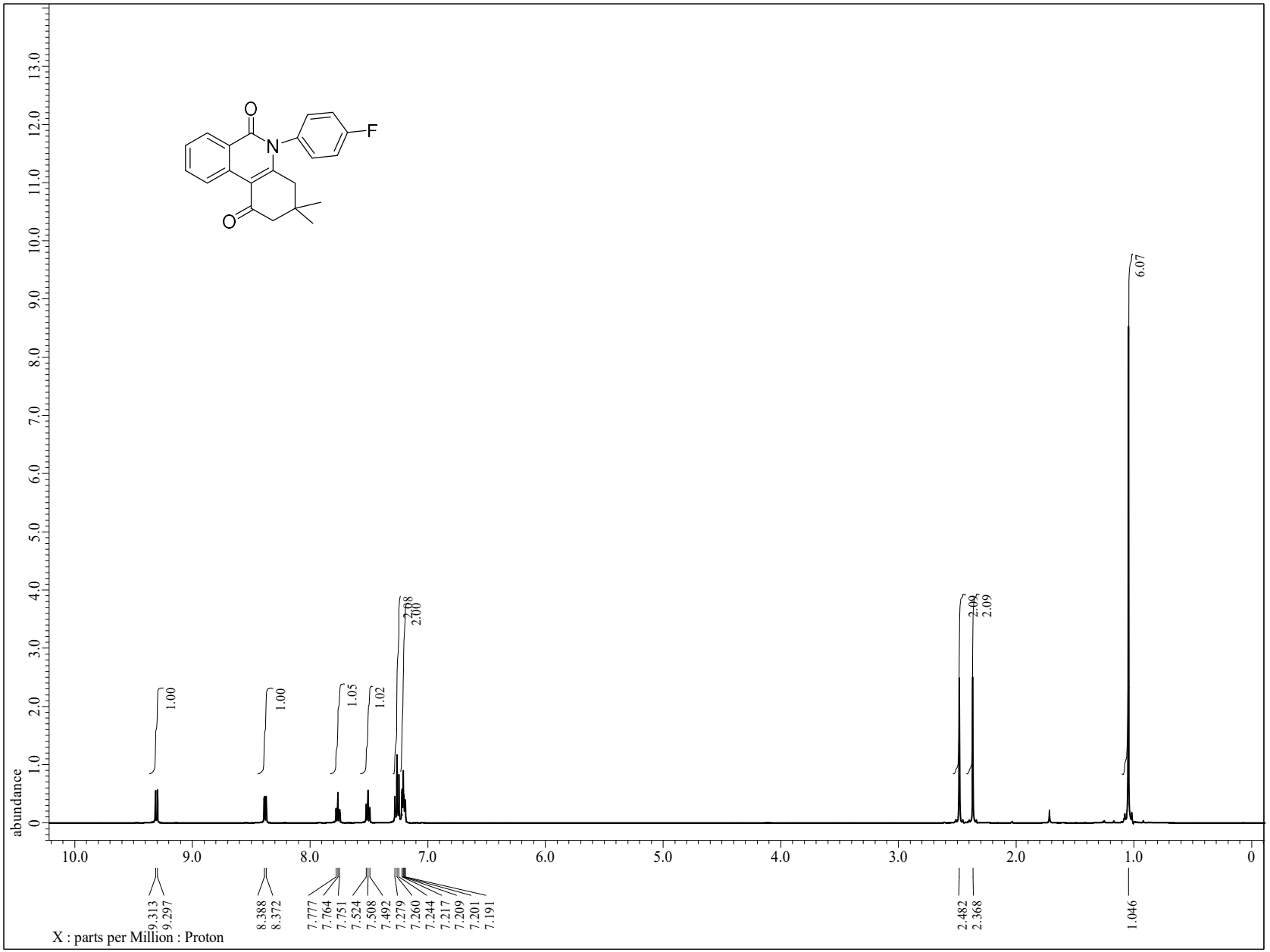

Figure S29: ^{1}H NMR (500 MHz, $CDCl_3$) of compound **6i**

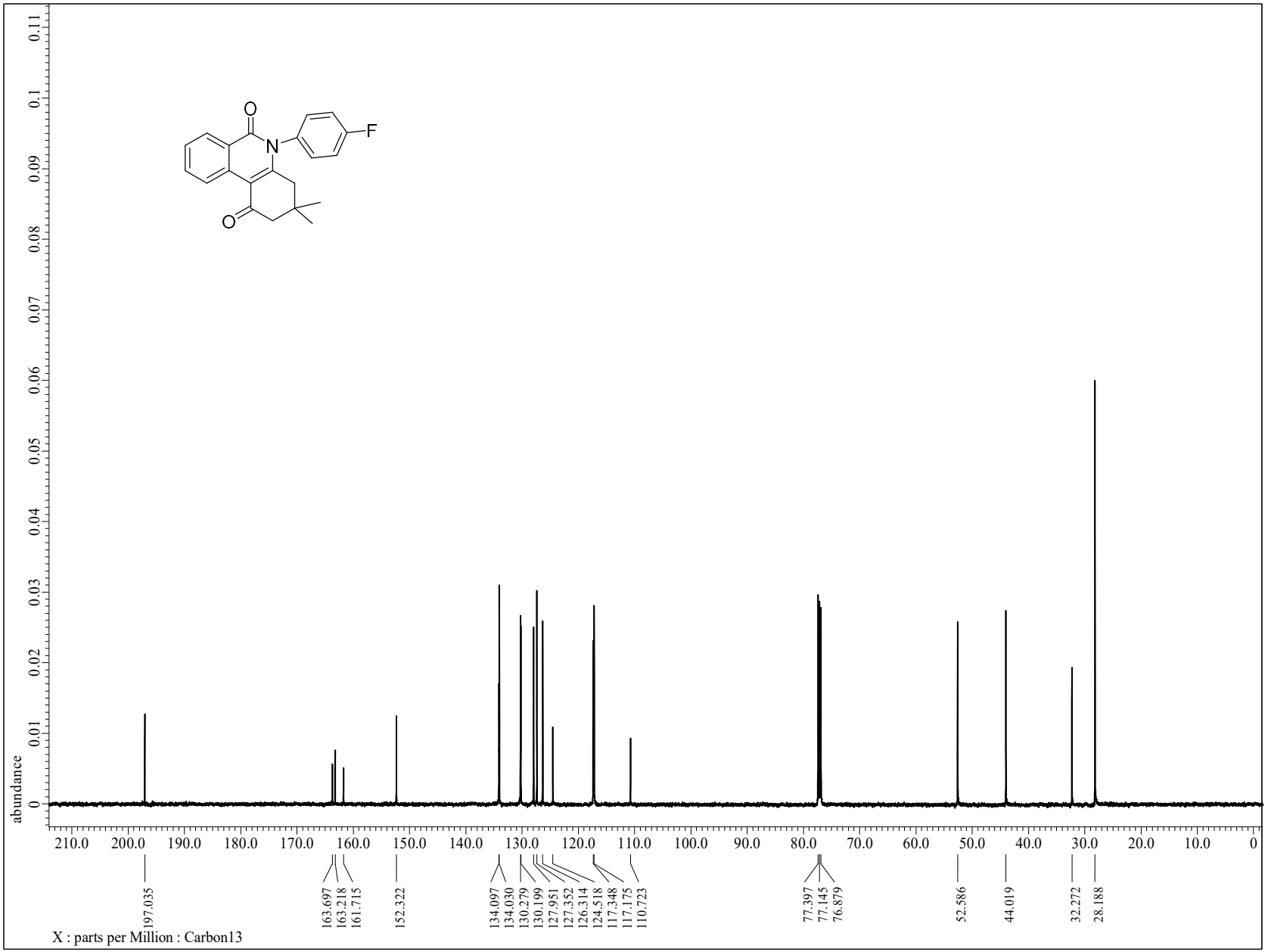

Figure S30: $^{13}C\{^{1}H\}$ NMR (125 MHz, $CDCl_3$) of compound **6i**

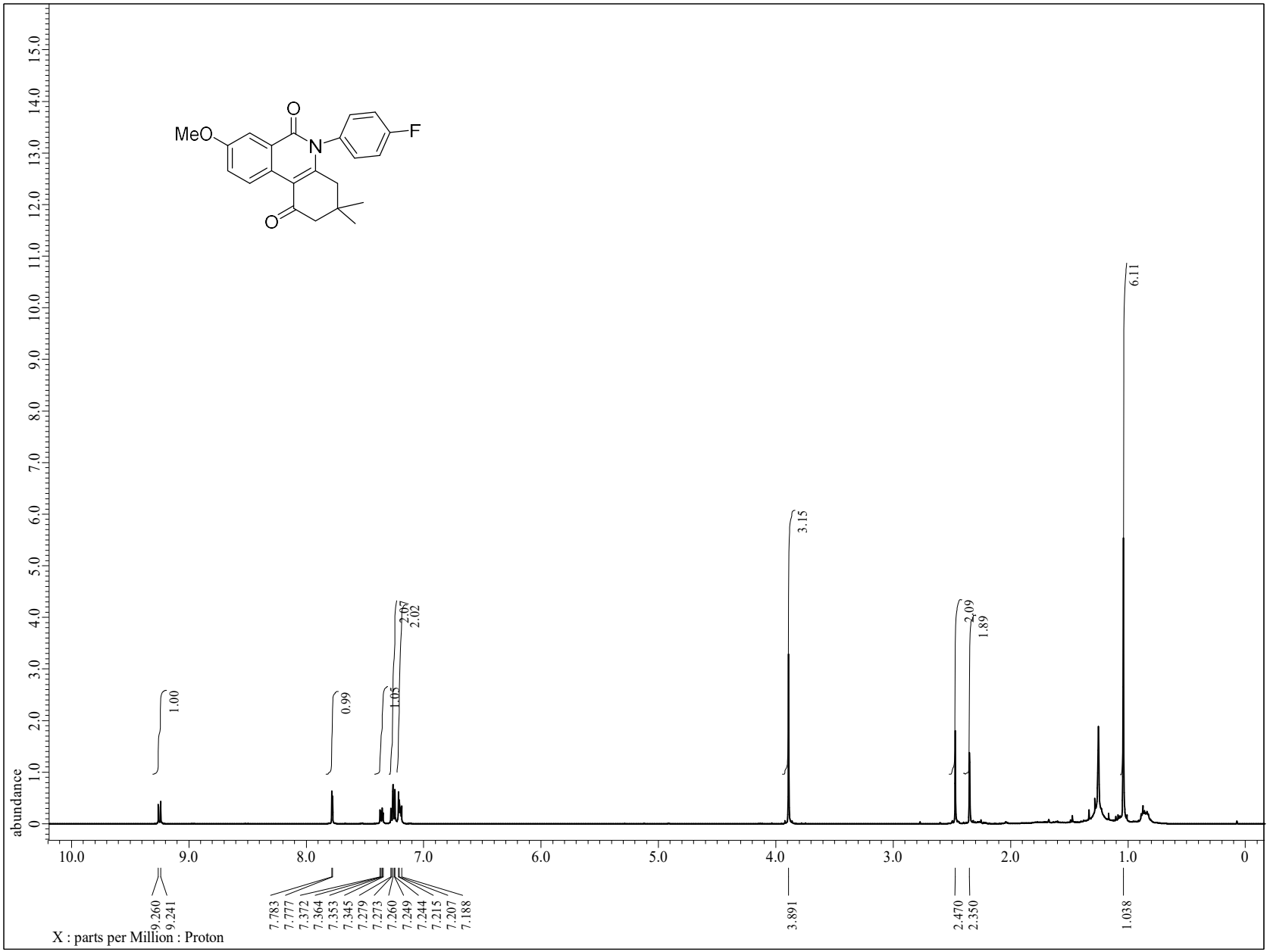

Figure S31: ^{1}H NMR (500 MHz, $CDCl_3$) of compound **6j**

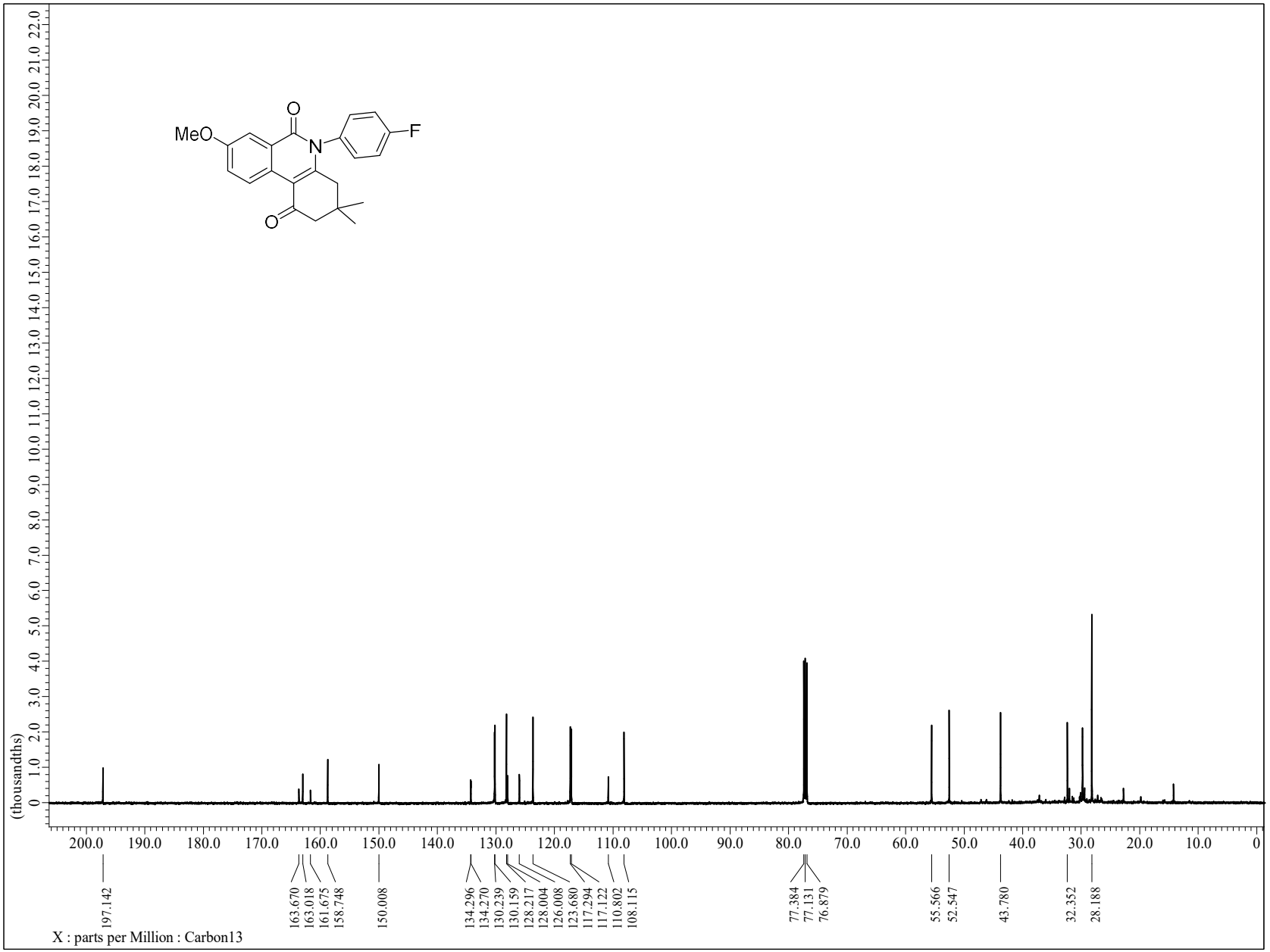

Figure S32: $^{13}C\{^{1}H\}$ NMR (125 MHz, $CDCl_3$) of compound **6j**

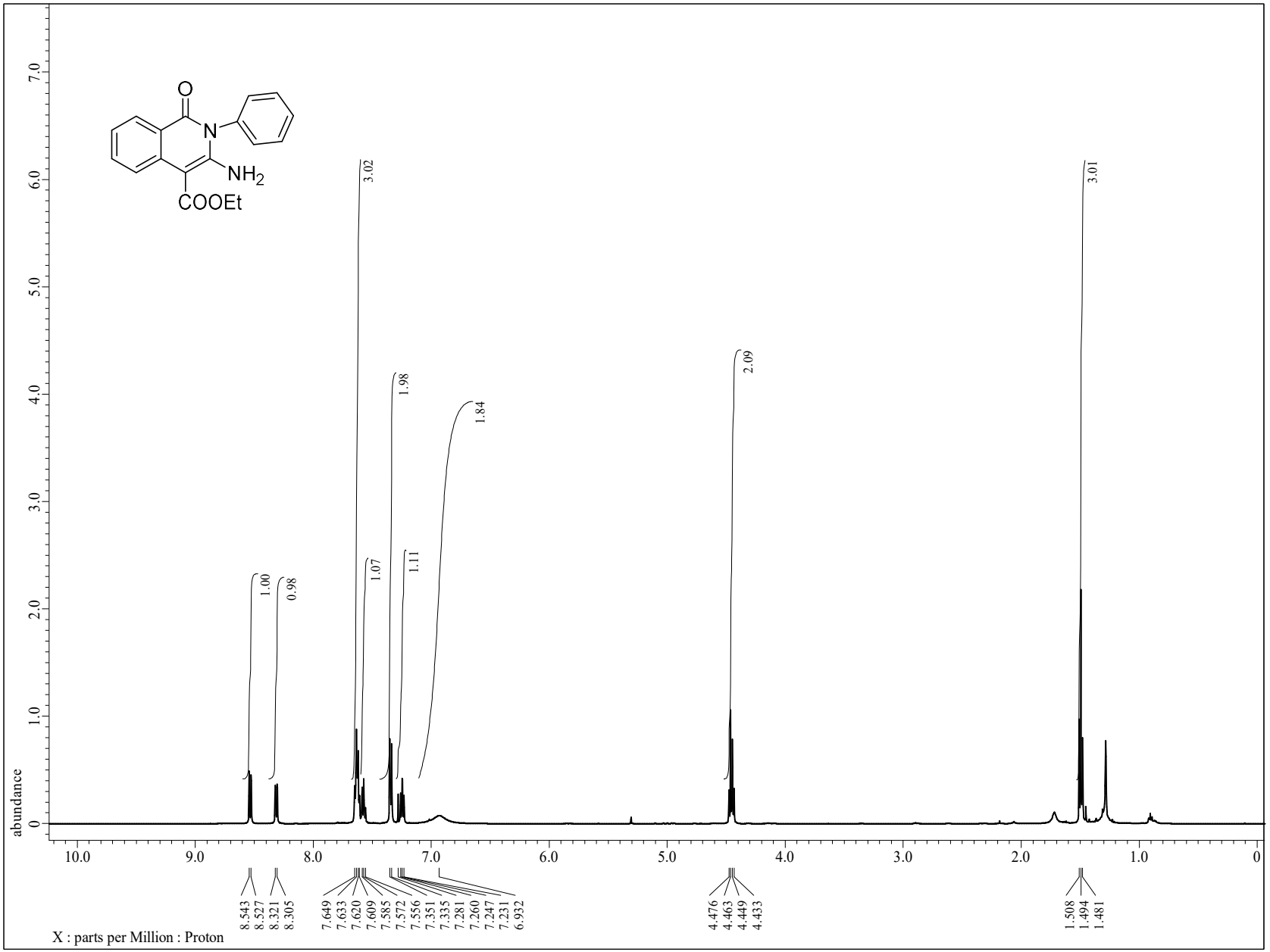

Figure S33: ^{1}H NMR (500 MHz, $CDCl_3$) of compound **7a**

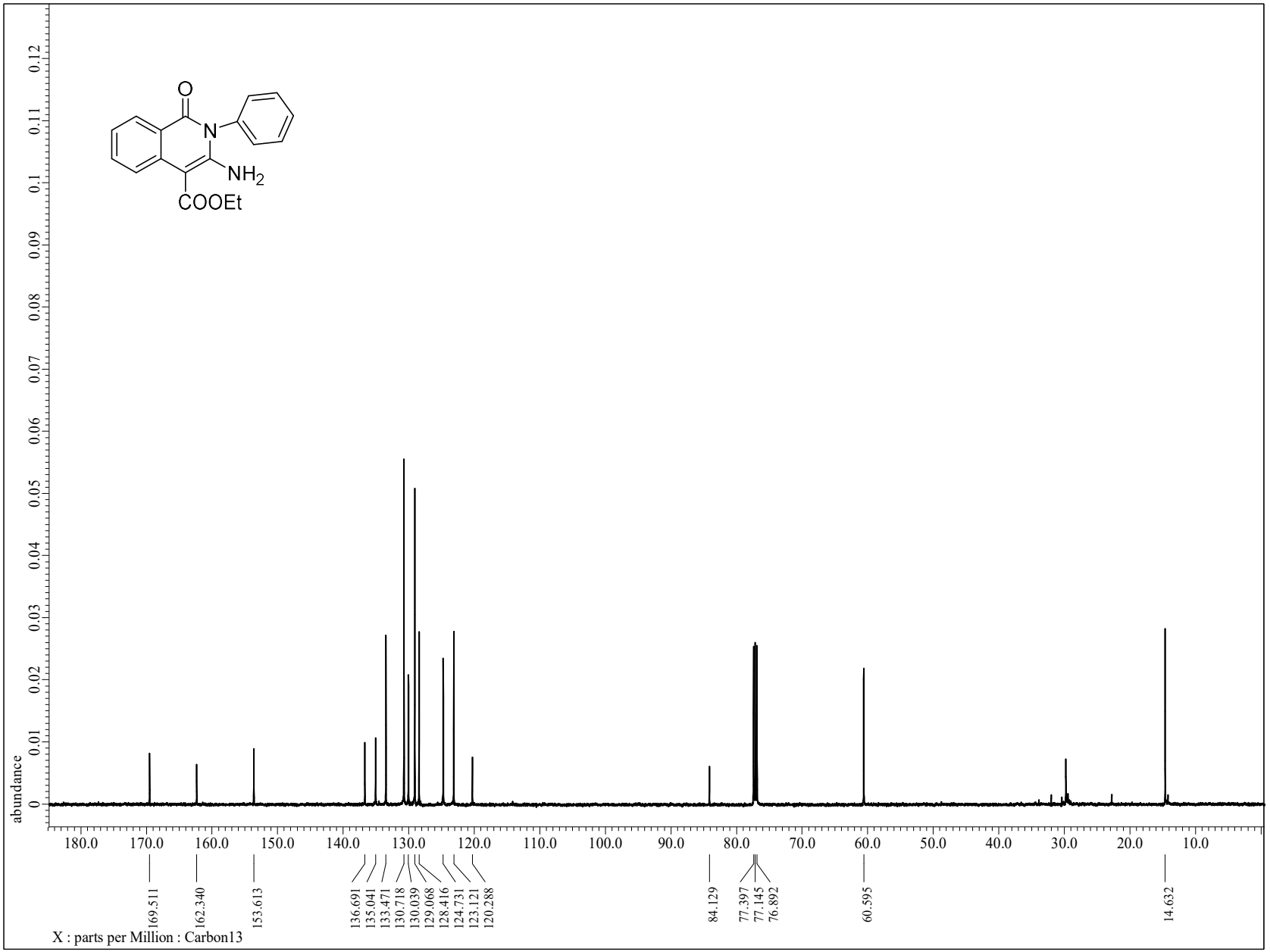

Figure S34: $^{13}C\{^{1}H\}$ NMR (125 MHz, $CDCl_3$) of compound **7a**

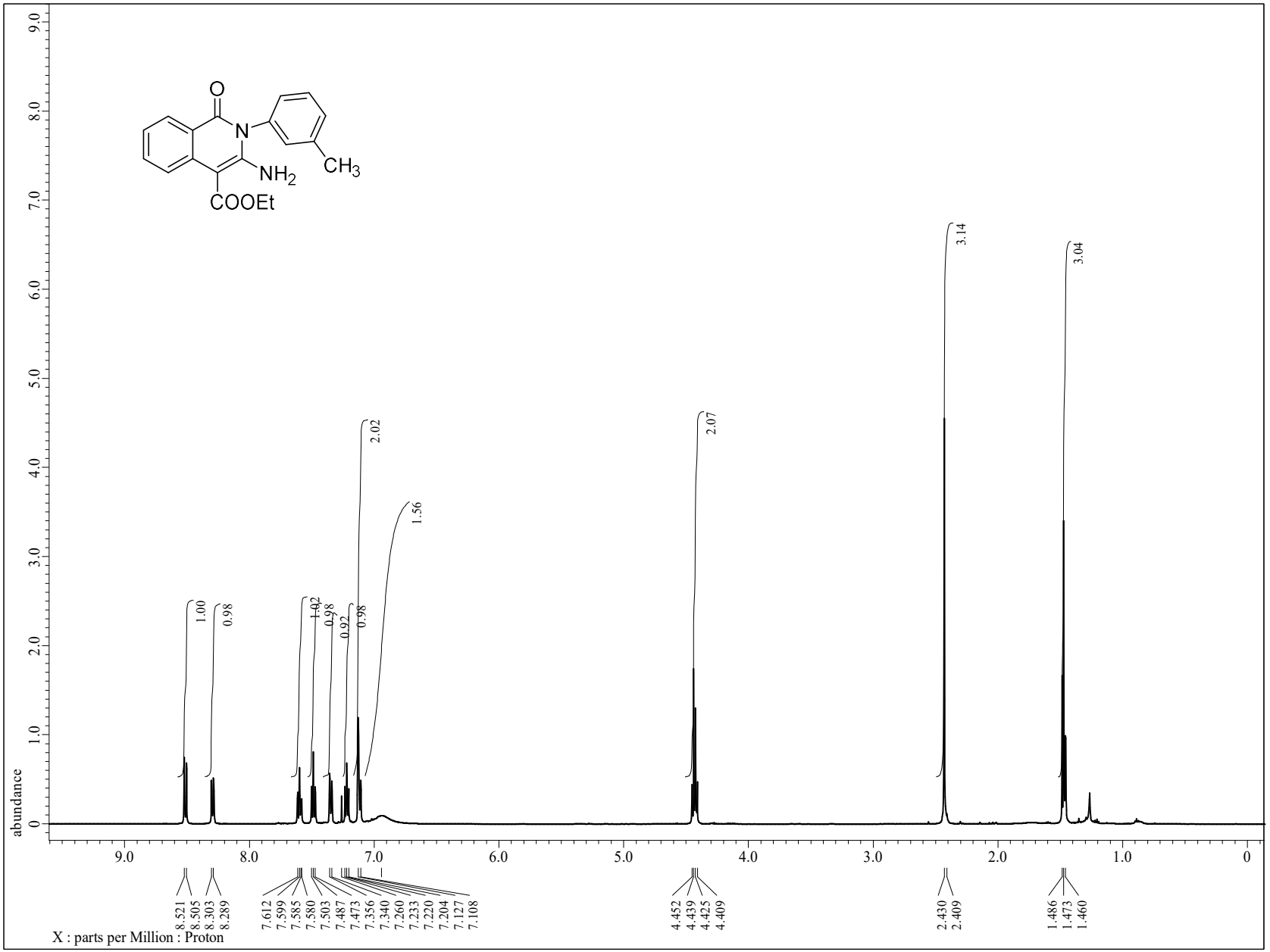

Figure S35: ^{1}H NMR (500 MHz, $CDCl_3$) of compound **7b**

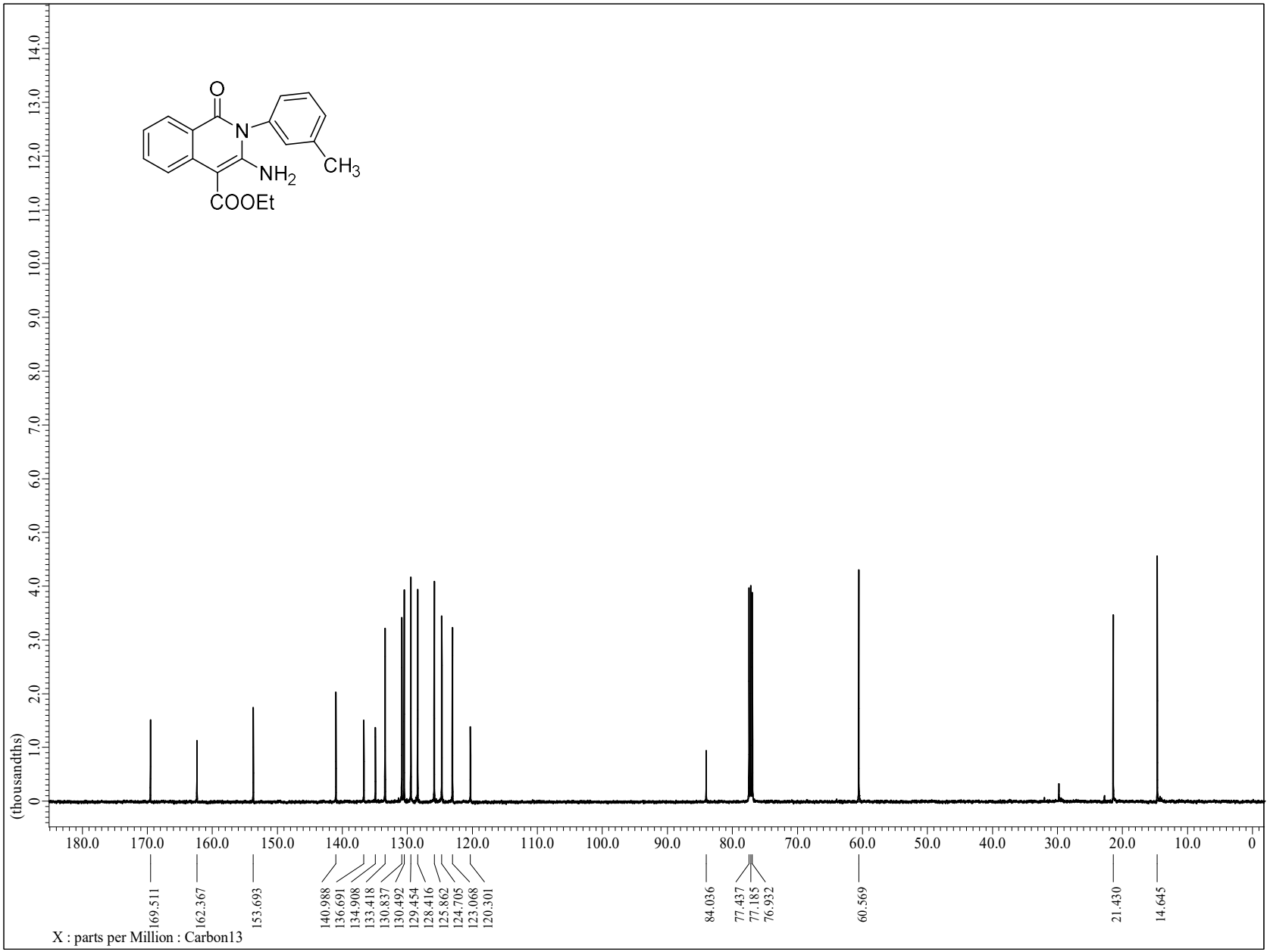

Figure S36: $^{13}C\{^{1}H\}$ NMR (125 MHz, $CDCl_3$) of compound **7b**

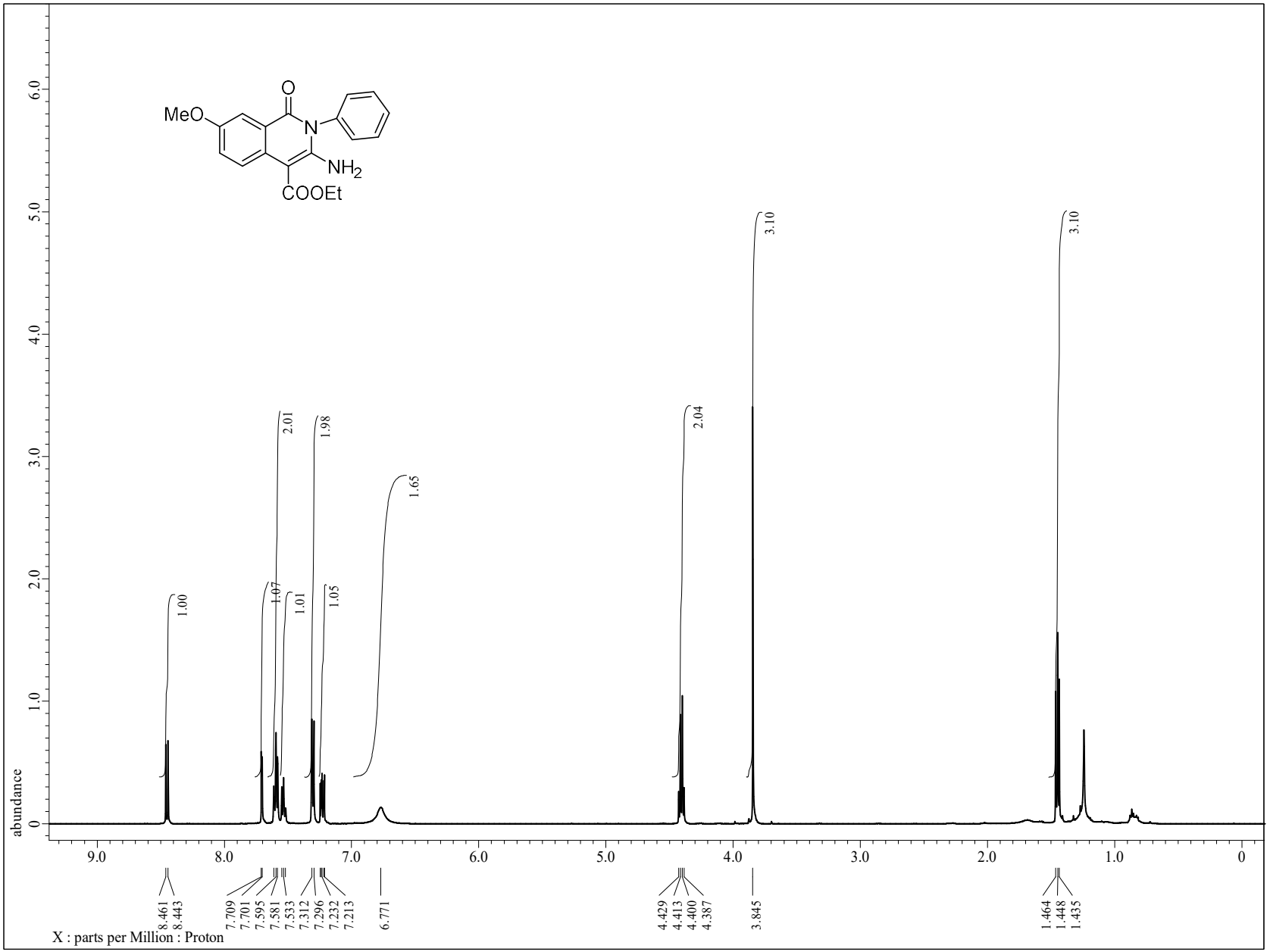

Figure S37: ^{1}H NMR (500 MHz, $CDCl_3$) of compound **7c**

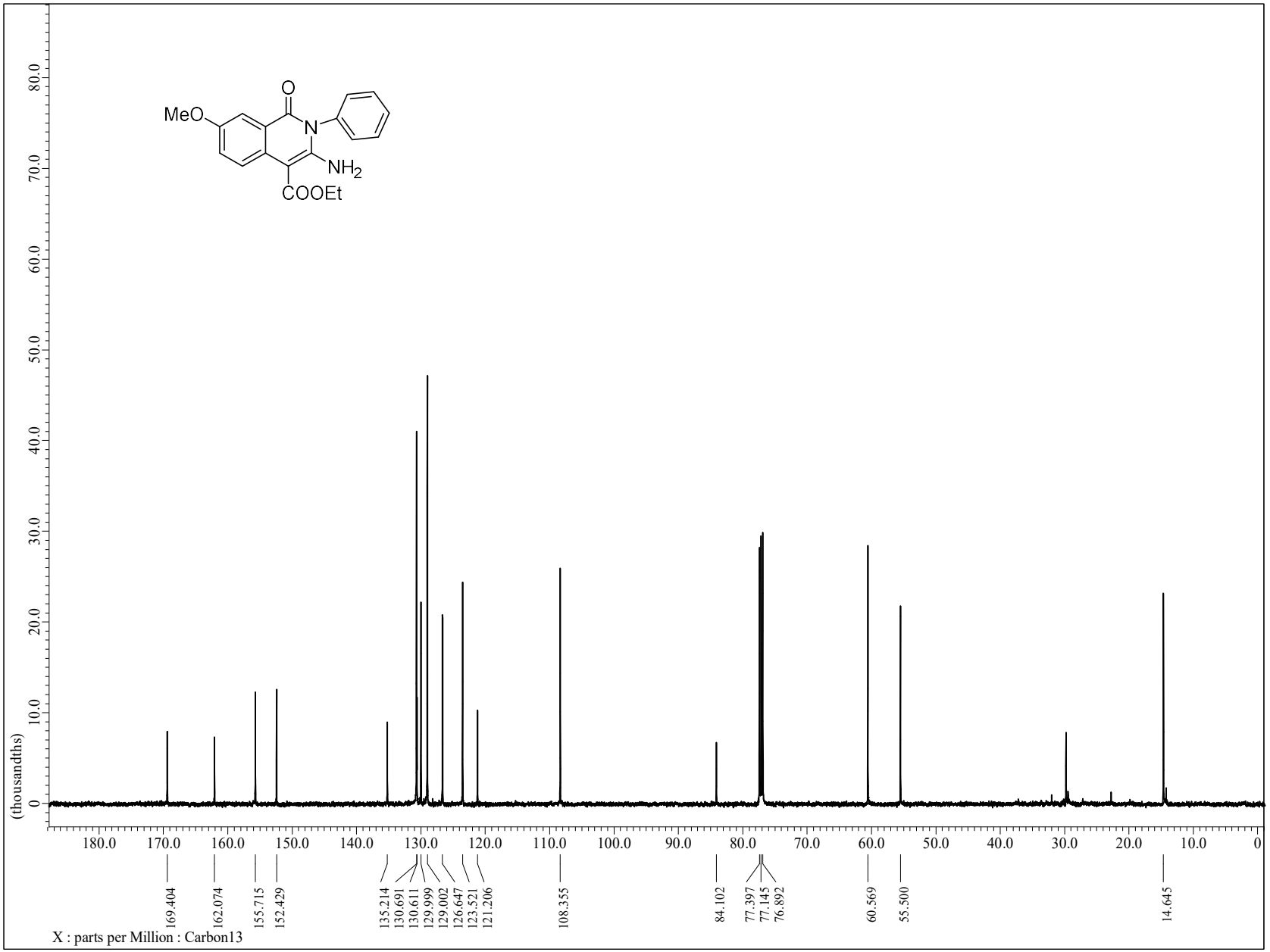

Figure S38: $^{13}C\{^{1}H\}$ NMR (125 MHz, $CDCl_3$) of compound **7c**

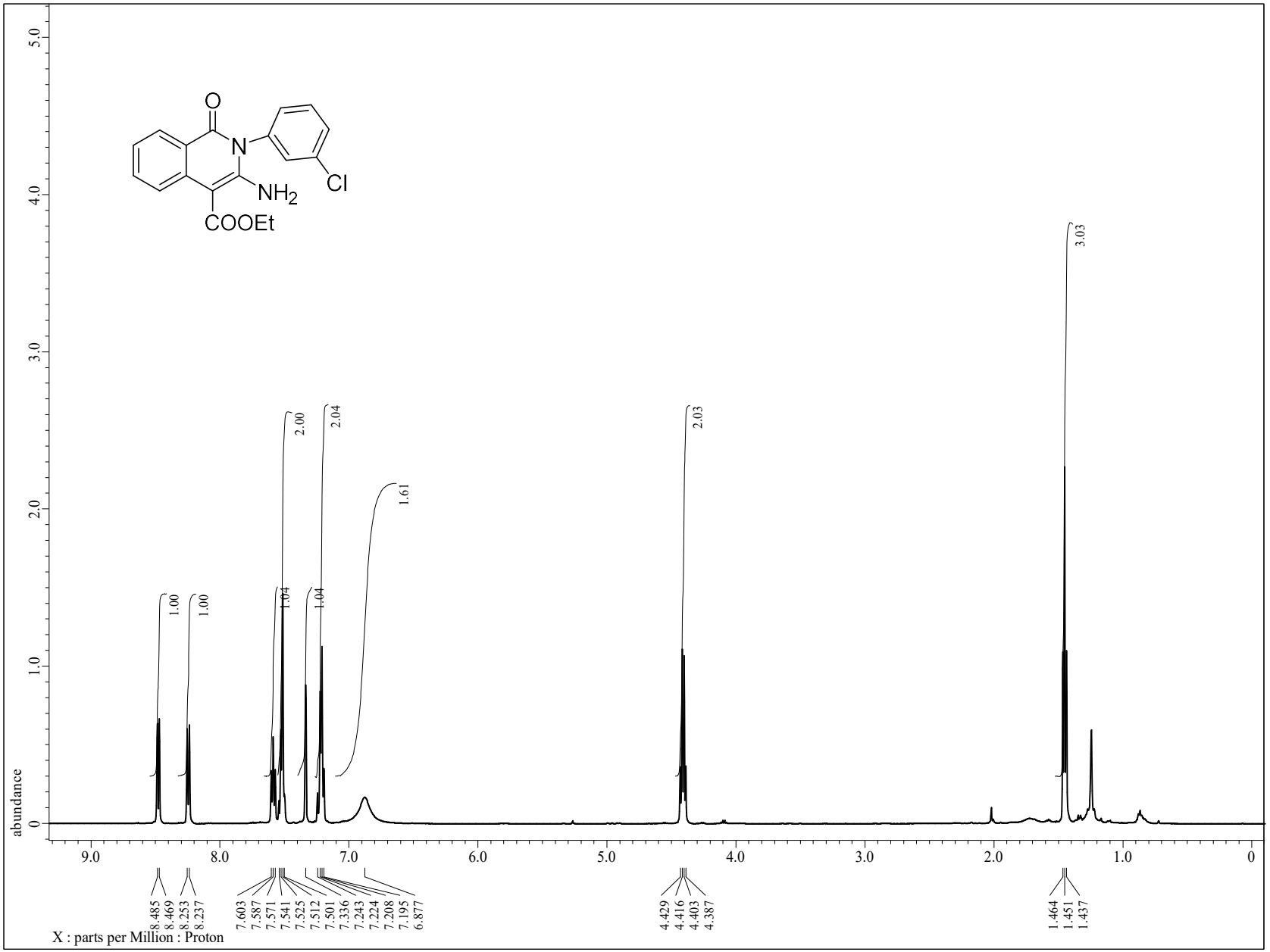

Figure S39: ^{1}H NMR (500 MHz, $CDCl_3$) of compound **7d**

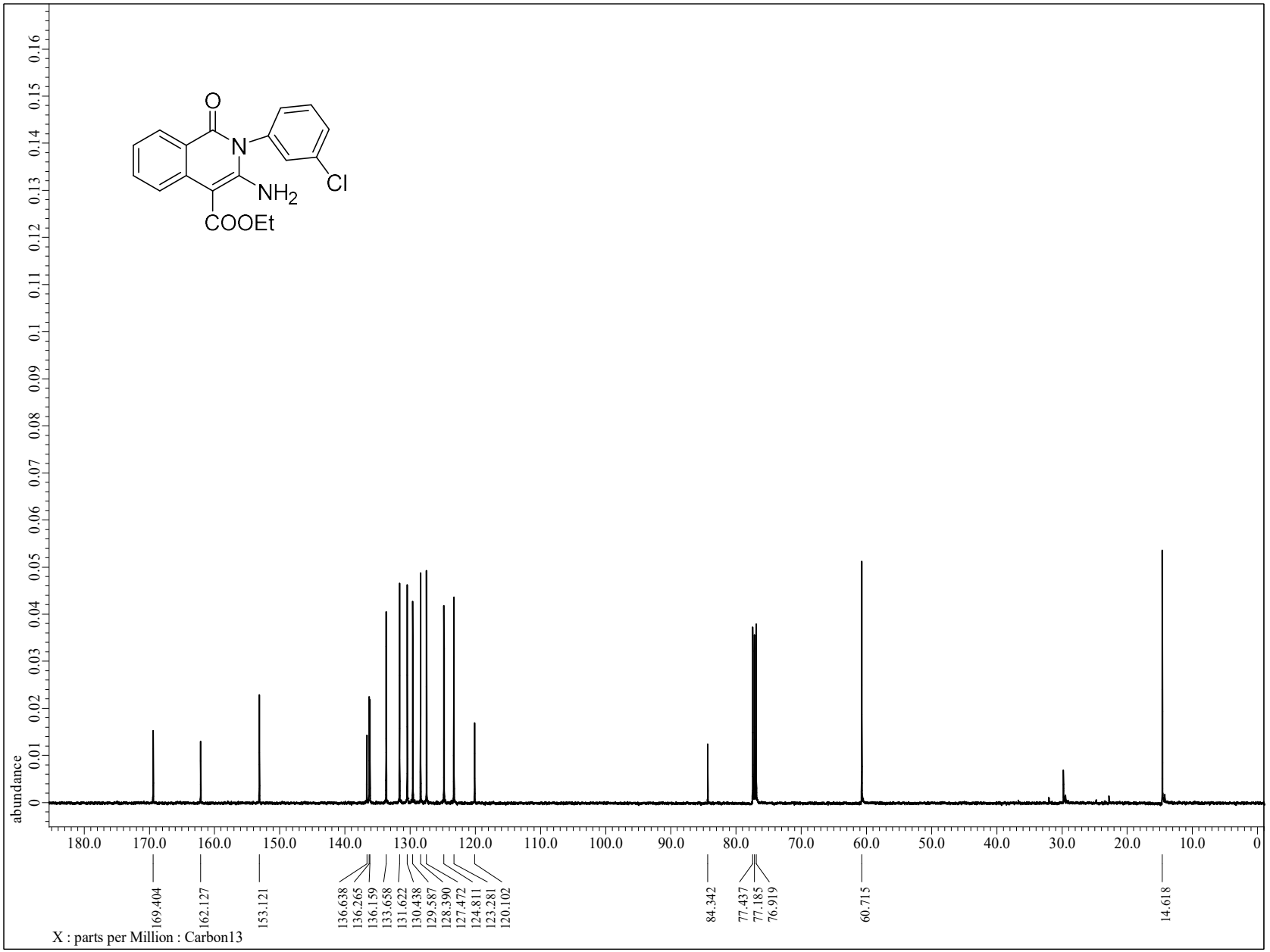

Figure S40: $^{13}C\{^{1}H\}$ NMR (125 MHz, $CDCl_3$) of compound **7d**

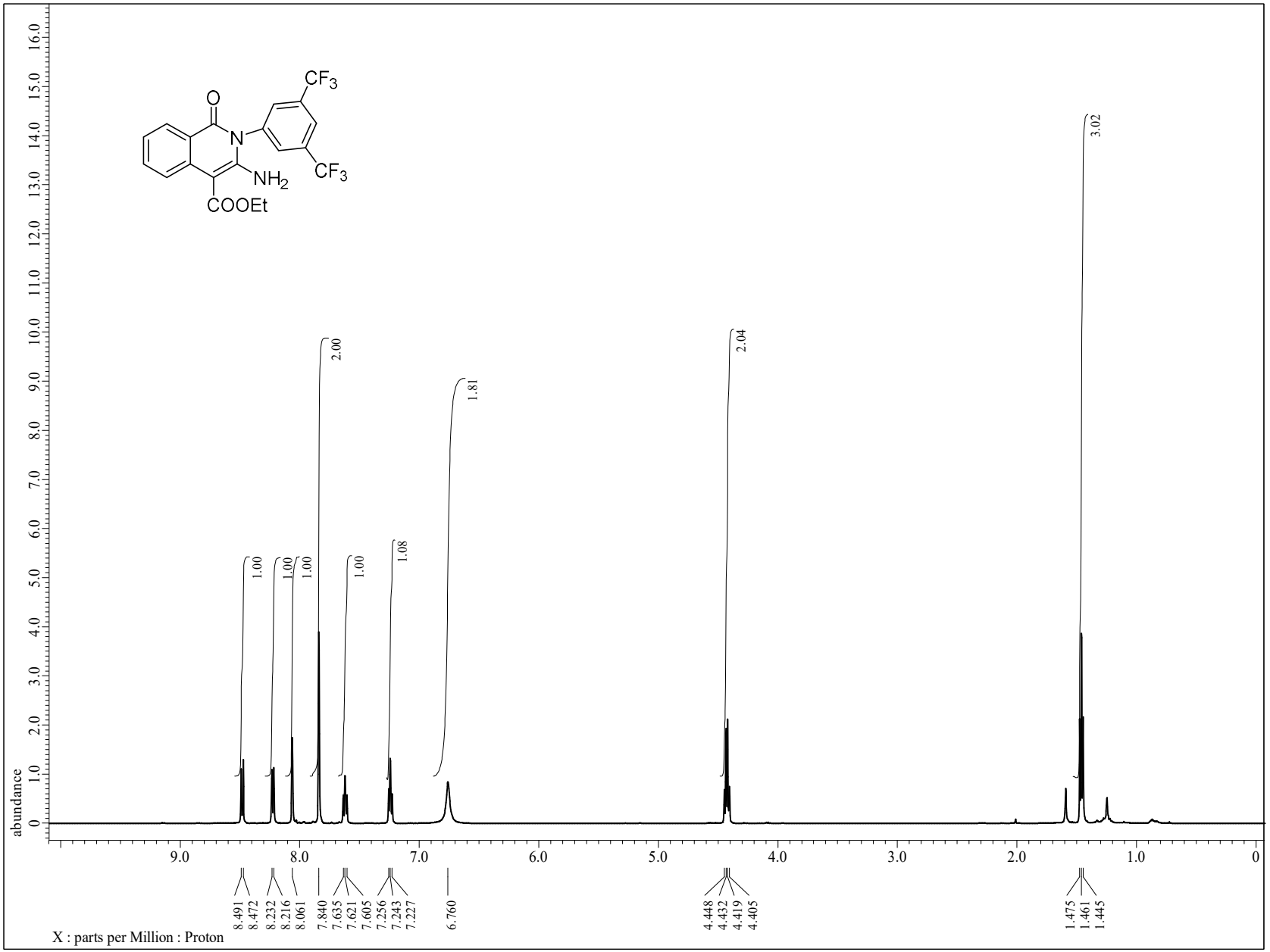

Figure S41: ^{1}H NMR (500 MHz, $CDCl_3$) of compound **7e**

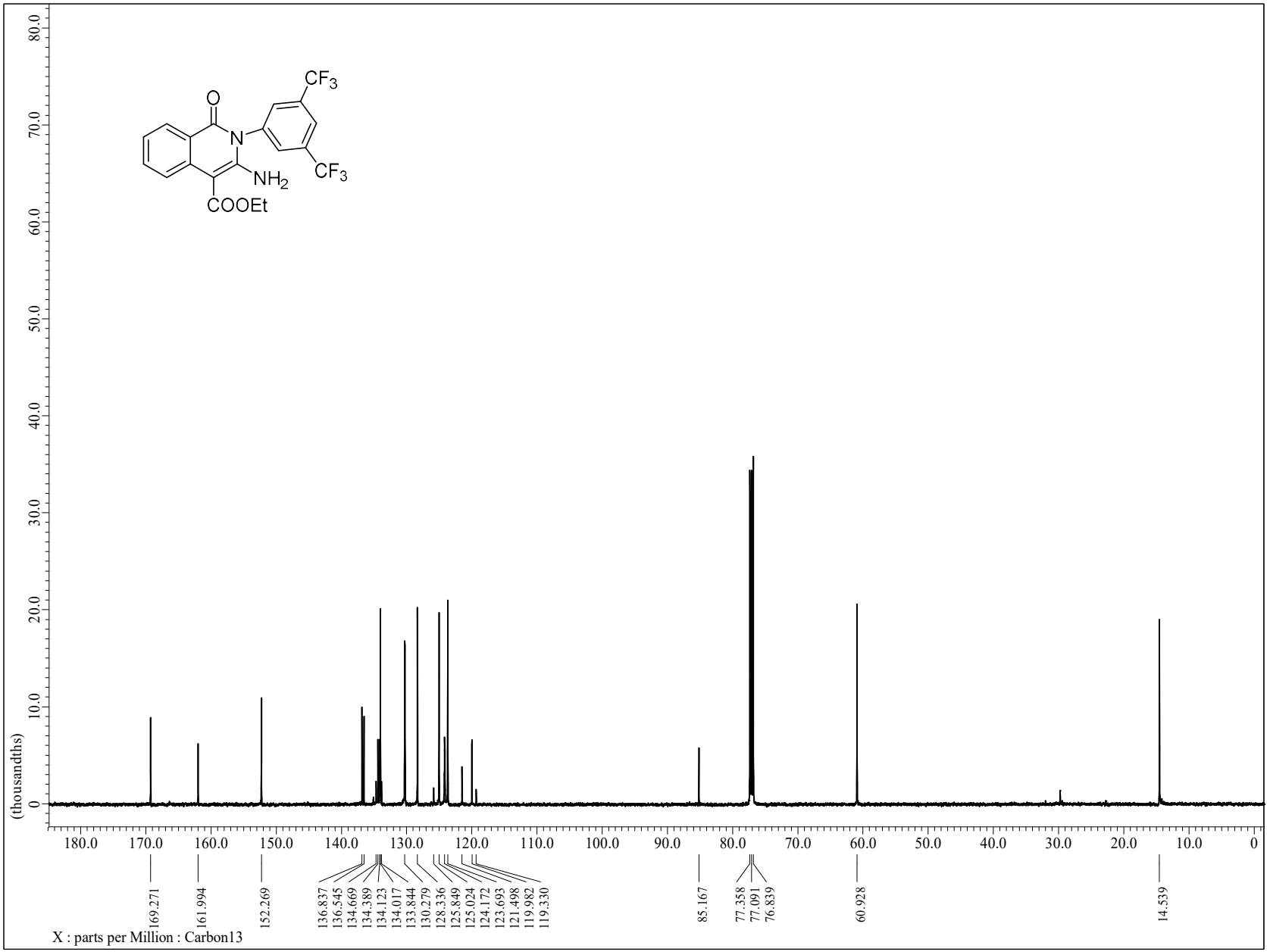

Figure S42: $^{13}C\{^{1}H\}$ NMR (125 MHz, $CDCl_3$) of compound **7e**

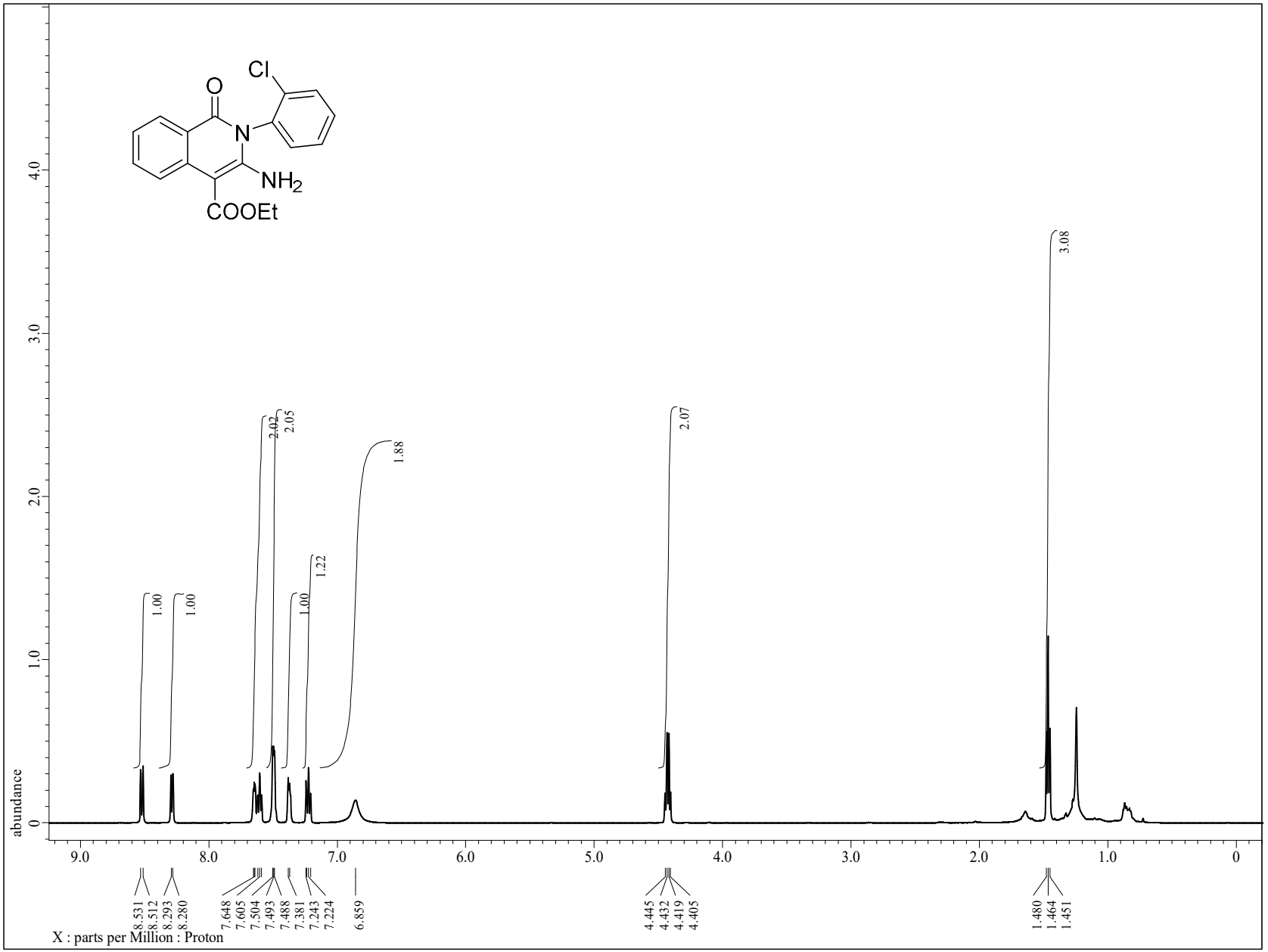

Figure S43: ^{1}H NMR (500 MHz, $CDCl_3$) of compound **7f**

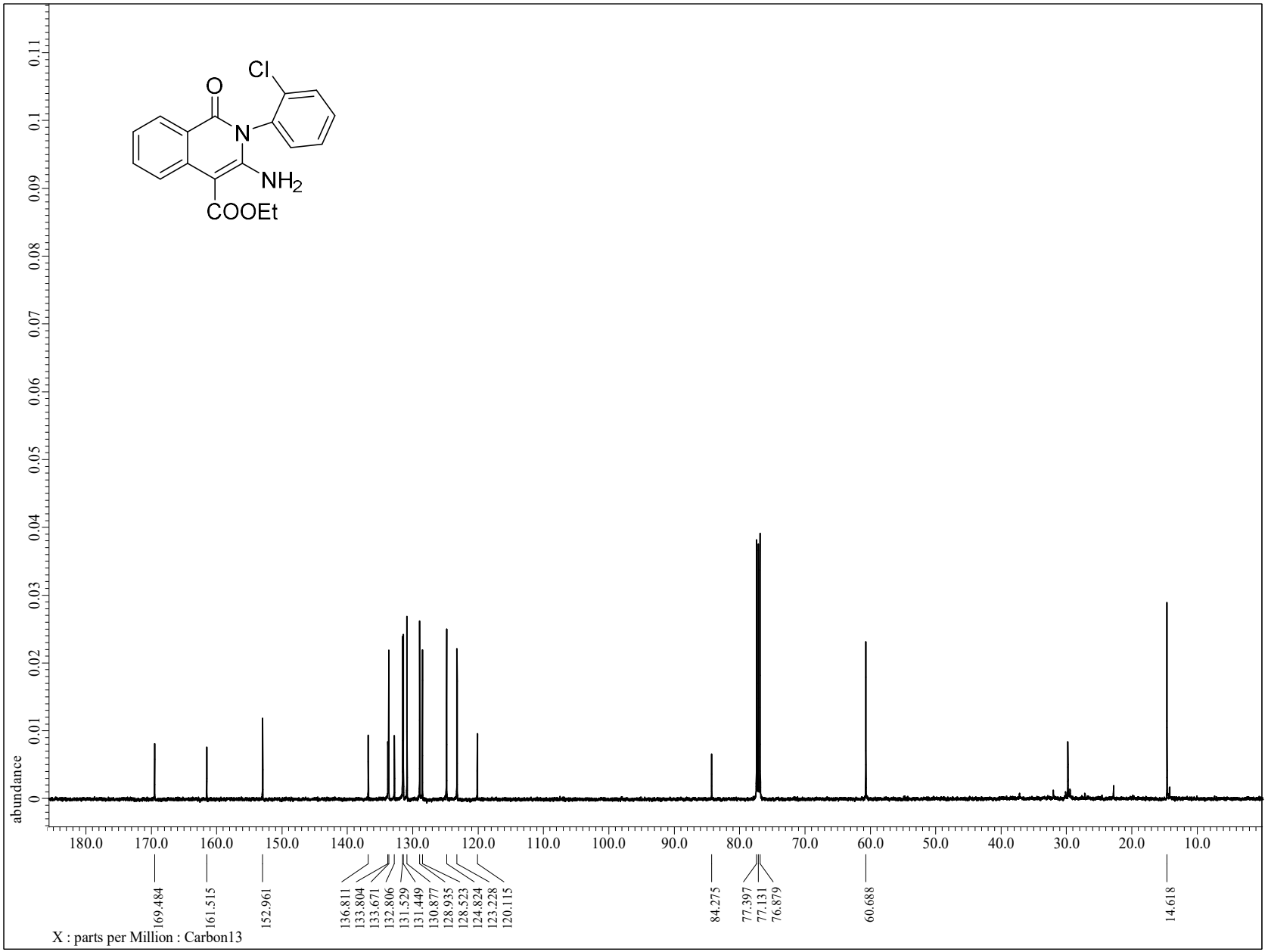

Figure S44: $^{13}C\{^{1}H\}$ NMR (125 MHz, $CDCl_3$) of compound **7f**

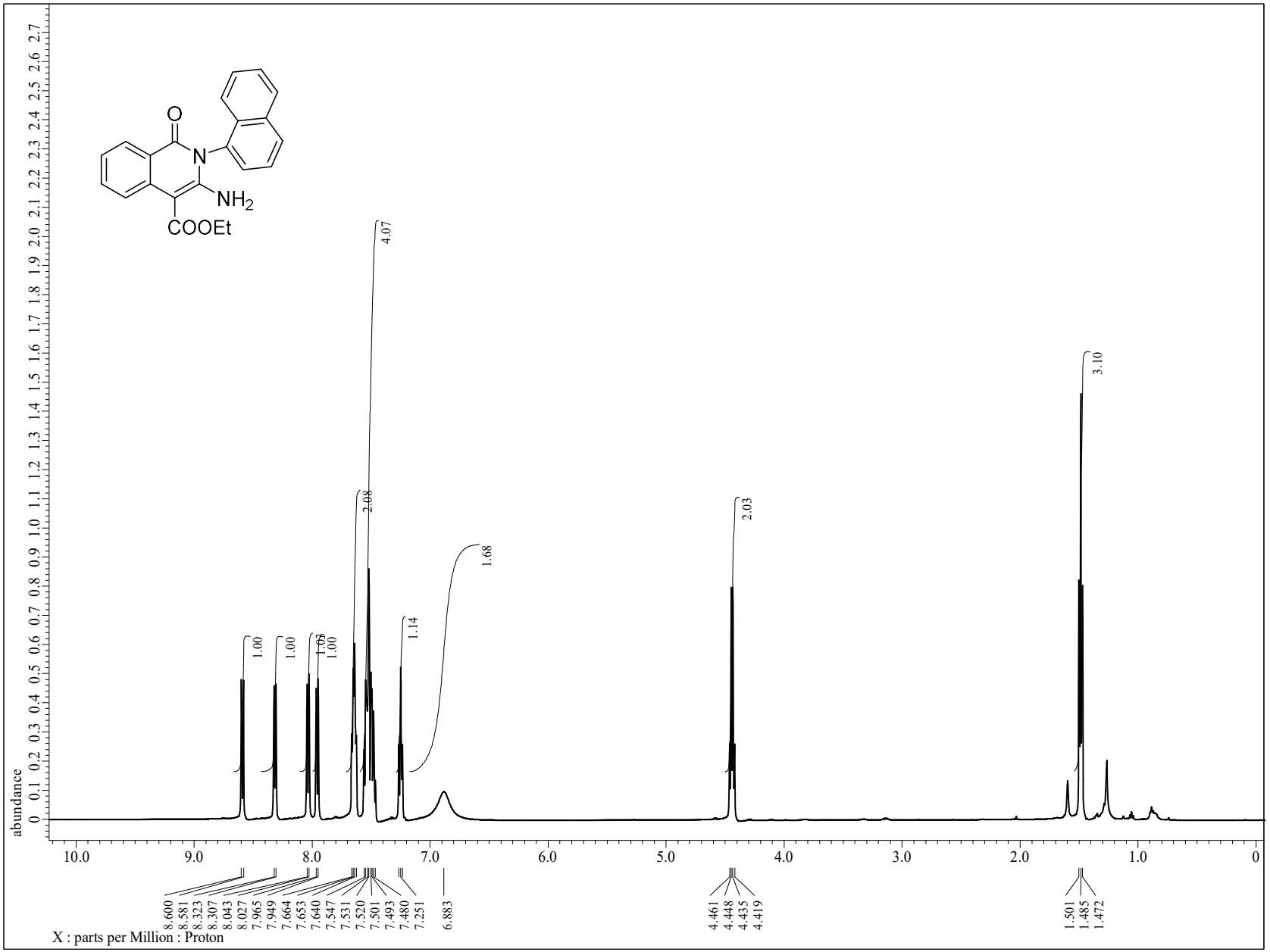

Figure S45: ^{1}H NMR (500 MHz, $CDCl_3$) of compound **7g**

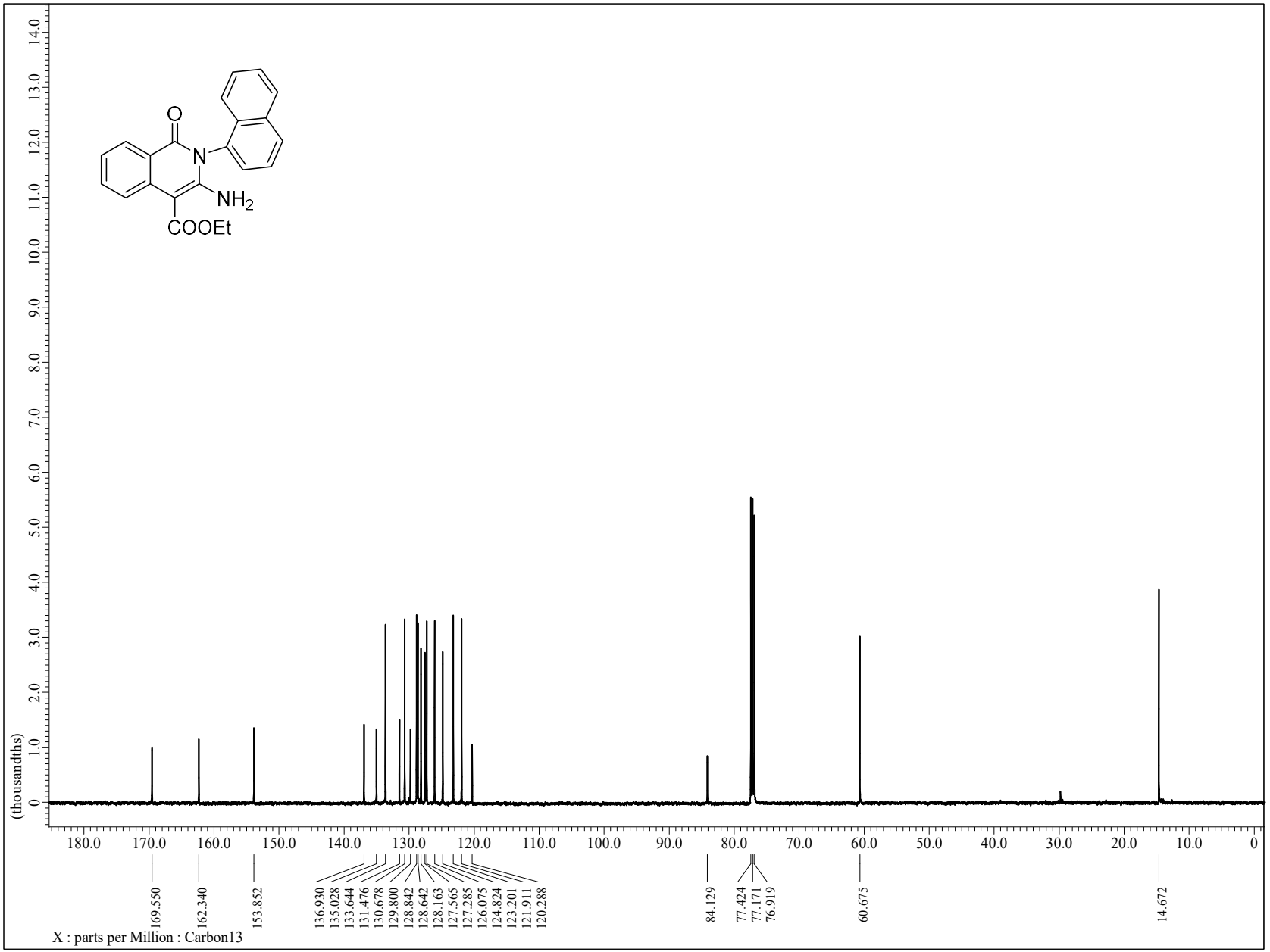

Figure S46: $^{13}C\{^{1}H\}$ NMR (125 MHz, $CDCl_3$) of compound **7g**

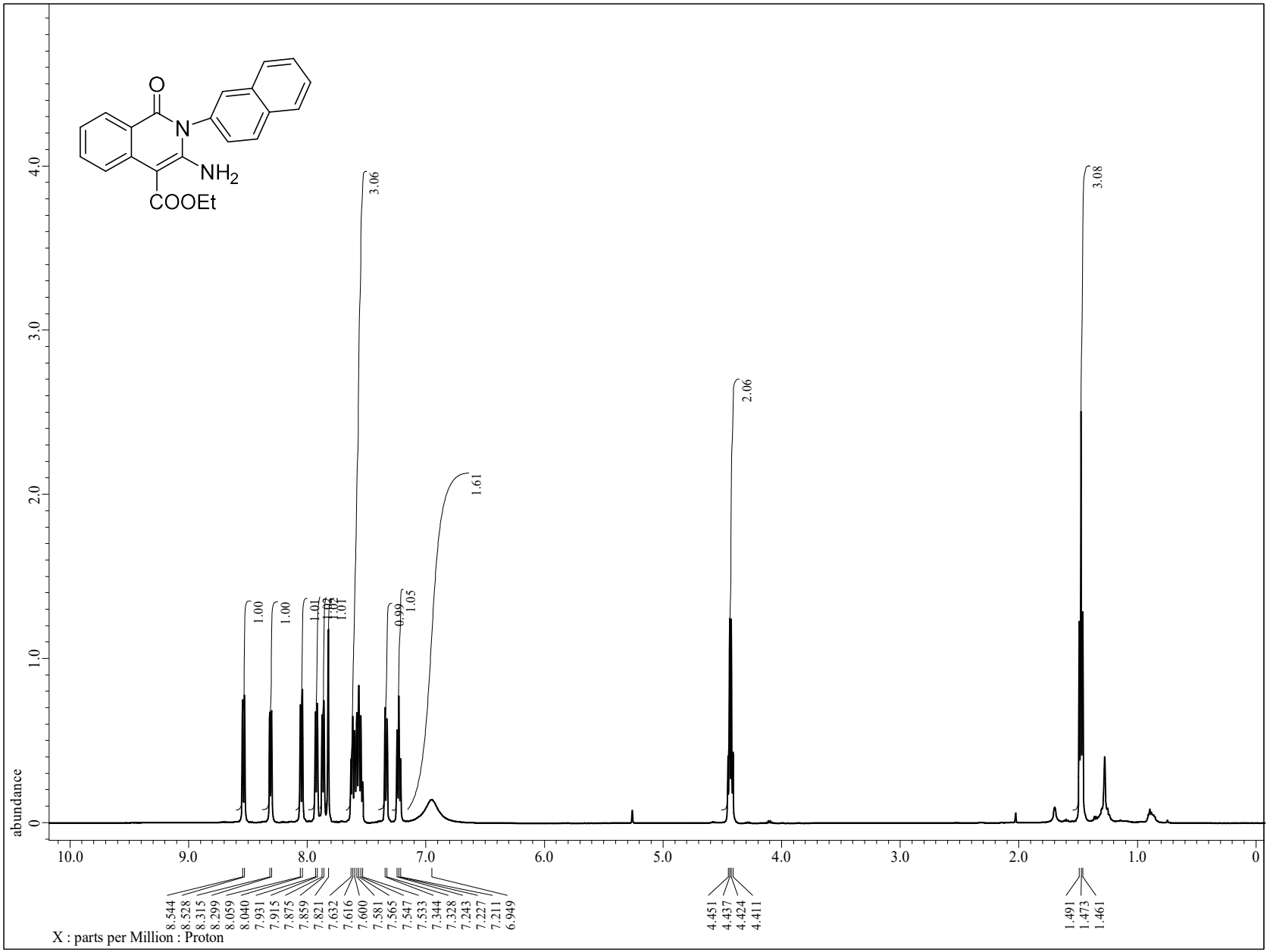

Figure S47: ^{1}H NMR (500 MHz, $CDCl_3$) of compound **7h**

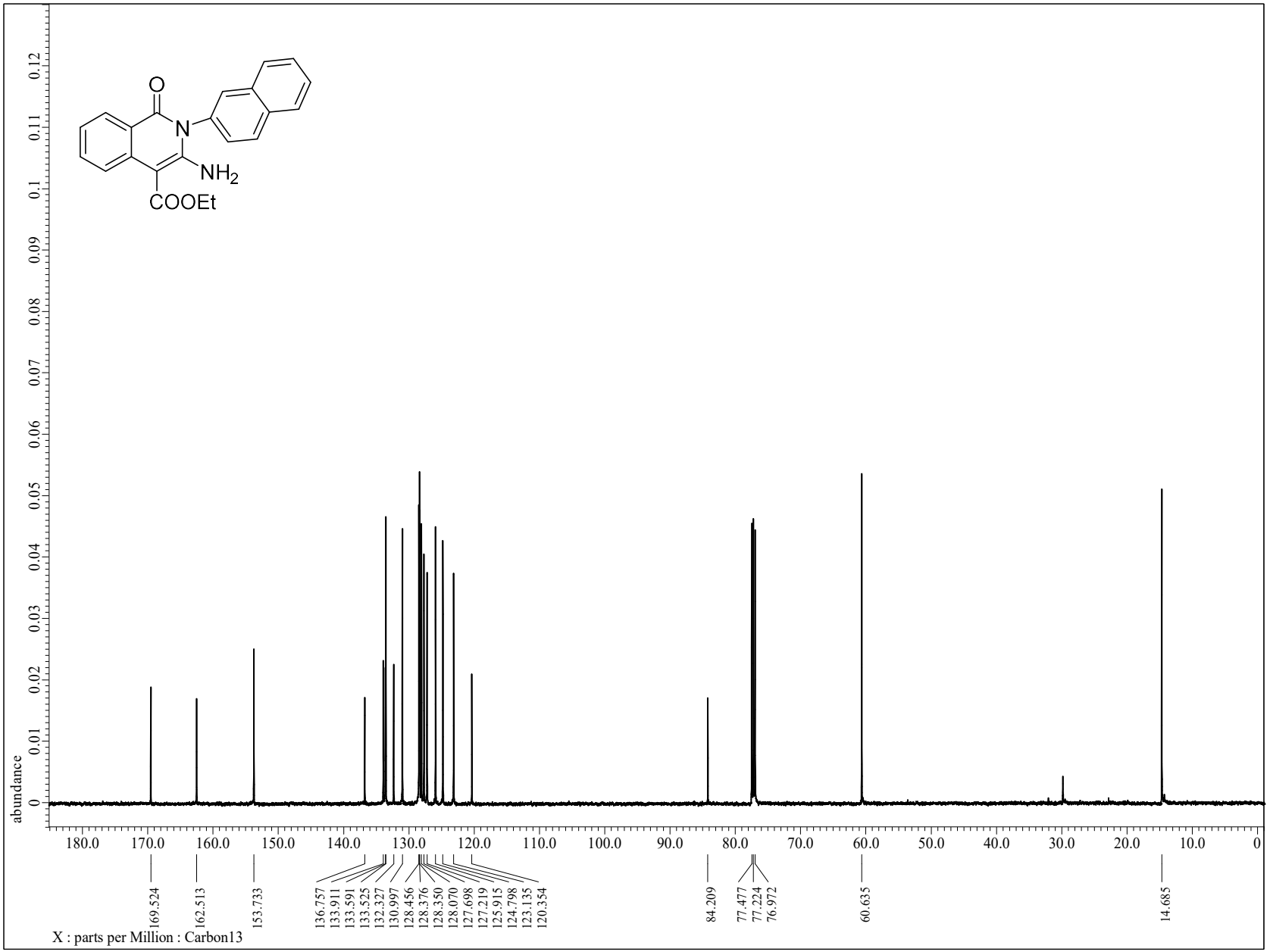

Figure S48: $^{13}C\{^{1}H\}$ NMR (125 MHz, $CDCl_3$) of compound **7h**

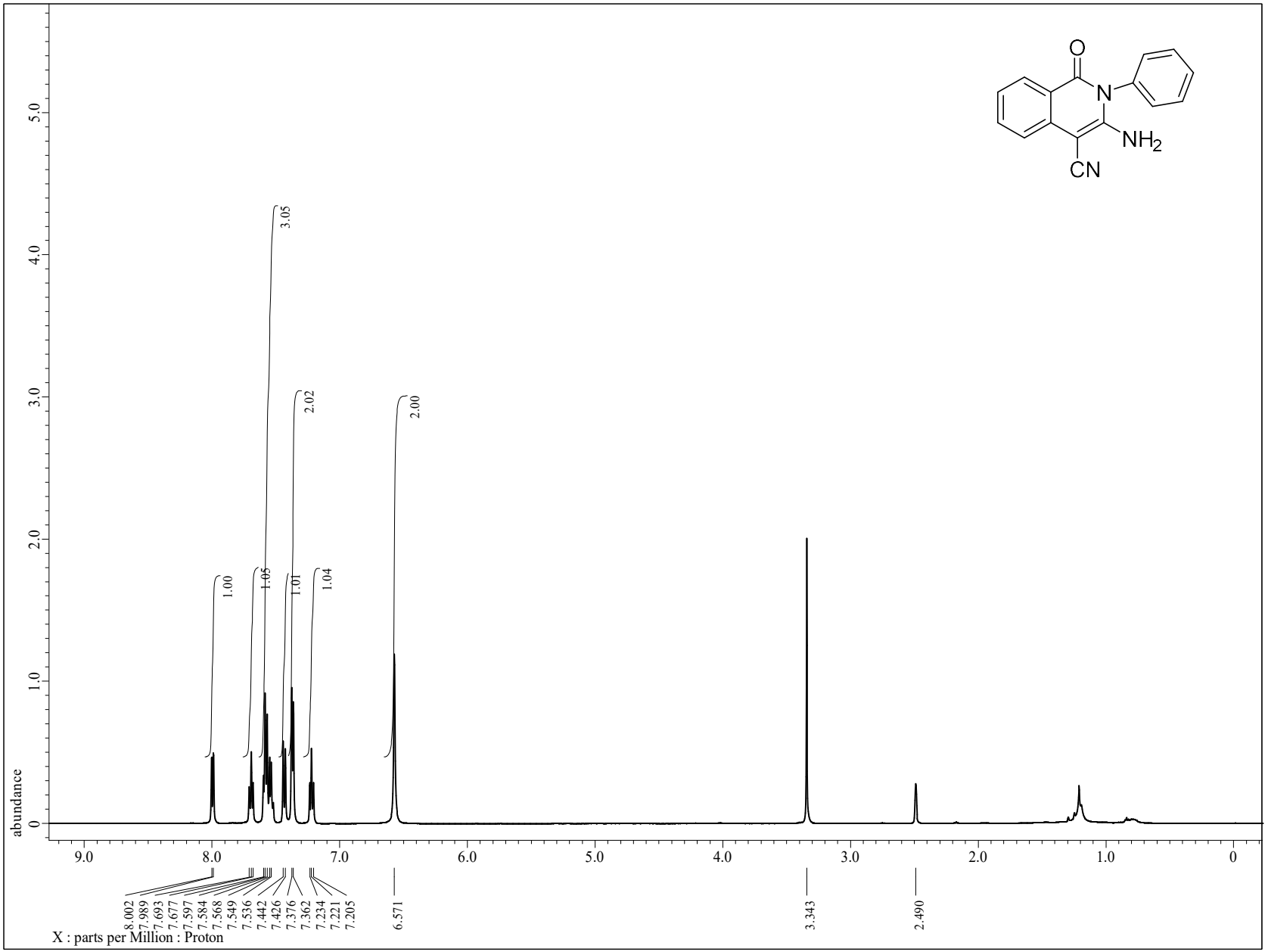

Figure S49: ^{1}H NMR (500 MHz, DMSO-d_6) of compound **8a**

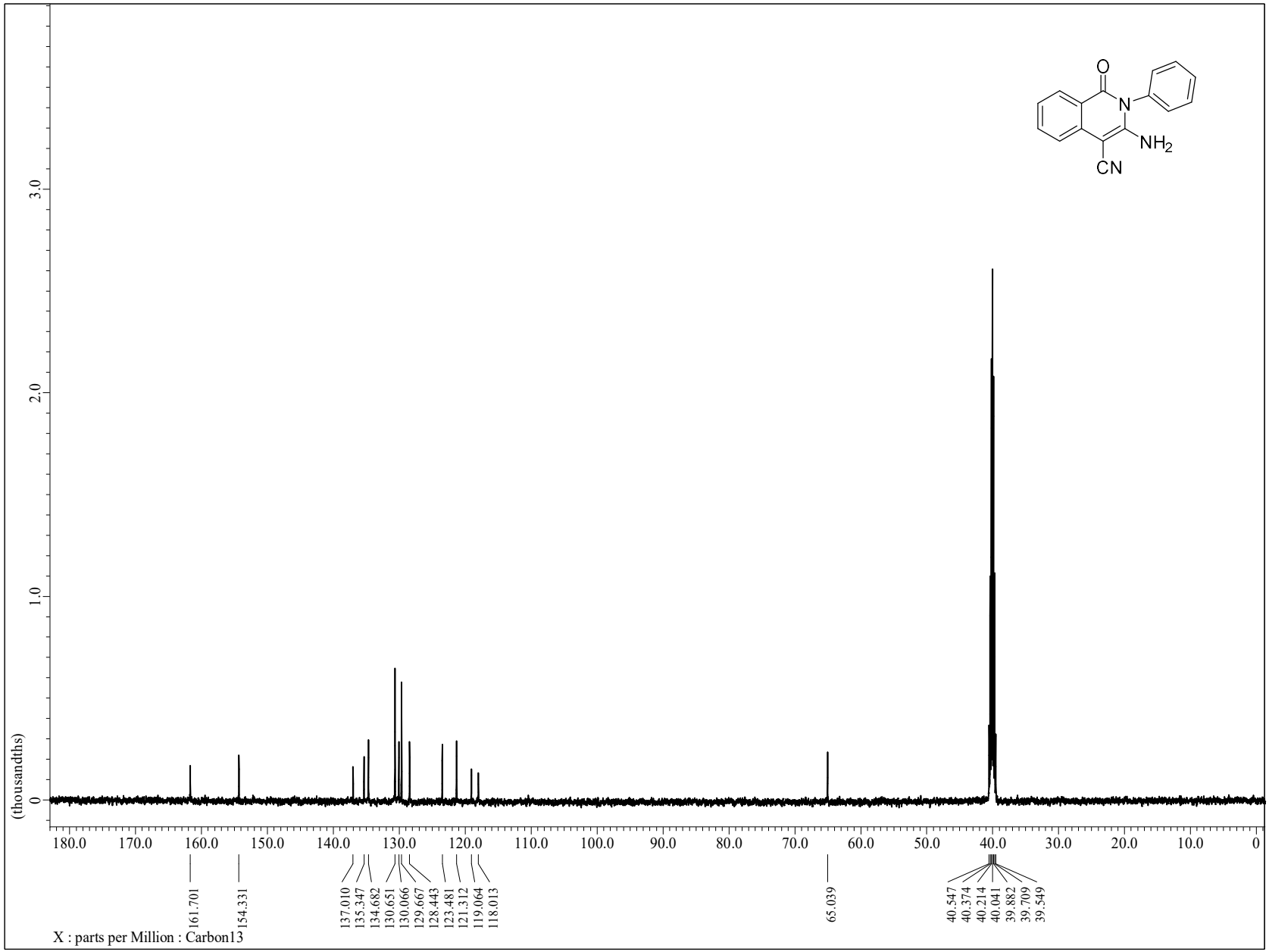

Figure S50: $^{13}C\{^{1}H\}$ NMR (125 MHz, DMSO-d_6) of compound **8a**

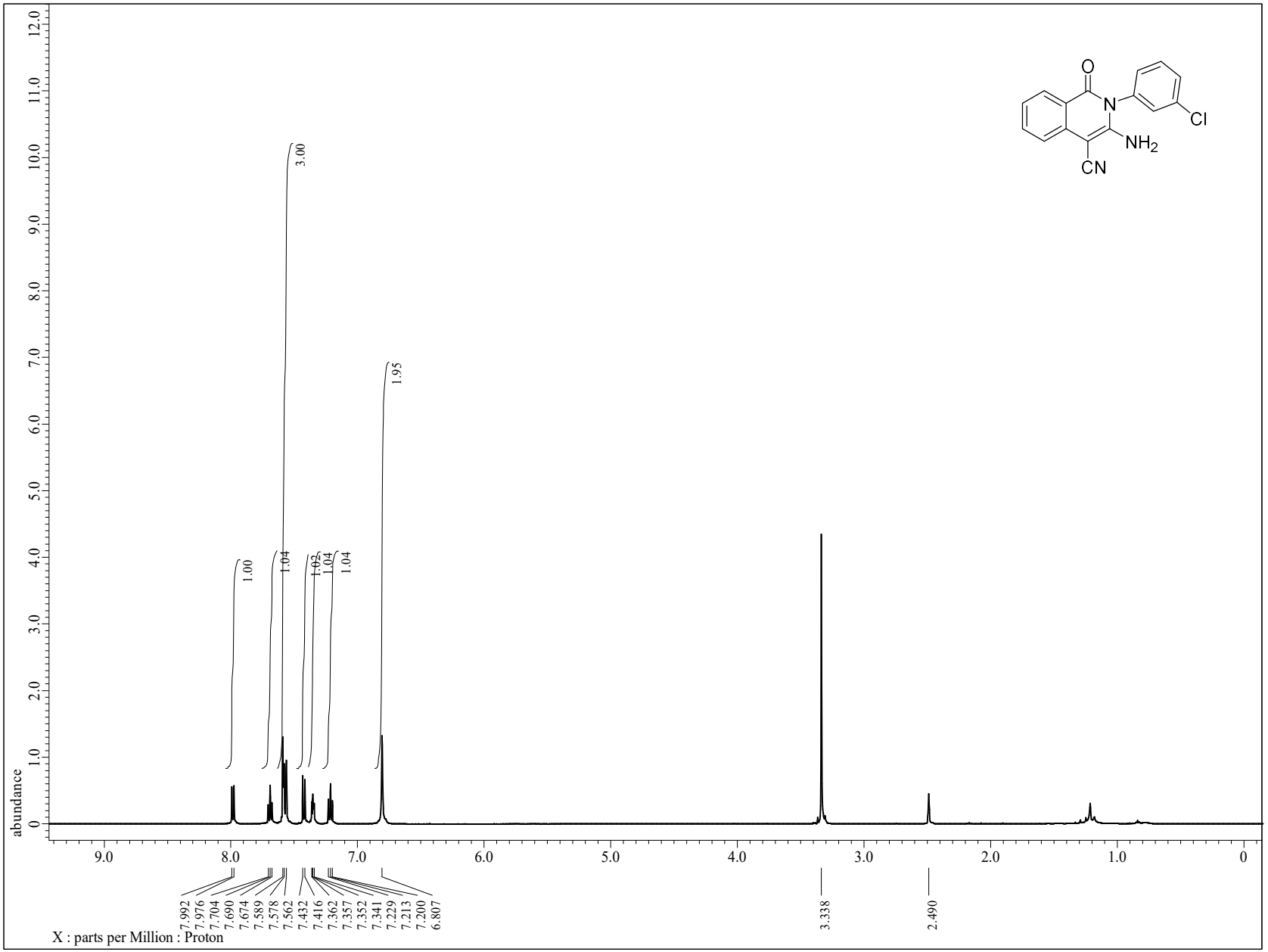

Figure S51: ^{1}H NMR (500 MHz, DMSO-d_6) of compound **8b**

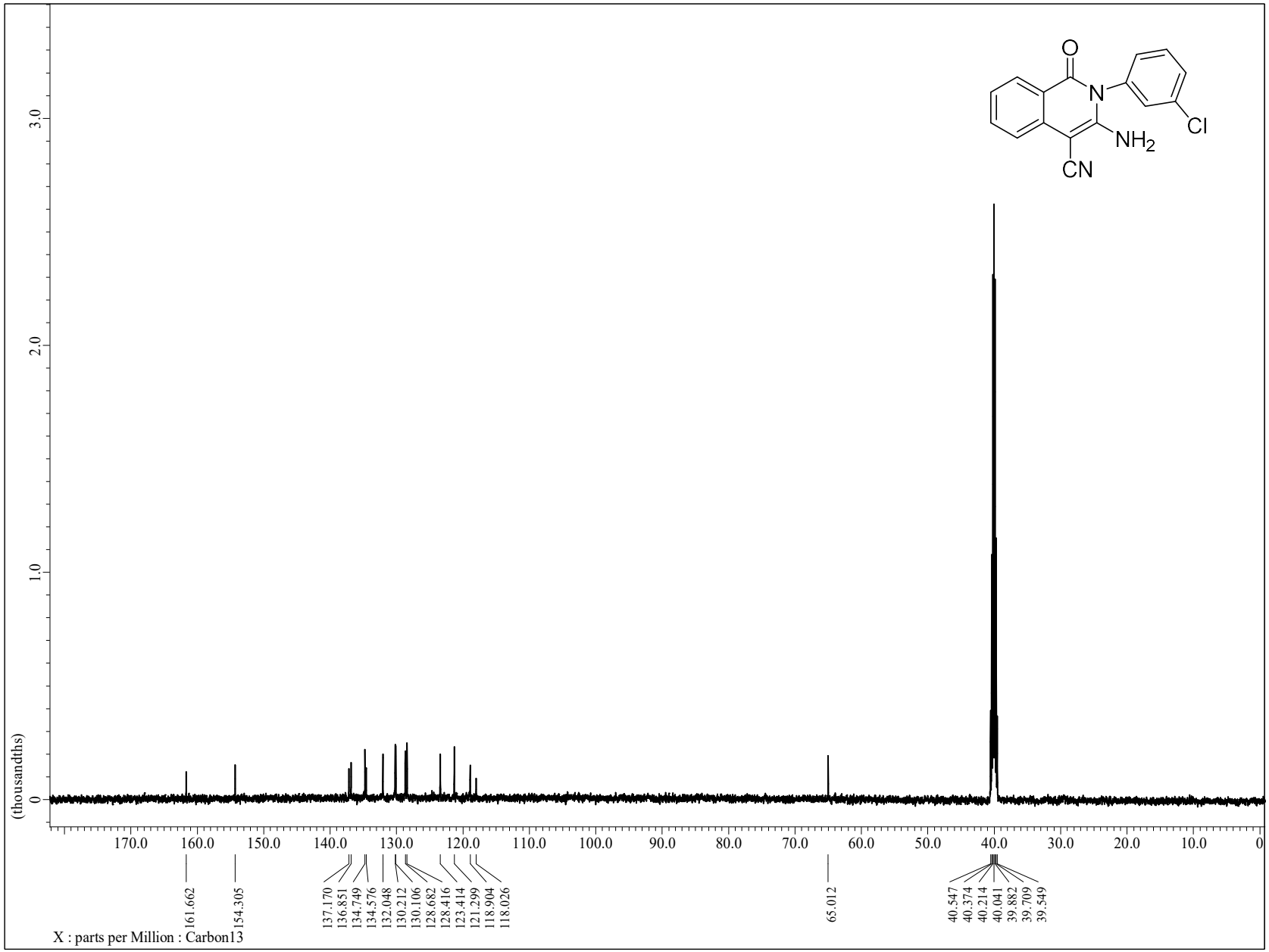

Figure S52: $^{13}C\{^{1}H\}$ NMR (125 MHz, DMSO-d_6) of compound **8b**

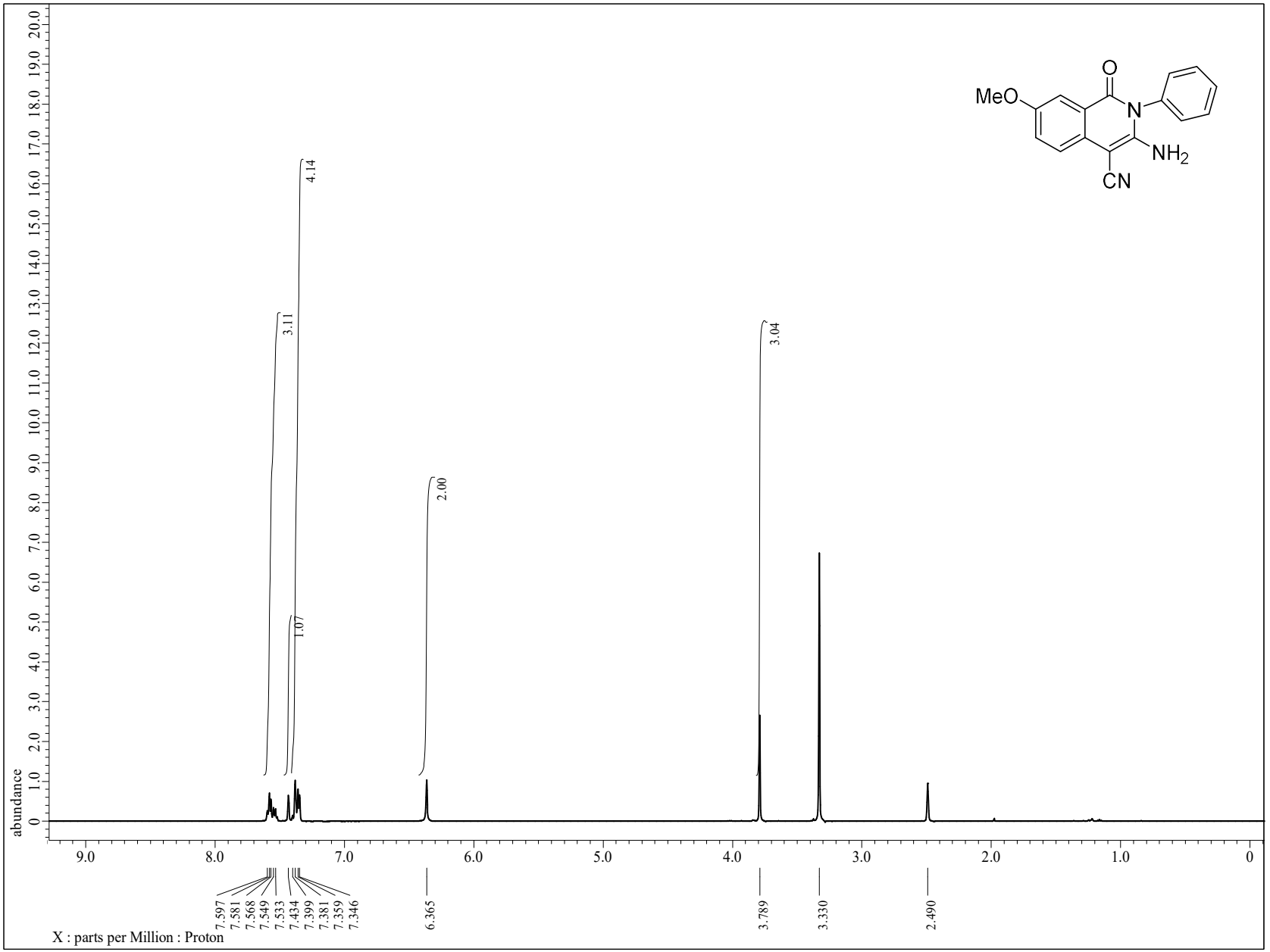

Figure S53: ^{1}H NMR (500 MHz, DMSO-d_6) of compound **8c**

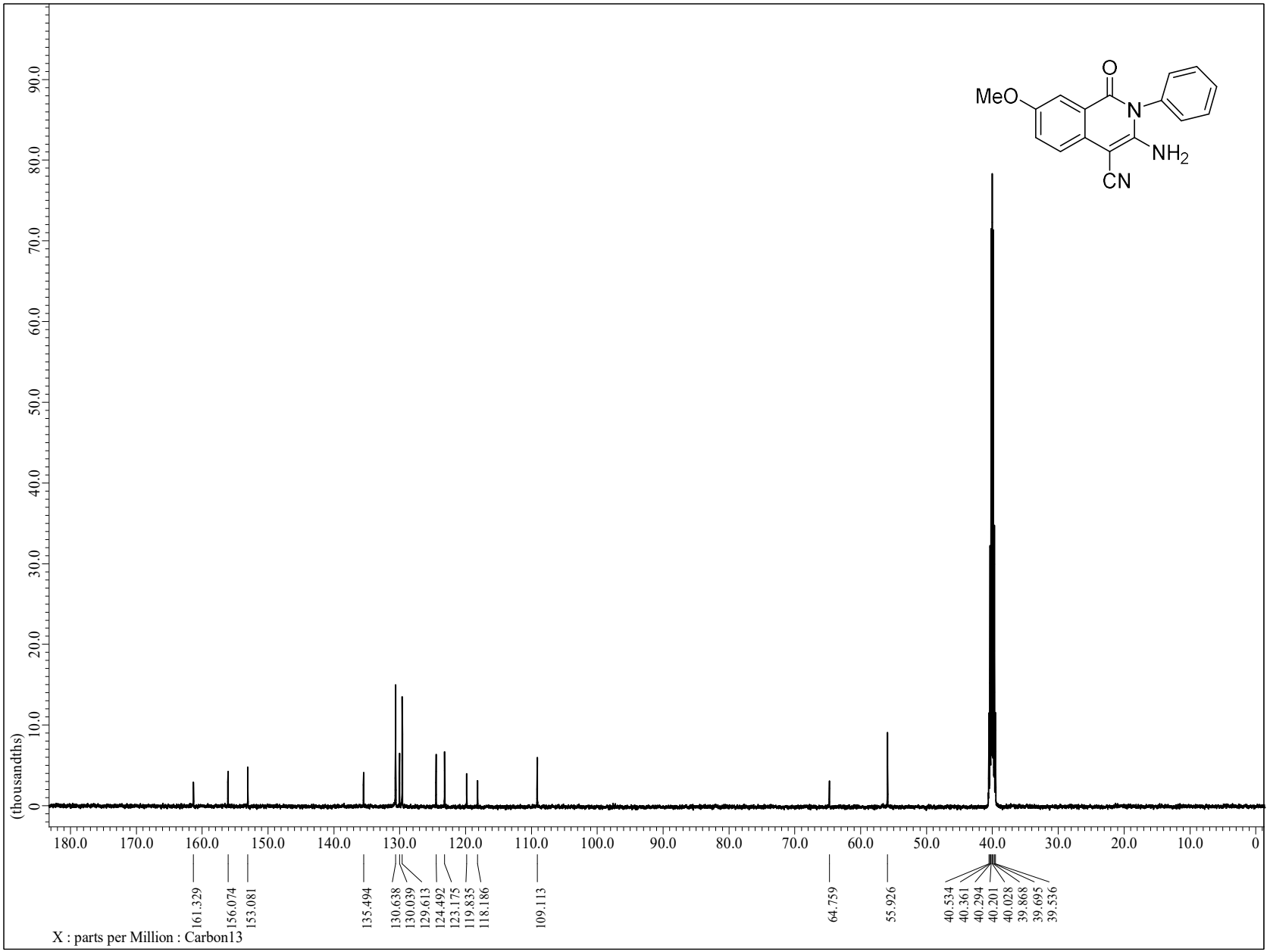

Figure S54: $^{13}C\{^{1}H\}$ NMR (125 MHz, DMSO-d_6) of compound **8c**

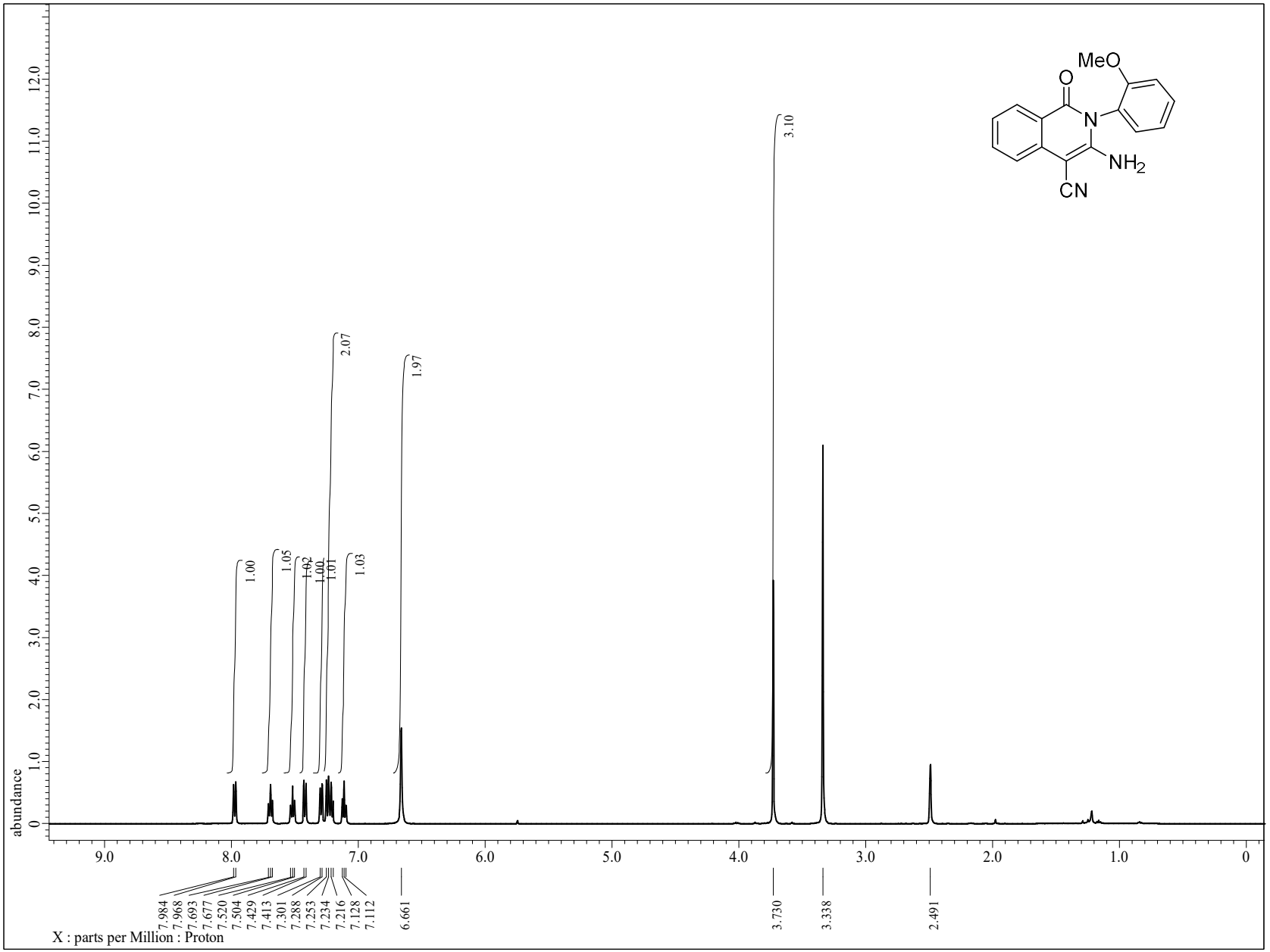

Figure S55: ^{1}H NMR (500 MHz, DMSO-d_6) of compound **8d**

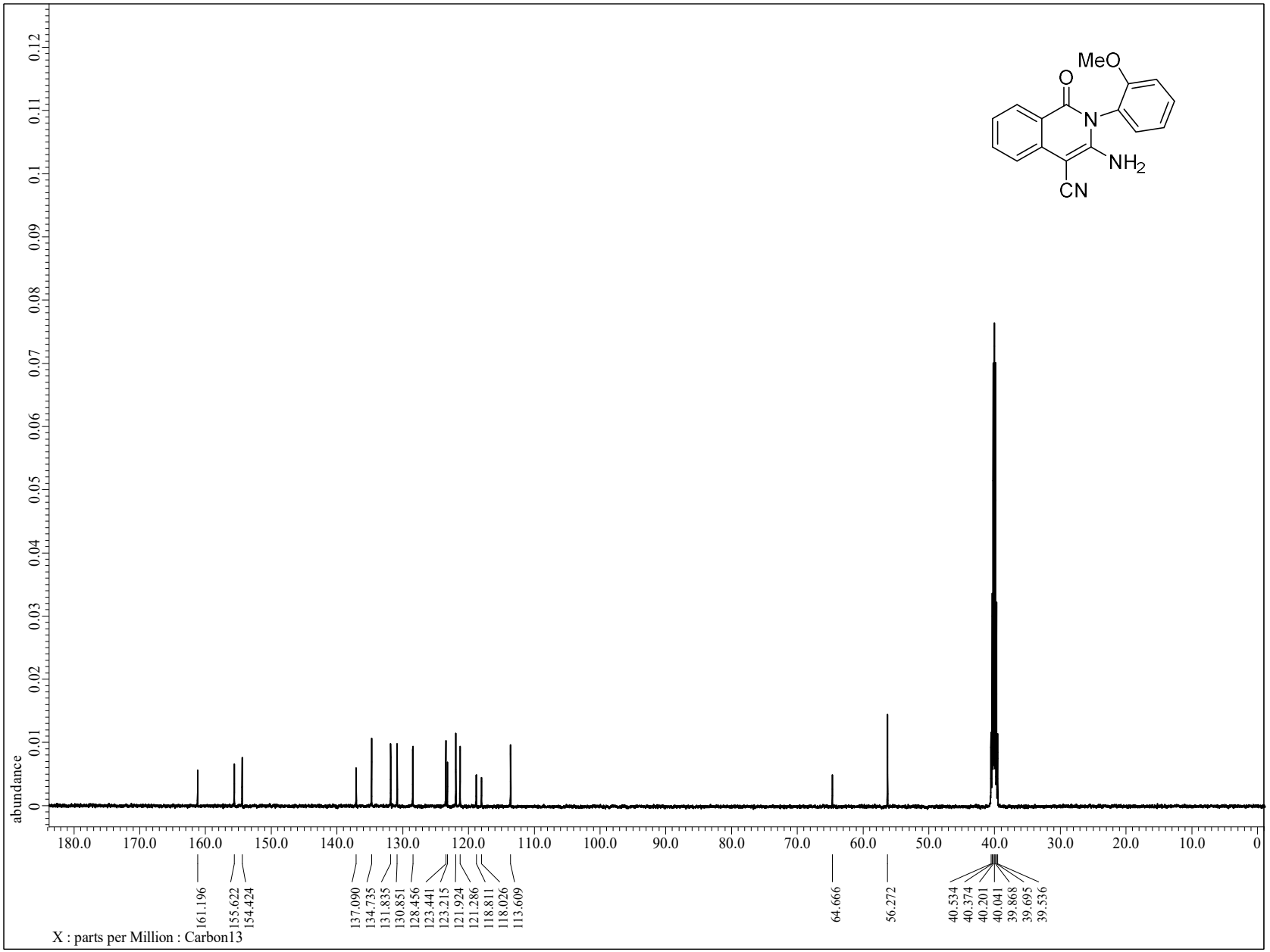

Figure S56: $^{13}C\{^{1}H\}$ NMR (125 MHz, DMSO-d_6) of compound **8d**

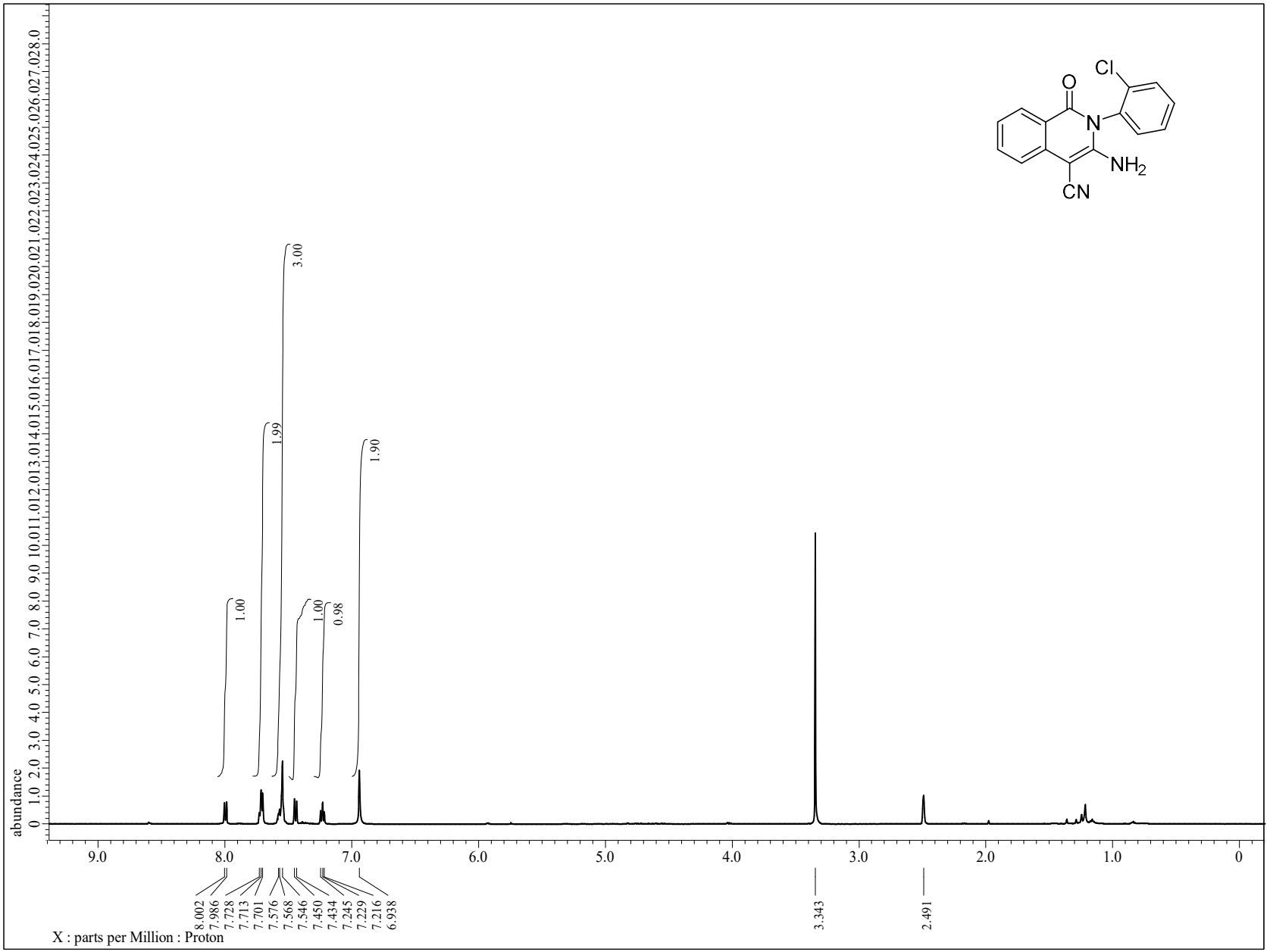

Figure S57: ^{1}H NMR (500 MHz, DMSO-d_6) of compound **8e**

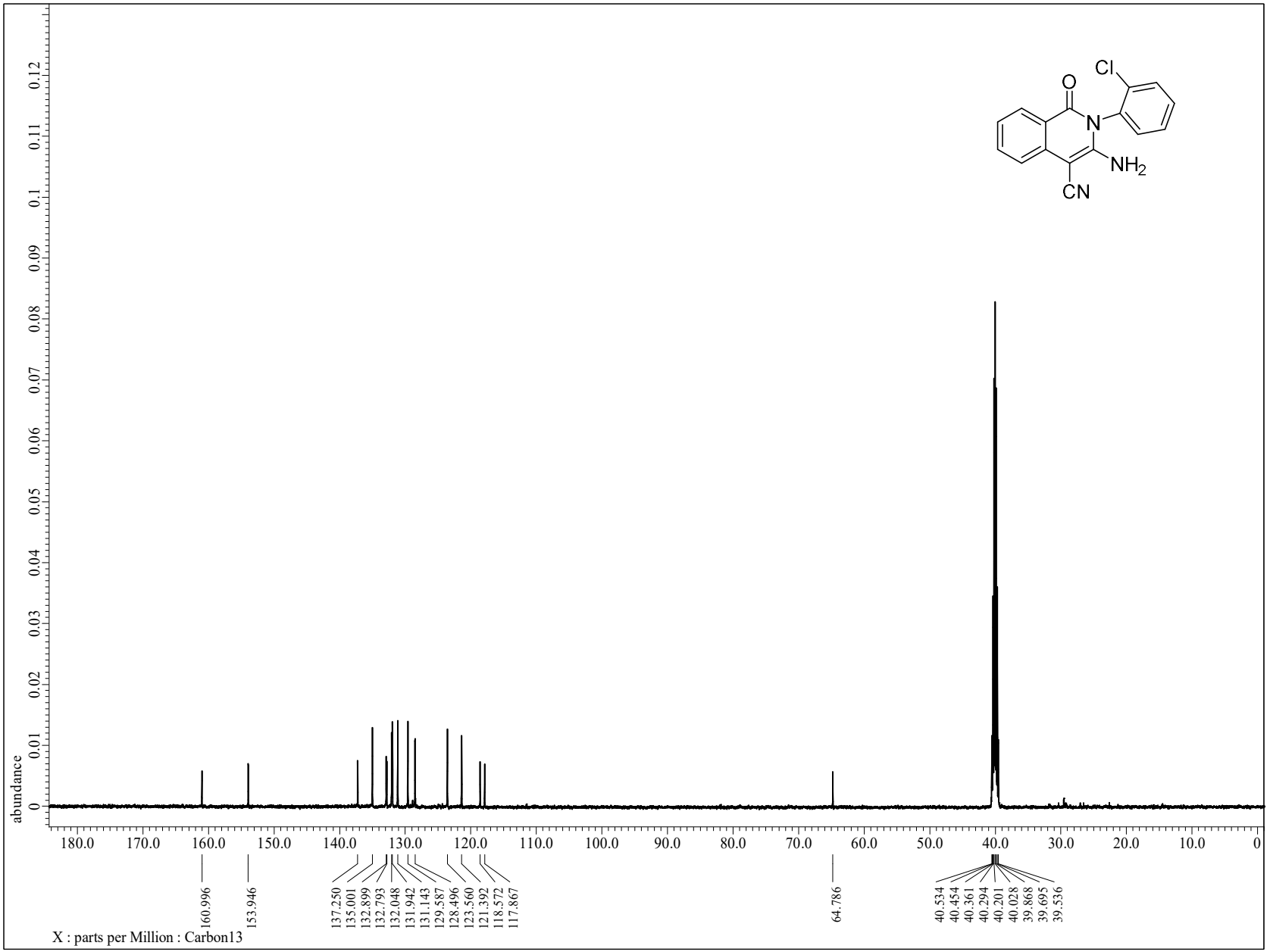

Figure S58: $^{13}C\{^{1}H\}$ NMR (125 MHz, DMSO-d_6) of compound **8e**

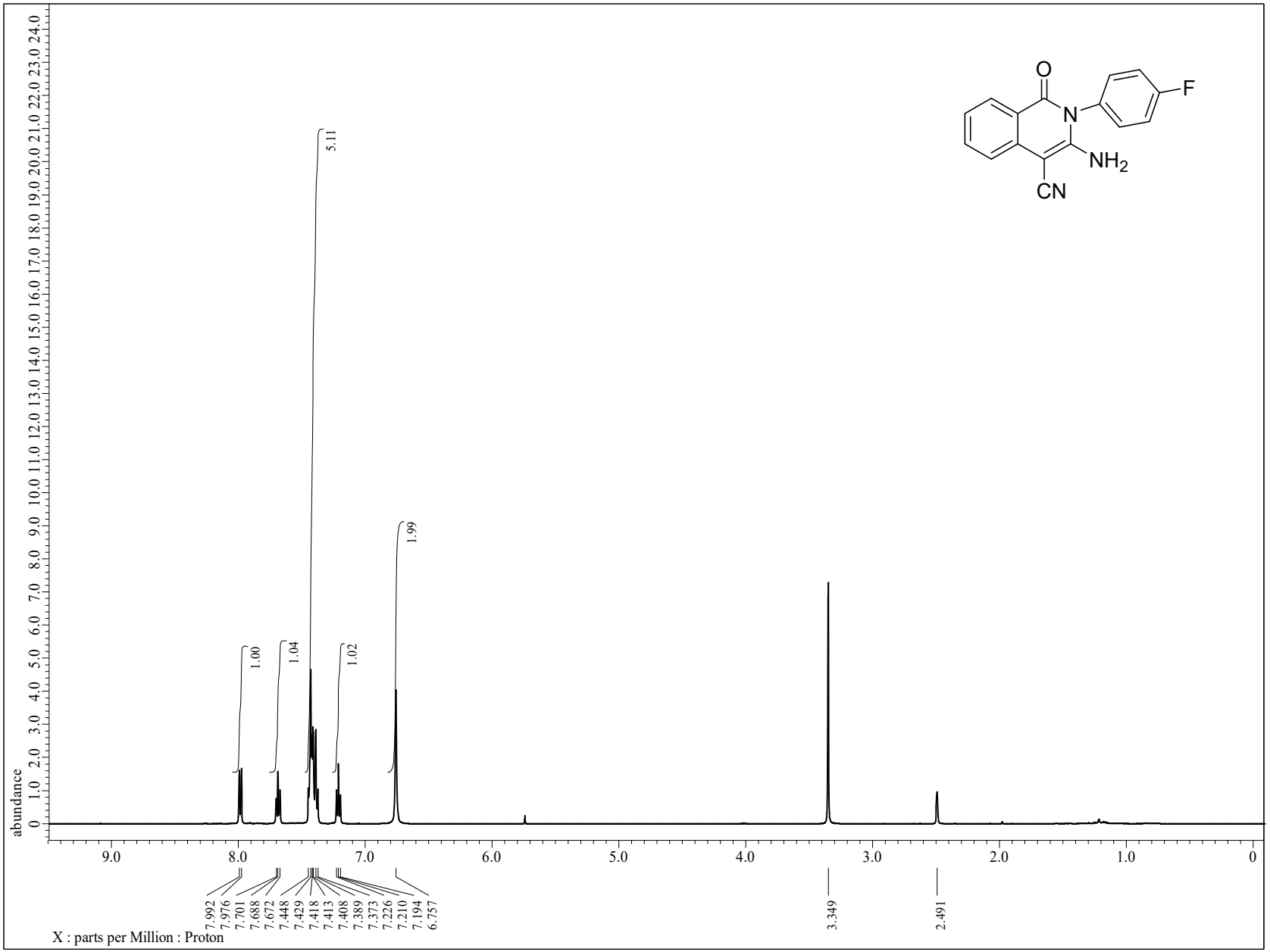

Figure S59: ^{1}H NMR (500 MHz, DMSO-d_6) of compound **8f**

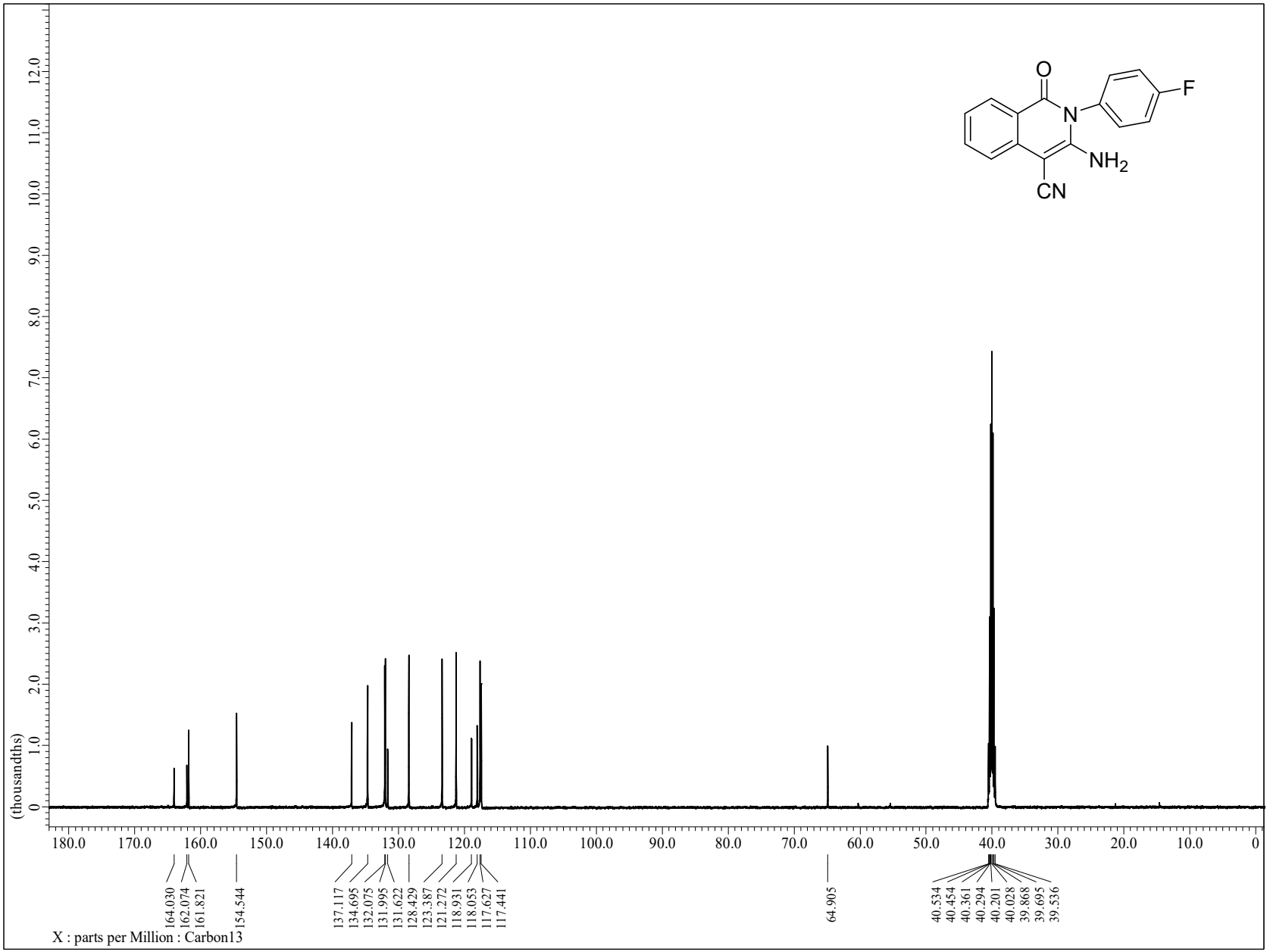

Figure S60: $^{13}C\{^{1}H\}$ NMR (125 MHz, DMSO-d_6) of compound **8f**

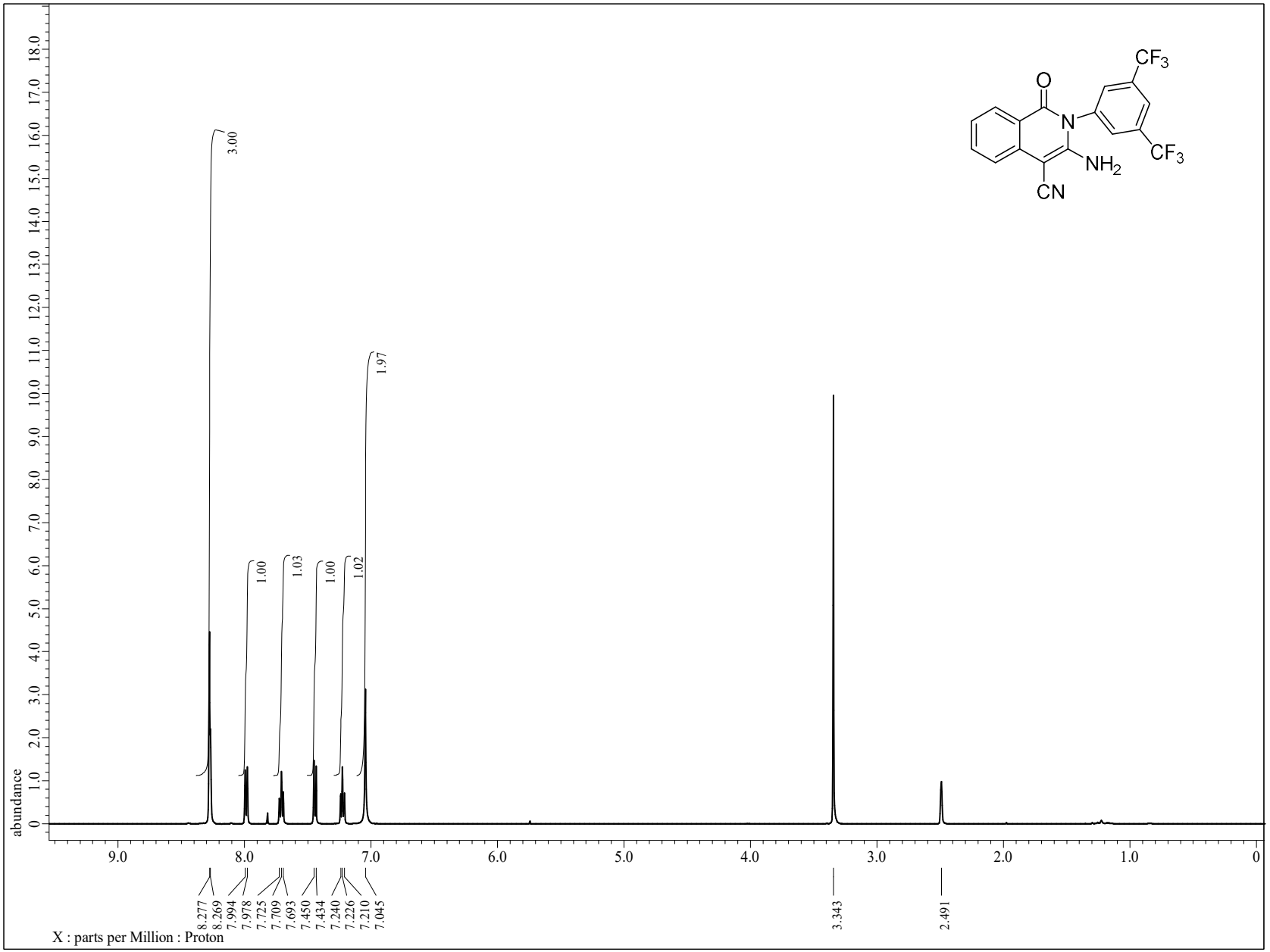

Figure S61: ^{1}H NMR (500 MHz, DMSO-d_6) of compound **8g**

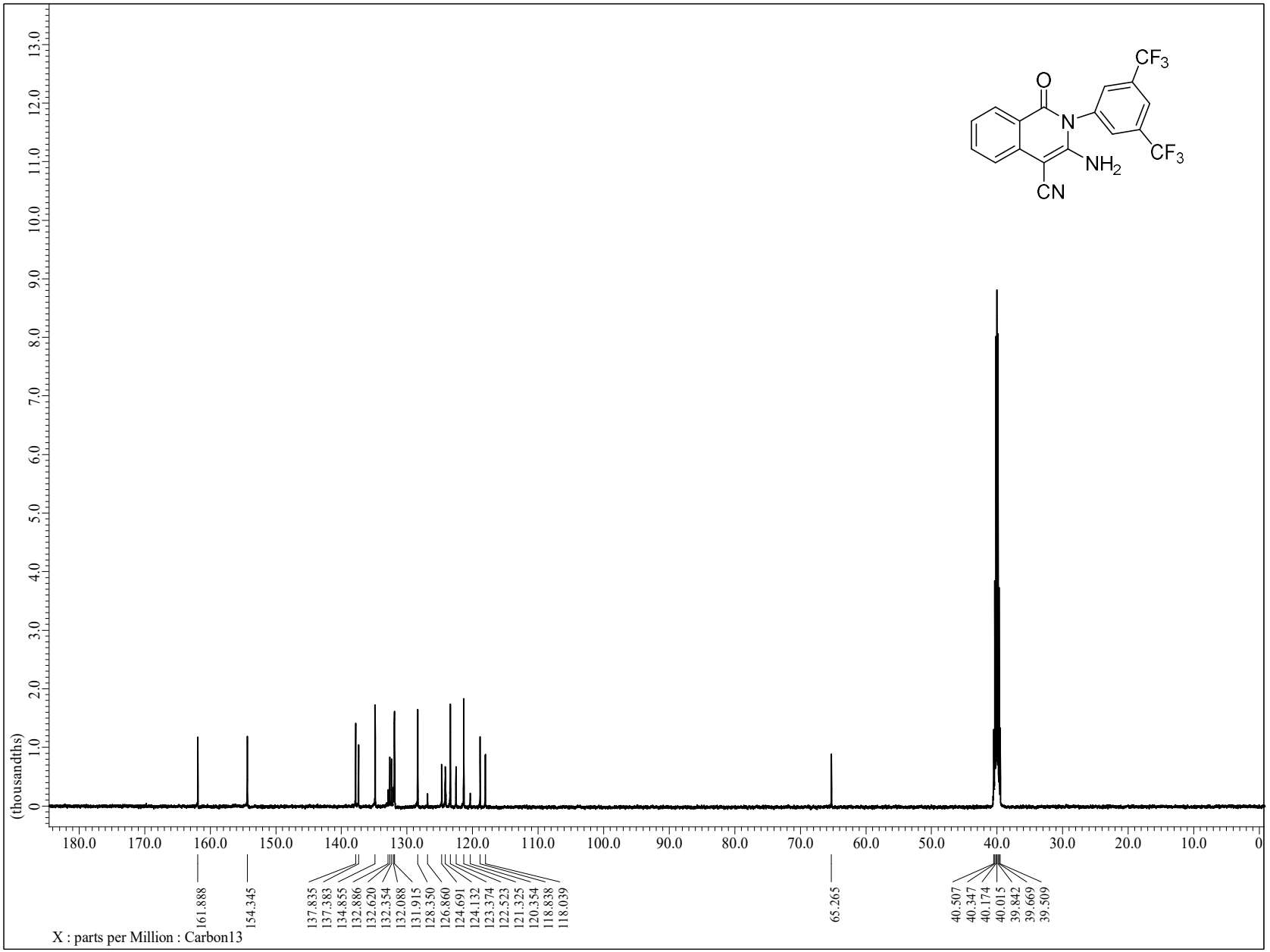

Figure S62: $^{13}C\{^{1}H\}$ NMR (125 MHz, DMSO-d_6) of compound **8g**

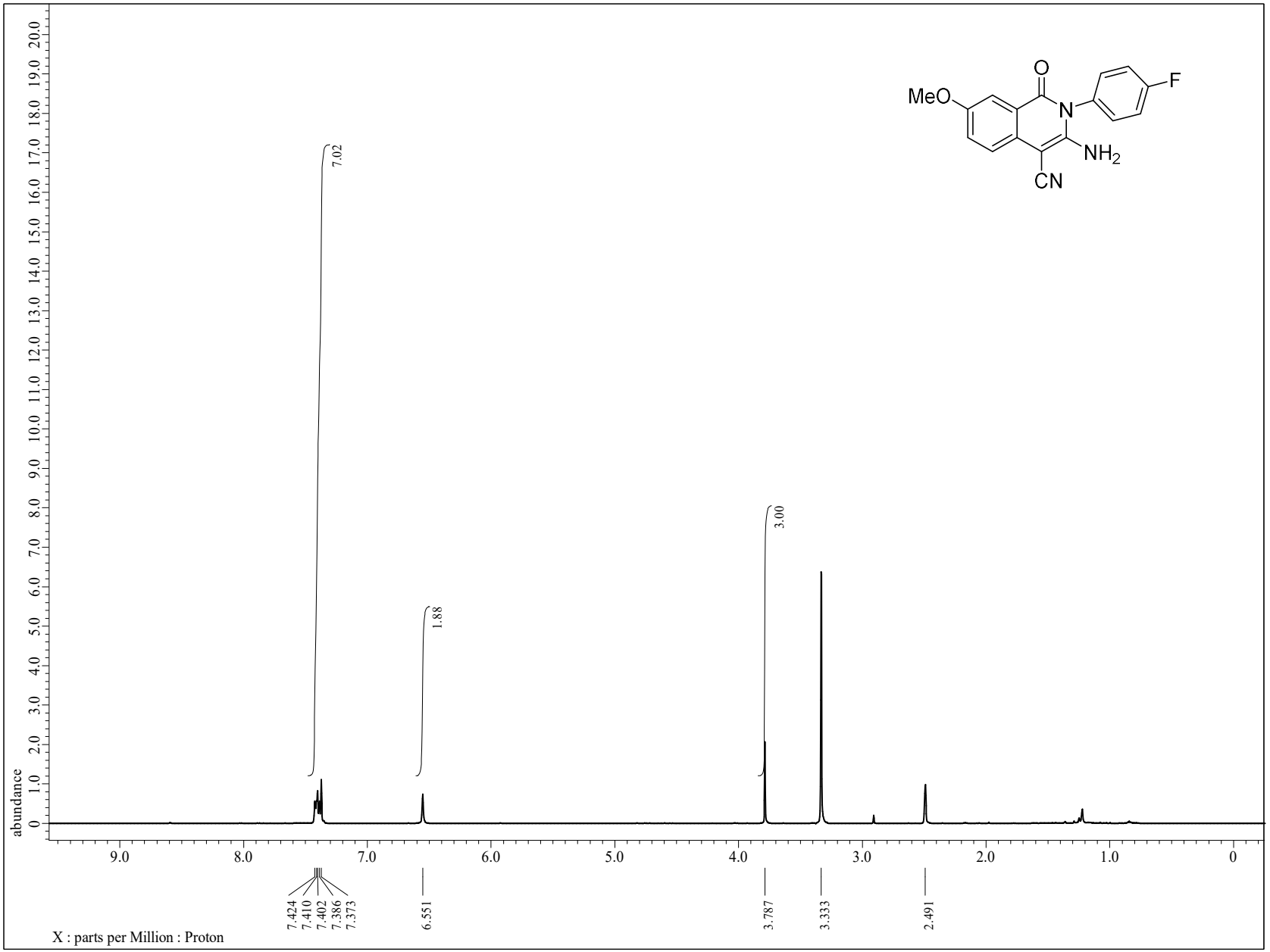

Figure S63: ^{1}H NMR (500 MHz, DMSO-d_6) of compound **8h**

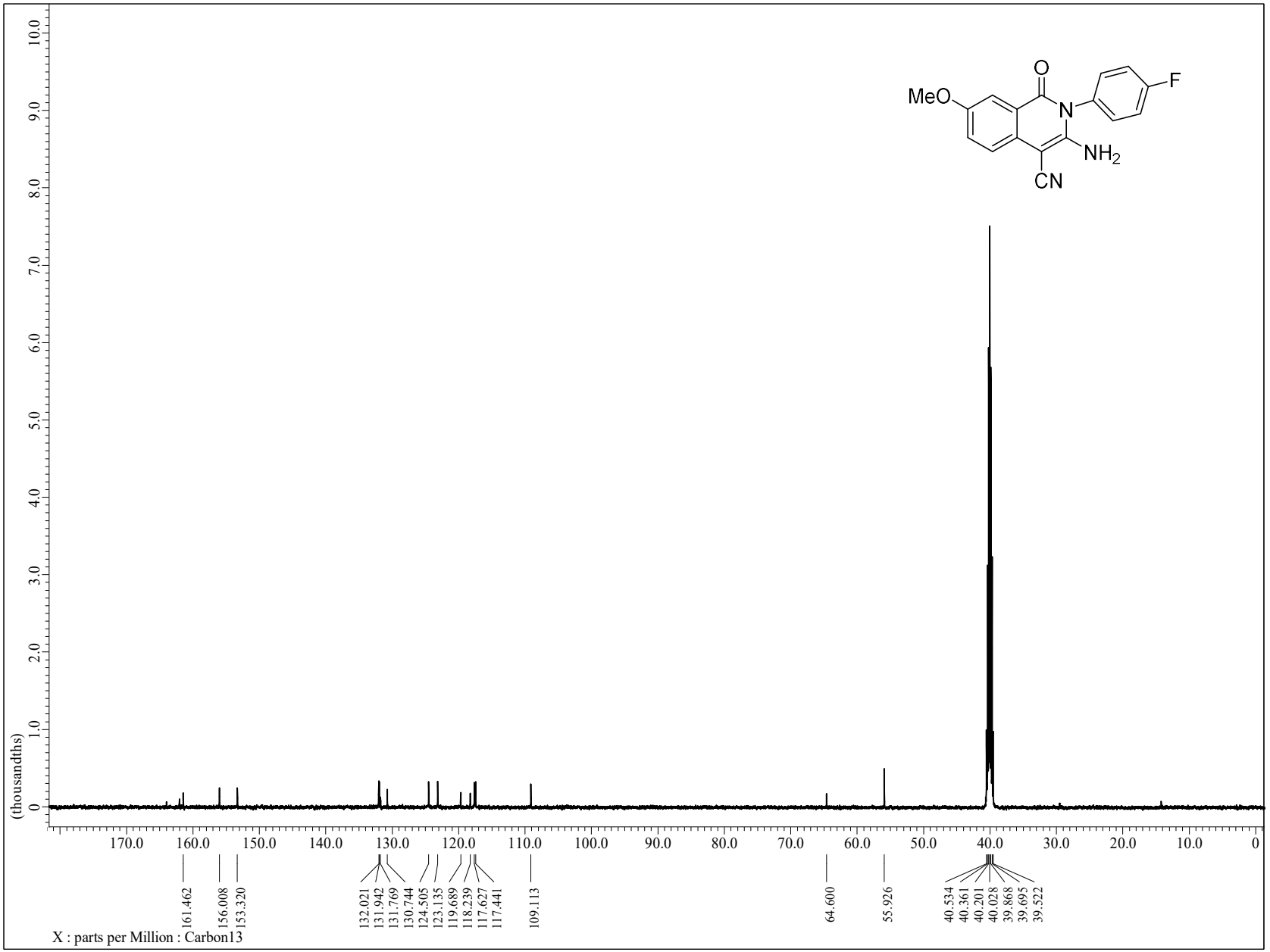

Figure S64: $^{13}C\{^{1}H\}$ NMR (125 MHz, DMSO-d_6) of compound **8h**

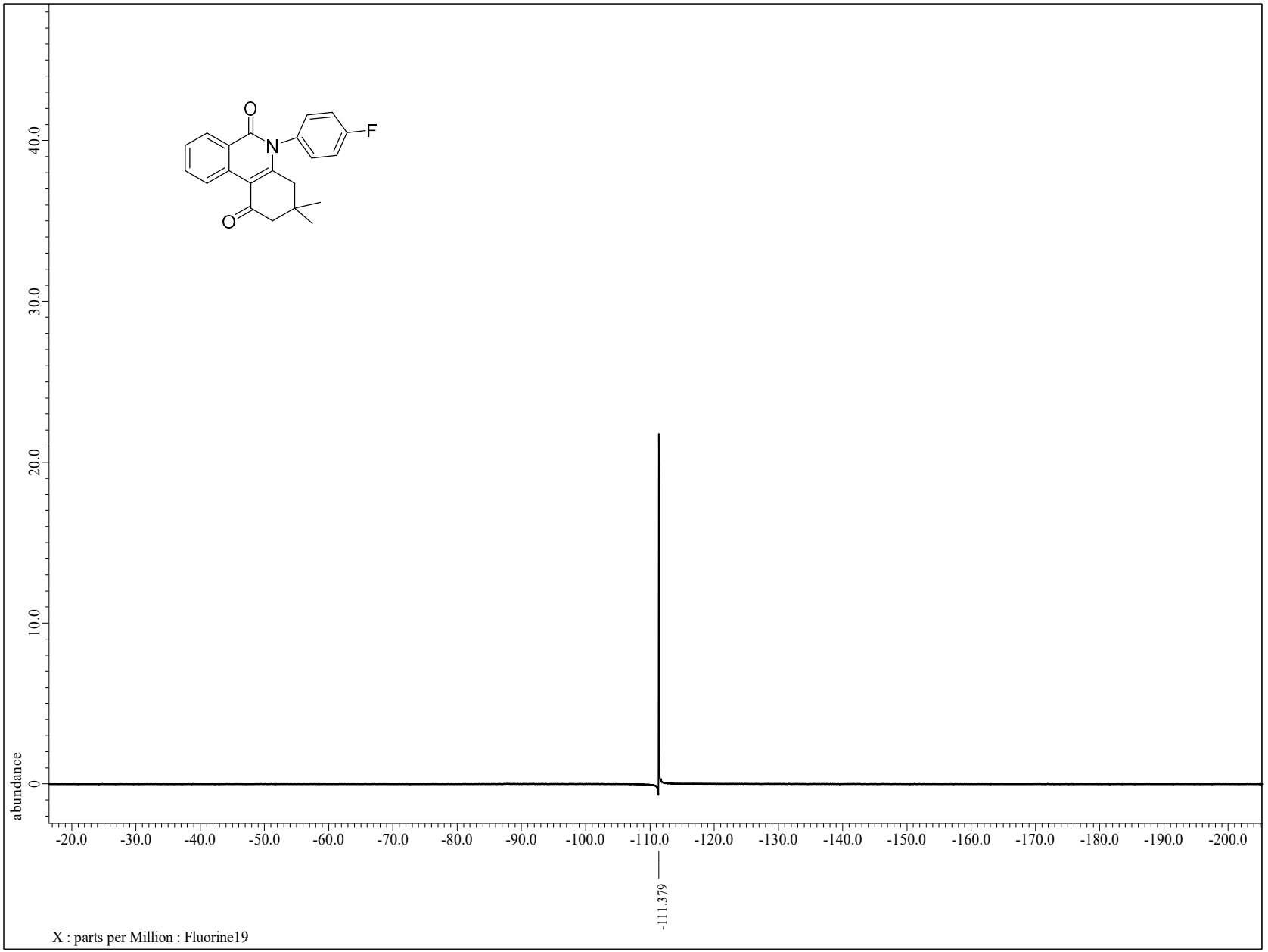

Figure S65: ^{19}F NMR (470 MHz, $CDCl_3$) of compound **6i**

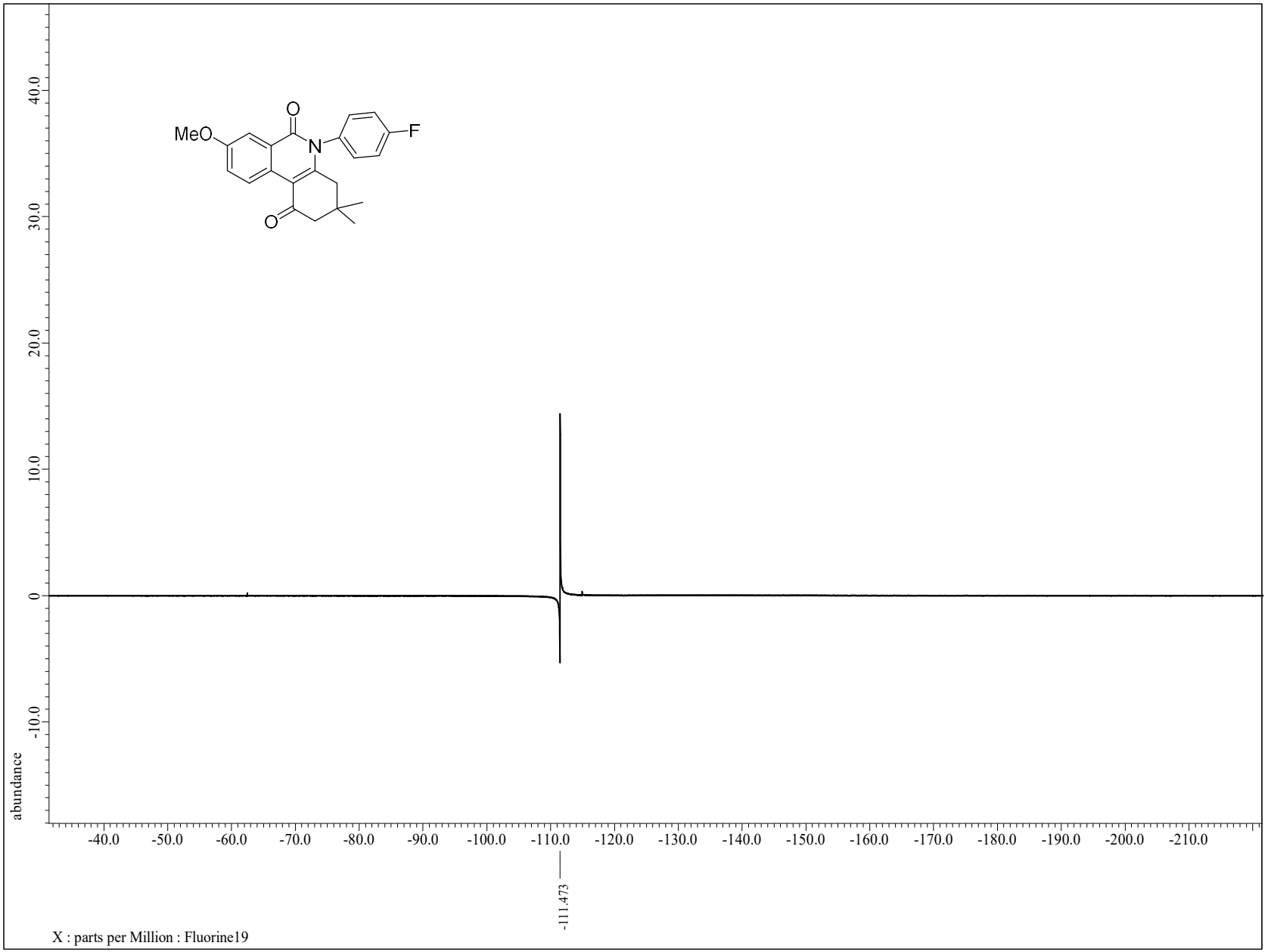

Figure S66: ^{19}F NMR (470 MHz, $CDCl_3$) of compound **6j**

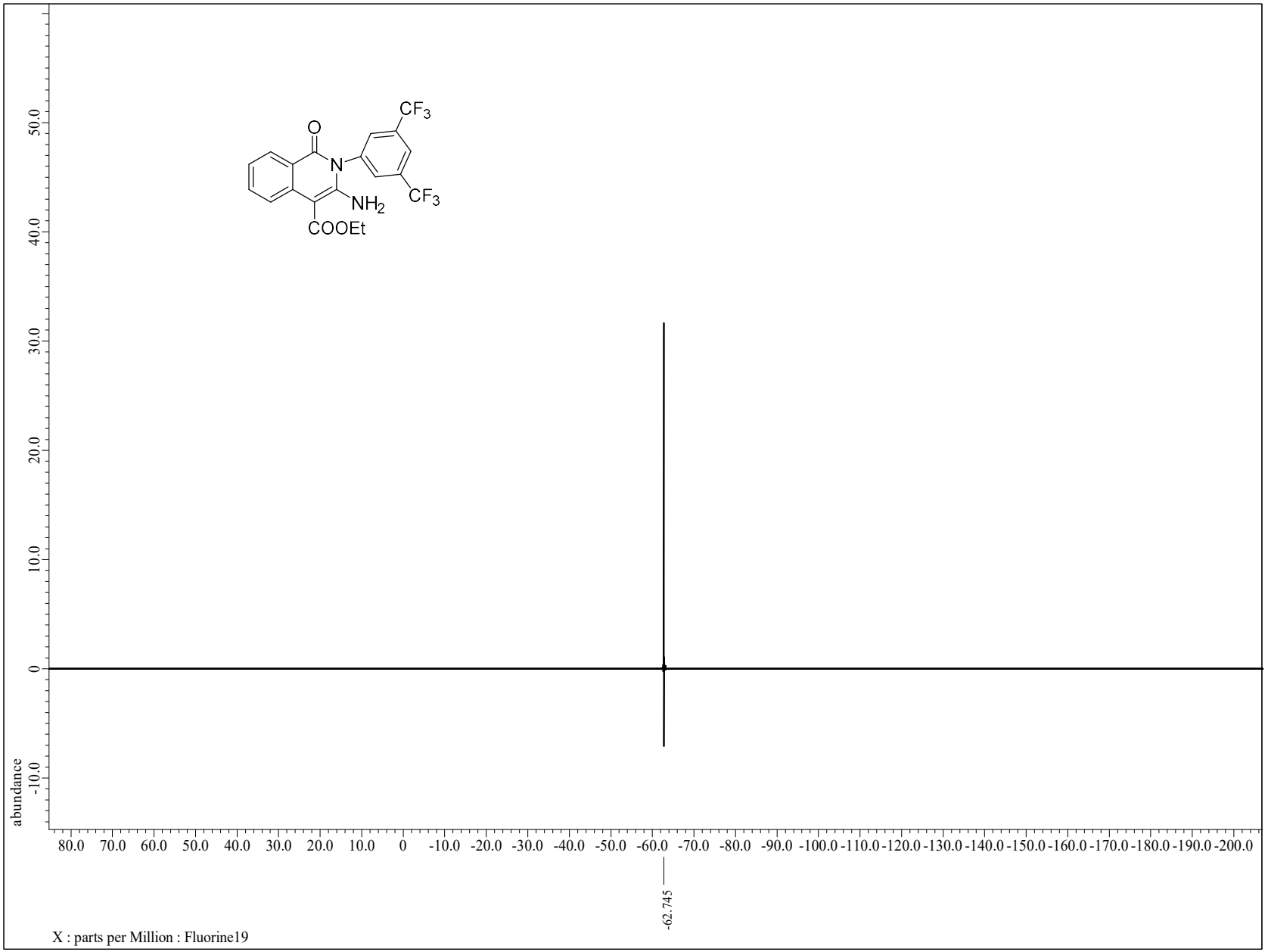

Figure S67: ^{19}F NMR (470 MHz, $CDCl_3$) of compound **7e**

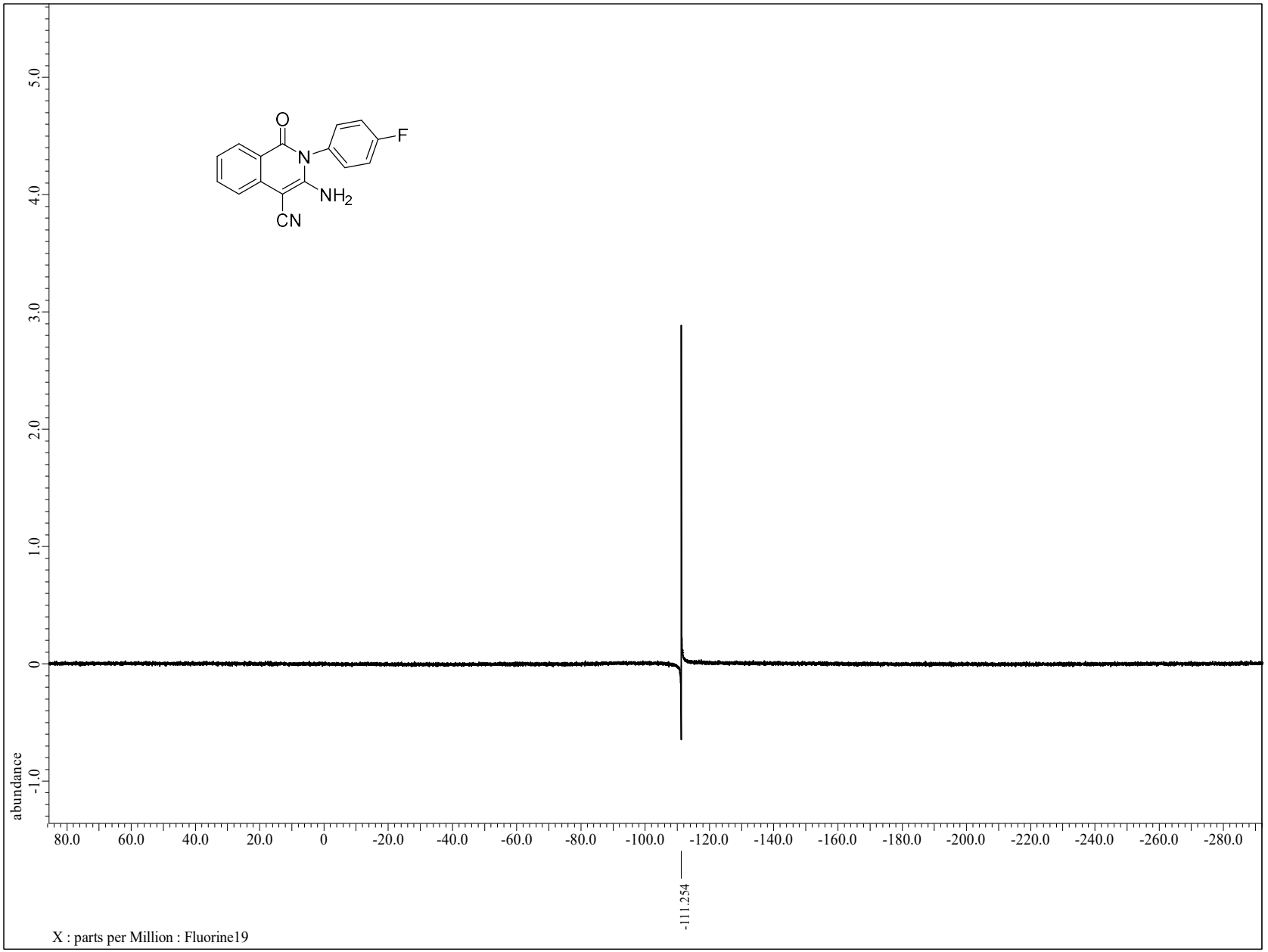

Figure S68: ^{19}F NMR (470 MHz, DMSO-d_6) of compound **8f**

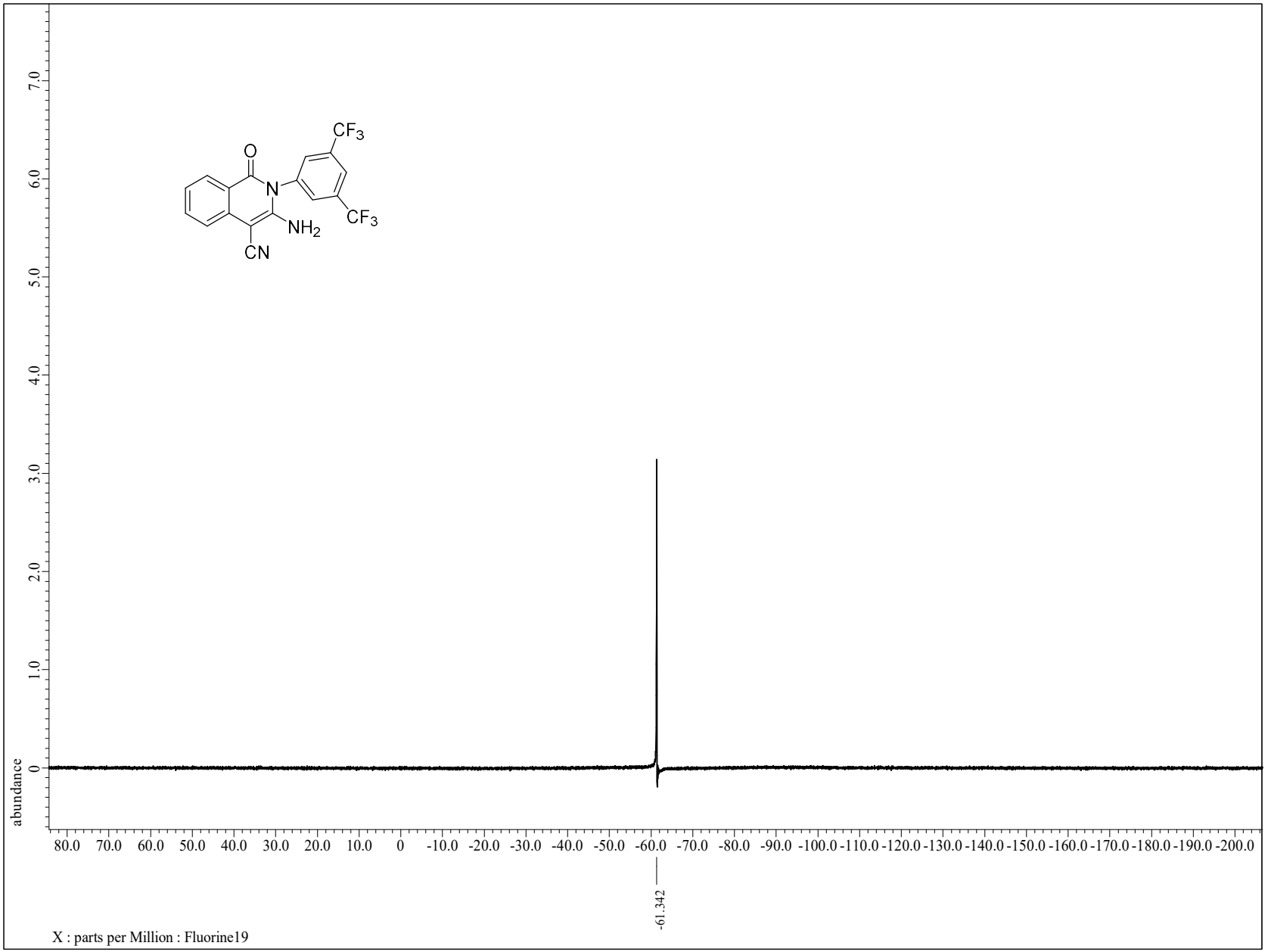

Figure S69: ^{19}F NMR (470 MHz, DMSO-d_6) of compound **8g**

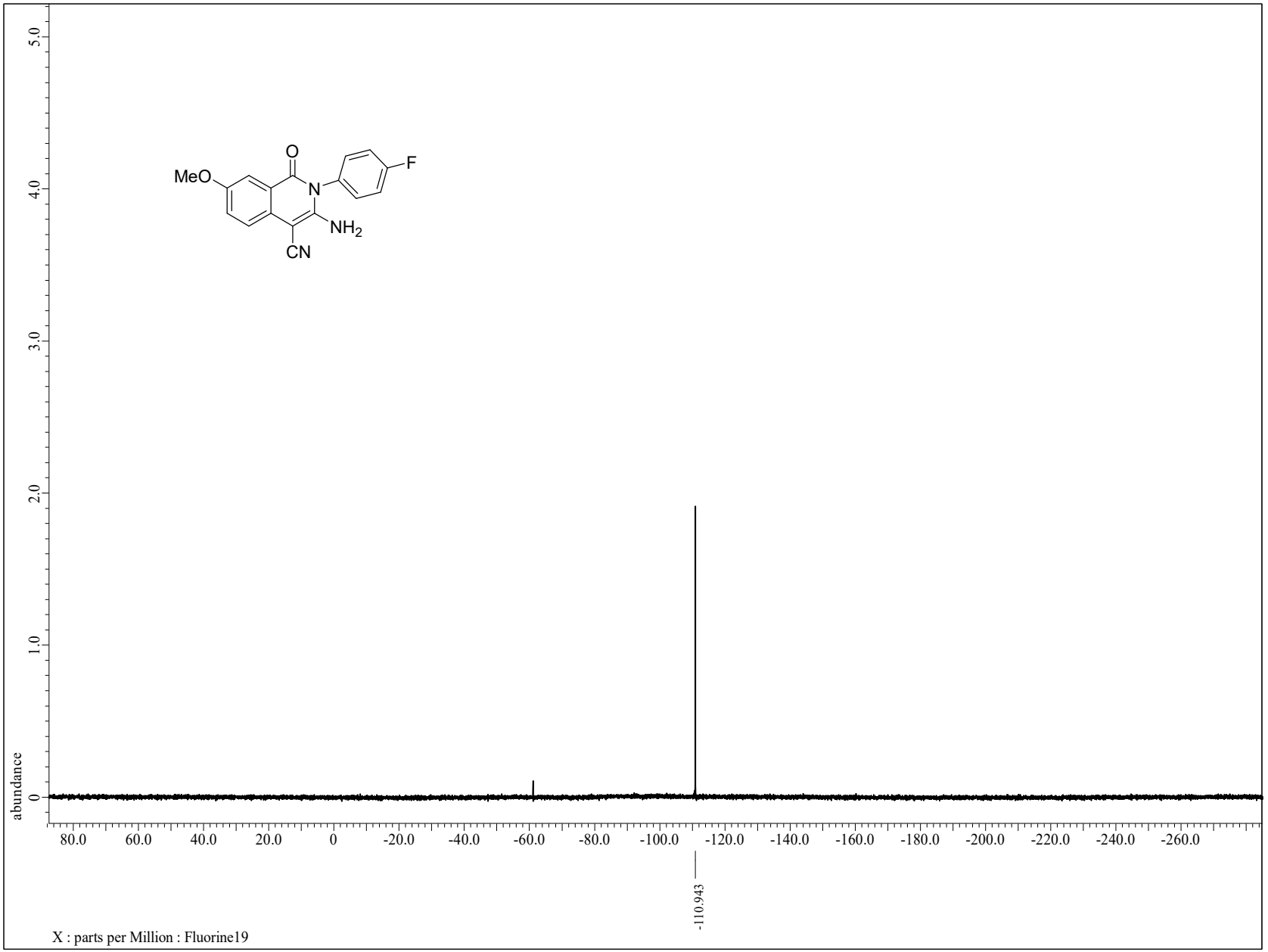

Figure S70: ^{19}F NMR (470 MHz, DMSO-d_6) of compound **8h**

Single Crystal X-Ray data and structure of compounds

Data Collection and Refinement:

Data of compounds were collected on Rigaku Oxford diffraction (XtaLAB Synergy-i) using graphite monochromated Mo*K*α radiation ($\lambda = 0.71073$ Å). The structures were solved by the direct method as the compound is containing Fluorine and then refined on $F2$ by the full matrix least-squares technique with the SHELX-86 set of software using the WinGX program package. All non-hydrogen atoms were refined anisotropically in respect to electron density and hydrogen atoms were treated as riding atoms using SHELX default parameters. The process has been validated through the IUCR site (International Union of Crystallography). Hence the crystals solved are validated. Further information on the crystal structures (excluding structure factors) have been given in **Table 1-9, Figure S67-S69** and also deposited in the Cambridge Crystallographic Data Centre as supplementary publication numbers of each compounds (**L2, 7f,** and **7h**). Copies of the data can be obtained free of charge upon application to CCDC, 12 Union Road, Cambridge CB2 1EZ, UK (fax: (+44) 1223-336-033. e-mail: deposit@ccdc.cam.ac.uk) or *via* internet.

Procedure for crystallization of compound L2

Compound **L2** single crystal was obtained by slow evaporation method: the compound **L2** (50 mg) was dissolved in ethanol (15 mL) solvent system and was kept in dark place at 25 ºC in the test tube. The needle-shaped colorless single crystal appeared after a month which was isolated in its initial state of growth and washed with *n*-pentane for several times.

Table S1: Crystallographic refinement data for compound **L2**

Empirical Formula	C23 H26 N5 O10
Formula Weight	532.49
Crystal System	Triclinic
Space group	P -1
a (Å)	5.59530(10)
b (Å)	10.6515(3)
c (Å)	11.0452(2)
α (°), β (°), γ(°)	92.586(2), 90.584(2), 101.290(2)
V (Å3)	644.76(2)
Z	1
Density (calc)	1.374
F(000)	280
Absorption coefficient	0.929 mm^-1
Crystal Size [mm]	0.30 x 0.24 x 0.22
Temperature (K)	293
Wavelength	1.54184 A
θ Min-Max [°]	4.007 to 68.030
Limiting indices	-6<=h<=6, -12<=k<=12, -13<=l<=13
Tot., UniqData, R(int)	10980 / 4383 [R(int) = 0.0266]
Obs. data [I > 2.0 σ(I)]	R1 = 0.0445, wR2 = 0.1211
Goodness-of-fit on F^2	1.083
R indices (all data)	R1 = 0.0460, wR2 = 0.1235
CCDC	**2251908**

Table S2: Bond lengths for compound **L2**

Number	Atom 1	Atom 2	Bond length
1	O(4)	C(6)	1.353(4)
2	O(4)	C(7)	1.445(4)
3	O(9)	C(14)	1.418(4)
4	O(9)	C(4)	1.441(3)
5	O(6)	C(10)	1.356(5)
6	O(6)	C(8)	1.427(4)
7	O(2)	C(2)	1.341(4)
8	O(2)	C(3)	1.444(4)
9	O(8)	C(12)	1.354(4)
10	O(8)	C(13)	1.431(4)
11	N(1)	C(15)	1.339(4)
12	N(1)	N(2)	1.347(4)
13	N(1)	C(14)	1.452(4)
14	O(3)	C(6)	1.191(4)
15	O(1)	C(2)	1.190(5)
16	N(2)	N(3)	1.303(4)
17	N(5)	C(19)	1.325(5)
18	N(5)	C(23)	1.346(5)
19	N(4)	C(18)	1.330(5)
20	N(4)	C(17)	1.465(5)
21	O(5)	C(10)	1.185(6)
22	N(3)	C(16)	1.362(5)

23	O(10)	C(18)	1.229(5)
24	C(13)	C(14)	1.516(4)
25	C(13)	C(8)	1.518(4)
26	C(2)	C(1)	1.490(5)
27	C(6)	C(5)	1.489(5)
28	C(4)	C(7)	1.518(4)
29	C(4)	C(3)	1.517(4)
30	C(7)	C(8)	1.528(4)
31	C(16)	C(15)	1.360(5)
32	C(16)	C(17)	1.498(5)
33	C(19)	C(20)	1.383(5)
34	C(19)	C(18)	1.500(5)
35	O(7)	C(12)	1.175(6)
36	C(20)	C(21)	1.368(5)
37	C(10)	C(9)	1.479(6)
38	C(12)	C(11)	1.488(7)
39	C(21)	C(22)	1.363(6)
40	C(22)	C(23)	1.361(6)

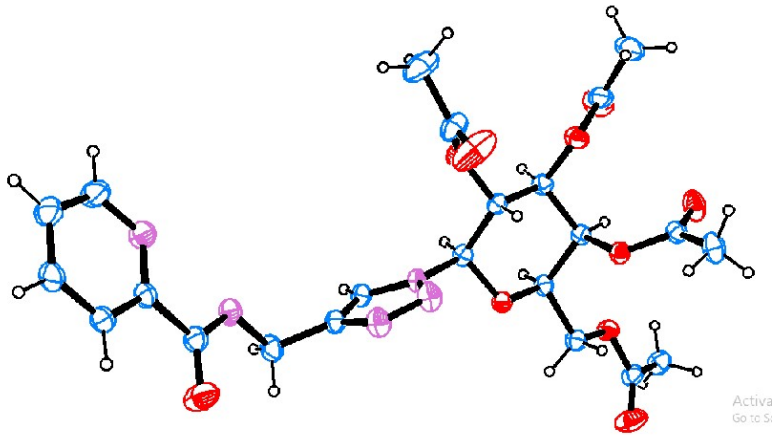

Figure S71: Molecular structure of compound **L2**, Thermal ellipsoids of carbon, nitrogen, and oxygen are set at 40% probability.

Table S3: Bond angles of compound **L2**

Number	Atom 1	Atom 2	Atom 3	Bond Angle
1	C(6)	O(4)	C(7)	116.4(2)
2	C(14)	O(9)	C(4)	112.8(2)
3	C(10)	O(6)	C(8)	118.1(3)
4	C(2)	O(2)	C(3)	114.8(3)
5	C(12)	O(8)	C(13)	118.2(3)
6	C(15)	N(1)	N(2)	110.8(3)
7	C(15)	N(1)	C(14)	127.7(3)
8	N(2)	N(1)	C(14)	121.3(2)
9	N(3)	N(2)	N(1)	106.9(3)
10	C(19)	N(5)	C(23)	116.9(3)
11	C(18)	N(4)	C(17)	121.9(3)
12	N(2)	N(3)	C(16)	109.1(3)
13	O(8)	C(13)	C(14)	109.4(2)

14	O(8)	C(13)	C(8)	107.3(2)
15	C(14)	C(13)	C(8)	108.2(2)
16	O(1)	C(2)	O(2)	121.9(3)
17	O(1)	C(2)	C(1)	125.6(3)
18	O(2)	C(2)	C(1)	112.5(3)
19	O(3)	C(6)	O(4)	123.4(3)
20	O(3)	C(6)	C(5)	125.2(3)
21	O(4)	C(6)	C(5)	111.4(3)
22	O(9)	C(4)	C(7)	111.0(2)
23	O(9)	C(4)	C(3)	103.3(2)
24	C(7)	C(4)	C(3)	114.7(3)
25	O(2)	C(3)	C(4)	107.2(3)
26	O(4)	C(7)	C(4)	109.4(2)
27	O(4)	C(7)	C(8)	108.2(2)
28	C(4)	C(7)	C(8)	109.9(2)
29	C(15)	C(16)	N(3)	108.0(3)
30	C(15)	C(16)	C(17)	128.9(3)
31	N(3)	C(16)	C(17)	123.1(3)
32	N(1)	C(15)	C(16)	105.1(3)
33	O(6)	C(8)	C(13)	105.7(2)
34	O(6)	C(8)	C(7)	111.4(2)
35	C(13)	C(8)	C(7)	111.7(2)
36	N(5)	C(19)	C(20)	122.9(3)
37	N(5)	C(19)	C(18)	117.3(3)

38	C(20)	C(19)	C(18)	119.8(3)
39	O(9)	C(14)	N(1)	106.2(2)
40	O(9)	C(14)	C(13)	109.5(2)
41	N(1)	C(14)	C(13)	112.8(2)
42	C(21)	C(20)	C(19)	118.8(4)
43	O(5)	C(10)	O(6)	123.1(4)
44	O(5)	C(10)	C(9)	127.4(4)
45	O(6)	C(10)	C(9)	109.5(4)
46	O(10)	C(18)	N(4)	124.5(4)
47	O(10)	C(18)	C(19)	120.4(3)
48	N(4)	C(18)	C(19)	115.0(3)
49	O(7)	C(12)	O(8)	123.0(4)
50	O(7)	C(12)	C(11)	125.5(4)
51	O(8)	C(12)	C(11)	111.5(4)
52	C(22)	C(21)	C(20)	119.0(4)
53	C(23)	C(22)	C(21)	119.0(4)
54	N(4)	C(17)	C(16)	112.6(3)
55	N(5)	C(23)	C(22)	123.4(4)

Procedure for crystallization of compound 7f

Compound **7f** single crystal was obtained by slow evaporation method: the compound **7f** (40 mg) was dissolved in ethanol (15 mL) solvent system and was kept in dark place at 25 ºC in the test tube. The block-shaped brown color single crystal appeared after 12-15 days which was isolated in its initial state of growth and washed with *n*-pentane for several times.

Table S4: Crystallographic refinement data for compound **7f**

Empirical Formula	C2.40 H2 Cl0.13 N0.27 O0.40
Formula Weight	45.70
Crystal System	Triclinic
Space group	P -1
a (Å)	7.5777(3)
b (Å)	9.5759(3)
c (Å)	12.1251(3)
α (°), *β* (°), *γ*(°)	99.690(2), 99.771(3), 107.825(3)
V (Å3)	802.38(5)
Z	15
Density (calc)	1.419
F(000)	356
Absorption coefficient	2.275 mm^-1
Crystal Size [mm]	0.24 x 0.24 x 0.20
Temperature (K)	293
Wavelength	1.54184 A
θ Min-Max [°]	3.806 to 67.989
Limiting indices	-9<=h<=9, -11<=k<=11, -14<=l<=14
Tot., UniqData, R(int)	6472 / 2882 [R(int) = 0.0203]
Obs. data [I > 2.0 σ(I)]	R1 = 0.0451, wR2 = 0.1301
Goodness-of-fit on F^2	1.055
R indices (all data)	R1 = 0.0541, wR2 = 0.1389
CCDC	**2251902**

Table S5: Bond lengths for compound **7f**

Number	Atom 1	Atom 2	Bond length
1	Cl	C(2)	1.726(2)
2	O(1)	C(15)	1.222(2)
3	O(2)	C(16)	1.219(2)
4	N(1)	C(15)	1.395(2)
5	N(1)	C(7)	1.396(2)
6	N(1)	C(1)	1.441(2)
7	O(3)	C(16)	1.313(19)
8	O(3)	C(17)	1.37(2)
9	N(2)	C(7)	1.340(3)
10	C(9)	C(10)	1.408(3)
11	C(9)	C(14)	1.410(3)
12	C(9)	C(8)	1.459(3)
13	C(8)	C(7)	1.386(3)
14	C(8)	C(16)	1.465(3)
15	C(1)	C(2)	1.382(3)
16	C(1)	C(6)	1.386(3)
17	C(14)	C(13)	1.400(3)
18	C(14)	C(15)	1.450(3)
19	C(2)	C(3)	1.389(3)
20	C(3)	C(4)	1.361(3)
21	C(16)	O(3B)	1.333(9)
22	C(10)	C(11)	1.368(3)
23	C(6)	C(5)	1.386(3)
24	C(13)	C(12)	1.364(3)

25	C(4)	C(5)	1.372(3)
26	C(11)	C(12)	1.379(3)
27	C(17)	C(18B)	1.478(16)
28	C(18)	C(17B)	1.256(12)
29	C(17B)	O(3B)	1.543(12)

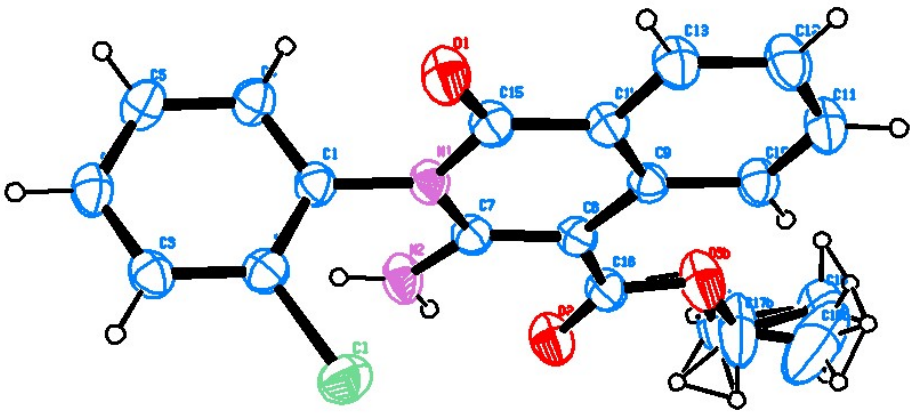

Figure S72: Molecular structure of compound **7f**, Thermal ellipsoids of carbon, nitrogen, and oxygen are set at 40% probability.

Table S6: Bond angles of compound **7f**

Number	Atom 1	Atom 2	Atom 3	Bond Angle
1	C(15)	N(1)	C(7)	123.64(16)
2	C(15)	N(1)	C(1)	116.65(15)
3	C(7)	N(1)	C(1)	119.71(15)
4	C(16)	O(3)	C(17)	115.7(15)
5	C(10)	C(9)	C(14)	115.72(17)
6	C(10)	C(9)	C(8)	125.25(17)

7	C(14)	C(9)	C(8)	119.02(17)
8	C(7)	C(8)	C(9)	118.61(16)
9	C(7)	C(8)	C(16)	116.16(17)
10	C(9)	C(8)	C(16)	125.22(17)
11	N(2)	C(7)	C(8)	124.68(18)
12	N(2)	C(7)	N(1)	114.36(17)
13	C(8)	C(7)	N(1)	120.96(16)
14	C(2)	C(1)	C(6)	119.62(18)
15	C(2)	C(1)	N(1)	120.29(18)
16	C(6)	C(1)	N(1)	120.09(17)
17	C(13)	C(14)	C(9)	121.48(18)
18	C(13)	C(14)	C(15)	116.76(18)
19	C(9)	C(14)	C(15)	121.76(17)
20	O(1)	C(15)	N(1)	118.96(18)
21	O(1)	C(15)	C(14)	125.07(18)
22	N(1)	C(15)	C(14)	115.96(16)
23	C(1)	C(2)	C(3)	120.73(19)
24	C(1)	C(2)	Cl	119.71(16)
25	C(3)	C(2)	Cl	119.56(16)
26	C(4)	C(3)	C(2)	118.9(2)
27	O(2)	C(16)	O(3)	115.5(9)
28	O(2)	C(16)	O(3B)	121.2(4)
29	O(2)	C(16)	C(8)	125.23(19)
30	O(3)	C(16)	C(8)	118.8(10)

31	O(3B)	C(16)	C(8)	113.5(4)
32	C(11)	C(10)	C(9)	121.53(19)
33	C(1)	C(6)	C(5)	119.2(2)
34	C(12)	C(13)	C(14)	120.7(2)
35	C(3)	C(4)	C(5)	121.28(19)
36	C(4)	C(5)	C(6)	120.2(2)
37	C(10)	C(11)	C(12)	121.9(2)
38	C(13)	C(12)	C(11)	118.6(2)
39	O(3)	C(17)	C(18B)	109.8(14)
40	C(18)	C(17B)	O(3B)	115.3(10)
41	C(16)	O(3B)	C(17B)	119.1(7)

Procedure for crystallization of compound 7h

Compound **7h** single crystal was obtained by slow evaporation method: the compound **7h** (50 mg) was dissolved in ethanol (25 mL) solvent system and was kept in dark place at 25 ^{o}C in the test tube. The prismatic shaped pale yellow color single crystal appeared after 20-25 days which was isolated in its initial state of growth and washed with *n*-pentane for several times.

Table S7: Crystallographic refinement data for compound **7h**

Empirical Formula	C22 H18 N2 O3
Formula Weight	358.38
Crystal System	Monoclinic
Space group	P 21/c
a (Å)	21.1372(5)
b (Å)	16.1045(4)

c (Å)	10.9027(4)
α (°), *β* (°), *γ*(°)	90, 100.168(3), 90
V (Å3)	3653.03(19)
Z	8
Density (calc)	1.303
F(000)	1504
Absorption coefficient	0.711 mm^-1
Crystal Size [mm]	0.26 x 0.20 x 0.18
Temperature (K)	293
Wavelength	1.54184 A
θ Min-Max [°]	3.471 to 68.304
Limiting indices	-25<=h<=16, -19<=k<=19, -13<=l<=13
Tot., UniqData, R(int)	32994 / 6645 [R(int) = 0.0351]
Obs. data [I > 2.0 σ(I)]	R1 = 0.1384, wR2 = 0.4517
Goodness-of-fit on F^2	2.023
R indices (all data)	R1 = 0.1587, wR2 = 0.4826
CCDC	**2251824**

Table S8: Bond lengths for compound **7h**

Number	Atom 1	Atom 2	Bond length
1	O(2)	C(3)	1.214(5)
2	O(3)	1C12	1.219(5)
3	N(2)	1C12	1.383(5)
4	N(2)	C(13)	1.391(5)

5	N(2)	C(14)	1.443(5)
6	O(6)	C(30)	1.231(5)
7	O(1)	C(3)	1.336(5)
8	O(1)	C(2)	1.455(6)
9	N(4)	C(29)	1.392(5)
10	N(4)	C(30)	1.398(5)
11	N(4)	C(37)	1.446(5)
12	O(5)	C(27)	1.235(6)
13	O(4)	C(27)	1.315(6)
14	O(4)	C(26)	1.457(7)
15	N(1)	C(13)	1.344(6)
16	N(3)	C(29)	1.332(6)
17	C(4)	C(13)	1.390(6)
18	C(4)	C(3)	1.462(6)
19	C(4)	C(5)	1.469(6)
20	C(32)	C(31)	1.392(6)
21	C(32)	C(33)	1.412(6)
22	C(32)	C(28)	1.473(6)
23	C(31)	C(36)	1.400(6)
24	C(31)	C(30)	1.461(6)
25	C(5)	C(6)	1.410(6)
26	C(5)	C(10)	1.411(6)
27	C(28)	C(29)	1.389(6)
28	C(28)	C(27)	1.449(6)

29	1C12	C(10)	1.442(6)
30	C(10)	C(9)	1.409(6)
31	C(37)	C(38)	1.341(7)
32	C(37)	C(39)	1.412(7)
33	C(46)	C(45)	1.400(8)
34	C(46)	C(40)	1.415(8)
35	C(46)	C(41)	1.443(7)
36	C(45)	C(44)	1.401(7)
37	C(45)	C(38)	1.441(7)
38	C(33)	C(34)	1.386(7)
39	C(9)	C(8)	1.363(7)
40	C(36)	C(35)	1.352(7)
41	C(6)	C(7)	1.362(7)
42	C(39)	C(40)	1.348(7)
43	C(35)	C(34)	1.373(7)
44	C(8)	C(7)	1.382(8)
45	C(42)	C(41)	1.303(10)
46	C(42)	C(43)	1.422(11)
47	C(44)	C(43)	1.376(9)
48	C(2)	C(1)	1.462(9)
49	C(26)	C(25)	1.450(11)
50	C(14)	C(17)	1.371(8)
51	C(14)	C(15)	1.400(8)
52	C(15)	C(18)	1.342(8)

53	C(17)	C(19)	1.560(8)
54	C(18)	C(20)	1.215(12)
55	C(19)	C(20)	1.3900
56	C(19)	C(23)	1.3900
57	C(20)	C(22)	1.3900
58	C(22)	C(21)	1.3900
59	C(21)	C(24)	1.3900
60	C(24)	C(23)	1.3900

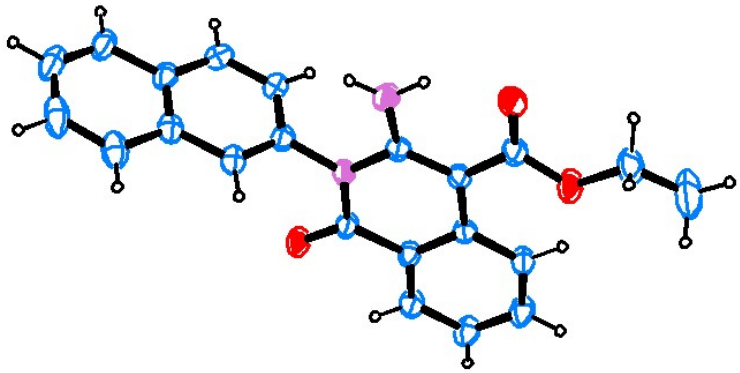

Figure S73: Molecular structure of compound **7h**, Thermal ellipsoids of carbon, nitrogen, and oxygen are set at 40% probability.

Table S9: Bond angles of compound **7h**

Number	Atom 1	Atom 2	Atom 3	Bond Angle
1	1C12	N(2)	C(13)	123.4(3)
2	1C12	N(2)	C(14)	116.7(3)
3	C(13)	N(2)	C(14)	119.8(3)
4	C(3)	O(1)	C(2)	117.6(4)
5	C(29)	N(4)	C(30)	123.0(3)
6	C(29)	N(4)	C(37)	120.9(3)

7	C(30)	N(4)	C(37)	115.9(3)
8	C(27)	O(4)	C(26)	120.1(4)
9	C(13)	C(4)	C(3)	117.2(4)
10	C(13)	C(4)	C(5)	118.1(4)
11	C(3)	C(4)	C(5)	124.7(4)
12	C(31)	C(32)	C(33)	115.9(4)
13	C(31)	C(32)	C(28)	119.0(4)
14	C(33)	C(32)	C(28)	125.1(4)
15	N(1)	C(13)	C(4)	123.4(4)
16	N(1)	C(13)	N(2)	115.1(4)
17	C(4)	C(13)	N(2)	121.5(4)
18	C(32)	C(31)	C(36)	121.7(4)
19	C(32)	C(31)	C(30)	121.5(4)
20	C(36)	C(31)	C(30)	116.7(4)
21	C(6)	C(5)	C(10)	115.6(4)
22	C(6)	C(5)	C(4)	126.2(4)
23	C(10)	C(5)	C(4)	118.2(4)
24	C(29)	C(28)	C(27)	117.4(4)
25	C(29)	C(28)	C(32)	118.7(4)
26	C(27)	C(28)	C(32)	123.9(4)
27	O(3)	1C12	N(2)	119.5(4)
28	O(3)	1C12	C(10)	124.3(4)
29	N(2)	1C12	C(10)	116.3(3)
30	C(9)	C(10)	C(5)	121.4(4)
31	C(9)	C(10)	1C12	116.2(4)
32	C(5)	C(10)	1C12	122.4(4)
33	O(6)	C(30)	N(4)	119.0(4)
34	O(6)	C(30)	C(31)	124.4(4)

35	N(4)	C(30)	C(31)	116.6(4)
36	O(2)	C(3)	O(1)	120.5(4)
37	O(2)	C(3)	C(4)	125.4(4)
38	O(1)	C(3)	C(4)	114.0(4)
39	N(3)	C(29)	C(28)	124.3(4)
40	N(3)	C(29)	N(4)	114.7(4)
41	C(28)	C(29)	N(4)	121.0(3)
42	C(38)	C(37)	C(39)	121.6(4)
43	C(38)	C(37)	N(4)	120.7(4)
44	C(39)	C(37)	N(4)	117.5(4)
45	C(45)	C(46)	C(40)	120.2(4)
46	C(45)	C(46)	C(41)	118.5(5)
47	C(40)	C(46)	C(41)	121.2(6)
48	C(46)	C(45)	C(44)	120.5(5)
49	C(46)	C(45)	C(38)	117.8(5)
50	C(44)	C(45)	C(38)	121.7(5)
51	C(34)	C(33)	C(32)	120.9(4)
52	C(37)	C(38)	C(45)	120.1(5)
53	O(5)	C(27)	O(4)	120.2(4)
54	O(5)	C(27)	C(28)	124.5(4)
55	O(4)	C(27)	C(28)	115.3(4)
56	C(8)	C(9)	C(10)	120.4(5)
57	C(35)	C(36)	C(31)	121.1(4)
58	C(7)	C(6)	C(5)	121.9(5)
59	C(40)	C(39)	C(37)	119.7(5)
60	C(36)	C(35)	C(34)	118.6(4)
61	C(35)	C(34)	C(33)	121.6(4)
62	C(39)	C(40)	C(46)	120.5(5)

63	C(9)	C(8)	C(7)	118.9(5)
64	C(41)	C(42)	C(43)	119.6(6)
65	C(42)	C(41)	C(46)	121.2(7)
66	C(43)	C(44)	C(45)	117.8(7)
67	C(6)	C(7)	C(8)	121.7(4)
68	O(1)	C(2)	C(1)	106.2(5)
69	C(44)	C(43)	C(42)	122.4(6)
70	C(25)	C(26)	O(4)	108.9(6)
71	C(17)	C(14)	C(15)	122.1(6)
72	C(17)	C(14)	N(2)	118.5(5)
73	C(15)	C(14)	N(2)	119.4(5)
74	C(18)	C(15)	C(14)	126.1(9)
75	C(14)	C(17)	C(19)	102.0(7)
76	C(20)	C(18)	C(15)	124.4(9)
77	C(20)	C(19)	C(23)	120.0
78	C(20)	C(19)	C(17)	135.3(6)
79	C(23)	C(19)	C(17)	104.7(6)
80	C(18)	C(20)	C(22)	129.7(6)
81	C(18)	C(20)	C(19)	110.2(6)
82	C(22)	C(20)	C(19)	120.0
83	C(20)	C(22)	C(21)	120.0
84	C(24)	C(21)	C(22)	120.0
85	C(21)	C(24)	C(23)	120.0
86	C(24)	C(23)	C(19)	120.0

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