Pd-catalyzed oxidative amination of 2-alkenylquinazolin-4(3*H*)-ones. Synthesis of methylene and vinyl derivatives of pyrrolo(pyrido)[2,1-*b*]quinazolinones

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Supporting Information

Detailed experimental procedures for all compounds and precursors, X-ray structure determination, $^{1}H/^{13}C$ NMR spectra for all compounds

Contents

X-ray crystallographic structure of 12f

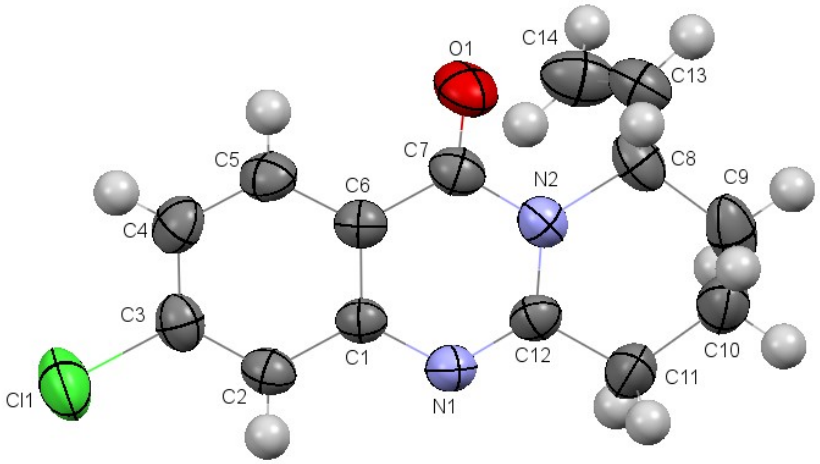


Figure S1. Molecular structure of compound **12f** according to X-ray diffraction data. Thermal ellipsoids are shown with 50 % probability level.

The colourless crystals of **12f** ($C_{14}H_{13}ClN_2O$) are orthorhombic. At 293 K a = 6.7519(6), b = 15.0413(13), c = 24.732(2) Å, V = 2511.8(4) Å^3, M_r = 260.71, Z = 8, space group *P*bca, d_{calc}= 1.379 g/cm^3, mμ(MoK_aα) = 0.293 mm^{-1}, F(000) = 1088. Intensities of 29777 reflections (2194 independent, R_{int}=0.039) were measured on the Bruker APEX II diffractometer (graphite monochromated MoK_α radiation, CCD detector, φ- and ω-scaning, $2\Theta_{max}$ = 50°). The structure was solved by direct method using SHELXTL package.[3] Positions of the hydrogen atoms were located from electron density difference maps and refined by "riding" model with $U_{iso} = 1.2U_{eq}$ of the carrier atom. Full-matrix least-squares refinement against F^2 in anisotropic approximation for non-hydrogen atoms using 2194 reflections was converged to wR_2 = 0.117 (R_1 = 0.047 for 1741 reflections with F>4σ(F), S = 1.087) (Figure S1).

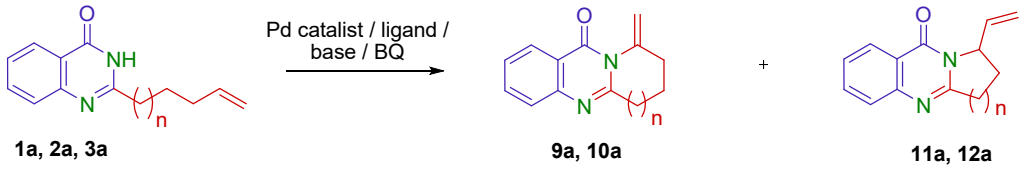
The partially saturated heterocycle of compound **12f** adopts a half-chair conformation (the puckering parameters[1] are: Q = 0.487(3), Θ = 43.6(4)^0, Ψ= 141.7(4)^0 (Figure S1). The C9 and C10 atoms deviate from the mean square plane of the remaining atoms of this cycle on 0.45 Å and -0.29 Å, respectively. The vinyl substituent is located in axial position (the C12–N2–C8–C13 torsion angle is 98.4(2)^0) and is turned in such a way that the C13=C14 double bond is almost *syn*-periplanar to the N2–C8 endocyclic bond (the N2–C8–C13–C14 torsion angle is -11.1(4)^0). It can be assumed that the orientation of the vinyl substituent is stabilized by the H14a…N2 attractive interaction (the H…N distance is 2.55 Å as compared with the van der Waals radii sum[2] of 2.67 Å), which cannot be considered as an intramolecular hydrogen bond, because the C14–H14…N angle is too sharp (100.2^0).

The final atomic coordinates, and crystallographic data for molecule **12f** have been deposited to with the Cambridge Crystallographic Data Centre, 12 Union Road, CB2 1EZ, UK (fax: +44-1223-336033; e-mail: deposit@ccdc.cam.ac.uk) and are available on request quoting the deposition numbers CCDC 2220181).

General Information

Commercially available reagents and solvents were used without further purification. The IR spectra of the compounds obtained were recorded on a Bruker Vertex 70 spectrometer in KBr pellets. The NMR spectra were recorded with Varian VXR-300 (400, 500, 600) instruments (300, 400, 500, 600 MHz for ^{1}H, 75, 101, 126, 151 MHz for ^{13}C) in $CDCl_3$ and DMSO-d_6 solutions, with TMS as an internal standard. Multiplets were assigned as s (singlet), d (doublet), t (triplet), dd (doublet of doublet), q (quartet), p (pentet), m (multiplet) and br.s (broad singlet). LC-MS spectra were recorded on an Agilent 1100 Series high performance liquid chromatograph equipped with a diode matrix with an Agilent LC\MSD SL mass selective detector. Mass spectrometric detection of samples were performed with an Infinity 1260 UHPLC system (Agilent Technologies, Waldbronn, Germany) coupled to an 6224 Accurate Mass TOF LC/MS system (Agilent Technologies, Singapore).

Table S1 Optimization of the reaction conditions for the oxidative amination of 2-alkenylquinazolin-4(3*H*)-ones **1a, 2a,3a**



1a, 2a, 3a **9a, 10a** **11a, 12a**

1a, 9a: n=0; **2a, 10a,11a:** n=1; **3a**,**12a**: n=2

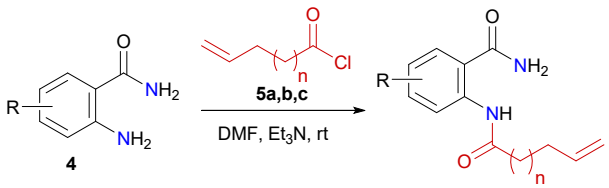
Experiment	Substrate	Catalyst (mol%)	Ligand (mol%)	Base (eq)	BQ (eq.)	Solvent	Substrate conversion, (%) [a,b]	Product
1	**1a**	$Pd(OAc)_2$ (5)	–	–	3	dioxane	5	**9a**
2	**1a**	$Pd(OAc)_2$ (5)	–	Cs_2CO_3 (2)	3	dioxane	5	**9a**
3	**1a**	$Pd(OAc)_2$ (5)	PPh_3 (11)	Cs_2CO_3 (2)	1	dioxane	45	**9a**
4	**1a**	$Pd(OAc)_2$ (5)	PPh_3 (11)	Cs_2CO_3 (2)	1,3	dioxane	54	**9a**
5	**1a**	$Pd(OAc)_2$ (5)	PPh_3 (11)	Cs_2CO_3 (2)	1,5	dioxane	60	**9a**
6	**1a**	$Pd(OAc)_2$ (5)	PPh_3 (11)	Cs_2CO_3 (2)	2	dioxane	92	**9a**
7	**1a**	$Pd(OAc)_2$ (10)	PPh_3 (21)	Cs_2CO_3 (2)	2	dioxane	100	**9a**
8	**1a**	$Pd(OAc)_2$ (5)	PPh_3 (11)	DIPEA(2)	2	dioxane	25	**9a**
9	**1a**	$Pd(dppf)_2Cl_2$(10)	–	Cs_2CO_3 (2)	4	dioxane	100	**9a**
10	**1a**	$Pd_2(dba)_3$ (10)	–	Cs_2CO_3 (2)	4	dioxane	100	**9a**
11	**2a**	$Pd(OAc)_2$ (10)	PPh_3 (21)	Cs_2CO_3 (2)	2	dioxane	0	–
12	**2a**	$Pd(OAc)_2$ (10)	PPh_3 (21)	KOH (2)	2	DMF	0	–
13	**2a**	$Pd(dppf)_2Cl_2$ (10)	–	Cs_2CO_3 (2)	2	dioxane	0	–
14	**2a**	$Pd(PPh_3)_2Cl_2$ (10)	–	*t*-BuONa (2)	2	toluene	90	**10a, 11a**
15	**2a**	$Pd(PPh_3)_2Cl_2$ (10)	–	*t*-BuONa (2)	3	toluene	100	**10a, 11a**
16	**3a**	$Pd(OAc)_2$ (10)	PPh_3 (21)	Cs_2CO_3 (2)	2	dioxane	0	–
17	**3a**	$Pd(PPh_3)_2Cl_2$ (10)	–	*t*-BuONa (2)	3	toluene	100	**12a**

[a] Reaction conditions: **1a-3a** (0.25 mmol), solvent (10.0 mL), 110 °C.

[b] Substrate conversion was determined by ^{1}H NMR spectroscopy.

General procedure 1 for the synthesis of amides (6a-i), (7a-i) and (8a-i)

2-Pent-4-enamidobenzamides (**6a-i**), 2-hex-5-enamidobenzamides (**7a-i**) and 2-hept-6-enamidobenzamides (**8a-i**) were synthesized by the previously reported procedure.[4]



5a, **6**: n = 1; **5b**, **7**: n = 2; **5c**, **8**: n = 3
4a,**6a**,**7a**,**8a**: R = H; **4b**,**6b**,**7b**,**8b**: R = 5-F;
4c,**6c**,**7c**,**8c**:R = 6-Me; **4d**,**6d**,**7d**,**8d**: R = 6-Cl;
4e,**6e**,**7e**,**8e**: R = 6-NO_2; **4f**,**6f**,**7f**,**8f**: R = 7-Cl;
4g,**6g**,**7g**,**8g**: R = 7-NO_2; **4h**,**6h**,**7h**,**8h**: R = 8-Me;
4i,**6i**,**7i**,**8i**: R = 8-F.

To a solution of amine **4** (1.5 mmol) and triethylamine (0.15 g, 1.5 mmol) in DMF (10 mL), acyl chloride **5** (1.5 mmol) was added dropwise at 0 °C. The resulting mixture was stirred at rt for 3–4 h and then left overnight. The solvent was removed *in vacuo*, and the residue was triturated with H_2O (20 mL). The crystalline product **6(7,8)** formed was filtered, dried, and used in the next without additional purification. An analytical sample of **6(7,8)** was obtained by *i*-PrOH or *t*-BuOMe (exception of 2-(hex-5-enoylamino)-4-nitrobenzamide (**7g**), which could not be isolated in the individual state).

2-(Pent-4-enoylamino)benzamide (6a)[4]

2-Fluoro-6-(pent-4-enoylamino)benzamide (6b) [4]

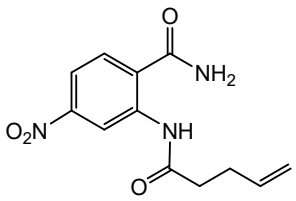
5-Methyl-2-(pent-4-enoylamino)benzamide (6c) [4]

5-Chloro-2-(pent-4-enoylamino)benzamide (6d)[4]

5-Nitro-2-(pent-4-enoylamino)benzamide (6e)[4]

4-Chloro-2-(pent-4-enoylamino)benzamide (6f) [4]

4-Nitro-2-(pent-4-enoylamino)benzamide (6g)



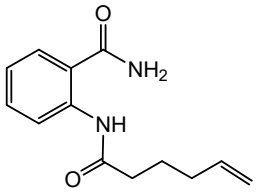
Followed the general procedure 1, using **4g** (272 mg), **5a** (178 mg). Light yellow solid (308 mg, 78% yield). Mp: 172–174 °C; **^{1}H NMR** (500 MHz, DMSO-d_6) δ 11.56 (s, 1H, NH), 9.26 (s, 1H, ArH), 8.47 (br.s, 1H, NH), 8.00–7.98 (m, 2H, ArH + NH), 7.91 (dd, J = 8.5, 1.5 Hz, 1H, ArH), 5.89–5.81 (m, 1H, =CH), 5.08 (dd, J = 17.0, 1.5 Hz, 1H, =CH_2), 4.98 (dd, J = 10.0, 1.5 Hz, 1H, =CH_2), 2.51-2.48 (m, 2H,

CH_2), 2.39–2.35 (m, 2H, CH_2); **^{13}C NMR** (150.8 MHz, DMSO-d_6) δ 171.5, 169.5, 149.5, 140.5, 137.5, 130.4, 125.7, 117.2, 116.0, 115.0, 36.9, 29.1; MS: m/z 264 (M+H); Anal. Calcd for $C_{12}H_{13}N_3O_4$: C, 54.75; H, 4.98; N, 15.96; found: C, 54.68; H, 4.95; N, 15.89.

3-Methyl-2-(pent-4-enoylamino)benzamide (6h) [4]

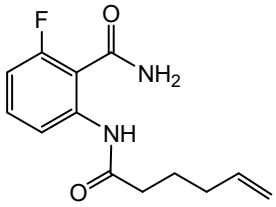
3-Fluoro-2-(pent-4-enoylamino)benzamide (6i) [4]

2-(Hex-5-enoylamino)benzamide (7a)



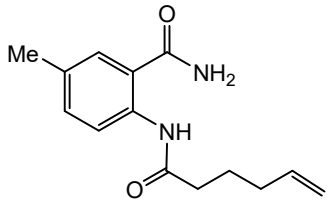
Followed the general procedure 1, using **4a** (204 mg), **5b** (199 mg). White solid (299 mg, 86% yield). Mp: 125–127 °C; **^{1}H NMR** (400 MHz, DMSO-d_6) δ 11.68 (br.s, 1H, NH), 8.47 (d, J = 8.0 Hz, 1H, ArH), 8.25 (br.s, 1H, NH), 7.78 (d, J = 8.0 Hz, 1H, ArH), 7.71 (br.s, 1H, NH), 7.47 (t, J = 8.0 Hz, 1H, ArH), 7.10 (t, J = 8.0 Hz, 1H, ArH), 5.86–5.76 (m, 1H, =CH), 5.06–4.97 (m, 2H, =CH_2), 2.34 (t, J = 7.6 Hz, 2H,CH_2); 2.07 (q, J = 7.6 Hz, 2H, CH_2); 1.70 (p, J = 7.6 Hz, 2H, CH_2); **^{13}C NMR** (150.8 MHz, DMSO-d_6) δ 171.3, 171.2, 140.1, 138.5, 132.6, 129.0, 122.7, 120.6, 120.0, 115.8, 37.3, 33.0, 24.5; MS: m/z 233 (M+H); Anal. Calcd for $C_{13}H_{16}N_2O_2$: C, 67.22; H, 6.94; N, 12.06; found: C, 67.17; H, 6.91; N, 12.05.

2-Fluoro-6-(hex-5-enoylamino)benzamide (7b)



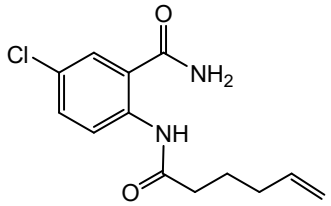
Followed the general procedure 1, using **4b** (231 mg), **5b** (199 mg). White solid (311 mg, 83% yield). Mp: 80–83 °C; **^{1}H NMR** (400 MHz, DMSO-d_6) δ 10.09 (br.s, 1H, NH), 8.00 (br.s, 1H, NH), 7.97 (br.s, 1H, NH), 7.91 (d, J = 8.4 Hz, 1H, ArH), 7.42 (dd, J = 8.4, 15.2 Hz, 1H, ArH), 7.01 (t, J = 8.4 Hz, 1H, ArH), 5.86–5.76 (m, 1H, =CH), 5.06-4.97 (m, 2H, =CH_2), 2.33 (t, J = 7.2 Hz, 2H, CH_2), 2.06 (q, J = 7.2 Hz, 2H, CH_2), 1.67 (p, J = 7.2 Hz, 2H, CH_2); **^{13}C NMR** (125.7 MHz, DMSO-d_6) δ 171.1, 165.4, 159.2 (d, $J_{C\text{-}F}$ = 246.3 Hz), 138.5 (d, $J_{C\text{-}F}$ = 7.5 Hz), 138.0, 131.4 (d, $J_{C\text{-}F}$ = 10.1 Hz), 117.9, 115.3, 114.5 (d, $J_{C\text{-}F}$ = 17.6 Hz), 110.7 (d, $J_{C\text{-}F}$ = 22.6 Hz), 36.1, 32.6, 24.1; MS: m/z 251 (M+H); Anal. Calcd for $C_{13}H_{15}FN_2O_2$: C, 62.39; H, 6.04; N, 11.19; found: C, 62.26; H, 6.00; N, 11.14.

2-(Hex-5-enoylamino)- 5-methylbenzamide (7c)



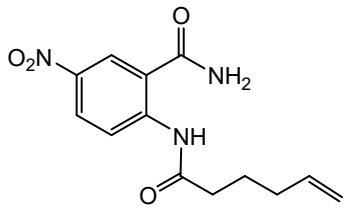
Followed the general procedure 1, using **4c** (225 mg), **5b** (199 mg). White solid (340 mg, 92% yield). Mp: 137–140 °C; **^{1}H NMR** (400 MHz, DMSO-d_6) δ 11.53 (br.s, 1H, NH), 8.35 (d, J = 8.4 Hz, 1H, ArH), 8.20 (br.s, 1H, NH), 7.67 (br.s, 1H, NH), 7.62 (s, 1H, CH), 7.28 (d, J = 8.4 Hz, 1H, ArH), 5.86–5.76 (m, 1H, =CH), 5.05-4.96 (m, 2H, =CH_2), 2.33-2.28 (m, 5H, CH_2+CH_3), 2.06 (q, J = 7.0 Hz, 2H, CH_2), 1.69 (p, J = 7.0 Hz, 2H, CH_2); **^{13}C NMR** (125.7 MHz, DMSO-d_6) δ 170.8, 170.5, 138.0, 137.2, 132.5, 131.2, 128.8, 120.1, 119.5, 115.2, 36.8, 32.4, 24.1, 20.3; MS: m/z 247 (M+H); Anal. Calcd for $C_{14}H_{18}N_2O_2$: C, 68.27; H, 7.37; N, 11.37; found: C, 68.22; H, 7.29; N, 11.32.

5-Chloro-2-(hex-5-enoylamino)benzamide (7d)



Followed the general procedure 1, using **4d** (256 mg), **5b** (199 mg). White solid (348 mg, 87% yield). Mp: 124–126 °C; **^{1}H NMR** (400 MHz, DMSO-d_6) δ 11.58 (br.s, 1H, NH), 8.47 (d, J = 9.2 Hz, 1H, ArH), 8.36 (br.s, 1H, NH), 7.86–7.85 (m, 2H, ArH + NH), 7.54 (dd, J = 9.2, 6.8 Hz, 1H, ArH), 5.85–5.75 (m, 1H, =CH), 5.05-4.96 (m, 2H, =CH_2), 2.34 (t, J = 7.2 Hz, 2H, CH_2), 2.06 (q, J = 7.2 Hz, 2H, CH_2), 1.67 (p, J = 7.2 Hz, 2H, CH_2); **^{13}C NMR** (125.7 MHz, DMSO-d_6) δ 170.9, 169.4, 138.4, 137.9, 131.7, 128.1, 126.0, 121.8, 121.2, 115.2, 36.7, 32.5, 23.9; MS: m/z 267 (M+H); Anal. Calcd for $C_{13}H_{15}ClN_2O_2$: C, 58.54; H, 5.67; N, 10.50; found: C, 58.51; H, 5.63; N, 10.46.

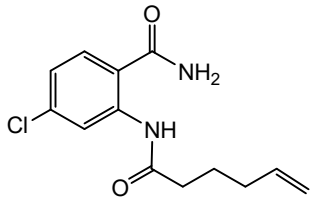
2-(Hex-5-enoylamino)-5-nitrobenzamide (7e)



Followed the general procedure 1, using **4e** (272 mg), **5b** (199 mg). Light yellow solid (332 mg, 80% yield). Mp: 126–129 °C; **^{1}H NMR** (400 MHz, DMSO-d_6) δ 12.07 (s, 1H, NH), 8.73–8.70 (m, 3H, 2ArH + NH), 8.38 (dd, J = 2.2, 9.4 Hz, 1H, ArH), 8.05 (br s, 1H, NH),), 5.86–5.76 (m, 1H, =CH), 5.06-4.97 (m, 2H, =CH_2), 2.43 (t, J = 7.2 Hz, 2H, CH_2), 2.08 (q, J = 7.2 Hz, 2H, CH_2), 1.71 (p, J = 7.2 Hz, 2H, CH_2); **^{13}C NMR** (125.7 MHz, DMSO-d_6) δ 171.7, 169.1, 145.3, 141.0, 137.9, 127.4, 124.4,

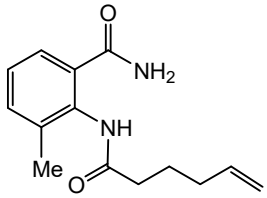
119.9, 119.0, 115.3, 36.9, 32.4, 23.7; MS: m/z 278 (M+H); Anal. Calcd for $C_{13}H_{15}N_3O_4$: C, 56.31; H, 5.45; N, 15.15; found: C, 56.25; H, 5.37; N, 15.11.

4-Chloro-2-(hex-5-enoylamino)benzamide (7f)



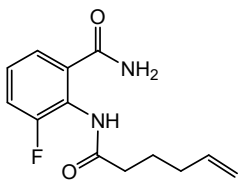
Followed the general procedure 1, using **4f** (256 mg), **5b** (199 mg). White solid (356 mg, 89% yield). Mp: 81–84 °C; **^{1}H NMR** (400 MHz, DMSO-d_6) δ 11.52 (s, 1H, NH), 8.46 (d, J = 8.8 Hz, 1H, ArH), 8.32 (br.s, 1H, NH), 7.85–7.79 (m, 2H, ArH + NH), 7.53 (d, J = 8.8 Hz, 1H, ArH), 5.85–5.75 (m, 1H, =CH), 5.05-4.96 (m, 2H, =CH_2), 2.34 (t, J = 7.2 Hz, 2H, CH_2), 2.07 (q, J = 7.2 Hz, 2H, CH_2), 1.69 (p, J = 7.2 Hz, 2H, CH_2); **^{13}C NMR** (150.8 MHz, DMSO-d_6) δ 171.7, 170.4, 141.5, 138.4, 137.1, 130.7, 122.4, 119.8, 118.2, 115.8, 37.3, 32.9, 24.4; MS: m/z 267 (M+H); Anal. Calcd for $C_{13}H_{15}ClN_2O_2$: C, 58.54; H, 5.67; N, 10.50; found: C, 58.52; H, 5.65; N, 10.42.

2-(Hex-5-enoylamino)-3-methylbenzamide (7h)



Followed the general procedure 1, using **4h** (225 mg), **5b** (199 mg). White solid (314 mg, 85% yield). Mp: 177–179 °C; **^{1}H NMR** (400 MHz, DMSO-d_6) δ 9.43 (s, 1H, NH), 7.54 (br.s, 1H, NH), 7.36–7.31 (m, 3H, ArH + NH), 7.18 (t, J = 8.8 Hz, 1H, ArH), 5.87–5.77 (m, 1H, =CH), 5.07-4.97 (m, 2H, =CH_2), 2.28 (t, J = 7.2 Hz, 2H, CH_2), 2.15 (s, 3H, CH_3), 2.07 (q, J = 7.2 Hz, 2H, CH_2), 1.67 (p, J = 7.2 Hz, 2H, CH_2); **^{13}C NMR** (150.8 MHz, DMSO-d_6) δ 171.6, 170.1, 138.7, 136.2, 134.4, 134.2, 132.2, 126.3, 126.1, 115.7, 35.5, 33.2, 24.9, 18.7; MS: m/z 247 (M+H); Anal. Calcd for $C_{14}H_{18}N_2O_2$: C, 68.27; H, 7.37; N, 11.37; found: C, 68.21; H, 7.35; N, 11.34.

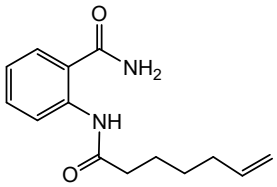
3-Fluoro-2-(hex-5-enoylamino)benzamide (7i)



Followed the general procedure 1, using **4i** (231 mg), **5b** (199 mg). White solid (270 mg, 72% yield). Mp: 176–178 °C; **^{1}H NMR** (300 MHz, DMSO-d_6) δ 9.51 (br.s, 1H, NH), 7.72 (br.s, 1H, NH), 7.48 (br.s, 1H, NH), 7.33–7.31 (m, 3H, ArH), 5.88–5.74 (m, 1H, CH), 5.06-4.95 (m, 2H, =CH_2), 2.29 (t, J =

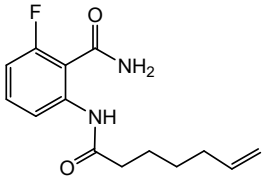
7.2 Hz, 2H, CH_2), 2.05 (q, J = 7.2 Hz, 2H, CH_2), 1.64 (p, J = 7.2 Hz, 2H, CH_2); **^{13}C NMR** (125.7 MHz, DMSO-d_6) δ 171.1, 168.0 (d, $J_{C\text{-}F}$ = 3.8 Hz), 157.0 (d,$^1J_{C\text{-}F}$ = 247.6 Hz), 138.2, 134.8, 126.9 (d, $J_{C\text{-}F}$ = 8.8 Hz), 123.6 (d, $J_{C\text{-}F}$ = 3.8 Hz), 123.6 (d, $J_{C\text{-}F}$ = 15.1 Hz), 117.3 (d, $J_{C\text{-}F}$ = 21.3 Hz), 115.2, 34.7, 32.5, 24.3; MS: m/z 251 (M+H); Anal. Calcd for $C_{13}H_{15}FN_2O_2$: C, 62.39; H, 6.04; N, 11.19; found: C, 62.34; H, 6.03; N, 11.12.

2-(Hept-6-enoylamino)benzamide (8a)



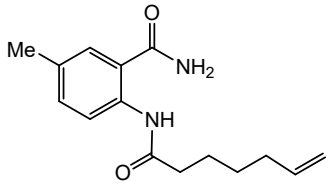
Followed the general procedure 1, using **4a** (204 mg), **5c** (220 mg). White solid (295 mg, 80% yield). Mp: 85-87 °C; **^{1}H NMR** (300 MHz, DMSO-d_6) δ 11.69 (br.s, 1H, NH), 8.47 (d, J = 7.6 Hz, 1H, ArH), 8.29 (br.s, 1H, NH), 7.79 (d, J = 7.6 Hz, 1H, ArH), 7.73 (br.s, 1H, NH), 7.47 (t, J = 7.6 Hz, 1H, ArH), 7.09 (t, J = 7.6 Hz, 1H, ArH), 5.86–5.72 (m, 1H, =CH), 4.99-4.93 (m, 2H, =CH_2), 2.33 (t, J = 7.5 Hz, 2H, CH_2), 2.04 (q, J = 7.5 Hz, 2H, CH_2), 1.61 (p, J = 7.5 Hz, 2H, CH_2), 1.39 (p, J = 7.5 Hz, 2H, CH_2); **^{13}C NMR** (150.8 MHz, DMSO-d_6) δ 171.4, 171.2, 140.2, 138.9, 132.6, 129.0, 122.6, 120.5, 119.9, 115.3, 37.8, 33.3, 28.2, 24.9; MS: m/z 247 (M+H); Anal. Calcd for $C_{14}H_{18}N_2O_2$: C, 68.27; H, 7.37; N, 11.37; found: C, 68.23; H, 7.29; N, 11.28.

2-Fluoro-6-(hept-6-enoylamino)benzamide (8b)



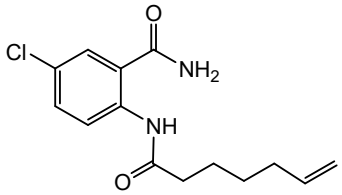
Followed the general procedure 1, using **4b** (231 mg), **5c** (220 mg). White solid (289 mg, 73% yield). Mp: 83–85 °C; **^{1}H NMR** (400 MHz, DMSO-d_6) δ 10.09 (s, 1H, NH), 8.00-7.91 (m, 3H, 2NH+ArH), 7.42 (dd, J = 8.6, 15.0 Hz, 1H, ArH), 7.00 (t, J = 8.6 Hz, 1H, ArH), 5.85–5.75 (m, 1H, =CH), 5.04-4.94 (m, 2H, =CH_2), 2.34 (t, J = 7.4 Hz, 2H, CH_2), 2.04 (q, J = 7.4 Hz, 2H, CH_2), 1.56 (p, J = 7.4 Hz, 2H, CH_2), 1.39 (p, J = 7.4 Hz, 2H, CH_2);**^{13}C NMR** (125.7 MHz, DMSO-d_6) δ 171.1, 165.3, 159.1 (d, $J_{C\text{-}F}$ = 246.2 Hz), 138.5, 138.4 (d, $J_{C\text{-}F}$ = 5.0 Hz), 131.4, 131.3, 117.8, 114.8, 110.6 (d, $^2J_{C\text{-}F}$ = 23.9 Hz), 36.5, 32.8, 27.7, 24.4; MS: m/z 265 (M+H); Anal. Calcd for $C_{14}H_{17}FN_2O_2$: C, 63.62; H, 6.48; N, 10.60; found: C, 63.55; H, 6.41; N, 10.57.

2-(Hept-6-enoylamino)- 5-methylbenzamide (8c)



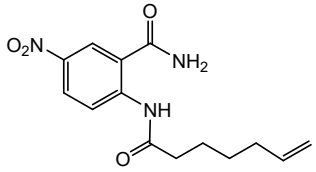
Followed the general procedure 1, using **4c** (225 mg), **5c** (220 mg). White solid (343 mg, 88% yield). Mp: 118–120 °C; **^{1}H NMR** (300 MHz, DMSO-d_6) δ 11.53 (br.s, 1H, NH), 8.34 (d, J = 8.7 Hz, 1H, ArH), 8.19 (br.s, 1H, NH), 7.66–7.61 (m, 2H, NH + ArH), 7.27 (d, J = 8.7 Hz, 1H, ArH), 5.85–5.71 (m, 1H, =CH), 5.03-4.92 (m, *2*H, =CH_2), 2.32-2.27 (m, 5H, CH_2 + CH_3), 2.03 (q, J = 7.2 Hz, 2H, CH_2), 1.59 (p, J = 7.2 Hz, 2H, CH_2), 1.38 (p, J = 7.2 Hz, 2H, CH_2); **^{13}C NMR** (125.7 MHz, DMSO-d_6) δ 171.3, 171.1, 138.9, 137.7, 133.0, 131.6, 129.2, 120.5, 119.9, 115.3, 37.8, 33.3, 28.2, 24.9, 20.8; MS: m/z 261 (M+H); Anal. Calcd for $C_{15}H_{20}N_2O_2$: C, 69.20; H, 7.74; N, 10.76; found: C, 69.16; H, 7.70; N, 10.72.

5-Chloro-2-(hept-6-enoylamino)benzamide (8d)



Followed the general procedure 1, using **4d** (256 mg), **5c** (220 mg). White solid (320 mg, 76% yield). Mp: 152–154 °C; **^{1}H NMR** (400 MHz, DMSO-d_6) δ 11.51 (br.s, 1H, NH), 8.46 (d, J = 8.8 Hz, 1H, ArH), 8.31 (br.s, 1H, NH), 7.85 (d, J = 2.4 Hz, 1H, ArH), 7.77 (br.s, 1H, NH), 7.53 (dd, J = 2.4, 8.8 Hz, 1H, ArH), 5.84–5.74 (m, 1H, =CH), 5.03-4.93 (m, 2H, =CH_2), 2.34 (t, J = 7.6 Hz, 2H, CH_2), 2.04 (q, J = 7.6 Hz, 2H, CH_2), 1.61 (p, J = 7.6 Hz, 2H, CH_2), 1.40 (p, J = 7.6 Hz, 2H, CH_2); **^{13}C NMR** (76 MHz, DMSO-d_6) δ 171.1, 169.6, 138.7, 138.4, 131.8, 128.2, 126.1, 121.8, 121.0, 114.8, 37.4, 33.0, 27.8, 24.4; MS: m/z 281 (M+H); Anal. Calcd for $C_{14}H_{17}ClN_2O_2$: C, 59.89; H, 6.10; N, 9.98; found: C, 59.83; H, 6.05; N, 9.97.

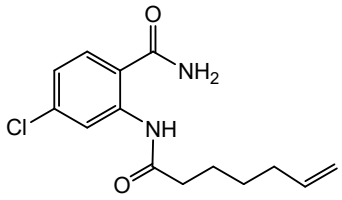
2-(Hept-6-enoylamino)-5-nitrobenzamide (8e)



Followed the general procedure 1, using **4e** (272 mg), **5c** (220 mg). Light yellow solid (323 mg, 74% yield). Mp: 135–137 °C; **^{1}H NMR** (300 MHz, DMSO-d_6) δ 12.07 (br.s, 1H, NH), 8.73-8.70 (m, 3H, 2ArH + NH), 8.36 (d, J = 9.3 Hz, 1H, ArH), 8.04 (br.s, 1H, NH), 5.86–5.72 (m, 1H, =CH), 5.04-4.93 (m, 2H, =CH_2), 2.43 (t, J = 7.2 Hz, 2H, CH_2), 2.04 (q, J = 7.2 Hz, 2H, CH_2), 1.62 (p, J = 7.2 Hz, 2H,

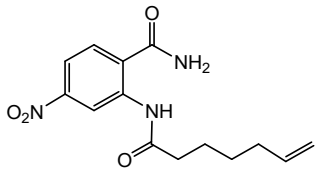
CH_2), 1.40 (p, J = 7.2 Hz, 2H, CH_2); **^{13}C NMR** (150.8 MHz, DMSO-d_6) δ 172.3, 169.6, 145.8, 141.5, 138.9, 128.0, 124.9, 120.4, 119.6, 115.4, 37.9, 33.3, 28.1, 24.6; MS: m/z 292 (M+H); Anal. Calcd for $C_{14}H_{17}N_3O_4$: C, 57.72; H, 5.88; N, 14.42; found: C, 57.69; H, 5.84; N, 14.39.

4-Chloro-2-(hept-6-enoylamino)benzamide (8f)



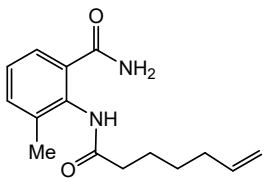
Followed the general procedure 1, using **4f** (256 mg), **5c** (220 mg). White solid (345 mg, 79% yield). Mp: 133–135 °C; **^{1}H NMR** (400 MHz, DMSO-d_6) δ 11.86 (br.s, 1H, NH), 8.60 (d, J = 1.6 Hz, 1H, ArH), 8.32 (br.s, 1H, NH), 7.84-7.80 (m, 2H, ArH + NH), 7.18 (dd, J = 1.6, 8.6 Hz, 1H, ArH), 5.84–5.74 (m, 1H, =CH), 5.03-4.93 (m, 2H, =CH_2), 2.36 (t, J = 7.2 Hz, 2H, CH_2), 2.05 (q, J = 7.2 Hz, 2H, CH_2), 1.61 (p, J = 7.2 Hz, 2H, CH_2), 1.40 (p, J = 7.2 Hz, 2H, CH_2); **^{13}C NMR** (125.7 MHz, DMSO-d_6) δ 171.9, 170.4, 141.5, 138.9, 137.1, 130.7, 122.4, 119.7, 118.1, 115.3, 37.8, 33.3, 28.1, 24.7; MS: m/z 281 (M+H); Anal. Calcd for $C_{14}H_{17}ClN_2O_2$: C, 59.89; H, 6.10; N, 9.98; found: C, 59.81; H, 6.07; N, 9.94.

2-(Hept-6-enoylamino)-4-nitrobenzamide (8g)



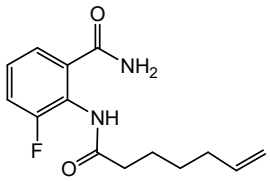
Followed the general procedure 1, using **4g** (272 mg), **5c** (220 mg). White solid (345 mg, 79% yield). Mp: 143–145 °C; **^{1}H NMR** (400 MHz, DMSO-d_6) 11.53 (br.s, 1H, NH), 9.28 (s, 1H, ArH), 8.48 (br.s, 1H, NH), 8.00-7.91 (m, 3H, 2ArH + NH), 5.85–5.75 (m, 1H, =CH), 5.04-4.94 (m, 2H, =CH_2), 2.40 (t, J = 6.8 Hz, 2H, CH_2), 2.05 (q, J = 6.8 Hz, 2H, CH_2), 1.63 (p, J = 6.8 Hz, 2H, CH_2), 1.41 (p, J = 6.8 Hz, 2H, CH_2); **^{13}C NMR** (125.7 MHz, DMSO-d_6) δ 171.72, 169.04, 148.97, 140.02, 138.39, 129.90, 125.07, 116.63, 114.85, 114.40, 37.10, 32.79, 27.60, 24.14; MS: m/z 292 (M+H); Anal. Calcd for $C_{14}H_{17}N_3O_4$: C, 57.72; H, 5.88; N, 14.42; found: C, 57.66; H, 5.84; N, 14.40.

2-(Hept-6-enoylamino)-3-methylbenzamide (8h)



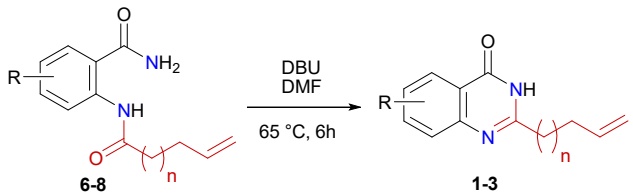
Followed the general procedure 1, using **4h** (225 mg), **5c** (220 mg). White solid (281 mg, 72% yield). Mp: 176–178 °C; **^{1}H NMR** (400 MHz, DMSO-d_6) δ 9.43 (br.s, 1H, NH), 7.55 (br.s, 1H, NH), 7.35–7.31 (m, 3H, 2ArH + NH), 7.19 (t, J = 7.2 Hz, 1H, ArH), 5.86–5.75 (m, 1H, =CH), 5.05-4.94 (m, 2H, =CH_2), 2.28 (t, J = 7.0 Hz, 2H, CH_2), 2.14 (s, 3H, CH_3), 2.05 (q, J = 7.0 Hz, 2H, CH_2), 1.59 (p, J = 7.0 Hz, 2H, CH_2), 1.40 (p, J = 7.2 Hz, 2H, CH_2); **^{13}C NMR** (100.6 MHz, DMSO-d_6) δ 171.7, 170.1, 139.1, 136.2, 134.5, 134.2, 132.2, 126.3, 126.1, 115.3, 35.9, 33.4, 28.3, 25.1, 18.7; MS: m/z 261 (M+H); Anal. Calcd for $C_{15}H_{20}N_2O_2$: C, 69.20; H, 7.74; N, 10.76; found: C, 69.17; H, 7.72; N, 10.71.

3-Fluoro-2-(hept-6-enoylamino)benzamide (8i)



Followed the general procedure 1, using **4i** (231 mg), **5c** (220 mg). White solid (321 mg, 81% yield). Mp: 150–152 °C; **^{1}H NMR** (400 MHz, DMSO-d_6) δ 9.53 (br.s, 1H, NH), 7.75 (br.s, 1H, NH), 7.50 (br.s, 1H, NH), 7.36–7.30 (m, 3H, ArH), 5.85–5.75 (m, 1H, =CH), 5.05-4.94 (m, 2H, =CH_2), 2.30 (t, J = 7.2 Hz, 2H, CH_2), 2.04 (q, J = 7.2 Hz, 2H, CH_2), 1.58 (p, J = 7.2 Hz, 2H, CH_2), 1.40 (p, J = 7.2 Hz, 2H, CH_2); **^{13}C NMR** (150.8 MHz, DMSO-d_6) δ 171.7, 168.6 (d, $J_{C\text{-}F}$ = 3.0 Hz), 157.5 (d, $J_{C\text{-}F}$ = 247.3 Hz), 139.1, 135.2, 127.4 (d, $J_{C\text{-}F}$ = 9.0 Hz), 124.2 (d, $J_{C\text{-}F}$ = 4.5 Hz), 124.1 (d, $J_{C\text{-}F}$ = 6.0 Hz), 117.8 (d, $J_{C\text{-}F}$ = 21.1 Hz), 115.2, 35.7, 33.4, 28.2, 25.0; MS: m/z 265 (M+H); Anal. Calcd for $C_{14}H_{17}FN_2O_2$: C, 63.62; H, 6.48; N, 10.60; found: C, 63.59; H, 6.44; N, 10.53.

General procedure 2 for the synthesis of 2-(but-3-en-1-yl)quinazolin-4(3*H*)-ones (1a-i), 2-(pent-4-en-1-yl)quinazolin-4(3*H*)-ones (2a-i) and 2-(hex-5-en-1-yl)quinazolin-4(3*H*)-ones (3a-i).

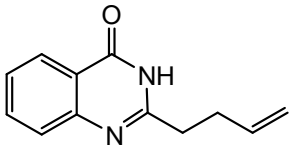


1,**6**: n = 1; **2**,**7**: n = 2; **3**,**8**: n = 3

1a,**2a**,**3a**: R = H; **1b**,**2b**,**3b**: R = 5-F; **1c**,**2c**,**3c**:R = 6-Me; **1d**,**2d**,**3d**: R = 6-Cl; **1e**,**2e3e**: R = 6-NO_2;**1f**,**2f**,**3f:** R = 7-Cl; **1g**,**2g**,**3g**: R = 7-NO_2; **1h**,**2h**,**3h**: R = 8-Me; **1i**,**2i**,**3i**: R = 8-F.

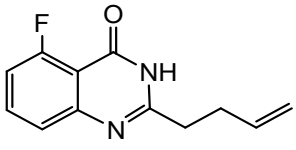
To a solution of corresponding benzamide **6-8 (**1.5 mmol) in DMF (10 ml), DBU was added (0.35 g, 2.25 mmol), followed by stirring the reaction mixture at 65-70 ºC for 6 h. After evaporation of the solvent in vacuo, water (10 ml) was added and the solution was then acidified with 2N hydrochloric acid until pH=6. The resulting precipitate was filtered off, washed with water, and dried in air.

2-(But-3-en-1-yl)quinazolin-4(3*H*)-one (1a)[4]



Followed the general procedure 2, using **6a** (327 mg). White solid (258 mg, 86% yield). Mp: 177–178 °C; **^{1}H NMR** (400 MHz, DMSO-d_6) δ 12.18 (s, 1H, NH), 8.08 (d, J = 8.0 Hz, 1H, ArH), 7.77 (t, J = 8.0 Hz, 1H, ArH), 7.60 (d, J = 8.0 Hz, 1H, ArH), 7.46 (t, J = 7.6 Hz, 1H, ArH), 5.92-5.82 (m, 1H, CH), 5.09 (d, J = 17.2 Hz, 1H, =CH_2), 4.98 (d, J = 10.4 Hz, 1H, =CH_2), 2.70 (t, J = 7.2 Hz, 2H, CH_2), 2.47–2.49 (m, 2H, CH_2); **^{13}C NMR** (125.7 MHz, DMSO-d_6) δ 161.8, 156.7, 148.9, 137.1, 134.2, 126.8, 125.9, 125.7, 120.9, 115.5, 33.7, 30.6; **HRMS** (ESI, m/z): Calcd. for $C_{12}H_{13}N_2O^+$ $[M+H]^+$, 201.1023; found: 201.1024.

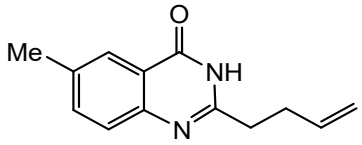
2-(But-3-en-1-yl)-5-fluoroquinazolin-4(3*H*)-one (1b) [4]



Followed the general procedure 2, using **6b** (354 mg). White solid (271 mg, 83% yield). Mp: 190–192 °C; **^{1}H NMR** (400 MHz, DMSO-d_6) δ 12.23 (br.s, 1H, NH), 7.73 (dd, J = 8.0, 14.0 Hz, 1H, ArH), 7.40 (d, J = 8.0 Hz, 1H, ArH), 7.17 (dd, J = 8.0, 10.8 Hz, 1H, ArH), 5.91-5.81 (m, 1H, CH), 5.06 (d, J = 17.6 Hz, 1H, =CH_2), 4.98 (d, J = 10.0 Hz, 1H, =CH_2), 2.67 (t, J = 7.6 Hz, 2H, CH_2), 2.48–2.46 (m, 2H, CH_2); **^{13}C NMR** (125.7 MHz, DMSO-d_6) δ 160.9 (d, J_{C-F} = 261.3 Hz), 159.5, 158.3, 151.5 137.5,

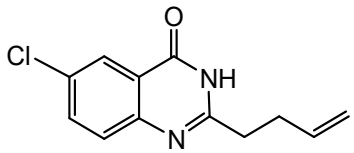
135.2 (d, $J_{C\text{-}F}$ = 10.0 Hz), 123.3, 116.0, 112.7 (d, $J_{C\text{-}F}$ = 20.0 Hz), 110.7 (d, $J_{C\text{-}F}$ = 6.3 Hz), 33.9, 30.9; **IR/cm^{-1}**: 2916, 1681, 1621, 1474, 1040, 891, 821; **HRMS** (ESI, m/z): Calcd. for $C_{12}H_{12}FN_2O^+$ $[M+H]^+$, 219.0928; found: 219.0925.

2-(But-3-en-1-yl)-6-methylquinazolin-4(3*H*)-one (1c)[4]



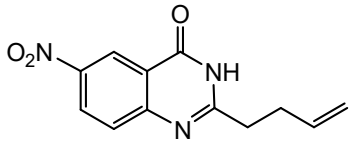
Followed the general procedure 2, using **6c** (348 mg). White solid (302 mg, 94% yield). Mp: 213–215 °C; **^{1}H NMR** (400 MHz, DMSO-d_6) δ 12.09 (br.s, 1H, NH), 7.86 (s, 1H, ArH), 7.59 (d, J = 8.4 Hz, 1H, ArH), 7.49 (d, J = 8.4 Hz, 1H, ArH), 5.92–5.82 (m, 1H, CH), 5.06 (d, J = 17.2 Hz, 1H, =CH_2), 4.97 (d, J = 10.4 Hz, 1H, =CH_2), 2.68 (t, J = 7.6 Hz, 2H, CH_2), 2.49–2.45 (m, 2H, CH_2), 2.42 (s, 3H, CH_3); **^{13}C NMR** (125.7 MHz, DMSO-d_6) δ 161.7, 155.8, 146.9, 137.2, 135.5, 135.5, 126.7, 125.0, 120.6, 115.6, 33.7, 30.6, 20.7; **IR/cm^{-1}**: 2895, 1674, 1617, 1488, 912,840; **HRMS** (ESI, m/z): Calcd. for $C_{13}H_{15}N_2O^+$ $[M+H]^+$, 215.1179; found: 215.1177.

2-(But-3-en-1-yl)-6-chloroquinazolin-4(3*H*)-one (1d)[4]



Followed the general procedure 2, using **6d** (379 mg). White solid (327 mg, 87% yield). Mp: 206–207 °C; **^{1}H NMR** (400 MHz, DMSO-d_6) δ 12.39 (s, 1H, NH), 7.99 (d, J = 2.2 Hz, 1H, ArH), 7.78 (dd, J = 8.8, 2.2 Hz, 1H, ArH), 7.61 (d, J = 8.8 Hz, 1H, ArH), 5.81–5.91 (m, 1H, =CH), 5.06 (d, J = 17.2 Hz, 1H, =CH_2), 4.97 (d, J = 10.0 Hz, 1H, =CH_2), 2.70 (t, J = 7.6 Hz, 2H, CH_2), 2.45–2.49 (m, 2H, CH_2); **^{13}C NMR** (125.7 MHz, DMSO-d_6) δ 160.7, 157.3, 147.5, 137.1, 134.2, 130.2, 129.0, 124.7, 122.1, 115.6, 33.7, 30.5; **HRMS** (ESI, m/z): Calcd. for $C_{12}H_{12}ClN_2O^+$ $[M+H]^+$, 235.0633; found: 235.0631.

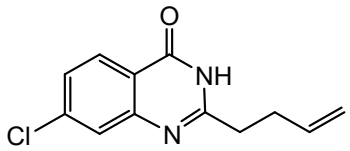
2-(But-3-en-1-yl)-6-nitroquinazolin-4(3*H*)-one (1e)[4]



Followed the general procedure 2, using **6e** (395 mg). Light yellow solid (316 mg, 86% yield). Mp: 220–222 °C; **^{1}H NMR** (400 MHz, DMSO-d_6) δ 12.67(s, 1H, NH), 8.72 (d, J = 2.6 Hz, 1H, ArH), 8.47 (dd, J = 8.8, 2.6 Hz, 1H, ArH), 7.74 (d, J = 8.8 Hz, 1H, ArH), 5.82–5.92 (m, 1H, =CH), 5.07 (dd, J = 1.6, 17.2 Hz, 1H, =CH_2), 4.99 (d, J = 1.6, 10.4 Hz, 1H, =CH_2), 2.74 (t, J = 7.6 Hz, 2H, CH_2), 2.47–2.53 (m, 2H, CH_2); **^{13}C NMR** (125.7 MHz, DMSO-d_6) δ 160.8, 160.7, 152.9, 144.2, 136.9, 128.4,

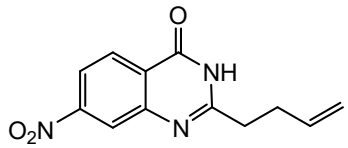
128.0, 121.7, 120.6, 115.7, 33.9, 30.3; **HRMS** (ESI, m/z): Calcd. for $C_{12}H_{12}N_3O_3^+$ $[M+H]^+$, 246.0873; found: 246.0870.

2-(But-3-en-1-yl)-7-chloroquinazolin-4(3*H*)-one (1f)[4]



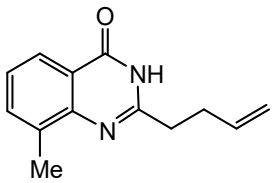
Followed the general procedure 2, using **6f** (379 mg). White solid (331 mg, 94% yield). Mp: 184–185 °C; **^{1}H NMR** (400 MHz, DMSO-d_6) δ 12.25 (s, 1H, NH), 8.06 (d, J = 8.8 Hz, 1H, ArH), 7.61 (s, H, ArH), 7.46 (d, J = 8.4 Hz, 1H, ArH), 5.82–5.92 (m, 1H, CH), 5.06 (d, J = 17.2 Hz, 1H, $=CH_2$), 4.98 (d, J = 10.4 Hz, 1H, $=CH_2$), 2.70 (t, J = 7.6 Hz, 2H, CH_2), 2.46–2.49 (m, 2H, CH_2); **^{13}C NMR** (150,8 MHz, DMSO-d_6) δ 161.5, 158.8, 150.3, 139.2, 137.4, 128.1, 126.5, 126.3, 120.0, 116.0, 34.1, 30.9; **IR/cm^{-1}**: 2910, 1682, 1620, 1603, 1428, 1072, 1001, 922, 878; **HRMS** (ESI, m/z): Calcd. for $C_{12}H_{12}ClN_2O^+$ $[M+H]^+$, 235.0633; found: 235.0635.

2-(But-3-en-1-yl)-7-nitroquinazolin-4(3*H*)-one (1g)



Followed the general procedure 2, using **6g** (395 mg). White solid (298 mg, 81% yield). Mp: 179–182 °C; **^{1}H NMR** (400 MHz, DMSO-d_6) δ 12.59 (s, 1H, NH), 8.27-8.25 (m, 2H, 2ArH), 8.14 (dd, J = 2.4, 8.8 Hz, 1H, ArH), 5.92–5.82 (m, 1H, CH), 5.07 (dd, J = 1.6, 17.2 Hz, 1H, $=CH_2$), 4.98 (d, J = 1.6, 10.0 Hz, 1H, $=CH_2$), 2.73 (t, J = 7.6 Hz, 2H, CH_2), 2.52–2.47 (m, 2H, CH_2); **^{13}C NMR** (150.8 MHz, DMSO-d_6) δ 161.1, 159.8, 151.4, 149.6, 137.4, 128.4, 125.6, 122.1, 119.9, 116.1, 34.1, 30.8; **HRMS** (ESI, m/z): Calcd. for $C_{12}H_{12}N_3O_3^+$ $[M+H]^+$, 246.0873; found: 246.0882.

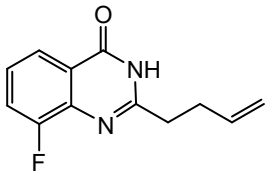
2-(But-3-en-1-yl)-8-methylquinazolin-4(3*H*)-one (1h) [4]



Followed the general procedure 2, using **6h** (348 mg). White solid (266 mg, 83% yield). Mp: 169–171 °C; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 11.21–11.31 (br.s, 1H, NH), 8.14 (d, J = 7.6 Hz, 1H, ArH), 7.64 (d, J = 7.2 Hz, H, ArH), 7.38 (t, J = 7.6 Hz, 1H, ArH), 5.93–6.03 (m, 1H, CH), 5.18 (d, J = 16.8 Hz, 1H, $=CH_2$), 5.08 (d, J = 10.4 Hz, 1H, $=CH_2$), 2.96 (t, J = 7.6 Hz, 2H, CH_2), 2.69–2.72 (m, 5H, CH_3 + CH_2); **^{13}C NMR** (125.7 MHz, DMSO-d_6) δ 164.2, 154.4, 147.2, 136.3, 135.3, 134.9, 125.5, 123.4, 119.9,

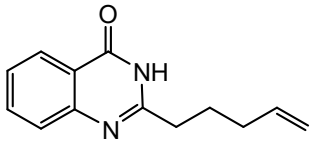
115.5, 34.3, 30.5, 17.2; **HRMS** (ESI, m/z): Calcd. for $C_{13}H_{15}N_2O^+$ $[M+H]^+$, 215.1179; found: 215.1181.

2-(But-3-en-1-yl)-8-fluoroquinazolin-4(3*H*)-one (1i)[4]



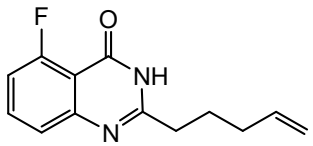
Followed the general procedure 2, using **6i** (354 mg). White solid (258 mg, 79% yield). Mp: 175–177 °C; **^{1}H NMR** (400 MHz, DMSO-d_6) δ 12.35 (br.s, 1H, NH), 7.88 (d, J = 8.0 Hz, 1H, ArH), 7.64 (dd, J = 8.0, 11.2 Hz, 1H, ArH), 7.44 (dt, J = 4.8, 8.0 Hz, 1H, ArH), 5.93–5.83 (m, 1H, CH), 5.08 (dd, J = 1.6, 17.2 Hz, 1H, =CH_2), 4.99 (d, J = 1.6, 10.0 Hz, 1H, =CH_2), 2.72 (t, J = 7.6 Hz, 2H, CH_2), 2.46–2.50 (m, 2H, CH_2); **^{13}C NMR** (150.8 MHz, DMSO-d_6) δ 161.5 (d, $J_{C\text{-}F}$ = 3.0 Hz), 158.2, 156.6 (d, $J_{C\text{-}F}$ = 252.0 Hz), 138.5 (d, $J_{C\text{-}F}$ = 10.5 Hz), 137.5, 126.4 (d, $J_{C\text{-}F}$ = 7.5 Hz), 123.4, 121.8 (d, $J_{C\text{-}F}$ = 3.0 Hz), 120.0 (d, $J_{C\text{-}F}$ = 19.5 Hz), 116.0, 34.4, 31.1; **HRMS** (ESI, m/z): Calcd. for $C_{12}H_{12}FN_2O^+$ $[M+H]^+$, 219.0928; found: 219.0925.

2-(Pent-4-en-1-yl)quinazolin-4(3*H*)-one (2a)



Followed the general procedure 2, using **7a** (348 mg). White solid (270 mg, 84%). Mp: 129–131 °C; **^{1}H NMR** (400 MHz, DMSO-d_6) δ 12.14 (br.s, 1H, NH), 8.07 (d, J = 8.0 Hz, 1H, ArH), 7.76 (t, J = 8.0 Hz, 1H, ArH), 7.59 (d, J = 8.0 Hz, 1H, ArH), 7.45 (t, J = 8.0 Hz, 1H, ArH), 5.88–5.78 (m, 1H, =CH), 5.06-4.97 (m, 2H, =CH_2), 2.60 (t, J = 7.6 Hz, 2H, CH_2), 2.09 (q, J = 7.6 Hz, 2H, CH_2), 1.82 (p, J = 7.6 Hz, 2H, CH_2); **^{13}C NMR** (125.7 MHz, DMSO-d_6) δ 162.2, 157.7, 149.4, 138.5, 134.7, 127.2, 126.4, 126.1, 121.3, 115.7, 34.4, 33.0, 26.3; **IR/cm^{-1}**: 2919, 1681, 1613, 1468, 1340, 1253, 916, 893; **HRMS** (ESI, m/z): Calcd. for $C_{13}H_{15}N_2O^+$ $[M+H]^+$, 215.1179; found: 215.1181.

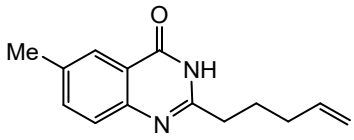
5-Fluoro-2-(pent-4-en-1-yl)quinazolin-4(3*H*)-one (2b)



Followed the general procedure 2, using **7b** (375 mg). White solid (296 mg, 85%). Mp: 138–141 °C; **^{1}H NMR** (400 MHz, DMSO-d_6) δ 12.18 (br.s, 1H, NH), 7.72 (dd, J = 8.0, 18.0 Hz, 1H, ArH), 7.39 (d,

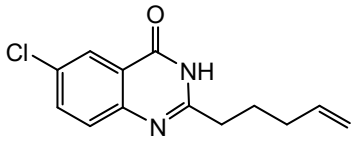
J = 8.0 Hz, 1H, ArH), 7.17 (dd, J = 8.0, 10.8 Hz, 1H, ArH), 5.86–5.76 (m, 1H, =CH), 5.05-4.95 (m, 2H, =CH_2), 2.57 (t, J = 7.2 Hz, 2H, CH_2), 2.08 (q, J = 7.2 Hz, 2H, CH_2), 1.79 (p, J = 7.2 Hz, 2H, CH_2); **^{13}C NMR** (150.8 MHz, DMSO-d_6) δ 161.0 (d, J_{C-F} = 262.4 Hz), 159.5 (d, J_{C-F} = 3.0 Hz), 158.9, 151.6 138.5, 135.3 (d, J_{C-F} = 10.6 Hz), 123.3 (d, J_{C-F} = 10.6 Hz), 115.7, 112.7 (d, J_{C-F} = 20.5 Hz), 110.8 (d, J_{C-F} = 6.0 Hz), 34.1, 33.0, 26.2; **HRMS** (ESI, m/z): Calcd. for $C_{13}H_{14}FN_2O^+$ $[M+H]^+$, 233.1085; found: 233.1082.

6-Methyl-2-(pent-4-en-1-yl)quinazolin-4(3*H*)-one (2c)



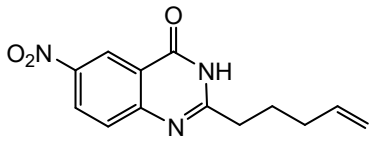
Followed the general procedure 2, using **7c** (369 mg). White solid (325 mg, 95%). Mp: 179–181 °C; **^{1}H NMR** (300 MHz, DMSO-d_6) δ 12.06 (br.s, 1H, NH), 7.84 (s, 1H, ArH), 7.57 (d, J = 8.1 Hz, 1H, ArH), 7.46 (d, J = 8.1 Hz, 1H, ArH), 5.87–5.74 (m, 1H, =CH), 5.04-4.94 (m, 2H, =CH_2), 2.56 (t, J = 7.4 Hz, 2H, CH_2), 2.40 (s, 3H, CH_3), 2.07 (q, J = 7.4 Hz, 2H, CH_2), 1.78 (p, J = 7.4 Hz, 2H, CH_2); **^{13}C NMR** (150.8 MHz, DMSO-d_6) δ 162.2, 156.7, 147.4, 138.5, 135.9, 135.9, 127.1, 125.5, 121.0, 115.7, 34.3, 33.1, 26.3, 21.2; **IR/cm^{-1}**: 2928, 1675, 1617, 1489, 1314, 1254, 1207, 992, 909; **HRMS** (ESI, m/z): Calcd. for $C_{14}H_{17}N_2O^+$ $[M+H]^+$, 229.1336; found: 229.1335.

6-Chloro-2-(pent-4-en-1-yl)quinazolin-4(3*H*)-one (2d)



Followed the general procedure 2, using **7d** (400 mg). White solid (343 mg, 92%). Mp: 184–186 °C; **^{1}H NMR** (400 MHz, DMSO-d_6) δ 12.27 (br.s, 1H, NH), 8.00 (s, 1H, ArH), 7.77 (d, J = 8.0 Hz, 1H, ArH), 7.61 (d, J = 8.0 Hz, 1H, ArH), 5.88–5.78 (m, 1H, =CH), 5.06-4.96 (m, 2H, =CH_2), 2.61 (t, J = 7.2 Hz, 2H, CH_2), 2.10 (q, J = 7.2 Hz, 2H, CH_2), 1.82 (p, J = 7.2 Hz, 2H, CH_2); **^{13}C NMR** (150.8 MHz, DMSO-d_6) δ 161.3, 158.4, 148.0, 138.5, .134.8, 130.6, 129.5, 125.1, 122.5, 115.8, 34.4, 33.0, 26.2; **IR/cm^{-1}**: 2892, 1674, 1615, 1469, 1312, 1252, 1151, 1207, 992, 924; **HRMS** (ESI, m/z): Calcd. for $C_{13}H_{14}ClN_2O^+$ $[M+H]^+$, 249.0789; found: 249.0788.

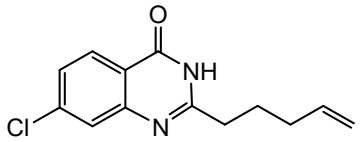
6-Nitro-2-(pent-4-en-1-yl)quinazolin-4(3*H*)-one (2e)



Followed the general procedure 2, using **7e** (416 mg). Light yellow solid (330 mg, 85%). Mp: 167–169 °C; **^{1}H NMR** (300 MHz, DMSO-d_6) δ 12.66 (br.s, 1H, NH), 8.73 (s, 1H, ArH), 8.48 (d, J = 9.0 Hz,

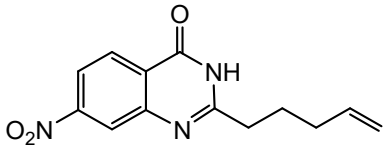
1H, ArH), 7.75 (d, J = 9.0 Hz, 1H, ArH), 5.87–5.74 (m, 1H, =CH), 5.06-4.95 (m, 2H, =CH_2), 2.64 (t, J = 7.2 Hz, 2H, CH_2), 2.09 (q, J = 7.2 Hz, 2H, CH_2), 1.82 (p, J = 7.2 Hz, 2H, CH_2); **^{13}C NMR** (150.8 MHz, DMSO-d_6) δ 161.8, 161.4, 153.6, 144.8, 138.4, 129.0, 128.7, 122.3, 121.3, 115.8, 34.6, 33.0, 26.1; **HRMS** (ESI, m/z): Calcd. for $C_{13}H_{14}N_3O_3^+$ $[M+H]^+$, 260.103; found: 260.1027.

7-Chloro-2-(pent-4-en-1-yl)quinazolin-4(3*H*)-one (2f)



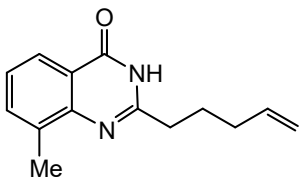
Followed the general procedure 2, using **7f** (400 mg). White solid (347 mg, 93%). Mp: 155–157 °C; **^{1}H NMR** (400 MHz, DMSO-d_6) δ 12.33 (br.s, 1H, NH), 8.06 (d, J = 8.4 Hz, 1H, ArH), 7.65 (d, J = 2.0 Hz, H, ArH), 7.49 (dd, J = 2.0, 8.4 Hz, 1H, ArH), 5.87–5.77 (m, 1H, CH), 5.06-4.96 (m, 2H, =CH_2), 2.60 (t, J = 7.2 Hz, 2H, CH_2), 2.09 (q, J = 7.2 Hz, 2H, CH_2), 1.81 (p, J = 7.2 Hz, 2H, CH_2); **^{13}C NMR** (150.8 MHz, DMSO-d_6) δ 161.8, 159.6, 150.5, 139.3, 138.5, 128.2, 126.6, 126.3, 120.1, 115.8, 34.44, 33.01 26.3; **HRMS** (ESI, m/z): Calcd. for $C_{13}H_{14}ClN_2O^+$ $[M+H]^+$, 249.0789; found: 249.0788.

7- Nitro-2-(pent-4-en-1-yl)quinazolin-4(3*H*)-one (2g)



Followed the general procedure 2, using crude **7g** (85% purity) (490 mg). White solid (311 mg, 80 %). Mp: 143–145 °C; **^{1}H NMR** (400 MHz, DMSO-d_6) δ 12.54 (br.s, 1H, NH), 8.30-8.28 (m, 2H, ArH), 8.17 (dd, J = 2.0, 8.4 Hz, H, ArH), 5.89–5.78 (m, 1H, CH), 5.07-4.97 (m, 2H, =CH_2), 2.65 (t, J = 7.2 Hz, 2H, CH_2), 2.12 (q, J = 7.2 Hz, 2H, CH_2), 1.84 (p, J = 7.2 Hz, 2H, CH_2); **^{13}C NMR** (150.8 MHz, DMSO-d_6) δ 161.2, 160.3, 151.5, 149.7, 138.4, 128.4, 125.6, 122.2, 120.0, 115.8, 34.4, 33.0, 26.1; **HRMS** (ESI, m/z): Calcd. for $C_{13}H_{14}N_3O_3^+$ $[M+H]^+$, 260.103; found: 260.1032.

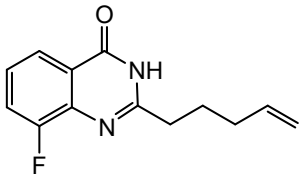
8-Methyl-2-(pent-4-en-1-yl)quinazolin-4(3*H*)-one (2h)



Followed the general procedure 2, using **7h** (369 mg). White solid (304mg, 89%). Mp: 135–138 °C; **^{1}H NMR** (400 MHz, DMSO-d_6) δ 12.15 (br.s, 1H, NH), 7.91 (d, J = 7.6 Hz, 1H, ArH), 7.62 (d, J = 7.6 Hz, H, ArH), 7.32 (t, J = 7.6 Hz, 1H, ArH), 5.89–5.79 (m, 1H, =CH), 5.07-4.97 (m, 2H, =CH_2), 2.62 (t, J = 7.4 Hz, 2H, CH_2), 2.50 (s, 3H, CH_3), 2.12 (q, J = 7.4 Hz, 2H, CH_2), 1.83 (p, J = 7.4 Hz, 2H, CH_2);**^{13}C NMR** (150.8 MHz, DMSO-d_6) δ 162.5, 155.4, 147.7, 138.6, 135.2, 135.0, 125.8, 123.8,

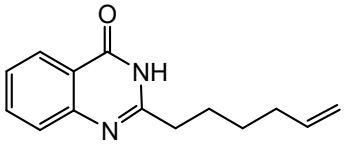
121.1, 115.7, 34.4, 33.0, 26.2, 17.6; **IR/cm^{-1}**: 2911, 1685, 1620, 1472, 1340, 1310, 1191, 996, 917; **HRMS** (ESI, m/z): Calcd. for $C_{14}H_{17}N_2O^+$ $[M+H]^+$, 229.1336; found: 229.1334.

8-Fluoro-2-(pent-4-en-1-yl)quinazolin-4(3*H*)-one (2i)



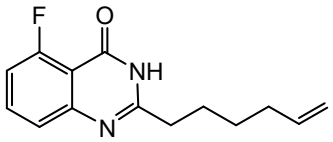
Followed the general procedure 2, using **7i** (375 mg). White solid (265 mg, 76%). Mp: 133–135 °C; **^{1}H NMR** (400 MHz, DMSO-d_6) δ 12.33 (br.s, 1H, NH), 7.87 (d, J = 7.8 Hz, 1H, ArH), 7.62 (dd, J = 7.8, 10.4 Hz, 1H, ArH), 7.42 (dt, J = 7.8, 4.8 Hz, 1H, ArH), 5.87–5.77 (m, 1H, =CH), 5.05-4.95 (m, 2H, =CH_2), 2.62 (t, J = 7.5 Hz, 2H, CH_2), 2.11 (q, J = 7.5 Hz, 2H, CH_2), 1.81 (p, J = 7.5 Hz, 2H, CH_2);**^{13}C NMR** (101 MHz, DMSO-d_6) δ 161.4, 158.6, 156.7 (d, $J_{C\text{-}F}$ = 251.0 Hz), 138.6 (d, $J_{C\text{-}F}$ = 12.1 Hz), 138.5, 126.5 (d, $J_{C\text{-}F}$ = 7.5 Hz), 123.0, 121.9 (d, $J_{C\text{-}F}$ = 5.0 Hz), 120.1 (d, $J_{C\text{-}F}$ = 18.1 Hz), 115.8, 34.6, 33.1, 26.4; **HRMS** (ESI, m/z): Calcd. for $C_{13}H_{14}FN_2O^+$ $[M+H]^+$, 233.1085; found: 233.1083.

2-(Hex-5-en-1-yl)quinazolin-4(3*H*)-one (3a)



Followed the general procedure 2, using **8a** (369 mg). White solid (291 mg, 85%). Mp: 138-142 °C; **^{1}H NMR** (400 MHz, DMSO-d_6) δ 12.16 (br.s, 1H, NH), 8.06 (d, J = 7.6 Hz, 1H, ArH), 7.74 (t, J = 7.6 Hz, 1H, ArH), 7.57 (d, J = 7.6 Hz, 1H, ArH), 7.43 (t, J = 7.6 Hz, 1H, ArH), 5.83–5.73 (m, 1H, =CH), 5.01-4.91 (m, 2H, =CH_2), 2.59 (t, J = 7.2 Hz, 2H, CH_2), 2.03 (q, J = 7.2 Hz, 2H, CH_2), 1.71 (p, J = 7.2 Hz, 2H, CH_2), 1.39 (p, J = 7.2 Hz, 2H, CH_2); **^{13}C NMR** (100.6 MHz, DMSO-d_6) δ 162.4, 157.9, 149.4, 139.0, 134.7, 127.2, 126.3, 126.2, 121.3, 115.3, 34.8, 33.3, 28.2, 26.8; **IR/cm^{-1}**: 2915, 1680, 1615, 1466, 1340, 1250, 1197, 1139, 995, 898; **HRMS** (ESI, m/z): Calcd. for $C_{14}H_{17}N_2O^+$ $[M+H]^+$, 229.1336; found: 229.1333.

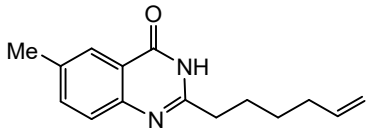
5-Fluoro-2-(hex-5-en-1-yl)quinazolin-4(3*H*)-one (3b)



Followed the general procedure 2, using **8b** (396 mg). White solid (303 mg, 82%). Mp: 146–148 °C; **^{1}H NMR** (400 MHz, DMSO-d_6) δ 12.18 (s, 1H, NH), 7.73 (dt, J = 7.8, 5.6 Hz, 1H, ArH), 7.39 (d, J = 7.8 Hz, 1H, ArH), 7.17 (dd, J = 7.8, 10.4 Hz, 1H, ArH), 5.85–5.74 (m, 1H, =CH), 5.03-4.93 (m, 2H, =CH_2), 2.57 (t, J = 7.2 Hz, 2H, CH_2), 2.05 (q, J = 7.2 Hz, 2H, CH_2), 1.71 (p, J = 7.2 Hz, 2H, CH_2),

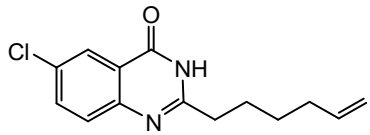
1.41 (p, J = 7.2 Hz, 2H, CH_2); **^{13}C NMR** (125.7 MHz, DMSO-d_6) δ 161.0 (d, J_{C-F} = 262.7 Hz), 159.5 (d, J_{C-F} = 5.0 Hz), 159.0, 151.6 138.9, 135.2 (d, J_{C-F} = 10.1 Hz), 123.3, 115.3, 112.7 (d, J_{C-F} = 20.2 Hz), 110.7 (d, $^4J_{C-F}$ = 6.3 Hz), 34.5, 33.37, 28.2, 26.6; **HRMS** (ESI, m/z): Calcd. for $C_{14}H_{16}FN_2O^+$ $[M+H]^+$, 247.1241; found: 247.1239.

2-(Hex-5-en-1-yl)-6-methylquinazolin-4(3*H*)-one (3c)



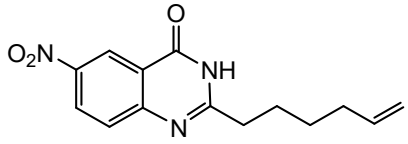
Followed the general procedure 2, using **8c** (390 mg). White solid (327 mg, 90%). Mp: 169-171 °C; **^{1}H NMR** (400 MHz, DMSO-d_6) δ 12.02 (s, 1H, NH), 7.86 (s, 1H, ArH), 7.58 (d, J = 8.4 Hz, 1H, ArH), 7.49 (d, J = 8.4 Hz, 1H, ArH), 5.85–5.75 (m, 1H, CH), 5.03-4.93 (m, 2H, =CH_2), 2.58 (t, J = 7.6 Hz, 2H, CH_2), 2.42 (s, 3H, CH_3), 2.06 (q, J = 7.2 Hz, 2H, CH_2), 1.72 (p, J = 7.2 Hz, 2H, CH_2), 1.42 (p, J = 7.2 Hz, 2H, CH_2); **^{13}C NMR** (125.7 MHz, DMSO-d_6) δ 162.8, 157.5, 148.0, 139.6, 136.6, 136.5, 127.7, 126.1, 121.6, 115.9, 35.3, 33.9, 28.8, 27.3, 21.8; **IR/cm^{-1}**: 2927, 1673, 1616, 1488, 1435, 1303, 1255, 1208, 991, 905; **HRMS** (ESI, m/z): Calcd. for $C_{15}H_{19}N_2O^+$ $[M+H]^+$, 243.1492; found: 243.149.

6-Chloro-2-(hex-5-en-1-yl)quinazolin-4(3*H*)-one (3d)



Followed the general procedure 2, using **8d** (420 mg). White solid (358 mg, 91%). Mp: 174-176 °C; **^{1}H NMR** (400 MHz, DMSO-d_6) δ 12.24 (br.s, 1H, NH), 7.98 (d, J = 2.4 Hz, 1H, ArH), 7.74 (dd, J = 8.8, 2.4 Hz, 1H, ArH), 7.58 (d, J = 8.4 Hz, 1H, ArH), 5.83–5.73 (m, 1H, =CH), 5.01-4.91 (m, 2H, =CH_2), 2.58 (t, J = 7.4 Hz, 2H, CH_2), 2.03 (q, J = 7.4 Hz, 2H, CH_2), 1.70 (p, J = 7.4 Hz, 2H, CH_2), 1.39 (p, J = 7.4 Hz, 2H, CH_2); **^{13}C NMR** (101 MHz, DMSO-d_6) δ 161.8, 159.0, 148.2, 139.0, 134.6, 130.4, 129.4, 125.2, 122.5, 115.3, 35.0, 33.3, 28.2, 26.7; **IR/cm^{-1}**: 2940, 1673, 1613, 1468, 1434, 1301, 1248, 1151, 992, 842; **HRMS** (ESI, m/z): Calcd. for $C_{14}H_{16}ClN_2O^+$ $[M+H]^+$, 263.0946; found: 263.0944.

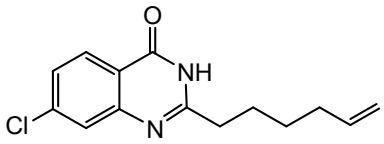
2-(Hex-5-en-1-yl)-6-nitroquinazolin-4(3*H*)-one (3e)



Followed the general procedure 2, using **8e** (437 mg). Light yellow solid (356 mg, 87%). Mp: 147-149 °C; **^{1}H NMR** (500 MHz, DMSO-d_6) δ 12.61 (s, 1H, NH), 8.71 (s, 1H, ArH), 8.45 (d, J = 9.0 Hz, 1H, ArH), 7.72 (d, J = 9.0 Hz, 1H, ArH), 5.83–5.74 (m, 1H, =CH), 5.01-4.92 (m, 2H, =CH_2), 2.63 (t, J =

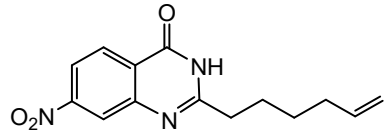
7.5 Hz, 2H, CH_2), 2.05 (q, *J* = 7.5 Hz, 2H, CH_2), 1.73 (p, *J* = 7.5 Hz, 2H, CH_2), 1.41 (p, *J* = 7.5 Hz, 2H, CH_2); **^{13}C NMR** (125.7 MHz, DMSO-d_6) δ 161.6, 161.0, 153.2, 144.4, 138.5, 128.6, 128.3, 121.9, 120.8, 114.9, 34.5, 32.8, 27.7, 26.1; **IR/cm^{-1}**: 2937, 1677, 1611, 1527, 1491,1341, 1237, 1069, 999, 924; **HRMS** (ESI, m/z): Calcd. for $C_{14}H_{16}N_3O^{3+}$ $[M+H]^+$, 274.1186; found: 274.1183.

7-Chloro-2-(hex-5-en-1-yl)quinazolin-4(3*H*)-one (3f)



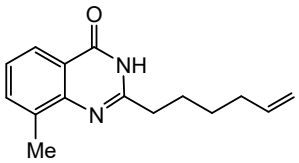
Followed the general procedure 2, using **8f** (420 mg). White solid (362 mg, 92%). Mp: 150–152 °C; **^{1}H NMR** (300 MHz, DMSO-d_6) δ 12.30 (br.s, 1H, NH), 8.06 (d, *J* = 8.4 Hz, 1H, ArH), 7.64 (d, *J* = 2.1 Hz, 1H, ArH), 7.48 (dd, *J* = 8.4, 2.1 Hz, 1H, ArH), 5.86–5.73 (m, 1H, =CH), 5.03-4.92 (m, 2H, =CH_2), 2.60 (t, *J* = 7.5 Hz, 2H, CH_2), 2.05 (q, *J* = 7.5 Hz, 2H, CH_2), 1.71 (p, *J* = 7.5 Hz, 2H, CH_2), 1.40 (p, *J* = 7.5 Hz, 2H, CH_2); **^{13}C NMR** (125.7 MHz, DMSO-d_6) δ 161.2, 159.2, 150.0, 138.9, 138.5, 127.8, 126.2, 125.9, 119.6, 114.9, 34.4, 32.8, 27.7, 26.2; **IR/cm^{-1}**: 2916, 1676, 1620, 1604, 1449, 1426, 1312, 1073, 991, 894; **HRMS** (ESI, m/z): Calcd. for $C_{14}H_{16}ClN_2O^+$ $[M+H]^+$, 263.0946; found: 263.0945.

2-(Hex-5-en-1-yl)-7-nitroquinazolin-4(3*H*)-one (3g)



Followed the general procedure 2, using **8g** (437 mg). White solid (348 mg, 85%). Mp: 139-141 °C; **^{1}H NMR** (400 MHz, DMSO-d_6) δ 12.56 (br.s, 1H, NH), 8.17 (d, *J* = 8.4 Hz, 1H, ArH), 5.86–5.75 (m, 1H, =CH), 5.04-4.94 (m, 2H, =CH_2), 2.65 (t, *J* = 7.4 Hz, 2H, CH_2), 2.05 (q, *J* = 7.4 Hz, 2H, CH_2), 1.75 (p, *J* = 7.4 Hz, 2H, CH_2), 1.43 (p, *J* = 7.4 Hz, 2H, CH_2); **^{13}C NMR** (125.7 MHz, DMSO-d_6) δ 161.3, 160.5, 151.5, 149.7, 138.9, 128.4, 125.6, 122.1, 119.9, 115.3, 34.8, 33.3, 28.1, 26.5; **HRMS** (ESI, m/z): Calcd. for $C_{14}H_{16}N_3O^{3+}$ $[M+H]^+$, 274.1186; found: 274.1183.

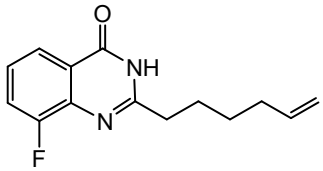
2-(Hex-5-en-1-yl)-8-methylquinazolin-4(3*H*)-one (3h)



Followed the general procedure 2, using **8h** (390 mg). White solid (287 mg, 79%). Mp: 119-121 °C; **^{1}H NMR** (600 MHz, DMSO-d_6) δ 12.10 (br.s, 1H, NH), 7.89 (dd, *J* = 7.8, 1.5 Hz, 1H, ArH), 7.57 (d, *J* = 7.8 Hz, H, ArH), 7.28 (t, *J* = 7.8 Hz, 1H, ArH), 5.80–5.73 (m, 1H, =CH), 4.99-4.90 (m, 2H, =CH_2), 2.59 (t, *J* = 7.5 Hz, 2H, CH_2), 2.03 (q, *J* = 7.5 Hz, 2H, CH_2), 1.73 (p, *J* = 7.5 Hz, 2H, CH_2), 1.40 (p, *J* =

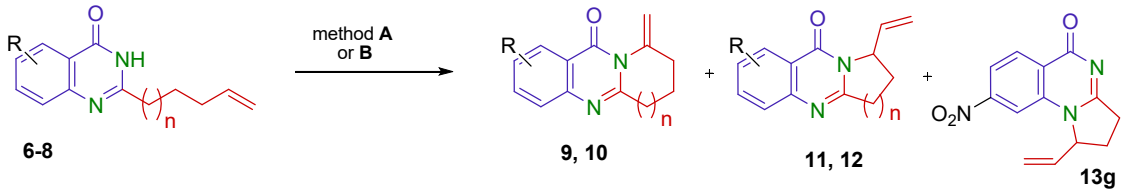
7.5 Hz, 2H, CH_2); **^{13}C NMR** (150.8 MHz, DMSO-d_6) δ 162.6, 156.6, 147.8, 139.0, 135.2, 135.0, 125.7, 123.8, 121.1, 115.2, 34.8, 33.3, 28.2, 26.6, 17.6; **HRMS** (ESI, m/z): Calcd. for $C_{15}H_{19}N_2O^+$ $[M+H]^+$, 243.1492; found: 243.1492.

8-Fluoro-2-(hex-5-en-1-yl)quinazolin-4(3*H*)-one (3i)



Followed the general procedure 2, using **8i** (396 mg).White solid (321 mg, 87%). Mp: 107-110 °C; **^{1}H NMR** (300 MHz, DMSO-d_6) δ 12.31 (br.s, 1H, NH), 7.87 (d, J = 8.1 Hz, 1H, ArH), 7.62 (dd, J = 8.1, 10.8 Hz, 1H, ArH), 7.42 (td, J = 8.1, 4.8 Hz, 1H, ArH),), 5.86–5.72 (m, 1H, =CH), 5.03-4.92 (m, 2H, $=CH_2$), 2.62 (t, J = 7.5 Hz, 2H, CH_2), 2.05 (q, J = 7.5 Hz, 2H, CH_2), 1.72 (p, J = 7.5 Hz, 2H, CH_2), 1.41 (p, J = 7.5 Hz, 2H, CH_2);**^{13}C NMR** (150.8 MHz, DMSO-d_6) δ 161.4 (d, $J_{C\text{-}F}$ = 4.5 Hz), 158.3, 156.6 (d, $J_{C\text{-}F}$ = 253.3 Hz), 138.9, 138.6 (d, $J_{C\text{-}F}$ = 12.0 Hz), 126.4 (d, $J_{C\text{-}F}$ = 7.5 Hz), 123.3, 121.9 (d, $J^{C\text{-}F}$ = 4.5 Hz), 120.1 (d, $J_{C\text{-}F}$ = 19.6 Hz), 115.3, 34.9, 33.3, 28.2, 26.7; **IR/cm^{-1}**: 2910, 1678, 1617, 1570, 1480, 1437, 1258, 1195, 1046, 999, 920, 893; **HRMS** (ESI, m/z): Calcd. for $C_{14}H_{16}FN_2O^+$ $[M+H]^+$, 247.1241; found: 247.1239.

Synthesis of 1-methylene-2,3-dihydropyrrolo[2,1-*b*]quinazolin-9(1*H*)-ones (9a-i), 9-methylene-8,9-dihydro-6*H*-pyrido[2,1-*b*]quinazolin-11(7*H*)-ones (10a-i), 1-vinyl-2,3-dihydropyrrolo[2,1-*b*]quinazolin-9(1*H*)-one (11a-c,e,h), 9-vinyl-8,9-dihydro-6*H*-pyrido[2,1-*b*]quinazolin-11(7*H*)-one (12a-i) and 8-nitro-1-vinyl-2,3-dihydropyrrolo[1,2-*a*]quinazolin-5(1*H*)-one (13g)



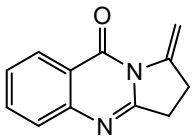
6, 9: n=0; **7, 10,11:** n=1; **8**,**12**: n=2

method **A:** $Pd(OAc)_2$,(10 mol %), PPh_3, (21 mol %), Cs_2CO_3 (2 eq), BQ, (2 eq), dioxane, 16h, 110 °C;
method **B:** $Pd(PPh_3)_2Cl_2$,(10 mol %), t-BuONa (2 eq), BQ (3 eq), toluene, 24-48h, 110 °C

Method A. To $Pd(OAc)_2$ (22 mg, 0.1 mmol) and PPh_3 (55 mg, 0.21 mmol) in dioxane (20 ml), corresponding 2-butenylquinazolinone **1a,c,d,f,h** (1.0 mmol), Cs_2CO_3 (652 mg, 2.0 mmol), and benzoquinone (652 mg, 2.0 mmol) were added. The stirred mixture was boiled for 16 h and then cooled, followed by evaporation of the solvent *in vacuo*, dilution of the residue with water (5 ml), and extraction with chloroform (3 x 20 ml). The organic layer was dried with Na_2SO_4 and the solvent was evaporated *in vacuo*. Pure product **9a-h** was chromatographed from the residue on silica gel eluting with $CHCl_3$: MeOH (100:1, v/v).

Method B. To $Pd(PPh_3)_2Cl_2$ (22 mg, 0.1 mmol) in toluene (20 ml), corresponding 2-butenyl(pentenyl)quinazolinone **1b,e,g,i** (**2a-i, 3a-i**) (1.0 mmol), *t*-BuONa (192 mg, 2.0 mmol), and benzoquinone (270 mg, 3.0 mmol) were added. The stirred mixture was boiled for 24-48 h and then cooled, followed by evaporation of the solvent *in vacuo*, dilution of the residue with water (5 ml), and extraction with chloroform (3 x 20 ml). The organic layer was dried with Na_2SO_4 and the solvent was evaporated *in vacuo*. Pure product was chromatographed from the residue on silica gel eluting with $CHCl_3$: MeOH (from 100:1, v/v).

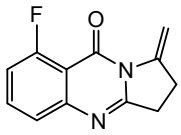
1-Methylene-2,3-dihydropyrrolo[2,1-*b*]quinazolin-9(1*H*)-one (9a)



Following the method A, using **1a** (200 mg). Light brown solid (127 mg, 64%). Mp 101-103 °C; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.32 (d, *J* = 7.6 Hz, 1H, 1ArH), 7.73 (t, *J* = 7.6 Hz, 1H, ArH), 7.62 (d, *J* = 7.6 Hz, 1H, 1ArH), 7.47 (t, *J* = 7.6 Hz, 1H, ArH), 6.45 (s, 1H, =CH_2), 5.03 (s, 1H, =CH_2), 3.14–3.10

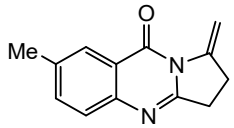
(m, 2H, CH_2), 2.92–2.86 (m, 2H, CH_2); **^{13}C NMR** (125.7 MHz, $CDCl_3$) δ 160.8, 158.9, 147.4, 143.3, 134.4, 126.9, 126.7, 126.6, 121.2, 100.5, 28.9, 25.9; **HRMS** (ESI, m/z): Calcd. for $C_{12}H_{11}N_2O^+$ $[M+H]^+$, 199.0866; found: 199.0865.

8-Fluoro-1-methylene-2,3-dihydropyrrolo[2,1-*b*]quinazolin-9(1*H*)-one (9b)



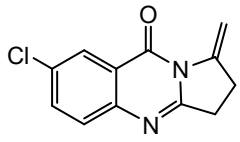
Following the method B, using 1b (218 mg). Light brown solid (117 mg, 54%). Mp: 150–152 °C; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.69-7.63 (m, 1H, 1ArH), 7.43 (d, J = 8.0 Hz, 1H, 1ArH), 7.12 (dd, J = 8.0 Hz, 10.4 Hz, 1H, ArH), 6.46 (s, 1H, =CH_2), 5.03 (s, 1H, =CH_2), 3.14–3.10 (m, 2H, CH_2), 2.93–2.89 (m, 2H, CH_2); **^{13}C NMR** (125.7 MHz, $CDCl_3$) δ 162.0 (d, J_{C-F} = 266.9 Hz), 159.9, 158.0, 149.6, 142.9, 134.8 (d, J_{C-F} = 12.1 Hz), 122.6 (d, J_{C-F} = 4.5 Hz), 113.5 (d, J_{C-F} = 21.1 Hz), 110.8, 101.0, 28.9, 25.8; **HRMS** (ESI, m/z): Calcd. for $C_{12}H_{10}FN_2O^+$ $[M+H]^+$, 217.0772; found: 217.0726.

7-Methyl-1-methylene-2,3-dihydropyrrolo[2,1-*b*]quinazolin-9(1*H*)-one (9c)



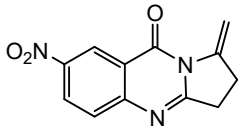
Following the method A, using **1c** (214 mg). Light brown solid (125 mg, 59%). Mp: 125-127 °C; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.03 (s, 1H, 1ArH), 7.48-7.42 (m, 2H, 2ArH), 6.35 (s, 1H, =CH_2), 4.95 (s, 1H, =CH_2), 3.05–3.01 (m, 2H, CH_2), 2.85–2.80 (m, 2H, CH_2); **^{13}C NMR** (125.7 MHz, $CDCl_3$) δ 160.7, 158.0, 145.3, 143.3, 136.6, 135.6, 126.4, 126.2, 120.8, 100.2, 28.7, 25.8, 21.2; **HRMS** (ESI, m/z): Calcd. for $C_{13}H_{13}N_2O^+$ $[M+H]^+$, 213.1023; found: 213.1014.

7-Chloro-1-methylene-2,3-dihydropyrrolo[2,1-*b*]quinazolin-9(1*H*)-one (9d)



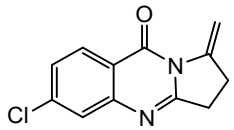
Following the method A, using **1d** (234.5 mg). White solid (135 mg, 58%). Mp: 141-143 °C; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.26 (d, J = 2.4 Hz, 1H, 1ArH), 7.65 (dd, J = 8.8, 2.4 Hz, 1H, ArH), 7.55 (d, J = 8.8 Hz, 1H, 1ArH), 6.42 (s, 1H, =CH_2), 5.04 (s, 1H, =CH_2), 3.13–3.09 (m, 2H, CH_2), 2.92–2.88 (m, 2H, CH_2); **^{13}C NMR** (125.7 MHz, DMSO-d_6) δ 160.9, 159.5, 146.5, 144.8, 135.0, 131.1, 129.2, 125.6, 122.5, 99.9, 28.7, 25.7; **HRMS** (ESI, m/z): Calcd. for $C_{12}H_{10}ClN_2O^+$ $[M+H]^+$, 233.0476; found: 233.0474.

1-Methylene-7-nitro-2,3-dihydropyrrolo[2,1-*b*]quinazolin-9(1*H*)-one (9e)



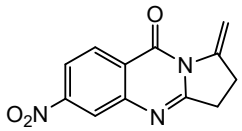
Following the method B, using **1e** (245 mg). Light yellow solid (100 mg, 41%). Mp: 194-196 °C; **^{1}H NMR** (300 MHz, $CDCl_3$) δ 9.21 (d, *J* = 2.1 Hz, 1H, 1ArH), 8.54 (dd, *J* = 9.0, 2.1 Hz, 1H, ArH), 7.76 (d, *J* = 9.0 Hz, 1H, 1ArH), 6.49 (s, 1H, =CH_2), 5.13 (s, 1H, =CH_2), 3.23–3.18 (m, 2H, CH_2), 2.99–2.94 (m, 2H, CH_2); **^{13}C NMR** (125.7 MHz, $CDCl_3$) δ 162.6, 159.4, 151.5, 145.7, 142.8, 128.5, 128.3, 123.5, 121.5, 101.9, 29.3, 25.6; **IR/cm^{-1}**: 2925, 1691, 1611, 1518, 1464, 1342, 1261, 1097, 1021; **HRMS** (ESI, m/z): Calcd. for $C_{12}H_{10}N_3O_3^+$ $[M+H]^+$, 244.0717; found: 244.0713.

6-Chloro-1-methylene-2,3-dihydropyrrolo[2,1-*b*]quinazolin-9(1*H*)-one (9f)



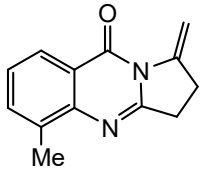
Following the method A, using **1f** (234.5 mg). White solid (130 mg,56 %). Mp: 129-131 °C; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.25 (d, *J* = 8.4 Hz, 1H, ArH), 7.62 (d, *J* = 1.6 Hz, 1H, ArH), 7.42 (dd, *J* = 1.6, 8.4 Hz, 1H, ArH), 6.43 (s, 1H, =CH_2), 5.05 (s, 1H, =CH_2), 3.15–3.11 (m, 2H, CH_2), 2.93–2.89 (m, 2H, CH_2);**^{13}C NMR** (150.8 MHz, $CDCl_3$) δ 160.3, 160.2, 148.4, 143.1, 140.6, 128.3, 127.2, 126.3, 119.7, 100.9, 29.0, 25.8; **IR/cm^{-1}**: 2924, 1680, 1601, 1462, 1261, 1096, 1020; **HRMS** (ESI, m/z): Calcd. for $C_{12}H_{10}ClN_2O^+$ $[M+H]^+$, 233.0476; found: 233.0475.

1-Methylene-6-nitro-2,3-dihydropyrrolo[2,1-*b*]quinazolin-9(1*H*)-one (9g)



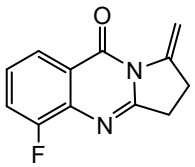
Following the method B, using **1g** (245 mg). Light yellow solid (109 mg, 45%). Mp: 207-209 °C; **^{1}H NMR** (300 MHz, $CDCl_3$) δ 8.51-8.48 (m, 2H, 2ArH), 8.25 (d, *J* = 8.4 Hz, 1H, 1ArH), 6.48 (s, 1H, =CH_2), 5.13 (s, 1H, =CH_2), 3.22–3.17 (m, 2H, CH_2), 2.99–2.93 (m, 2H, CH_2);**^{13}C NMR** (125.7 MHz, $CDCl_3$) δ 161.3, 159.4, 151.5, 148.0, 142.9, 128.7, 125.4, 122.4, 120.3, 101.8, 29.1, 25.7; **IR/cm^{-1}**: 2926, 1686, 1608,1525, 1340, 1306, 907; **HRMS** (ESI, m/z): Calcd. for $C_{12}H_{10}N_3O_3^+$ $[M+H]^+$, 244.0717; found: 244.0713.

5-Methyl-1-methylene-2,3-dihydropyrrolo[2,1-*b*]quinazolin-9(1*H*)-one (9h)



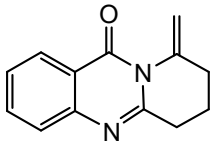
Following the method A, using **1h** (214 mg). Light brown solid (125 mg, 59%). Mp: 120-121 °C; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.20 (d, *J* = 7.6 Hz, 1H, 1ArH), 7.58 (d, *J* = 7.6 Hz, 1H, ArH), 7.36 (t, *J* = 7.6 Hz, 1H, 1ArH), 6.46–6.44 (m, 1H, =CH_2), 5.04–5.03 (m, 1H, =CH_2), 3.17–3.13 (m, 2H, CH_2), 2.93–2.88 (m, 2H, CH_2); **^{13}C NMR** (150.8 MHz, $CDCl_3$) δ 161.3, 157.6, 146.1, 143.4, 135.1, 135.0, 126.0, 124.5, 121.1, 100.4, 29.1, 25.9, 17.5; **IR/cm^{-1}**: 2963, 1684, 1614, 1454, 1335, 1277, 1148, 1073, 875; **HRMS** (ESI, m/z): Calcd. for $C_{13}H_{13}N_2O^+$ $[M+H]^+$, 213.1023; found: 213.1023.

5-Fluoro-1-methylene-2,3-dihydropyrrolo[2,1-*b*]quinazolin-9(1*H*)-one (9i)



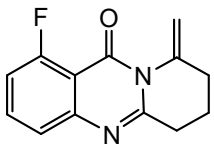
Following the method B, using **1i** (218 mg). White solid (124 mg, 57%). Mp: 142-144 °C; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.12 (d, *J* = 8.0 Hz, 1H, 1ArH), 7.50-7.39 (m, 2H, 2ArH), 6.45 (s, 1H, =CH_2), 5.07 (s, 1H, =CH_2), 3.21–3.17 (m, 2H, CH_2), 2.95–2.91 (m, 2H, CH_2); **^{13}C NMR** (125.7 MHz, $CDCl_3$) δ 159.4 (d, $J_{C\text{-}F}$ = 2.5 Hz), 159.2, 156.1 (d, $J_{C\text{-}F}$ = 255.2 Hz), 142.7, 136.3 (d, $J_{C\text{-}F}$ = 11.3 Hz), 126.1 (d, $J_{C\text{-}F}$ = 7.5 Hz), 122.7, 121.9 (d, $J_{C\text{-}F}$ = 5.0 Hz), 119.4 (d, $J_{C\text{-}F}$ = 18.9 Hz), 110.6, 28.7, 25.3; **IR/cm^{-1}**: 2963, 1690, 1614, 1448, 1339, 1260, 1096, 1020, 864; **HRMS** (ESI, m/z): Calcd. for $C_{12}H_{10}FN_2O^+$ $[M+H]^+$, 217.0772; found: 217.0722.

9-Methylene-6,7,8,9-tetrahydropyrido[2,1-*b*]quinazolin-11-one (10a)



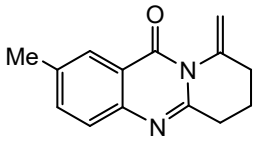
Following the method B, using **2a** (214 mg). White solid (114 mg, 54%). Mp 76-–78 °C; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.31 (d, *J* = 8.0 Hz, 1H, ArH), 7.73 (t, *J* = 8.0 Hz, 1H, ArH), 7.61 (d, *J* = 8.0 Hz, 1H, ArH), 7.46 (t, *J* = 8.0 Hz, 1H, ArH), 5.59 (s, 1H, =CH_2), 5.45 (s, 1H, =CH_2), 2.85-2.83 (m, 2H, CH_2), 2.67-2.64 (m, 2H, CH_2), 2.03–1.98 (m, 2H, CH_2); **^{13}C NMR** (150.8 MHz, DMSO-d_6) δ 160.3, 155.8, 146.8, 136.9, 134.4, 127.4, 126.6, 126.5, 121.3, 112.5, 31.7, 29.6, 18.3; **IR/cm^{-1}**: 2950, 1677, 1586, 1566, 1474, 1394, 1335, 1246, 1172, 921; **HRMS** (ESI, m/z): Calcd. for $C_{13}H_{13}N_2O^+$ $[M+H]^+$, 213.1023; found: 213.1022.

1-Fluoro-9-methylene-6,7,8,9-tetrahydropyrido[2,1-*b*]quinazolin-11-one (10b)



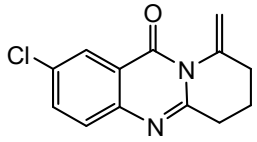
Following the method B, using **2b** (232 mg). White solid (117 mg, 56%). Mp: 85–86°C (decom.); **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.63 (dt, J = 5.0, 8.3 Hz, 1H, ArH), 7.38 (d, J = 8.3 Hz, 1H, ArH), 7.07 (dd, J = 8.3, 10.5 Hz, 1H, ArH), 5.57 (s, 1H, =CH_2), 5.43 (s, 1H, =CH_2), 2.81-2.78 (m, 2H, CH_2), 2.64-2.61 (m, 2H, CH_2), 2.01–1.95 (m, 2H, CH_2); **^{13}C NMR** (150.8 MHz, $CDCl_3$) δ 161.7 (d, $J_{C\text{-}F}$ = 265.4 Hz), 157.3 (d, $J_{C\text{-}F}$ = 4.5 Hz), 156.8, 149.0, 136.3, 134.7 (d, $J_{C\text{-}F}$ = 10.6 Hz), 122.6 (d, $J_{C\text{-}F}$ = 3.0 Hz), 113.1 (d, $J_{C\text{-}F}$ = 21.1 Hz), 112.8, 111.0 (d, $J_{C\text{-}F}$ = 6.0 Hz), 31.7, 29.7, 18.2; **HRMS** (ESI, m/z): Calcd. for $C_{13}H_{12}FN_2O^+$ $[M+H]^+$, 231.0928; found: 231.0926.

2-Methyl-9-methylene-6,7,8,9-tetrahydropyrido[2,1-*b*]quinazolin-11-one (10c)



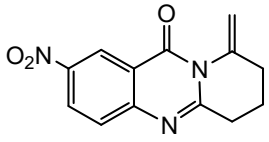
Following the method B, using **2c** (228 mg). Light yellow oil (86 mg, 38%). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.07 (s, 1H, 1ArH), 7.53-7.48 (m, 2H, 2ArH), 5.55 (s, 1H, =CH_2), 5.42 (s, 1H, =CH_2), 2.82-2.78 (m, 2H, CH_2), 2.64-2.61 (m, 2H, CH_2), 2.46 (s, 3H, CH_3), 2.01–1.94 (m, 2H, CH_2); **^{13}C NMR** (150.8 MHz, $CDCl_3$) δ 160.3, 154.8, 144.8, 137.0, 136.5, 135.8, 126.8, 126.5, 121.0, 112.4, 31.7, 29.7, 21.3, 18.3; **IR/cm^{-1}**: 2922, 1689, 1604, 1490, 1348, 1314, 1274, 1170, 1078, 896; **HRMS** (ESI, m/z): Calcd. for $C_{14}H_{15}N_2O^+$ $[M+H]^+$, 227.1179; found: 227.1178.

7-Chloro-9-methylene-6,7,8,9-tetrahydropyrido[2,1-*b*]quinazolin-11-one (10d)



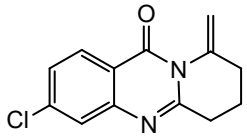
Following the method B, using **2d** (248.5 mg). White solid (141 mg, 57%). Mp: 109-111 °C; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.25 (d, J = 2.2 Hz, 1H, 1ArH), 7.65 (dd, J = 2.2, 8.4 Hz, 1H, ArH), 7.54 (d, J = 8.4 Hz, 1H, 1ArH), 5.58 (s, 1H, =CH_2), 5.46 (s, 1H, =CH_2), 2.84-2.81 (m, 2H, CH_2), 2.67-2.63 (m, 2H, CH_2), 2.04–1.97 (m, 2H, CH_2); **^{13}C NMR** (150.8 MHz, $CDCl_3$) δ 159.2, 156.0, 145.3, 136.7, 134.7, 132.1, 128.3, 126.6, 122.3, 112.7, 31.7, 29.5, 18.2; **HRMS** (ESI, m/z): Calcd. for $C_{13}H_{12}ClN_2O^+$ $[M+H]^+$, 247.0633; found: 247.0632.

9-Methylene-2-nitro-6,7,8,9-tetrahydropyrido[2,1-*b*]quinazolin-11-one (10e)



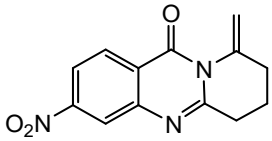
Following the method B, using **2e** (259 mg). Light yellow solid (100 mg, 39%). Mp: 169–171 °C; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 9.17 (d, *J* = 2.4 Hz, 1H, 1ArH), 8.51 (dd, *J* = 8.8, 2.4 Hz, 1H, 1ArH), 7.73 (d, *J* = 8.8 Hz, 1H, 1ArH), 5.64 (s, 1H, =CH_2), 5.52 (s, 1H, =CH_2), 2.91-2.88 (m, 2H, CH_2), 2.72-2.68 (m, 2H, CH_2), 2.09–2.02 (m, 2H, CH_2); **^{13}C NMR** (125.7 MHz, $CDCl_3$) δ 158.9, 158.6, 150.5, 144.9, 135.8, 127.9, 127.8, 123.6, 120.9, 112.7, 31.5, 28.9, 17.7; **IR/cm^{-1}**: 2958, 1690, 1598, 1573, 1520, 1344, 1262, 1166, 1125, 920, 855; **HRMS** (ESI, m/z): Calcd. for $C_{13}H_{12}N_3O_3^+$ $[M+H]^+$, 258.0873; found: 258.0873.

Chloro-9-methylene-6,7,8,9-tetrahydropyrido[2,1-*b*]quinazolin-11-one (10f)



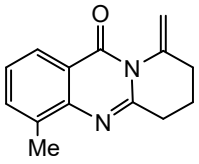
Following the method B, using **2f** (248.5 mg). White solid (138 mg, 56%). Mp: 127-129 °C; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.24 (d, *J* = 8.4 Hz, 1H, 1ArH), 7.62 (d, *J* = 1.6 Hz, 1H, ArH), 7.41 (dd, *J* = 1.6, 8.4 Hz, 1H, 1ArH), 5.59 (s, 1H, =CH_2), 5.47 (s, 1H, =CH_2), 2.86-2.82 (m, 2H, CH_2), 2.69-2.65 (m, 2H, CH_2), 2.06–1.98 (m, 2H, CH_2); **^{13}C NMR** (125.7 MHz, $CDCl_3$) δ 159.2, 156.6, 147.4, 140.0, 136.2, 128.4, 126.5, 125.8, 119.3, 112.1, 31.3, 29.0, 17.7; **HRMS** (ESI, m/z): Calcd. for $C_{13}H_{12}ClN_2O^+$ $[M+H]^+$, 247.0633; found: 247.0632.

9-Methylene-3-nitro-6,7,8,9-tetrahydropyrido[2,1-*b*]quinazolin-11-one (10g)



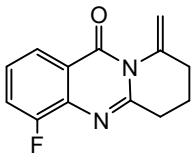
Following the method B, using **2g** (259 mg). Light yellow solid (97 mg, 37%). Mp: 133-135 °C; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.47-8.45 (m, 2H, 2ArH), 8.21 (dd, *J* = 1.6, 8.8 Hz, 1H, 1ArH), 5.63 (s, 1H, =CH_2), 5.52 (s, 1H, =CH_2), 2.91-2.87 (m, 2H, CH_2), 2.71-2.67 (m, 2H, CH_2), 2.09–2.02 (m, 2H, CH_2); **^{13}C NMR** (100.6 MHz, $CDCl_3$) δ 159.1, 158.1, 151.5, 147.5, 136.5, 129.3, 125.5, 122.4, 120.0, 113.1, 31.8, 29.4, 18.2; **HRMS** (ESI, m/z): Calcd. for $C_{13}H_{12}N_3O_3^+$ $[M+H]^+$, 258.0873; found: 258.0872.

4-Methyl-9-methylene-6,7,8,9-tetrahydropyrido[2,1-*b*]quinazolin-11-one (10h)



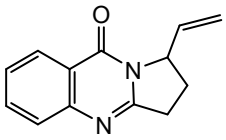
Following the method B, using **2h** (228 mg). Light yellow solid (79 mg, 35%). Mp: 79-81 °C; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.15 (d, *J* = 8.0 Hz, 1H, ArH), 7.56 (d, *J* = 8.0 Hz, 1H, ArH), 7.32 (t, *J* = 8.0 Hz, 1H, ArH), 5.58 (s, 1H, =CH_2), 5.43 (s, 1H, =CH_2), 2.87-2.83 (m, 2H, CH_2), 2.70-2.60 (m, 5H, CH_3 + CH_2), 2.03-1.96 (m, 2H, CH_2); **^{13}C NMR** (100.6 MHz, $CDCl_3$) δ 160.7, 154.3, 145.5, 137.1, 135.2, 134.9, 125.9, 125.0, 121.3, 112.3, 31.9, 29.7, 18.4, 17.3; **IR/cm^{-1}**: 2949, 1691, 1602, 1525, 1456, 1348, 1276; **HRMS** (ESI, m/z): Calcd. for $C_{14}H_{15}N_2O^+$ $[M+H]^+$, 227.1179; found: 227.1178.

4-Fluoro-9-methylene-6,7,8,9-tetrahydropyrido[2,1-*b*]quinazolin-11-one (10i)



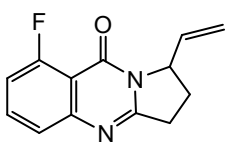
Following the method B, using **2i** (232 mg). White solid (127 mg, 55%). Mp: 111-113 °C; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.10 (d, *J* = 8.0 Hz, 1H, 1ArH), 7.48 (t, *J* = 8.0 Hz, 1H, ArH), 7.40 (dt, *J* = 4.8, 8.0 Hz, 1H, 1ArH), 5.60 (s, 1H, =CH_2), 5.49 (s, 1H, =CH_2), 2.93-2.90 (m, 2H, CH_2), 2.70-2.66 (m, 2H, CH_2), 2.07-1.99 (m, 2H, CH_2); **^{13}C NMR** (150.8 MHz, $CDCl_3$) δ 159.4 (d, J_{C-F} = 3.0 Hz), 156.6, 156.6 (d, J_{C-F} = 254.9 Hz), 136.8, 136.4 (d, J_{C-F} = 12.1 Hz), 126.4 (d, J_{C-F} = 7.5 Hz), 123.3, 122.9 (d, J_{C-F} = 4.5 Hz), 119.7 (d, $^2J_{C-F}$ = 19.6 Hz), 112.8, 31.9, 29.5, 18.2; **IR/cm^{-1}**: 2956, 1691, 1605, 1571, 1521, 1482, 1351, 1252; **HRMS** (ESI, m/z): Calcd. for $C_{13}H_{12}FN_2O^+$ $[M+H]^+$, 231.0928; found: 231.093.

1-Vinyl-2,3-dihydropyrrolo[2,1-*b*]quinazolin-9(1*H*)-one (11a)



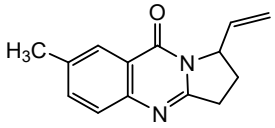
Following the method B, using **2a** (214 mg). Colourless oil (21 mg, 10%). **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.28 (d, *J* = 7.8 Hz, 1H, 1ArH), 7.73 (t, *J* = 7.8 Hz, 1H, 1ArH), 7.65 (d, *J* = 7.8 Hz, 1H, 1ArH), 7.44 (t, *J* = 7.8 Hz, 1H, 1ArH), 6.00-5.93 (m, 1H, =CH_2), 5.29-5.24 (m, 2H, CH + =CH_2), 5.17 (d, *J* = 17.0 Hz, 1H, =CH_2), 3.27–3.20 (m, 1H, CH_2), 3.07-3.02 (m, 1H, CH_2), 2.49-2.41 (m, 1H, CH_2), 2.16-2.11 (m, 1H, CH_2); **^{13}C NMR** (150.8 MHz, $CDCl_3$) δ 160.5, 159.2, 149.0, 134.2, 134.1, 126.8, 126.6, 126.3, 120.9, 116.4, 60.1, 30.7, 26.4; **HRMS** (ESI, m/z): Calcd. for $C_{13}H_{13}N_2O^+$ $[M+H]^+$, 213.1023; found: 213.1022.

8-Fluoro-1-vinyl-2,3-dihydropyrrolo[2,1-*b*]quinazolin-9(1*H*)-one (11b)



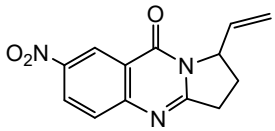
Following the method B, using **2b** (232 mg). White solid (39 mg, 15%). Mp 107-109 °C; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.63 (dt, *J* = 5.6, 8.0 Hz, 1H, 1ArH), 7.42 (dd, *J* = 0.8, 8.0 Hz, 1H, 1ArH), 7.06 (ddd, *J* = 0.8, 8.0, 10.8 Hz, 1H, 1ArH), 5.97-5.89 (m, 1H, $=CH_2$), 5.27-5.18 (m, 3H, CH + $=CH_2$), 3.26–3.17 (m, 1H, CH_2), 3.05-2.98 (m, 1H, CH_2), 2.47-2.37 (m, 1H, CH_2), 2.15-2.09 (m, 1H, CH_2);**^{13}C NMR** (125.7 MHz, $CDCl_3$) δ 161.2 (d, J_{C-F} = 265.2 Hz), 159.6, 157.1 (d, J_{C-F} = 2.5 Hz), 150.8, 134.0 (d, J_{C-F} = 10.1 Hz), 133.2, 122.2 (d, J_{C-F} = 3.8 Hz), 116.4, 112.4 (d, J_{C-F} = 21.4 Hz), 110.2 (d, J_{C-F} = 6.3 Hz), 59.7, 30.3, 25.6; **HRMS** (ESI, m/z): Calcd. for $C_{13}H_{12}FN_2O^+$ $[M+H]^+$, 231.0928; found: 231.0935.

7-Methyl-1-vinyl-2,3-dihydropyrrolo[2,1-*b*]quinazolin-9(1*H*)-one (11c)



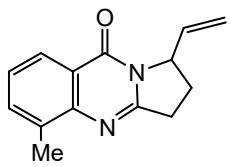
Following the method B, using **2c** (228 mg). Light yellow solid (72 mg, 32%). Mp: 60-62 °C; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.05 (s, 1H, ArH), 7.53-7.52 (m, 2H, 2ArH), 5.98-5.90 (m, 1H, $=CH_2$), 5.28-5.20 (m, 2H, CH + $=CH_2$), 5.13 (d, *J* = 17.6 Hz, 1H, $=CH_2$), 3.25–3.15 (m, 1H, CH_2), 3.04-2.98 (m, 1H, CH_2), 2.48-2.37 (m, 1H, CH_2), 2.14-2.08 (m, 1H, CH_2); **^{13}C NMR** (101.6 MHz, $CDCl_3$) δ 160.5, 158.4, 147.9, 136.5, 135.7, 134.1, 126.5, 126.1, 120.5, 116.3, 60.1, 30.6, 26.5, 21.2; **HRMS** (ESI, m/z): Calcd. for $C_{14}H_{15}N_2O^+$ $[M+H]^+$, 227.1179; found: 227.1176.

7-Nitro-1-vinyl-2,3-dihydropyrrolo[2,1-*b*]quinazolin-9(1*H*)-one (11e)



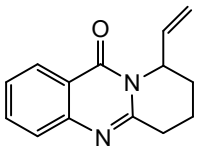
Following the method B, using **2e** (259 mg). Light yellow solid (80 mg, 31%). Mp: 123-125 °C; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 9.16 (s, 1H, 1ArH); 8.54 (d, *J* = 10.0 Hz, 1H, 1ArH); 7.78 (d, *J* = 10.0 Hz, 1H, 1ArH); 6.03-5.94 (m, 1H, $=CH_2$), 5.35-5.31 (m, 2H, CH + $=CH_2$), 5.23 (d, *J* = 17.2 Hz, 1H, $=CH_2$), 3.36–3.26 (m, 1H, CH_2), 3.17-3.10 (m, 1H, CH_2), 2.58-2.48 (m, 1H, CH_2), 2.25-2.19 (m, 1H, CH_2); **^{13}C NMR** (125.7 MHz, $CDCl_3$) δ 162.4, 158.7, 152.7, 144.9, 132.9, 127.9, 127.8, 122.8, 120.6, 116.7, 60.2, 30.6, 25.7; **HRMS** (ESI, m/z): Calcd. for $C_{13}H_{12}N_3O_3^+$ $[M+H]^+$, 258.0873; found: 258.0870.

5-Methyl-1-vinyl-2,3-dihydropyrrolo[2,1-*b*]quinazolin-9(1*H*)-one (11h)



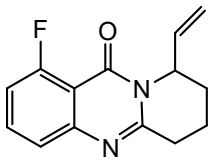
Following the method B, using **2h** (228 mg). Light brown solid (75 mg, 33%). Mp: 60-62 °C; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.16 (d, *J* = 8 Hz, 1H, 1ArH), 7.59 (d, *J* = 8 Hz, 1H, 1ArH), 7.34 (t, *J* = 8 Hz, 1H, 1ArH), 6.02-5.94 (m, 1H, =CH_2), 5.31-5.15 (m, 3H, CH + =CH_2), 3.31–3.21 (m, 1H, CH_2), 3.12-3.05 (m, 1H, CH_2), 2.62 (s, 3H, CH_3), 2.50-2.40 (m, 1H, CH_2), 2.18-2.12 (m, 1H, CH_2); **^{13}C NMR** (125.7 MHz, $CDCl_3$) δ 160.3, 157.4, 147.2, 134.7, 134.3, 133.7, 125.2, 123.8, 120.3, 115.8, 59.5, 30.3, 26.0, 17.2; **HRMS** (ESI, m/z): Calcd. for $C_{14}H_{15}N_2O^+$ $[M+H]^+$, 227.1179; found: 227.1178.

9-Vinyl-6,7,8,9-tetrahydropyrido[2,1-*b*]quinazolin-11-one (12a)



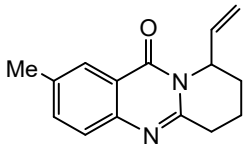
Following the method B, using **3a** (228 mg). Colourless oil (151 mg, 67%). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.27 (d, *J* = 8.0 Hz, 1H, 1ArH), 7.75 (t, *J* = 8.0 Hz, 1H, ArH), 7.66 (d, *J* = 8.0 Hz, 1H, 1ArH), 7.45 (t, *J* = 8.0 Hz, 1H, ArH), 5.95–5.87 (m, 1H, =CH), 5.67–5.61 (m, 1H, CH), 5.22 (d, *J* = 10.4 Hz, 1H, =CH_2), 4.87 (d, *J* = 17.2 Hz, 1H, =CH_2), 3.17–2.94 (m, 2H, CH_2), 2.21-1.88 (m, 4H, 2CH_2); **^{13}C NMR** (150.8 MHz, $CDCl_3$) δ 161.6, 154.7, 147.4, 136.2, 134.3, 126.9, 126.4, 126.1, 120.5, 115.9, 52.7, 31.1, 26.6, 15.7; **HRMS** (ESI, m/z): Calcd. for $C_{14}H_{15}N_2O^+$ $[M+H]^+$, 227.1179; found: 227.118.

1-Fluoro-9- vinyl-6,7,8,9-tetrahydropyrido[2,1-*b*]quinazolin-11-one (12b).



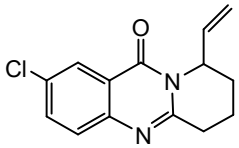
Following the method B, using **3b** (246 mg). White solid (183 mg, 75%). Mp: 92-94 °C; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.62 (dt, *J* = 8.3, 5.5 Hz, 1H, 1ArH), 7.38 (d, *J* = 8.3 Hz, 1H, 1ArH), 7.05 (dd, *J* = 8.3, 10.0 Hz, 1H, ArH), 5.91–5.84 (m, 1H, =CH), 5.61–5.57 (m, 1H, CH), 5.22-5.20 (m, 1H, =CH_2), 4.92-4.89 (m, 1H, =CH_2), 3.06–3.01 (m, 1H, CH_2), 2.94-2.87 (m, 1H, CH_2), 2.17-2.12 (m, 1H, CH_2), 2.05-1.85 (m, 3H, 1CH_2+2CH_2); **^{13}C NMR** (150.8 MHz, $CDCl_3$) δ 161.3 (d, $^1J_{C\text{-}F}$ = 266.9 Hz), 158.5 (d, $J_{C\text{-}F}$ = 4.5 Hz), 155.9, 149.4, 135.9, 134.5 (d, $J_{C\text{-}F}$ = 10.6 Hz), 122.3 (d, $J_{C\text{-}F}$ = 4.5 Hz), 116.1, 112.5 (d, $J_{C\text{-}F}$ = 21.1 Hz), 110.3 (d, $J_{C\text{-}F}$ = 6.0 Hz), 52.4, 31.0, 26.5, 15.5; **IR/cm^{-1}**: 2926, 1689, 1620, 1574, 1514, 1480, 1465, 1449, 1336, 1249, 1207, 1024, 999; **HRMS** (ESI, m/z): Calcd. for $C_{14}H_{14}FN_2O^+$ $[M+H]^+$, 245.1085; found: 245.1095.

2-Methyl-9-vinyl-6,7,8,9-tetrahydropyrido[2,1-*b*]quinazolin-11-one (12c).



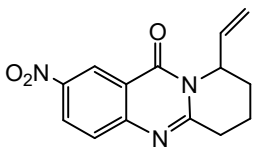
Following the method B, using **3c** (242 mg). Light brown oil (163 mg, 68%). **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.04 (s, 1H, ArH), 7.54 (d, *J* = 8.3 Hz, 1H, ArH), 7.50 (d, *J* = 8.3 Hz, 1H, ArH), 5.92–5.85 (m, 1H, =CH), 5.63–5.60 (m, 1H, CH), 5.18 (dd, *J* = 1.5, 10.0 Hz, 1H, $=CH_2$), 4.83 (dd, *J* = 1.5, 17.0 Hz, 1H, $=CH_2$), 3.07–3.02 (m, 1H, CH_2), 2.95-2.88 (m, 1H, CH_2), 2.46 (s, 3H, CH_3), 2.15-2.11 (m, 1H, CH_2), 2.03–1.94 (m, 2H, CH_2), 1.90-1.85 (m, 1H, CH_2); **^{13}C NMR** (125.7 MHz, $CDCl_3$) δ 161.1, 153.3, 144.8, 135.8, 135.7, 135.3, 125.8, 125.7, 119.7, 115.2, 52.2, 30.6, 26.1, 20.7, 15.2; **IR/cm^{-1}**: 3433, 2929, 1686, 1645, 1587, 1524, 1490; **HRMS** (ESI, m/z): Calcd. for $C_{15}H_{17}N_2O^+$ $[M+H]^+$, 241.1336; found: 241.1332.

7-Chloro-9-vinyl-6,7,8,9-tetrahydropyrido[2,1-*b*]quinazolin-11-one (12d).



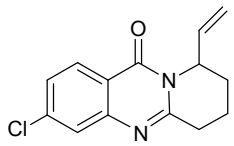
Following the method B, using **3d** (262.5 mg). Light yellow oil (167 mg, 64%). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.22 (d, *J* = 2.5 Hz, 1H, 1ArH), 7.66 (dd, *J* = 9.0, 2.5 Hz, 1H, ArH), 7.55 (d, *J* = 9.0 Hz, 1H, 1ArH), 5.93–5.85 (m, 1H, =CH), 5.62–5.58 (m, 1H, CH), 5.22 (d, *J* = 11.2 Hz, 1H, $=CH_2$), 4.86 (d, *J* = 17.2 Hz, 1H, $=CH_2$), 3.10–3.03 (m, 1H, CH_2), 2.97-2.89 (m, 1H, CH_2), 2.18-2.14 (m, 1H, CH_2), 2.05–1.88 (m, 3H, CH_2); **^{13}C NMR** (125.7 MHz, $CDCl_3$) δ 160.7, 155.2, 146.0, 136.1, 134.9, 131.9, 128.3, 126.4, 121.5, 116.2, 53.1, 31.3, 26.6, 15.7; **HRMS** (ESI, m/z): Calcd. for $C_{14}H_{14}ClN_2O^+$ $[M+H]^+$, 261.0789; found: 261.0784.

2-Nitro-9-vinyl-6,7,8,9-tetrahydropyrido[2,1-*b*]quinazolin-11-one (12e).



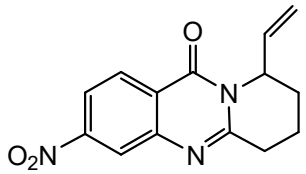
Following the method B, using **3e** (273 mg). Yellow solid (136 mg, 50%). Mp: 124-127 °C; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 9.13 (d, *J* = 2.4 Hz, 1H, 1ArH), 8.51 (dd, *J* = 2.4, 9.0 Hz, 1H, ArH), 7.70 (d, *J* = 9.0 Hz, 1H, 1ArH), 5.95–5.87 (m, 1H, =CH), 5.63–5.59 (m, 1H, CH), 5.26 (d, *J* = 10.4 Hz, 1H, $=CH_2$), 4.89 (d, *J* = 17.2 Hz, 1H, $=CH_2$), 3.15-2.95 (m, 2H, CH_2), 2.21-1.90 (m, 4H, $2CH_2$); **^{13}C NMR** (150.8 MHz, $CDCl_3$) δ 160.5, 158.7, 151.4, 145.1, 135.5, 128.4, 128.0, 123.8, 120.3, 116.4, 53.3, 31.4, 26.4, 15.4; **HRMS** (ESI, m/z): Calcd. for $C_{14}H_{14}N_3O_3^+$ $[M+H]^+$, 272.103; found: 272.1026.

3-Chloro-9-vinyl-6,7,8,9-tetrahydropyrido[2,1-*b*]quinazolin-11-one (12f).



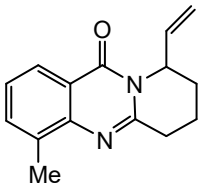
Following the method B, using **3f** (262.5 mg). White solid (180 mg, 69%). Mp: 105-107 °C; **^{1}H NMR** (300 MHz, $CDCl_3$) δ 8.18 (d, *J* = 8.4 Hz, 1H, 1ArH), 7.60 (d, *J* = 1.8 Hz, 1H, ArH), 7.37 (dd, J^1 = 8.4, 1.8 Hz, 1H, 1ArH), 5.95–5.84 (m, 1H, =CH), 5.62–5.56 (m, 1H, CH), 5.22 (dd, *J* = 1.4, 10.5 Hz, 1H, $=CH_2$), 4.86 (dd, *J* = 1.4, 14.1 Hz, 1H, $=CH_2$), 3.10–2.87 (m, 2H, CH_2), 2.18–1.86 (m, 4H, $2CH_2$); **^{13}C NMR** (100.6 MHz, $CDCl_3$) δ 161.0, 156.1, 148.3, 140.4, 136.0, 128.4, 126.7, 126.0, 118.9, 116.0, 52.9, 31.2, 26.5, 15.5; **IR/cm^{-1}**: 3333, 2953, 1676, 1600, 1576, 1556, 1466, 1392, 1319, 1150, 1073, 1001, 944, 917; **HRMS** (ESI, m/z): Calcd. for $C_{14}H_{14}ClN_2O^+$ $[M+H]^+$, 261.0789; found: 261.0785.

3-Nitro-9-vinyl-6,7,8,9-tetrahydropyrido[2,1-*b*]quinazolin-11-one (12g).



Following the method B, using **3g** (273 mg). Yellow solid (171 mg, 63%). Mp: 104-105 °C; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.44 (d, *J* = 2.0 Hz, 1H, ArH), 7.40 (d, *J* = 8.6 Hz, 1H, ArH), 8.16 (dd, *J* = 2.0, 8.6 Hz, 1H, ArH), 5.94–5.86 (m, 1H, =CH), 5.61–5.57 (m, 1H, CH), 5.24 (dd, *J* = 1.6, 10.6 Hz, 1H, $=CH_2$), 4.87 (dd, *J* = 1.6, 17.2 Hz, 1H, $=CH_2$), 3.14–3.07 (m, 1H, CH_2), 3.02-2.93 (m, 1H, CH_2), 2.19-2.15 (m, 1H, CH_2), 2.07-1.89 (m, 3H, CH_2); **^{13}C NMR** (150.8 MHz, $CDCl_3$) δ 160.4, 157.2, 151.6, 147.8, 135.6, 128.8, 124.4, 122.2, 119.6, 116.3, 53.3, 31.2, 26.4, 15.4; **HRMS** (ESI, m/z): Calcd. for $C_{14}H_{14}N_3O_3^+$ $[M+H]^+$, 272.103; found: 272.1028.

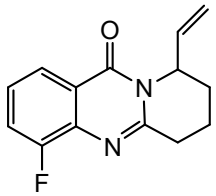
4-Methyl-9-vinyl-6,7,8,9-tetrahydropyrido[2,1-*b*]quinazolin-11-one (12h).



Following the method B, using **3h** (242 mg). White solid (173 mg, 72%). Mp: 68-69 °C; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.13 (d, *J* = 7.6 Hz, 1H, ArH), 7.57 (d, *J* = 7.6 Hz, 1H, ArH), 7.31 (t, *J* = 7.6 Hz, 1H, ArH), 5.95–5.87 (m, 1H, =CH), 5.64–5.61 (m, 1H, CH), 5.20 (dd, *J* = 10.4, 1.6 Hz, 1H, $=CH_2$), 4.87 (dd, *J* = 17.4, 1.6 Hz, 1H, $=CH_2$), 3.13–3.06 (m, 1H, CH_2), 3.00-2.91 (m, 1H, CH_2), 2.60 (s, 3H, CH_3), 2.17-2.12 (m, 1H, CH_2), 2.06-1.86 (m, 3H, CH_2); **^{13}C NMR** (125.7 MHz, $CDCl_3$) δ 162.2, 153.5, 146.2, 136.5, 135.1, 134.9, 125.7, 124.7, 120.6, 115.9, 52.8, 31.5, 26.8, 17.4, 16.0; **IR/cm^{-1}**:

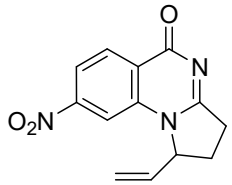
2951, 1676, 1595, 1572, 1461, 1393, 1337, 1205, 1075, 1017, 918; **HRMS** (ESI, m/z): Calcd. for $C_{15}H_{17}N_2O^+$ $[M+H]^+$, 241.1336; found: 241.1333.

4-Fluoro-9-vinyl-6,7,8,9-tetrahydropyrido[2,1-*b*]quinazolin-11-one (12i).



Following the method B, using **3i** (246 mg). White solid (168 mg, 69%). Mp: 96-98 °C; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.02 (d, *J* = 8.0 Hz, 1H, 1ArH), 7.43 (ddd, *J* = 10.4, 8.0, 1.2 Hz, 1H, ArH), 7.33 (dt, *J* = 8.0, 4.8 Hz, 1H, 1ArH), 5.92–5.84 (m, 1H, =CH), 5.63–5.56 (m, 1H, CH), 5.20 (dd, *J* = 10.4, 1.2 Hz, 1H, $=CH_2$), 4.85 (dd, *J* = 17.6, 1.2 Hz, 1H, $=CH_2$), 3.15-3.08 (m, 1H, CH_2), 3.02-2.94 (m, 1H, CH_2), 2.19-2.11 (m, 1H, CH_2), 2.06–1.84 (m, 2H, $1CH_2$ + $2CH_2$); **^{13}C NMR** (100.6 MHz, $CDCl_3$) δ 160.7, (d, $J_{C\text{-}F}$ = 3.0 Hz), 156.4 (d, $J_{C\text{-}F}$ = 254.5 Hz), 155.6, 137.0 (d, $J_{C\text{-}F}$ = 11.1 Hz), 135.93, 126.0 (d, $J_{C\text{-}F}$ = 8.0 Hz), 122.4 (d, $J_{C\text{-}F}$ = 5.0 Hz), 119.5 (d, $J_{C\text{-}F}$ = 19.1 Hz), 117.2, 116.0, 53.0, 31.3, 26.5, 15.5; **HRMS** (ESI, m/z): Calcd. for $C_{14}H_{14}FN_2O^+$ $[M+H]^+$, 245.1085; found: 245.1083.

8-Nitro-1-vinyl-2,3-dihydropyrrolo[1,2-*a*]quinazolin-5(1*H*)-one (13g)



Following the method B, using **2g** (259 mg). Yellow oil (75 mg, 29%). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.23 -8.18 (m, 2H, 2ArH); 7.91 (d, *J* = 8.4 Hz, 1H, 1ArH); 5.73-5.64 (m, 1H, $=CH_2$), 5.33 (d, *J* = 17.2 Hz, 1H, $=CH_2$), 5.22 (d, *J* = 10.0 Hz, 1H, $=CH_2$), 4.87 (q, *J* = 7.2 Hz, 1H, CH), 2.79-2.63 (m, 2H, CH_2), 2.61-2.53 (m, 1H, CH_2), 2.13-2.03 (m, 1H, CH_2); **^{13}C NMR** (150.8 MHz, $CDCl_3$) δ 174.4, 150.3, 142.0, 135.9, 134.6, 122.9, 121.7, 120.6, 117.3, 115.3, 63.8, 30.4, 26.7; **HRMS** (ESI, m/z): Calcd. for $C_{13}H_{12}N_3O_3^+$ $[M+H]^+$, 258.0873; found: 258.0869.

References

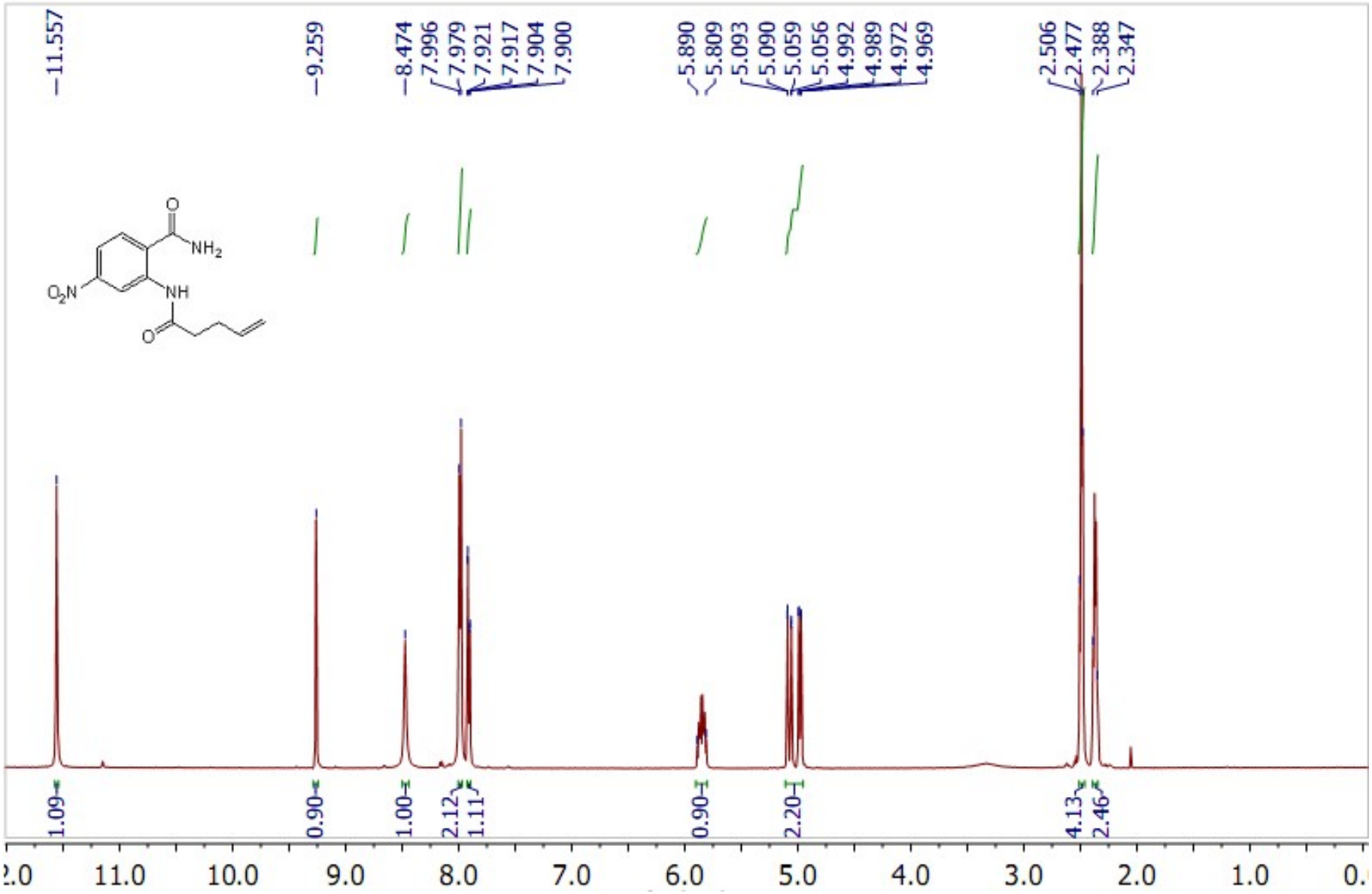
1 D. Cremer and J.A. Pople, General definition of ring puckering coordinates. *J. Amer. Chem. Soc*., 1975, **97** (6), 1354-1358.

2 Y.V. Zefirov, Reduced intermolecular contacts and specific interactions in molecular crystals, *Crystallogr. Rep.* 1997, **42**, 865–886.

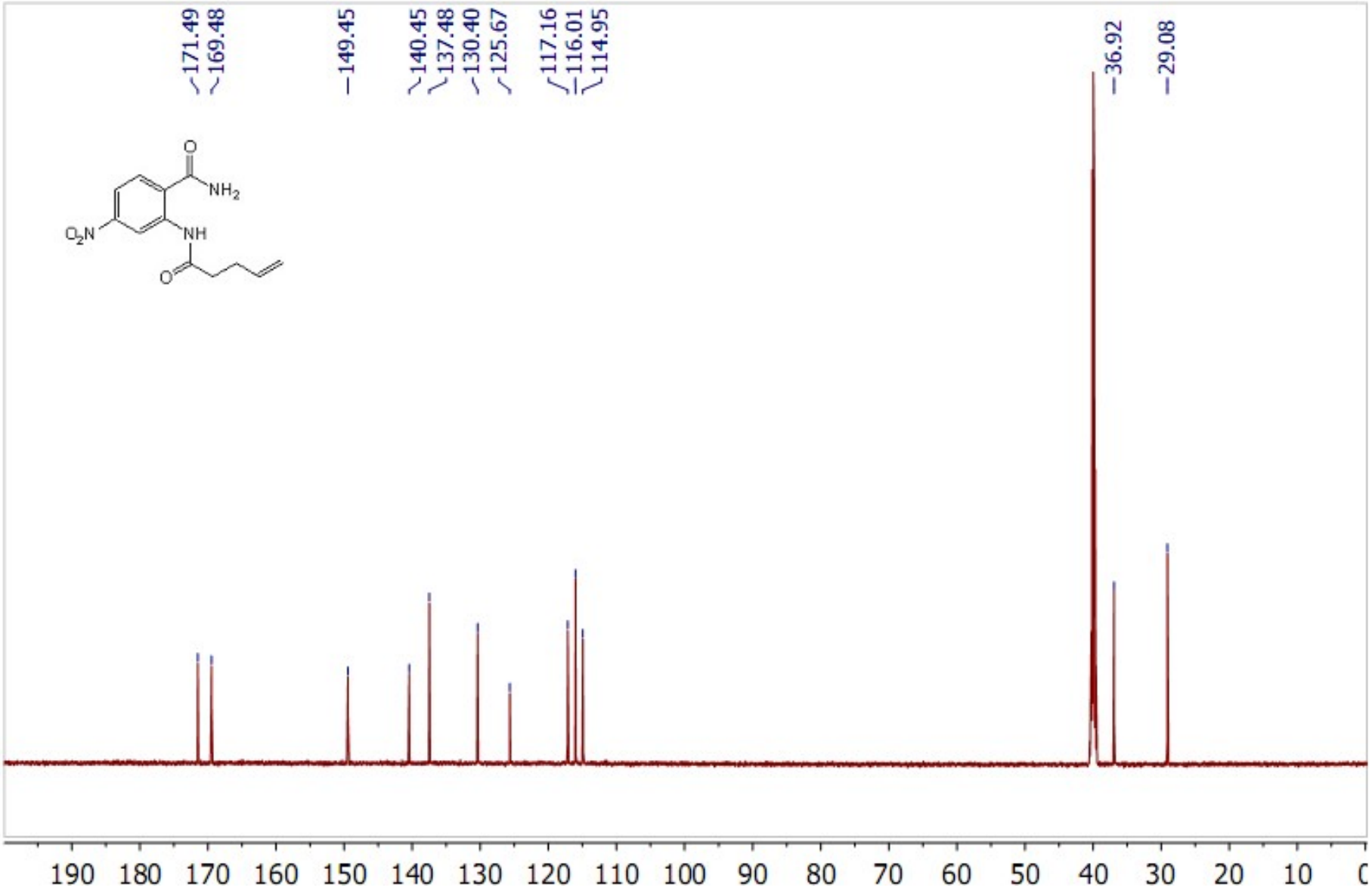
3 Sheldrick G. M., *Acta Crystallogr., Sect. A*, 2008**,** **64**, 112. http://dx.doi.org/10.1107/S0108767307043930.

4 A.I. Vaskevich, N.O. Savinchuk, R.I. Vaskevich, E.B. Rusanov, O.O. Grygorenko and M.V. Vovk, The PIFA-Initiated Oxidative Cyclization of 2-(3-Butenyl)quinazolin-4(3*H*)-ones – an Efficient Approach to 1-(Hydroxymethyl)-2,3-dihydropyrrolo[1,2-*a*]quinazolin-5(1*H*)-ones, *Beilstein J. Org. Chem*. 2021, **17**, 2787-2794.

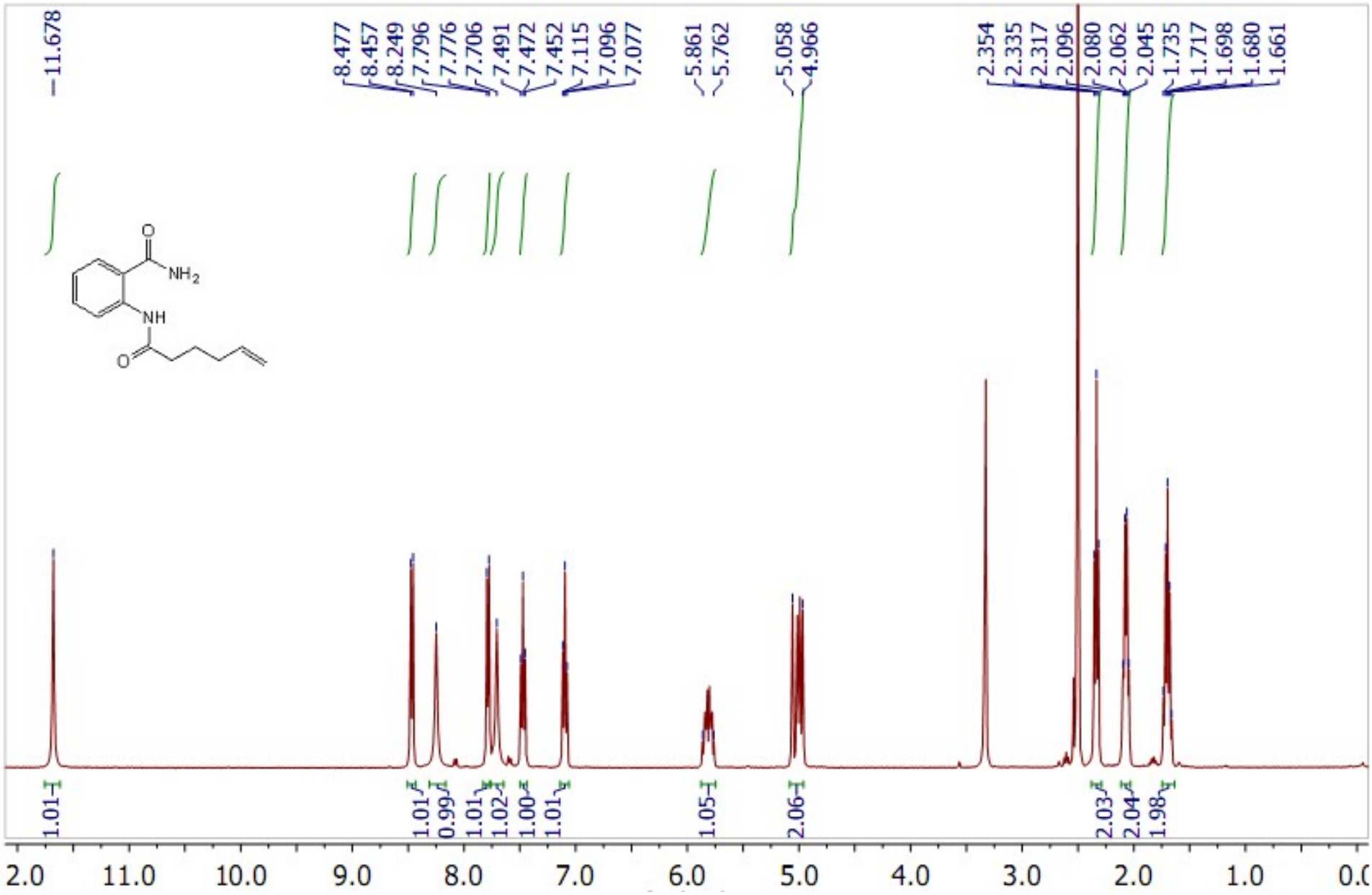
^{1}H NMR spectrum (500 MHz, DMSO-d6) of compound 6g



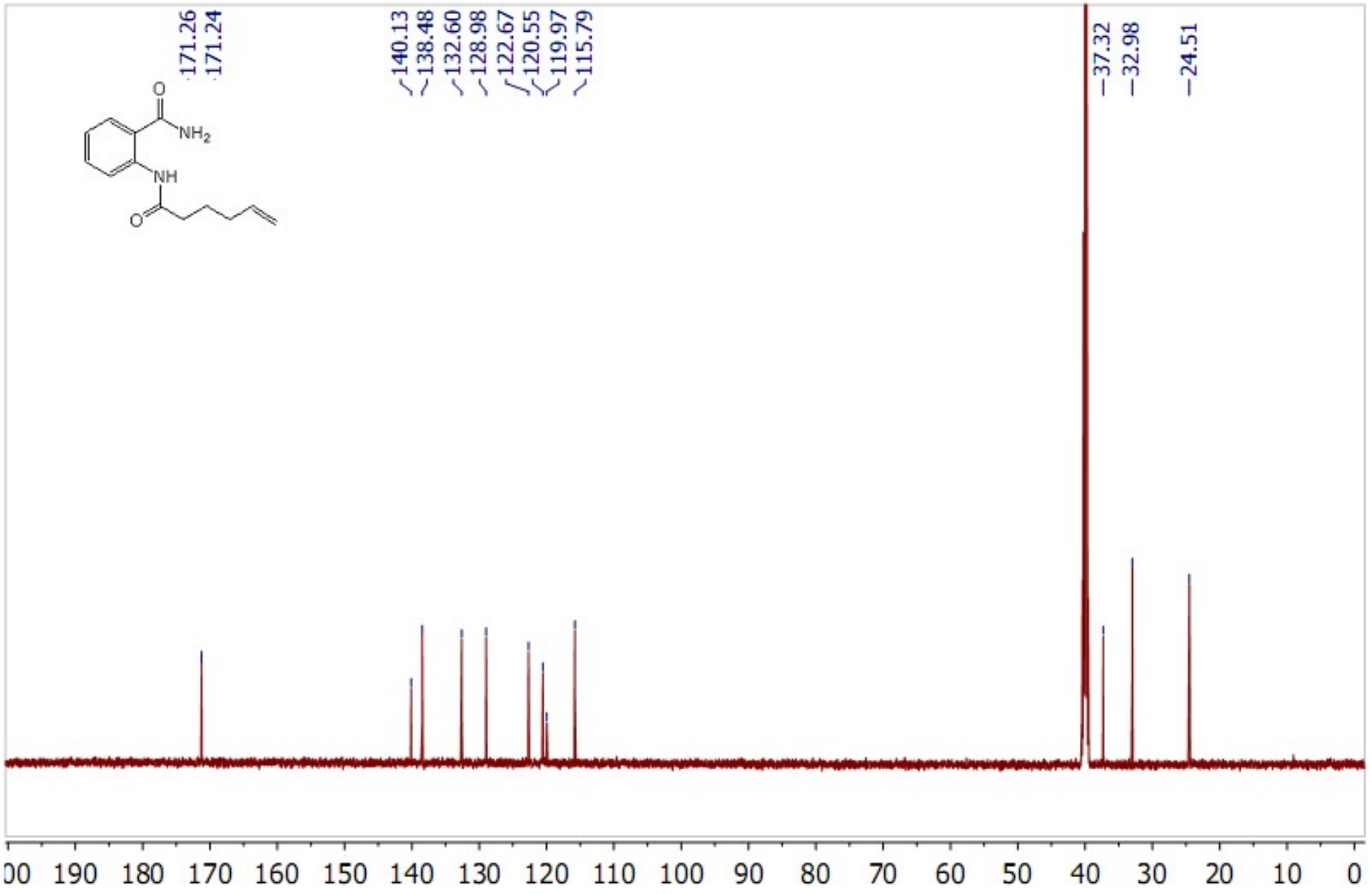
^{13}C NMR spectrum (151 MHz, DMSO-d6) of compound 6g



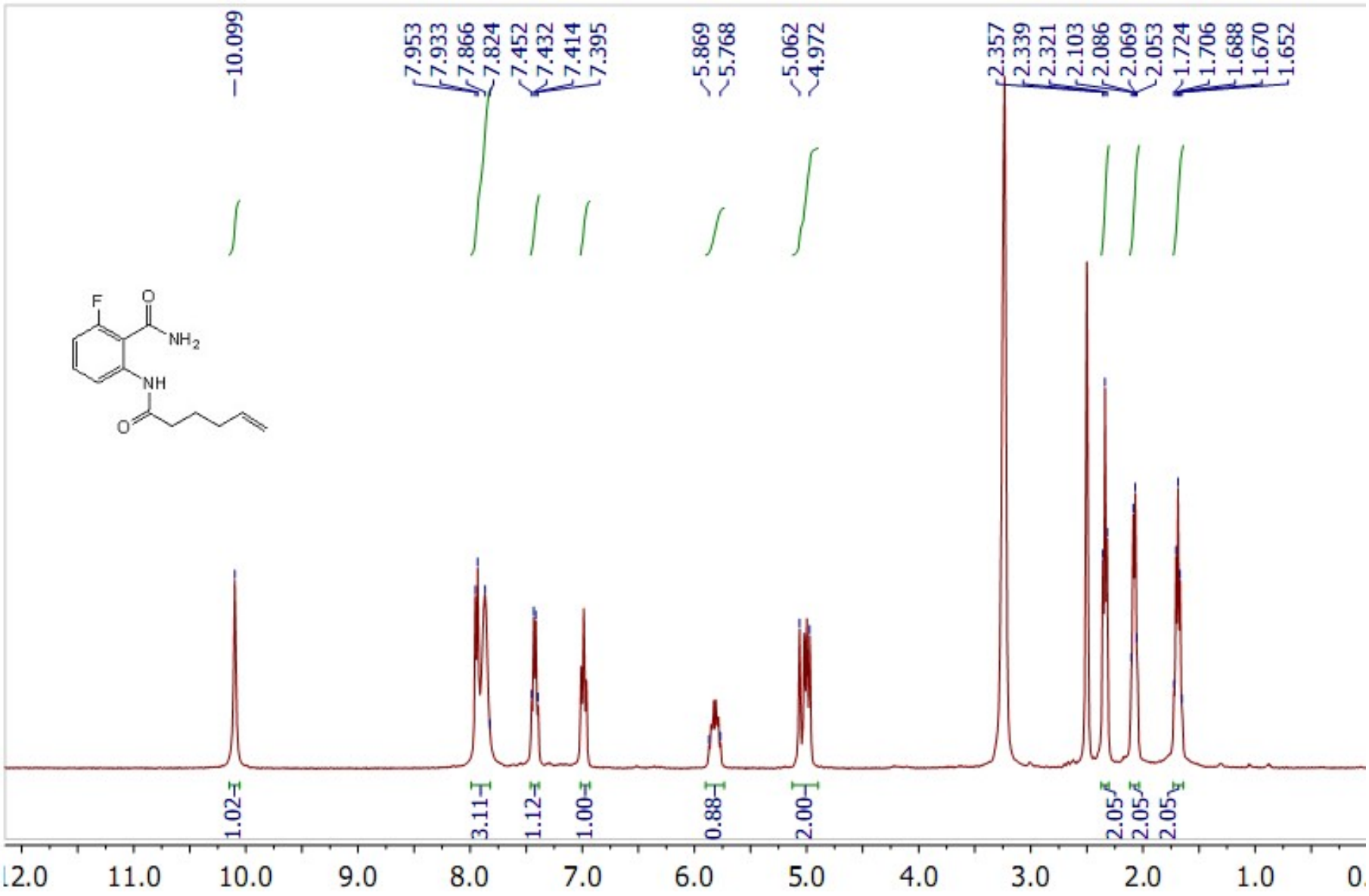
^{1}H NMR spectrum (400 MHz, DMSO-d6) of compound 7a



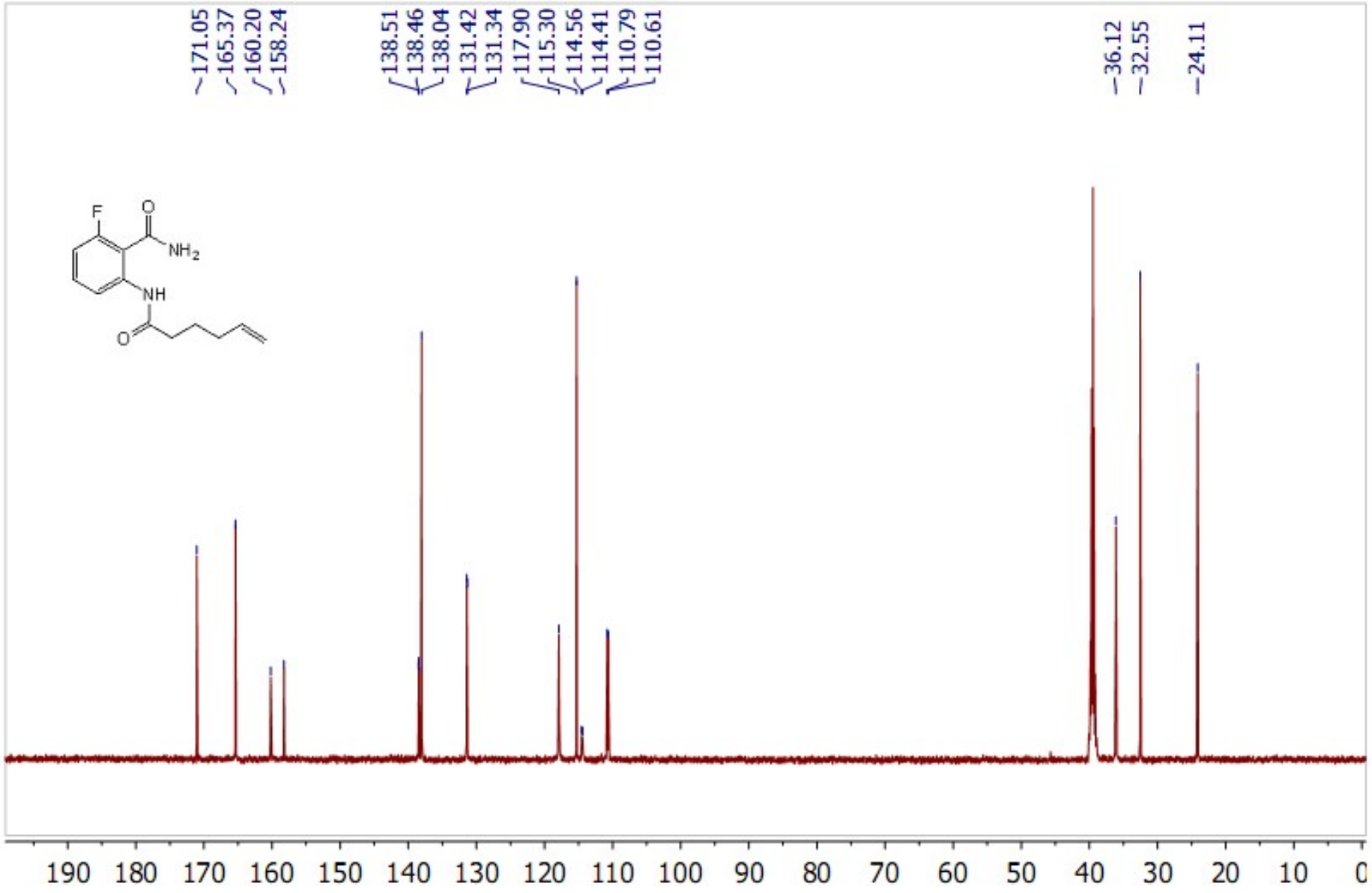
^{13}C NMR spectrum (151 MHz, DMSO-d6) of compound 7a



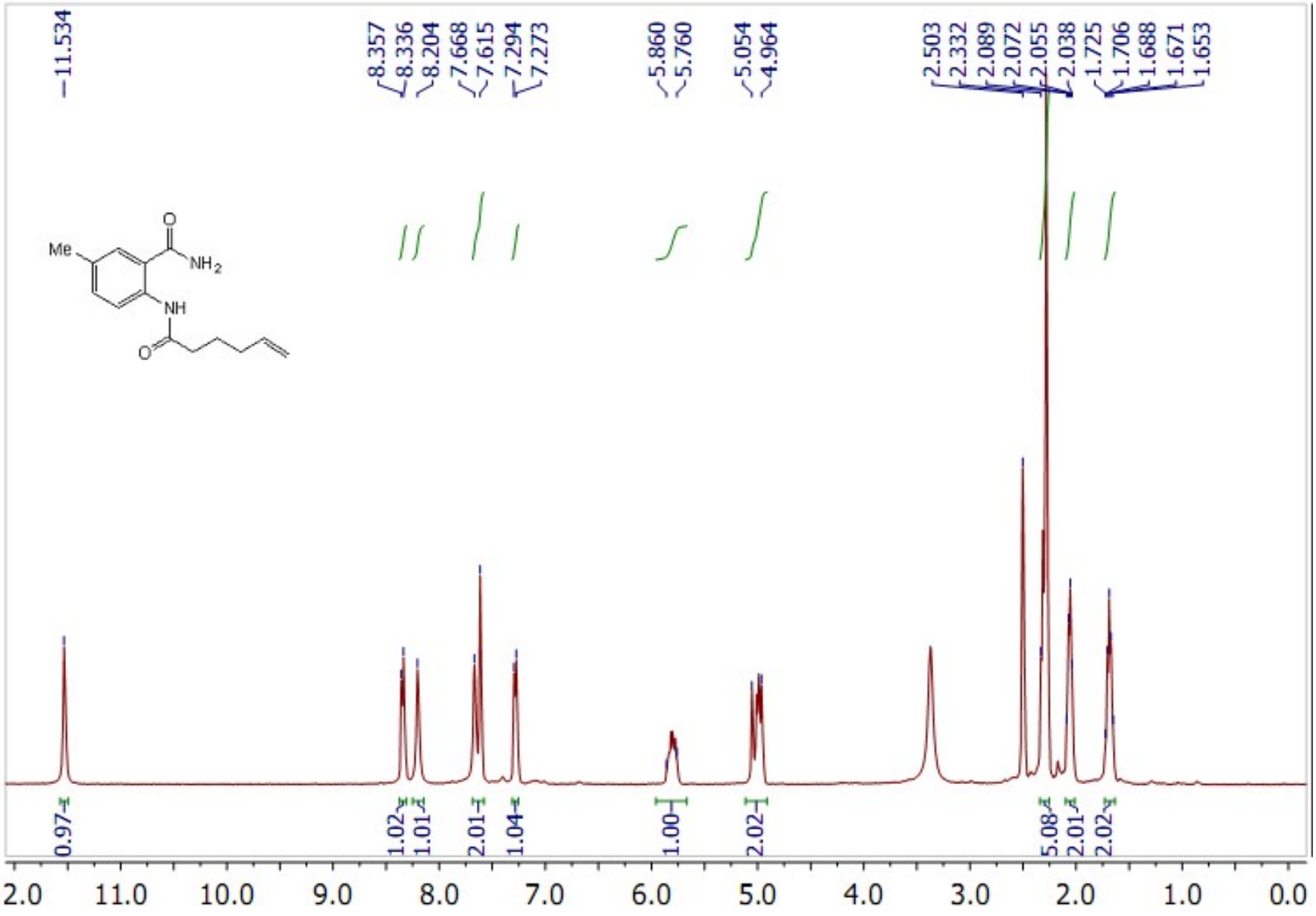
^{1}H NMR spectrum (400 MHz, DMSO-d6) of compound 7b



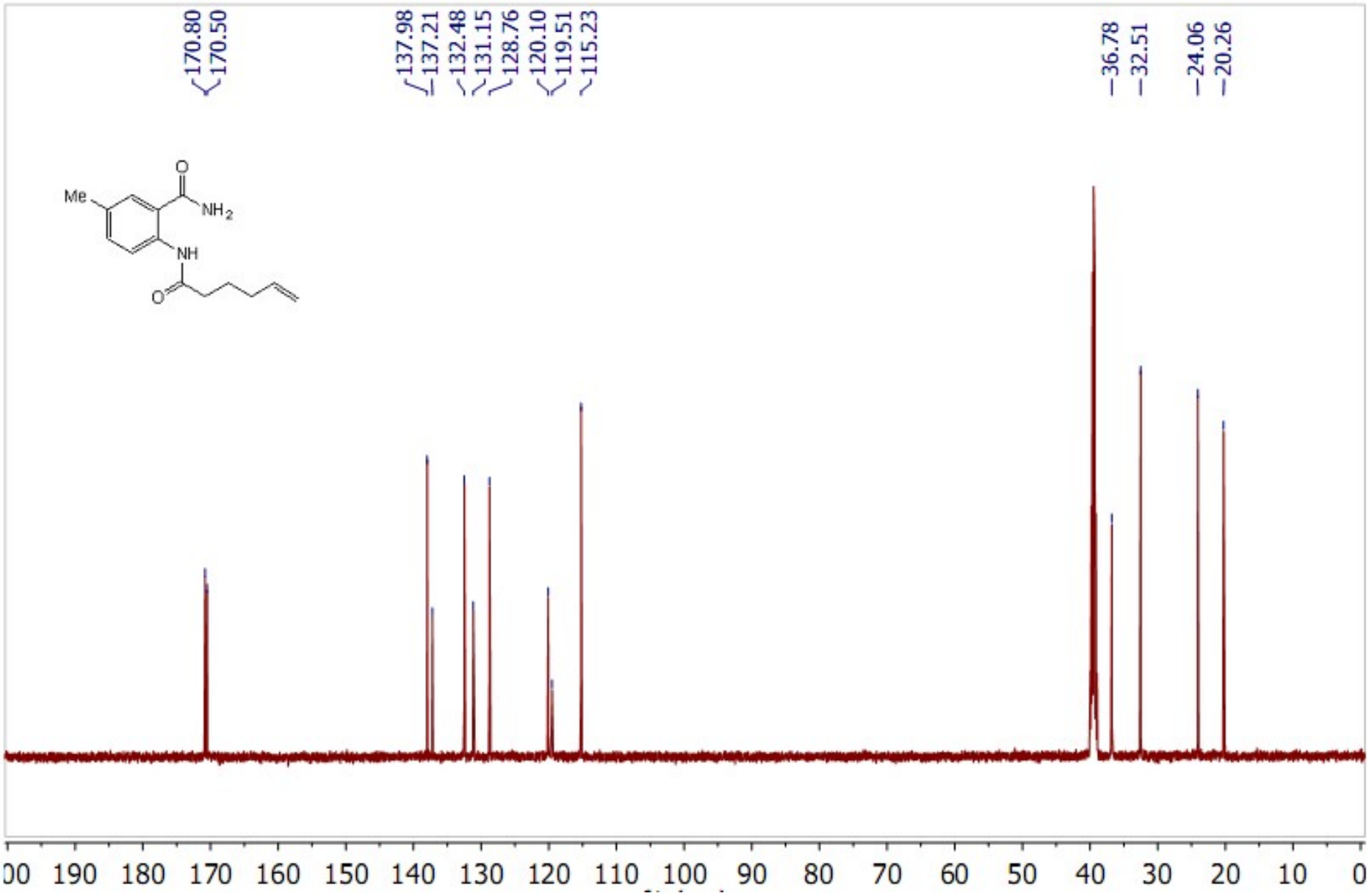
^{13}C NMR spectrum (126 MHz, DMSO-d6) of compound 7b



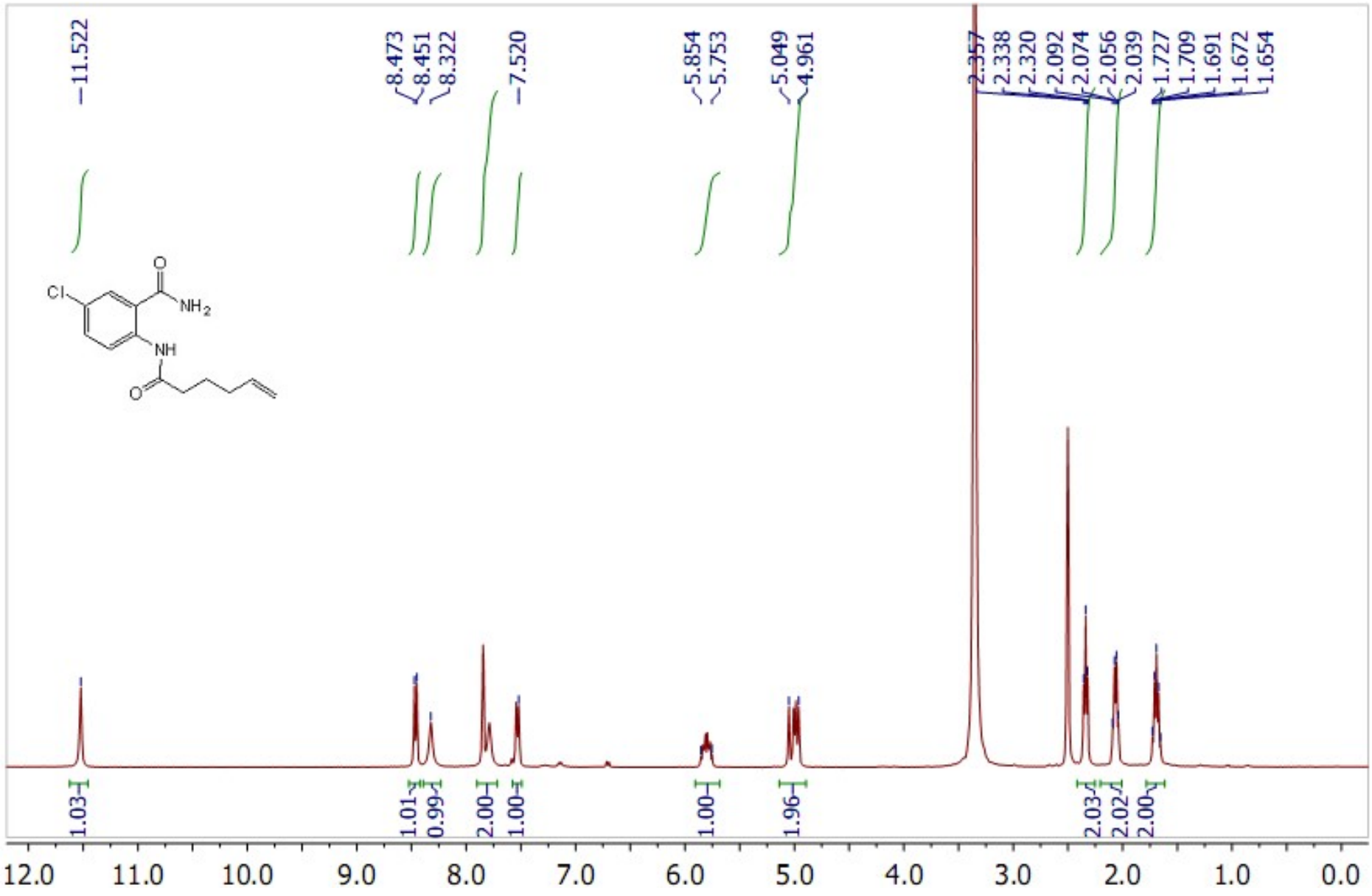
^{1}H NMR spectrum (400 MHz, DMSO-d6) of compound 7c



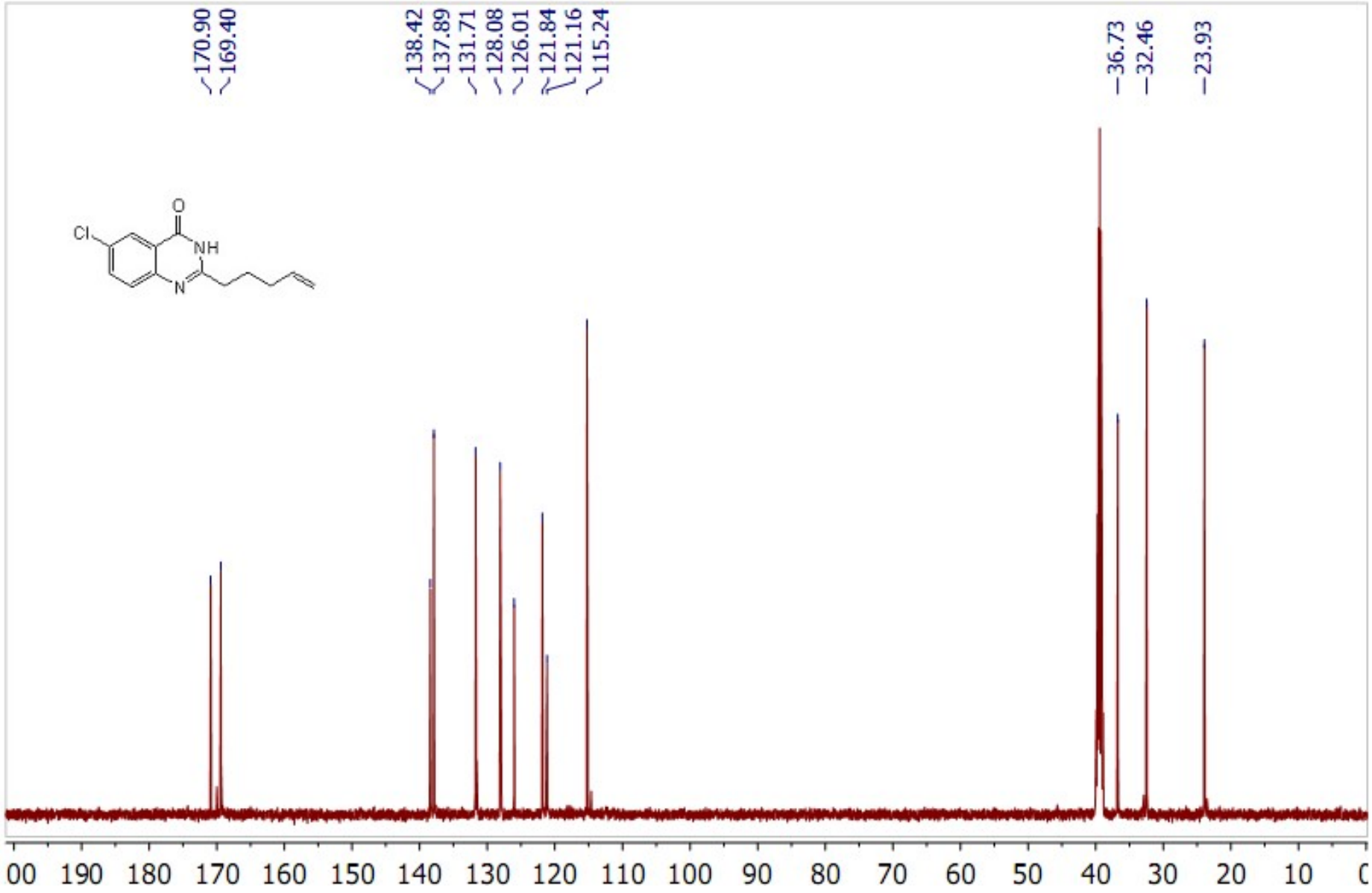
^{13}C NMR spectrum (126 MHz, DMSO-d6) of compound 7c



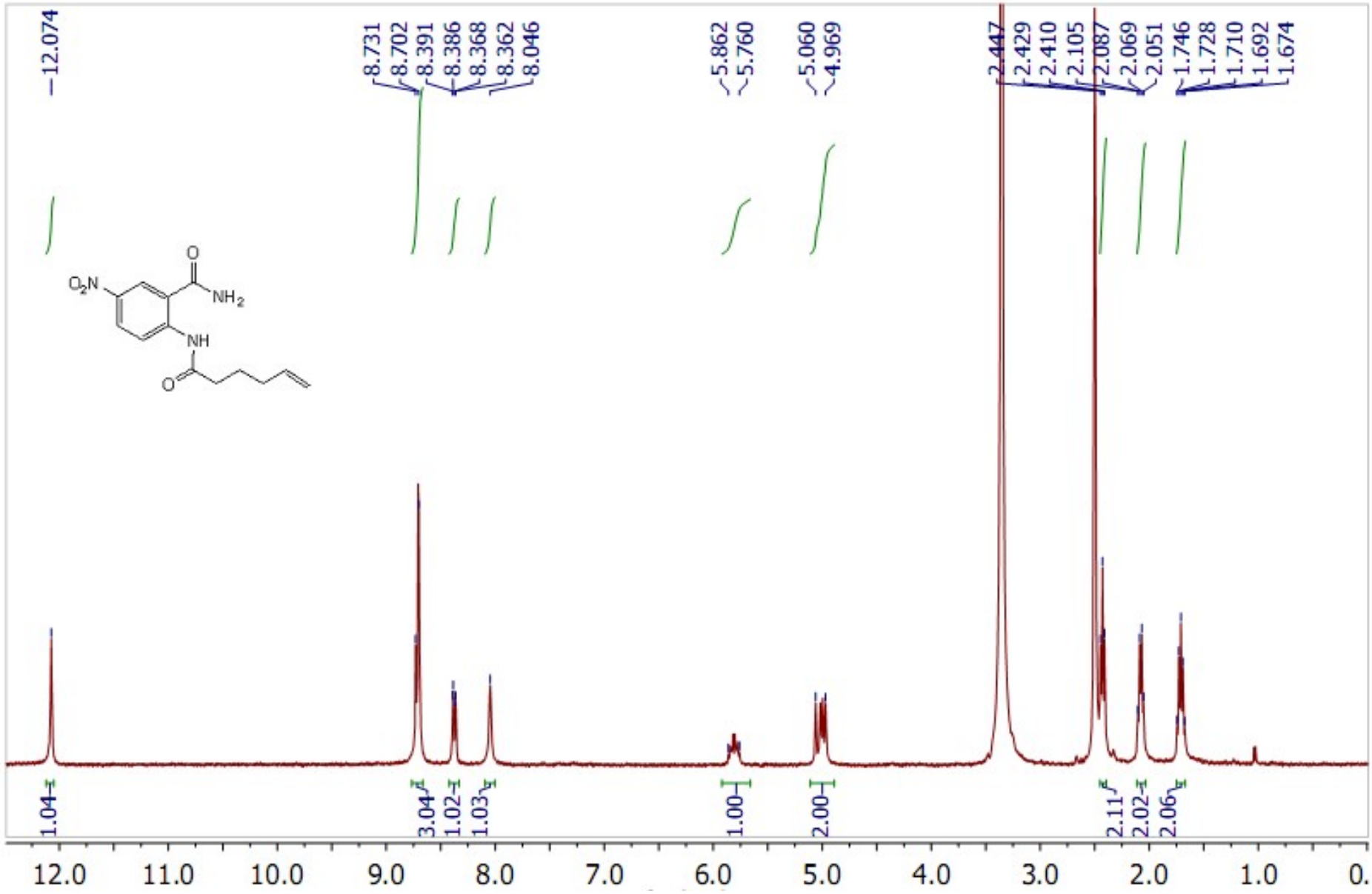
^{1}H NMR spectrum (400 MHz, DMSO-d6) of compound 7d



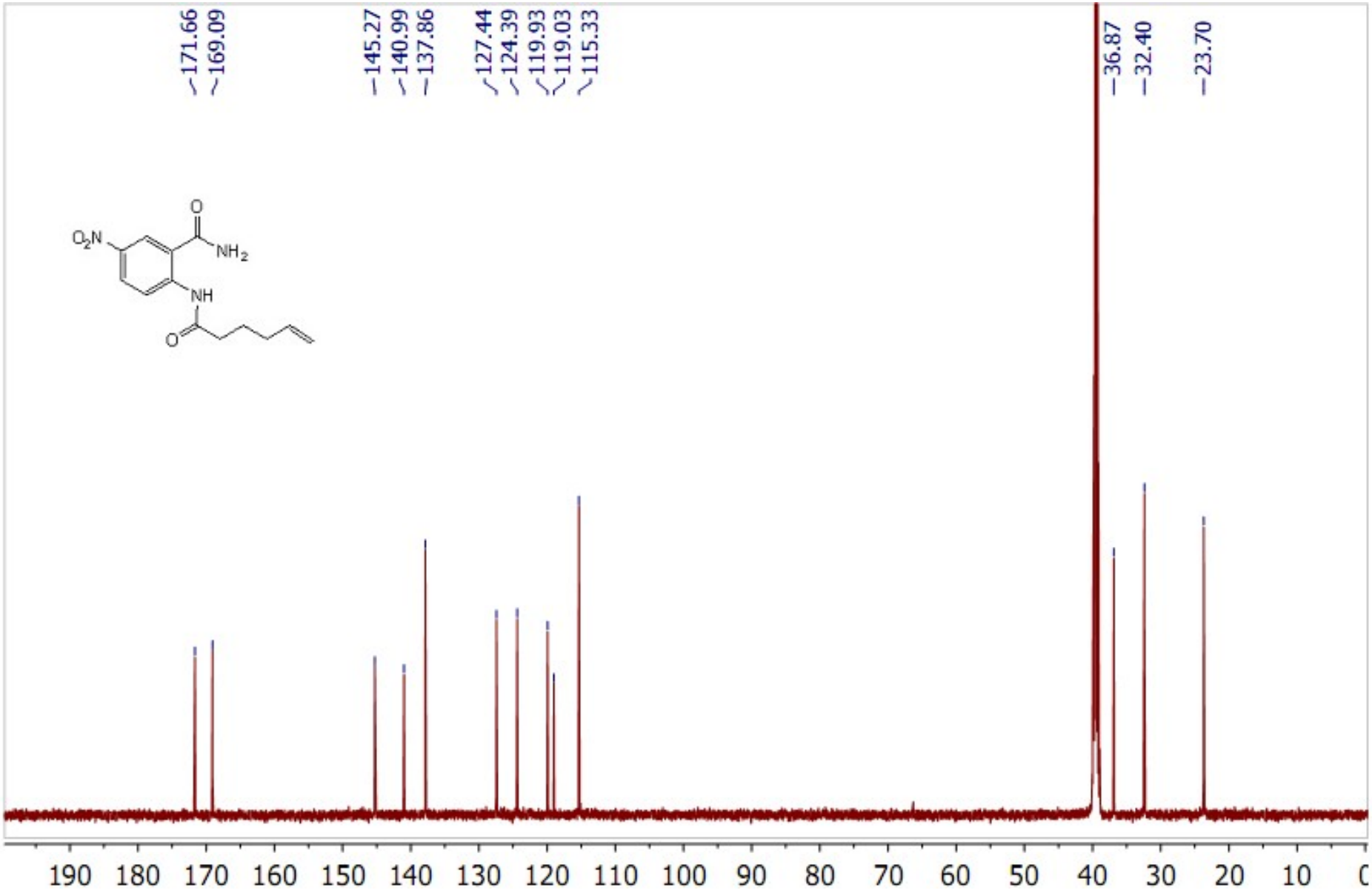
^{13}C NMR spectrum (126 MHz, DMSO-d6) of compound 7d



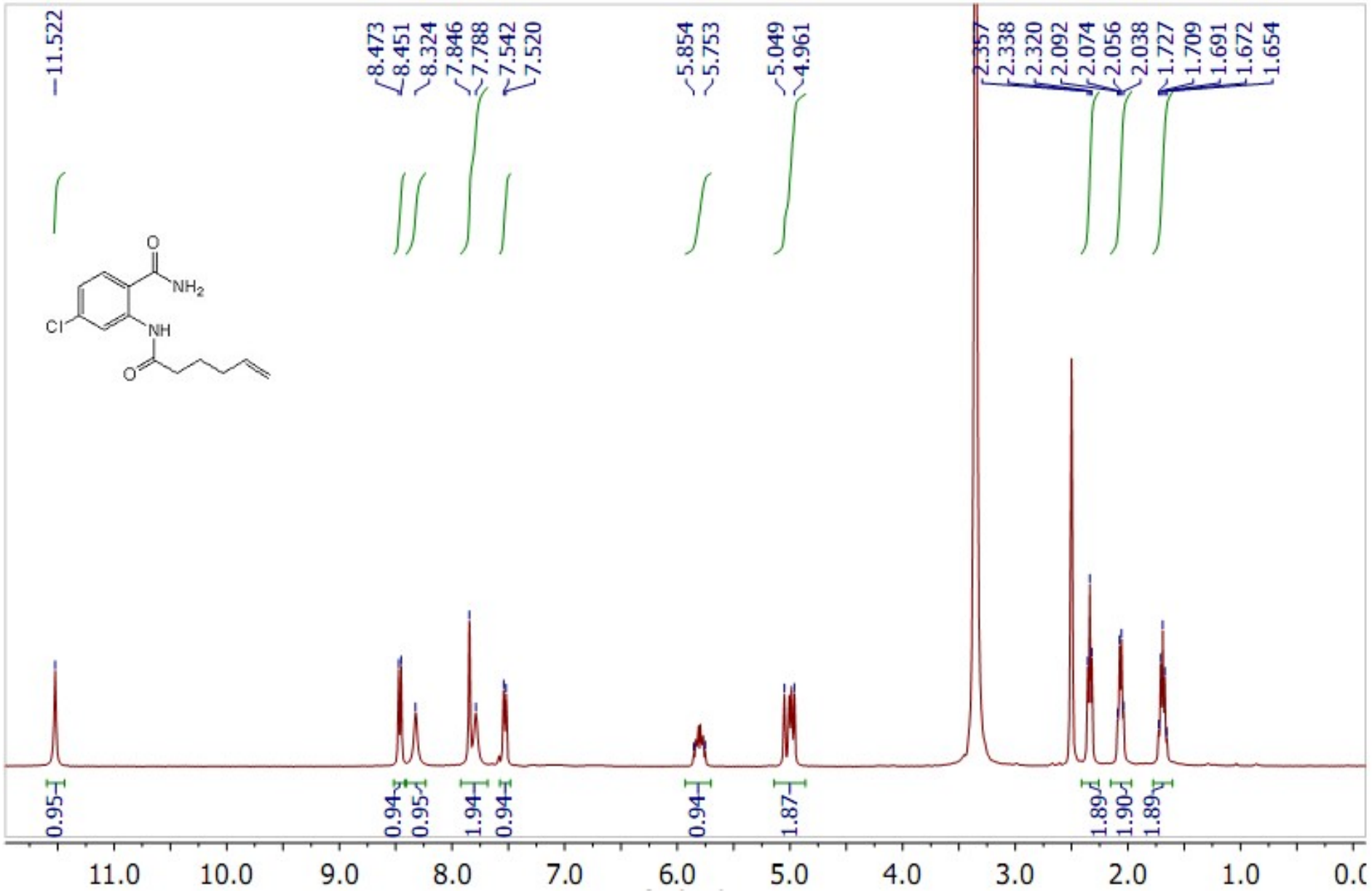
^{1}H NMR spectrum (400 MHz, DMSO-d6) of compound 7e



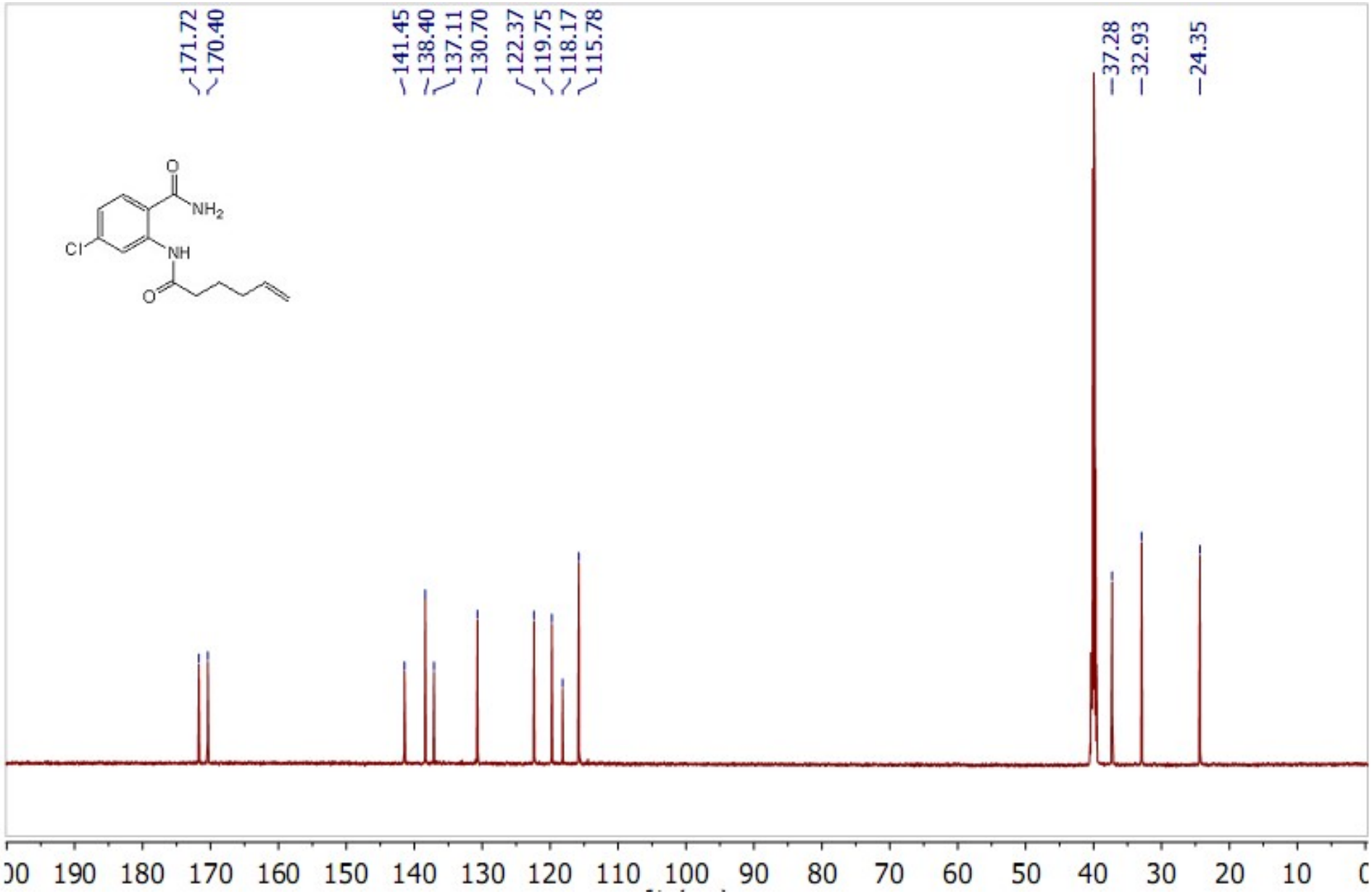
^{13}C NMR spectrum (126 MHz, DMSO-d6) of compound 7e



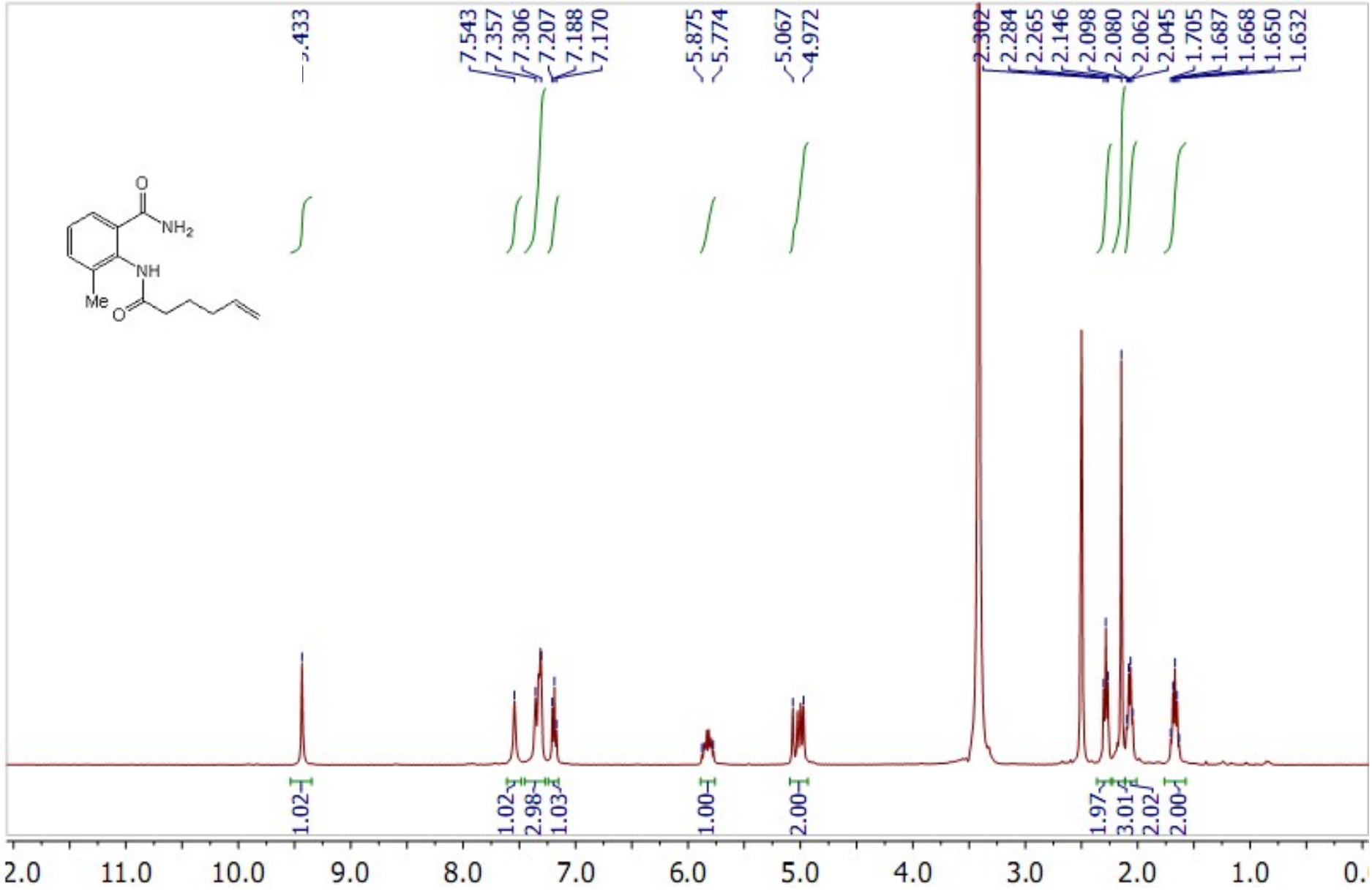
^{1}H NMR spectrum (400 MHz, DMSO-d6) of compound 7f



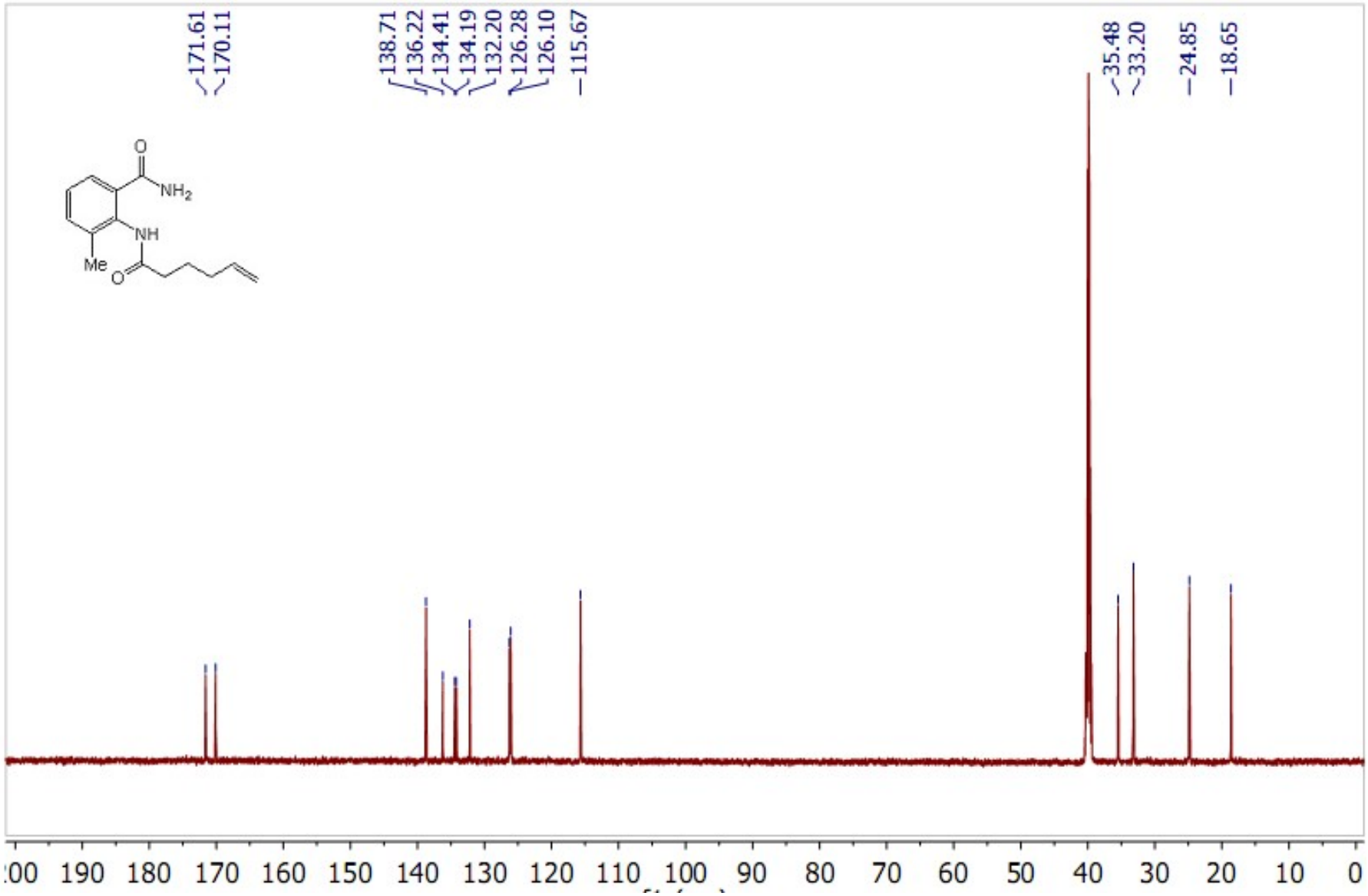
^{13}C NMR spectrum (151 MHz, DMSO-d6) of compound 7f



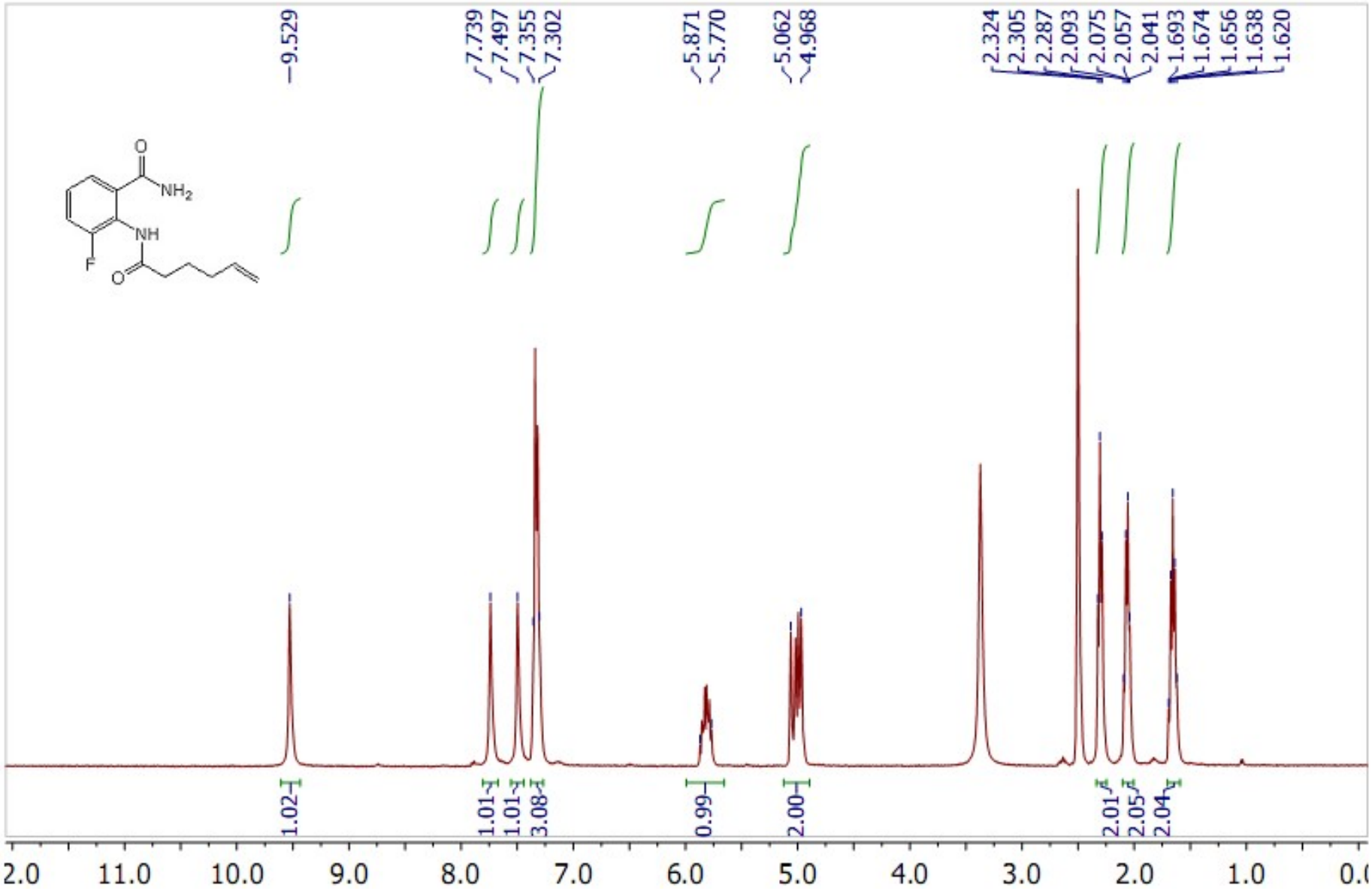
^{1}H NMR spectrum (400 MHz, DMSO-d6) of compound 7h



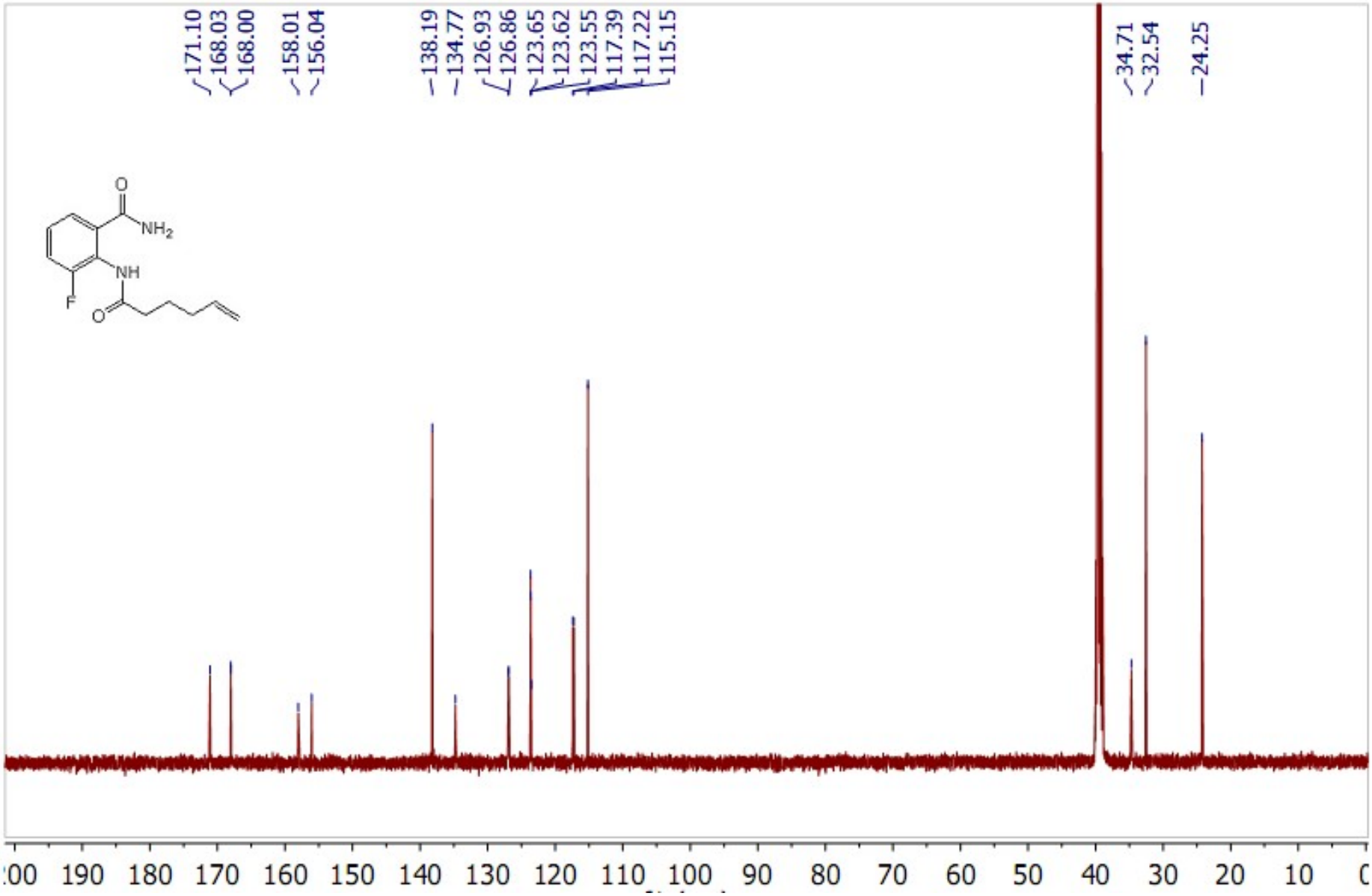
^{13}C NMR spectrum (151 MHz, DMSO-d6) of compound 7h



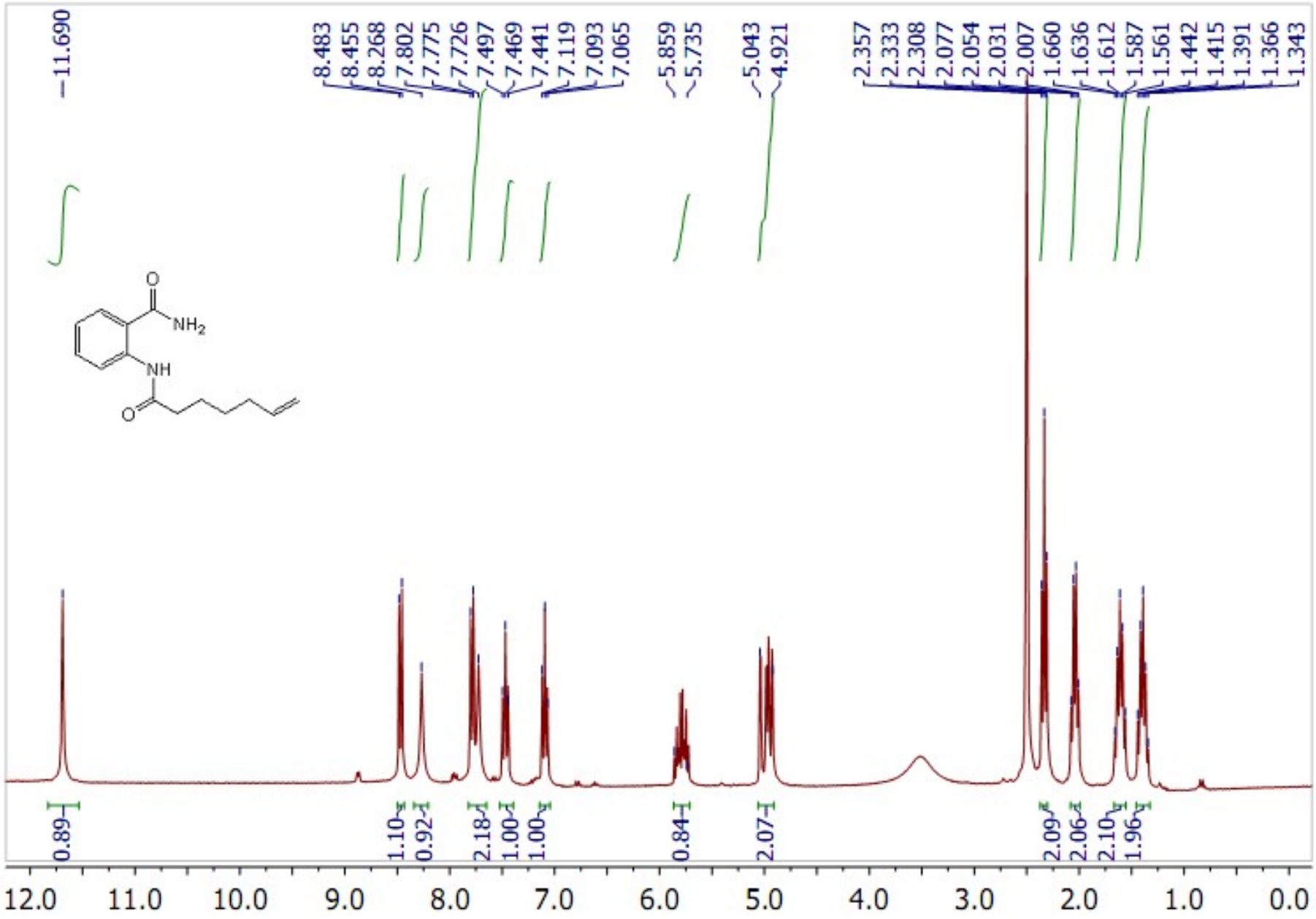
^{1}H NMR spectrum (400 MHz, DMSO-d6) of compound 7i



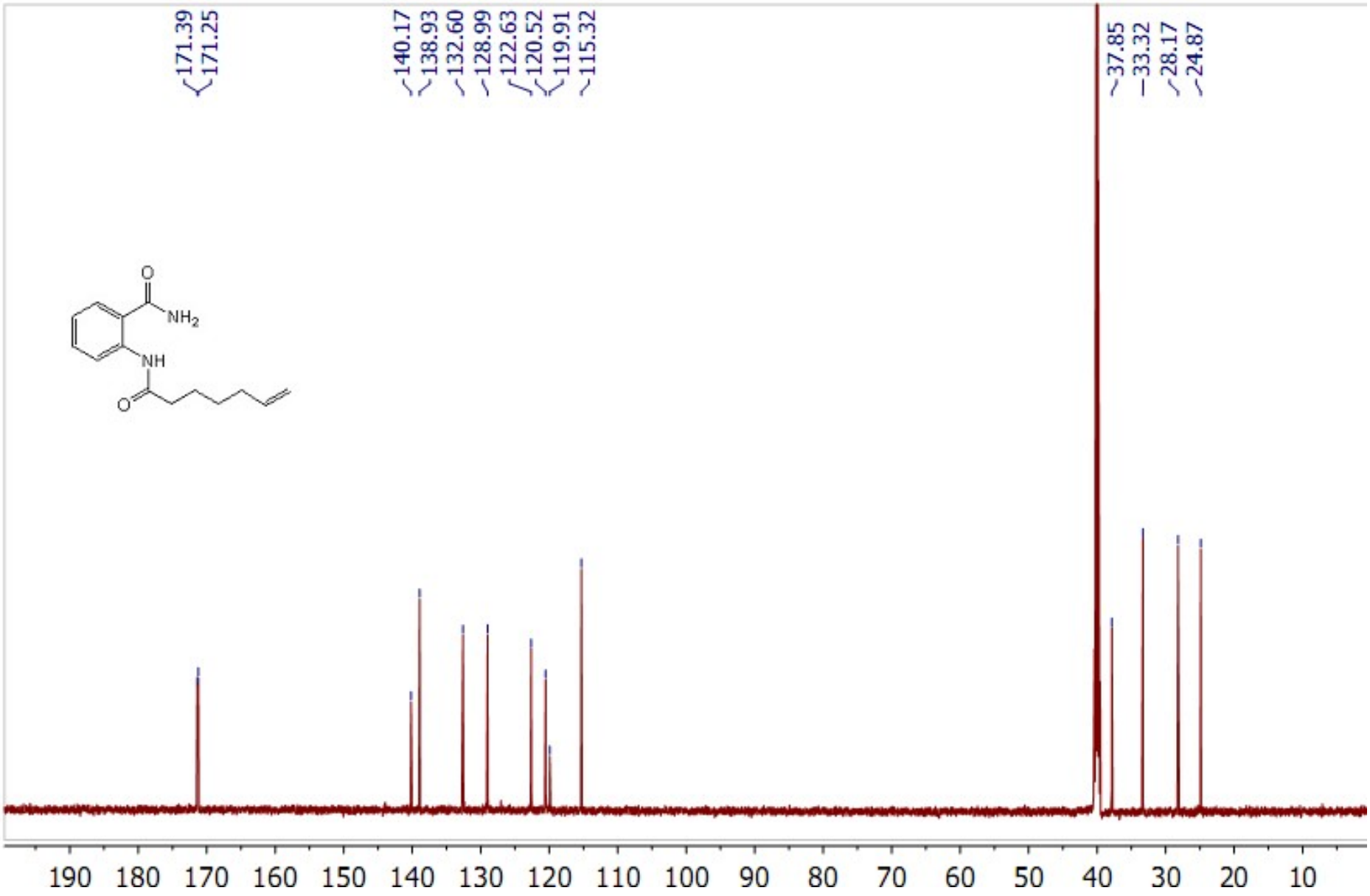
^{13}C NMR spectrum (126 MHz, DMSO-d6) of compound 7i



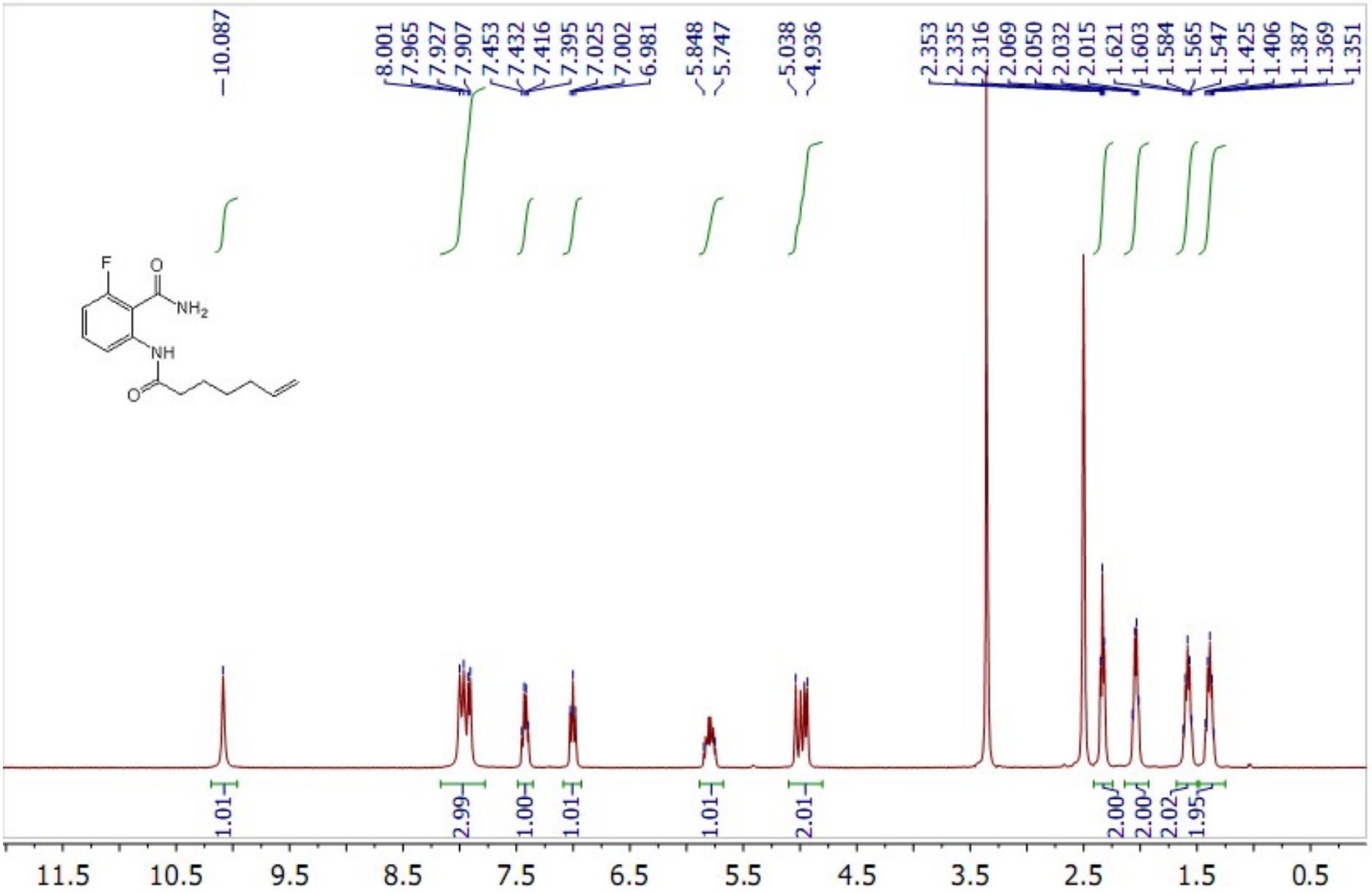
^{1}H NMR spectrum (300 MHz, DMSO-d6) of compound 8a



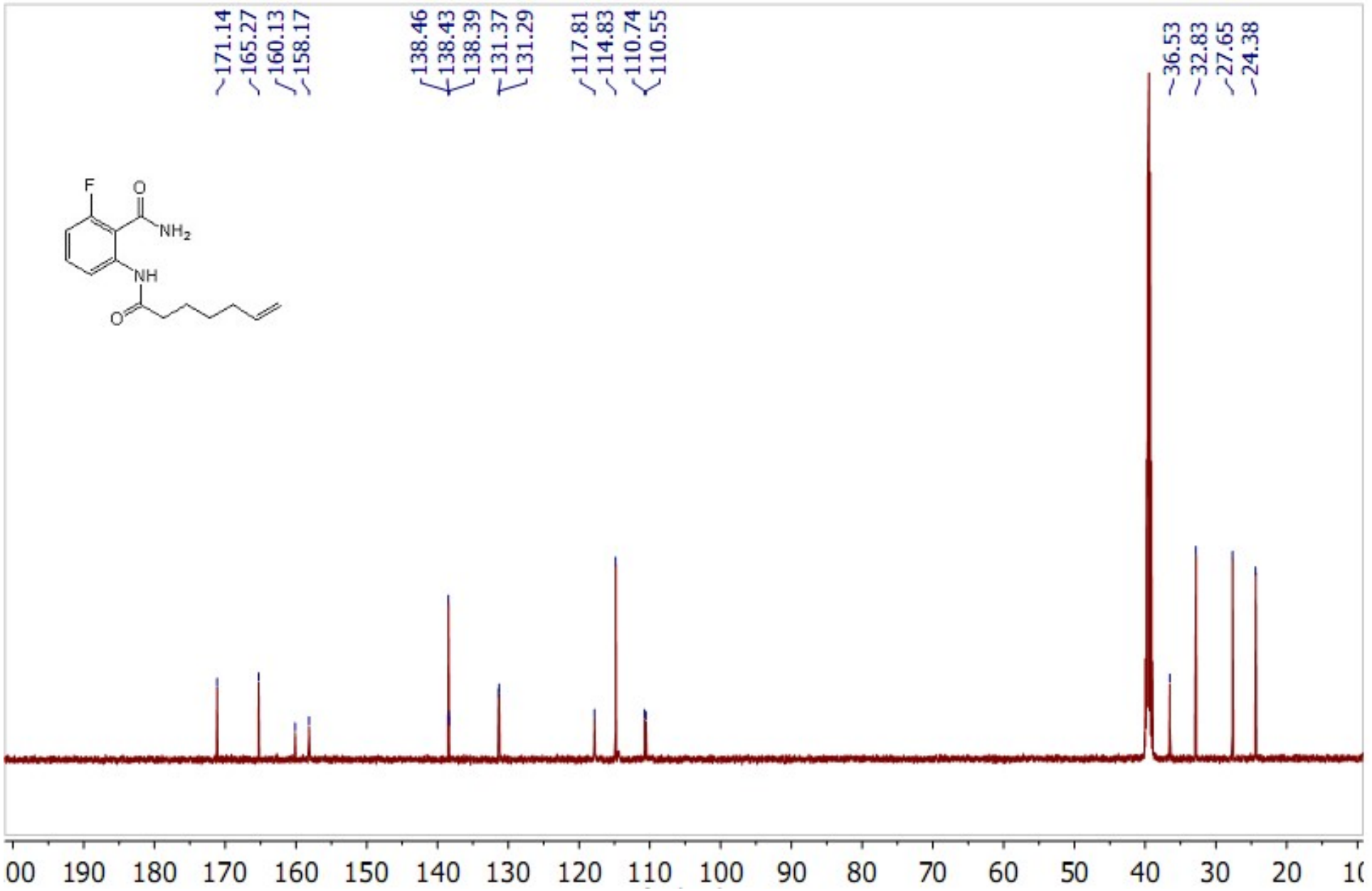
^{13}C NMR spectrum (151 MHz, DMSO-d6) of compound 8a



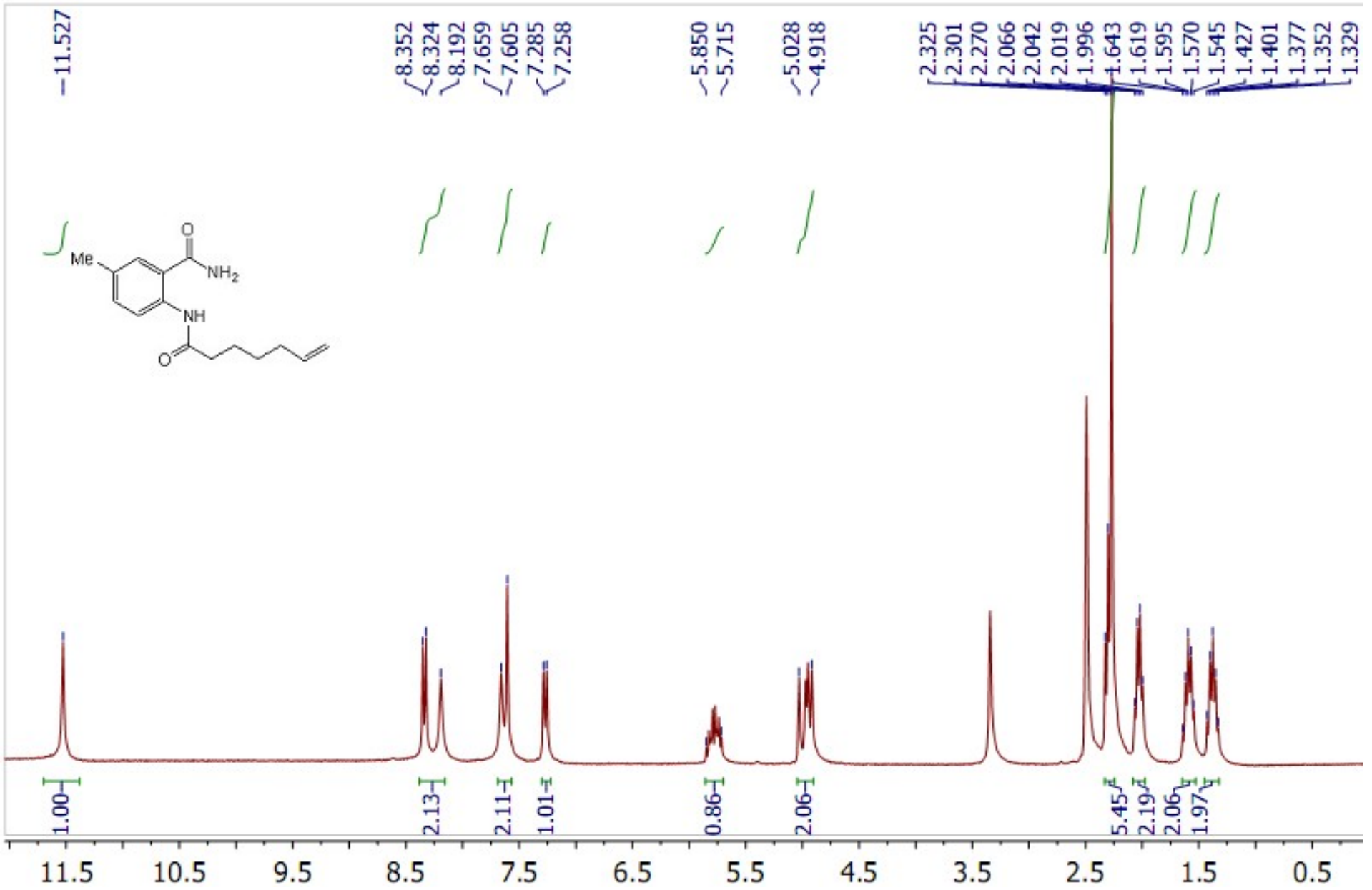
^{1}H NMR spectrum (400 MHz, DMSO-d6) of compound 8b



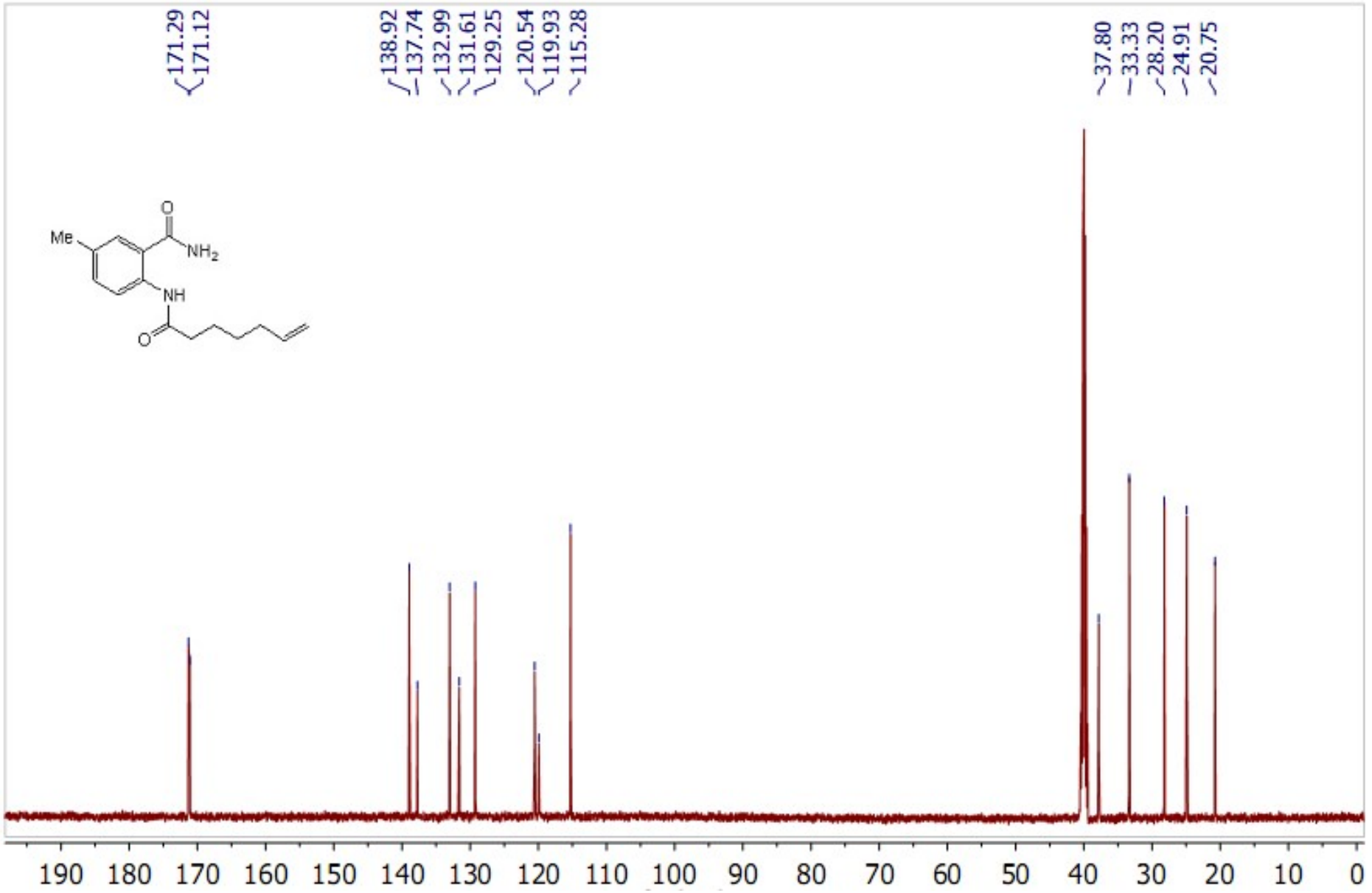
^{13}C NMR spectrum (126 MHz, DMSO-d6) of compound 8b



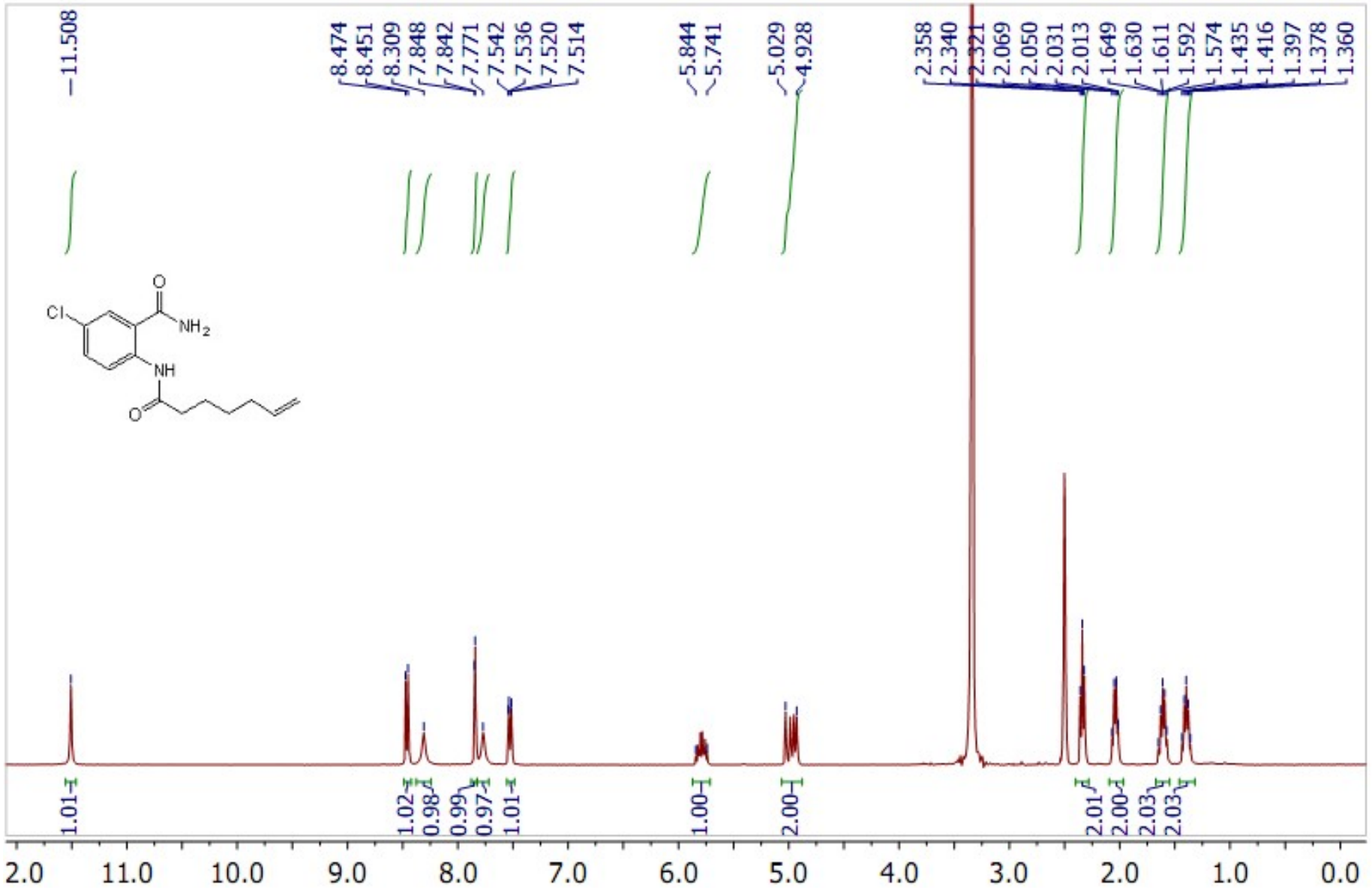
^{1}H NMR spectrum (300 MHz, DMSO-d6) of compound 8c



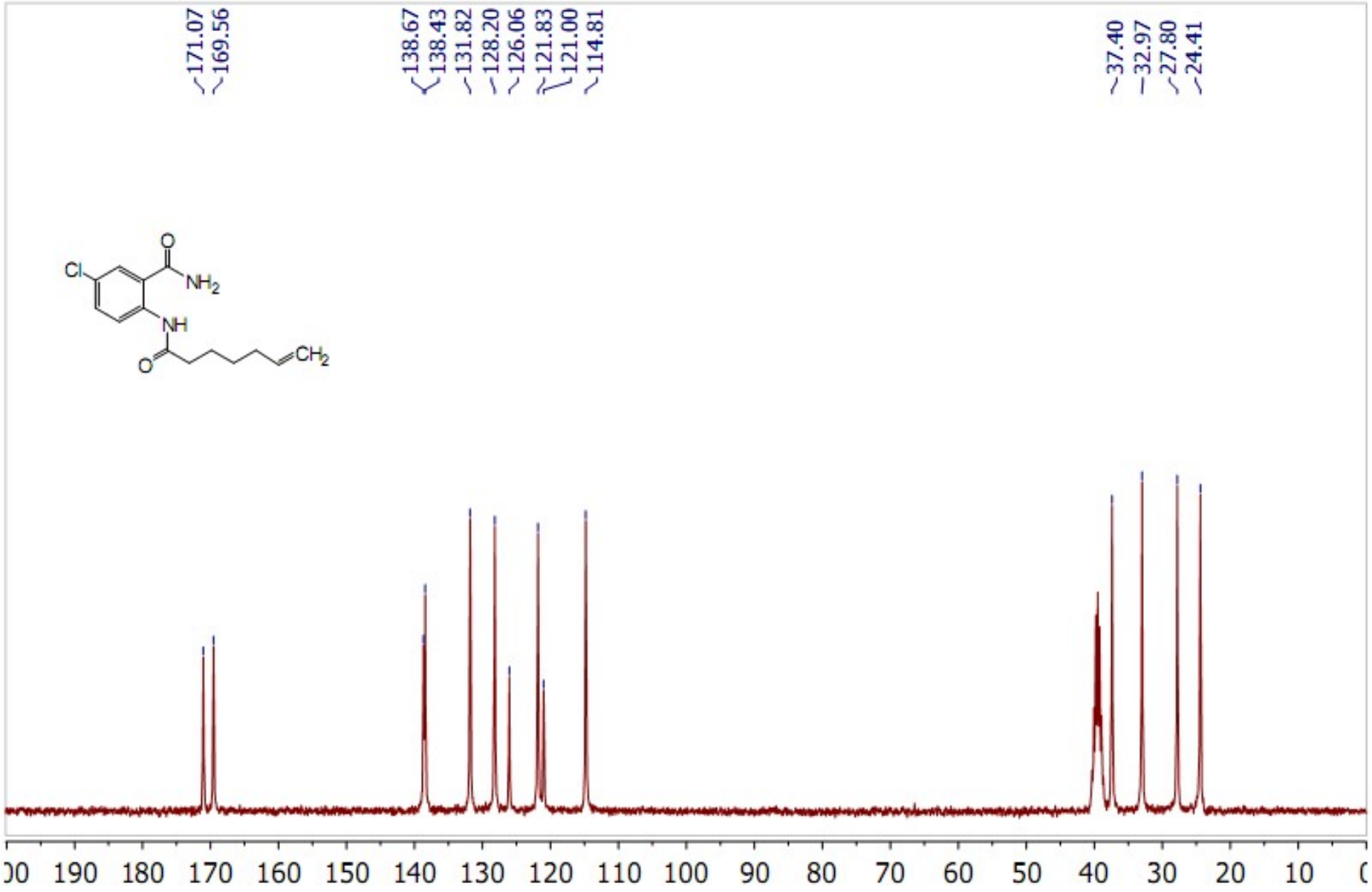
^{13}C NMR spectrum (126 MHz, DMSO-d6) of compound 8c



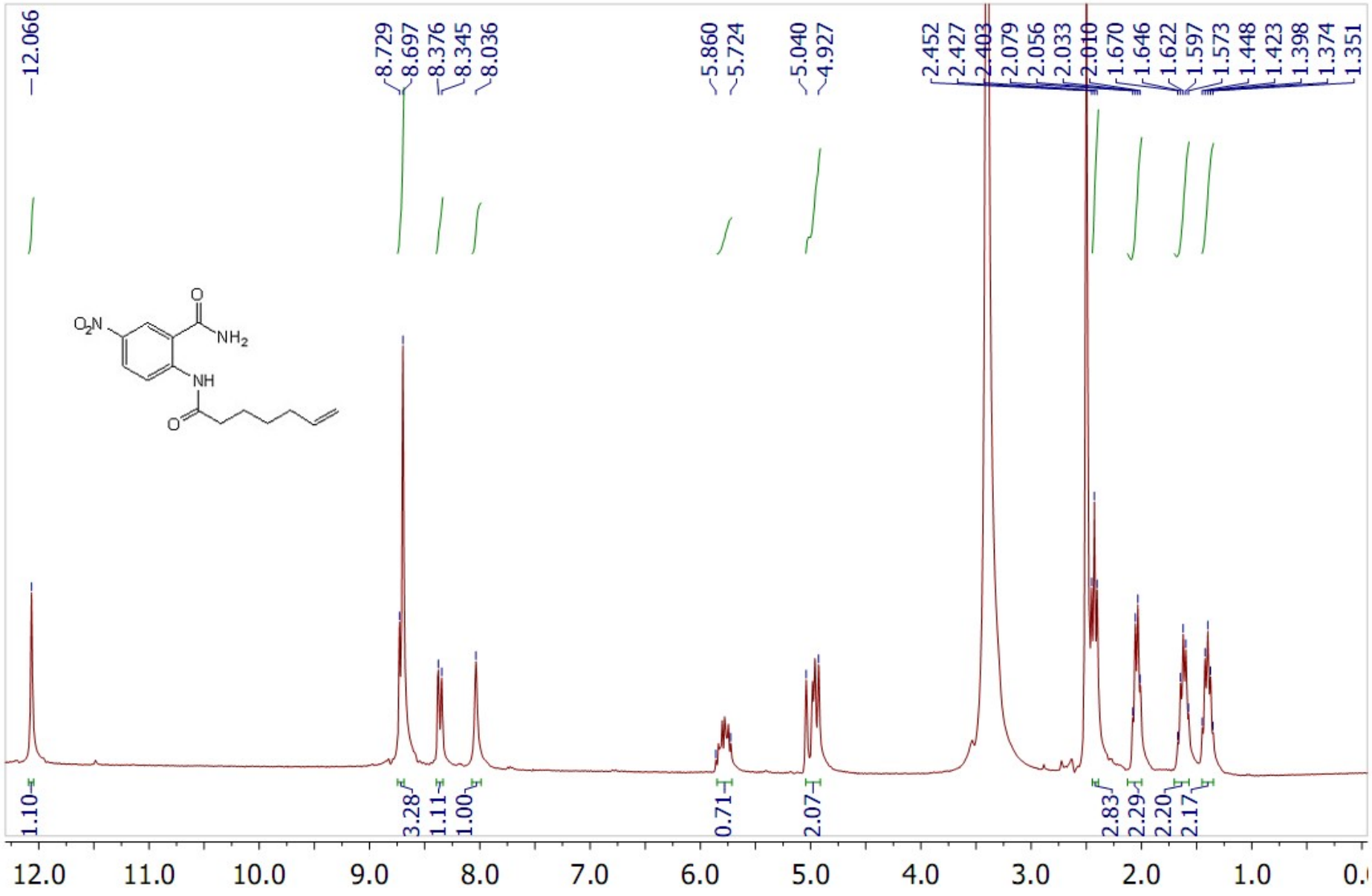
^{1}H NMR spectrum (400 MHz, DMSO-d6) of compound 8d



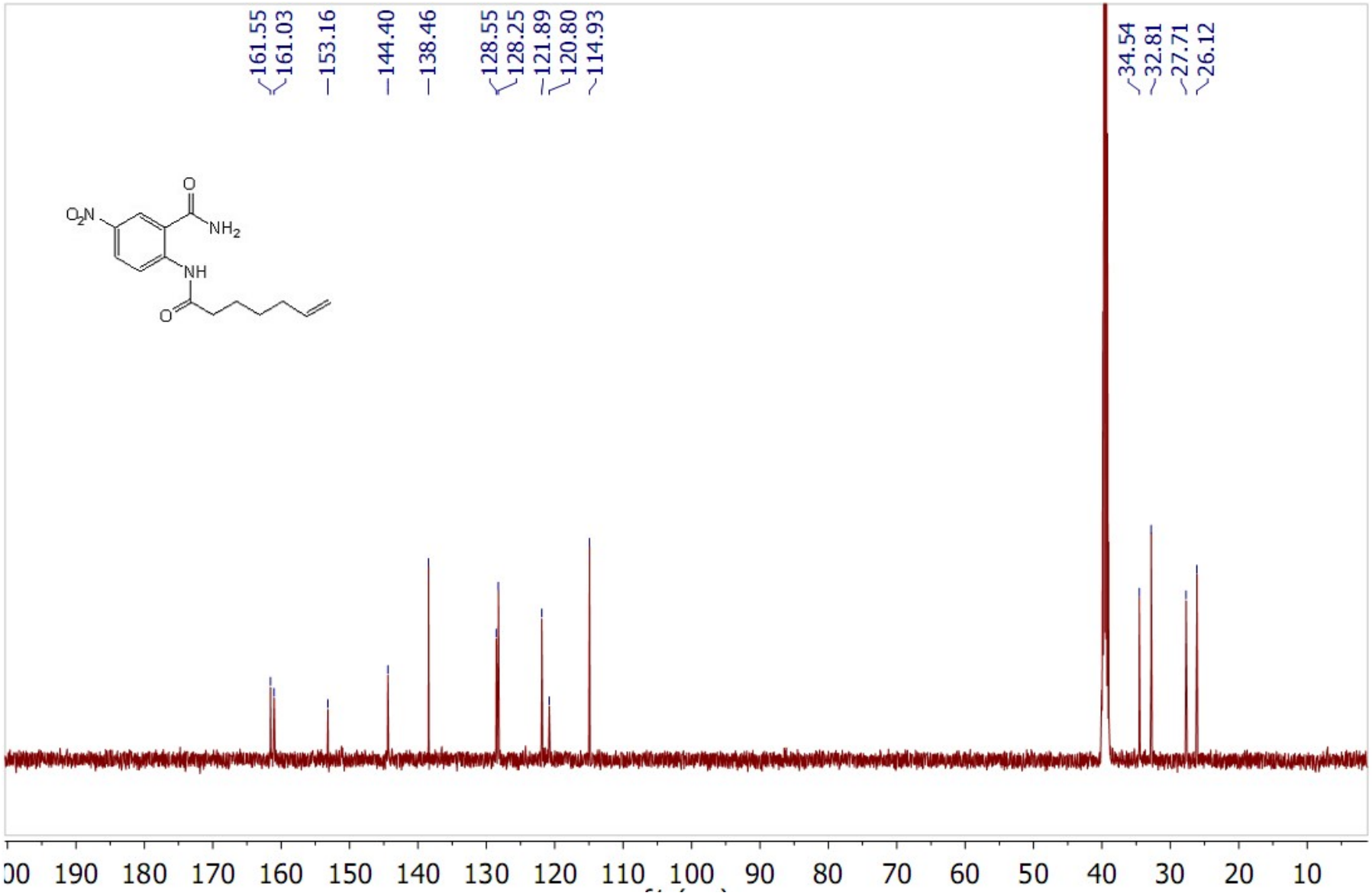
^{13}C NMR spectrum (76 MHz, DMSO-d6) of compound 8d



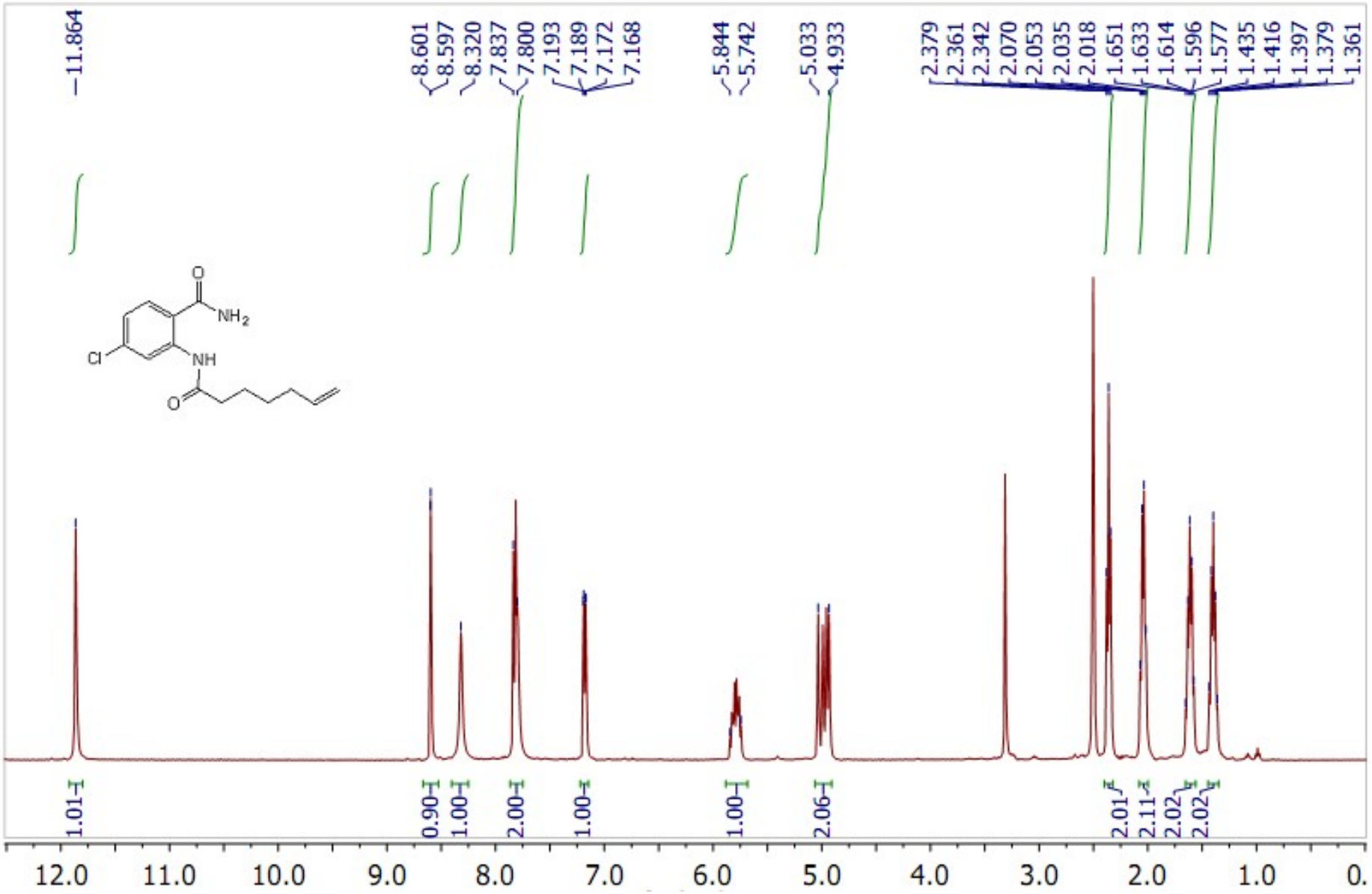
^{1}H NMR spectrum (300 MHz, DMSO-d6) of compound 8e



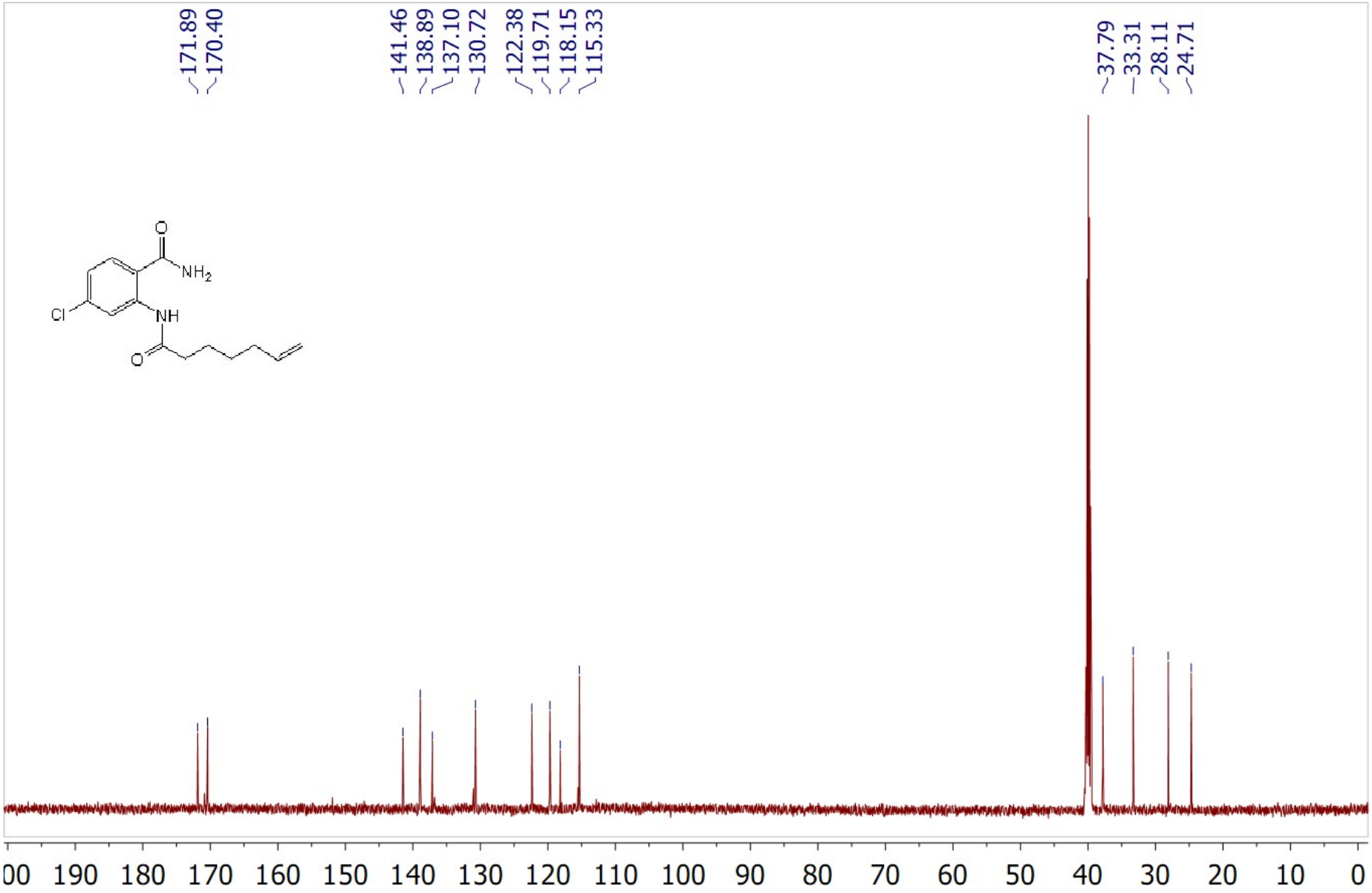
^{13}C NMR spectrum (151 MHz, DMSO-d6) of compound 8e



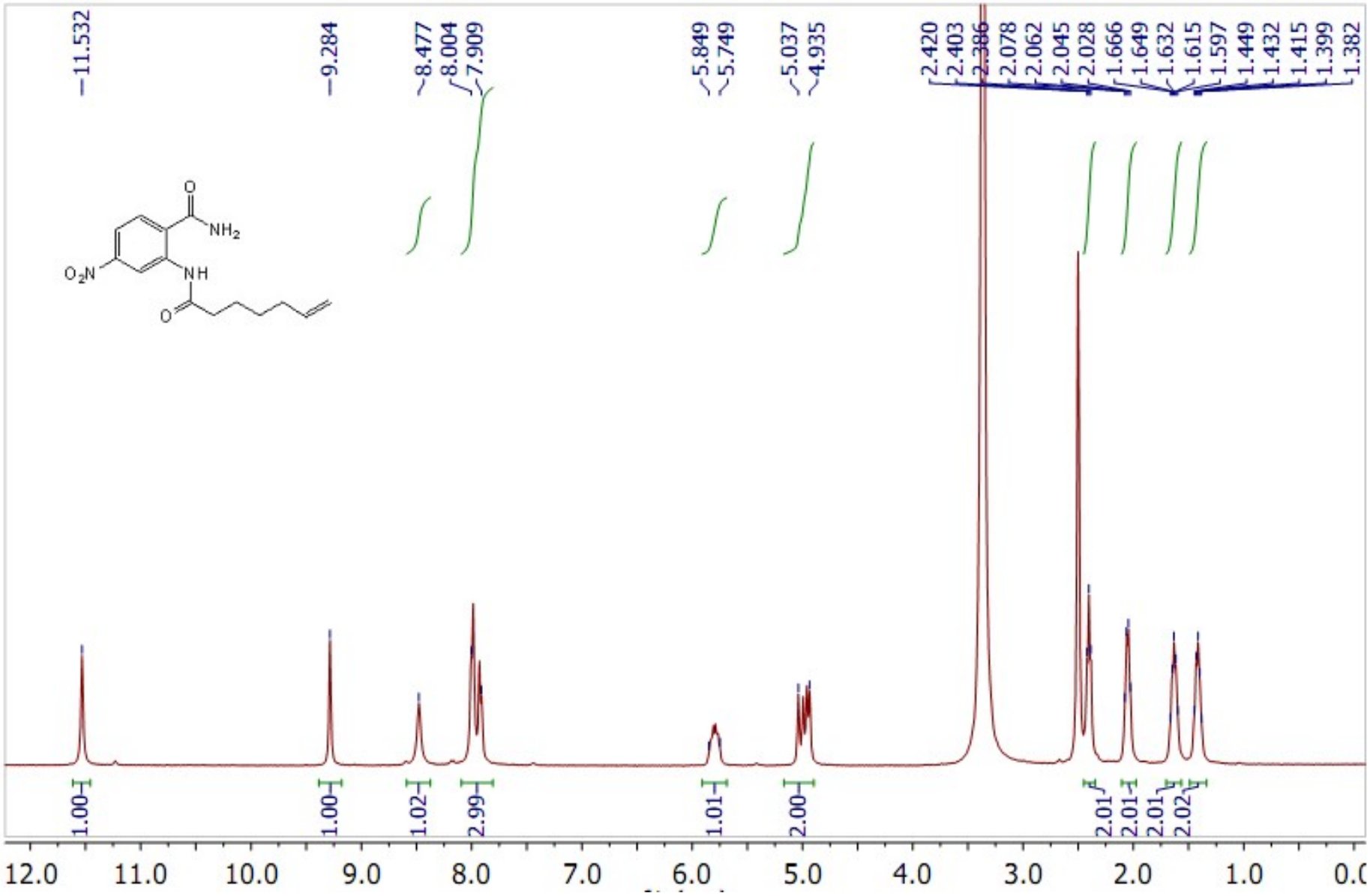
^{1}H NMR spectrum (400 MHz, DMSO-d6) of compound 8f



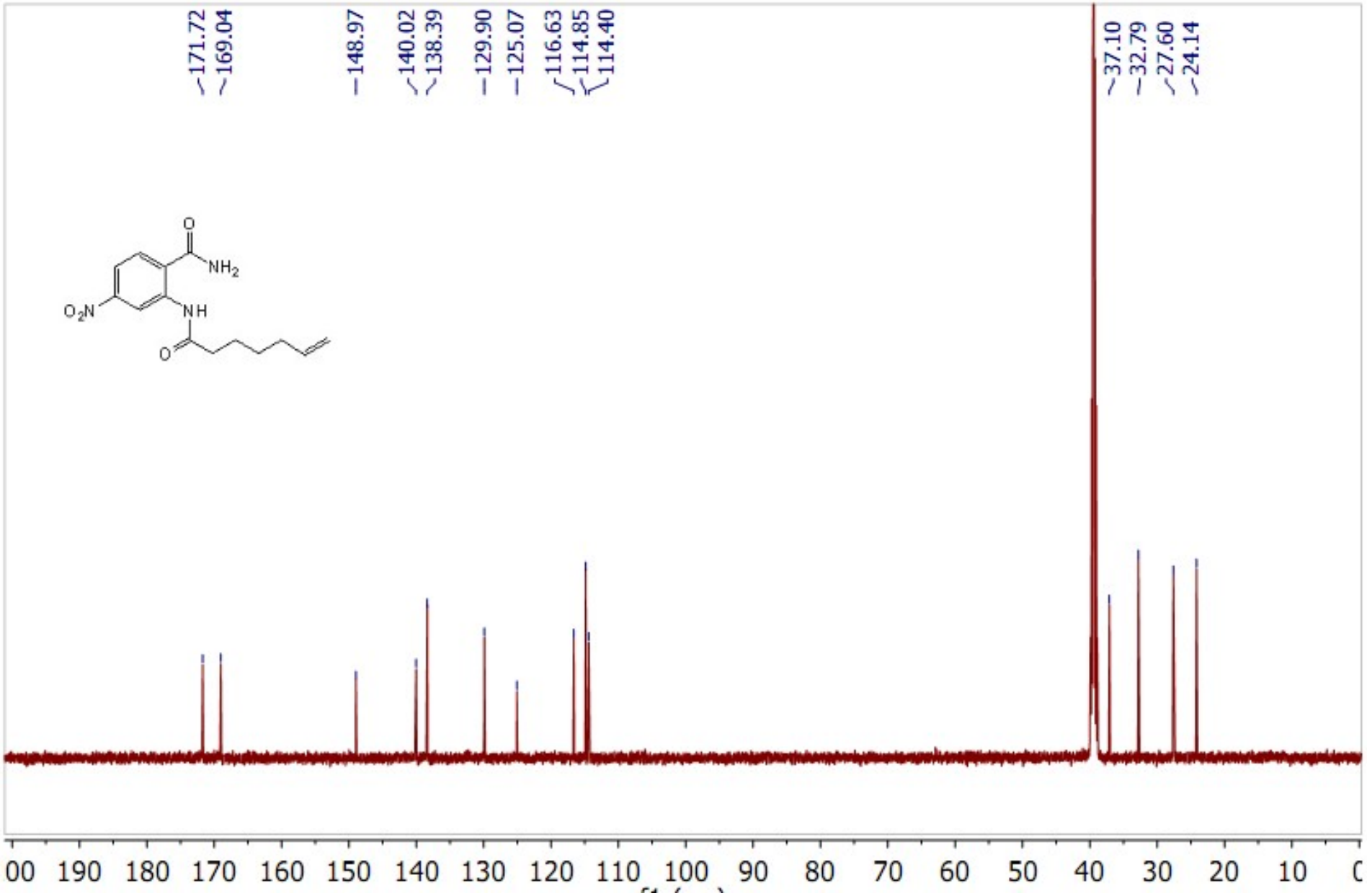
^{13}C NMR spectrum (126 MHz, DMSO-d6) of compound 8f



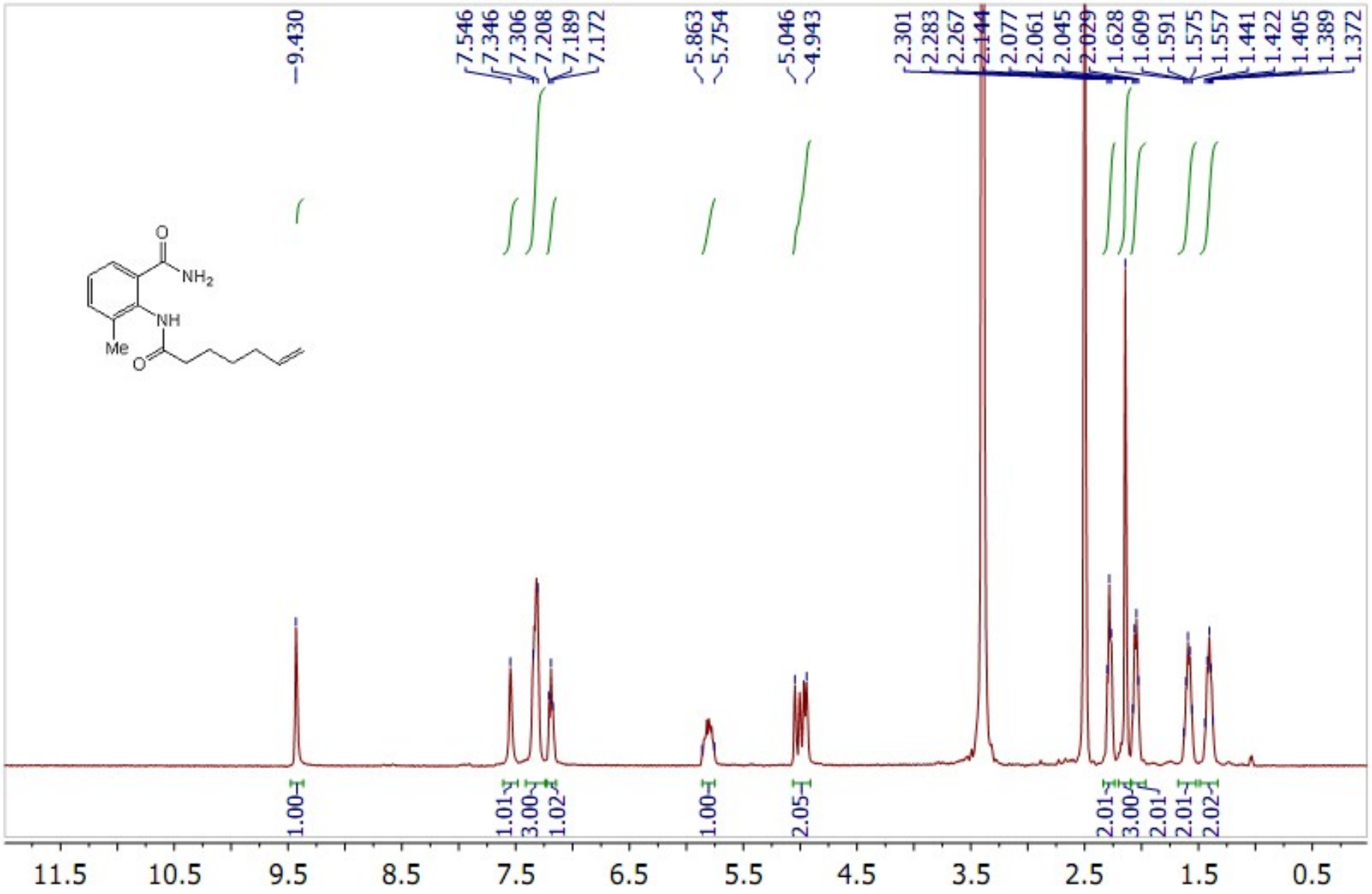
^{1}H NMR spectrum (400 MHz, DMSO-d6) of compound 8g



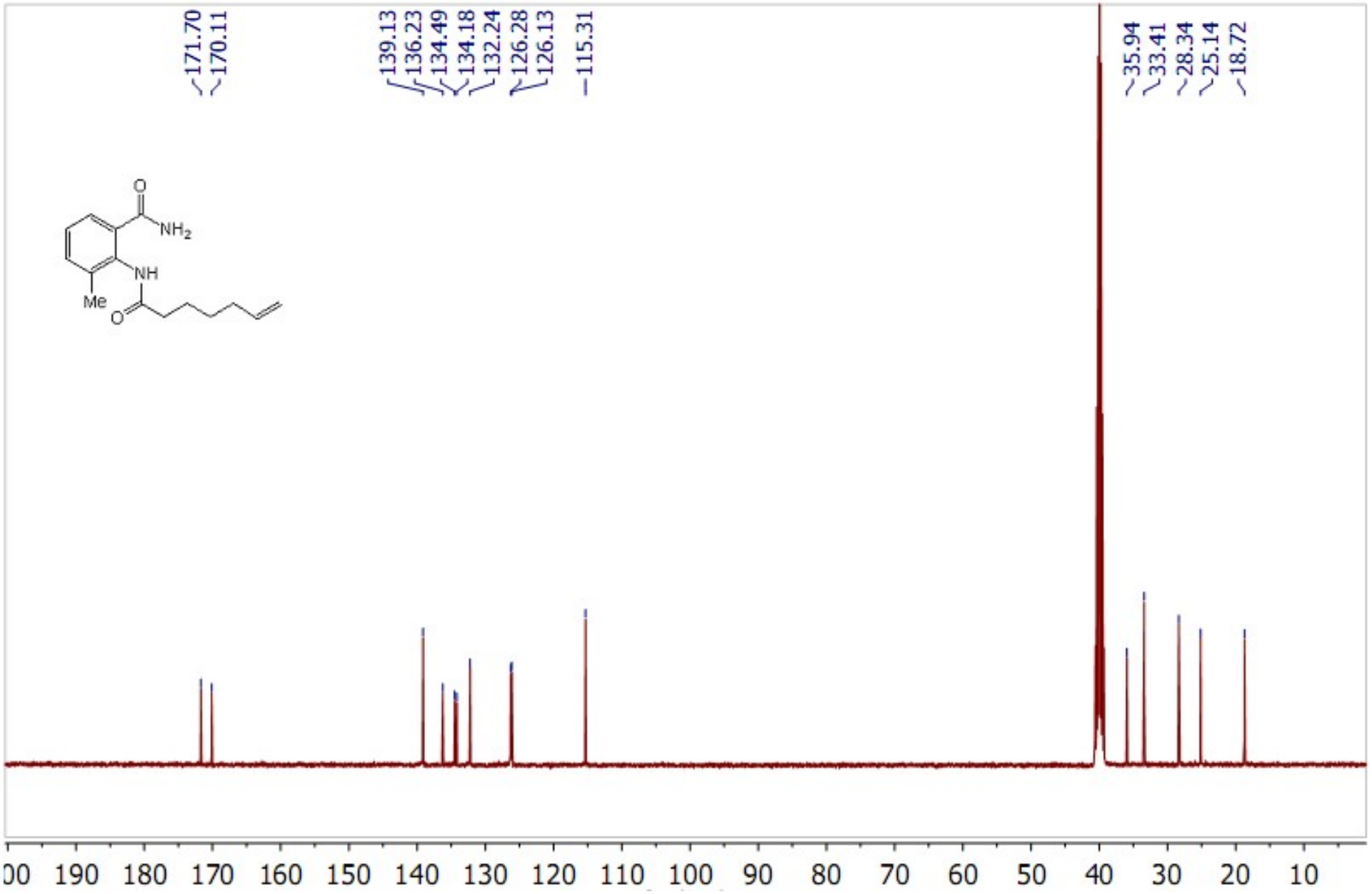
^{13}C NMR spectrum (126 MHz, DMSO-d6) of compound 8g



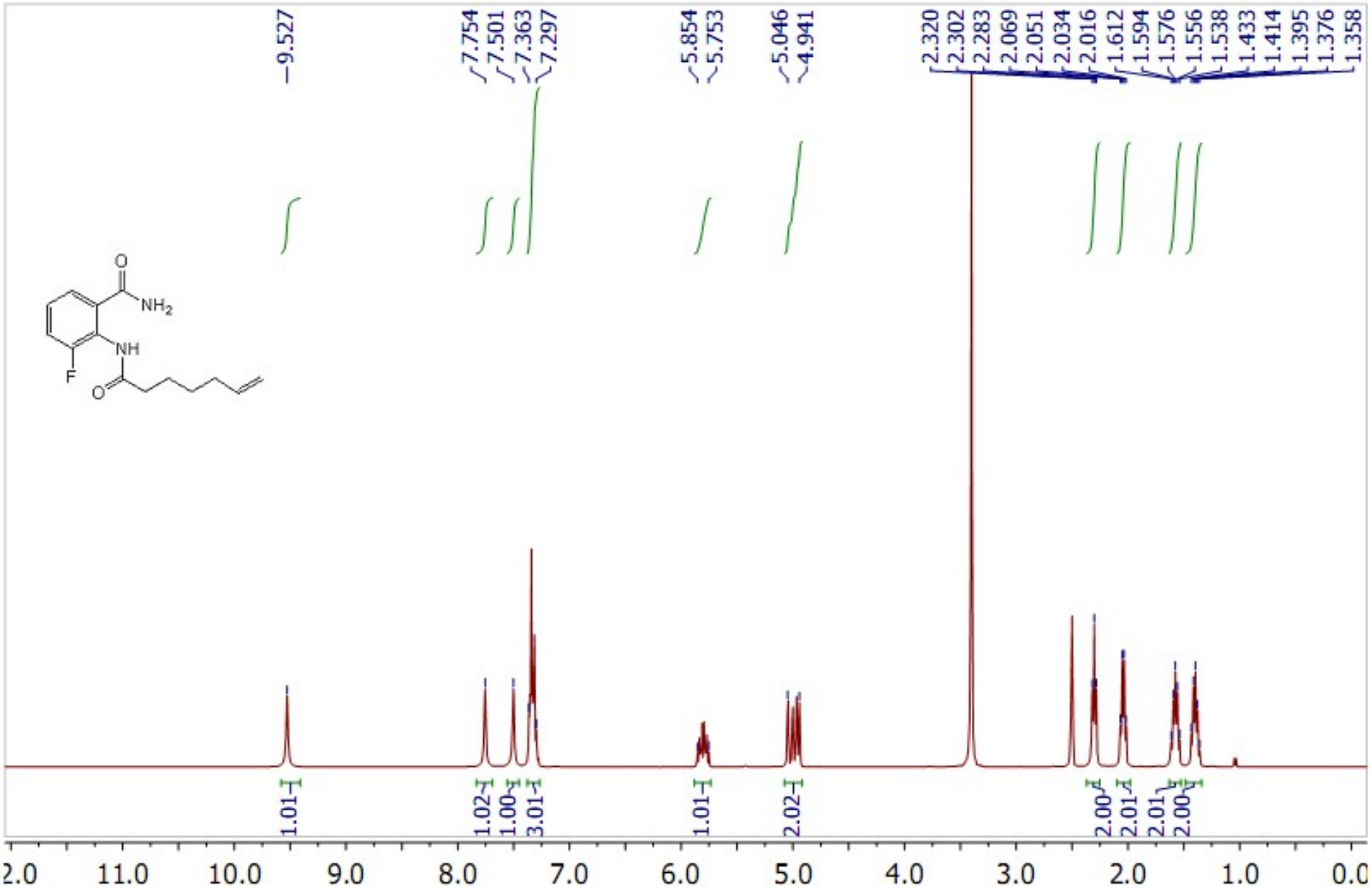
^{1}H NMR spectrum (400 MHz, DMSO-d6) of compound 8h



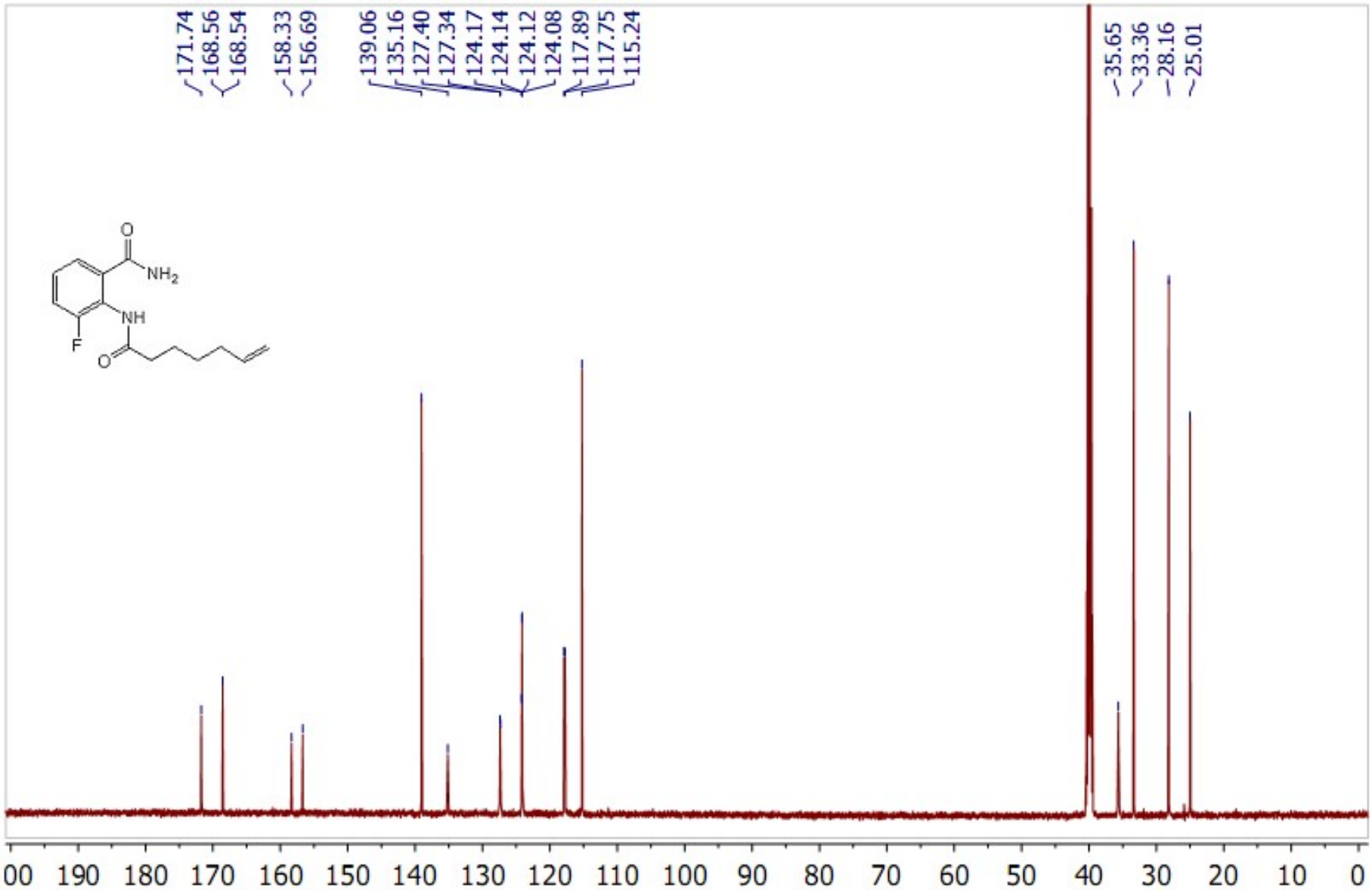
^{13}C NMR spectrum (101 MHz, DMSO-d6) of compound 8h



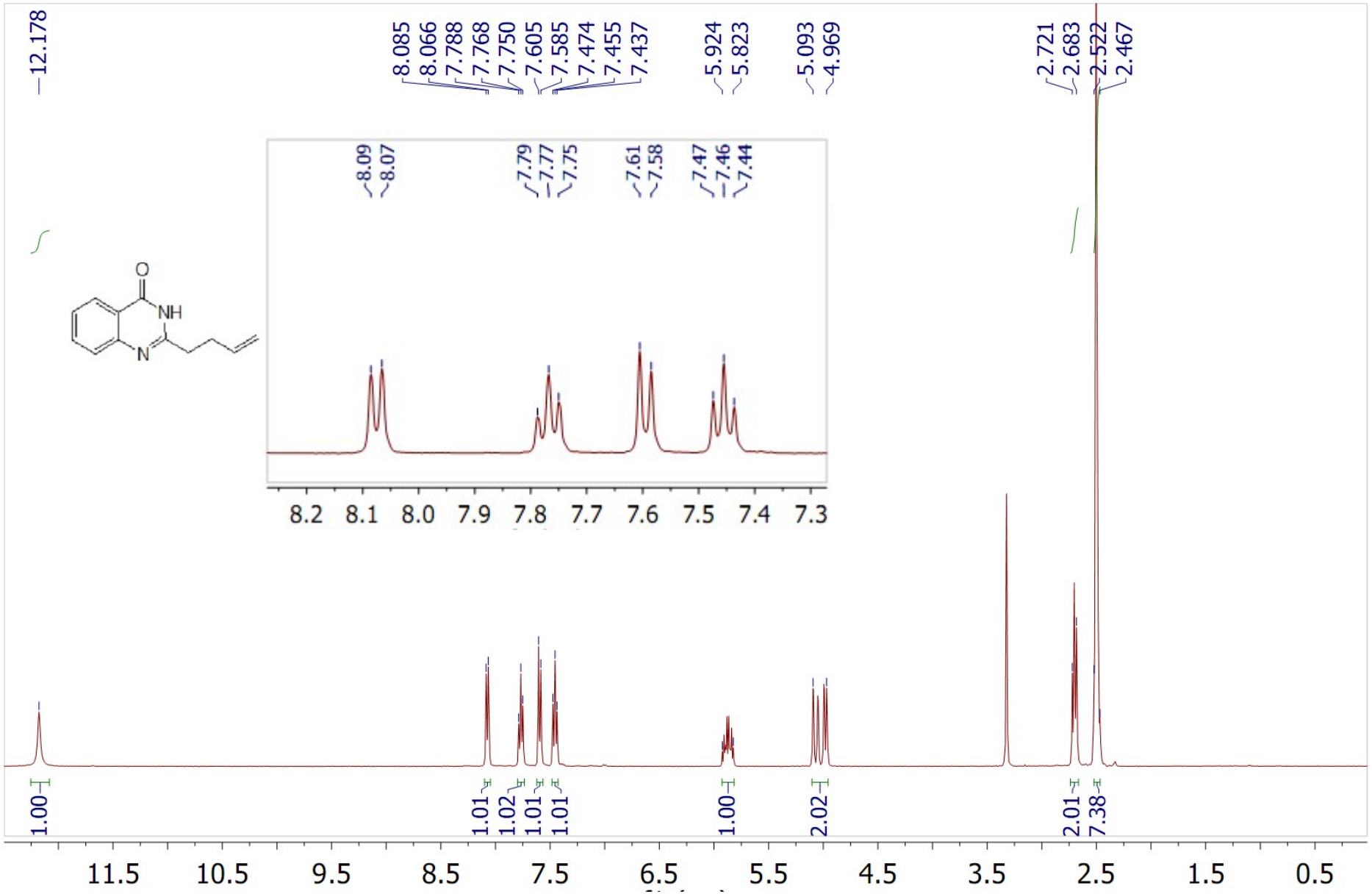
^{1}H NMR spectrum (400 MHz, DMSO-d6) of compound 8i



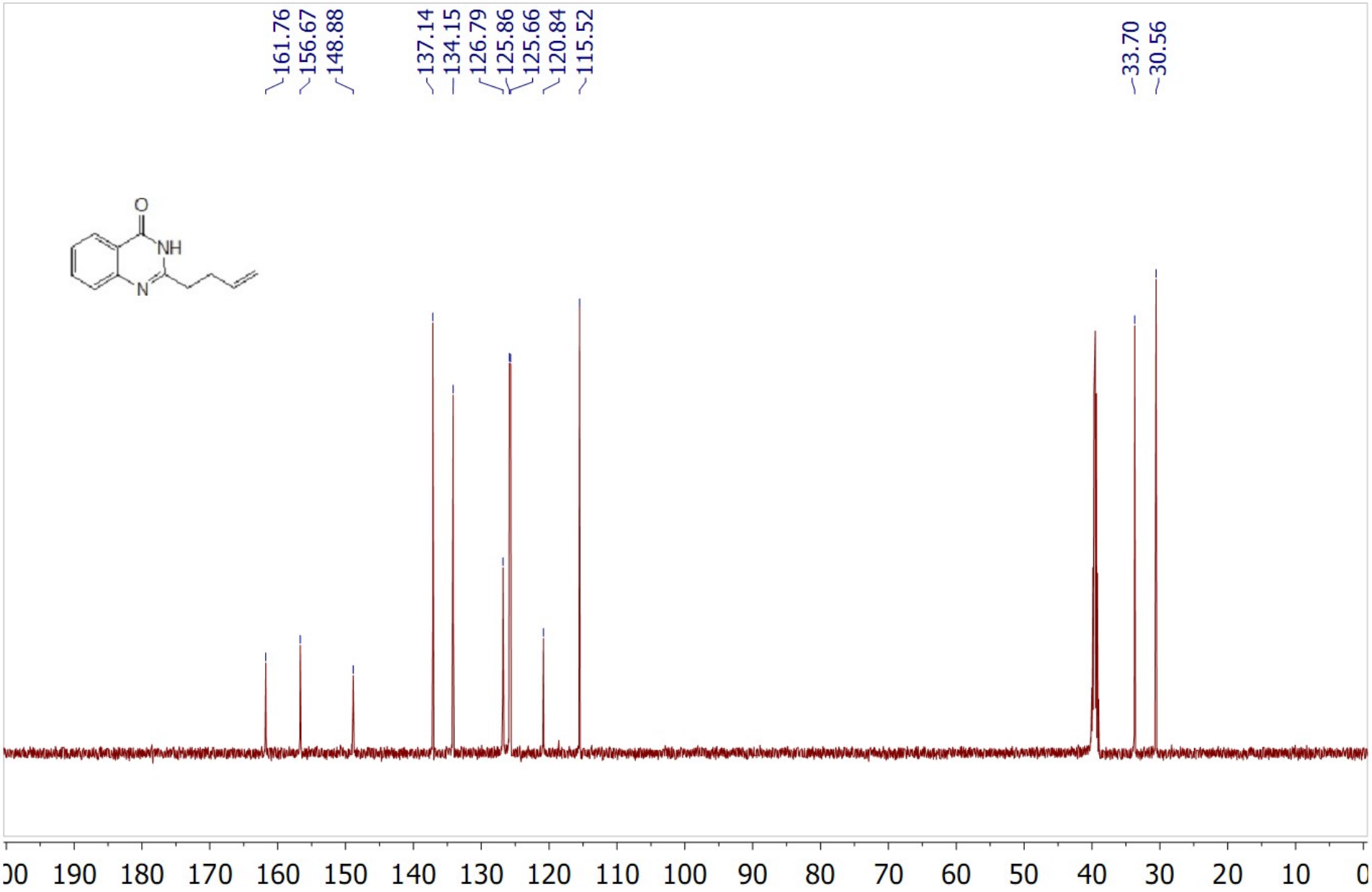
^{13}C NMR spectrum (151 MHz, DMSO-d6) of compound 8i



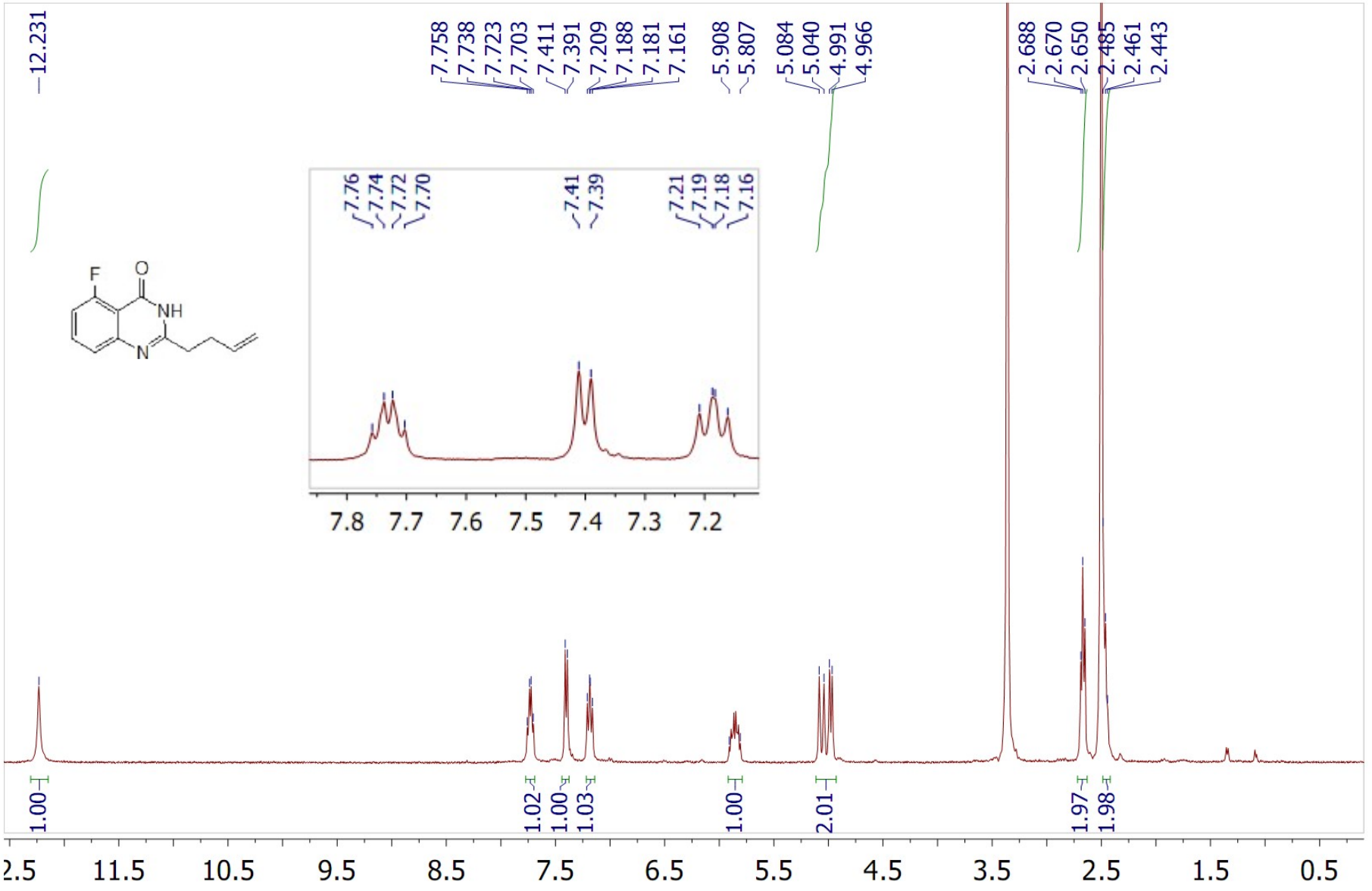
^{1}H NMR spectrum (400 MHz, DMSO-d6) of compound 1a



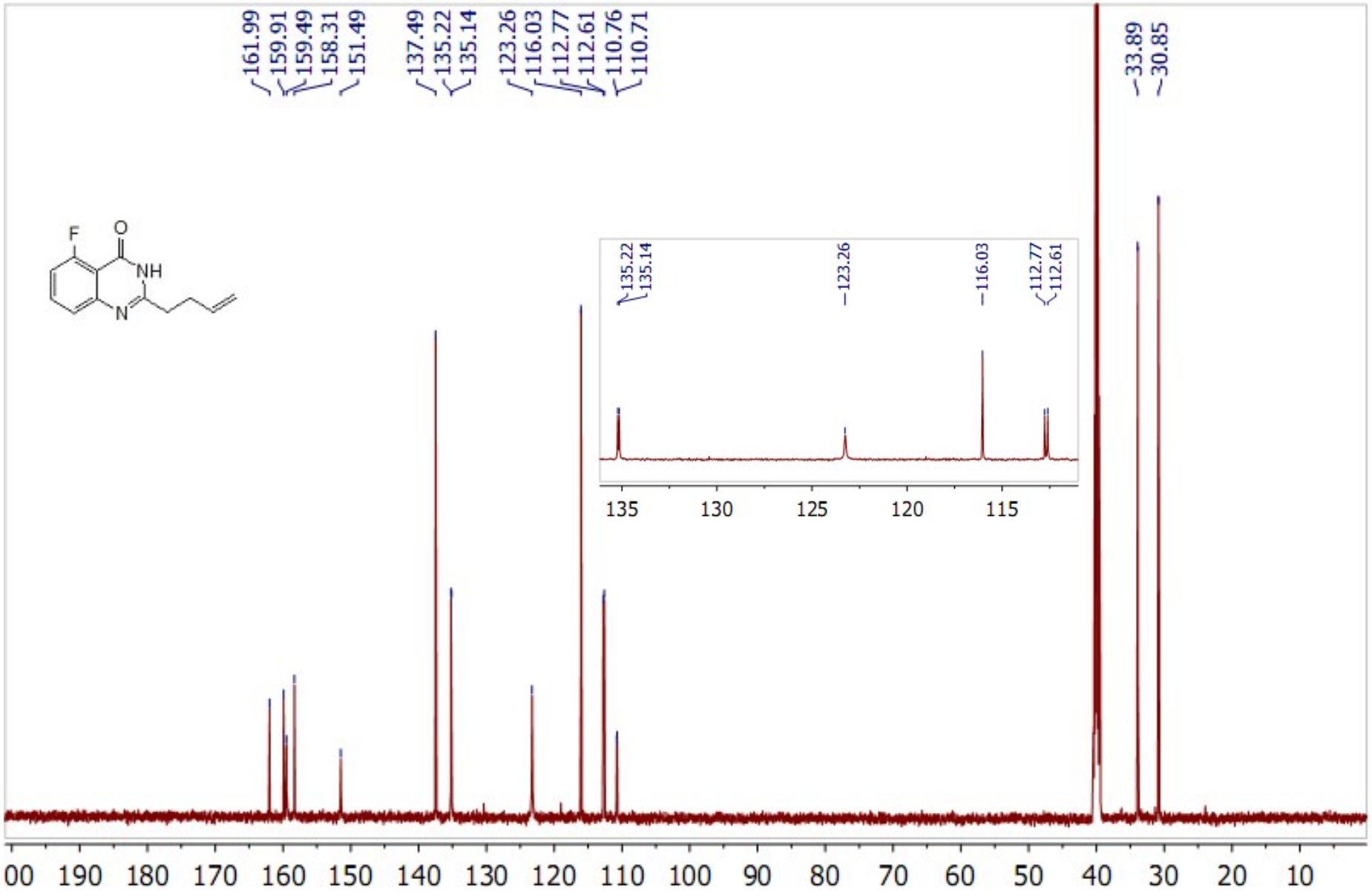
^{13}C NMR spectrum (126 MHz, DMSO-d6) of compound 1a



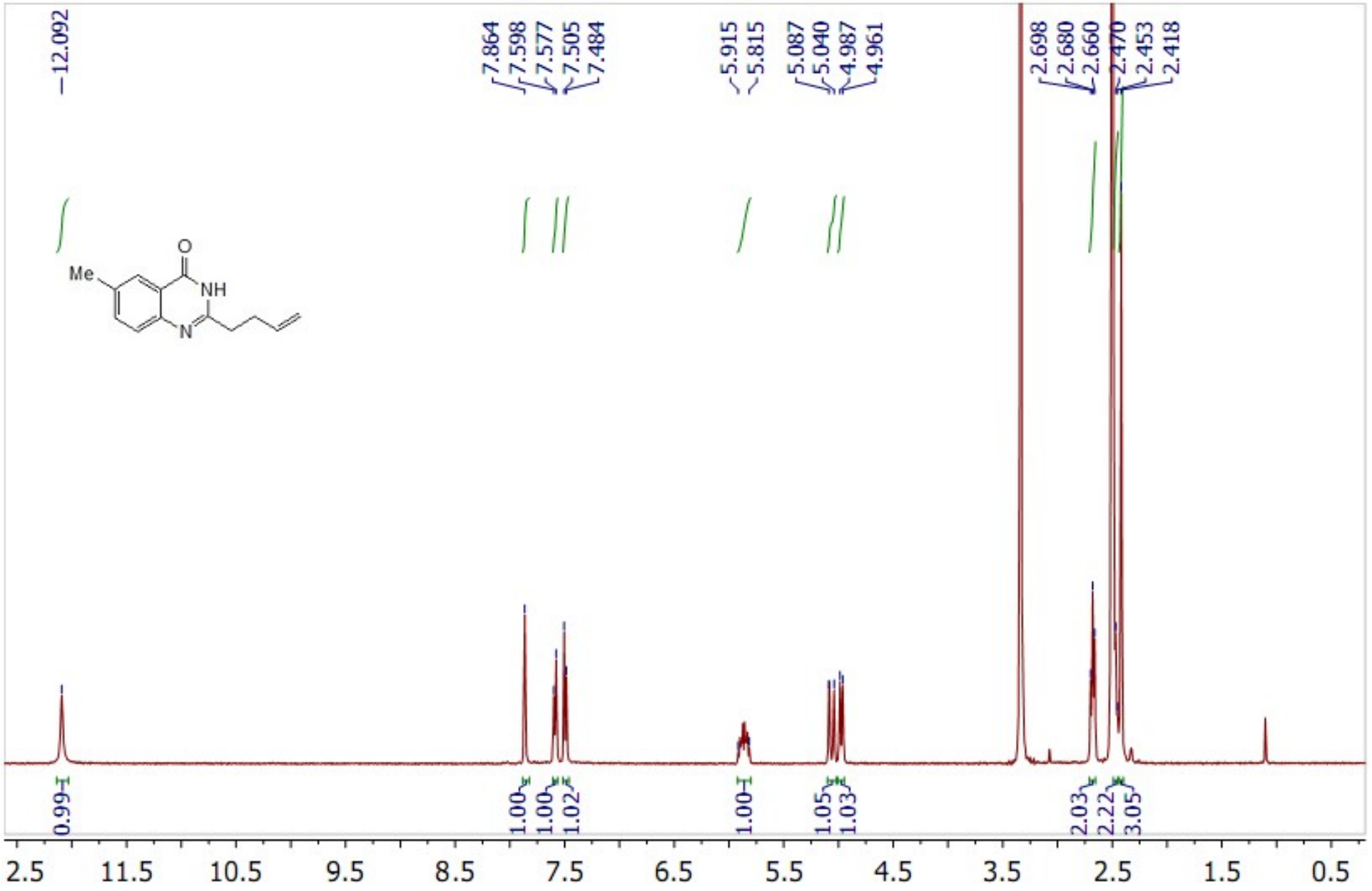
^{1}H NMR spectrum (400 MHz, DMSO-d6) of compound 1b



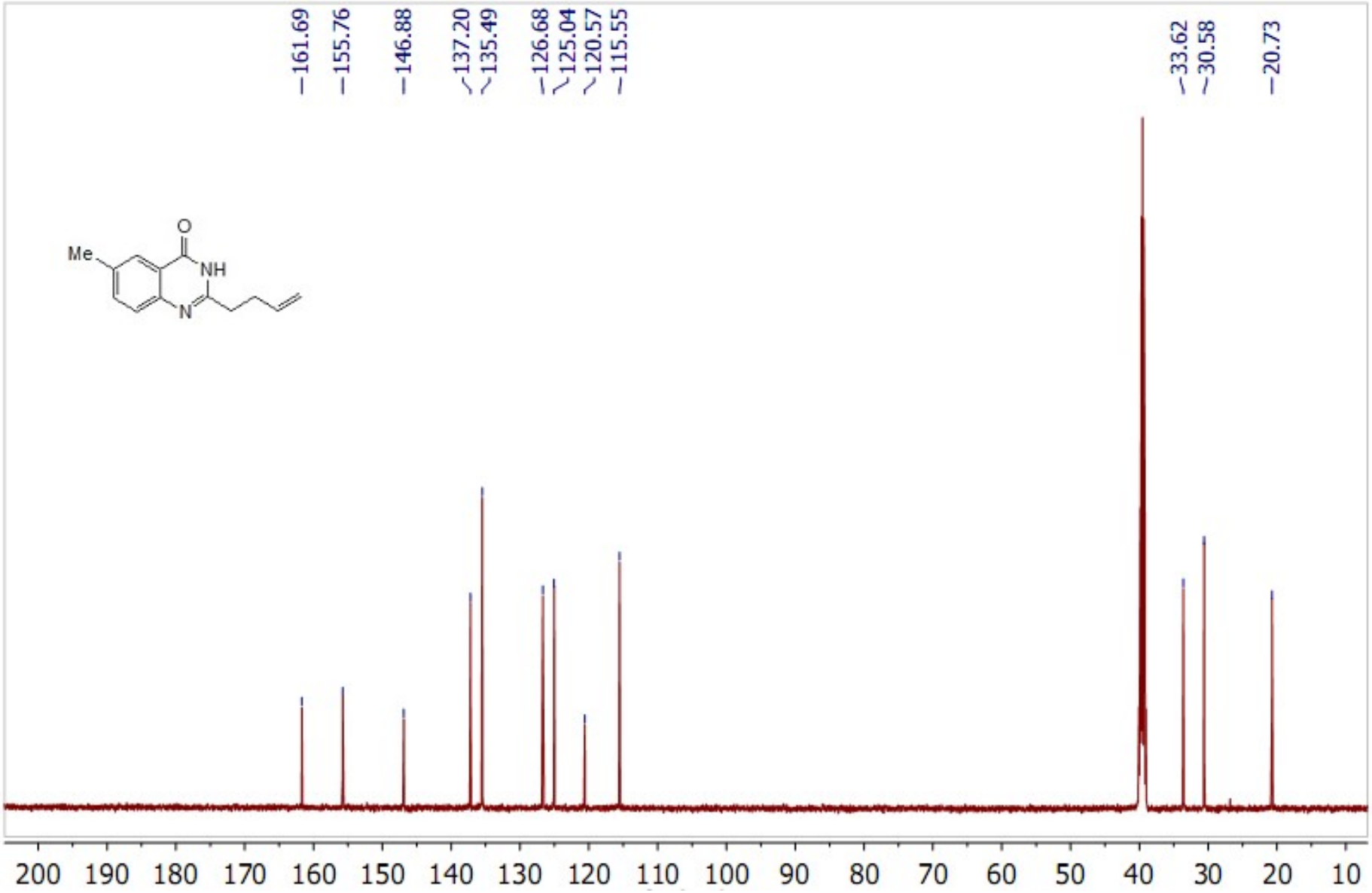
^{13}C NMR spectrum (126 MHz, DMSO-d6) of compound 1b



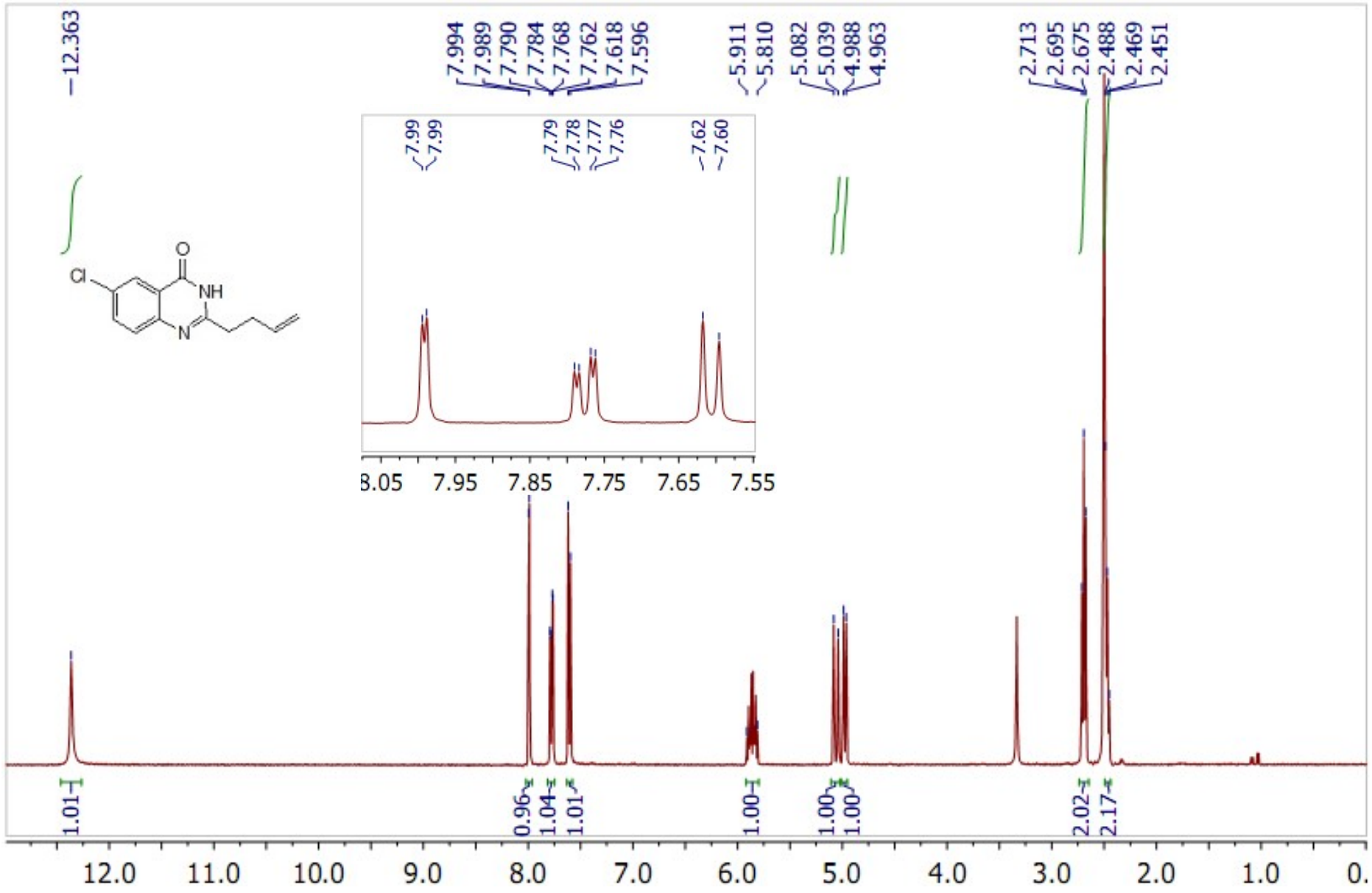
^{1}H NMR spectrum (400 MHz, DMSO-d6) of compound 1c



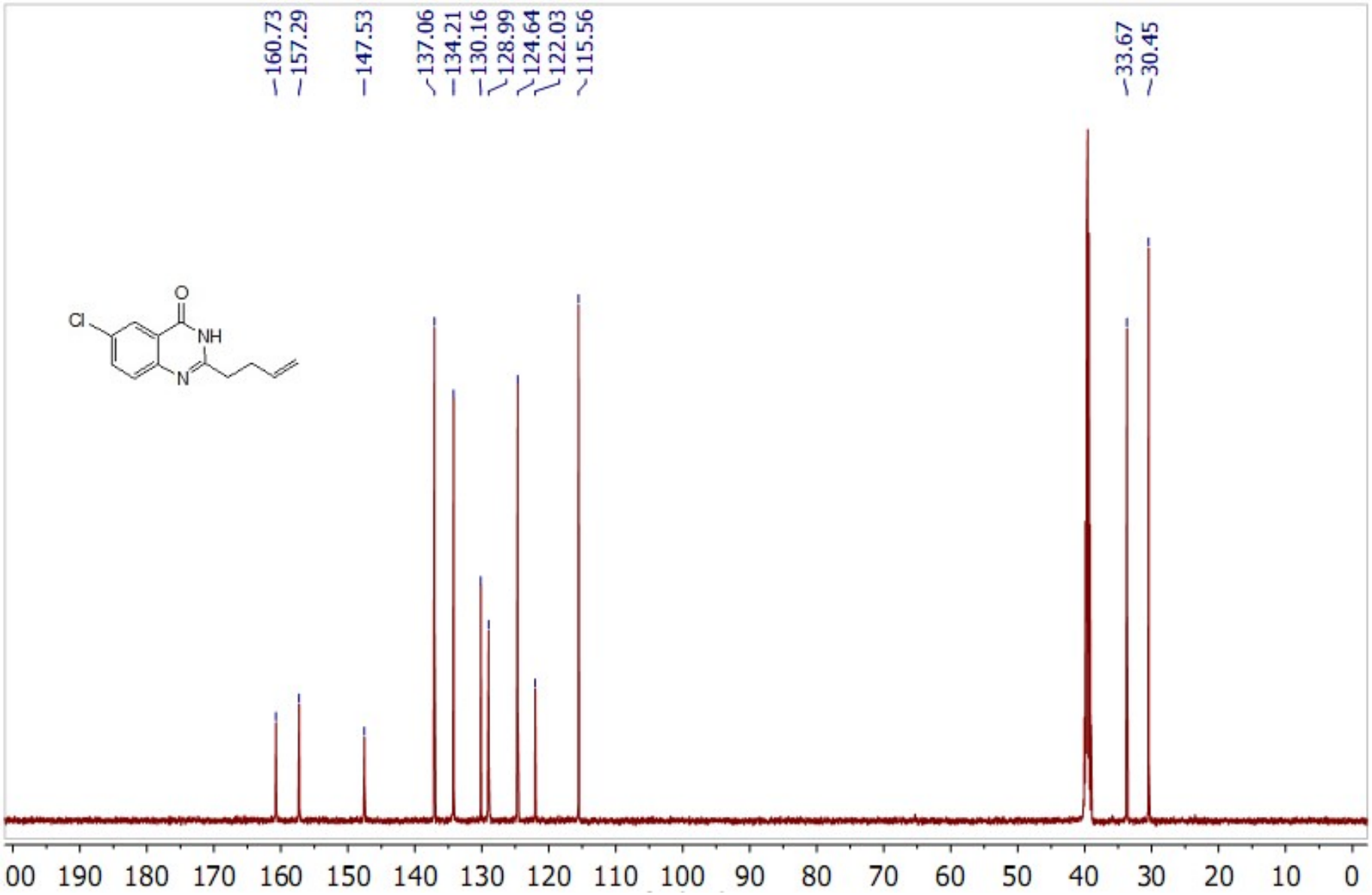
^{13}C NMR spectrum (126 MHz, DMSO-d6) of compound 1c



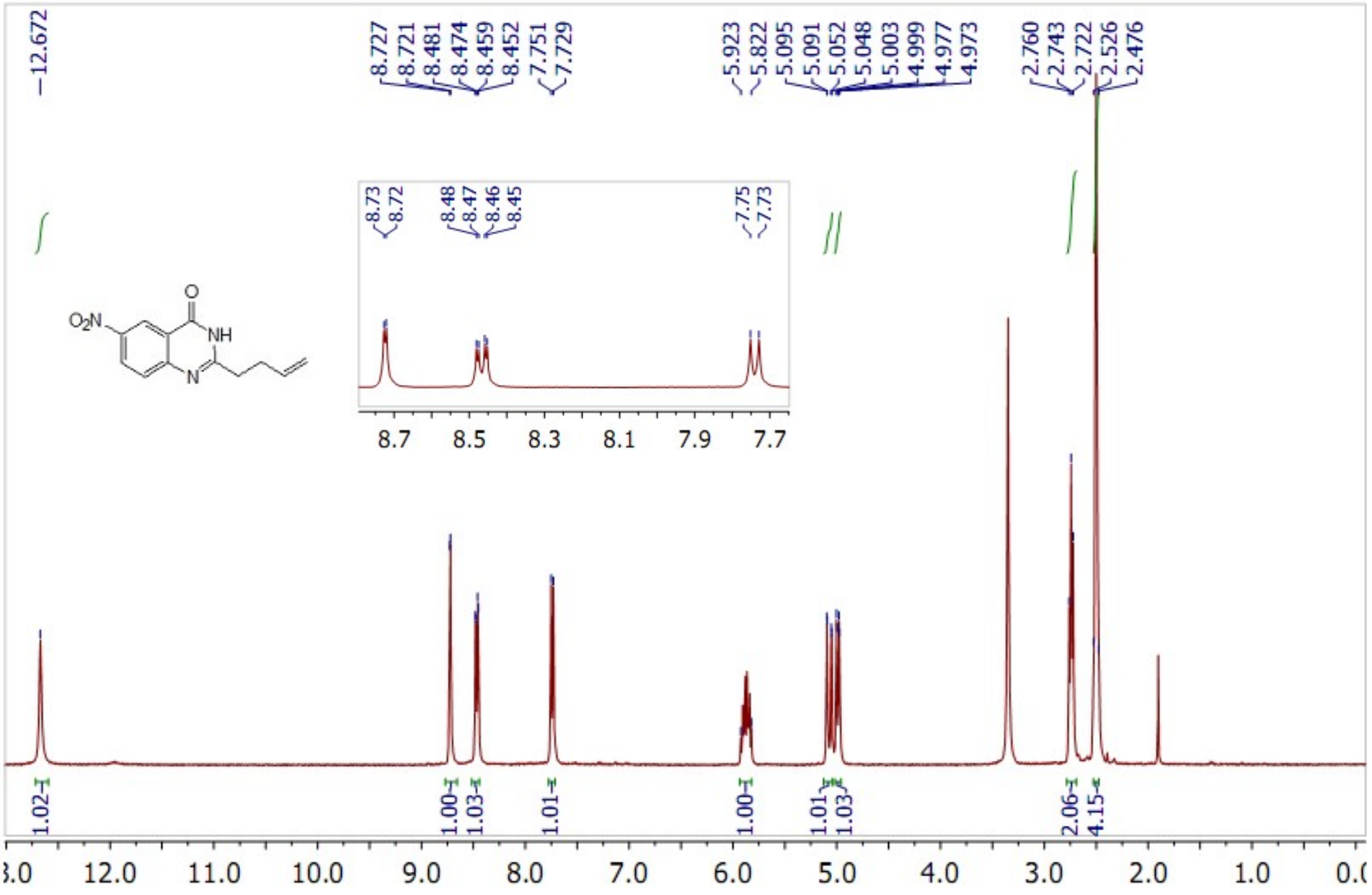
^{1}H NMR spectrum (400 MHz, DMSO-d6) of compound 1d



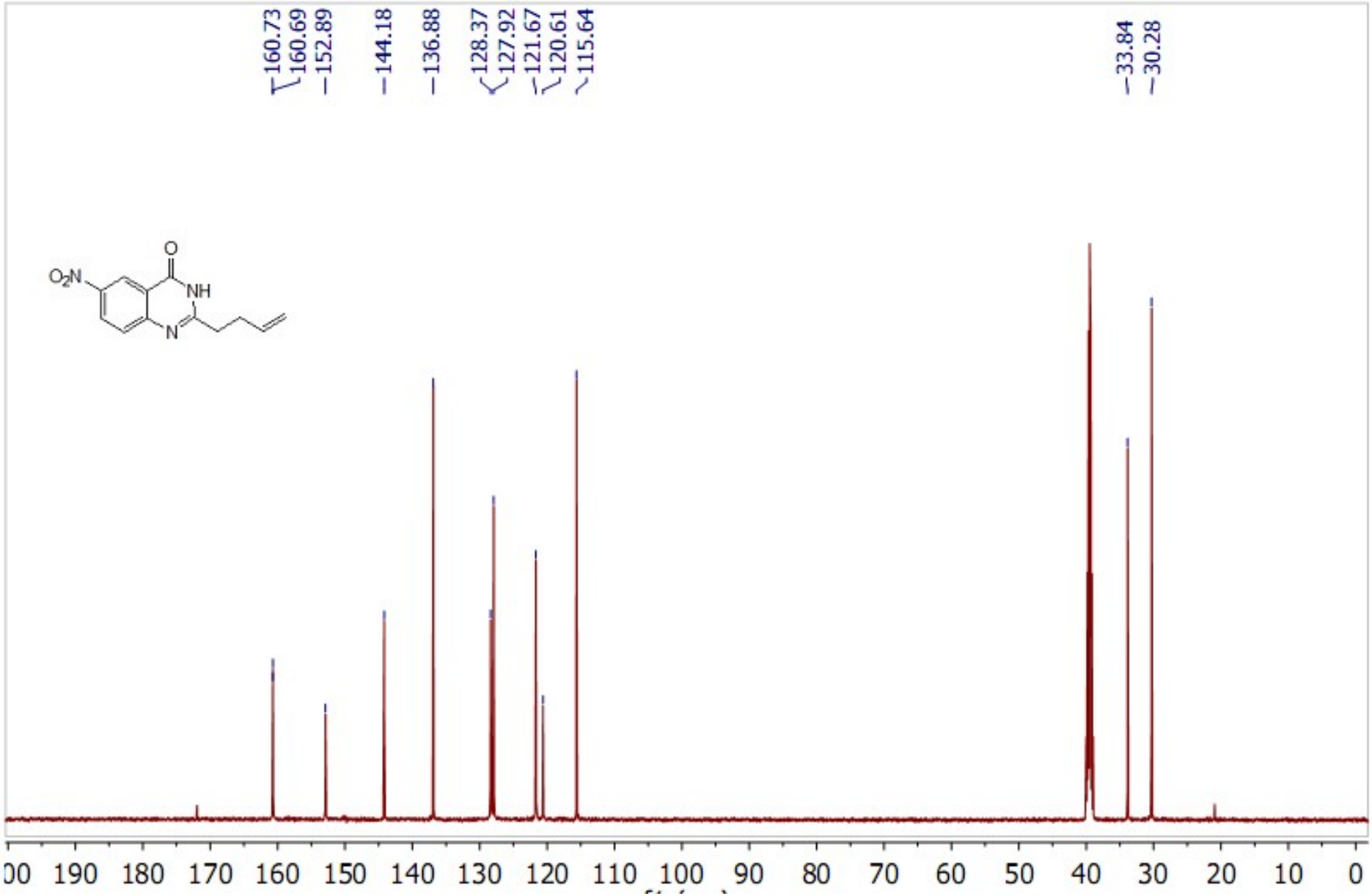
^{13}C NMR spectrum (126 MHz, DMSO-d6) of compound 1d



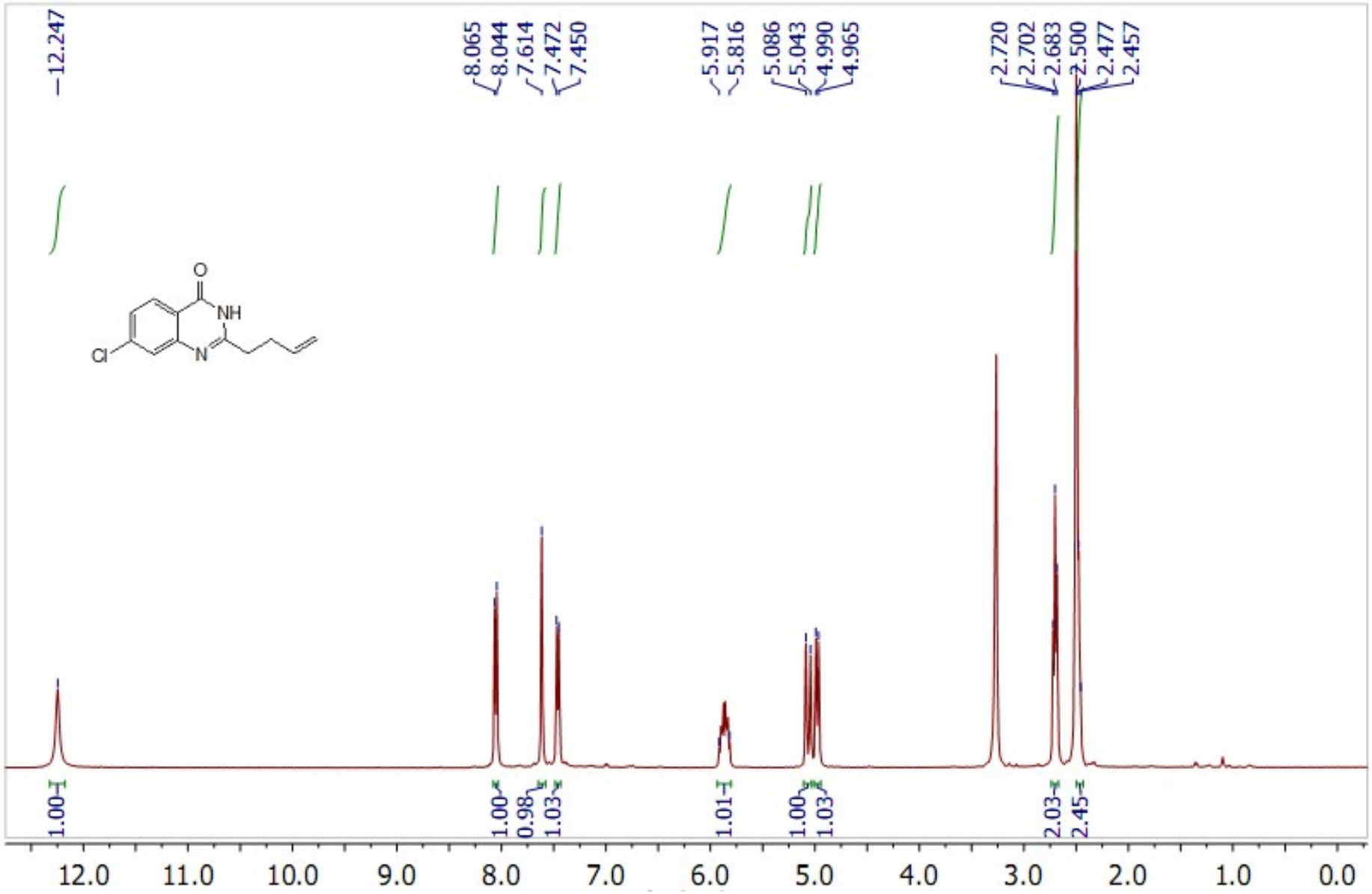
^{1}H NMR spectrum (400 MHz, DMSO-d6) of compound 1e



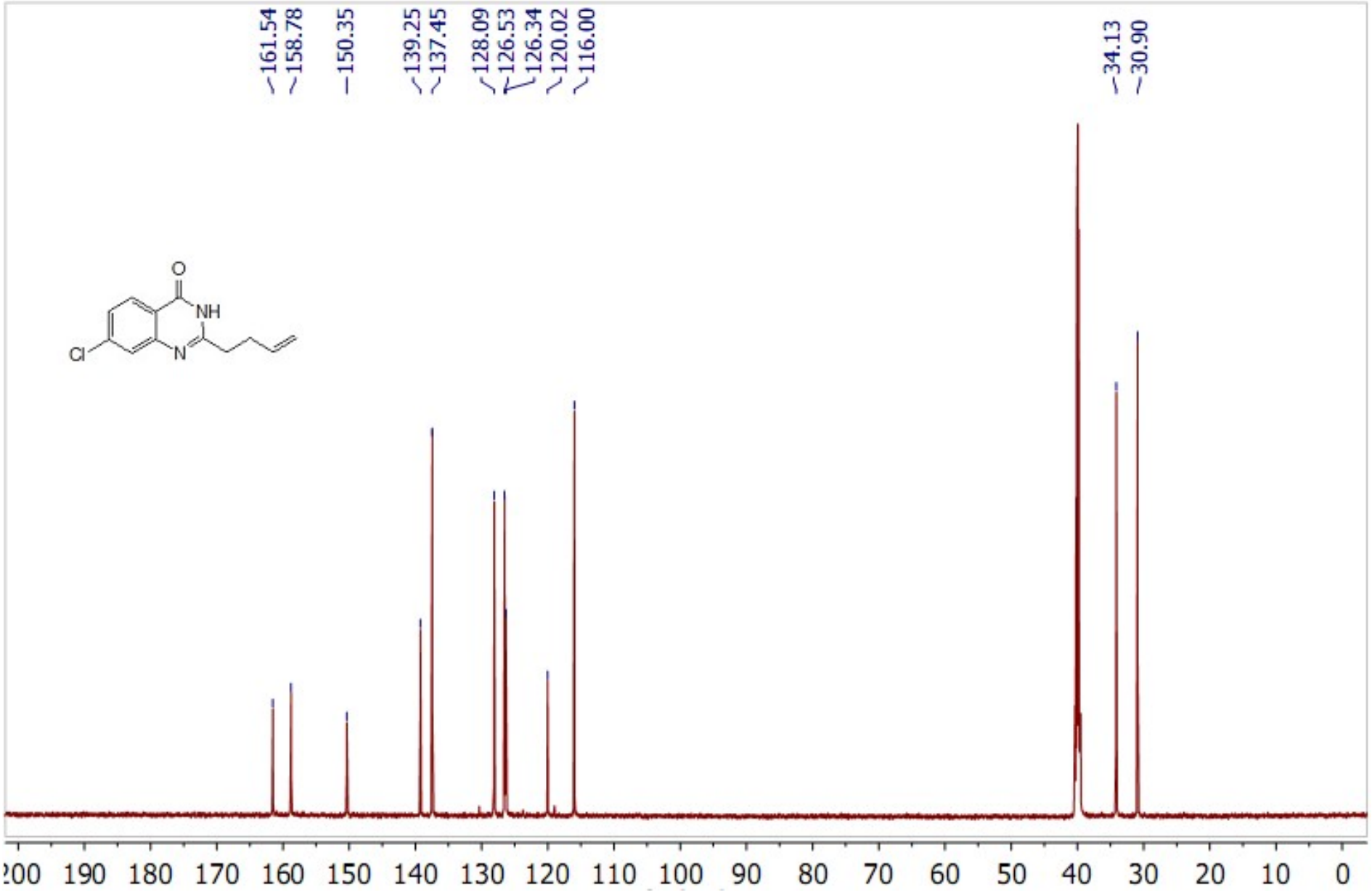
^{13}C NMR spectrum (126 MHz, DMSO-d6) of compound 1e



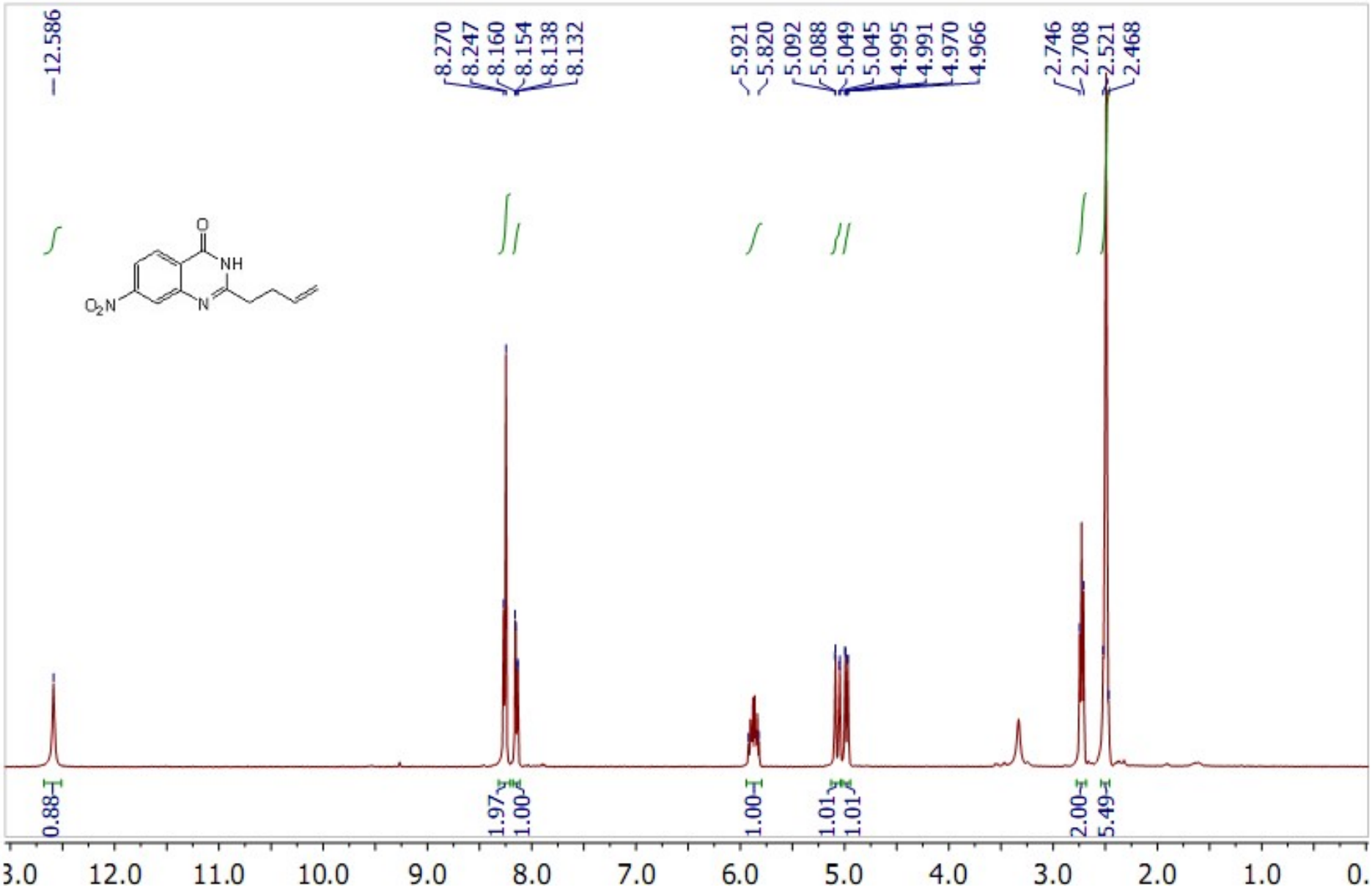
^{1}H NMR spectrum (400 MHz, DMSO-d6) of compound 1f



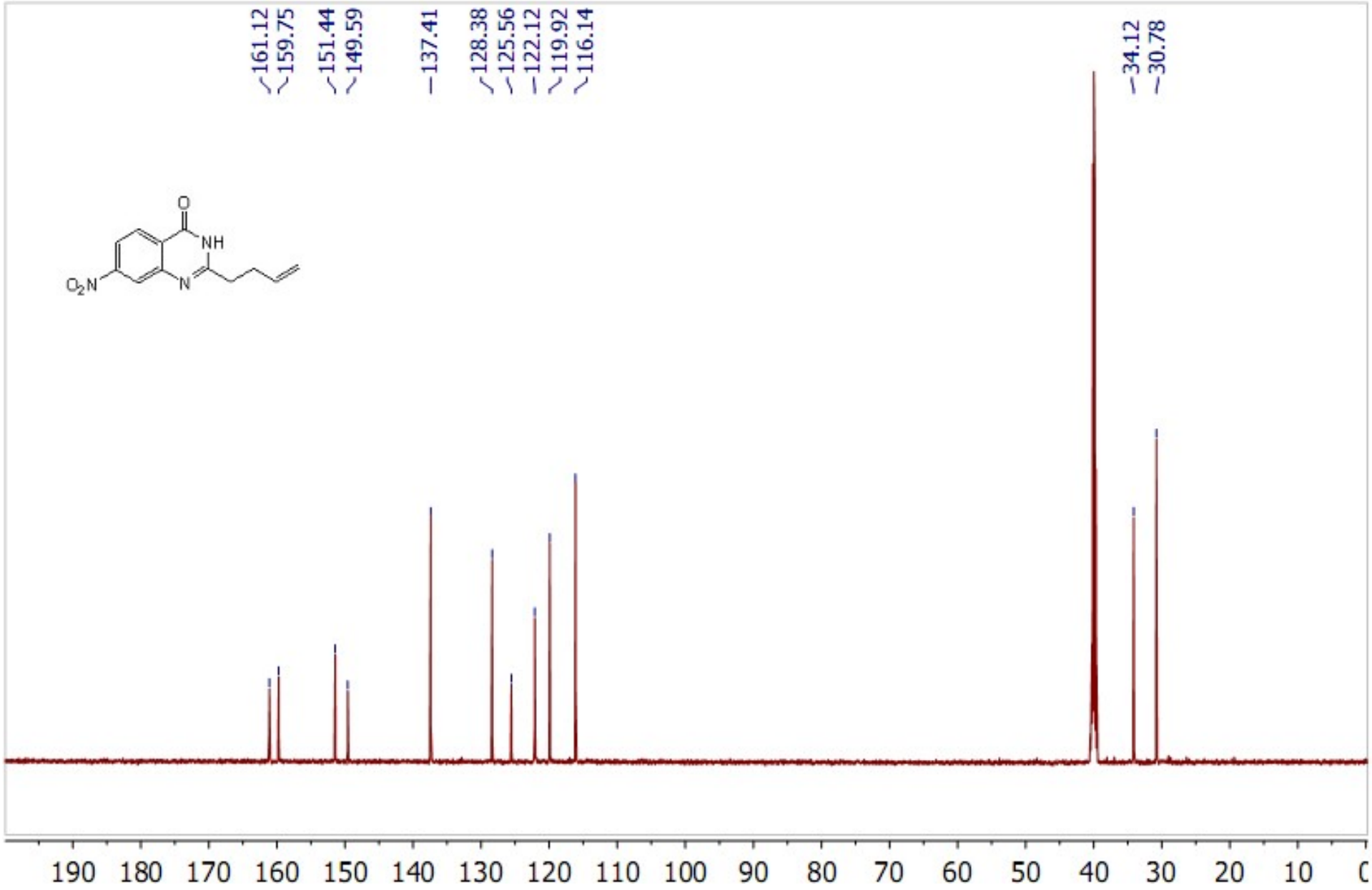
^{13}C NMR spectrum (151 MHz, DMSO-d6) of compound 1f.



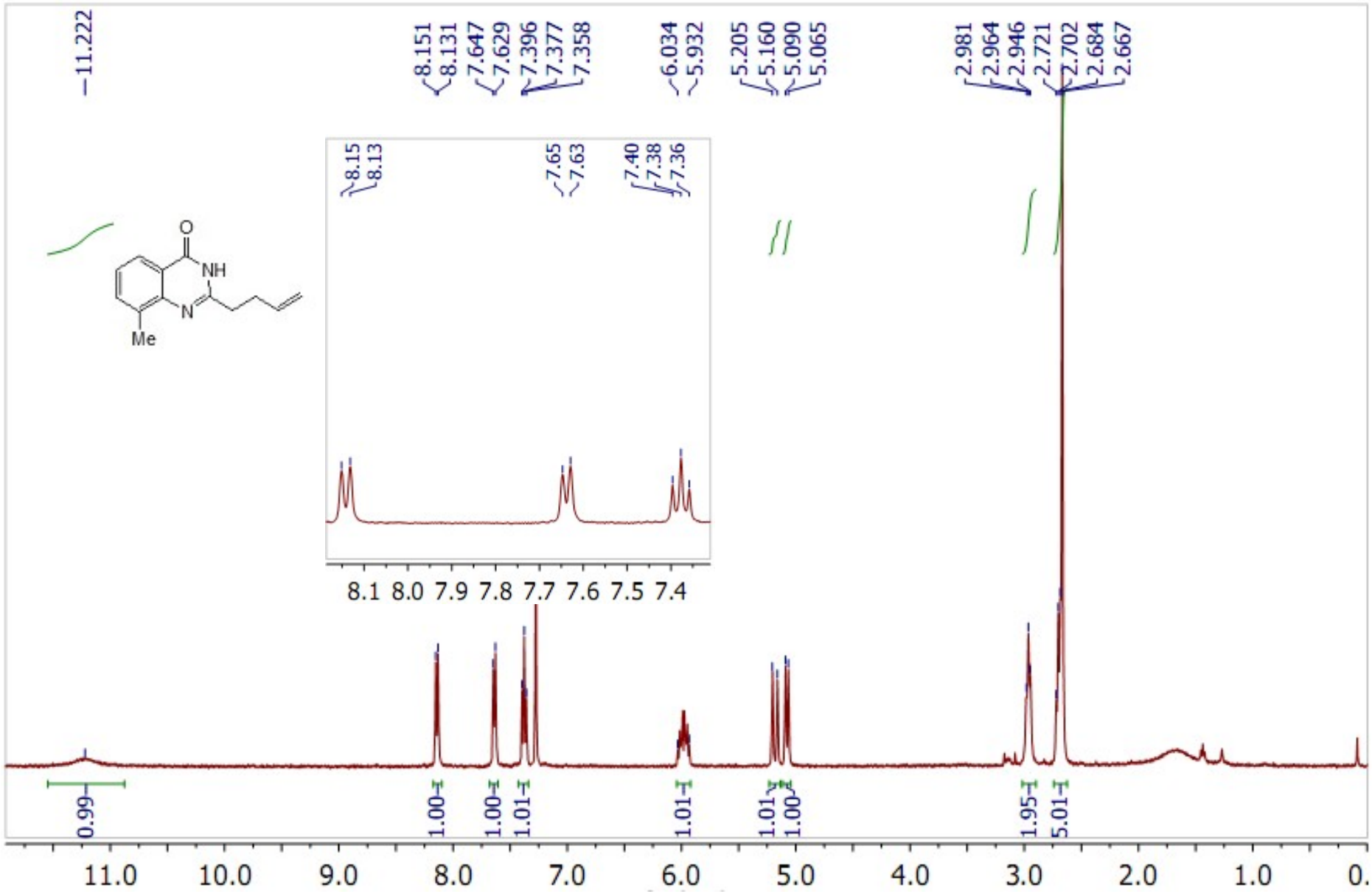
^{1}H NMR spectrum (400 MHz, DMSO-d6) of compound 1g



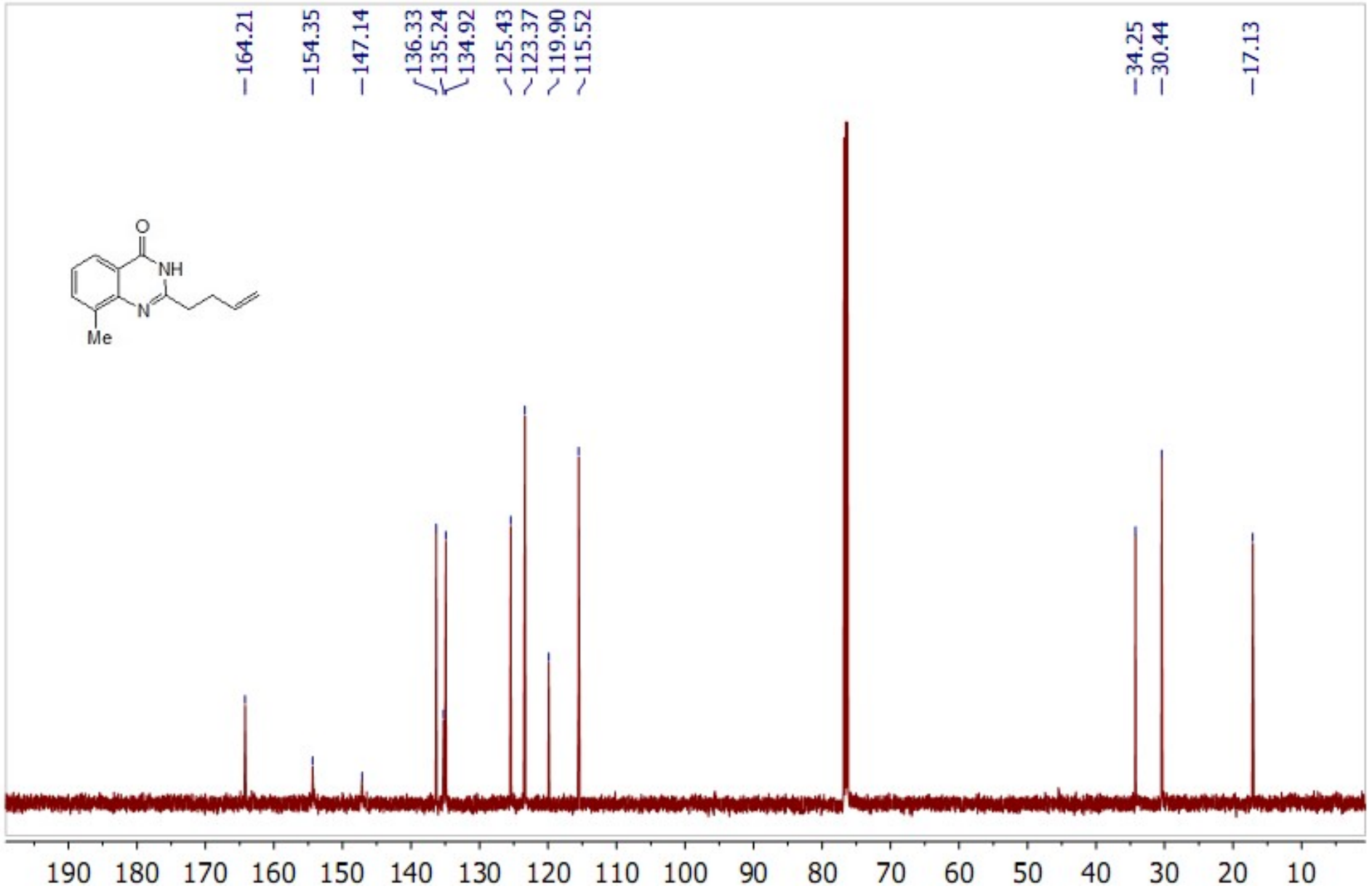
^{13}C NMR spectrum (151 MHz, DMSO-d6) of compound 1g



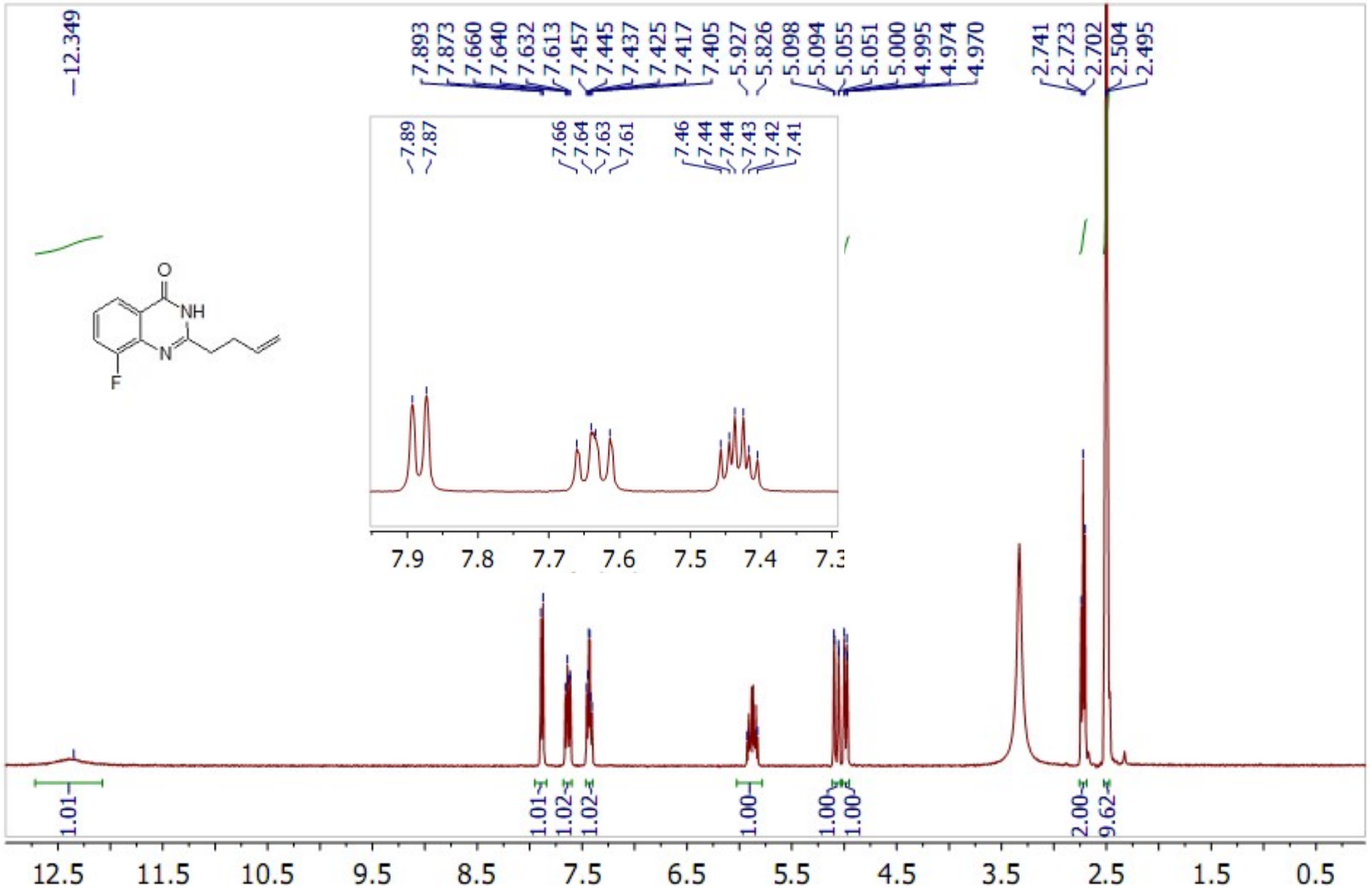
^{1}H NMR spectrum (400 MHz, $CDCl_3$) of compound 1h



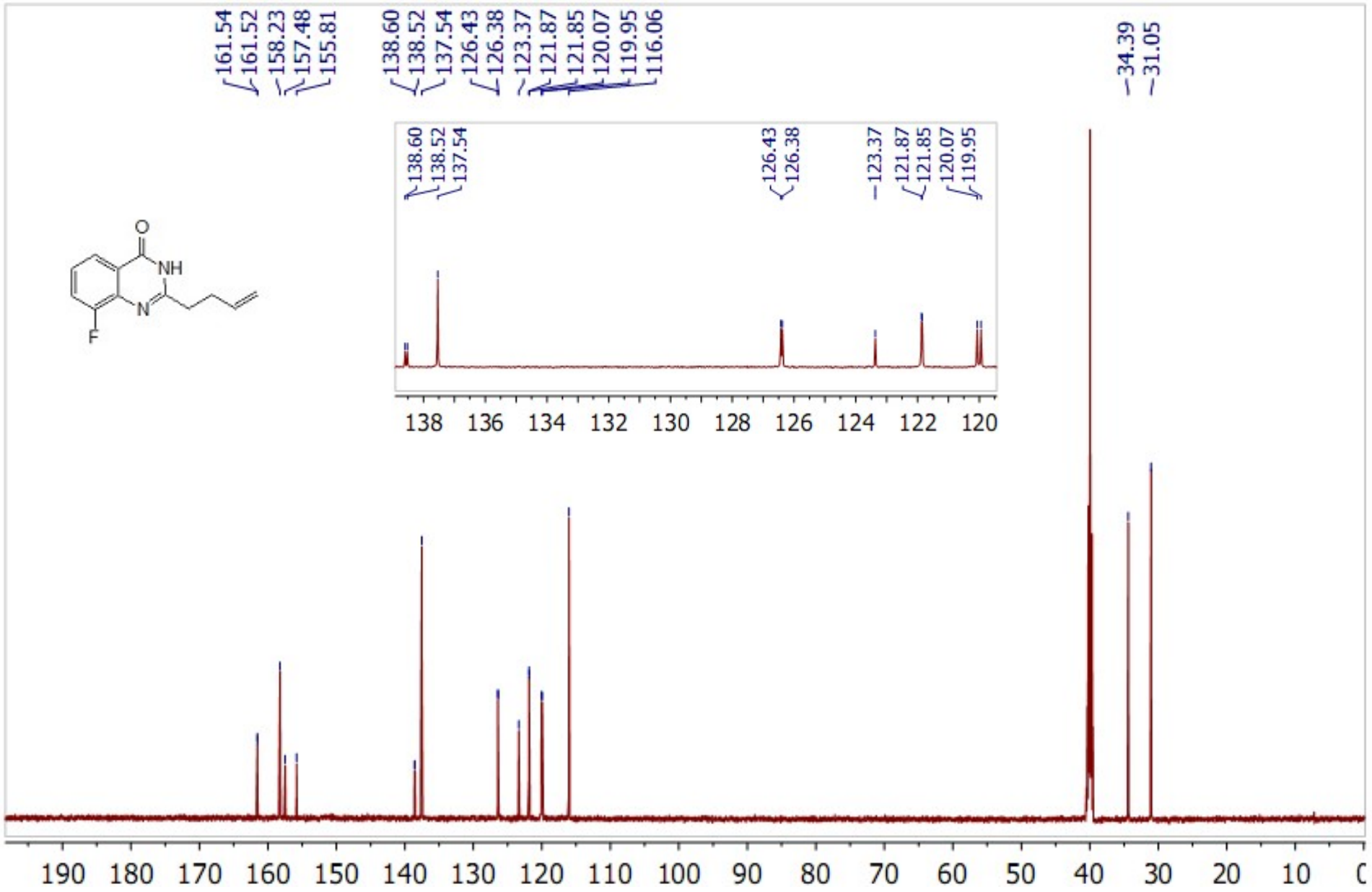
^{13}C NMR spectrum (126 MHz, $CDCl_3$) of compound 1h



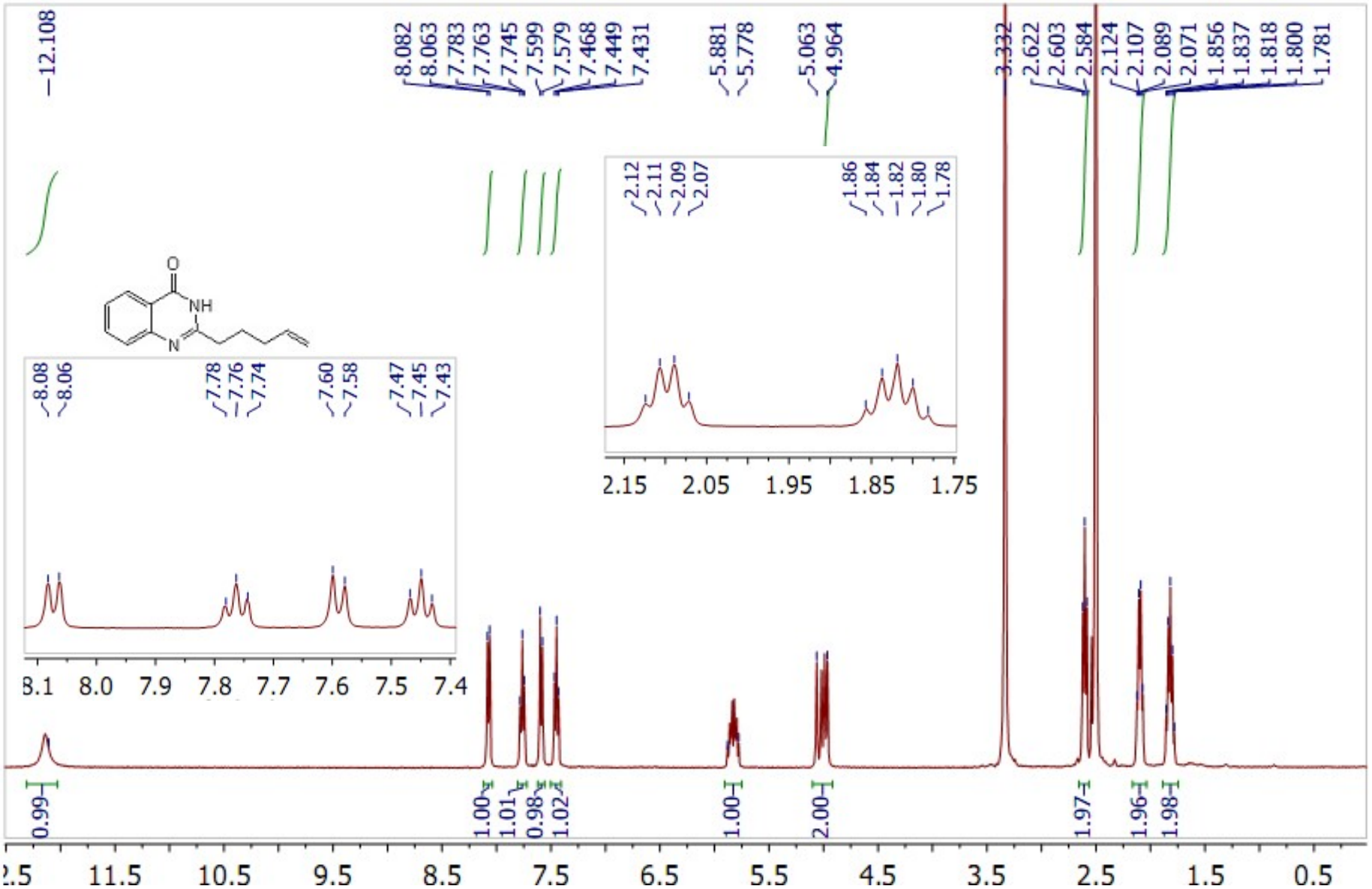
^{1}H NMR spectrum (400 MHz, DMSO-d6) of compound 1i



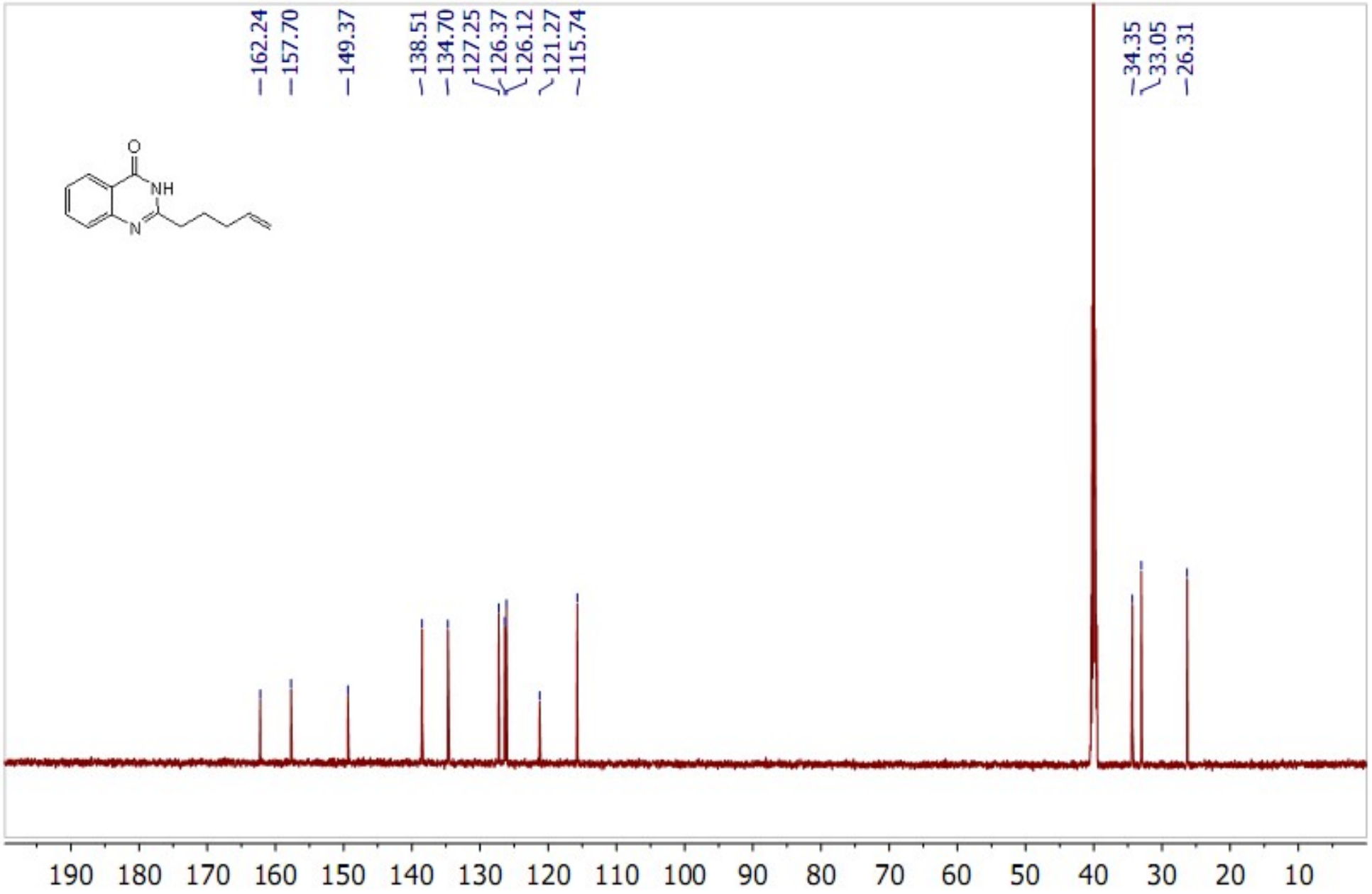
^{13}C NMR spectrum (151 MHz, DMSO-d6) of compound 1i



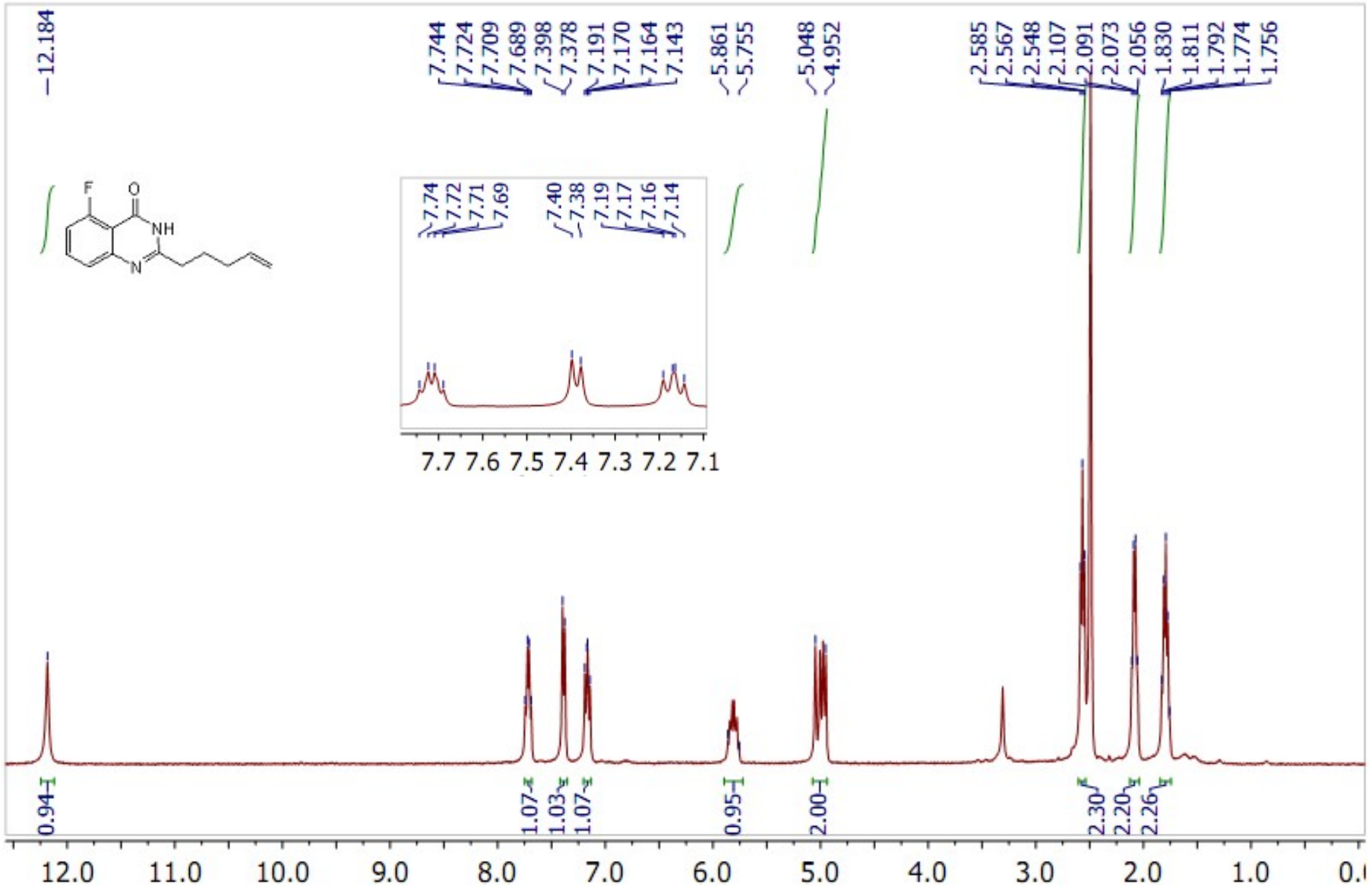
^{1}H NMR spectrum (400 MHz, DMSO-d6) of compound 2a



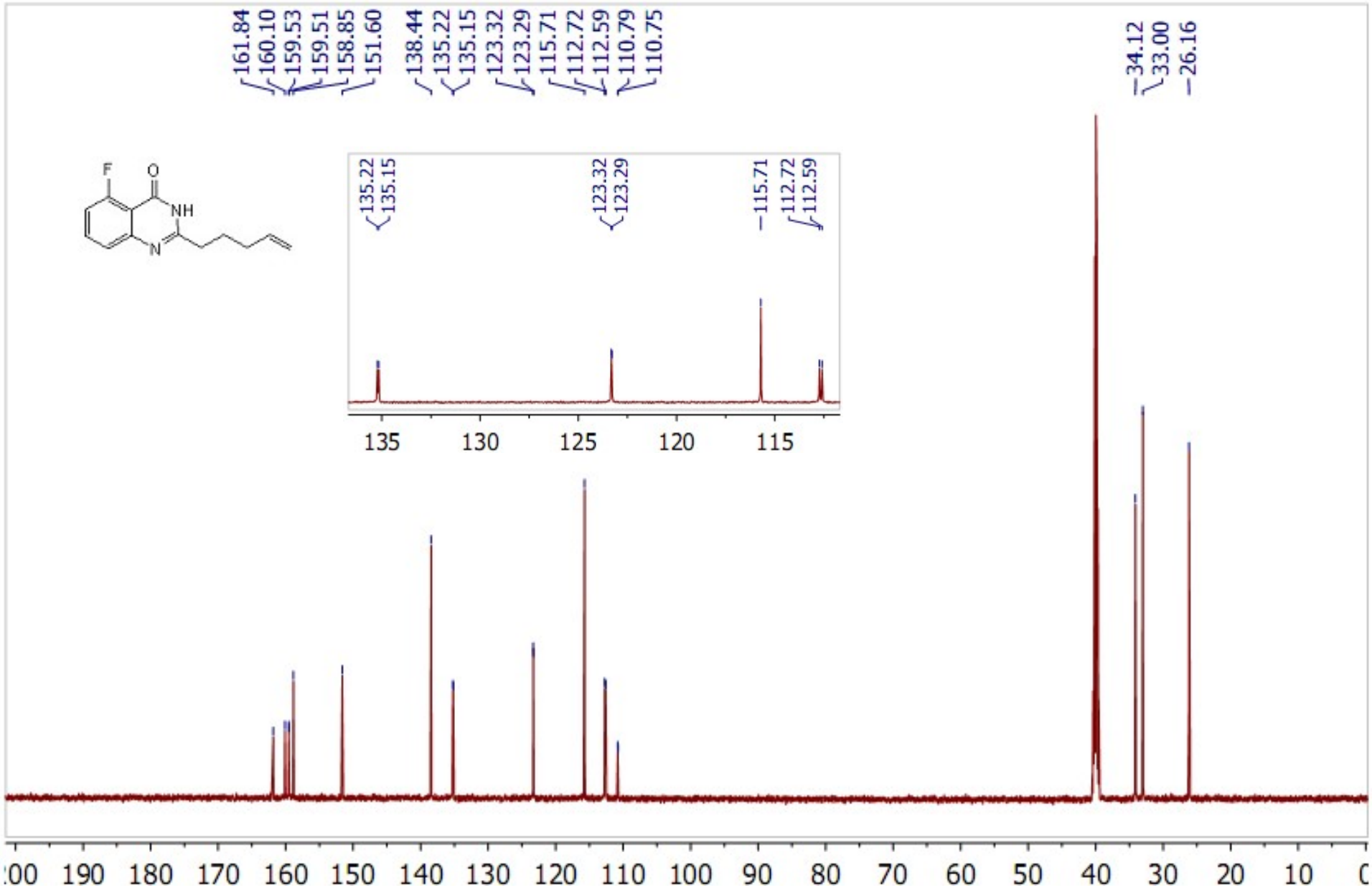
^{13}C NMR spectrum (126 MHz, DMSO-d6) of compound 2a



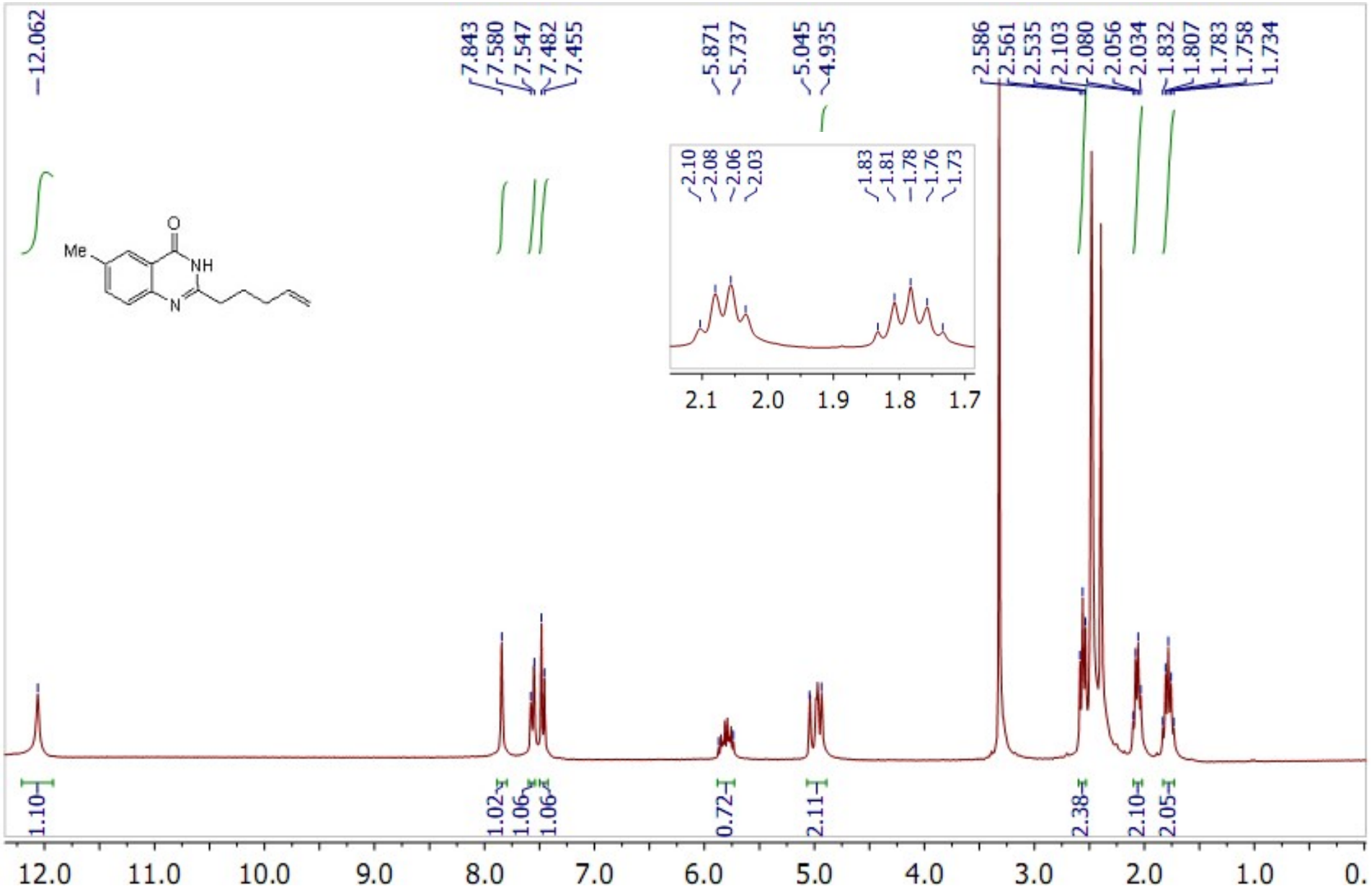
^{1}H NMR spectrum (400 MHz, DMSO-d6) of compound 2b



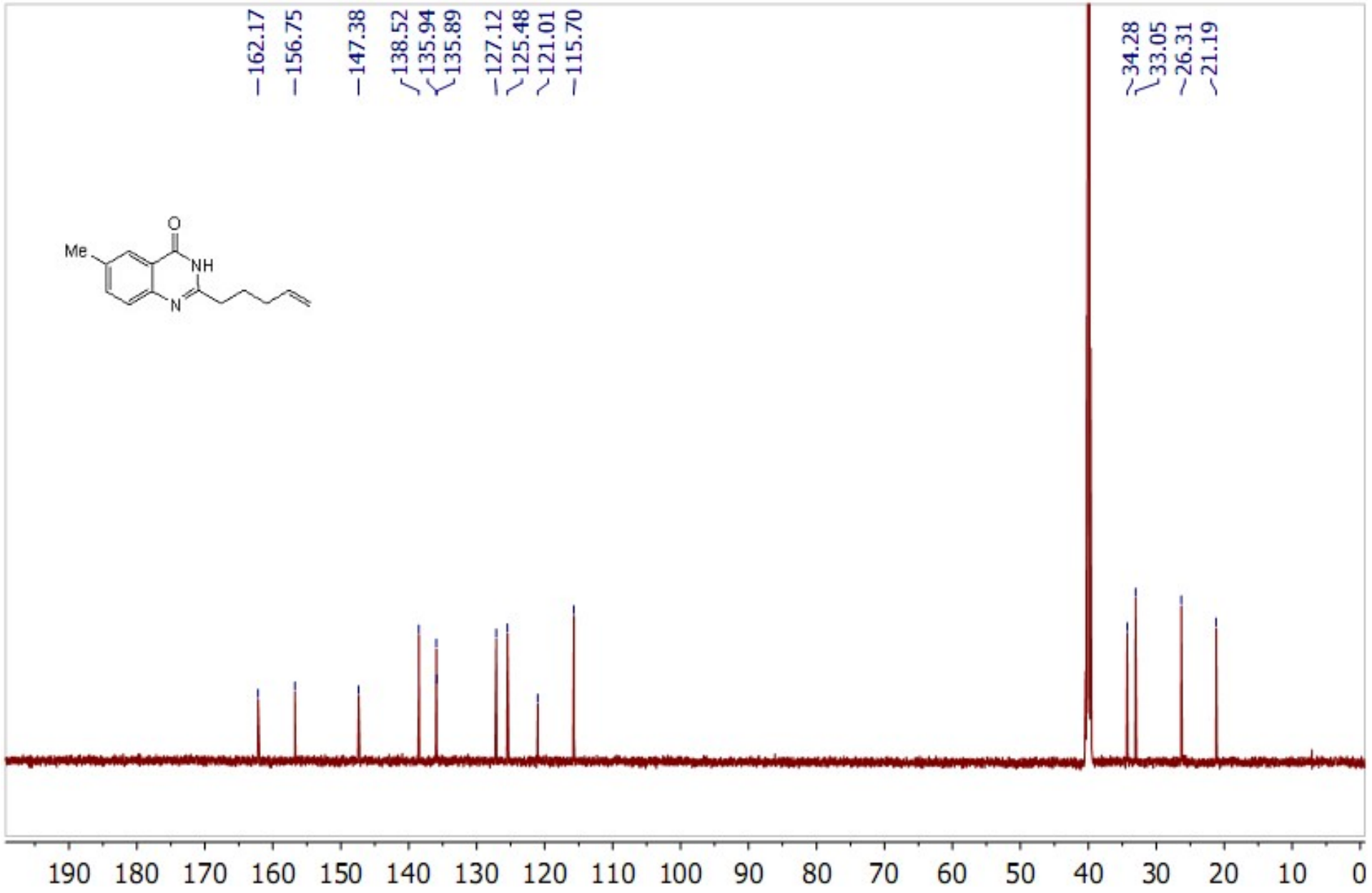
^{13}C NMR spectrum (151 MHz, DMSO-d6) of compound 2b



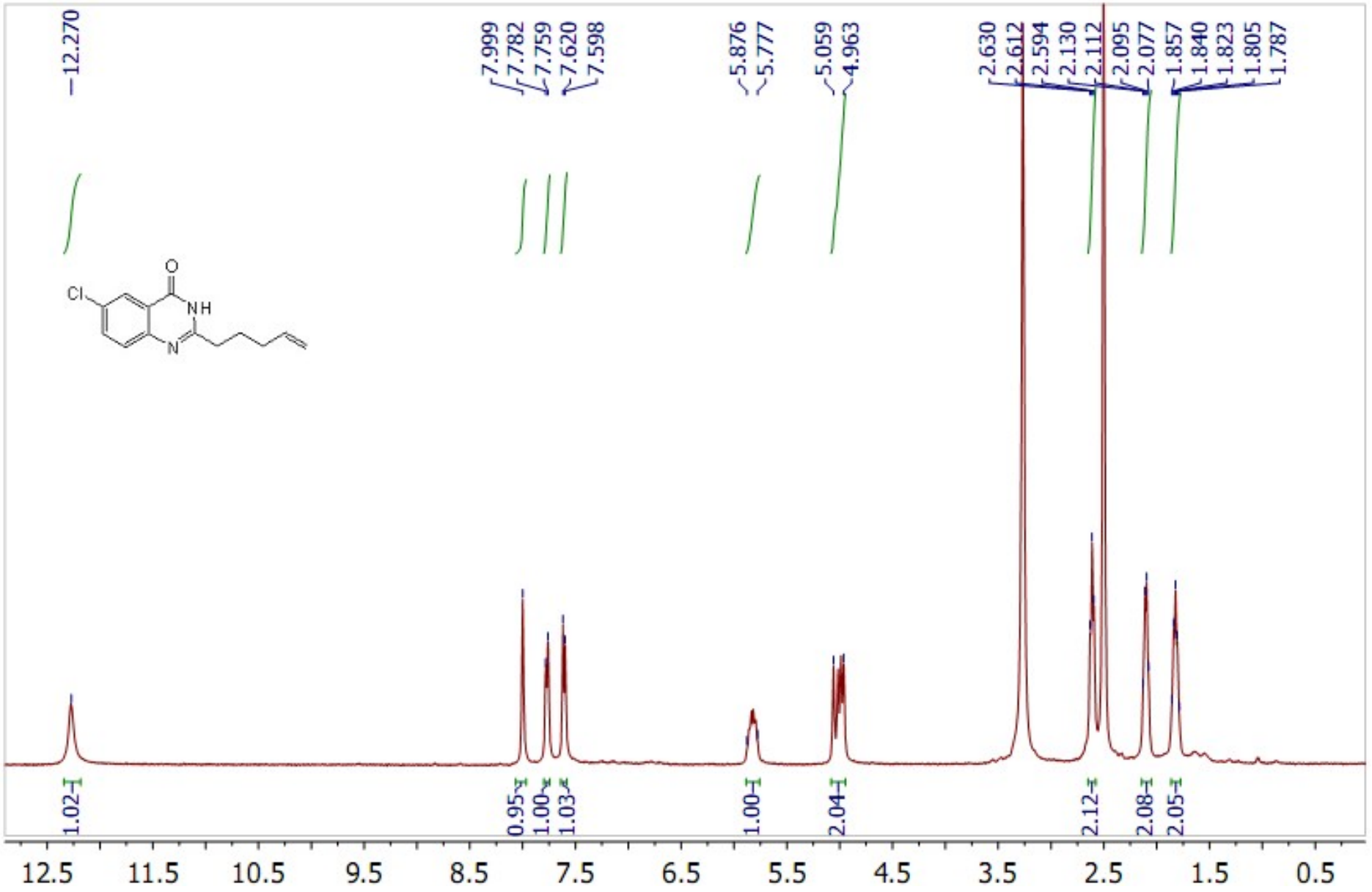
^{1}H NMR spectrum (300 MHz, DMSO-d6) of compound 2c



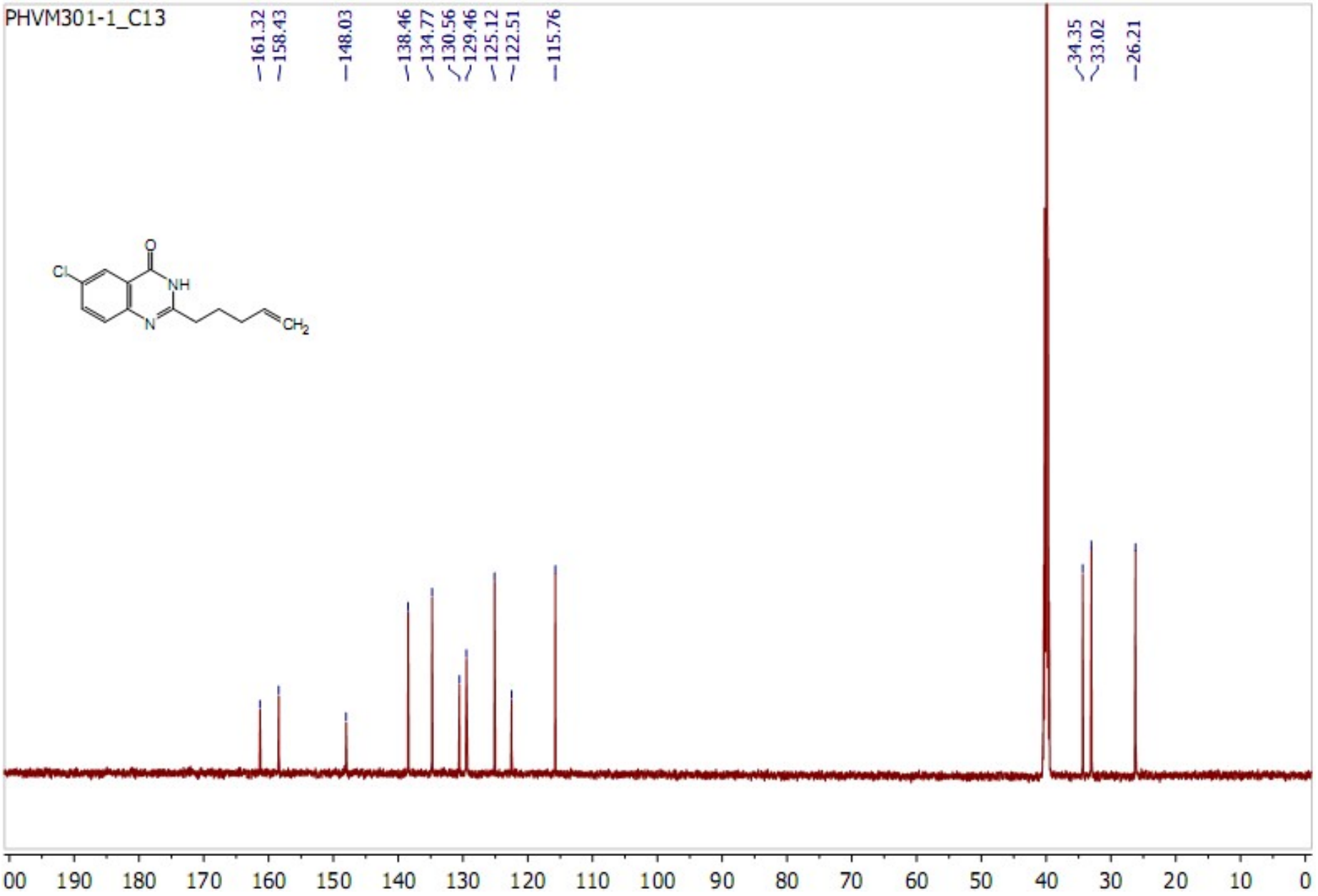
^{13}C NMR spectrum (151 MHz, DMSO-d6) of compound 2c



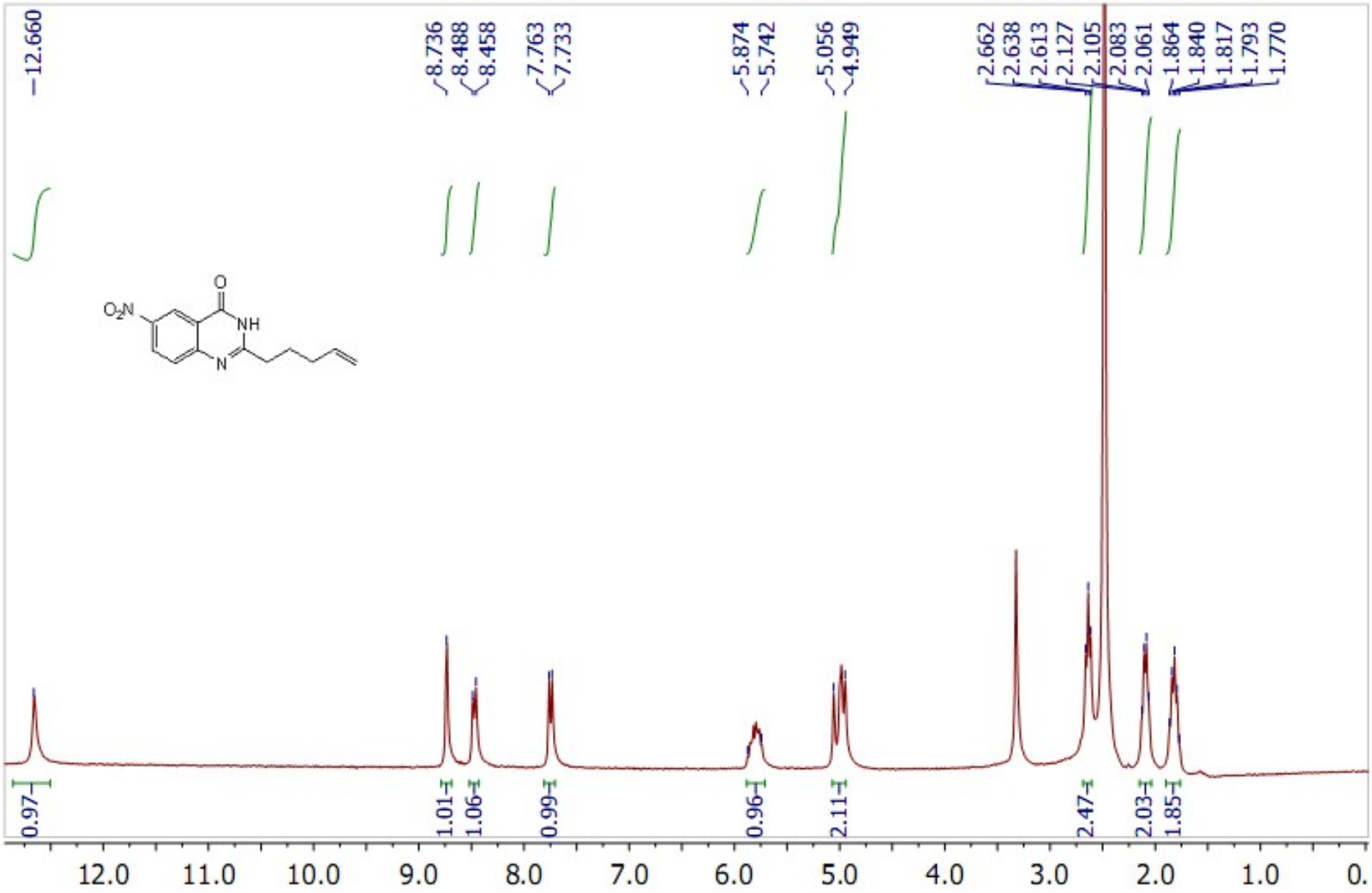
^{1}H NMR spectrum (400 MHz, DMSO-d6) of compound 2d



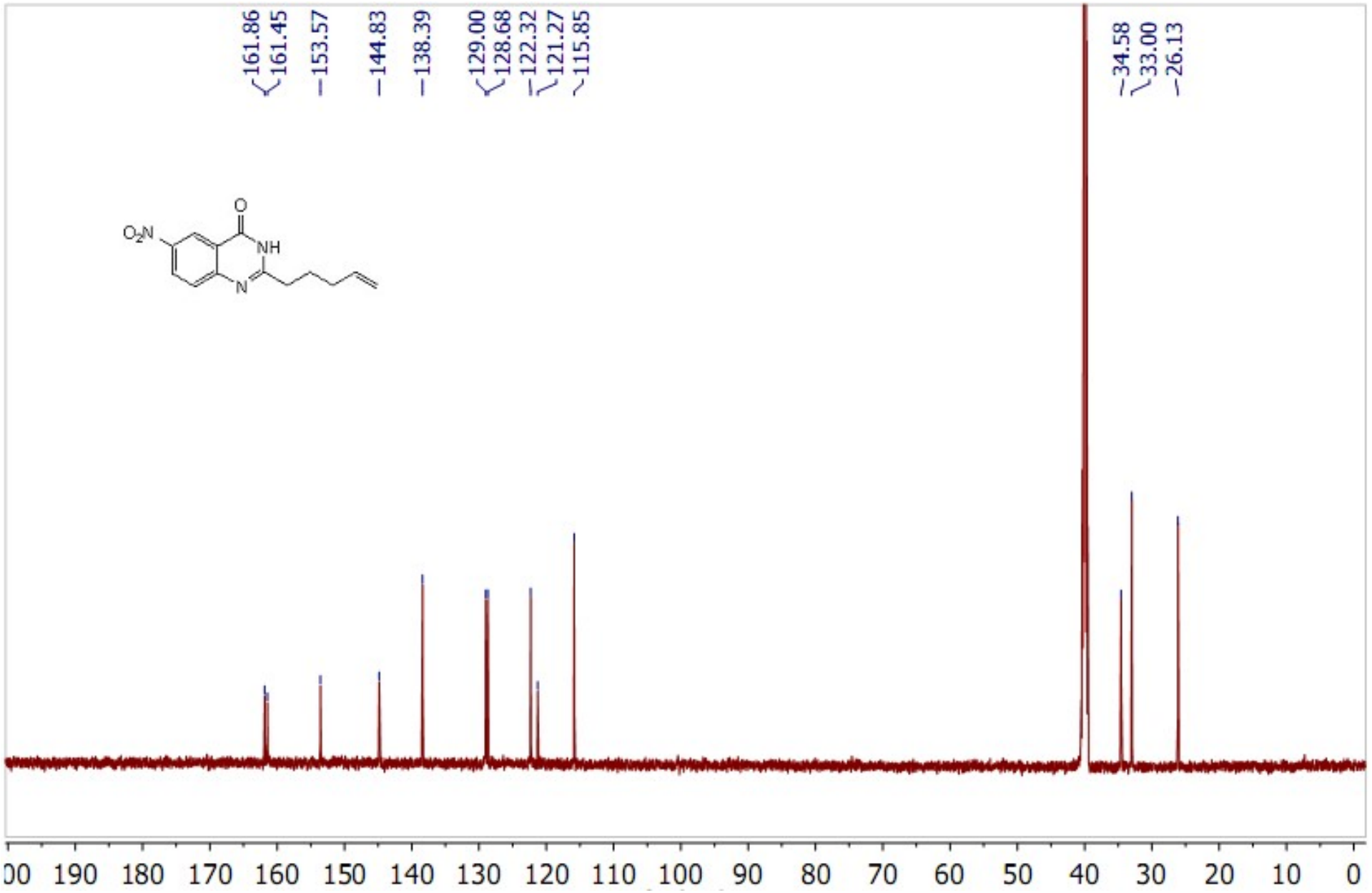
^{13}C NMR spectrum (151 MHz, DMSO-d6) of compound 2d



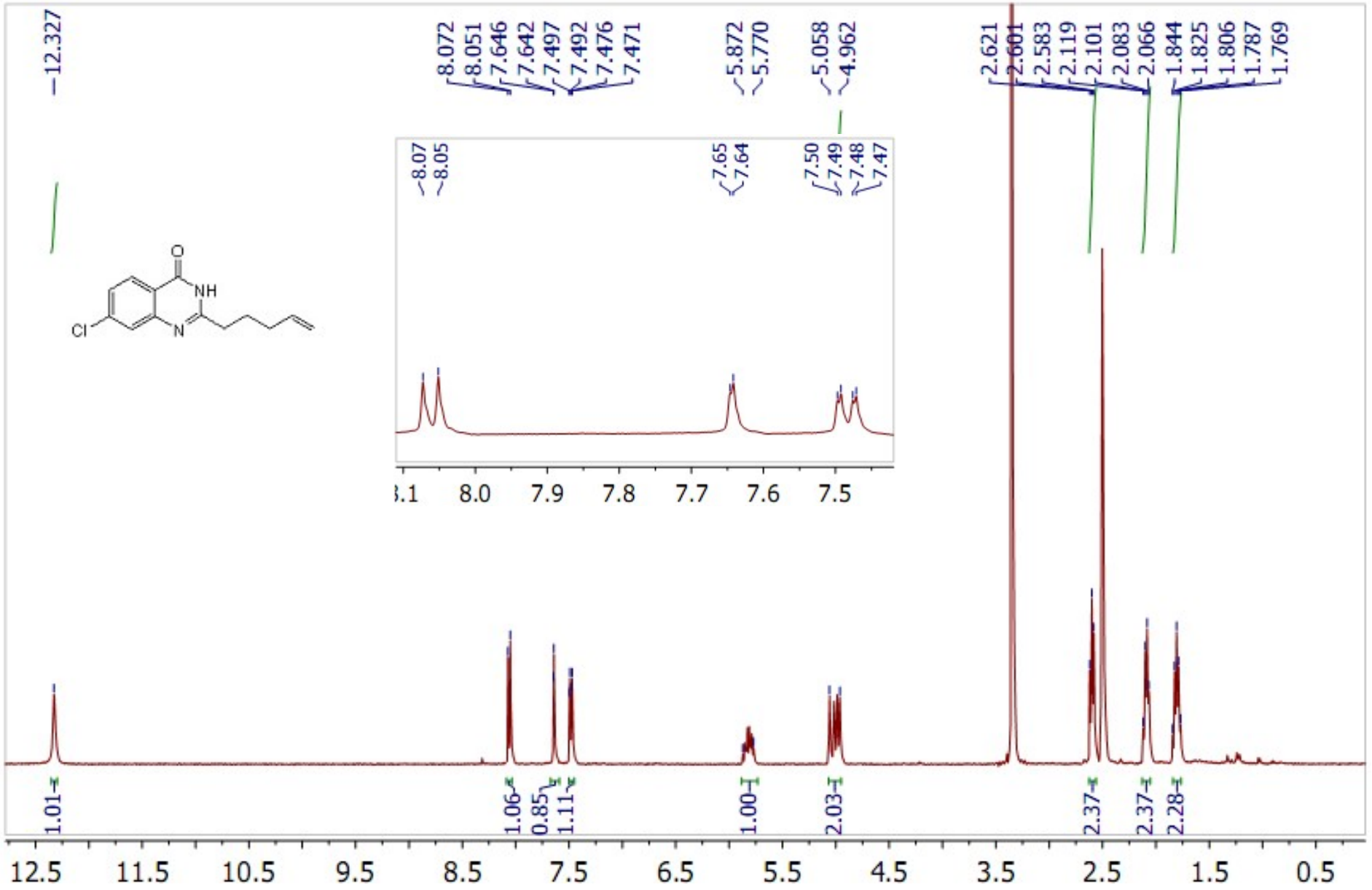
^{1}H NMR spectrum (300 MHz, DMSO-d6) of compound 2e



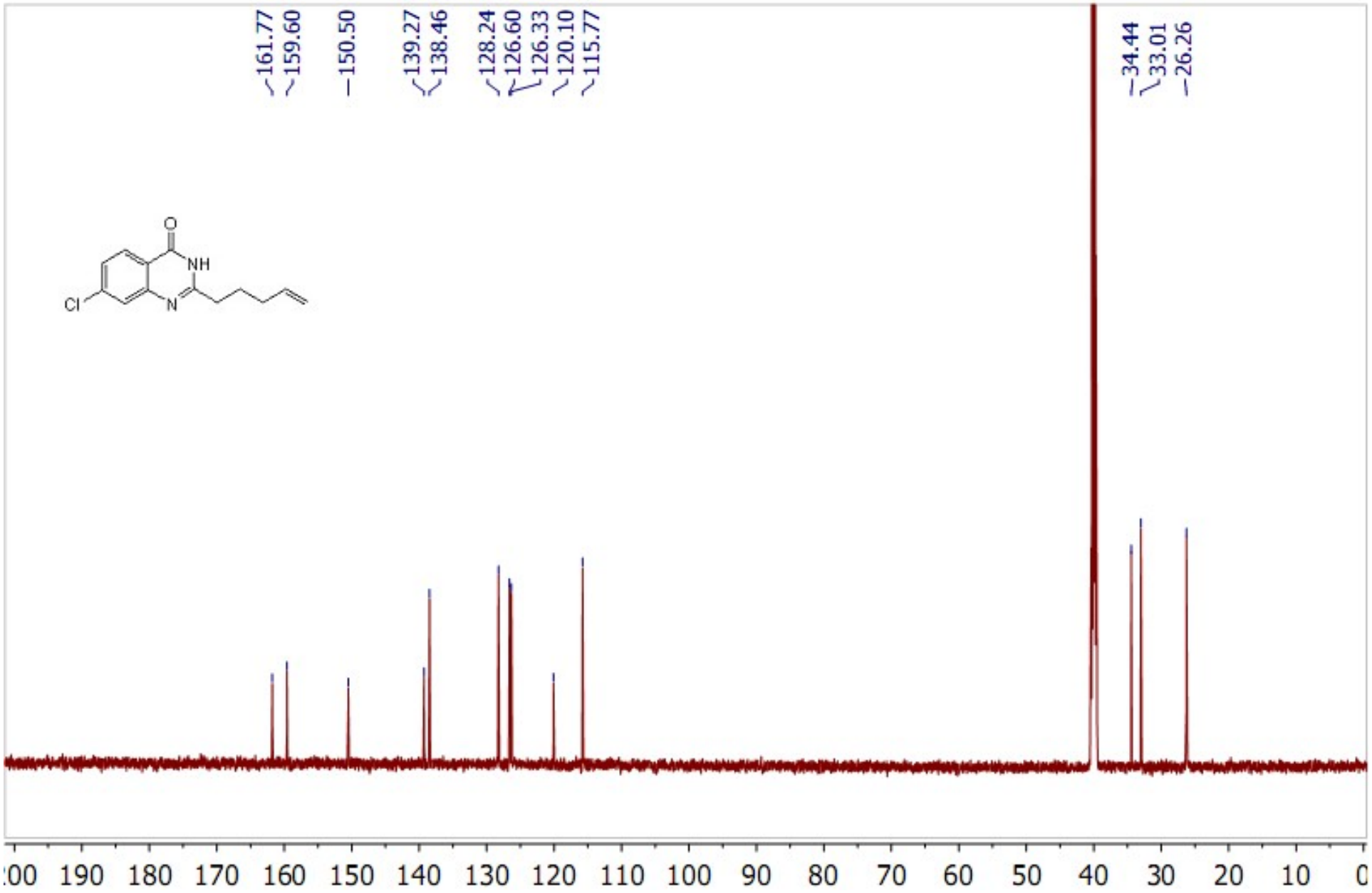
^{13}C NMR spectrum (151 MHz, DMSO-d6) of compound 2e



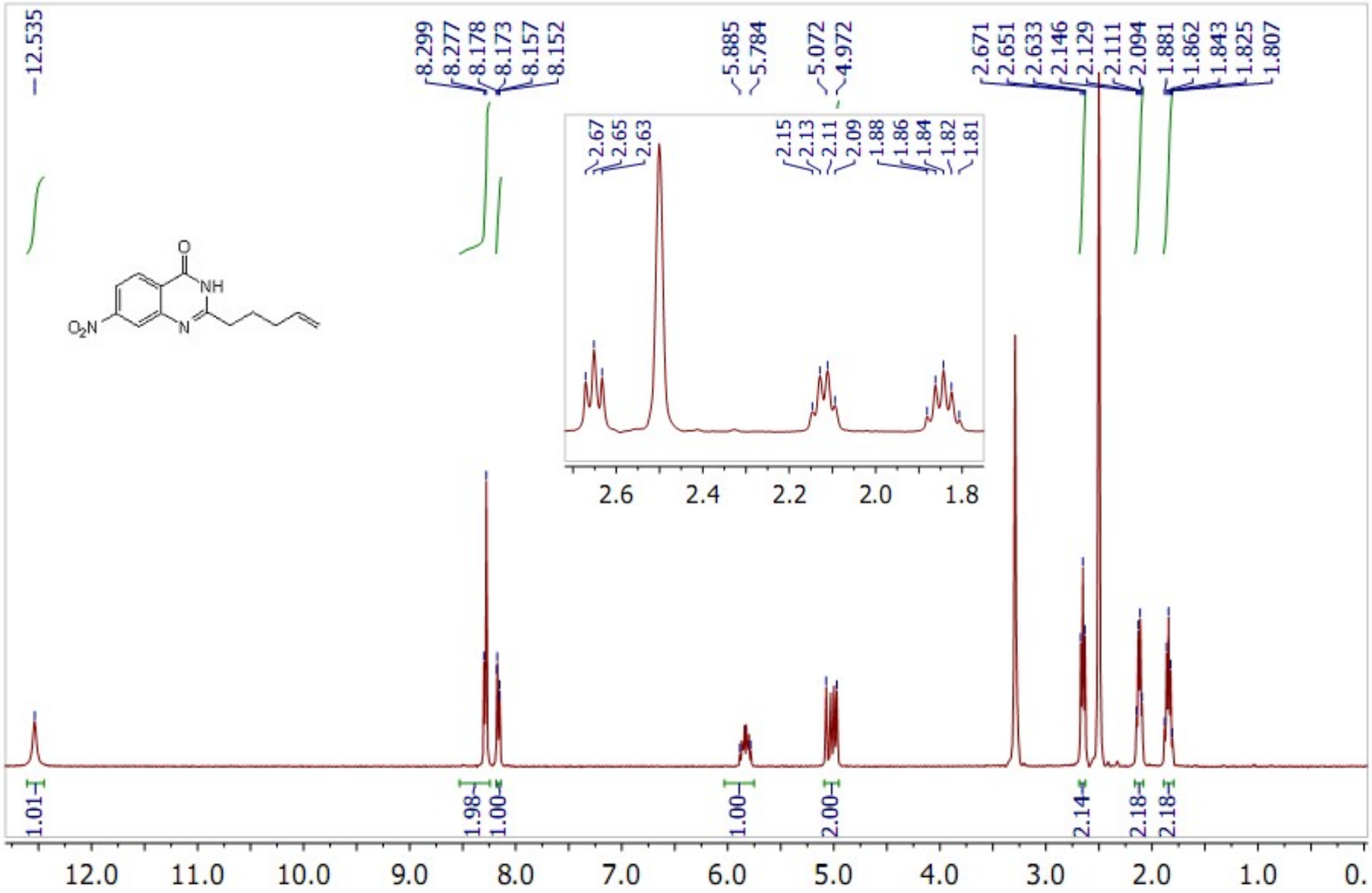
^{1}H NMR spectrum (400 MHz, DMSO-d6) of compound 2f



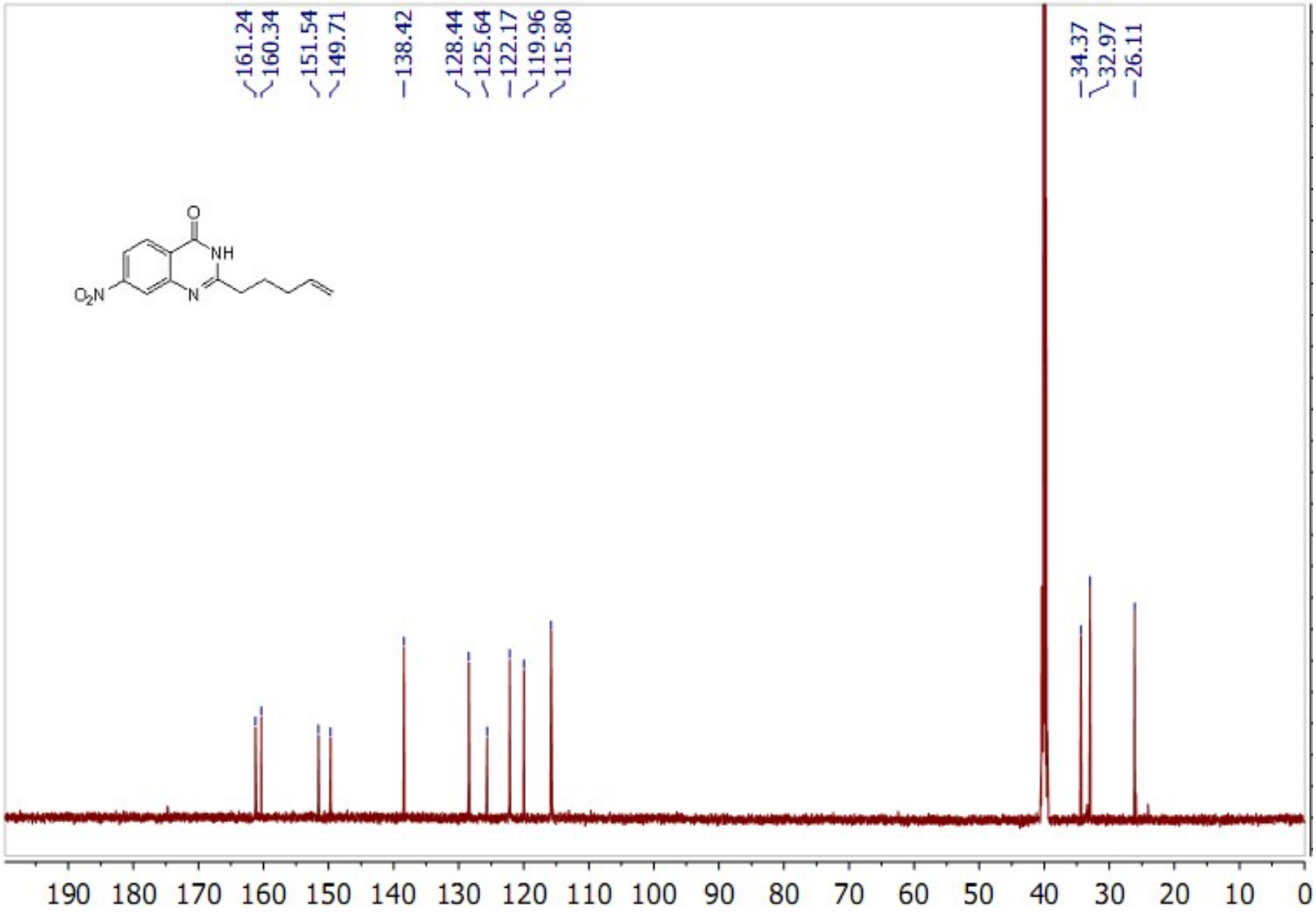
^{13}C NMR spectrum (151 MHz, DMSO-d6) of compound 2f



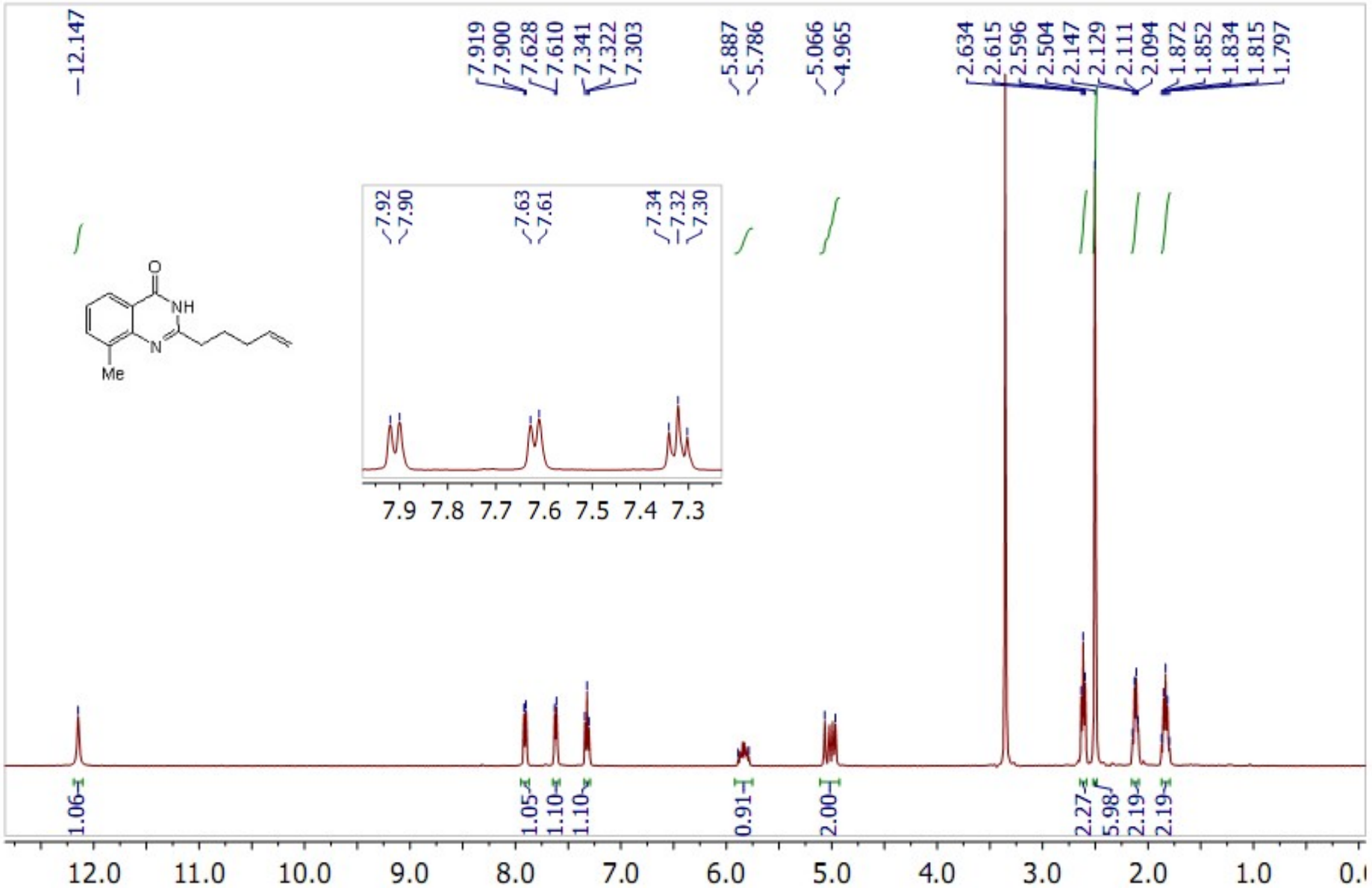
^{1}H NMR spectrum (400 MHz, DMSO-d6) of compound 2g



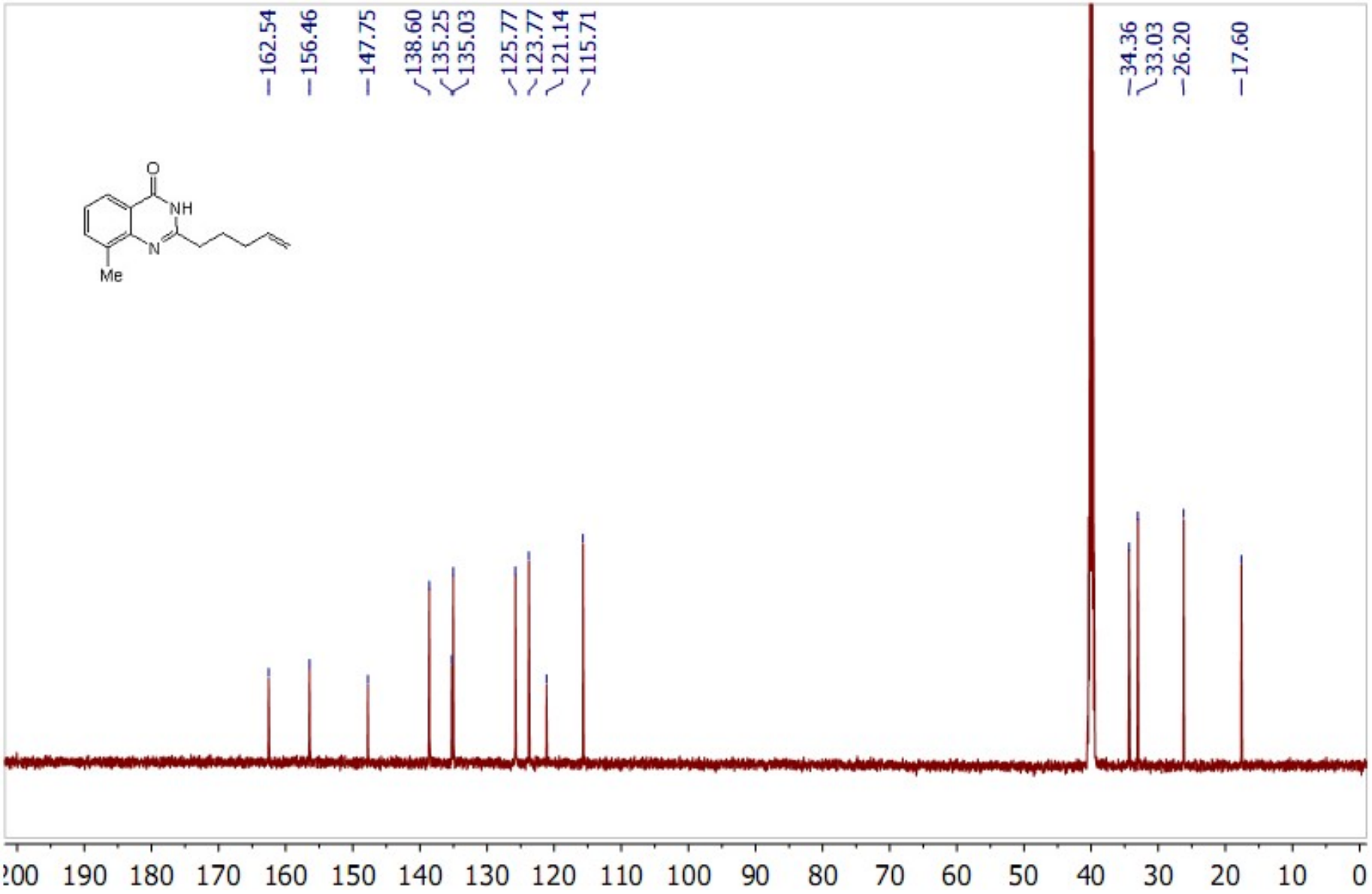
^{13}C NMR spectrum (151 MHz, DMSO-d6) of compound 2g



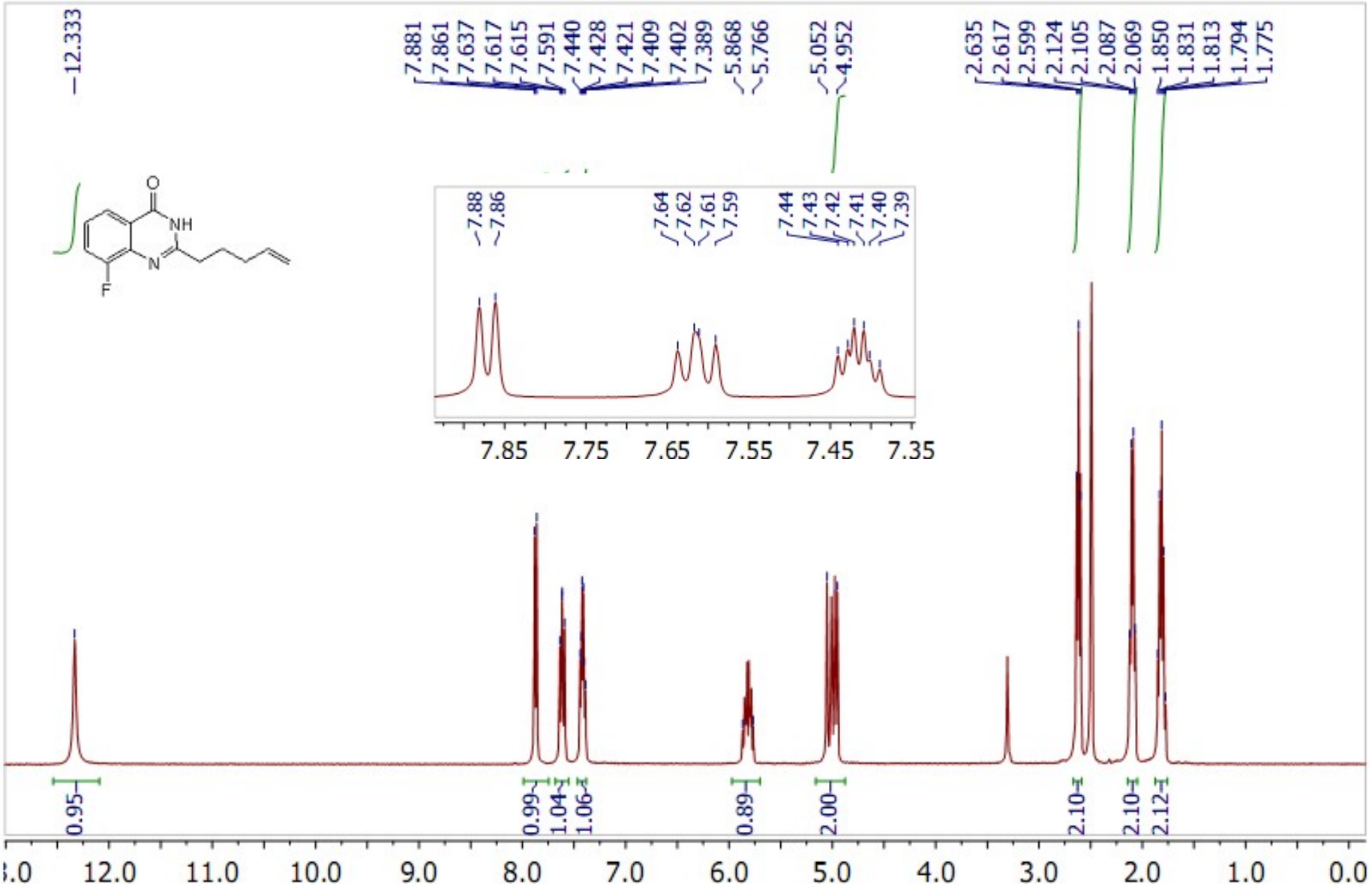
^{1}H NMR spectrum (400 MHz, DMSO-d6) of compound 2h



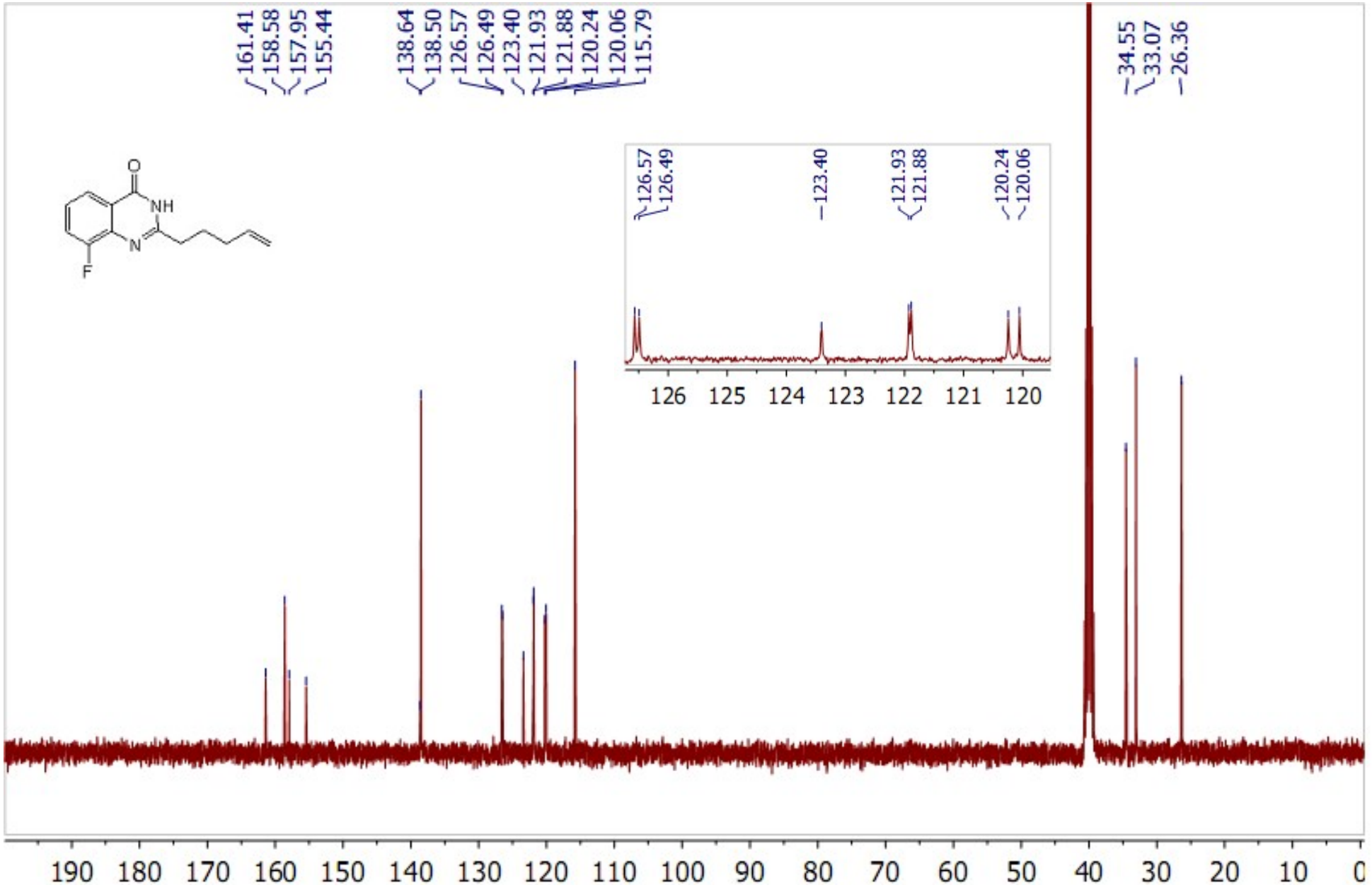
^{13}C NMR spectrum (151 MHz, DMSO-d6) of compound 2h



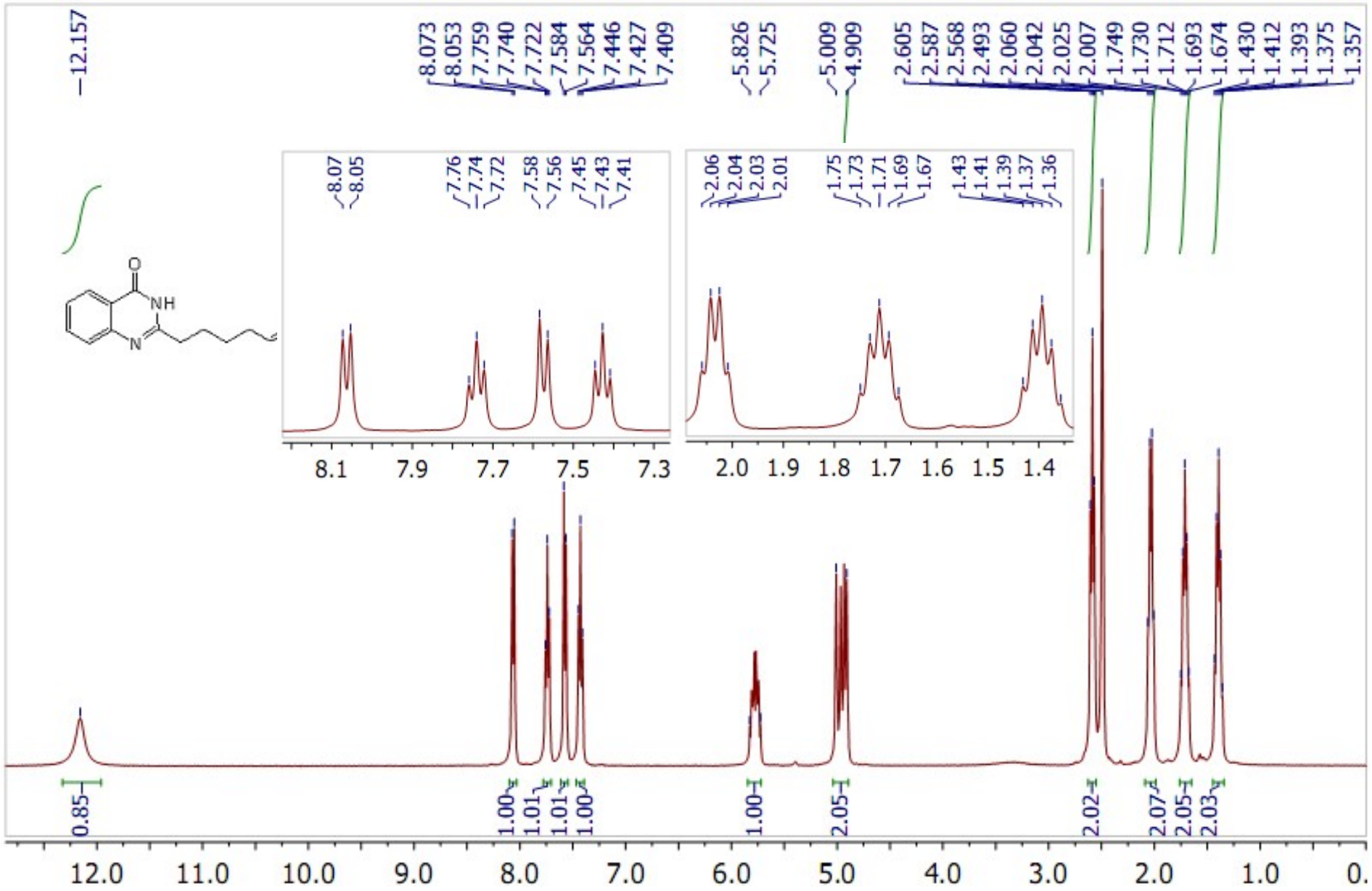
^{1}H NMR spectrum (400 MHz, DMSO-d6) of compound 2i



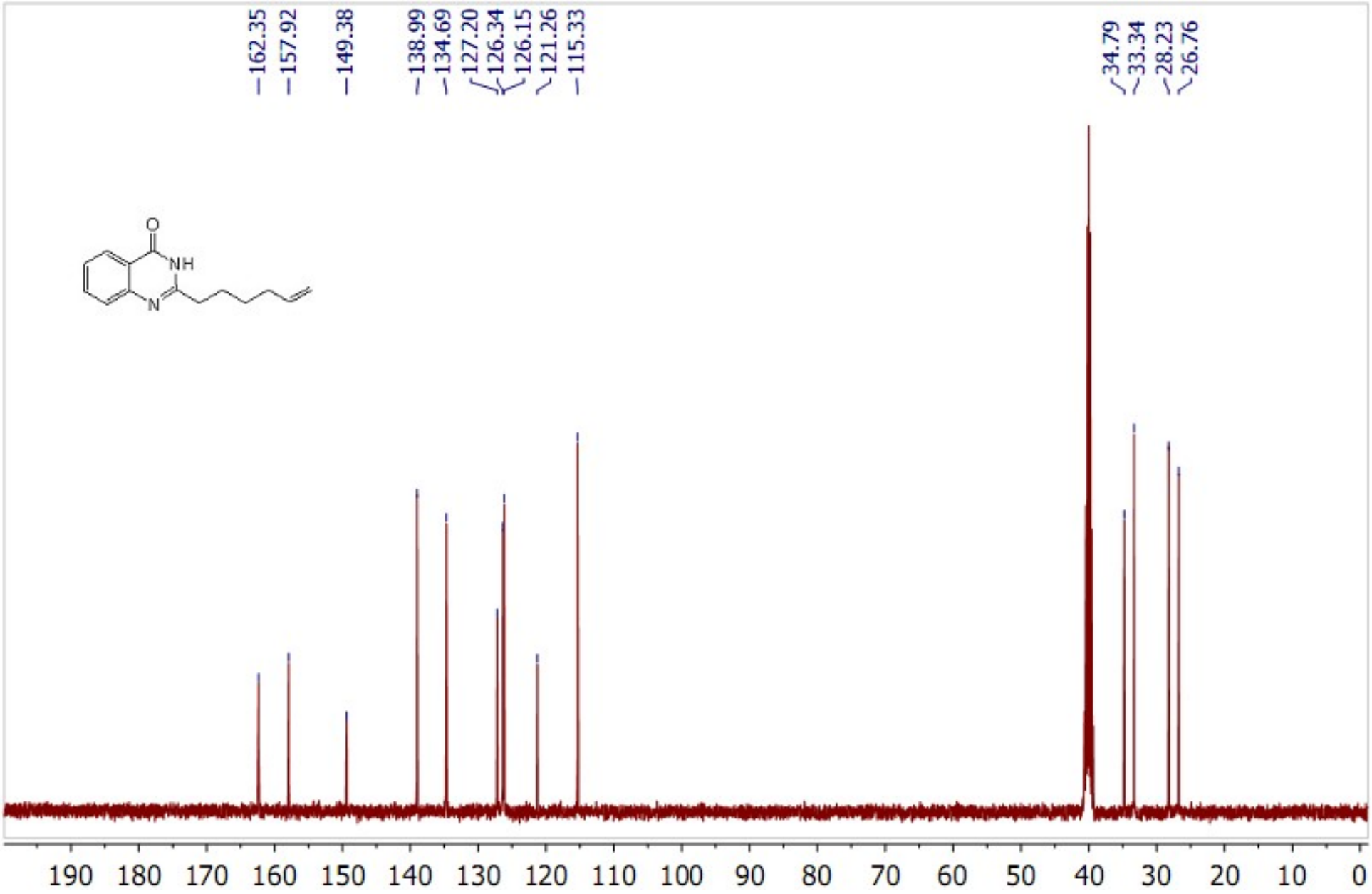
^{13}C NMR spectrum (101 MHz, DMSO-d6) of compound 2i



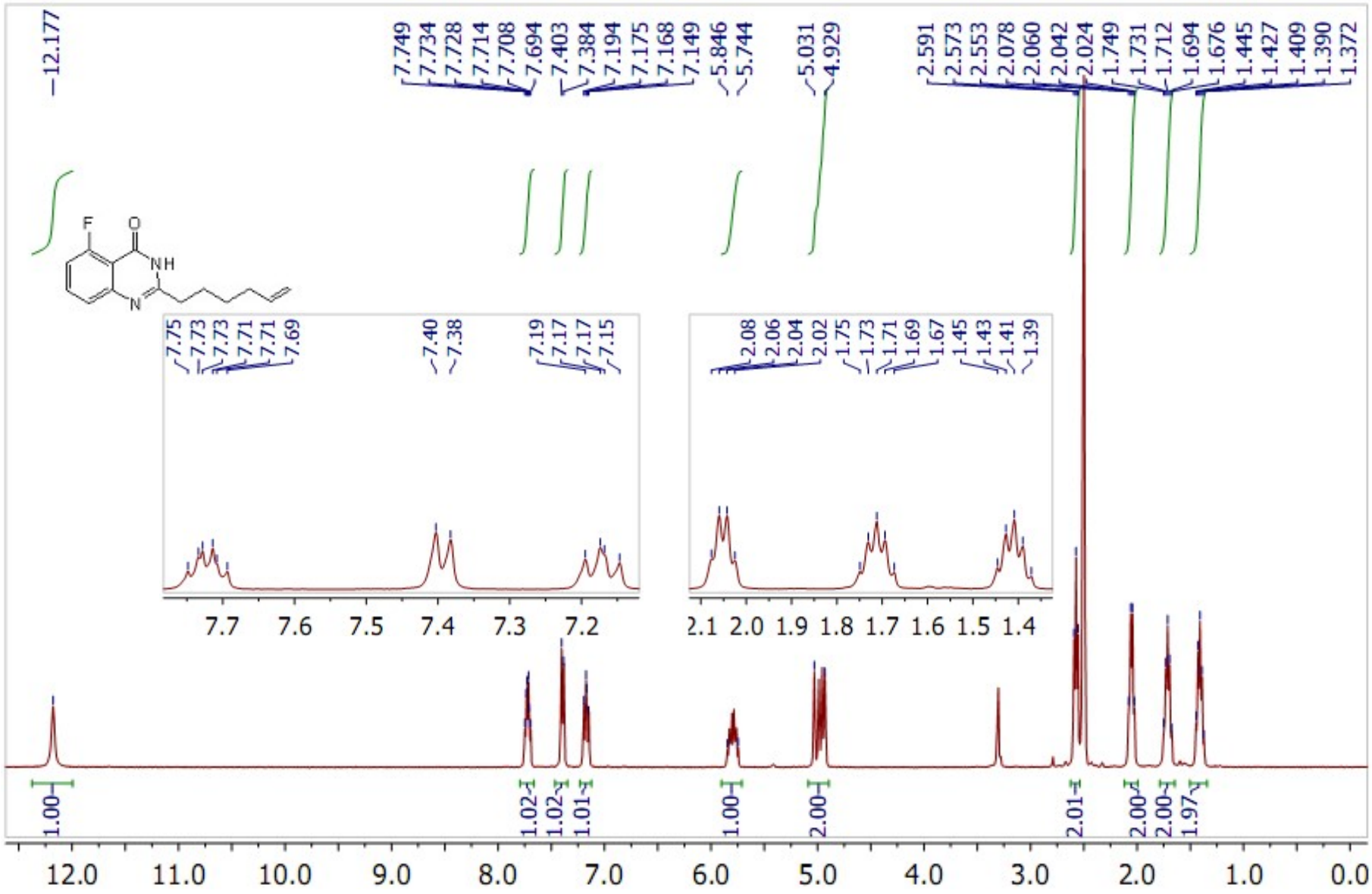
^{1}H NMR spectrum (400 MHz, DMSO-d6) of compound 3a



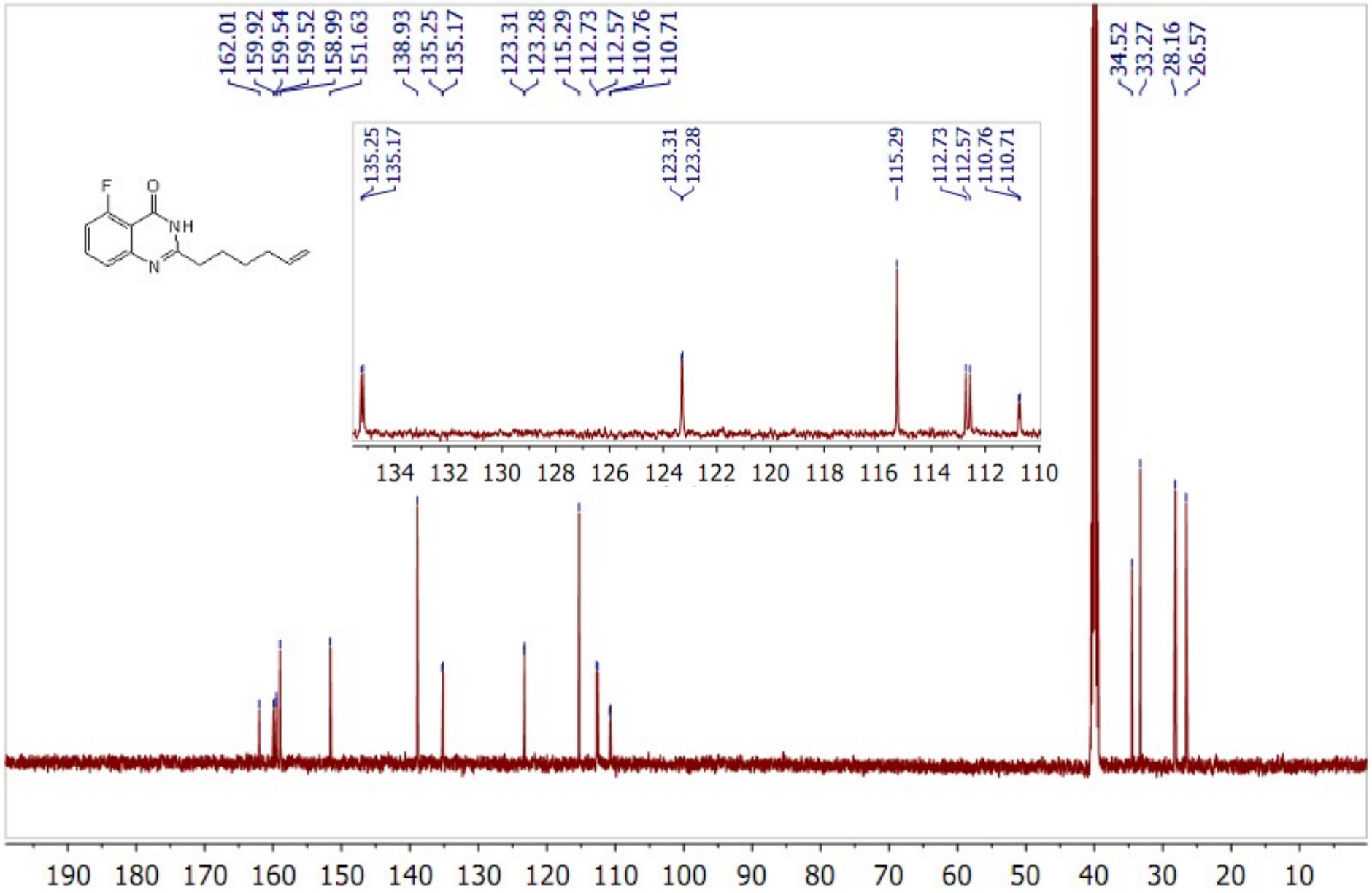
^{13}C NMR spectrum (101 MHz, DMSO-d6) of compound 3a



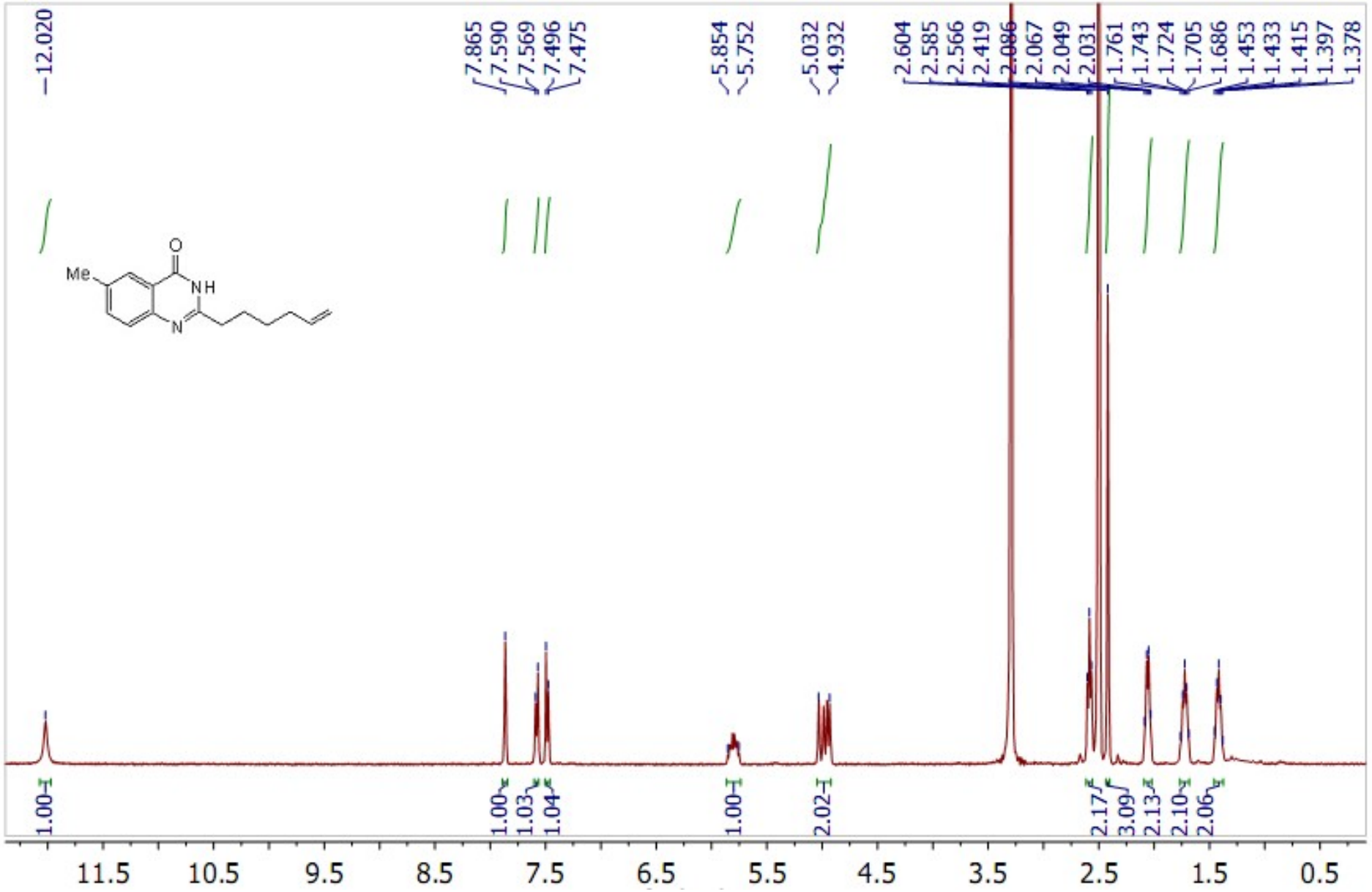
^{1}H NMR spectrum (400 MHz, DMSO-d6) of compound 3b



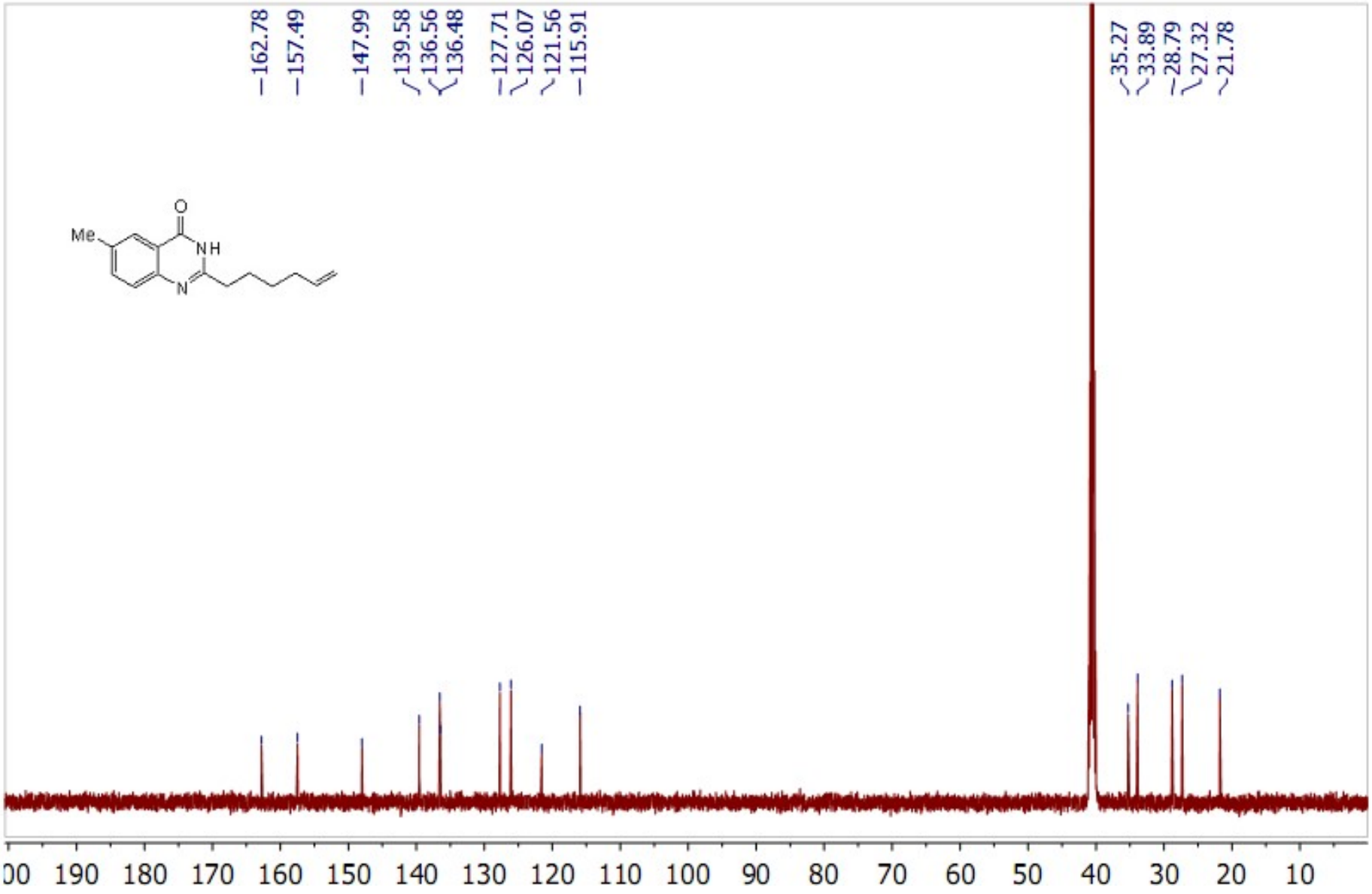
^{13}C NMR spectrum (126 MHz, DMSO-d6) of compound 3b



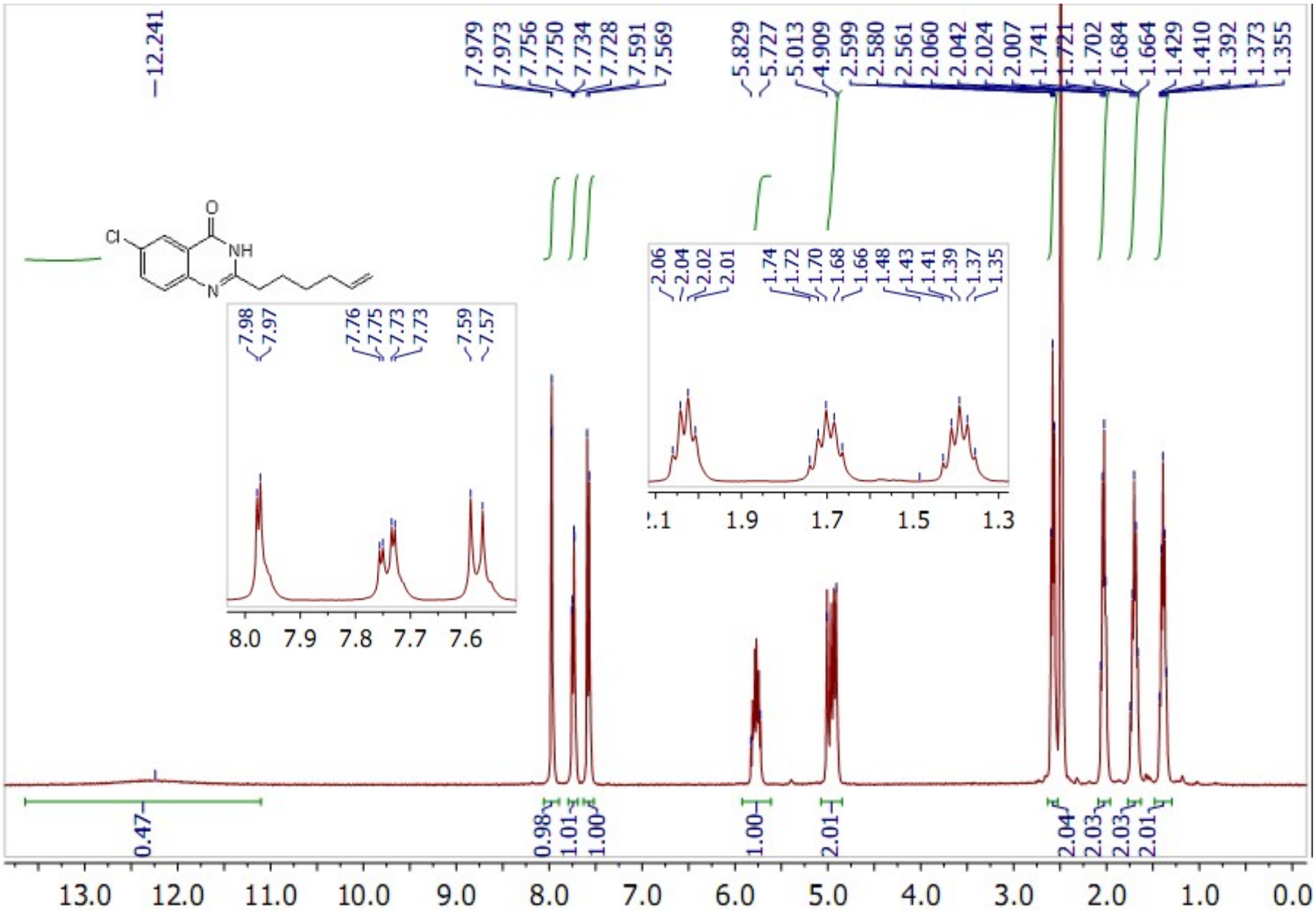
^{1}H NMR spectrum (400 MHz, DMSO-d6) of compound 3c



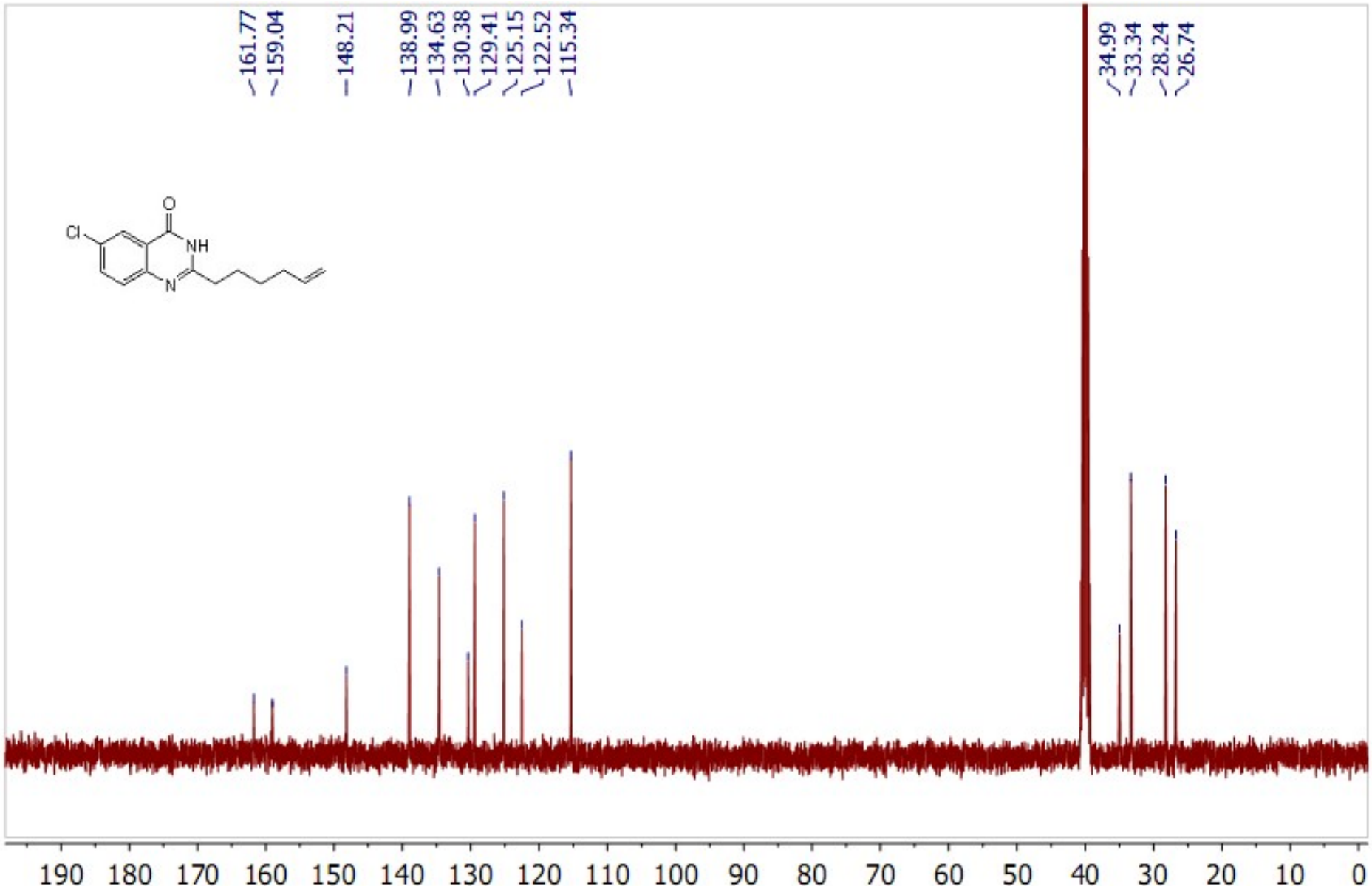
^{13}C NMR spectrum (126 MHz, DMSO-d6) of compound 3c



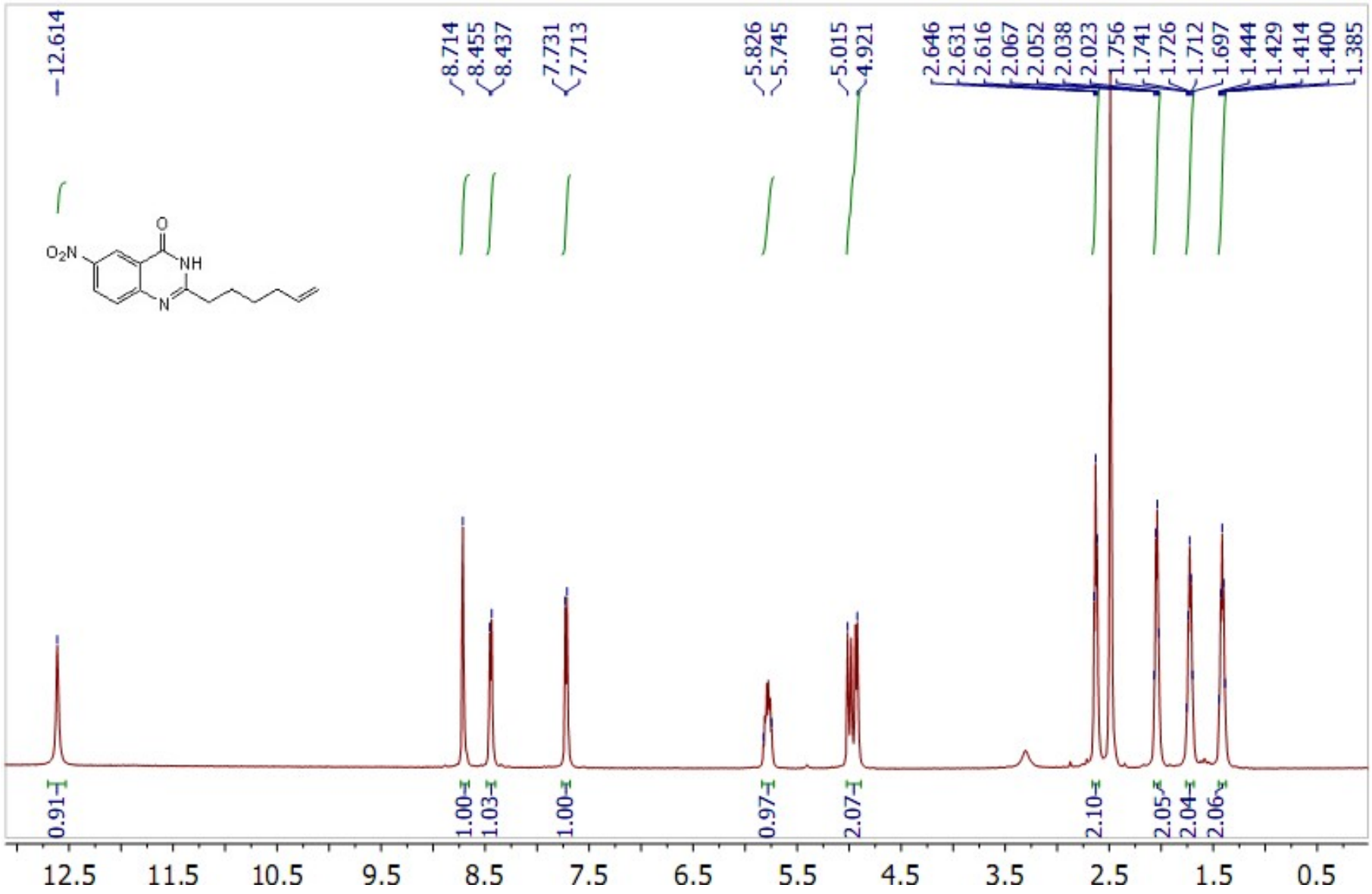
^{1}H NMR spectrum (400 MHz, DMSO-d6) of compound 3d



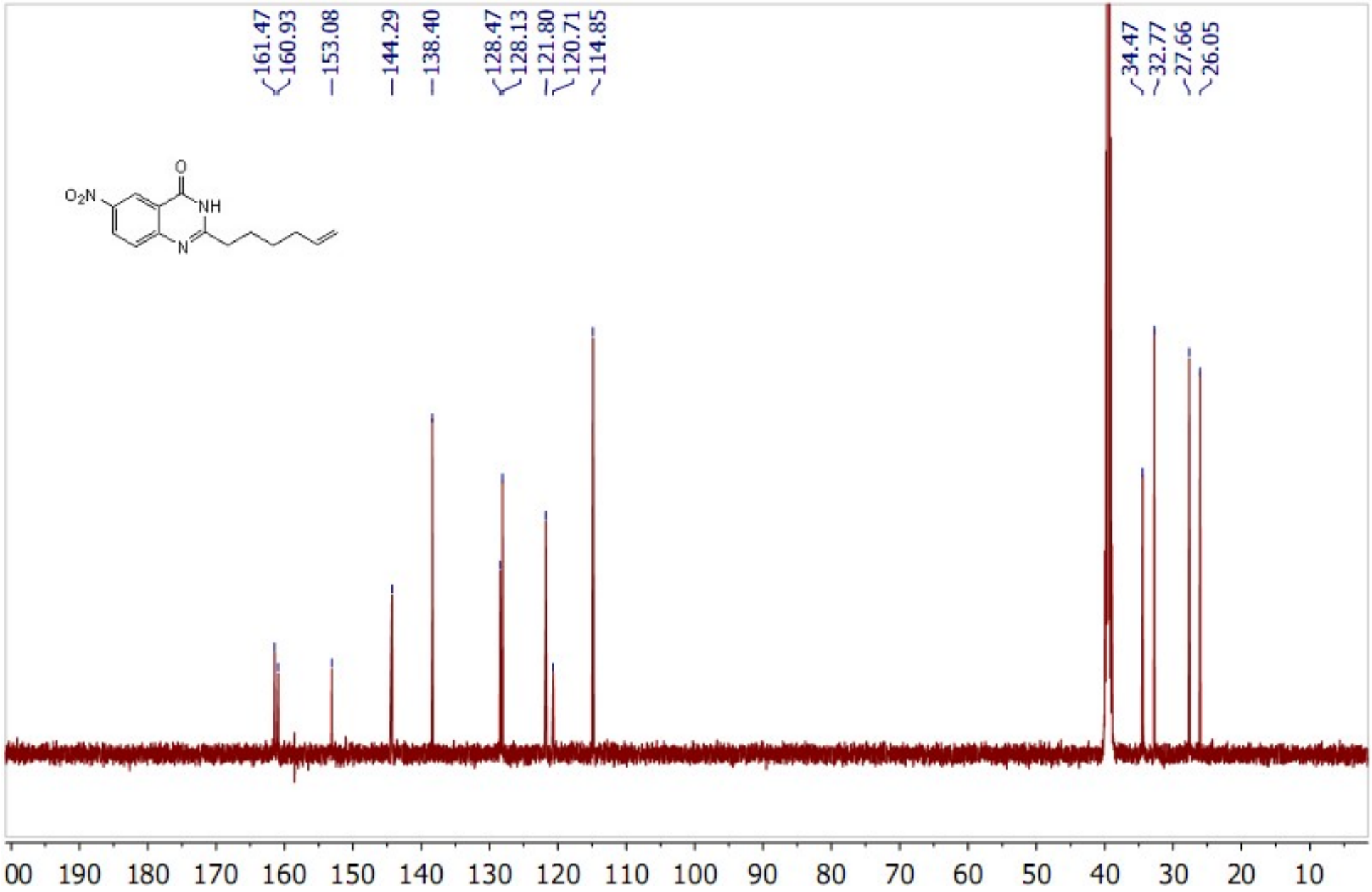
^{13}C NMR spectrum (101 MHz, DMSO-d6) of compound 3d



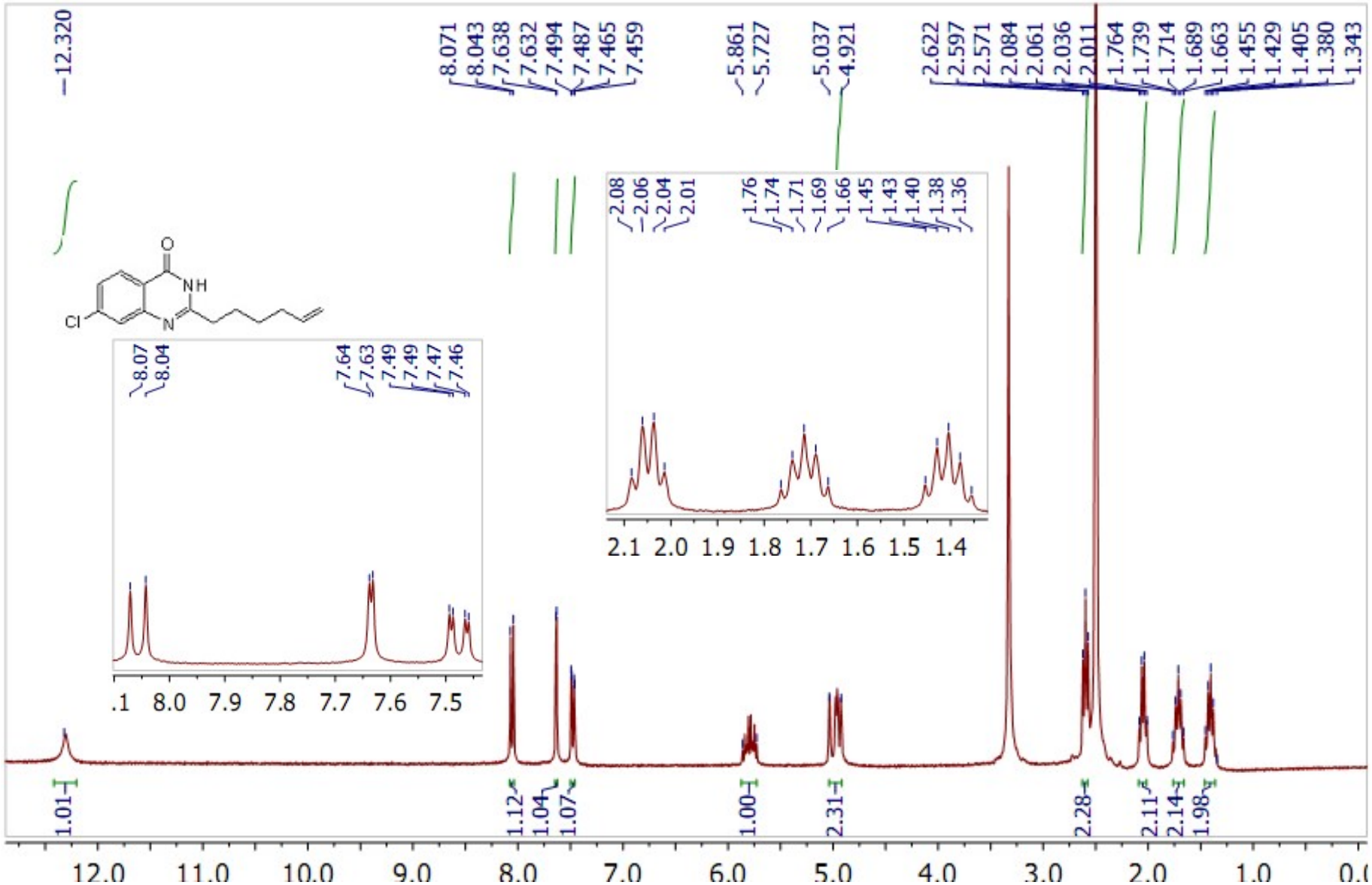
^{1}H NMR spectrum (500 MHz, DMSO-d6) of compound 3e



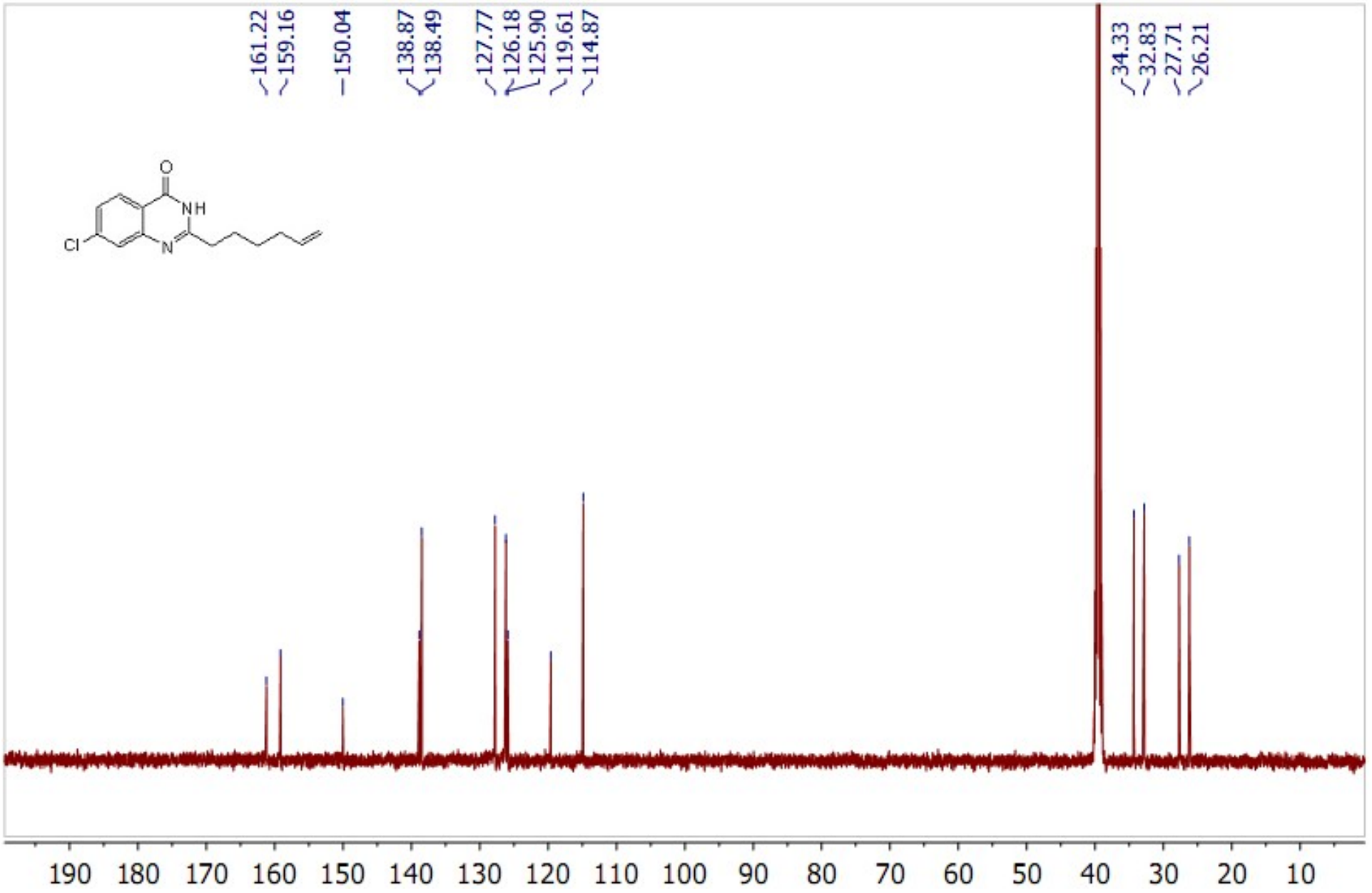
^{13}C NMR spectrum (126 MHz, DMSO-d6) of compound 3e



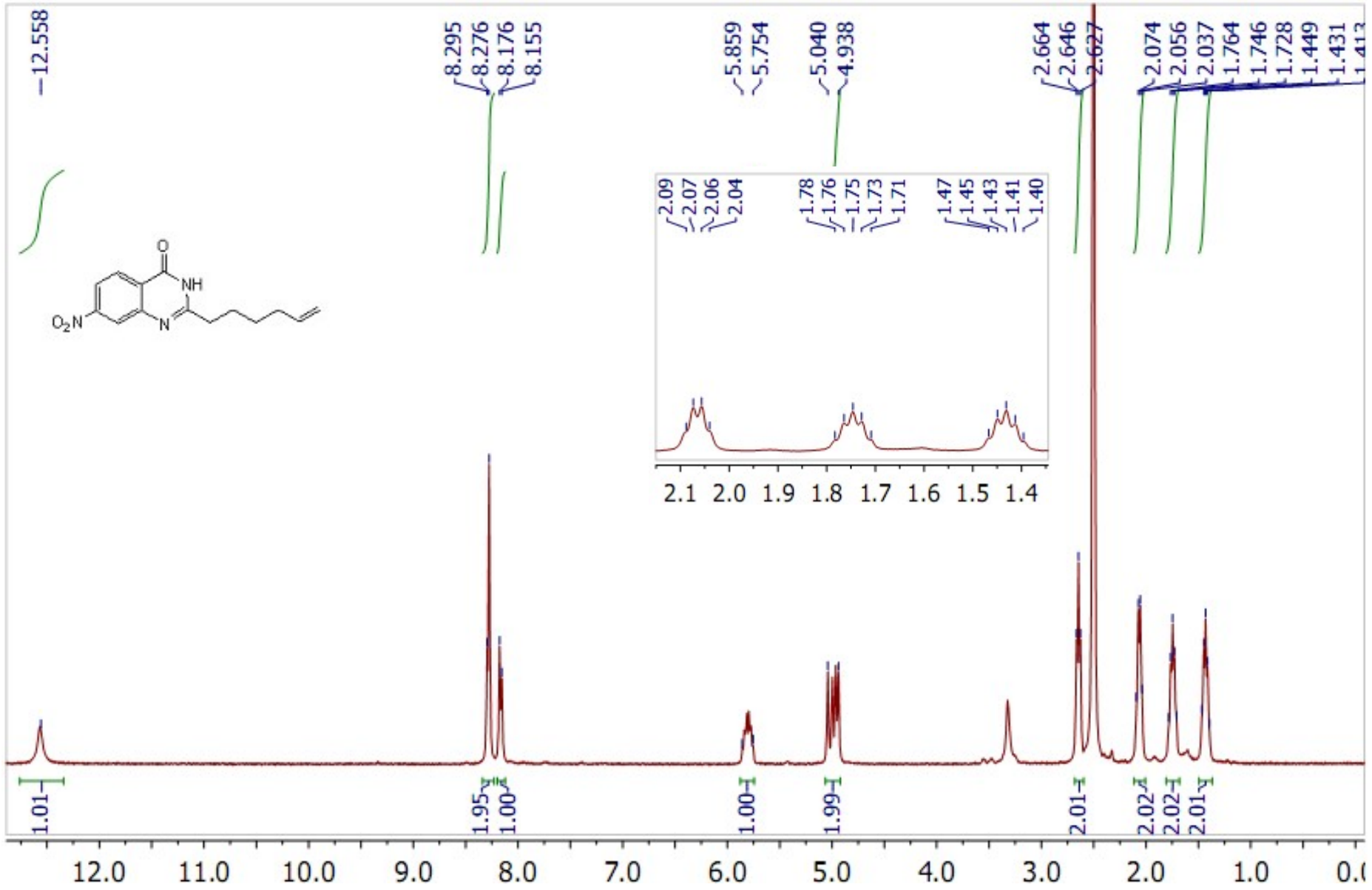
^{1}H NMR spectrum (300 MHz, DMSO-d6) of compound 3f



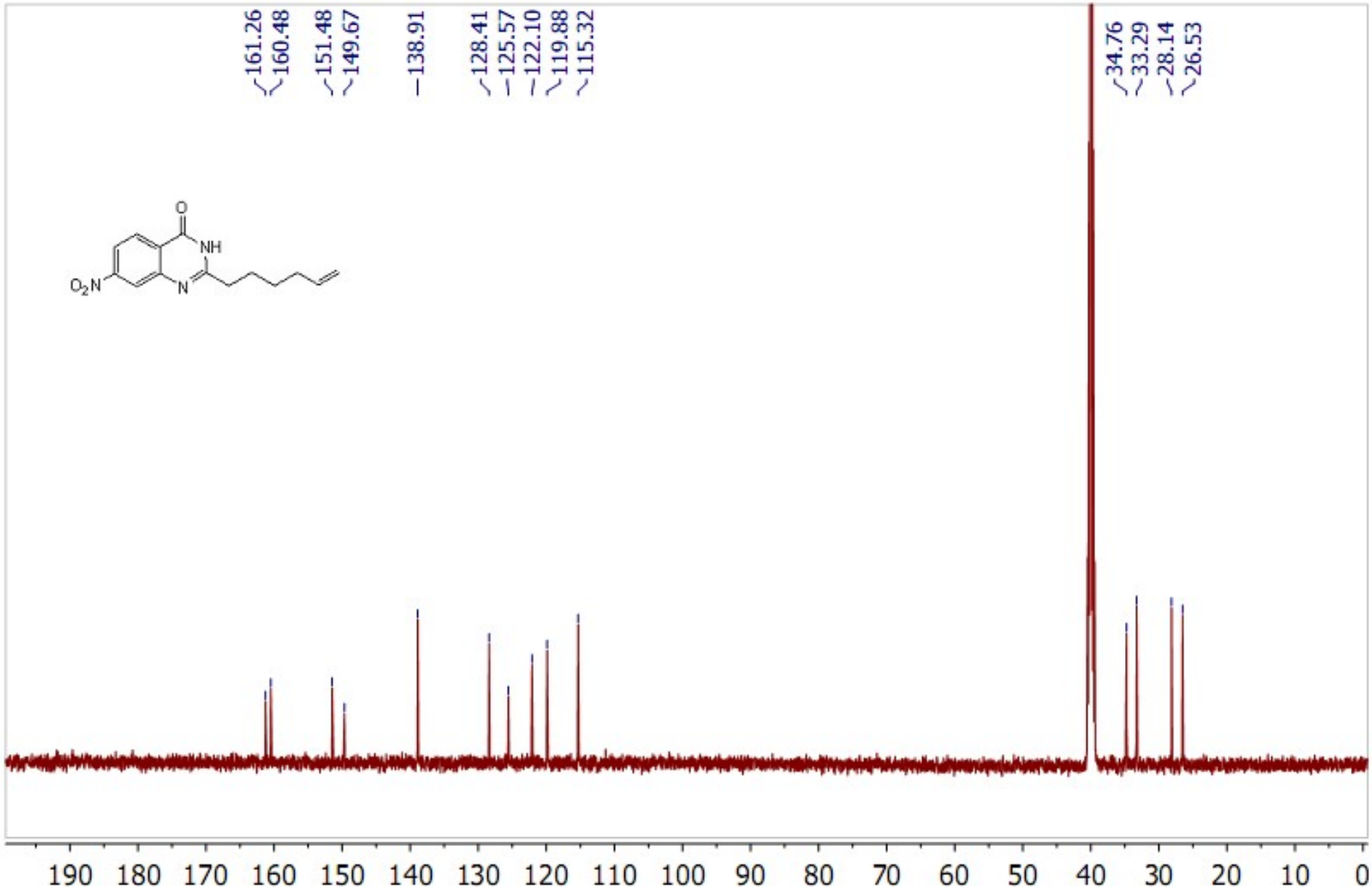
^{13}C NMR spectrum (126 MHz, DMSO-d6) of compound 3f



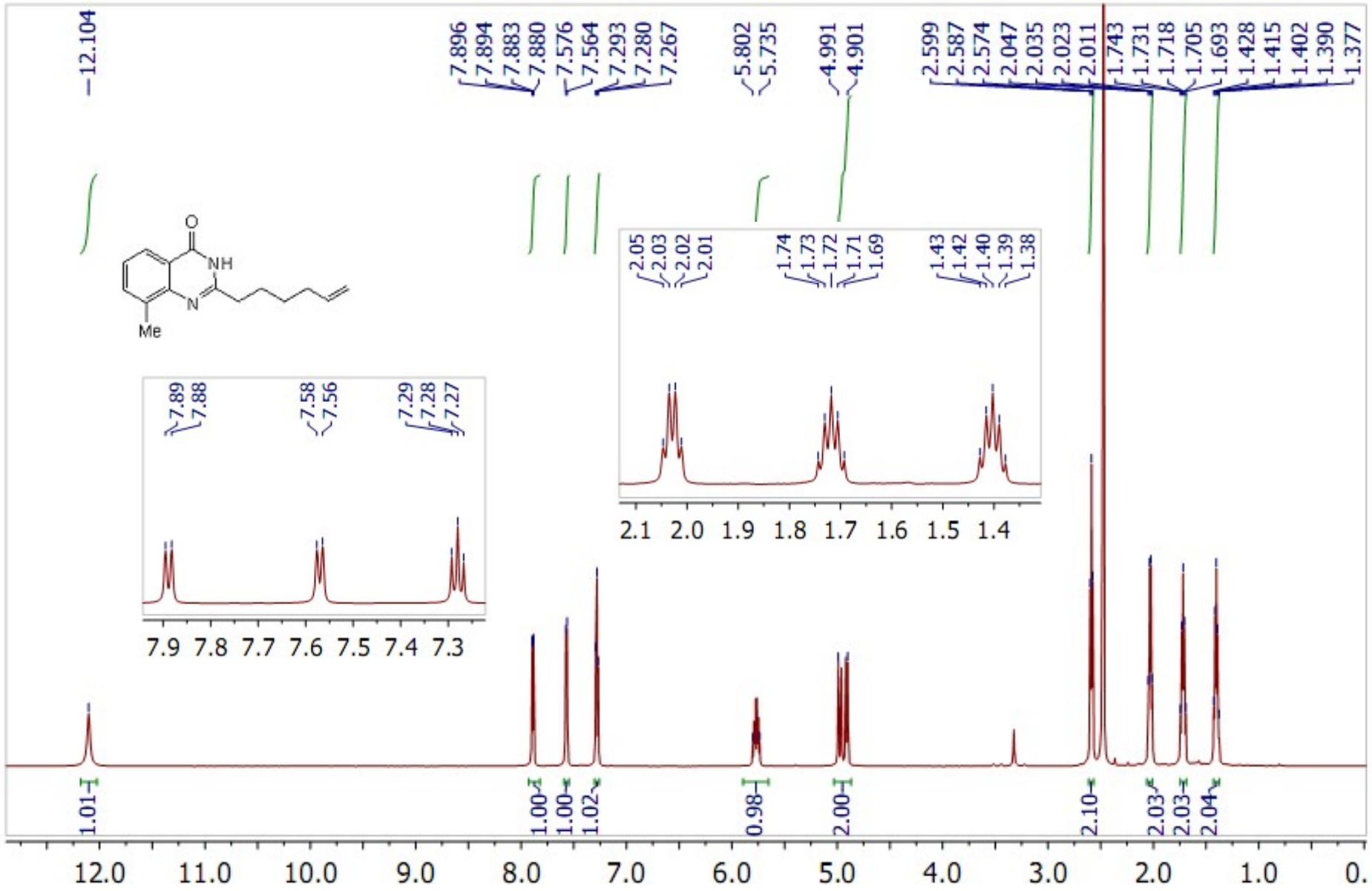
^{1}H NMR spectrum (400 MHz, DMSO-d6) of compound 3g



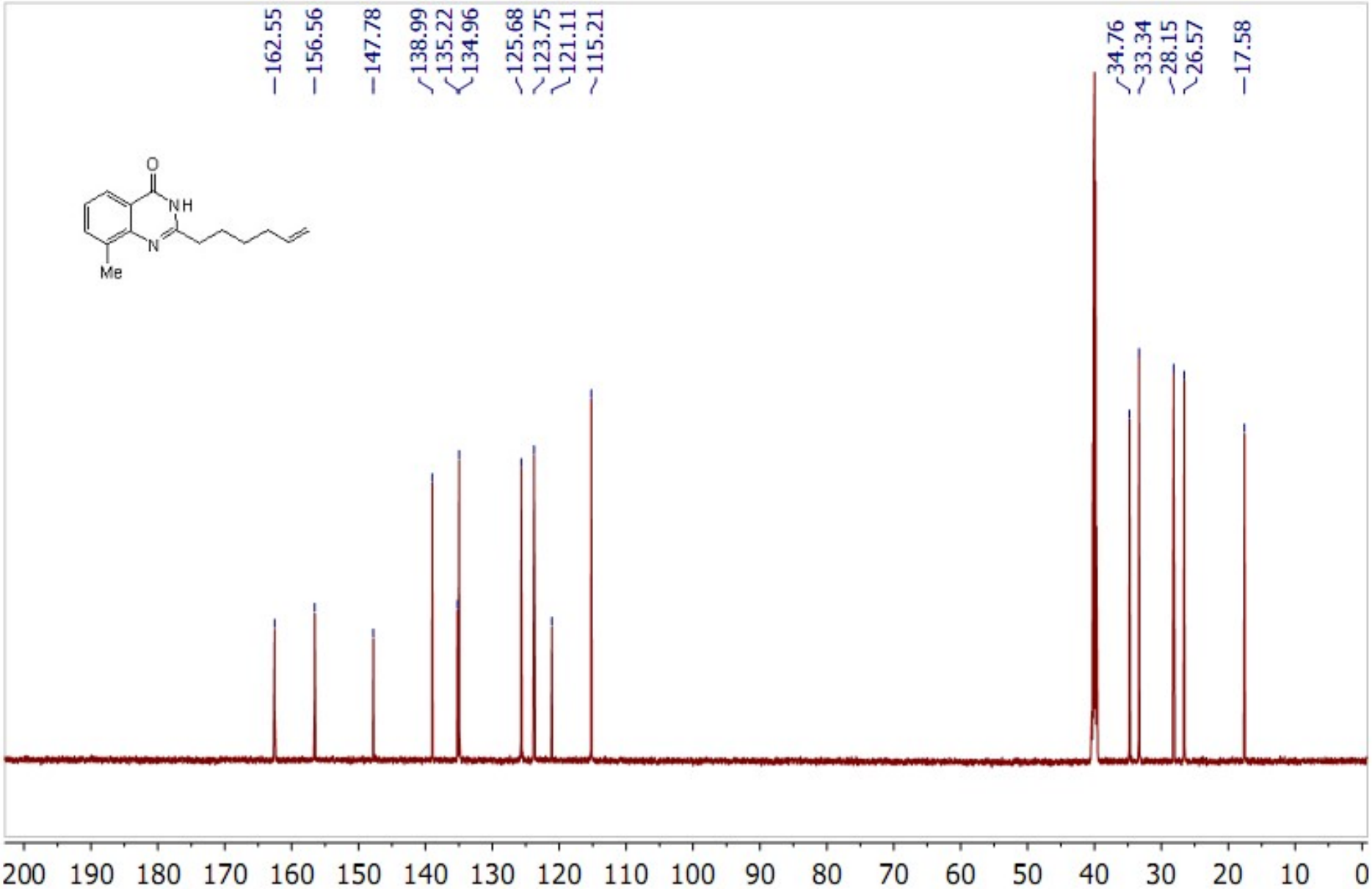
^{13}C NMR spectrum (126 MHz, DMSO-d6) of compound 3g



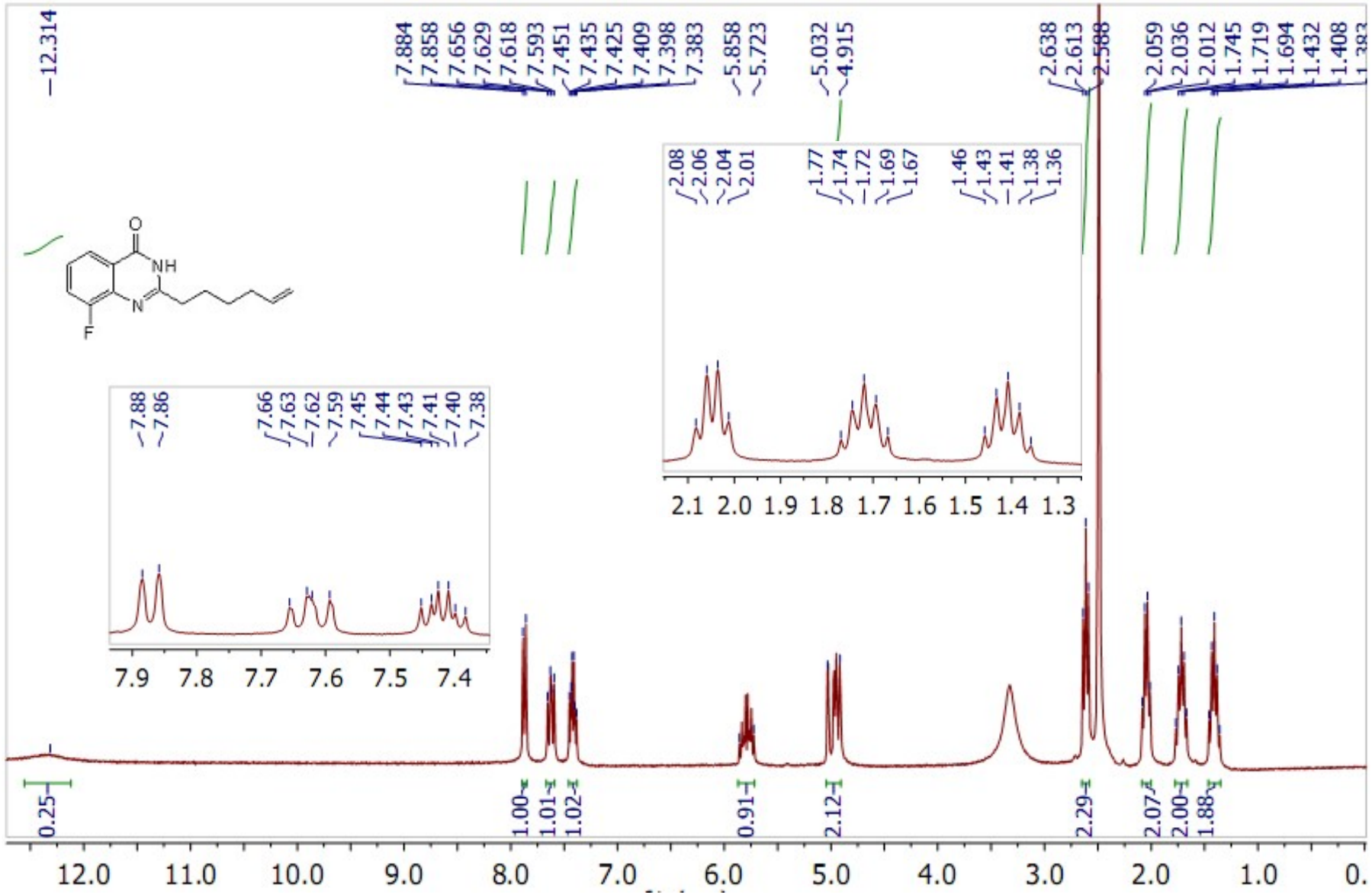
^{1}H NMR spectrum (600 MHz, DMSO-d6) of compound 3h



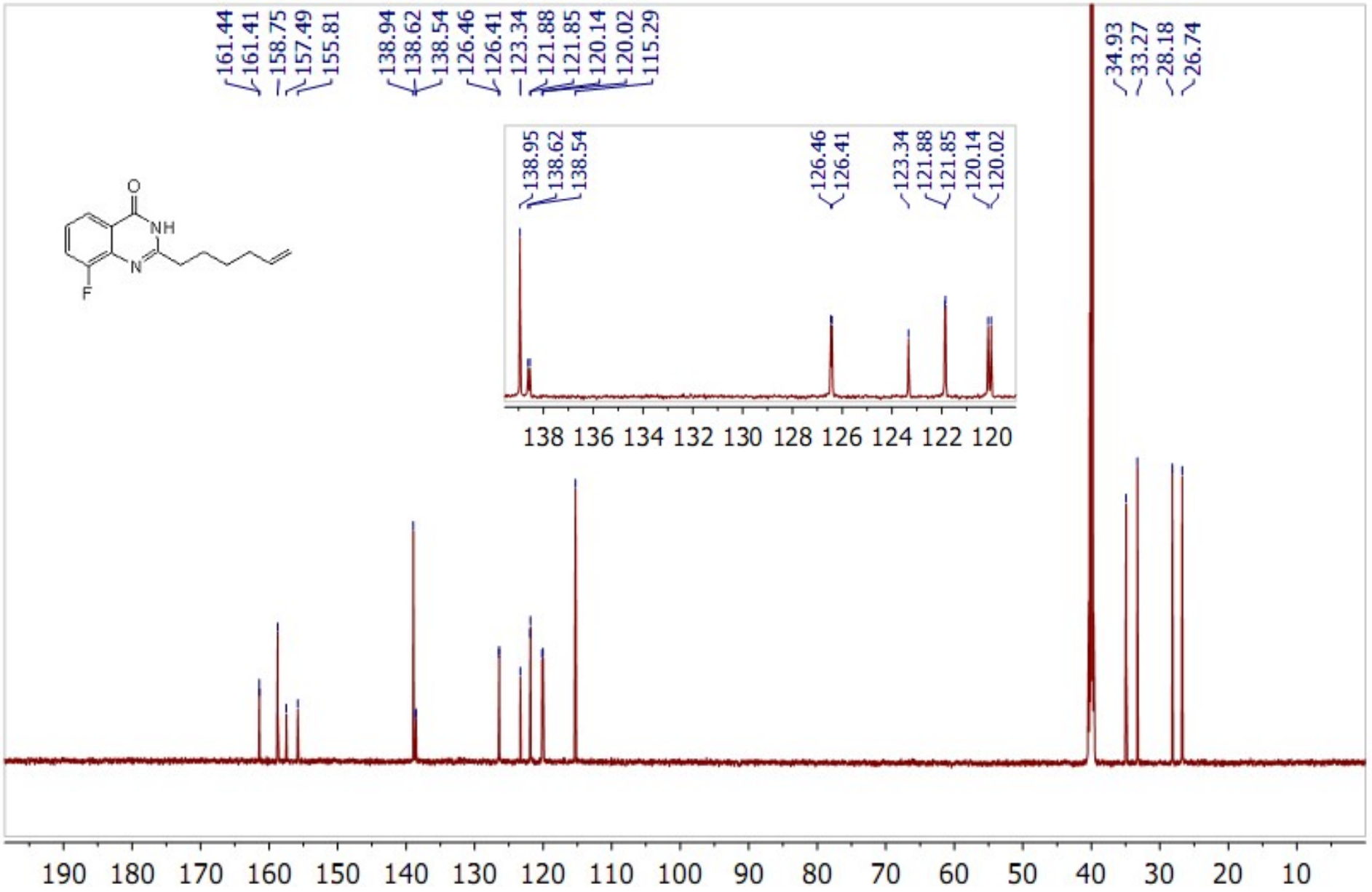
^{13}C NMR spectrum (151 MHz, DMSO-d6) of compound 3h



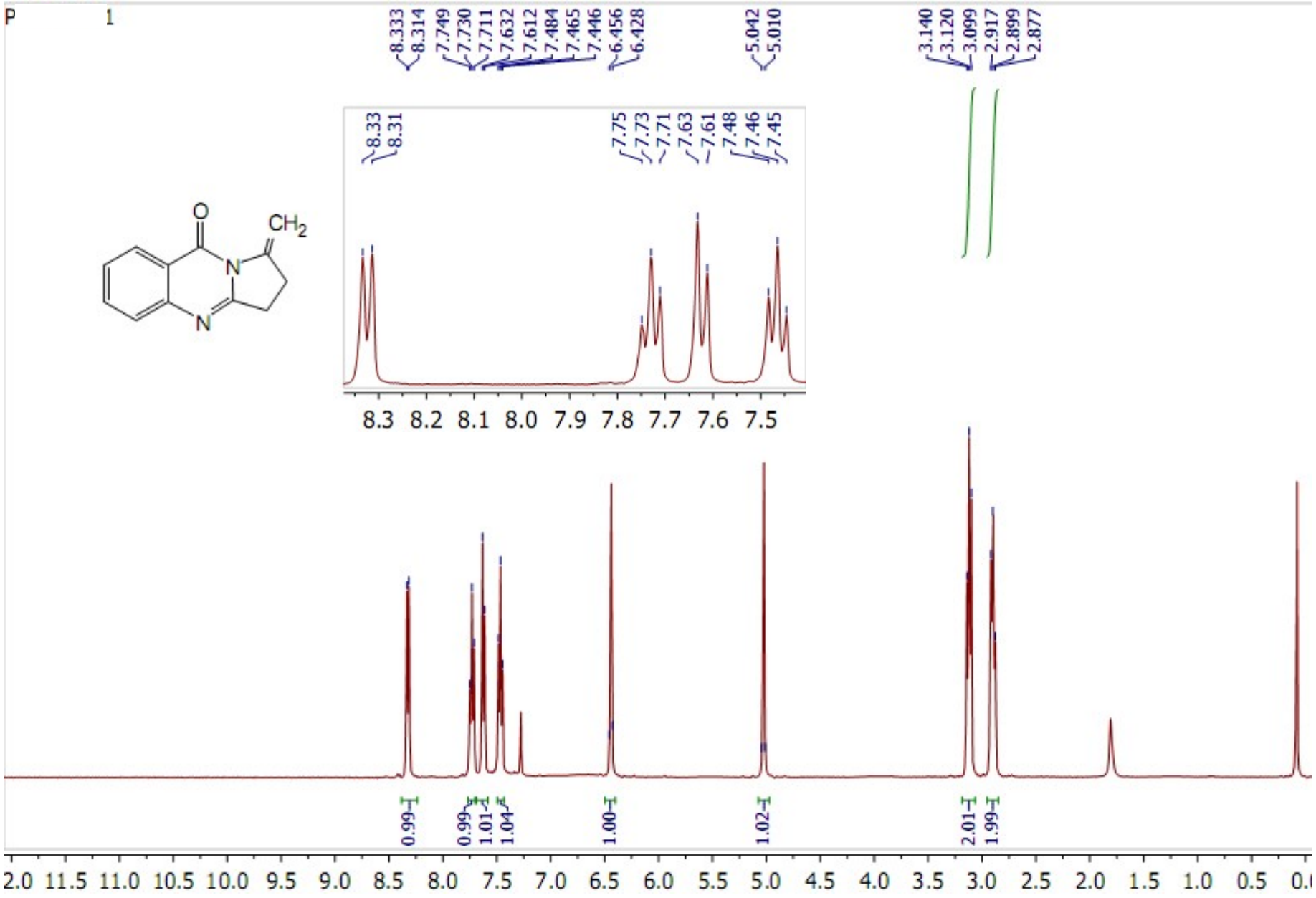
^{1}H NMR spectrum (300 MHz, DMSO-d6) of compound 3i



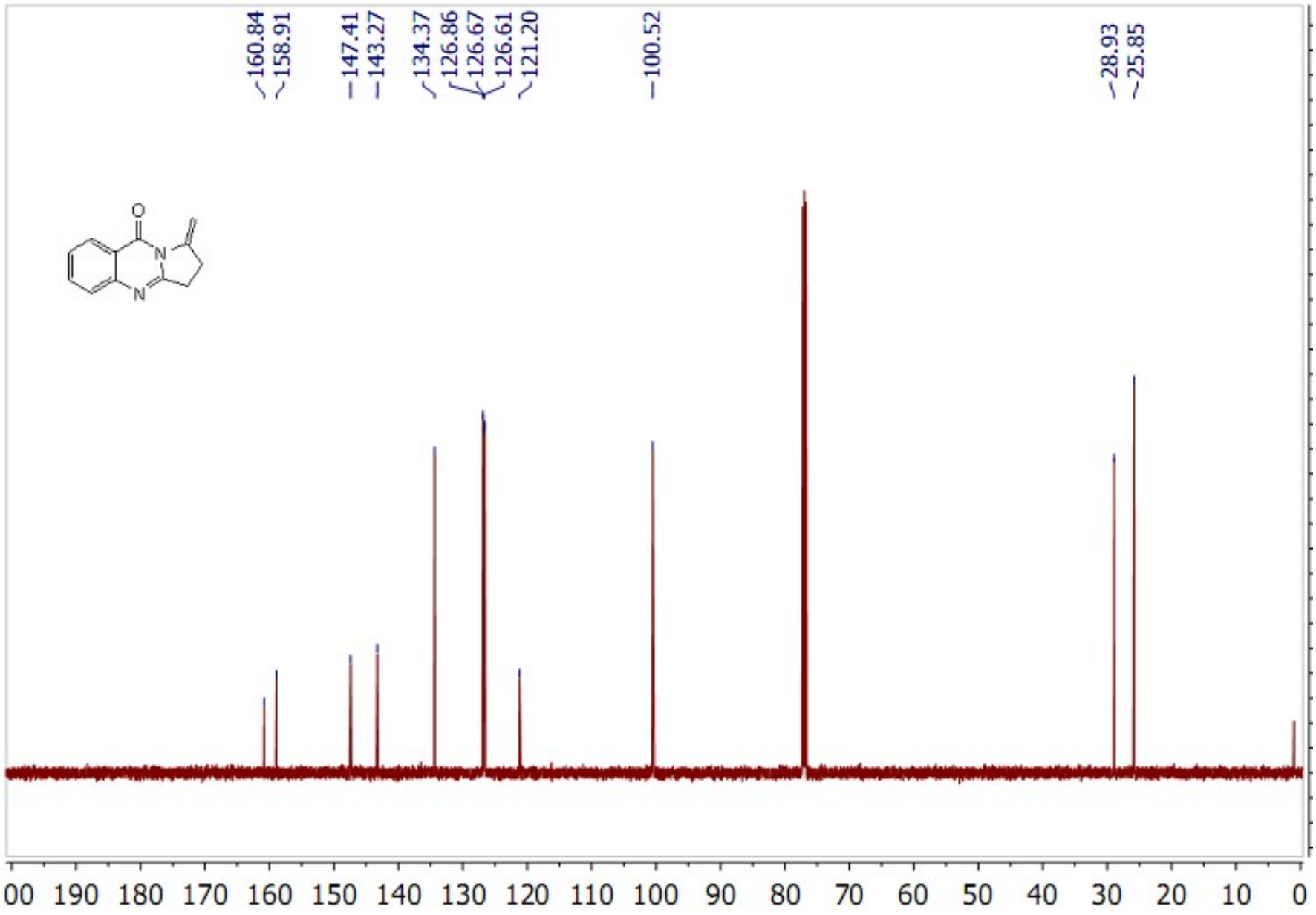
^{13}C NMR spectrum (151 MHz, DMSO-d6) of compound 3i



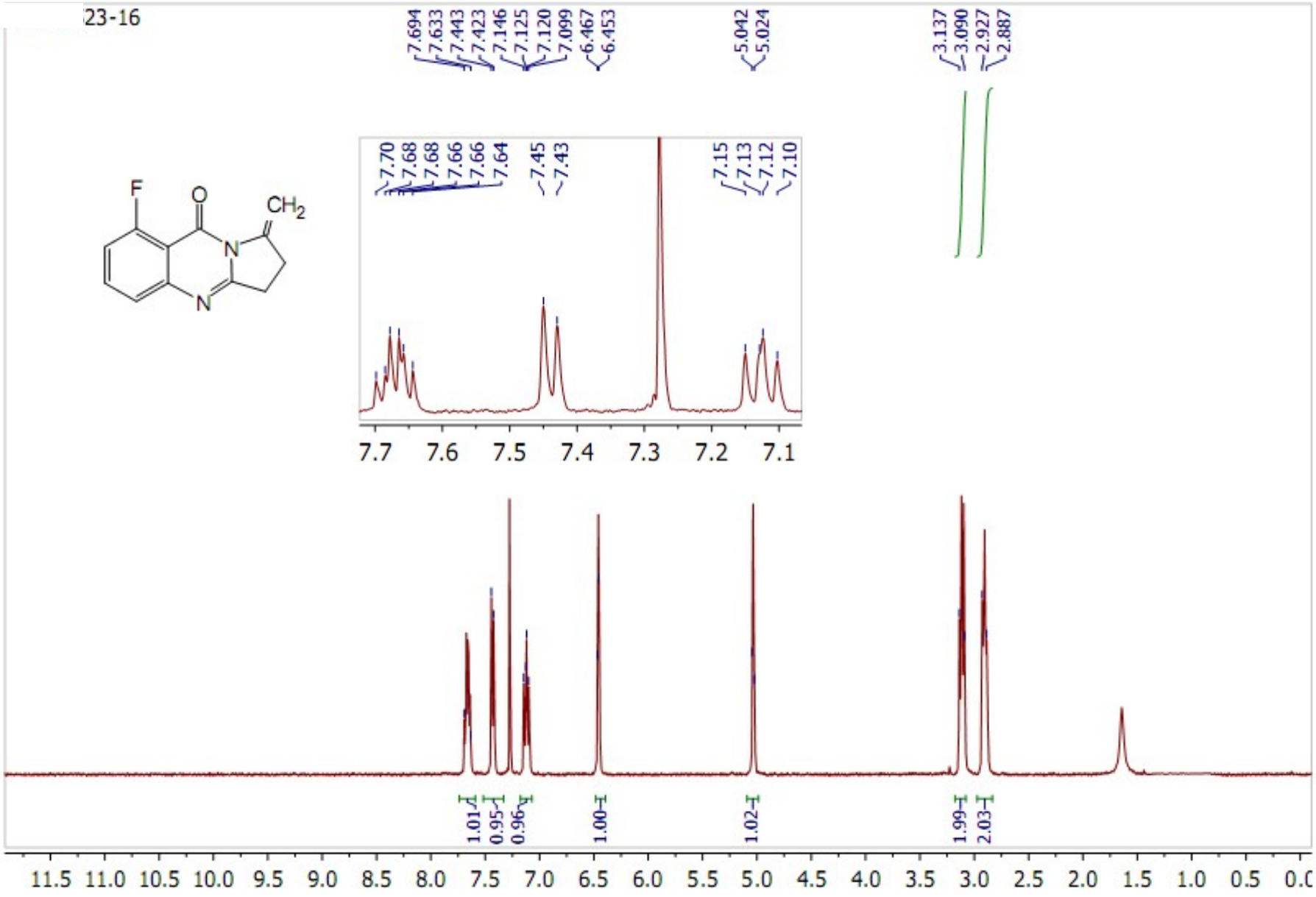
^{1}H NMR spectrum (400 MHz, $CDCl_3$) of compound 9a



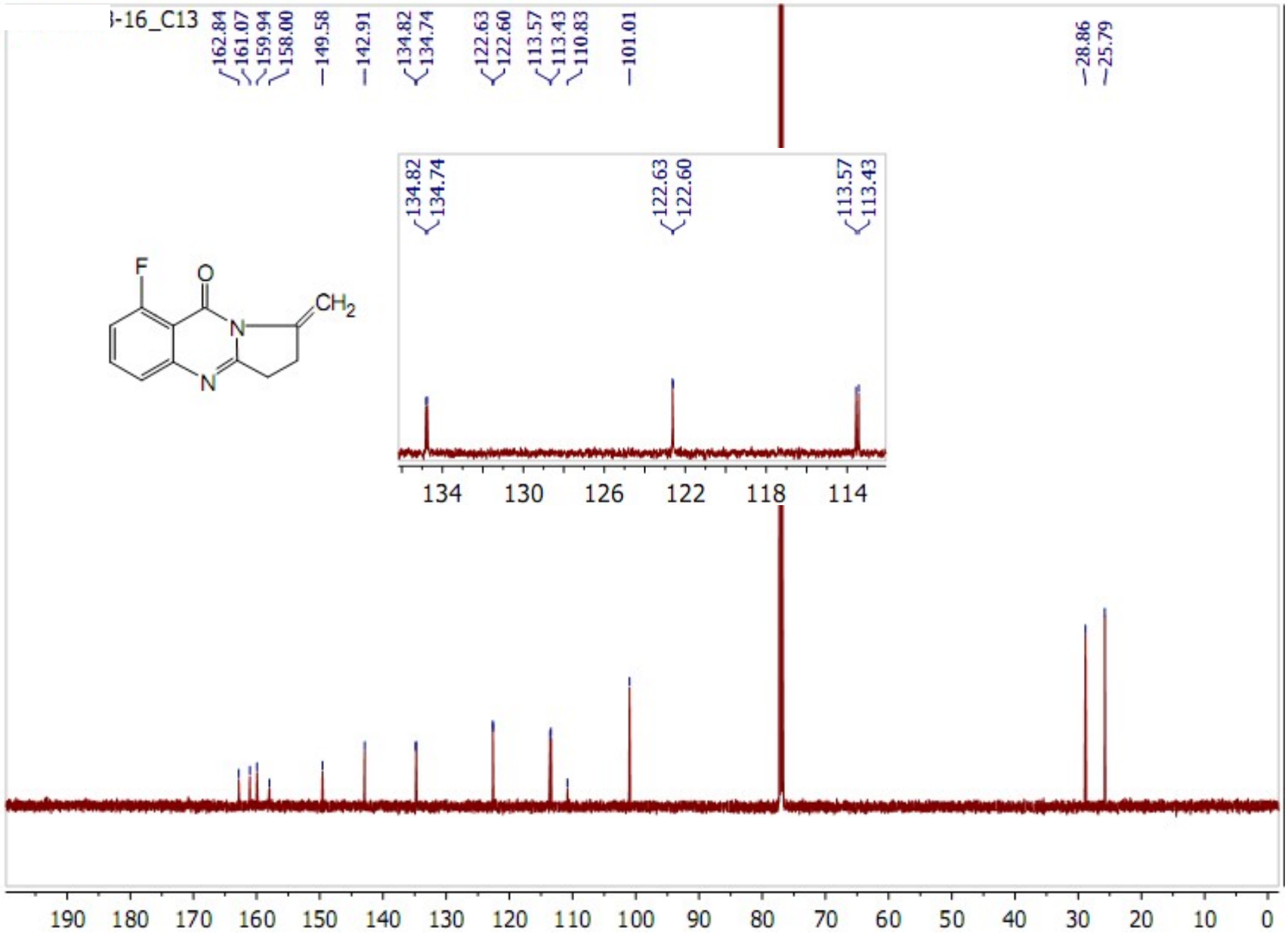
^{13}C NMR spectrum (126 MHz, $CDCl_3$) of compound 9a



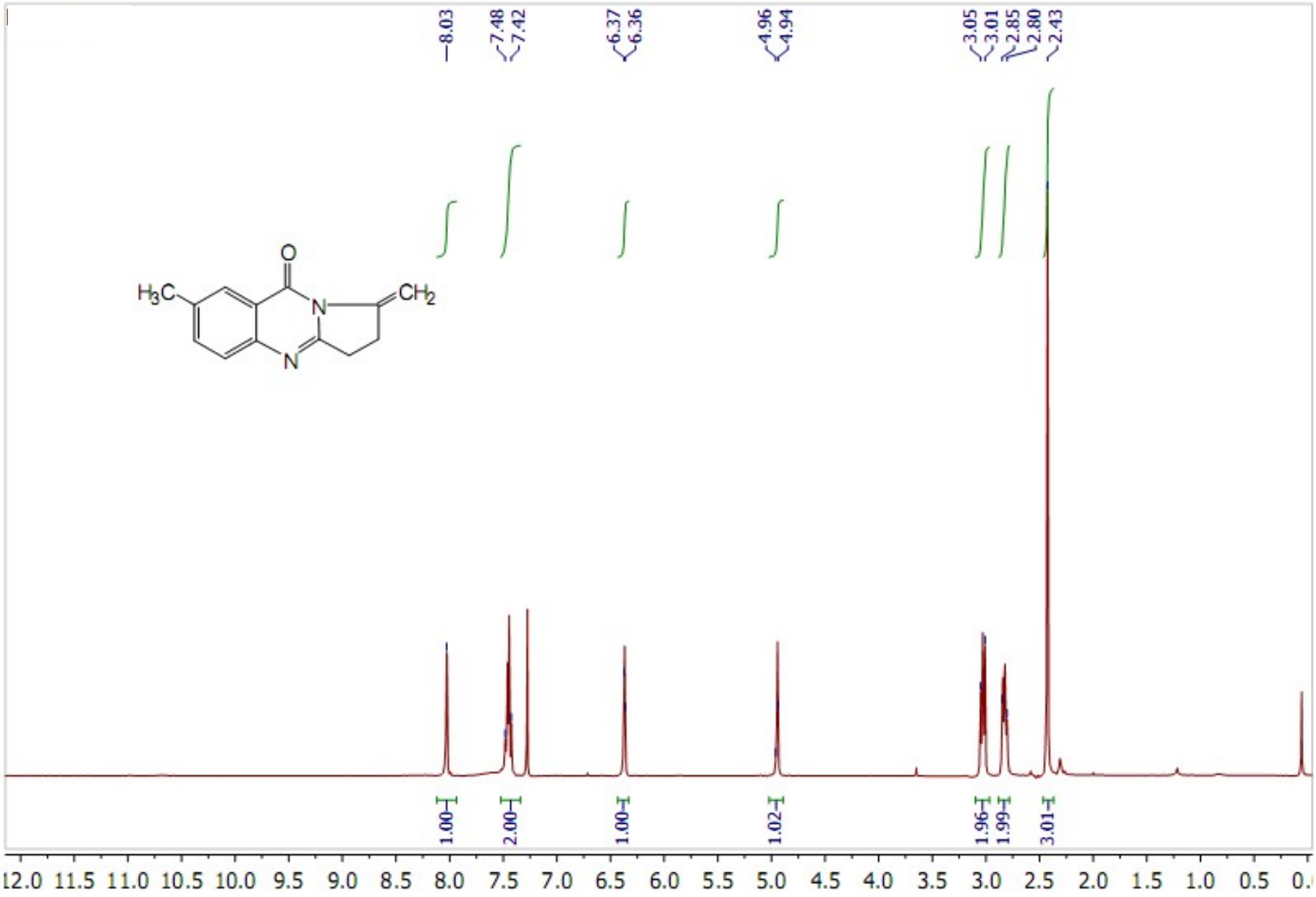
^{1}H NMR spectrum (400 MHz, $CDCl_3$) of compound 9b



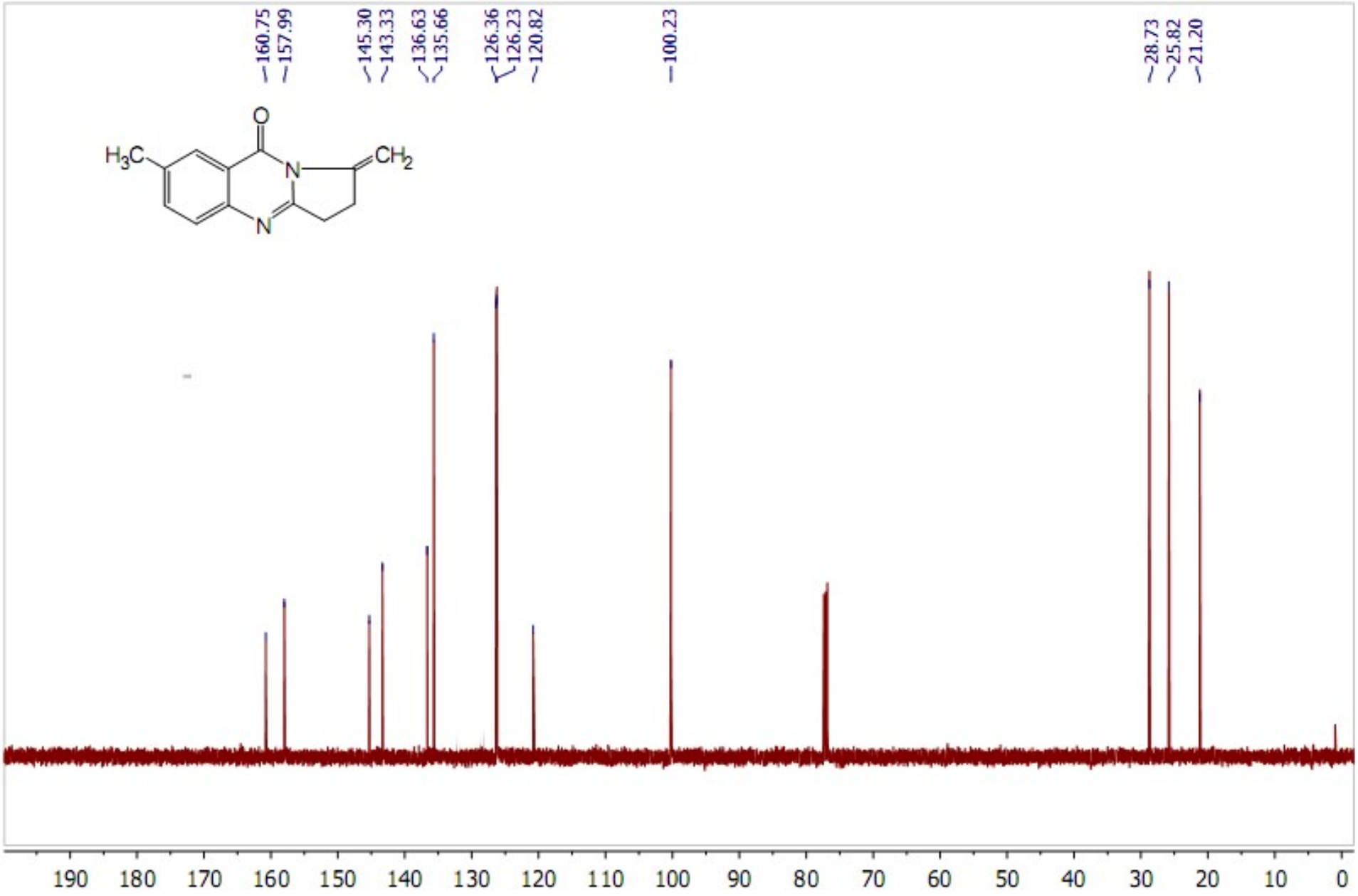
^{13}C NMR spectrum (126 MHz, $CDCl_3$) of compound 9b



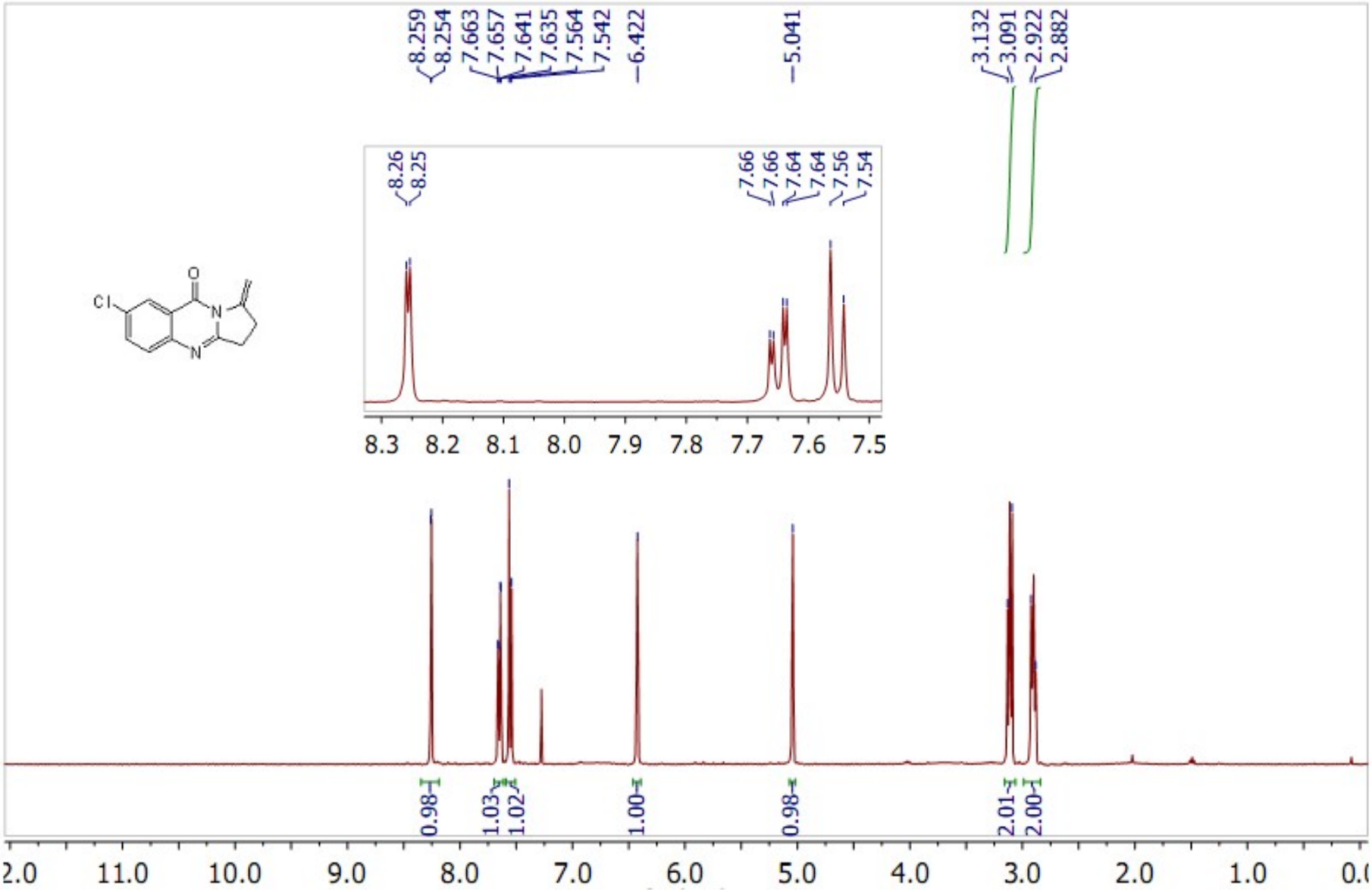
^{1}H NMR spectrum (400 MHz, $CDCl_3$) of compound 9c



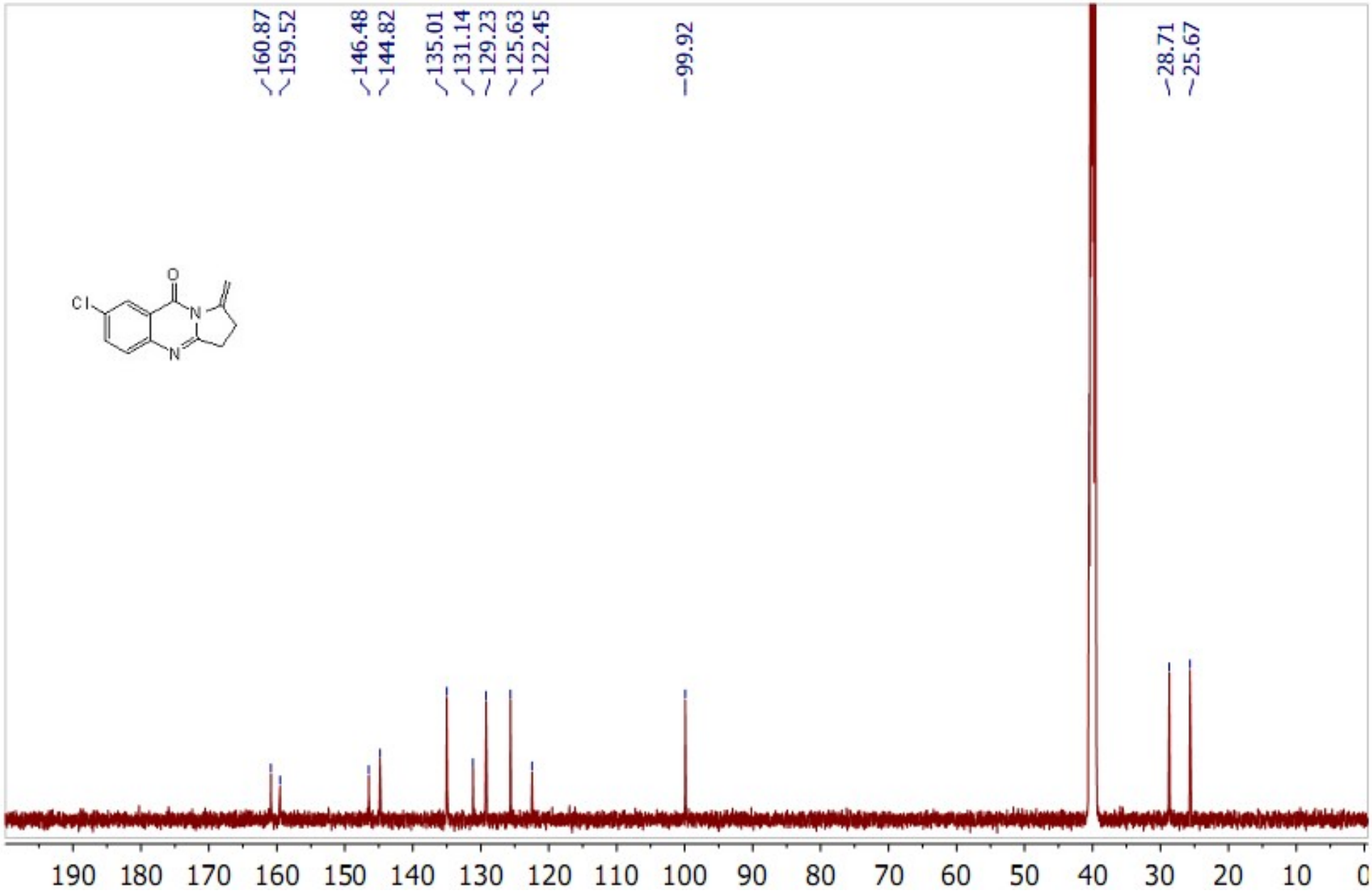
^{13}C NMR spectrum (126 MHz, $CDCl_3$) of compound 9c



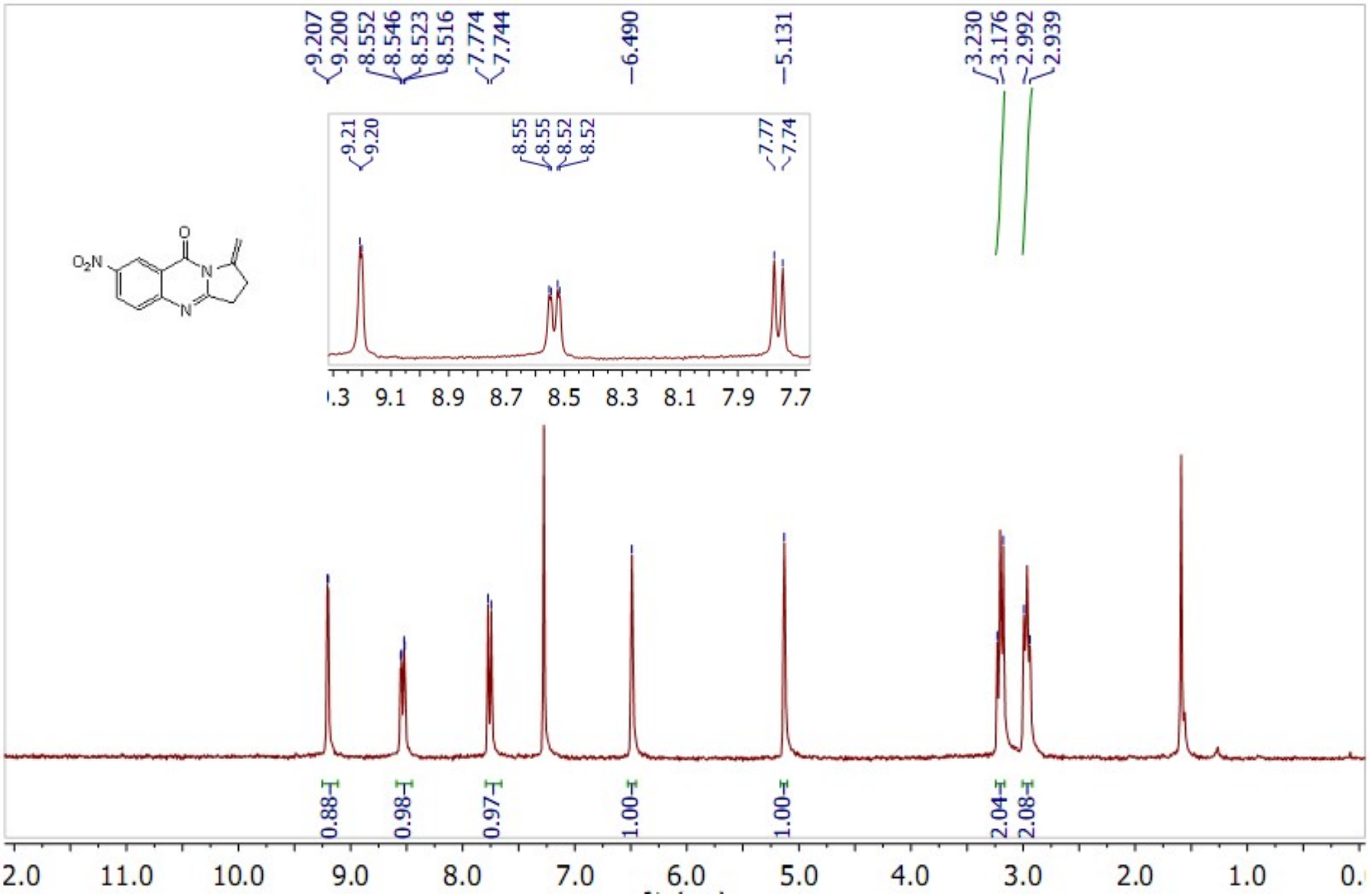
^{1}H NMR spectrum (400 MHz, $CDCl_3$) of compound 9d



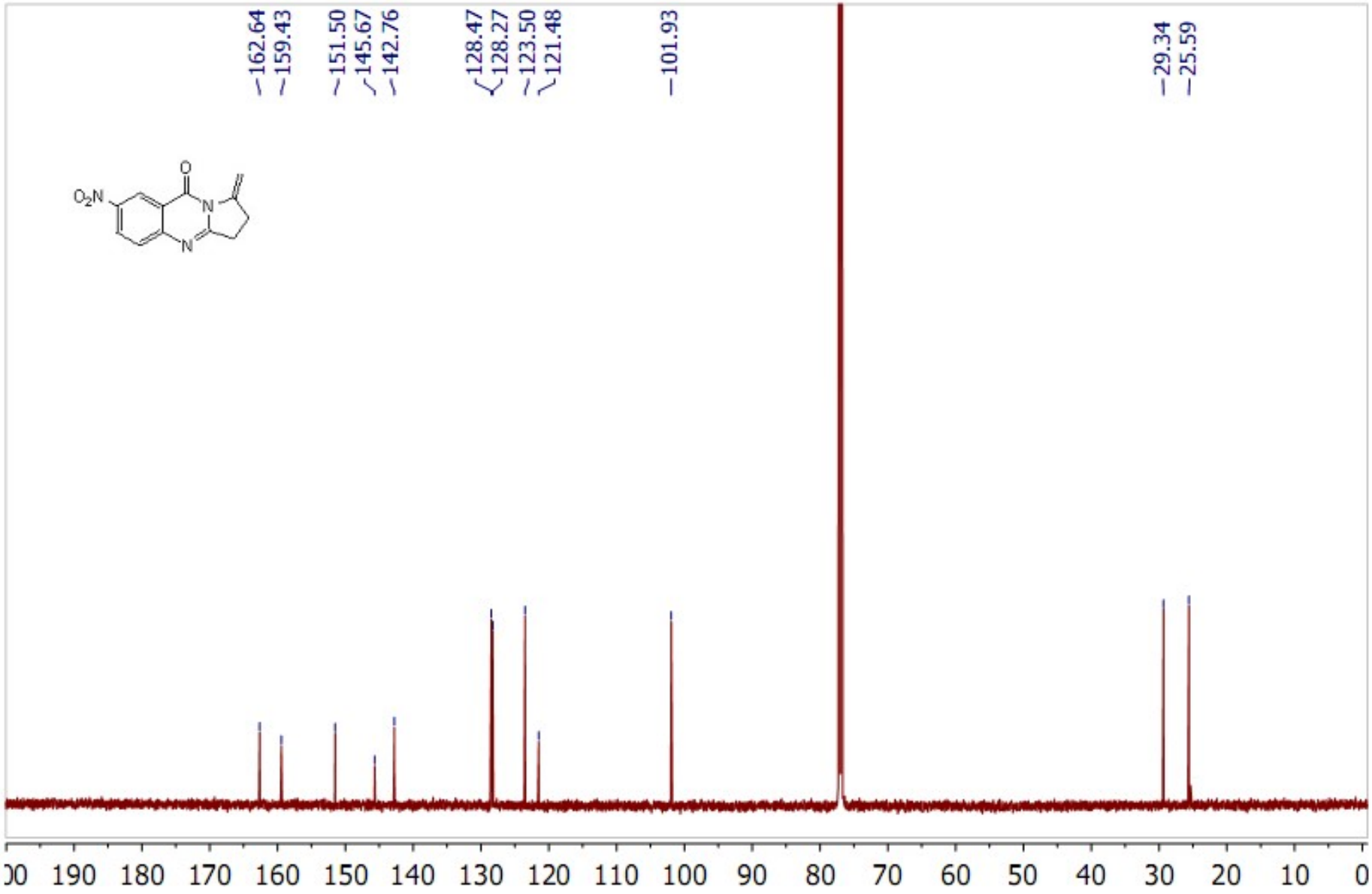
^{13}C NMR spectrum (126 MHz, DMSO-d6) of compound 9d



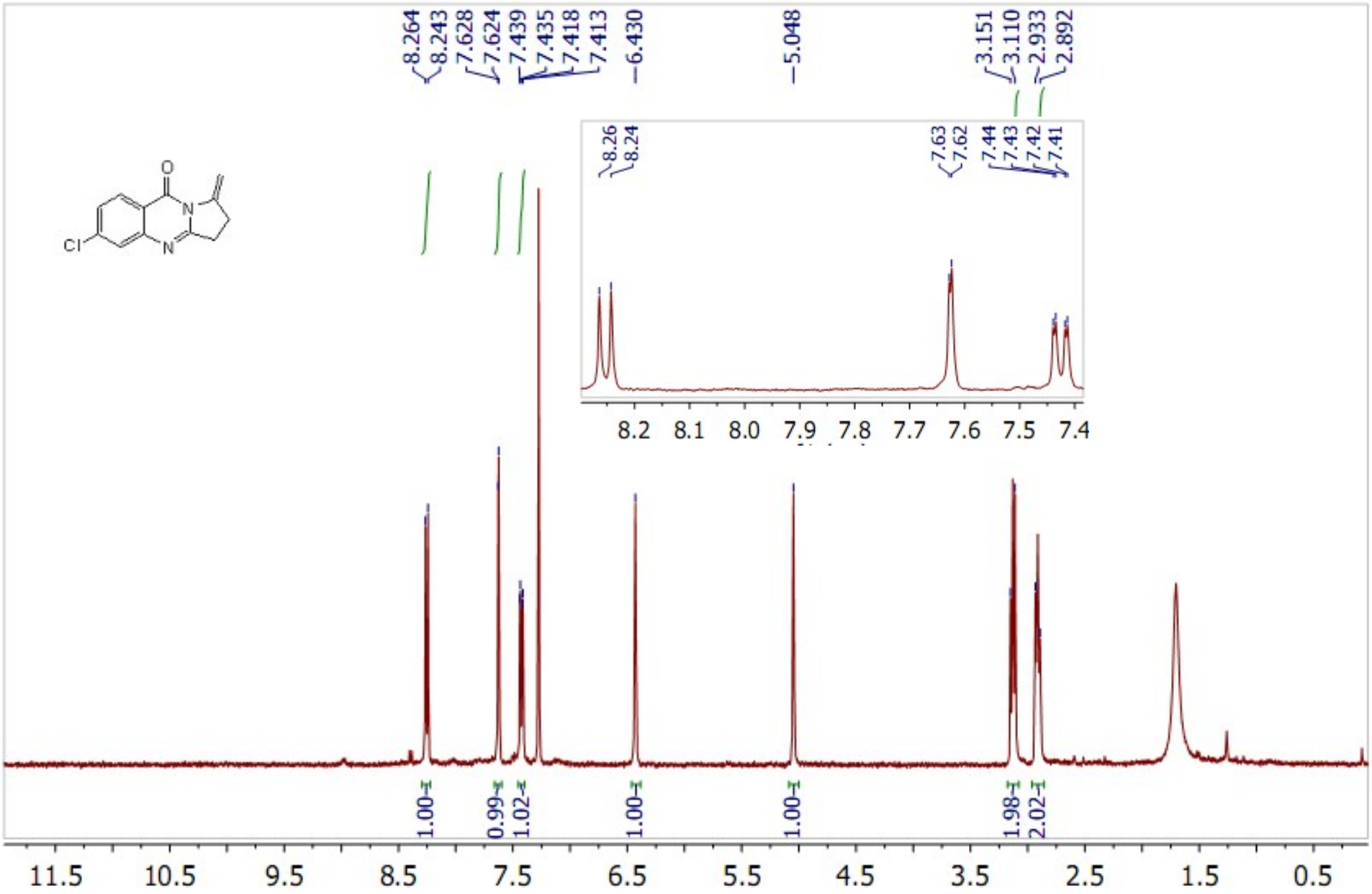
^{1}H NMR spectrum (300 MHz, $CDCl_3$) of compound 9e



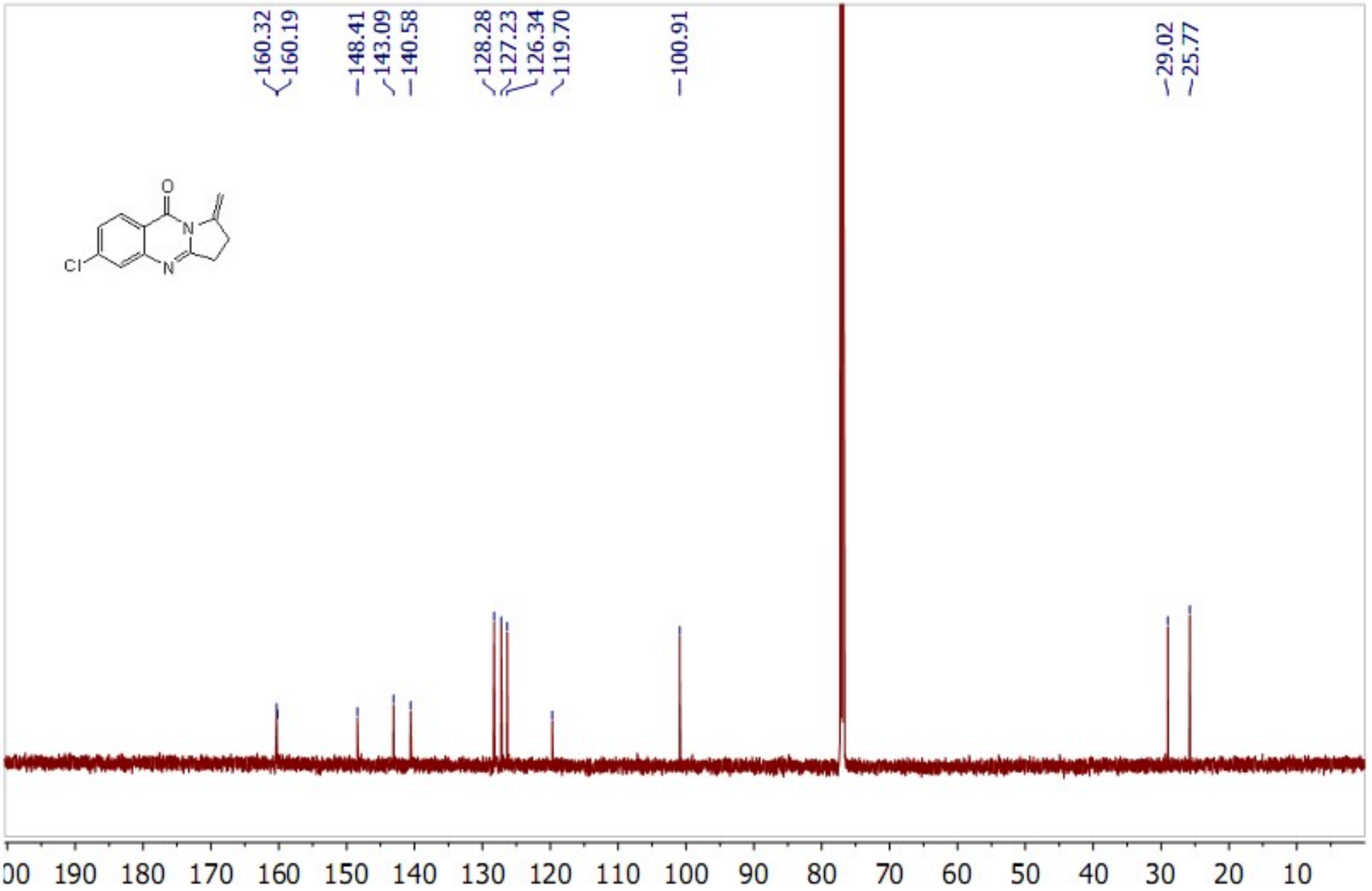
^{13}C NMR spectrum (126 MHz, $CDCl_3$) of compound 9e



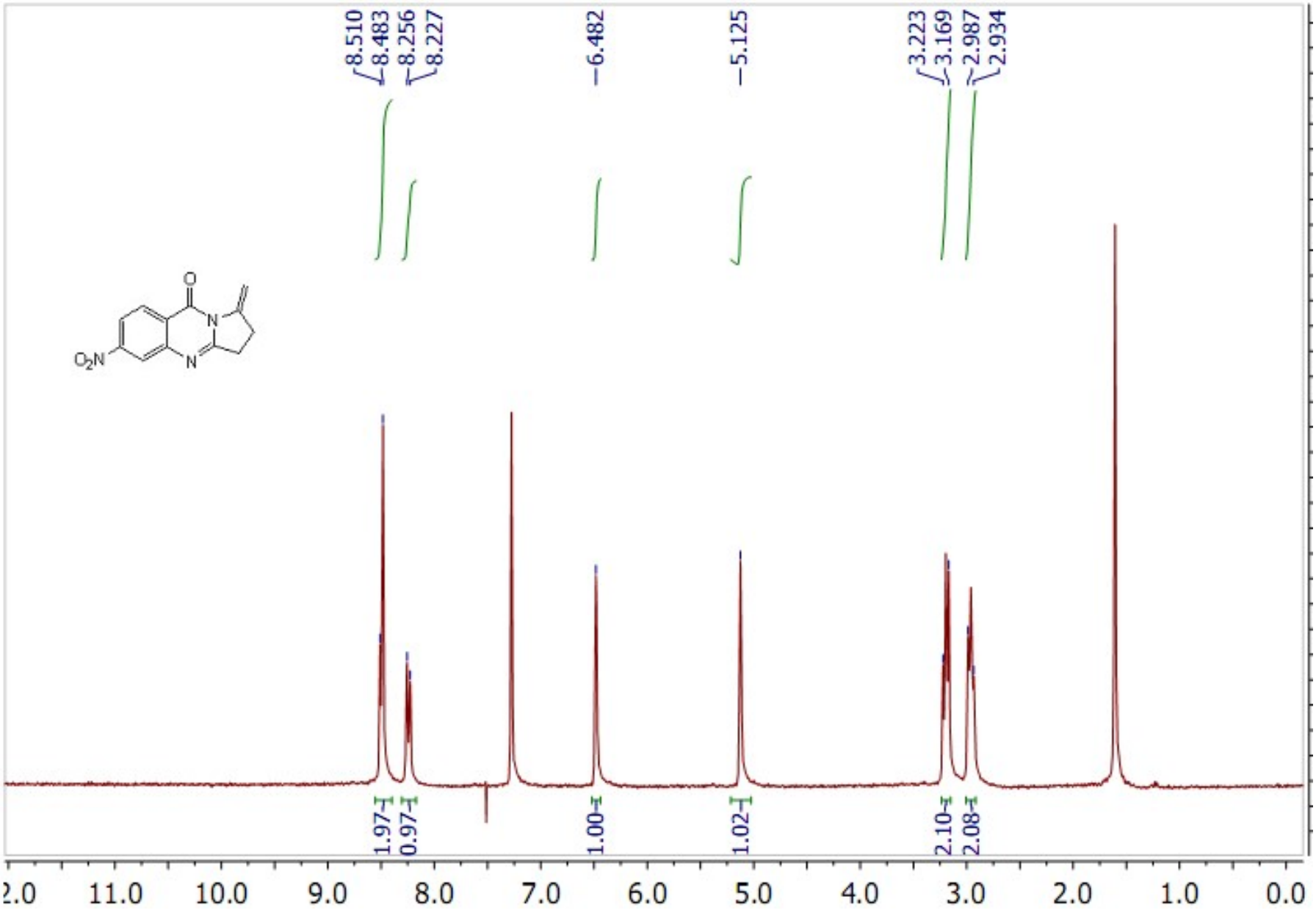
^{1}H NMR spectrum (400 MHz, $CDCl_3$) of compound 9f



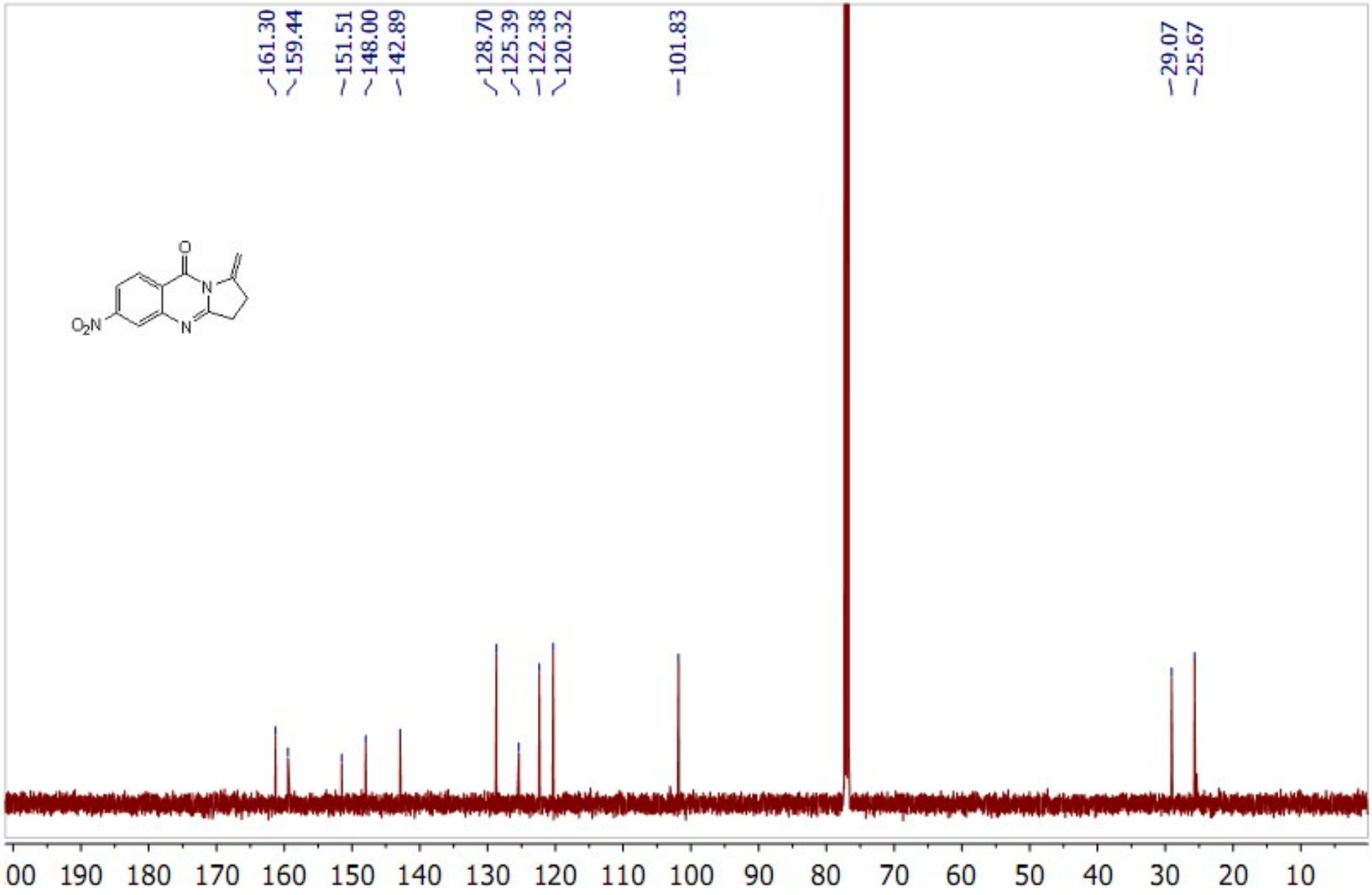
^{13}C NMR spectrum (151 MHz, $CDCl_3$) of compound 9f



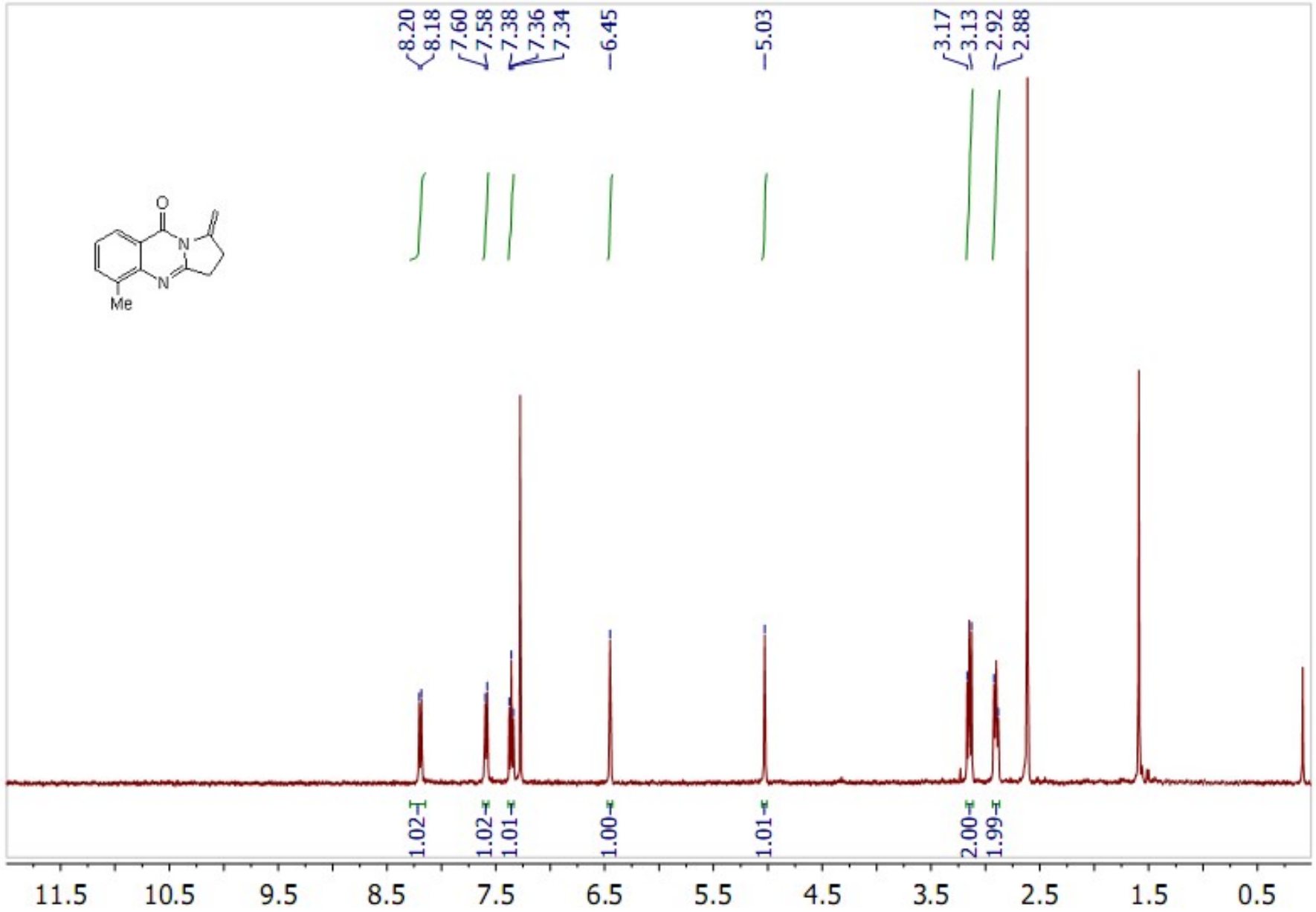
^{1}H NMR spectrum (300 MHz, $CDCl_3$) of compound 9g



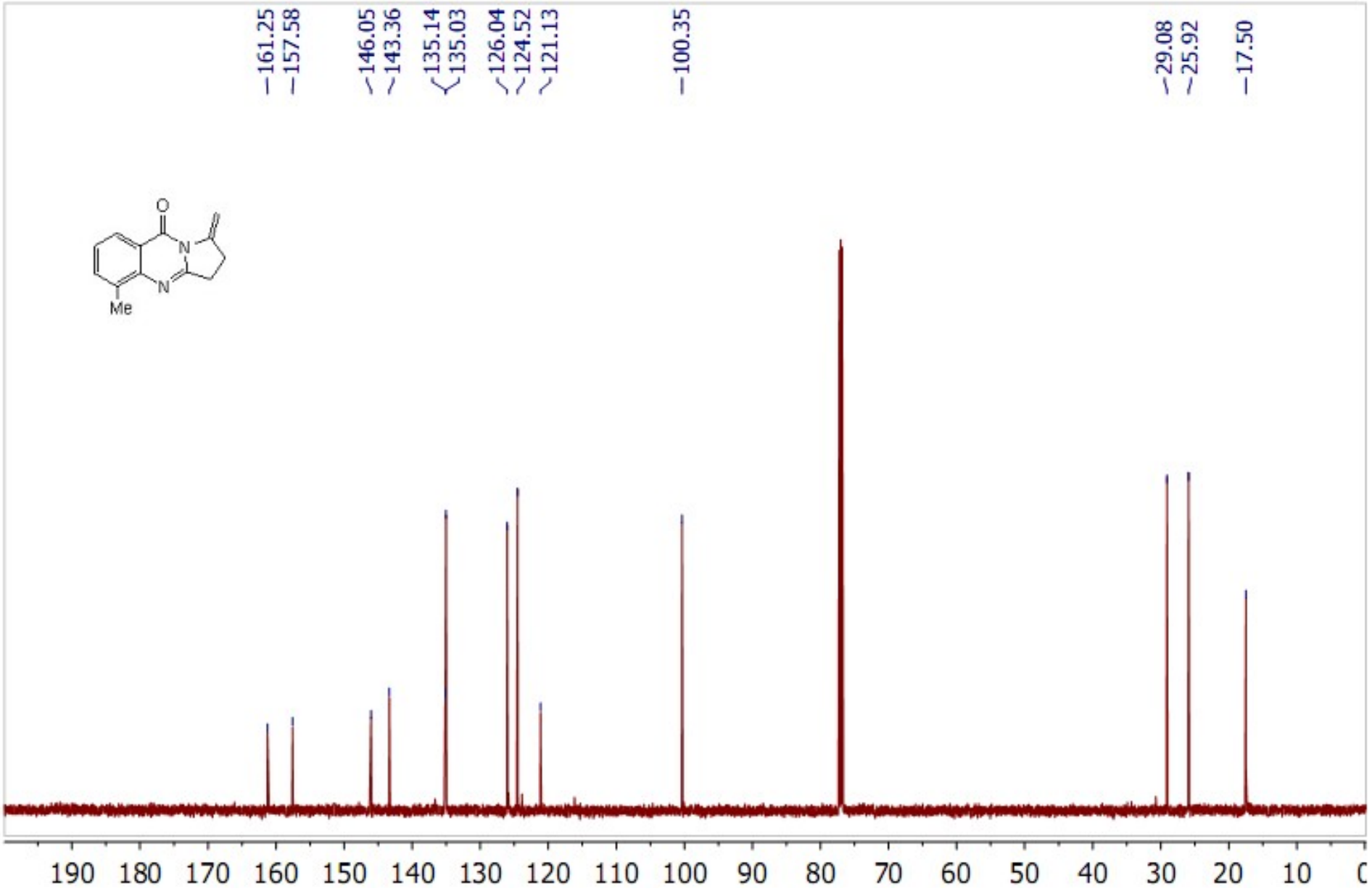
^{13}C NMR spectrum (126 MHz, $CDCl_3$) of compound 9g



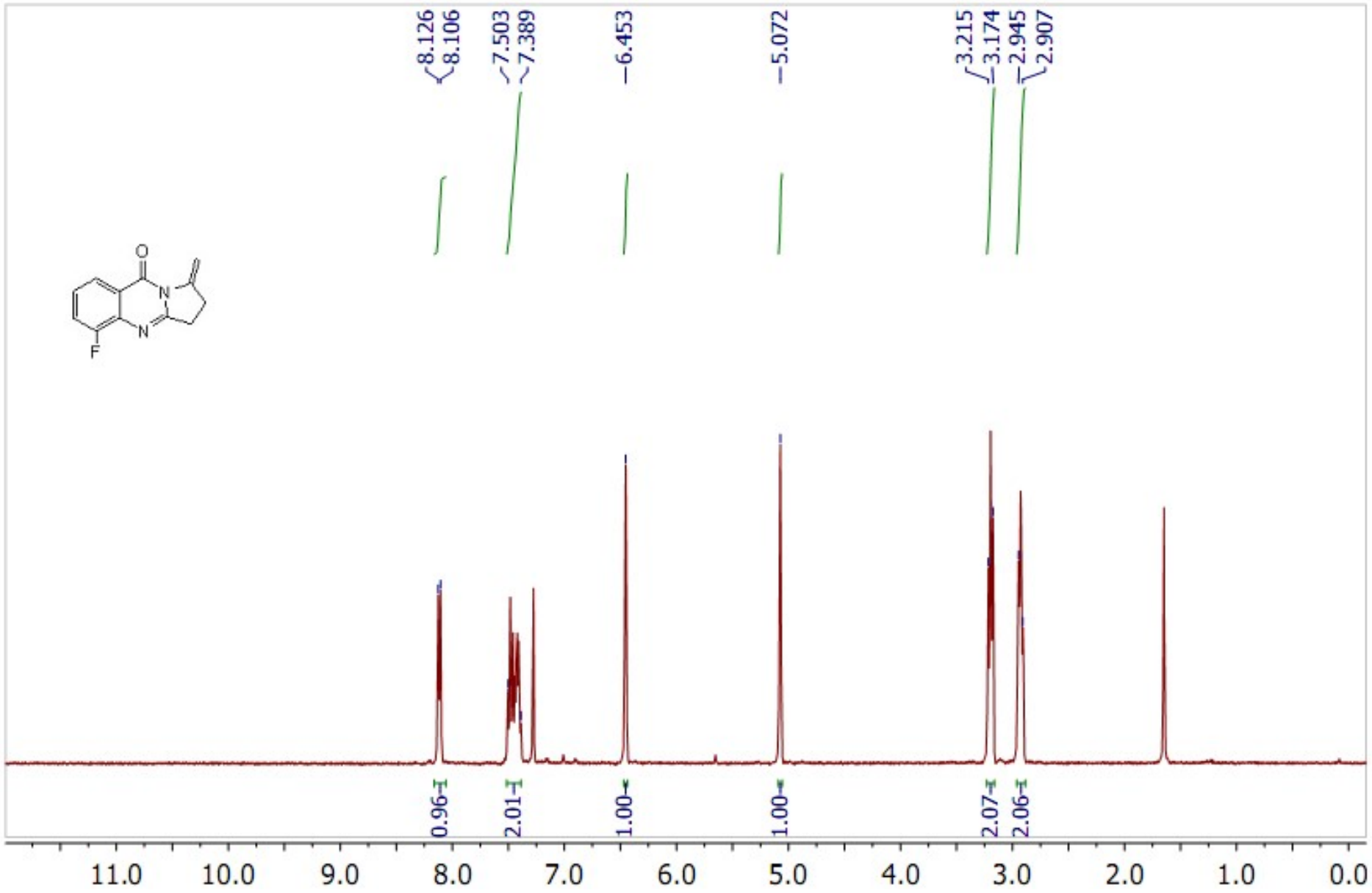
^{1}H NMR spectrum (400 MHz, $CDCl_3$) of compound 9h



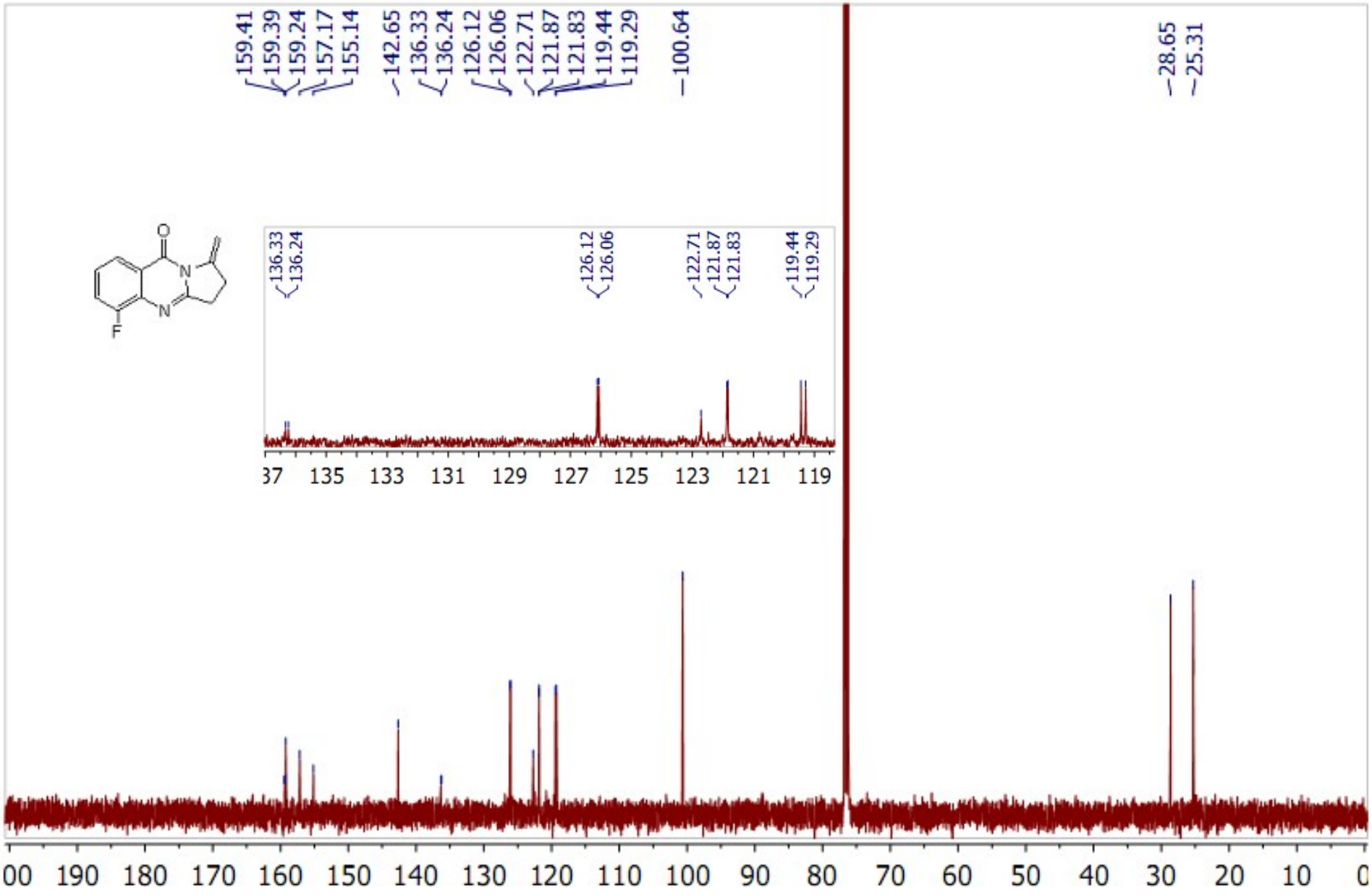
^{13}C NMR spectrum (151 MHz, $CDCl_3$) of compound 9h



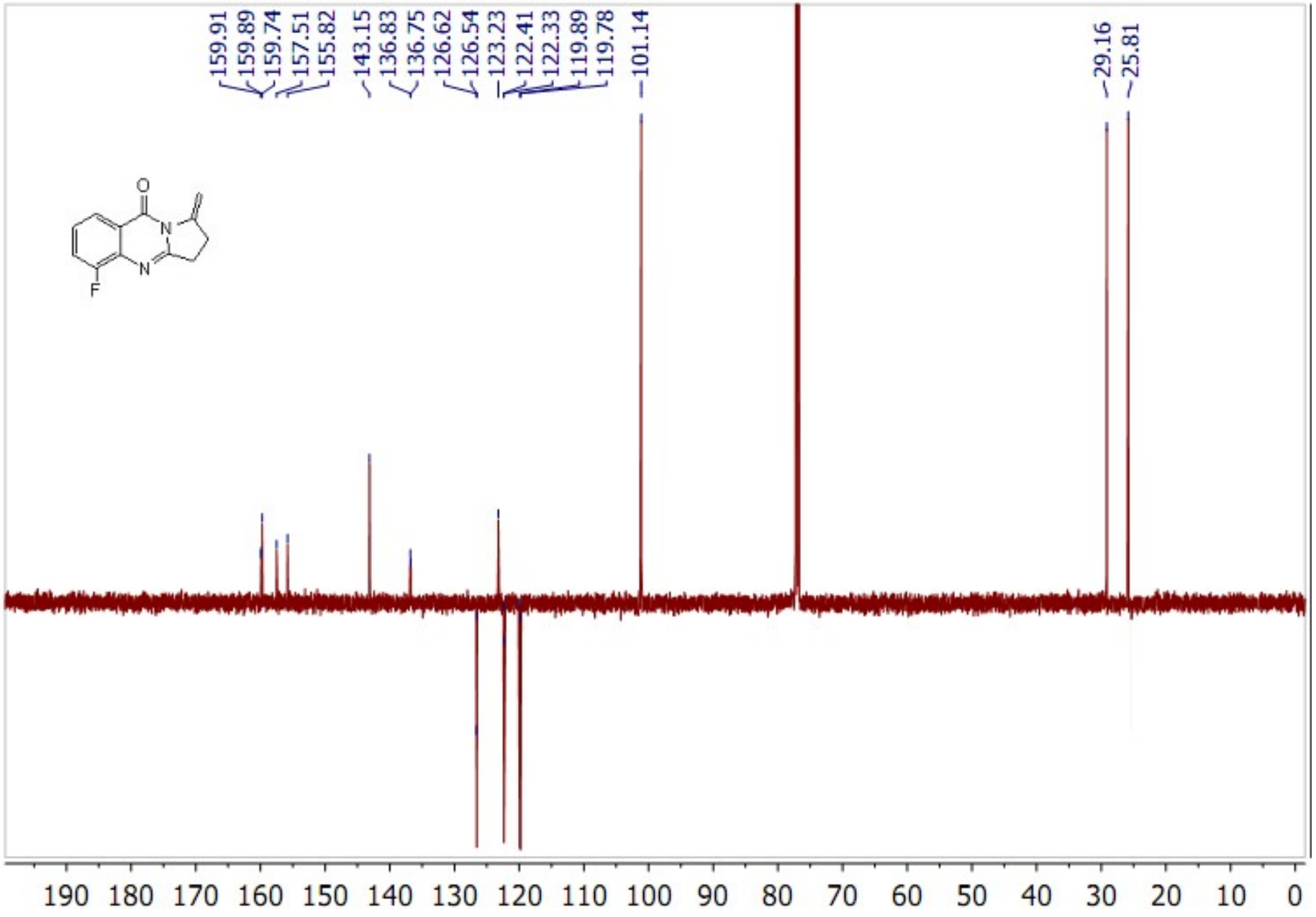
^{1}H NMR spectrum (400 MHz, $CDCl_3$) of compound 9i



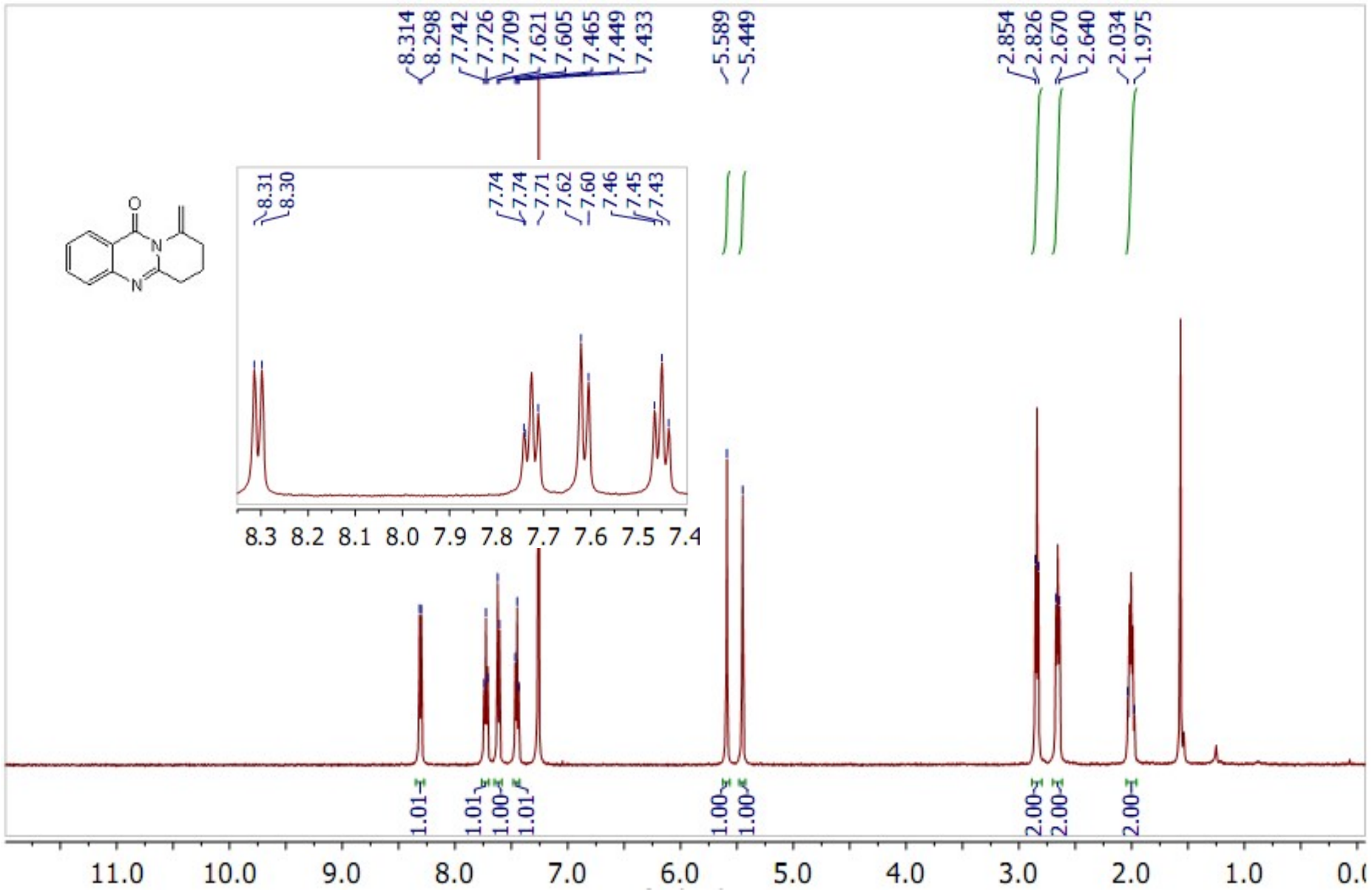
^{13}C NMR spectrum (126 MHz, $CDCl_3$) of compound 9i



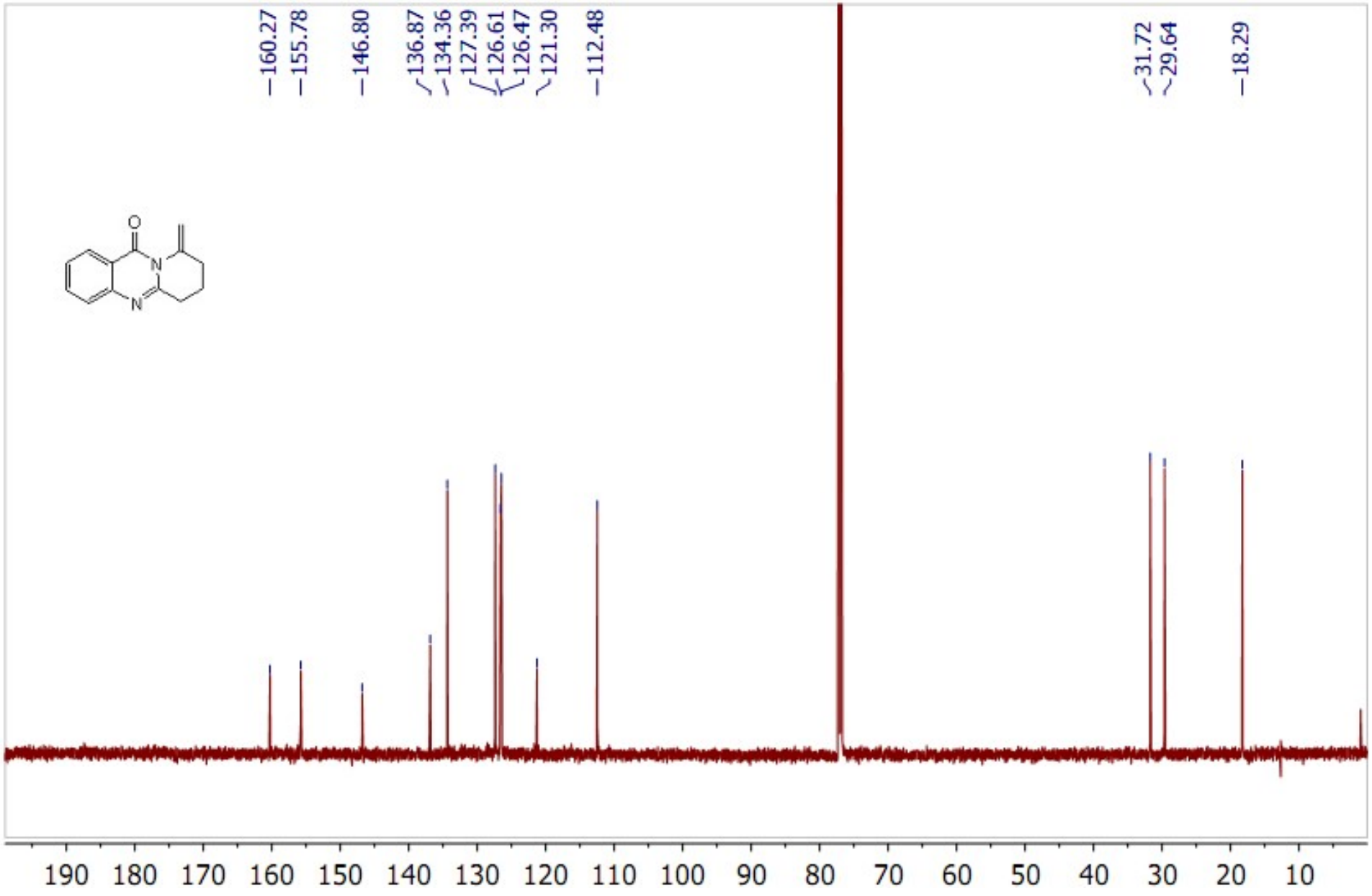
^{13}C/APT NMR spectrum (151 MHz, $CDCl_3$) of compound 9i



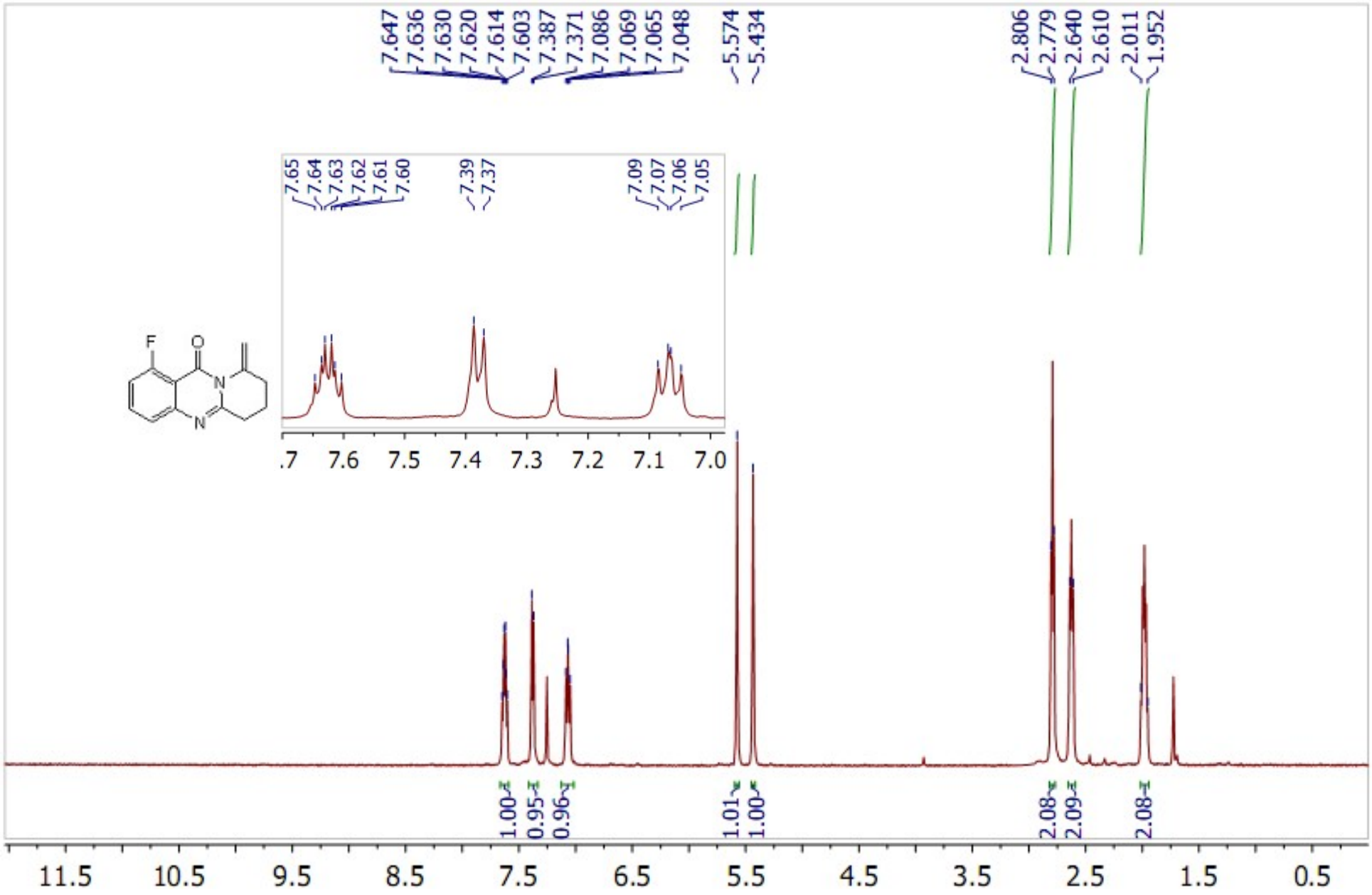
^{1}H NMR spectrum (500 MHz, $CDCl_3$) of compound 10a



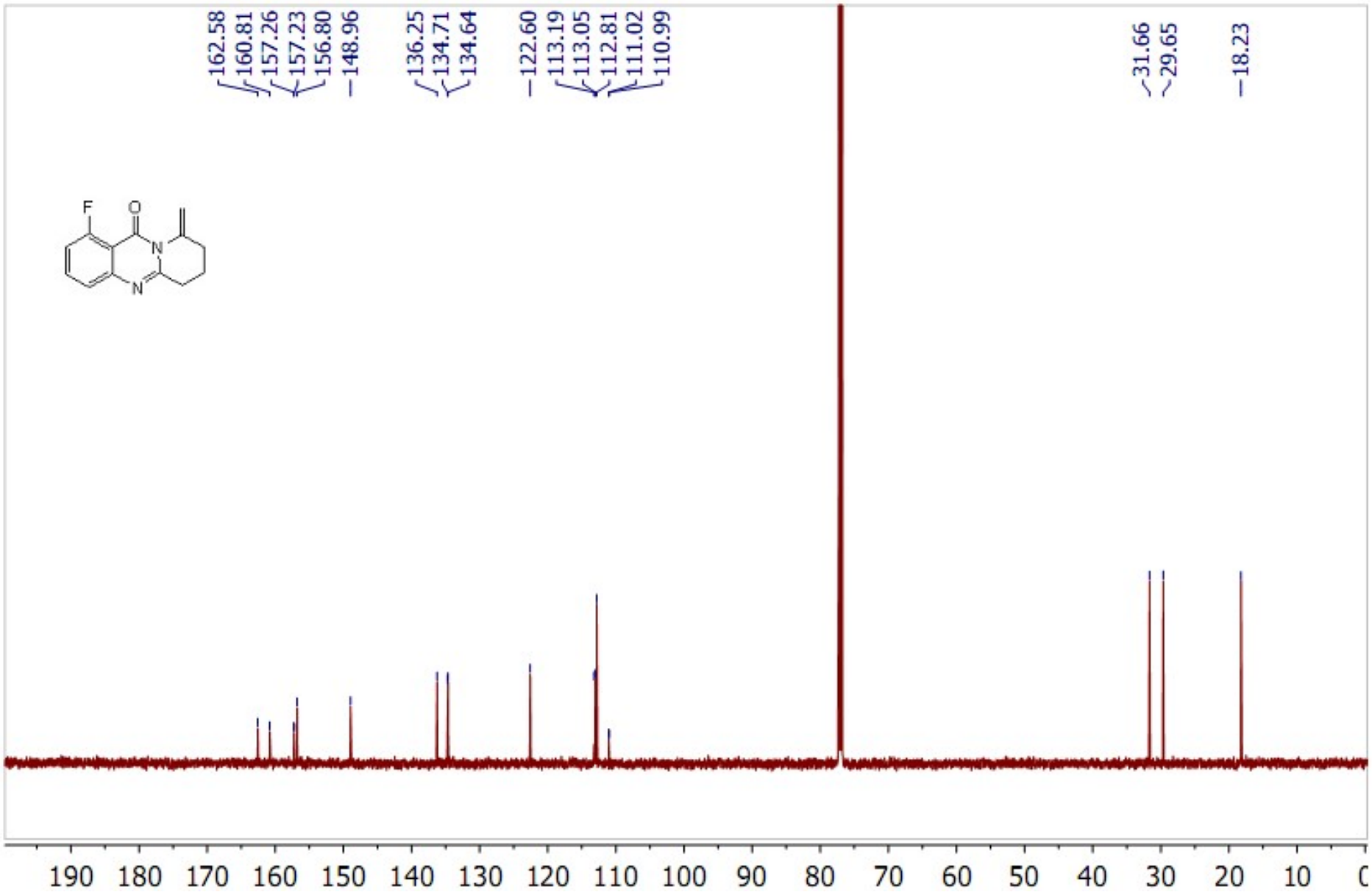
^{13}C NMR spectrum (151 MHz, $CDCl_3$) of compound 10a



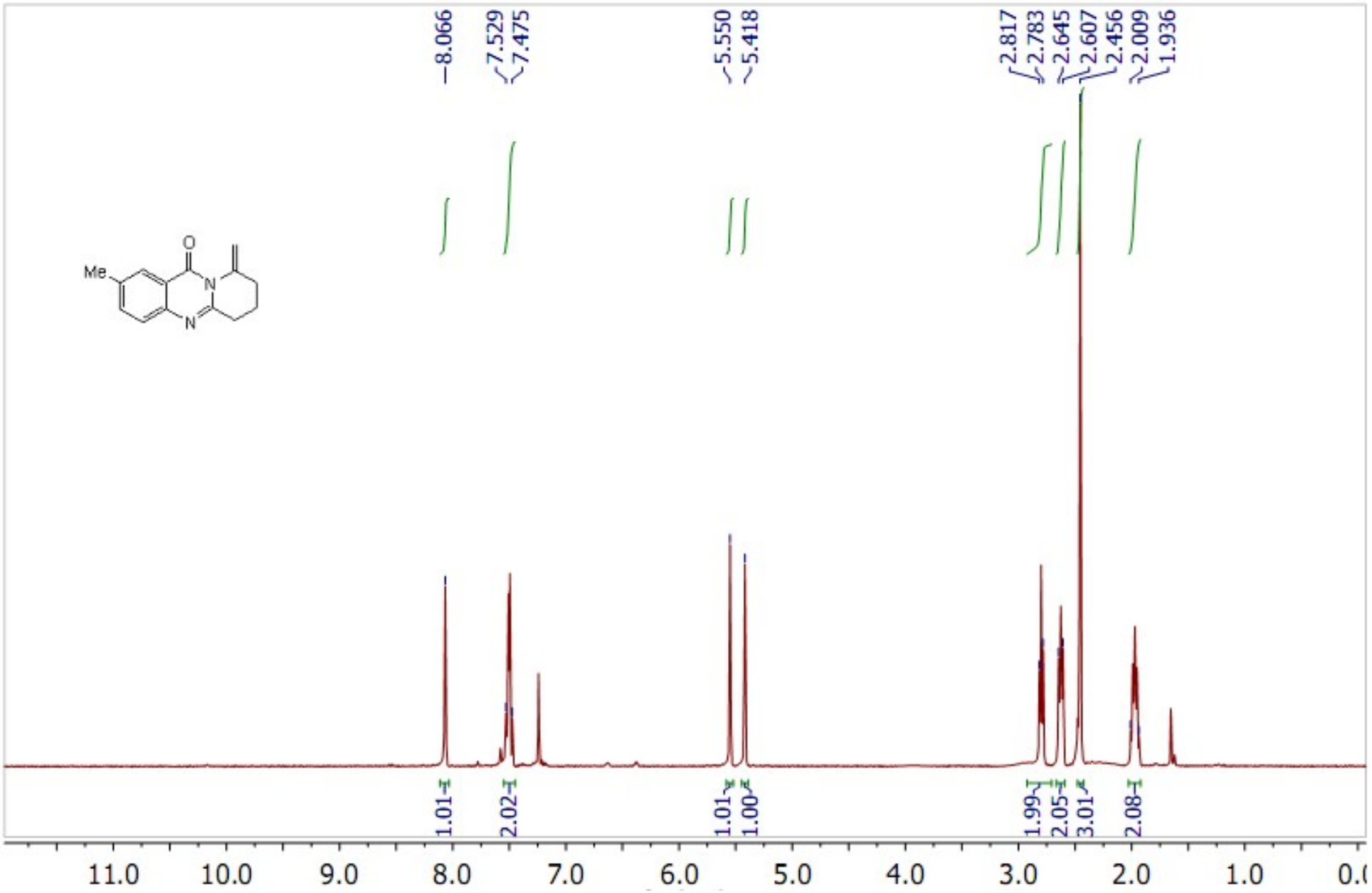
^{1}H NMR spectrum (500 MHz, $CDCl_3$) of compound 10b



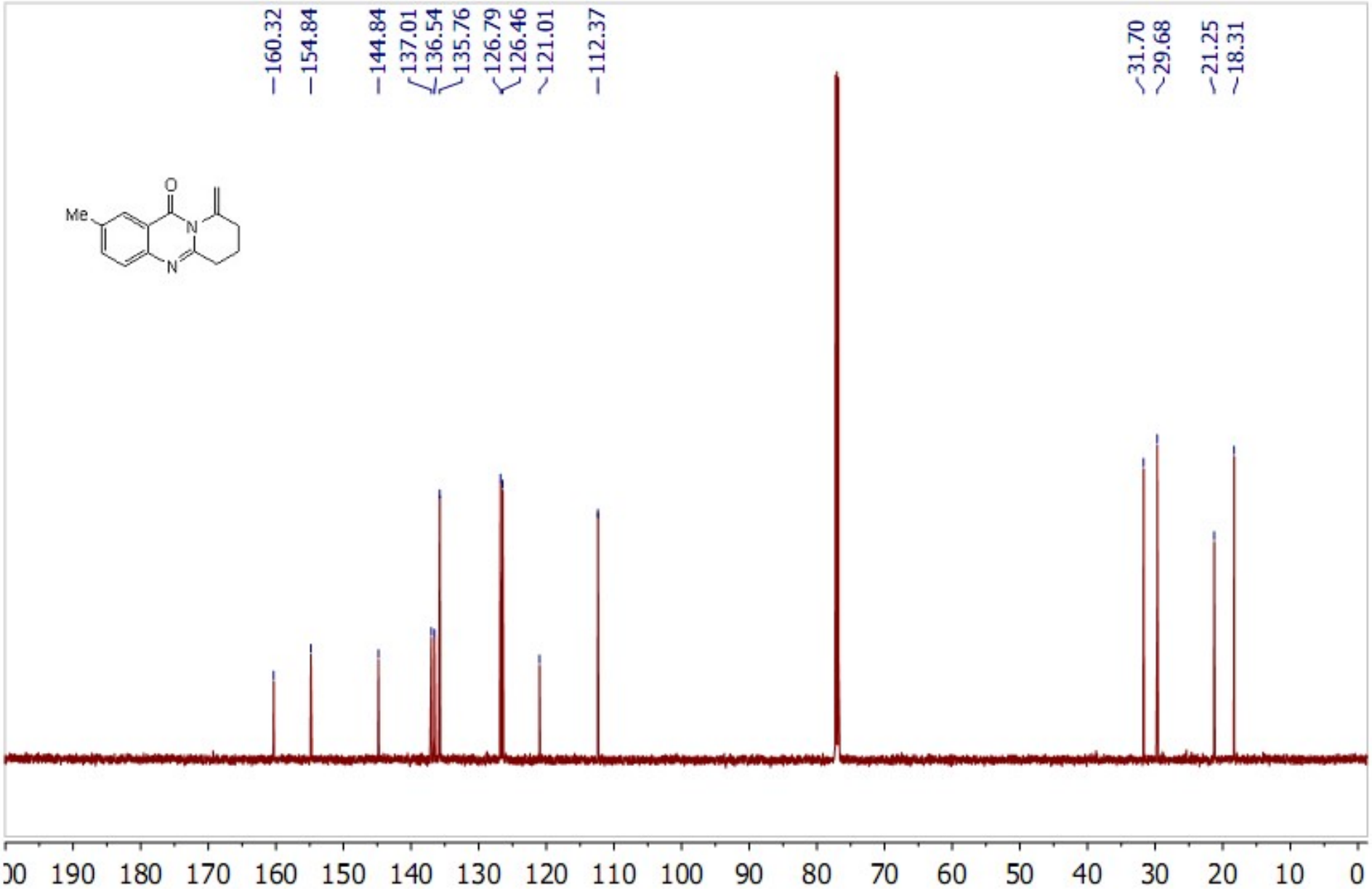
^{13}C NMR spectrum (151 MHz, $CDCl_3$) of compound 10b



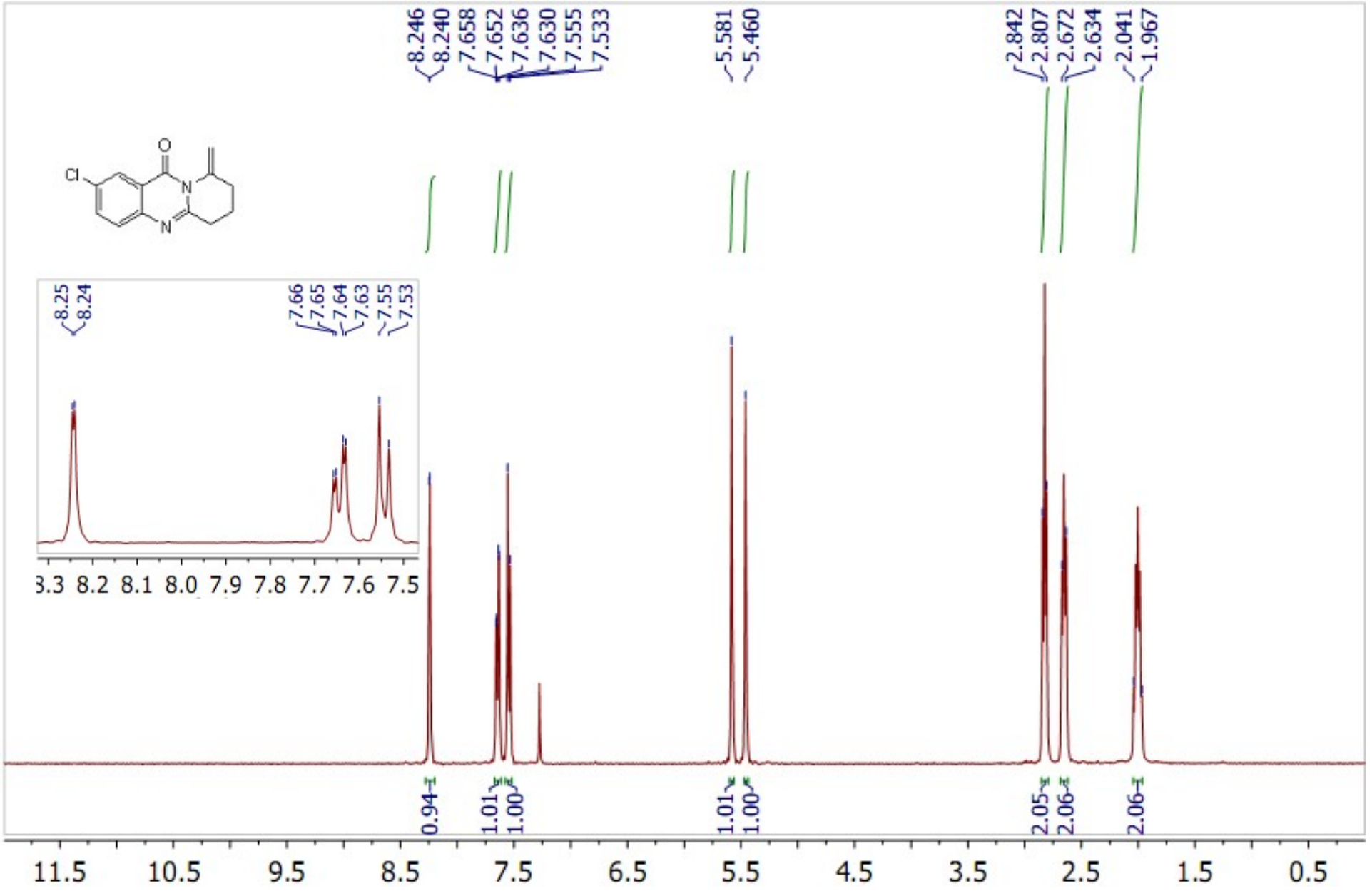
^{1}H NMR spectrum (400 MHz, $CDCl_3$) of compound 10c



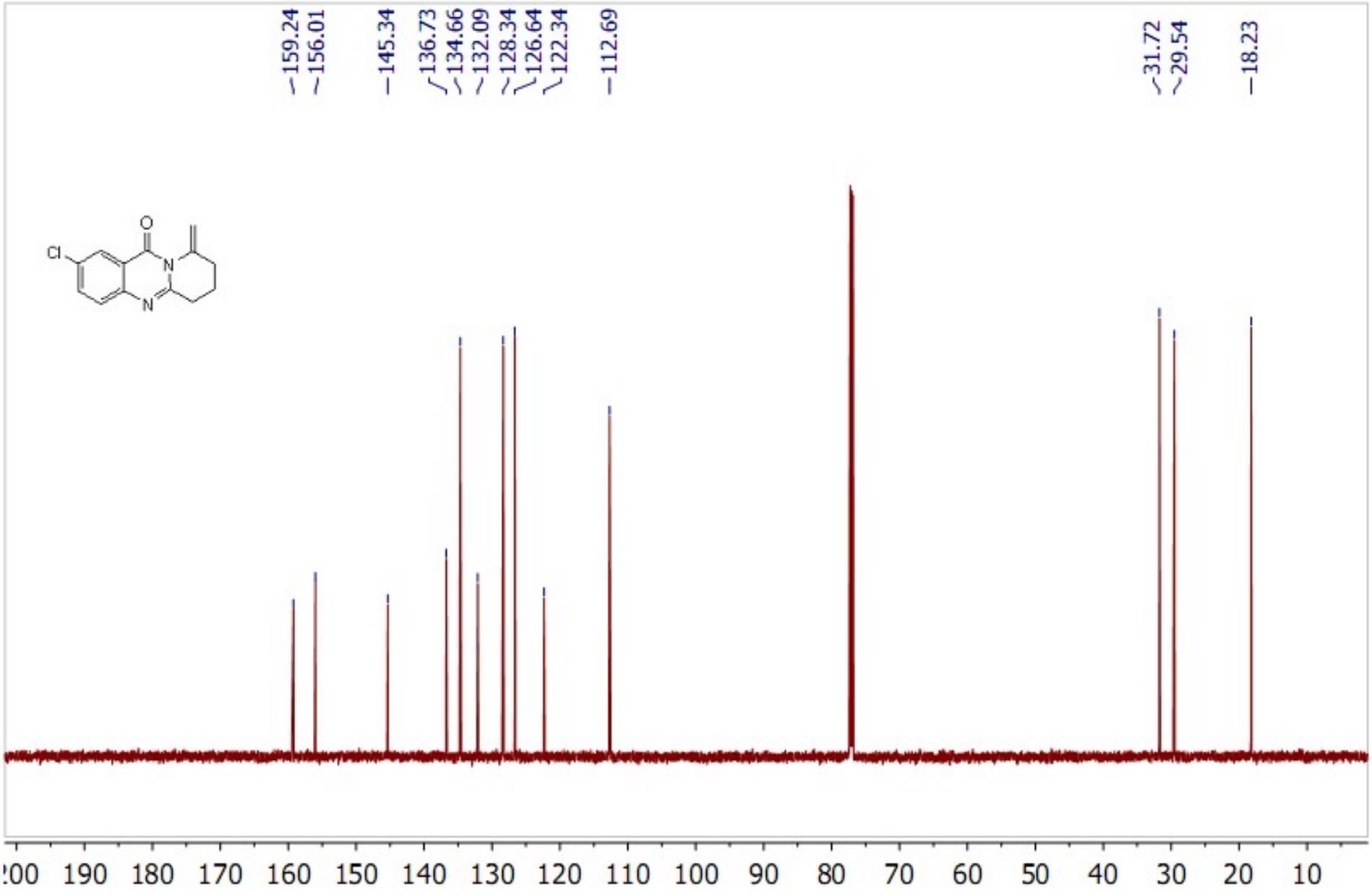
^{13}C NMR spectrum (151 MHz, $CDCl_3$) of compound 10c



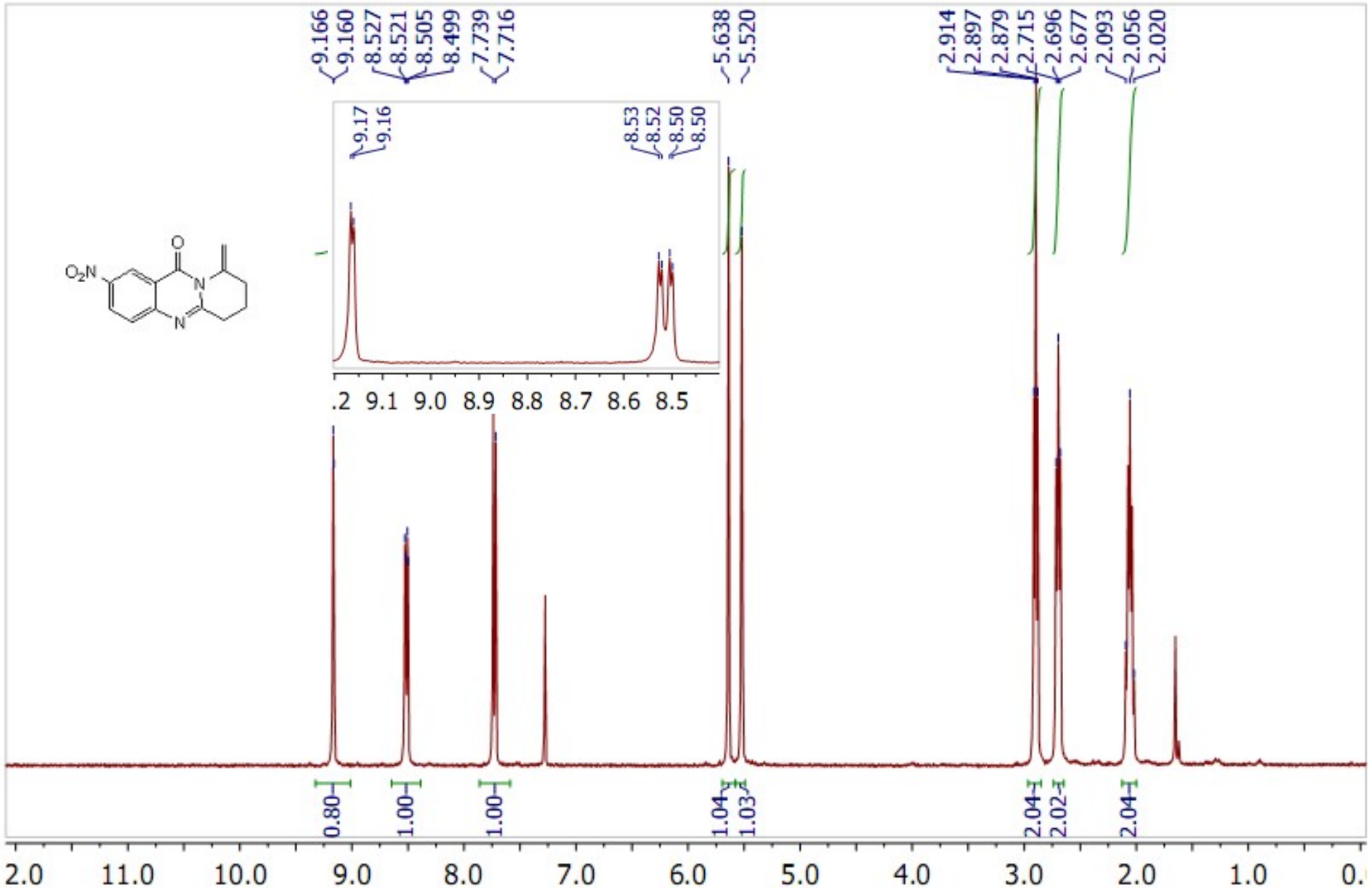
^{1}H NMR spectrum (400 MHz, $CDCl_3$) of compound 10d



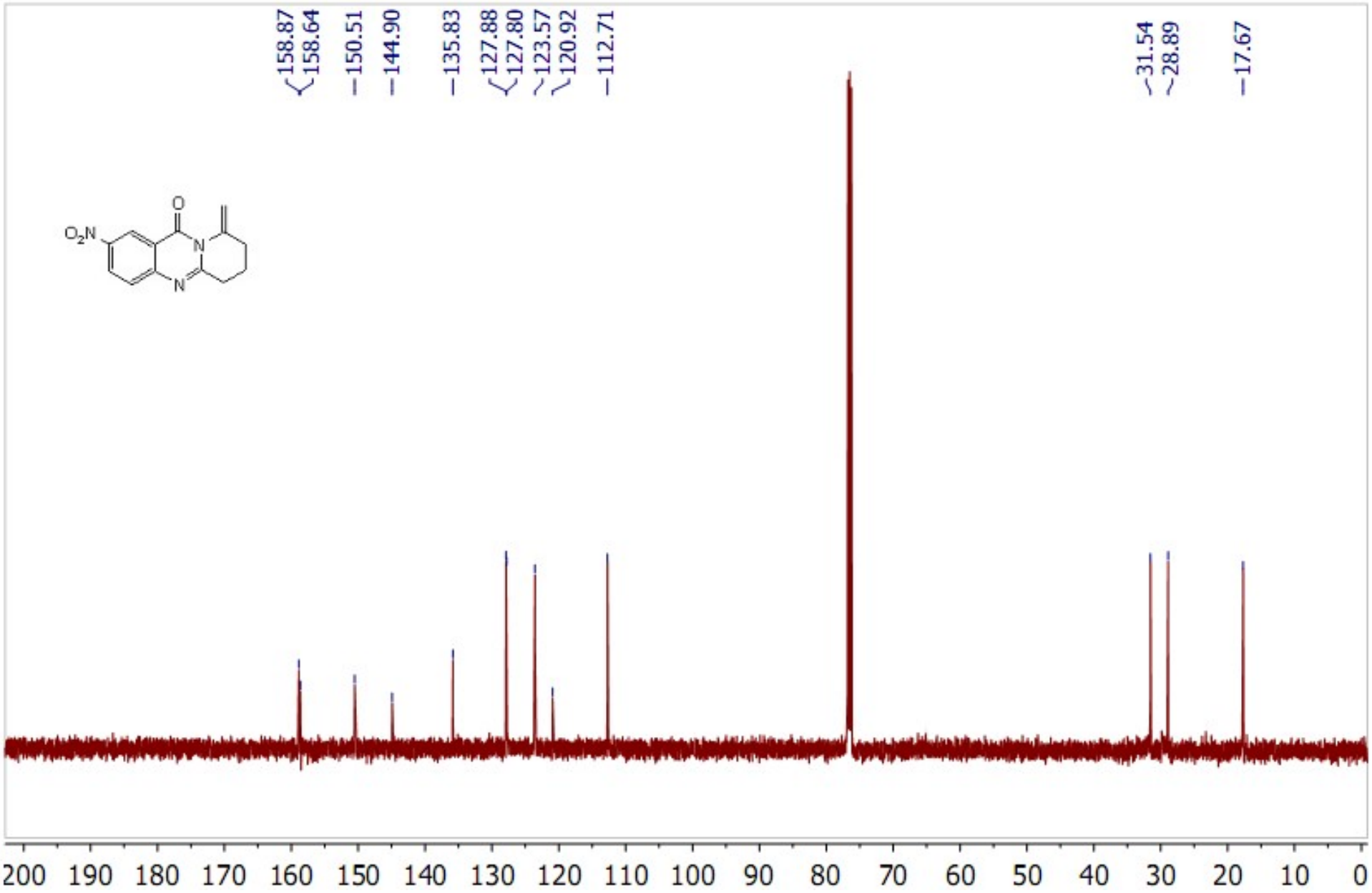
^{13}C NMR spectrum (151 MHz, $CDCl_3$) of compound 10d



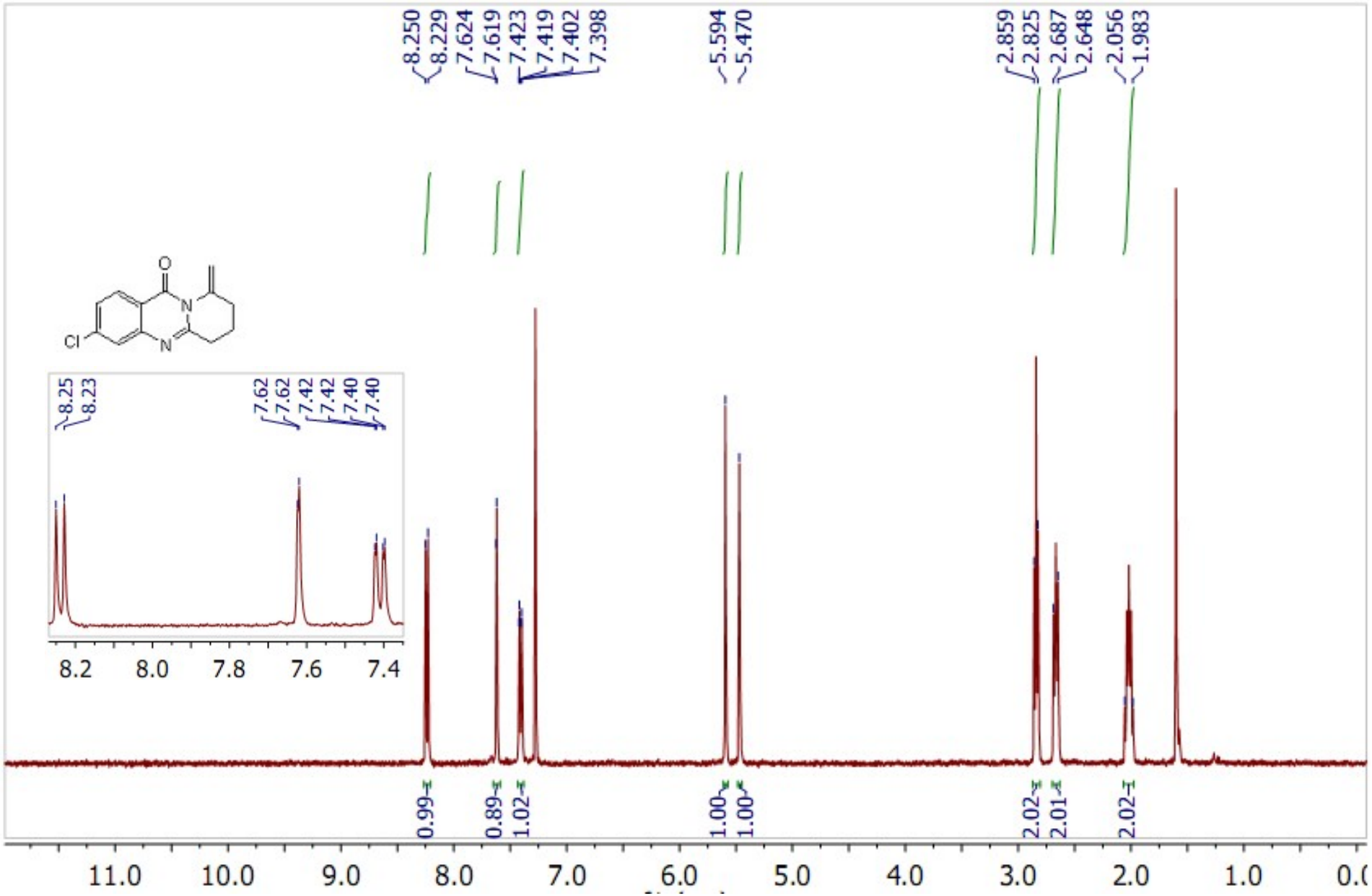
^{1}H NMR spectrum (400 MHz, $CDCl_3$) of compound 10e



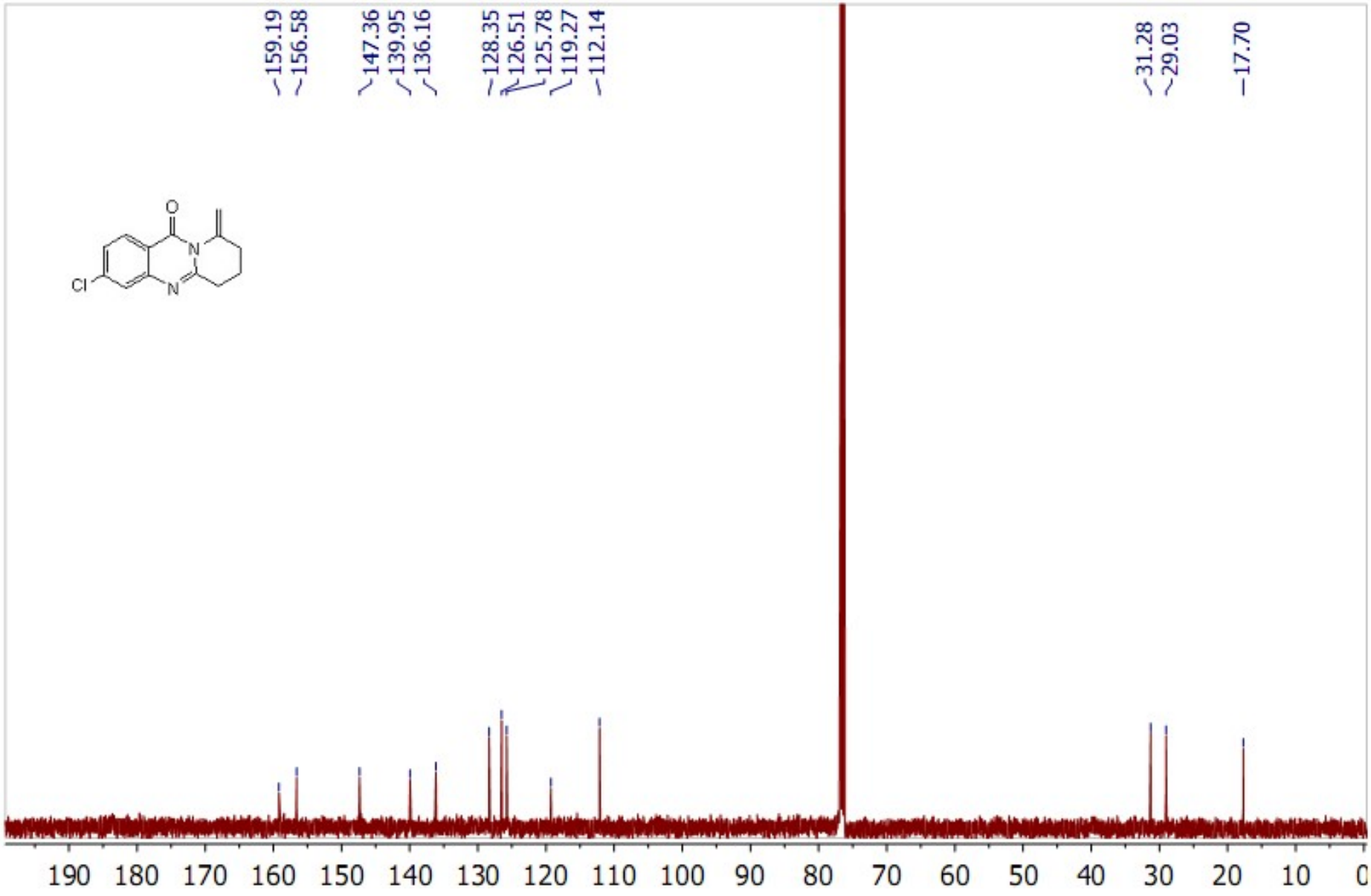
^{13}C NMR spectrum (126 MHz, $CDCl_3$) of compound 10e



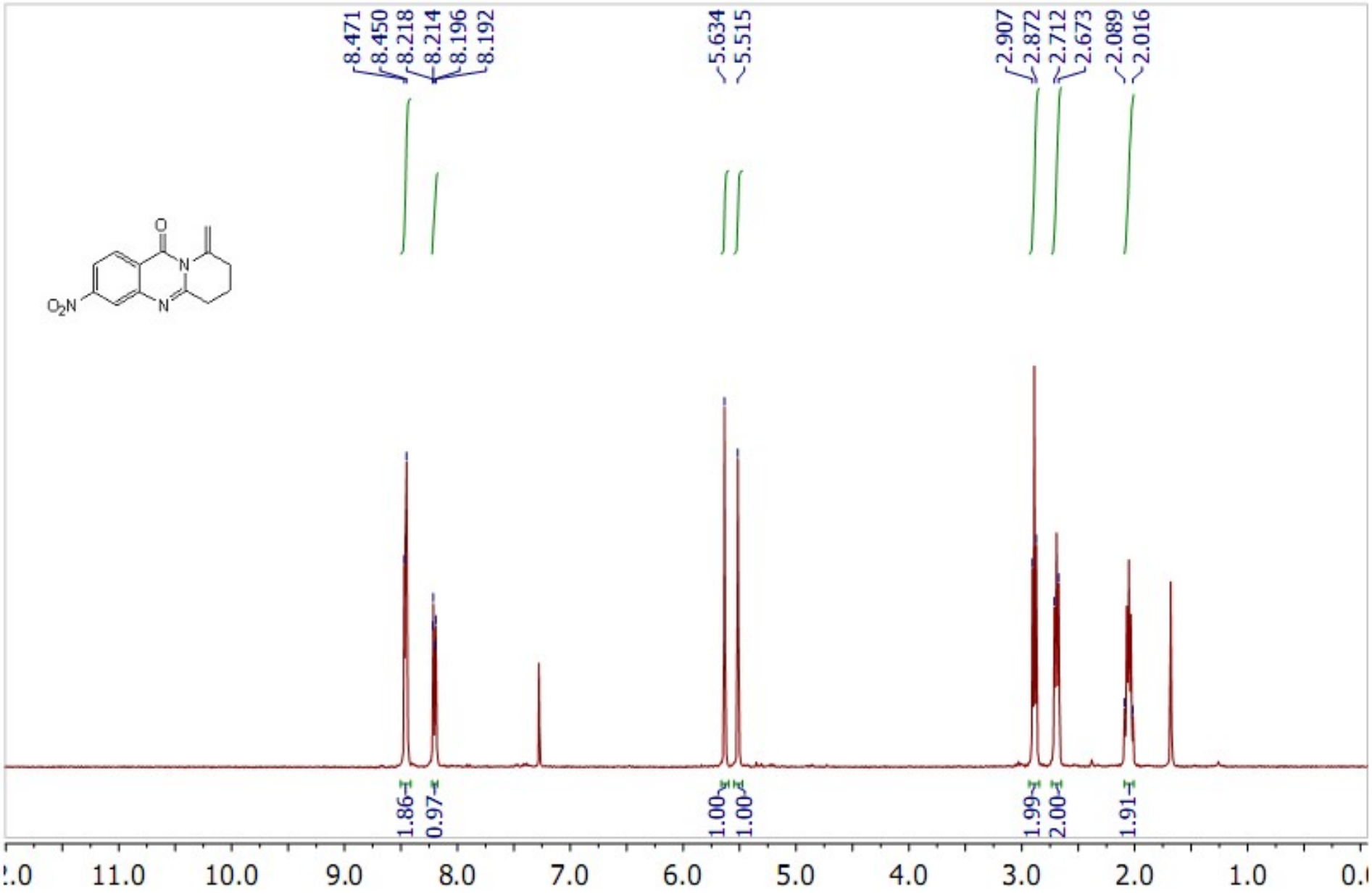
^{1}H NMR spectrum (400 MHz, $CDCl_3$) of compound 10f



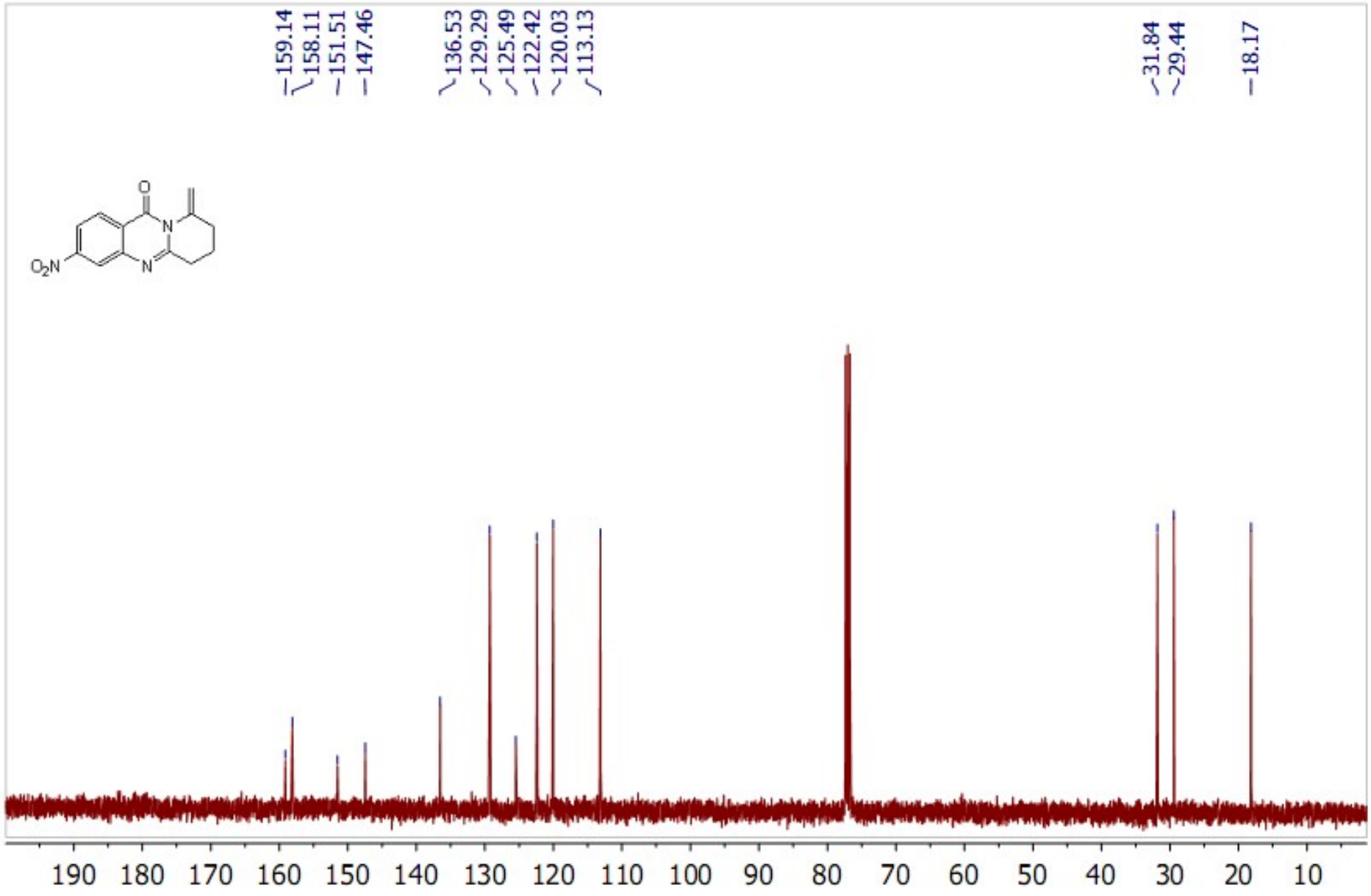
^{13}C NMR spectrum (126 MHz, $CDCl_3$) of compound 10f.



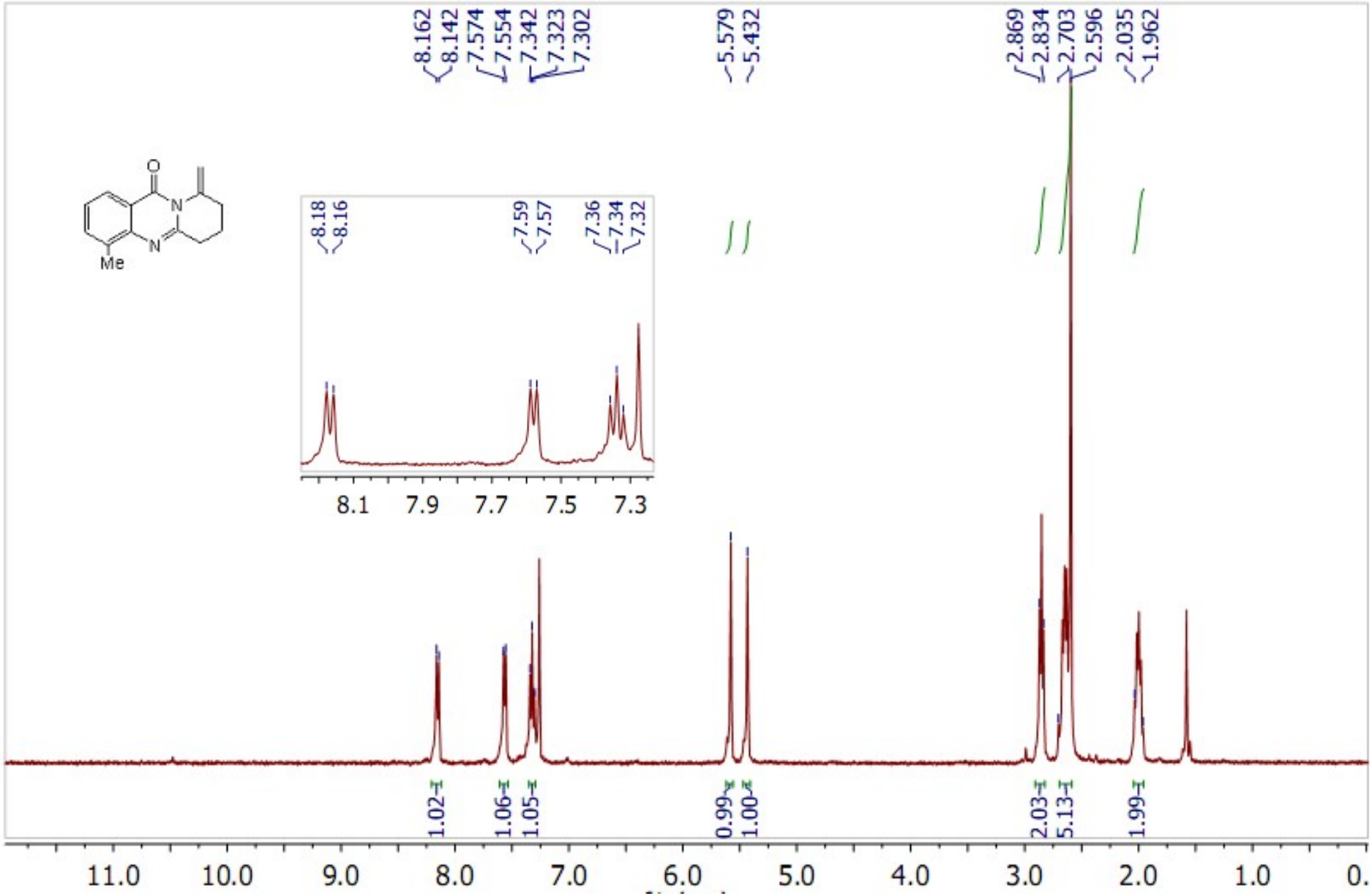
^{1}H NMR spectrum (400 MHz, $CDCl_3$) of compound 10g



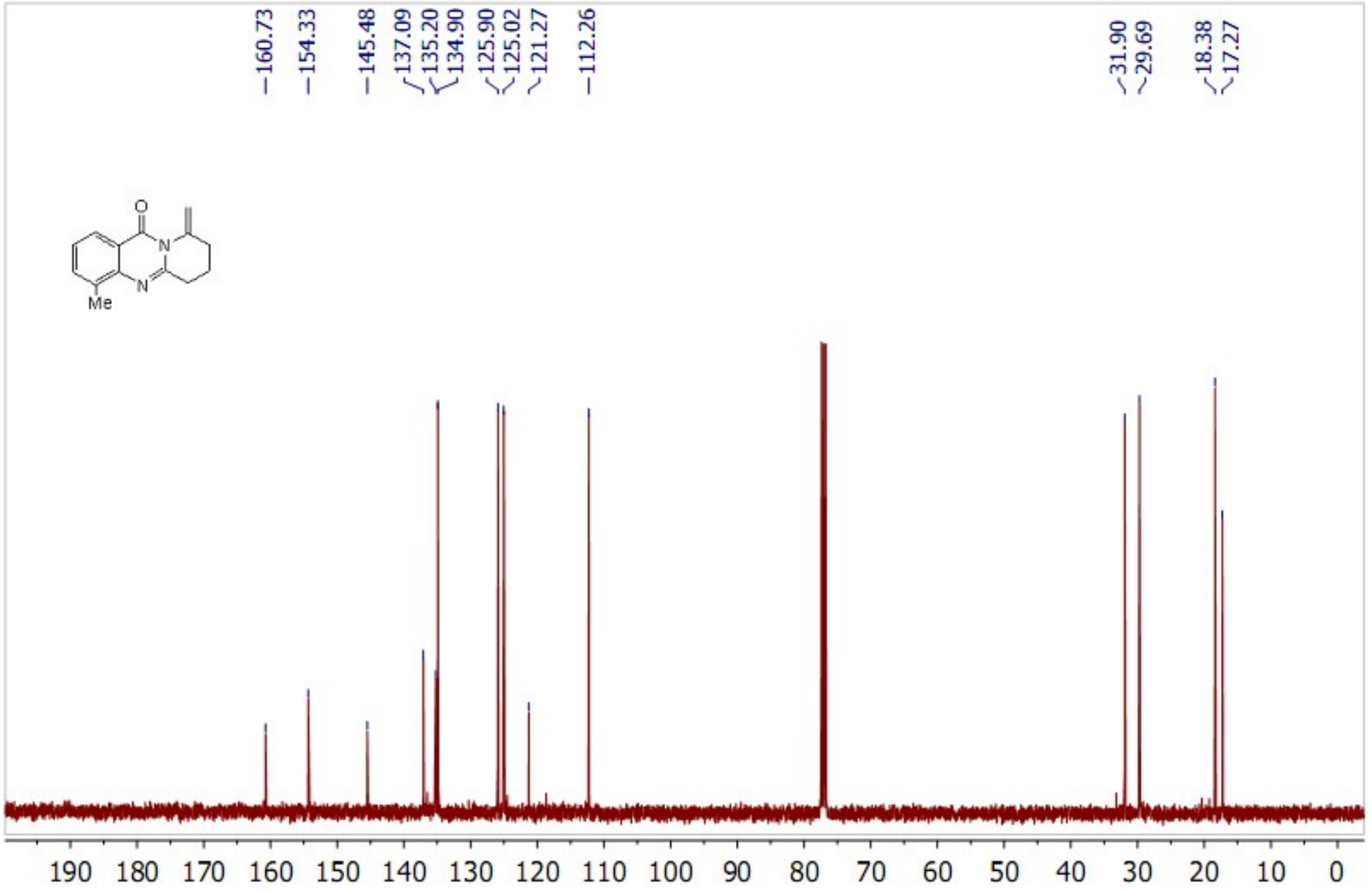
^{13}C NMR spectrum (101 MHz, $CDCl_3$) of compound 10g



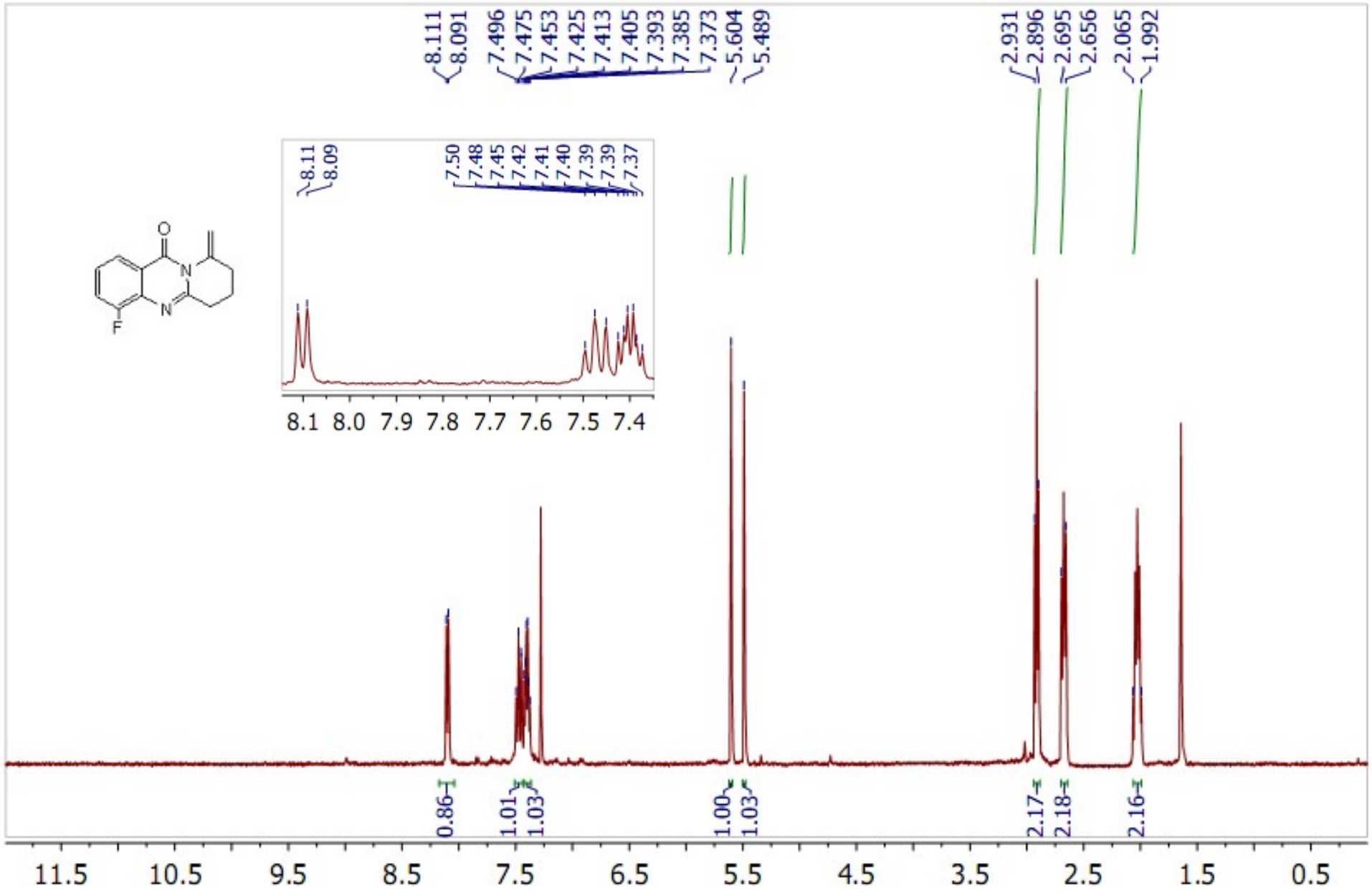
^{1}H NMR spectrum (400 MHz, $CDCl_3$) of compound 10h



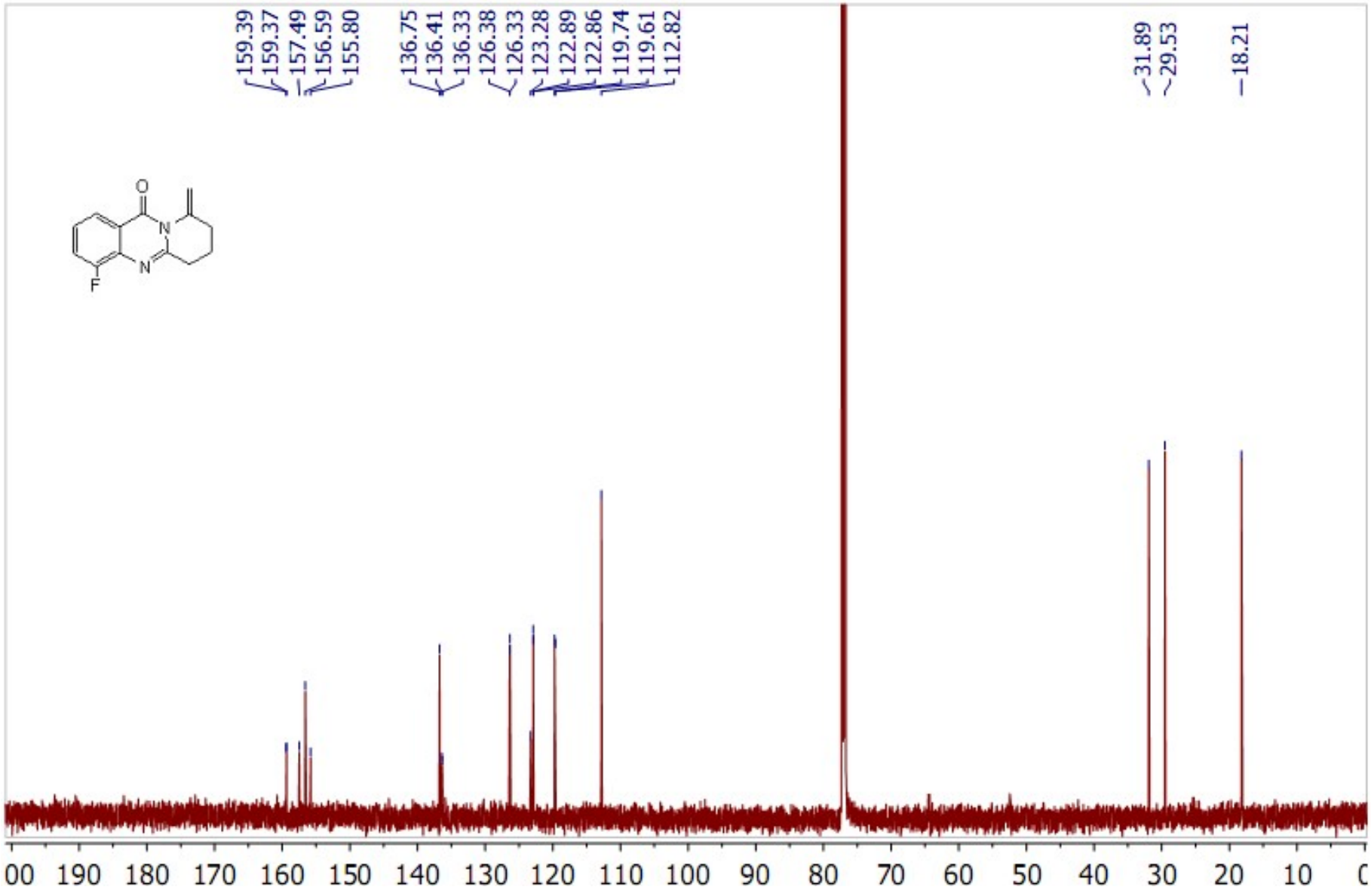
^{13}C NMR spectrum (101 MHz, $CDCl_3$) of compound 10h



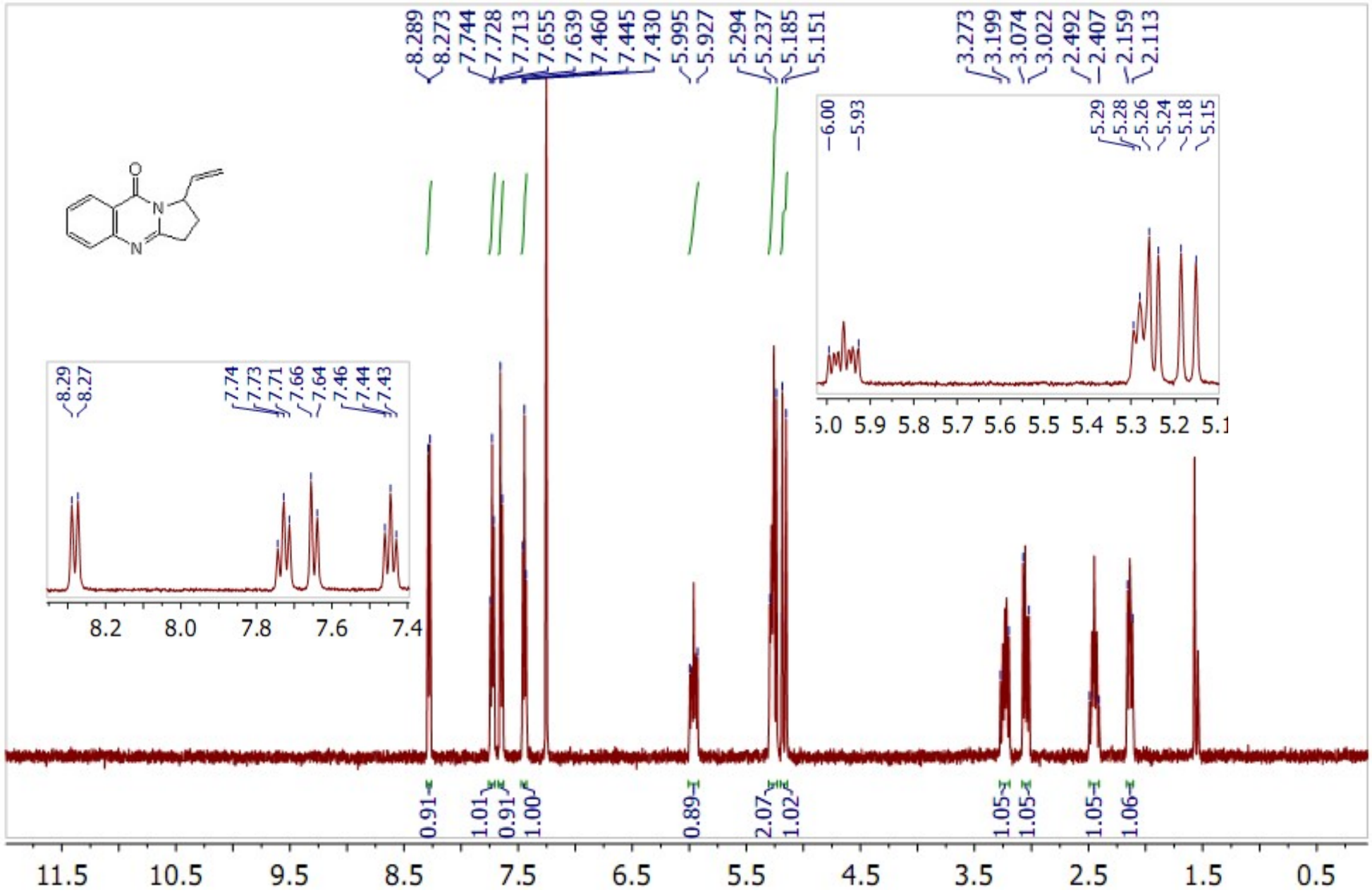
^{1}H NMR spectrum (400 MHz, $CDCl_3$) of compound 10i



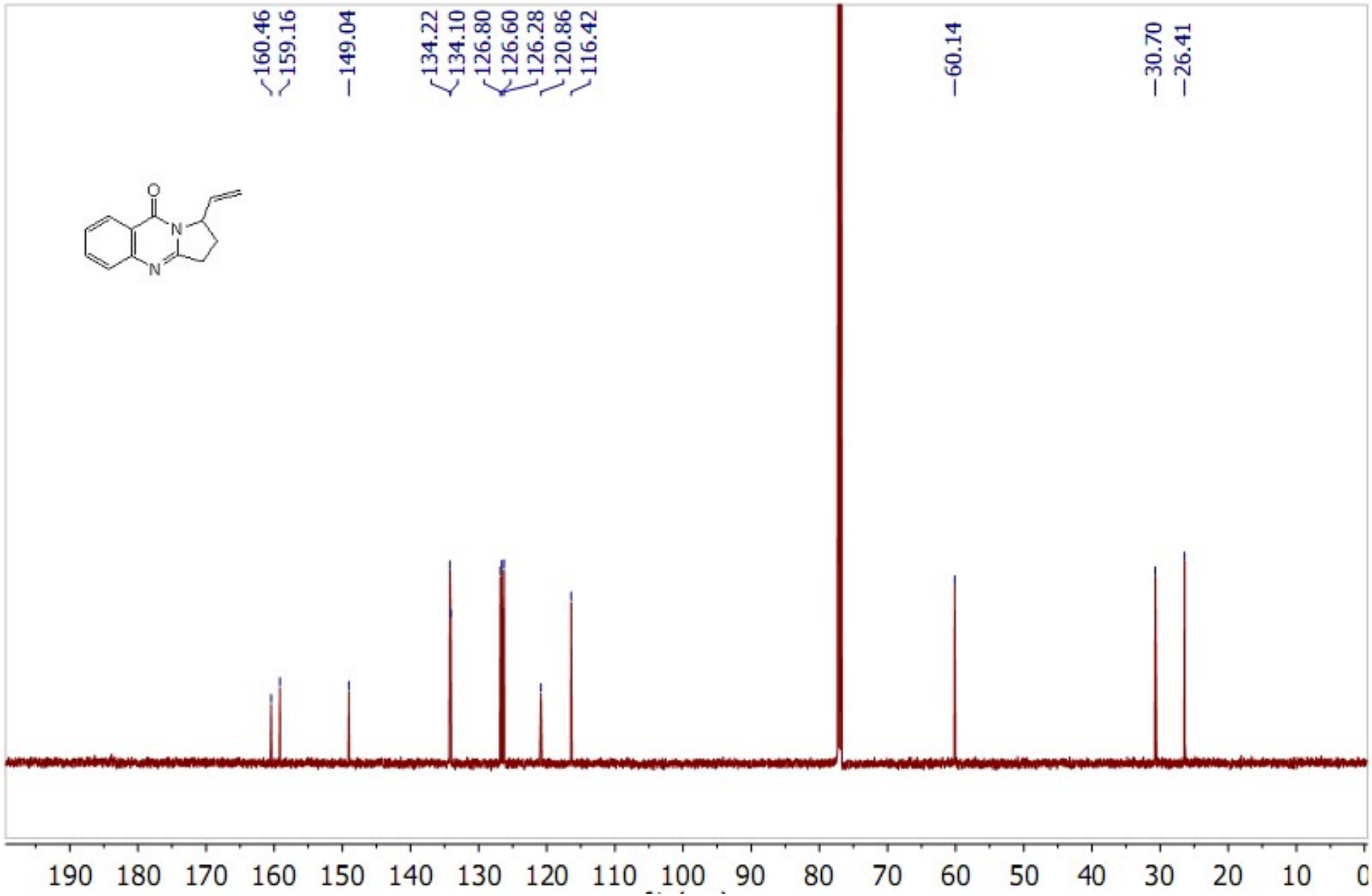
^{13}C NMR spectrum (151 MHz, $CDCl_3$) of compound 10i



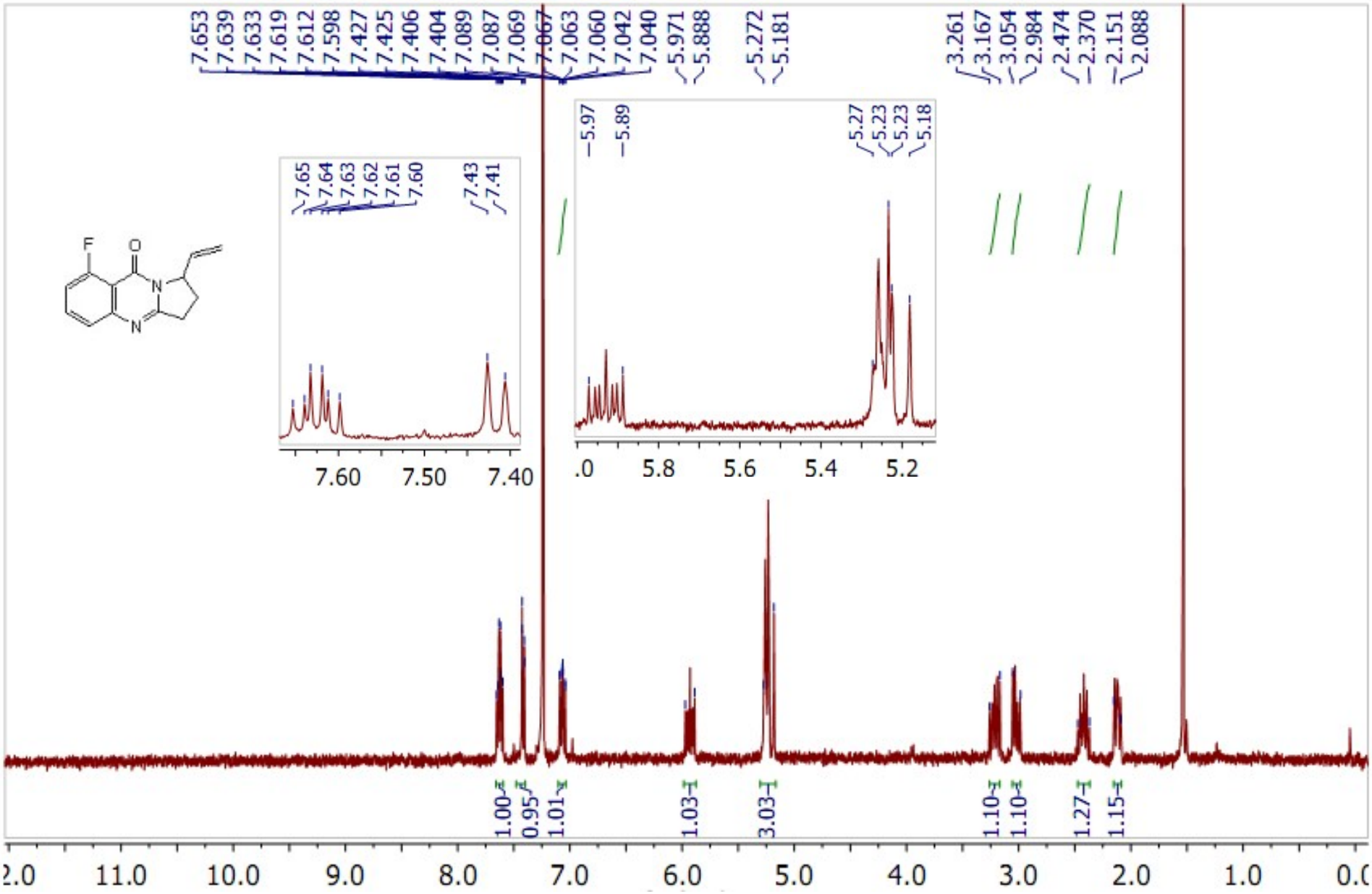
^{1}H NMR spectrum (500 MHz, $CDCl_3$) of compound 11a



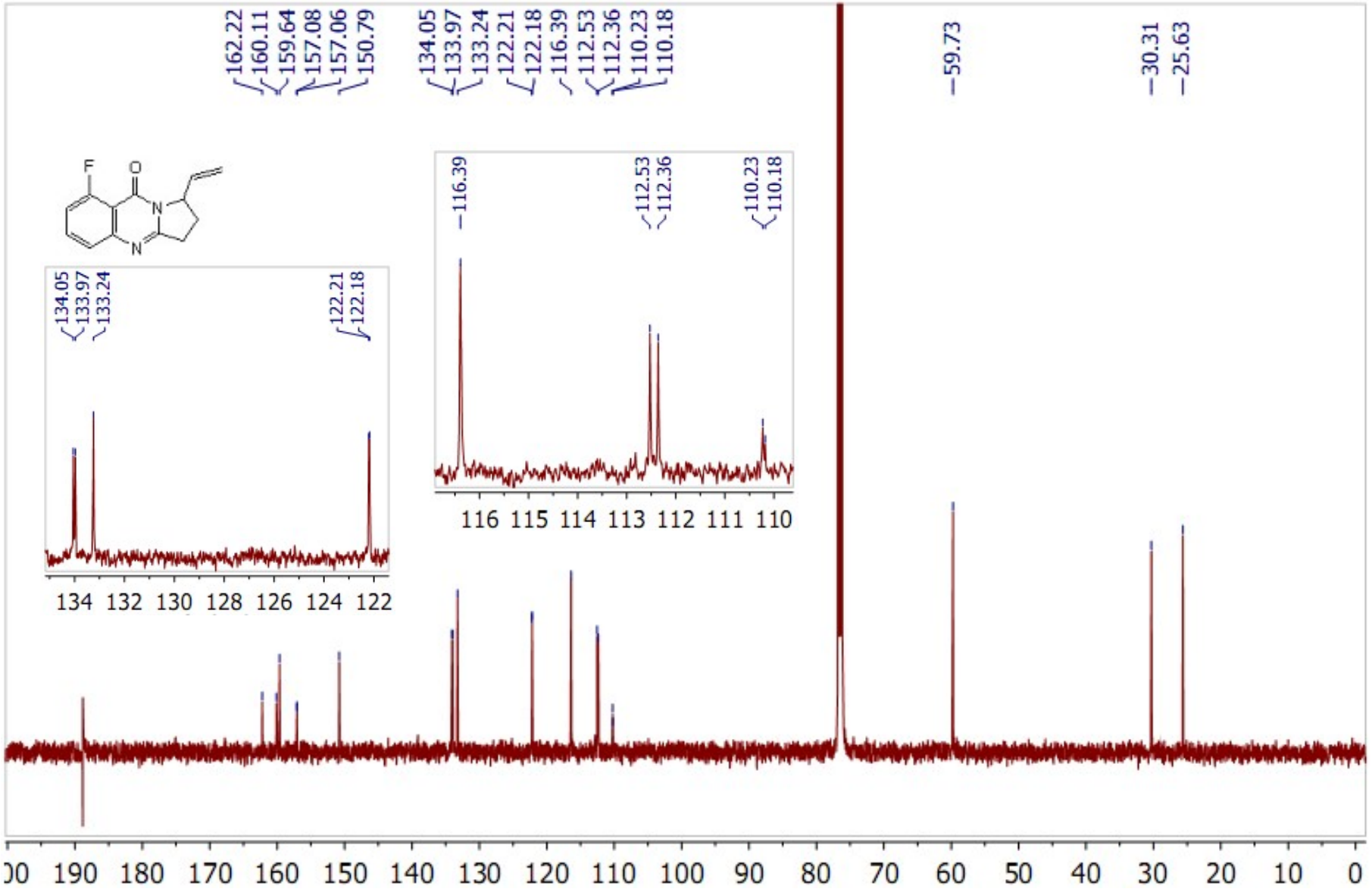
^{13}C NMR spectrum (151 MHz, $CDCl_3$) of compound 11a



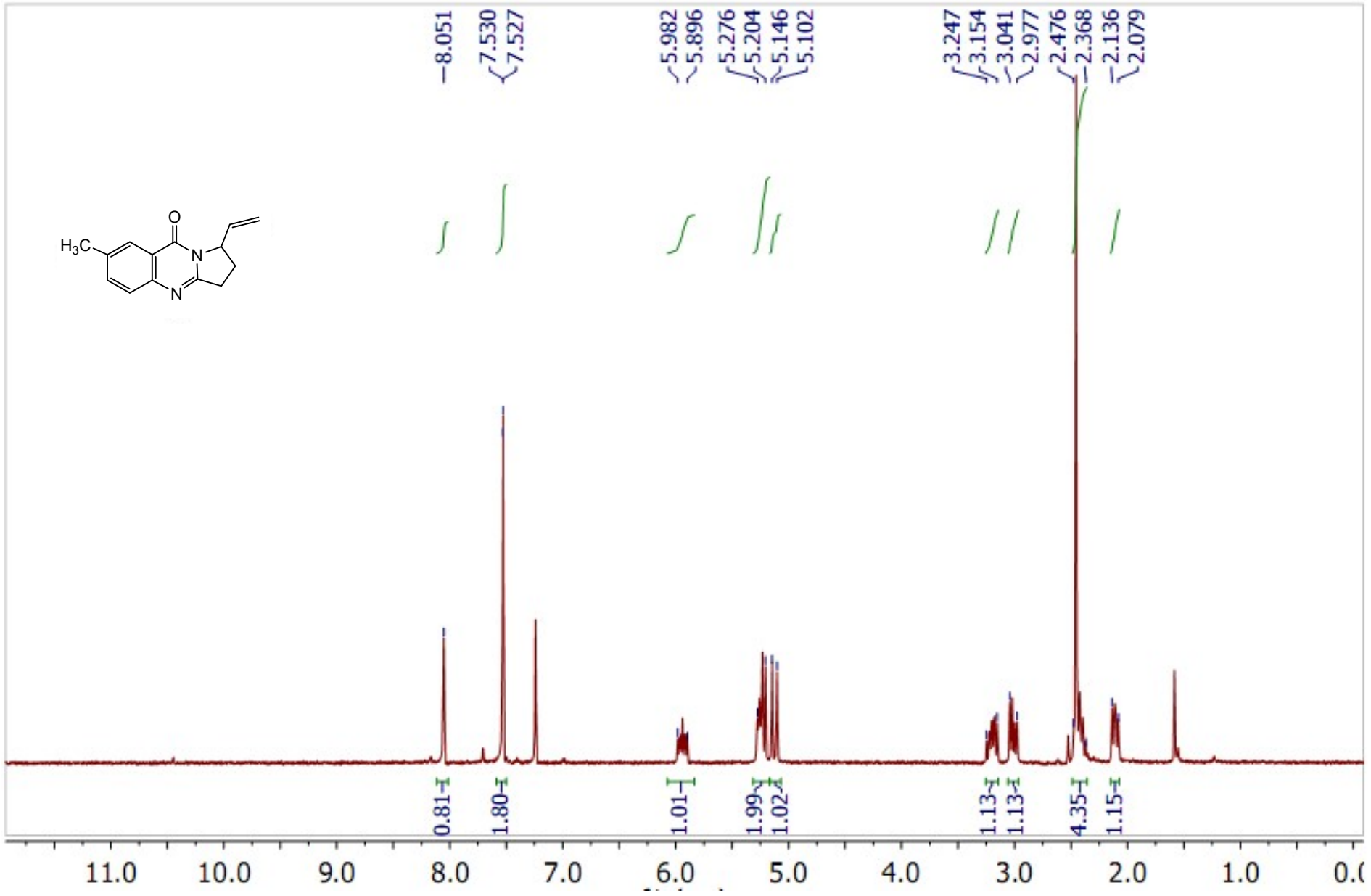
^{1}H NMR spectrum (400 MHz, $CDCl_3$) of compound 11b



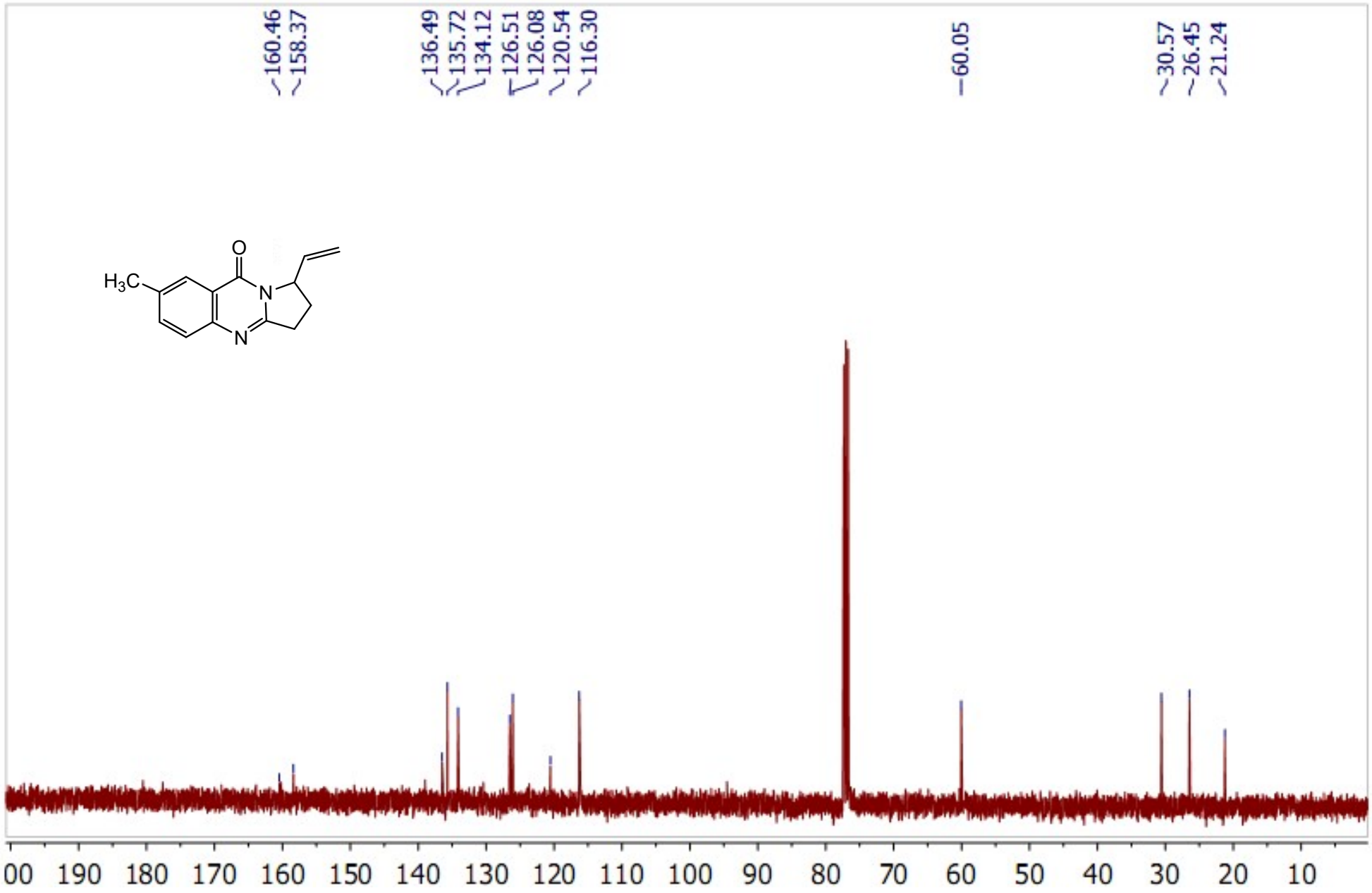
^{13}C NMR spectrum (126 MHz, $CDCl_3$) of compound 11b



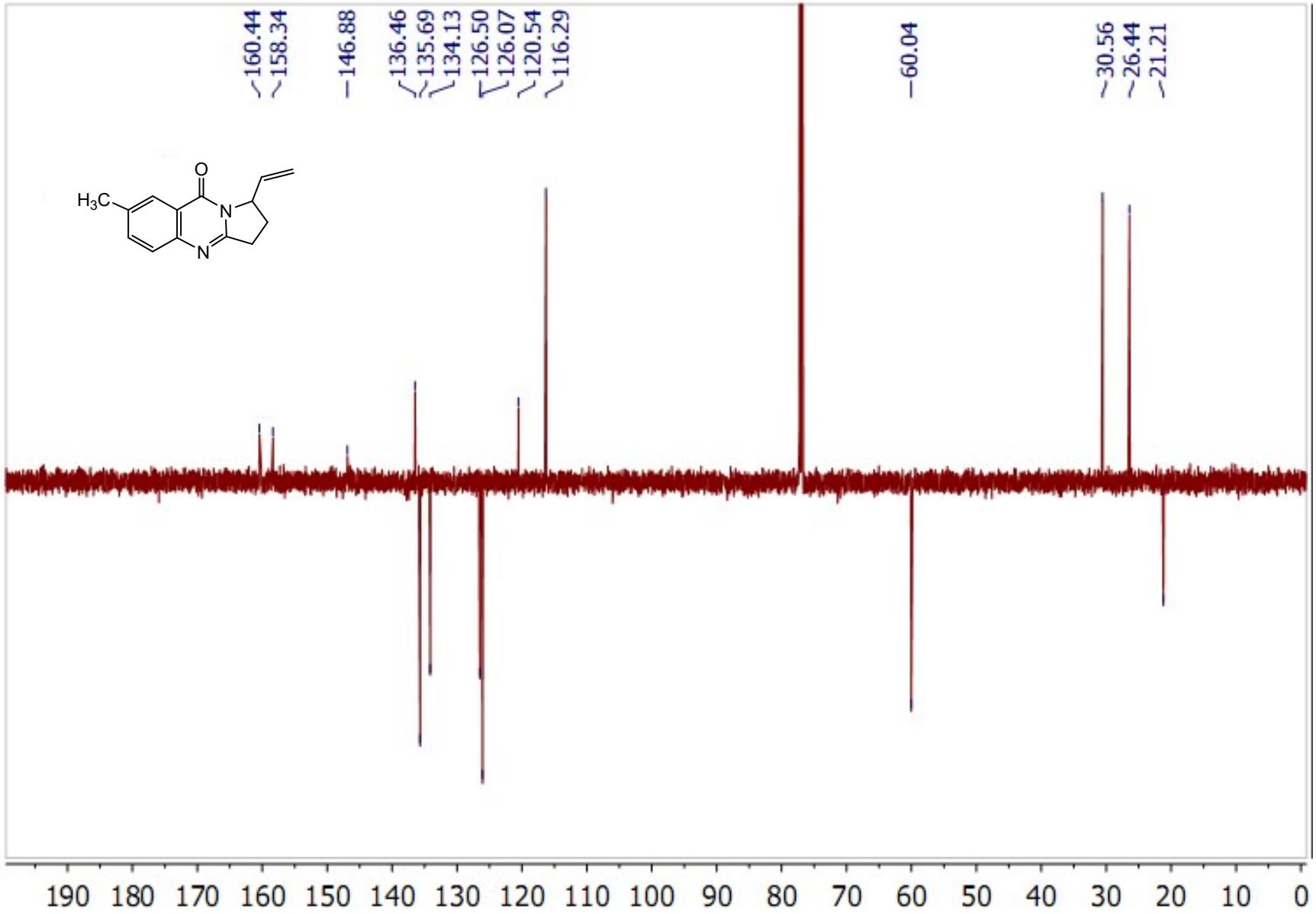
^{1}H NMR spectrum (400 MHz, $CDCl_3$) of compound 11c



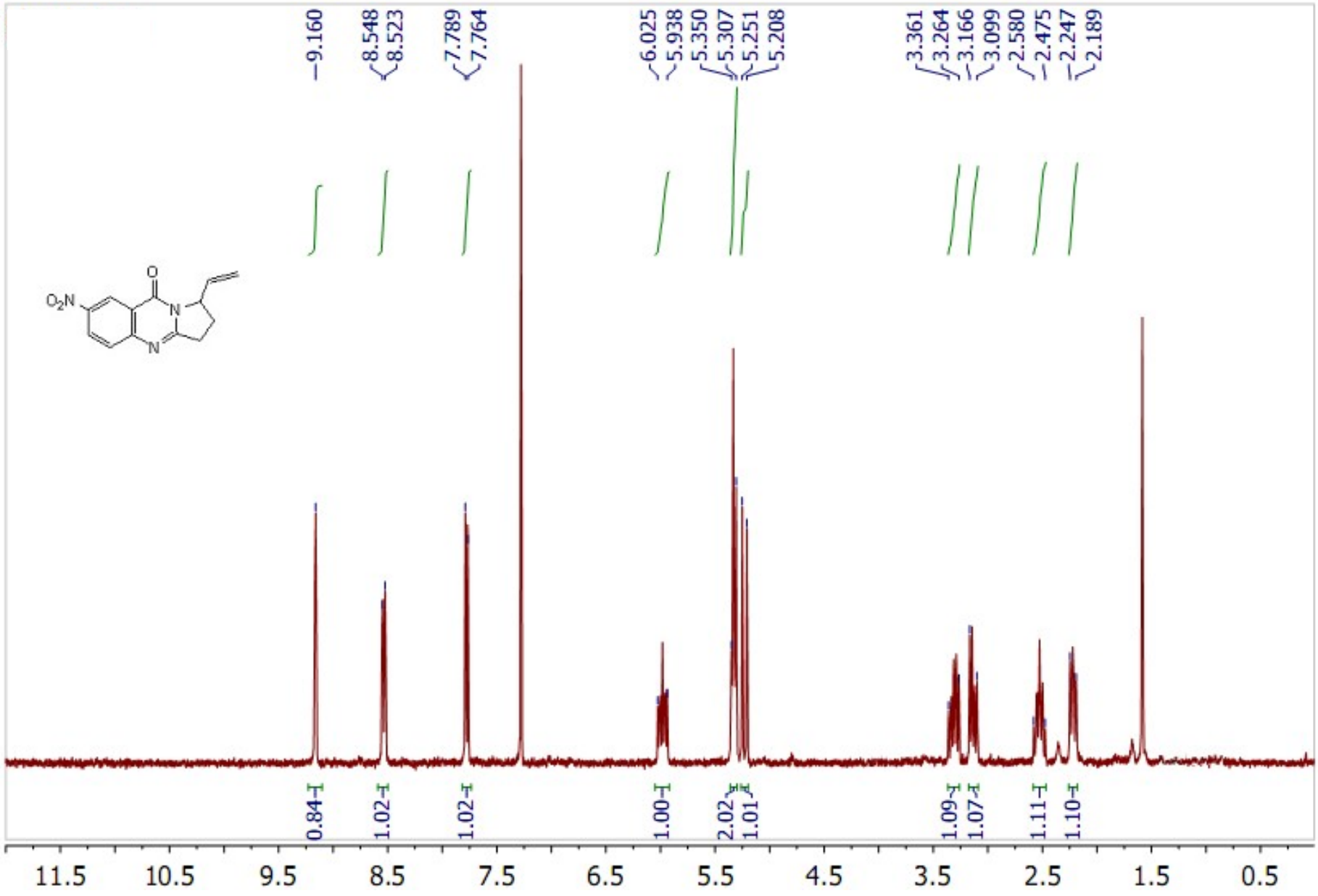
^{13}C NMR spectrum (101 MHz, $CDCl_3$) of compound 11c



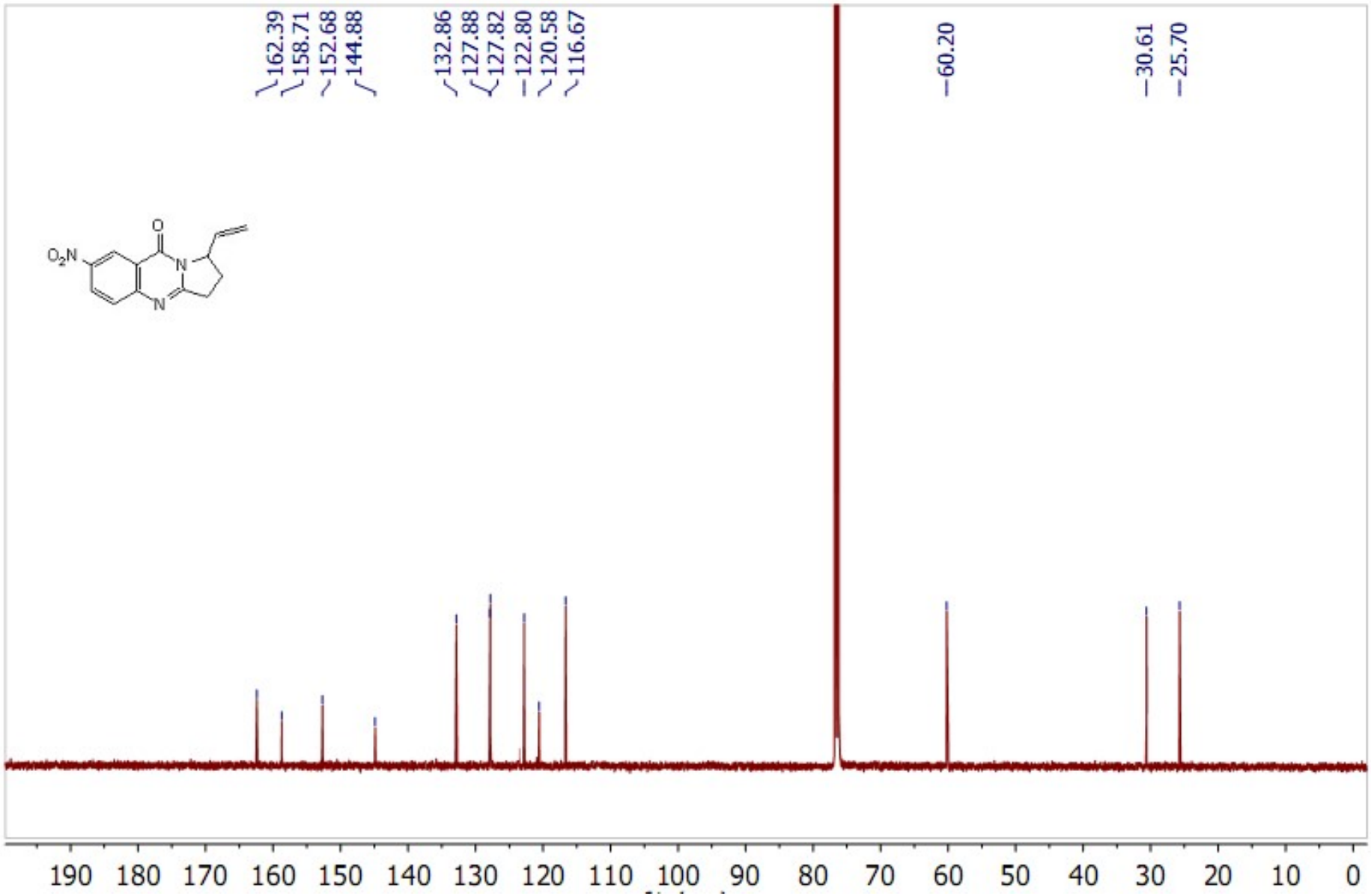
13C/APT NMR spectrum (151 MHz, $CDCl_3$) of compound 11c



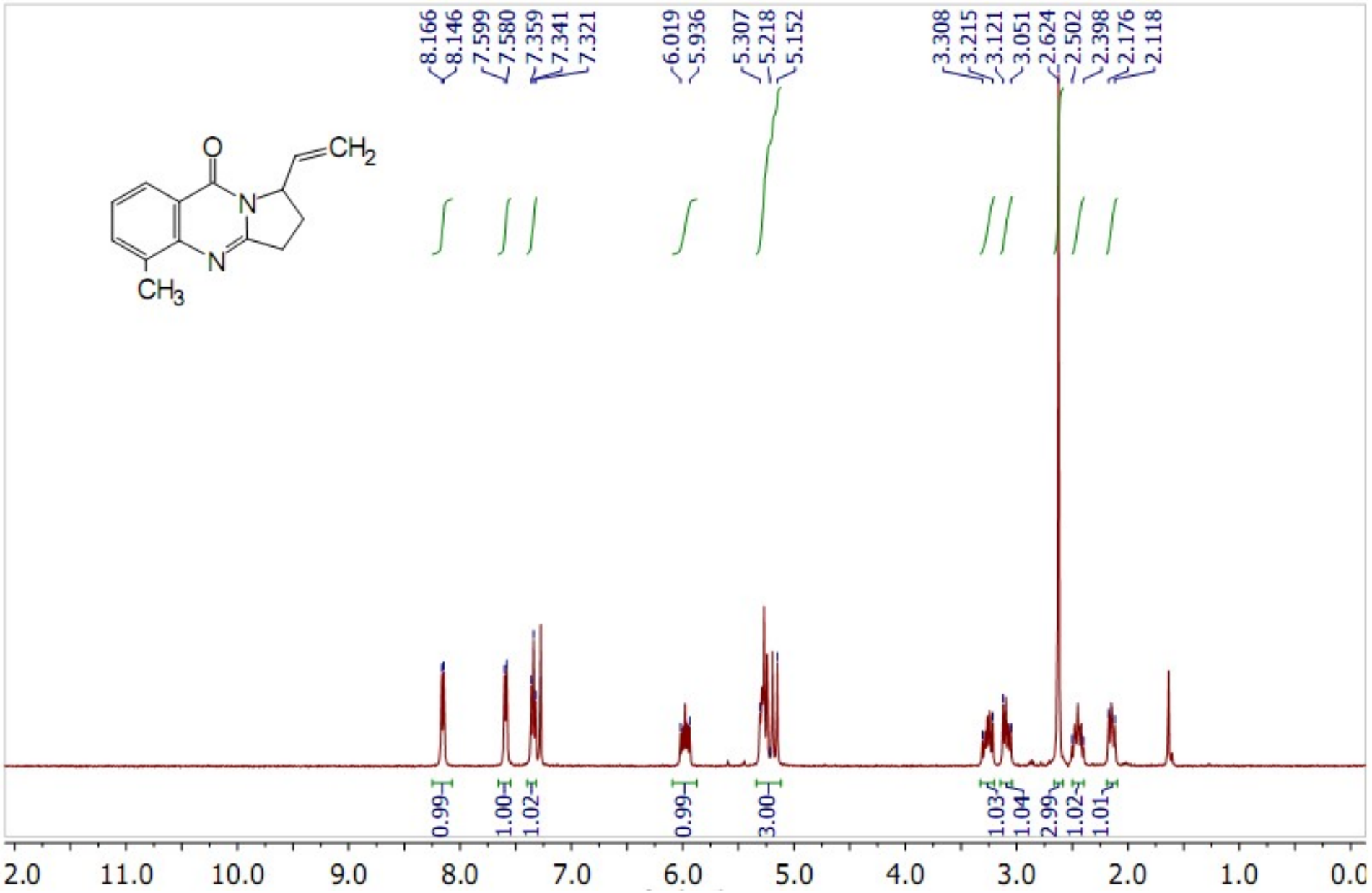
^{1}H NMR spectrum (400 MHz, $CDCl_3$) of compound 11e



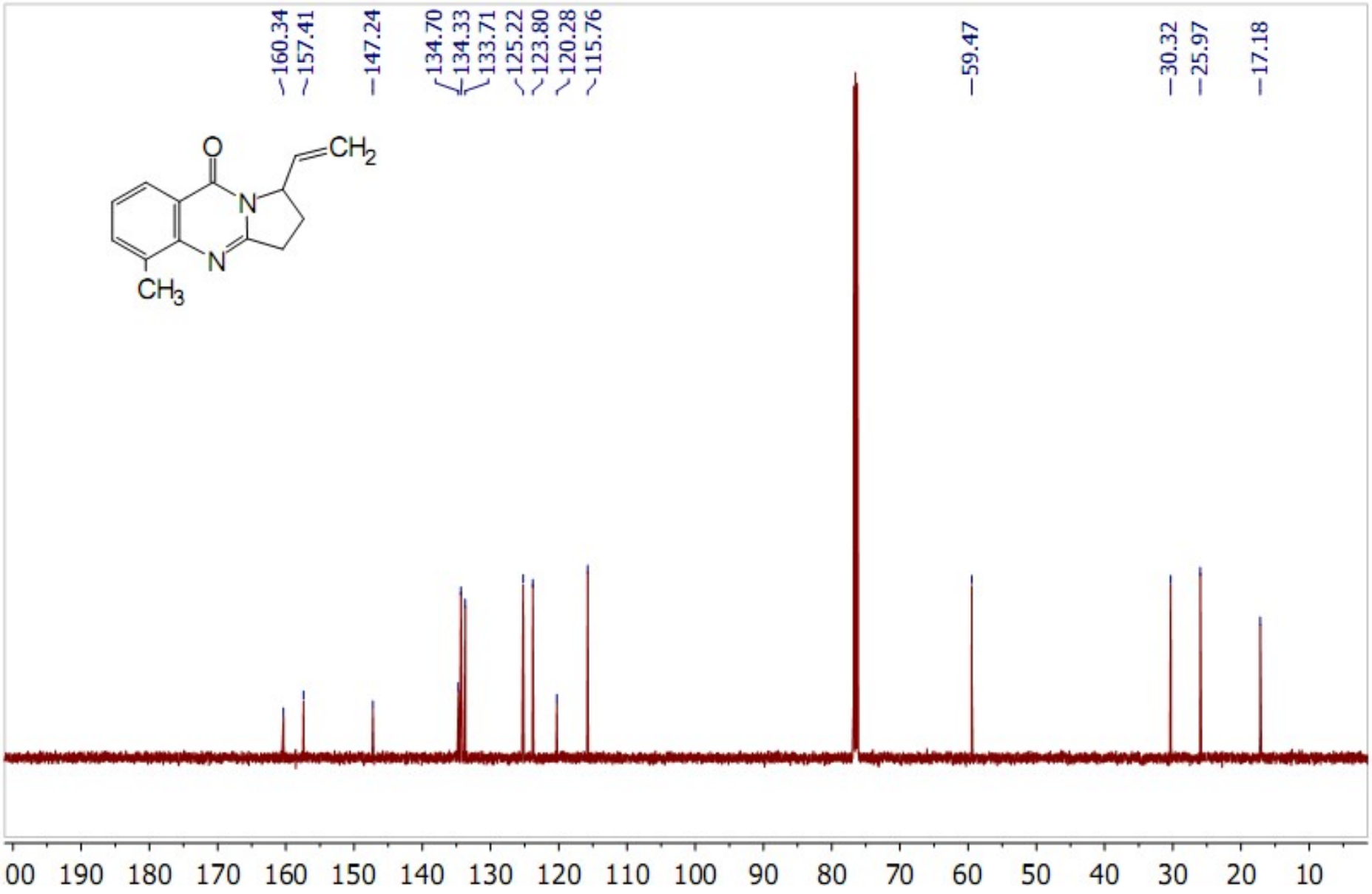
^{13}C NMR spectrum (126 MHz, $CDCl_3$) of compound 11e



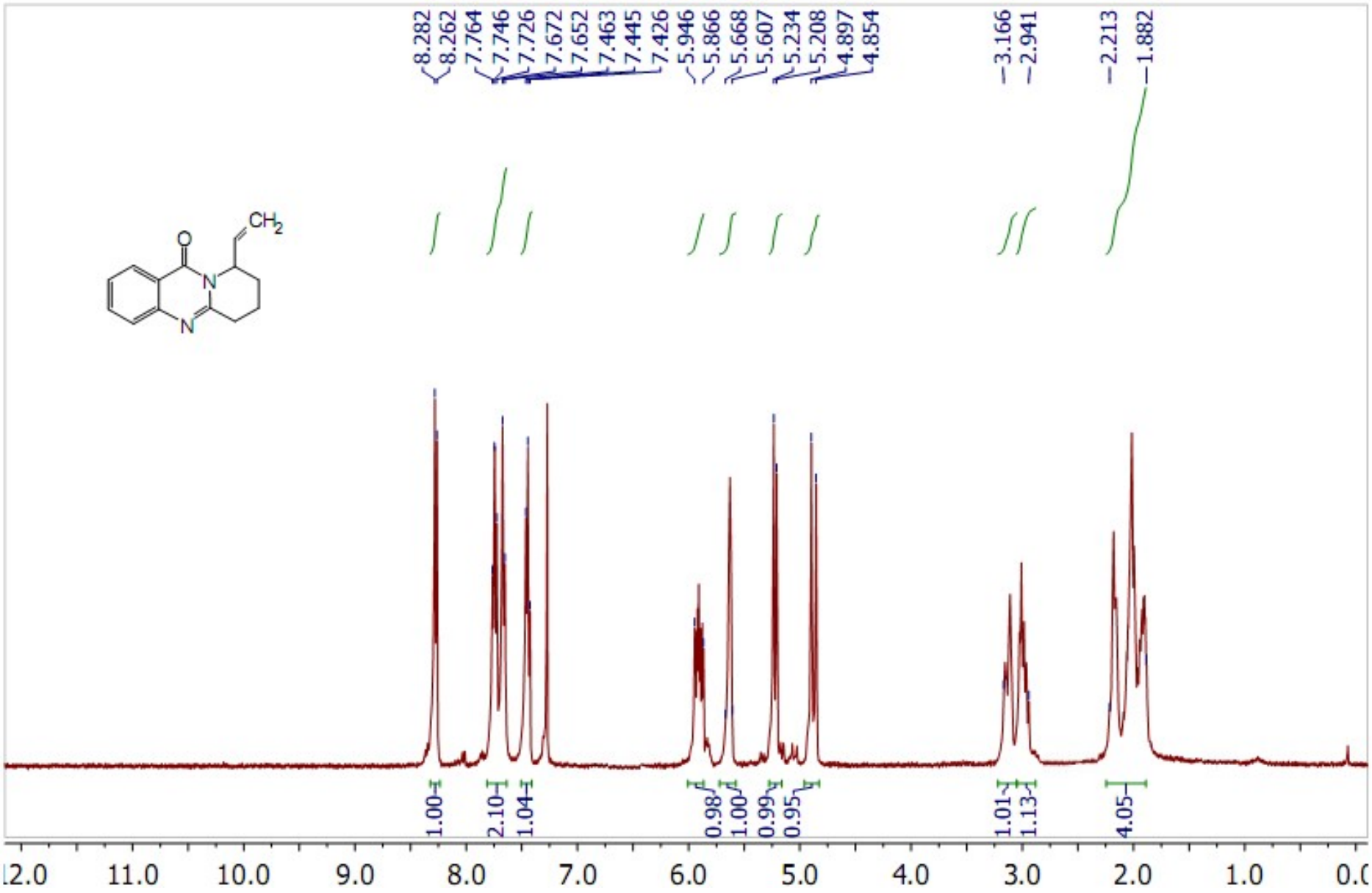
^{1}H NMR spectrum (400 MHz, $CDCl_3$) of compound 11h



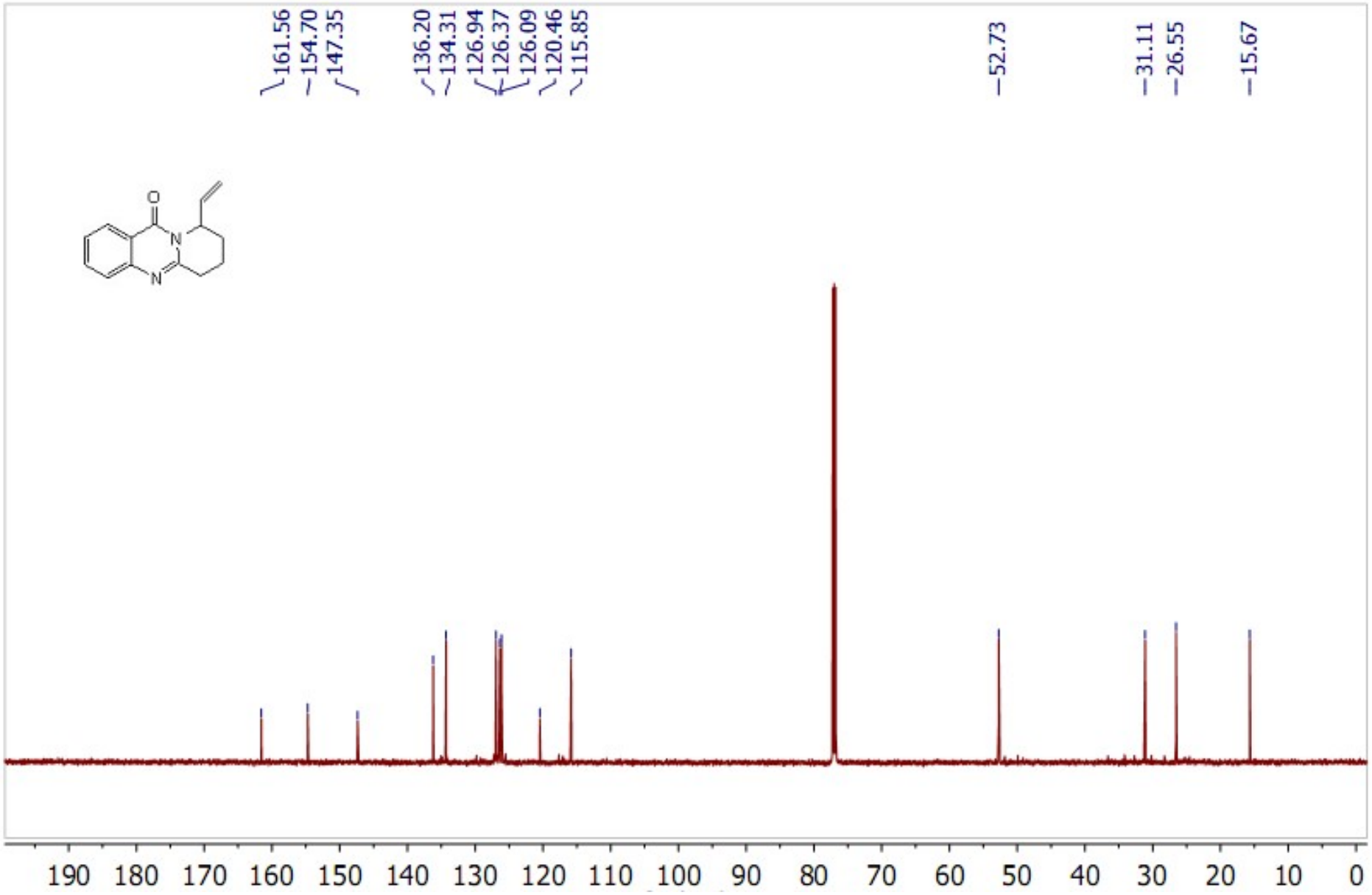
^{13}C NMR spectrum (126 MHz, $CDCl_3$) of compound 11h



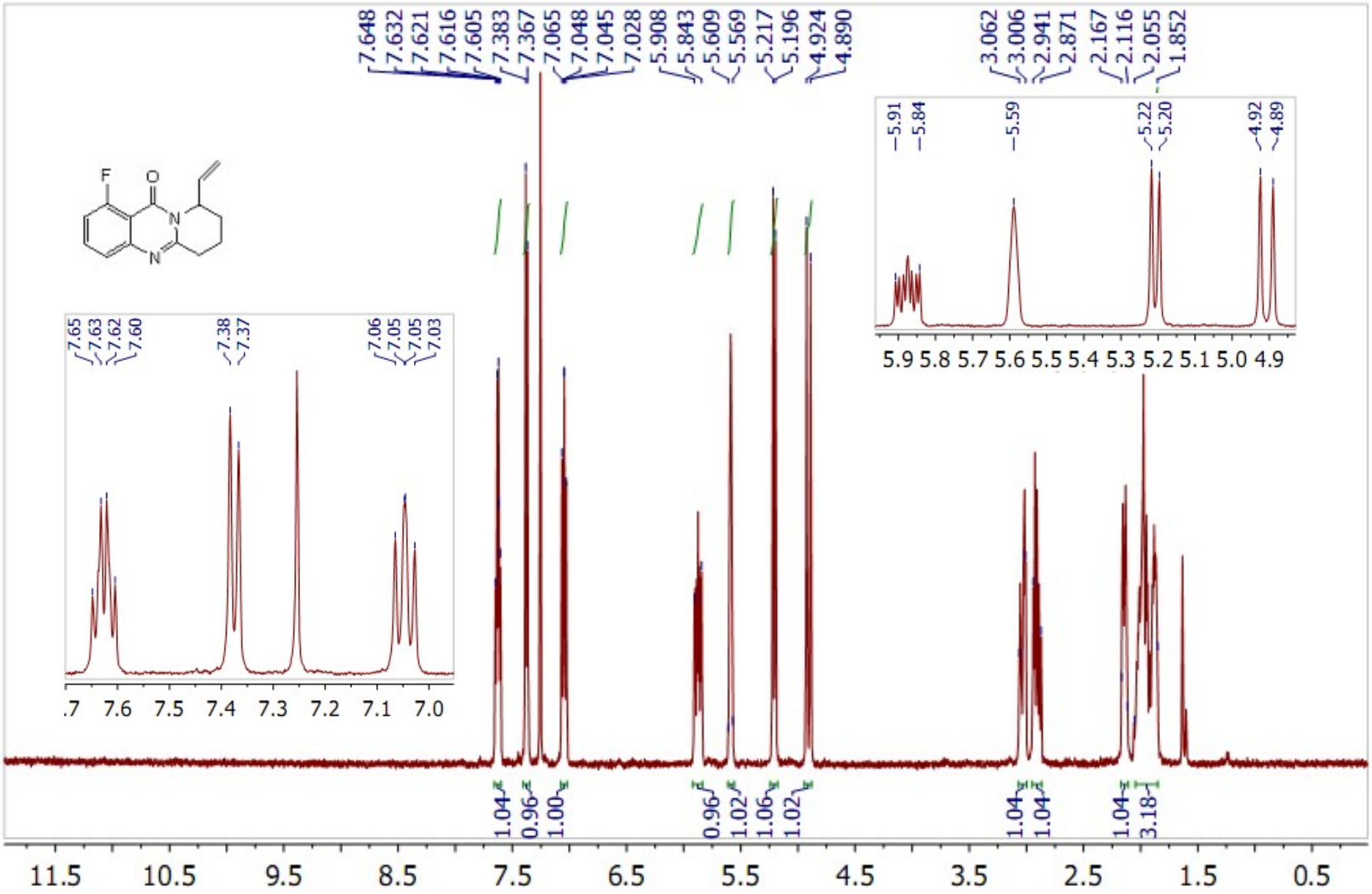
^{1}H NMR spectrum (400 MHz, $CDCl_3$) of compound 12a



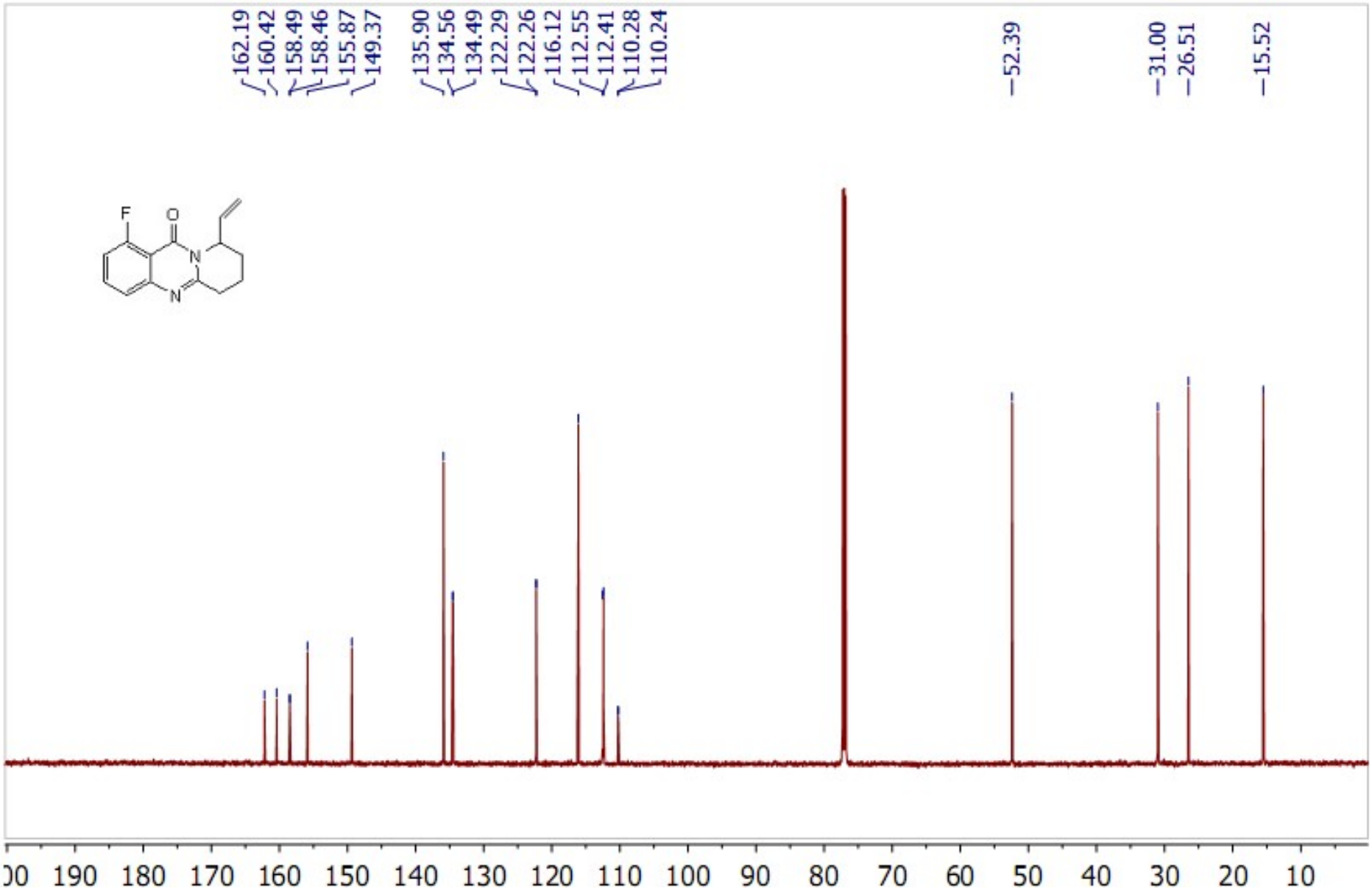
^{13}C NMR spectrum (151 MHz, $CDCl_3$) of compound 12a



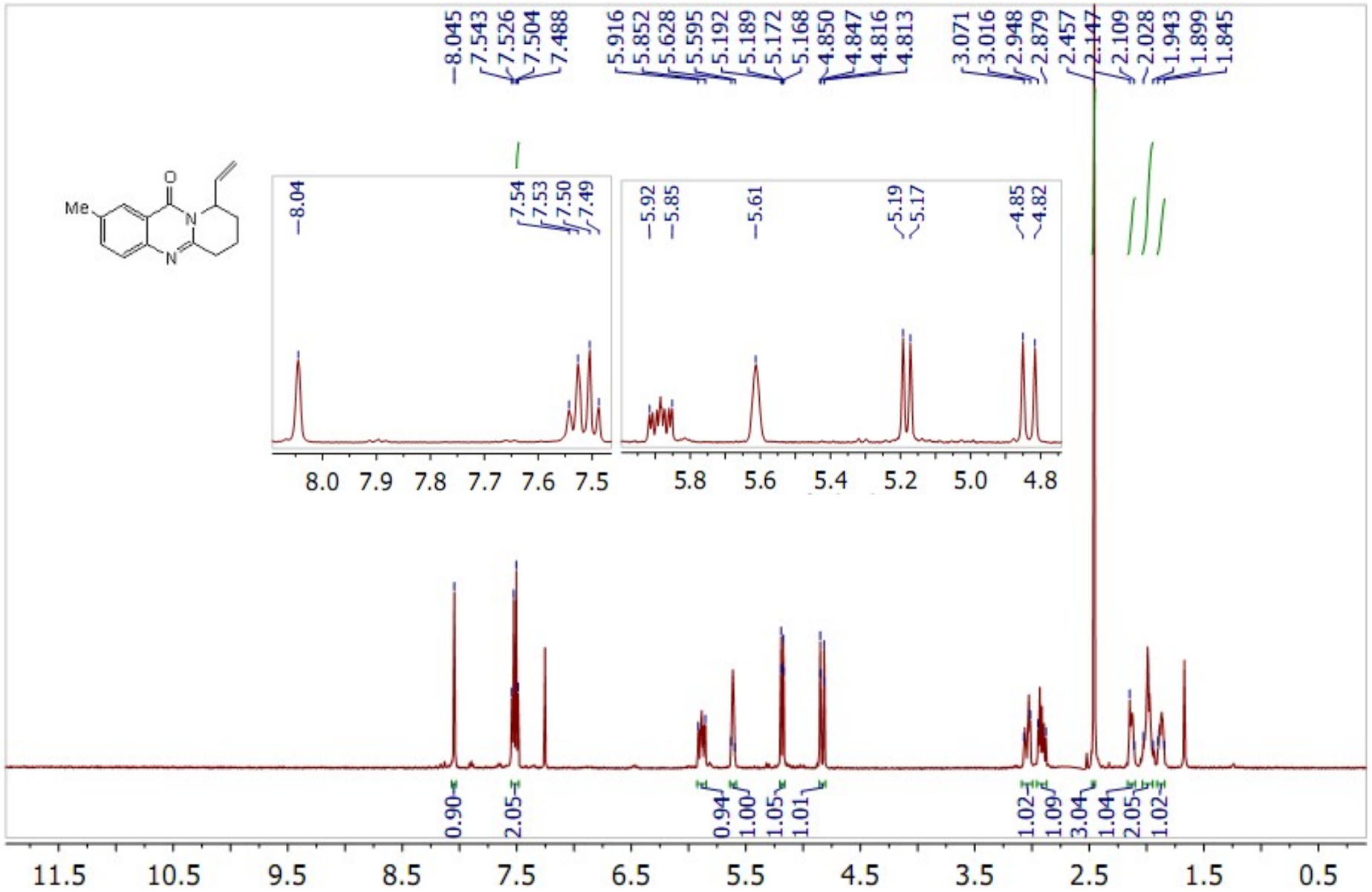
^{1}H NMR spectrum (500 MHz, $CDCl_3$) of compound 12b



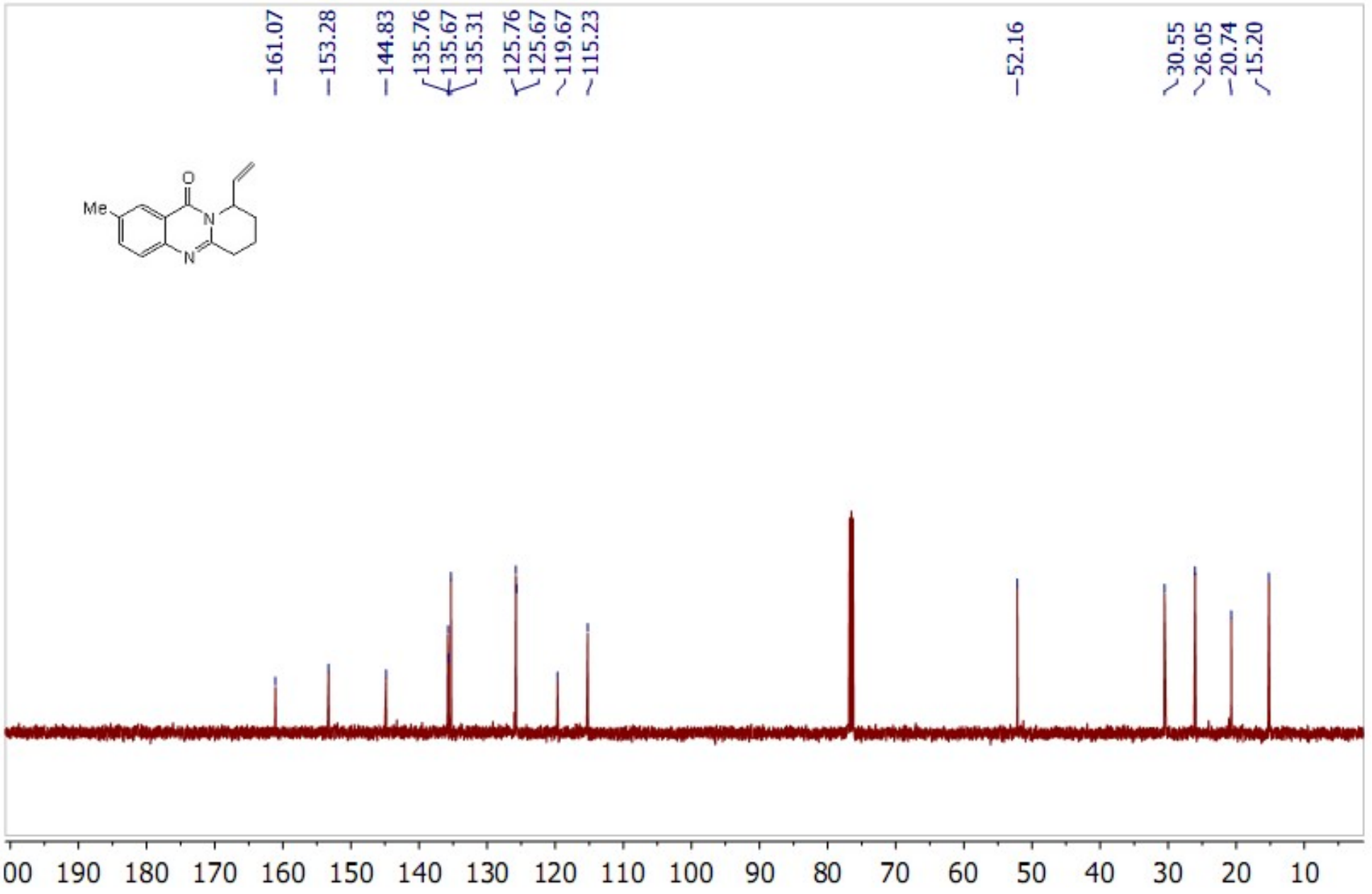
^{13}C NMR spectrum (151 MHz, $CDCl_3$) of compound 12b



^{1}H NMR spectrum (500 MHz, $CDCl_3$) of compound 12c



^{13}C NMR spectrum (126 MHz, $CDCl_3$) of compound 12c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135.76
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125.67
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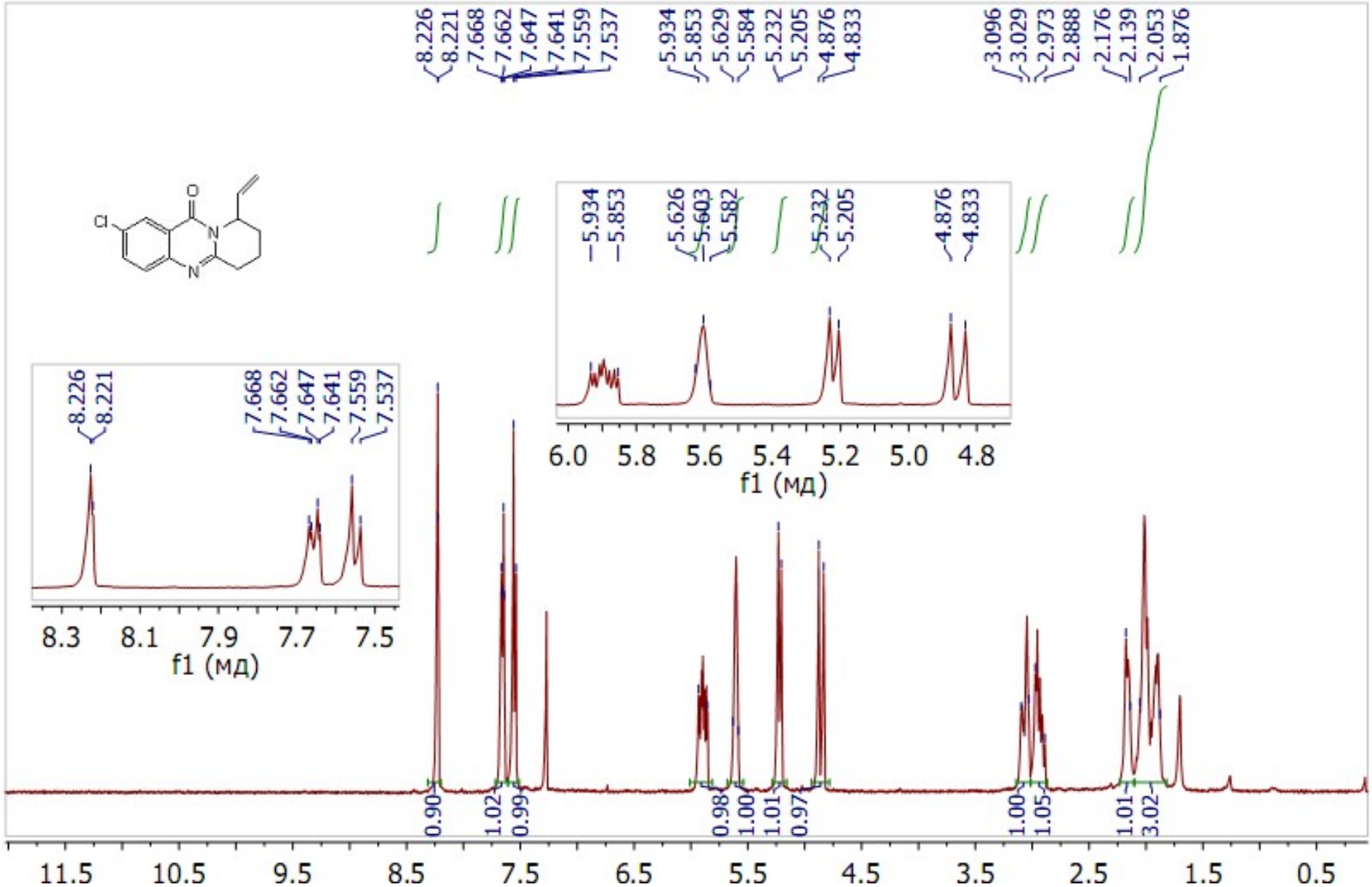
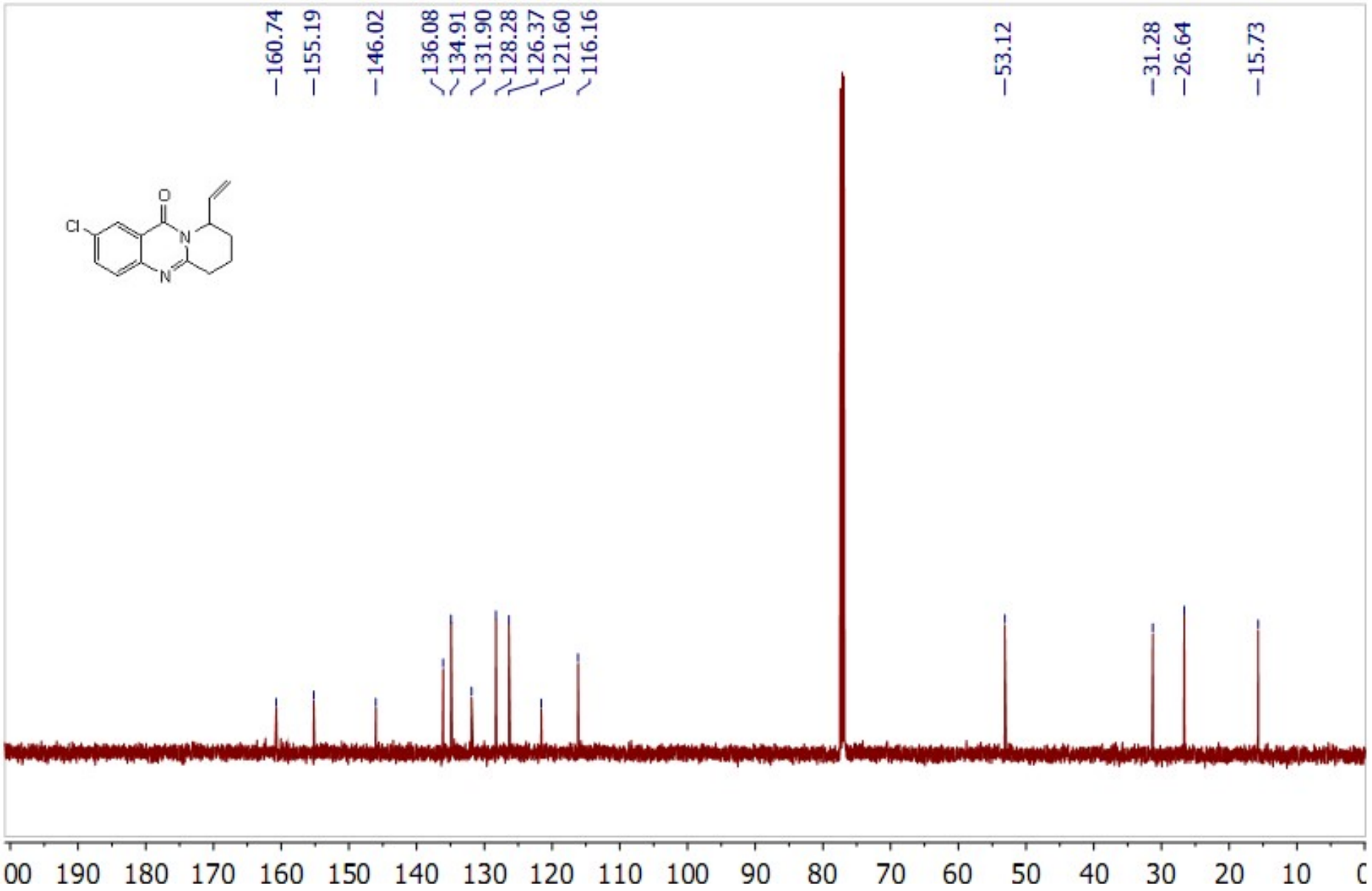
115.23
52.16
30.55
26.05
20.74
15.20
Me
O
N
N
00 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10

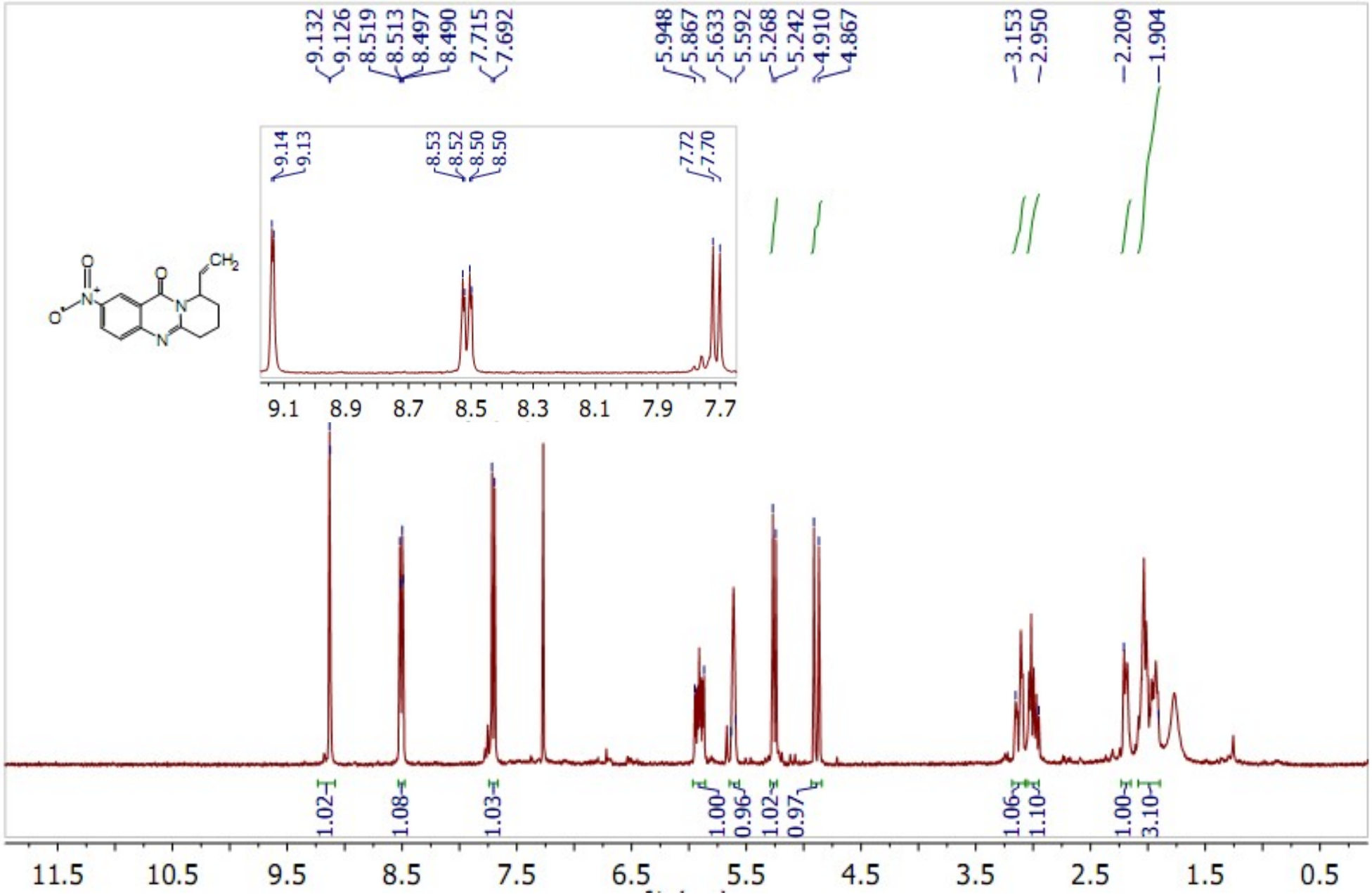
^{1}H NMR spectrum (400 MHz, $CDCl_3$) of compound 12d



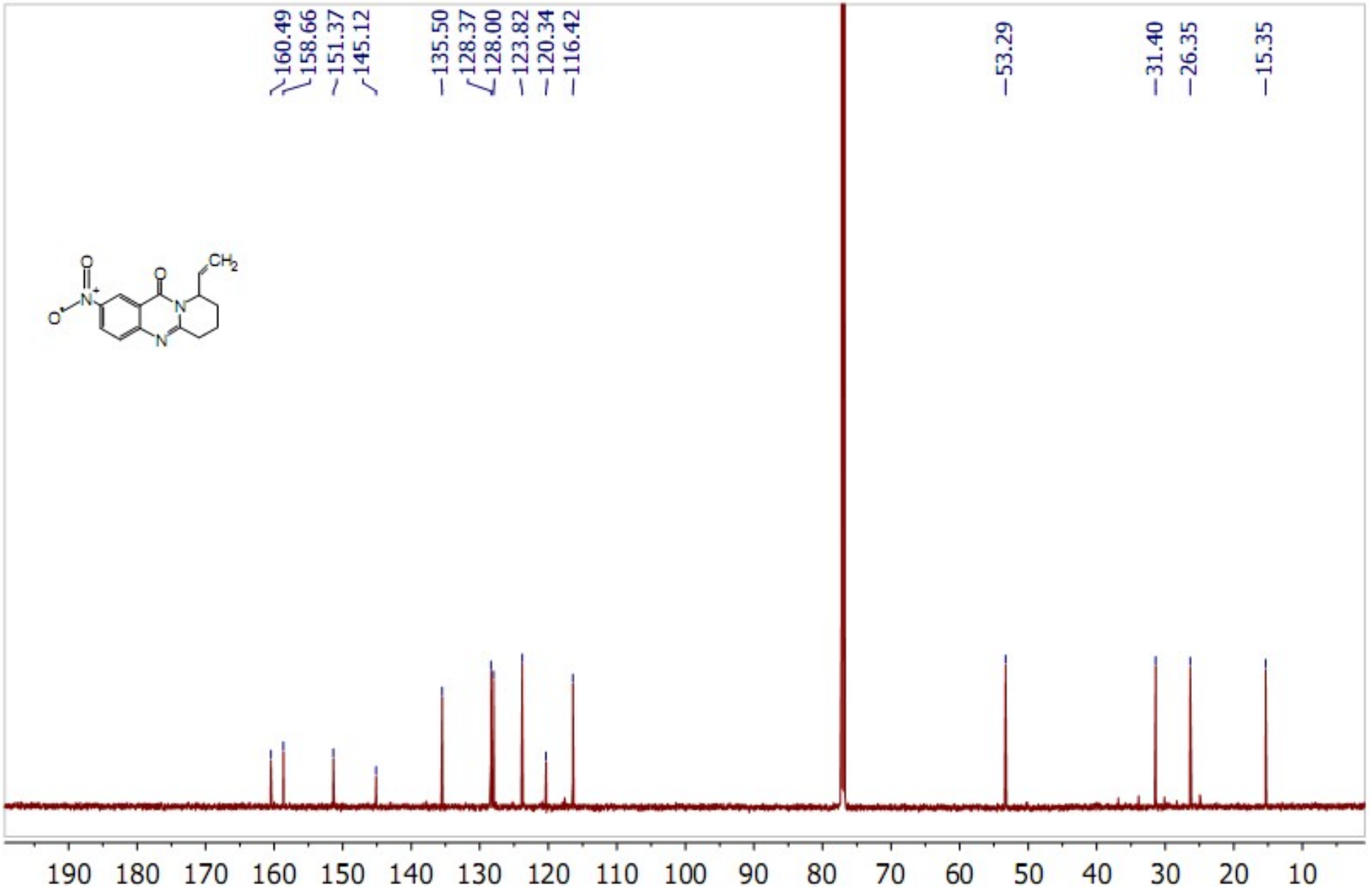
^{13}C NMR spectrum (126 MHz, $CDCl_3$) of compound 12d



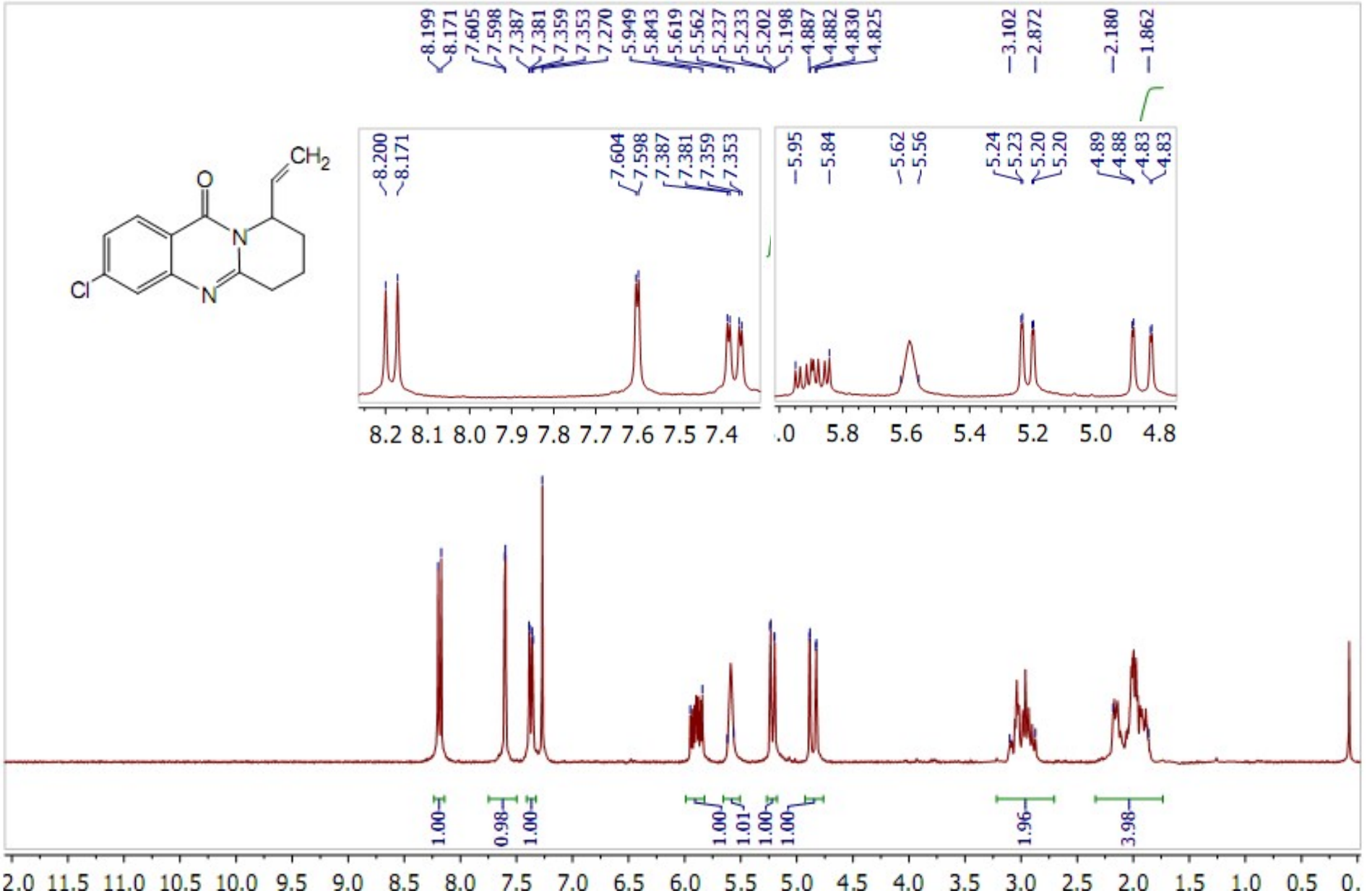
^{1}H NMR spectrum (400 MHz, $CDCl_3$) of compound 12e



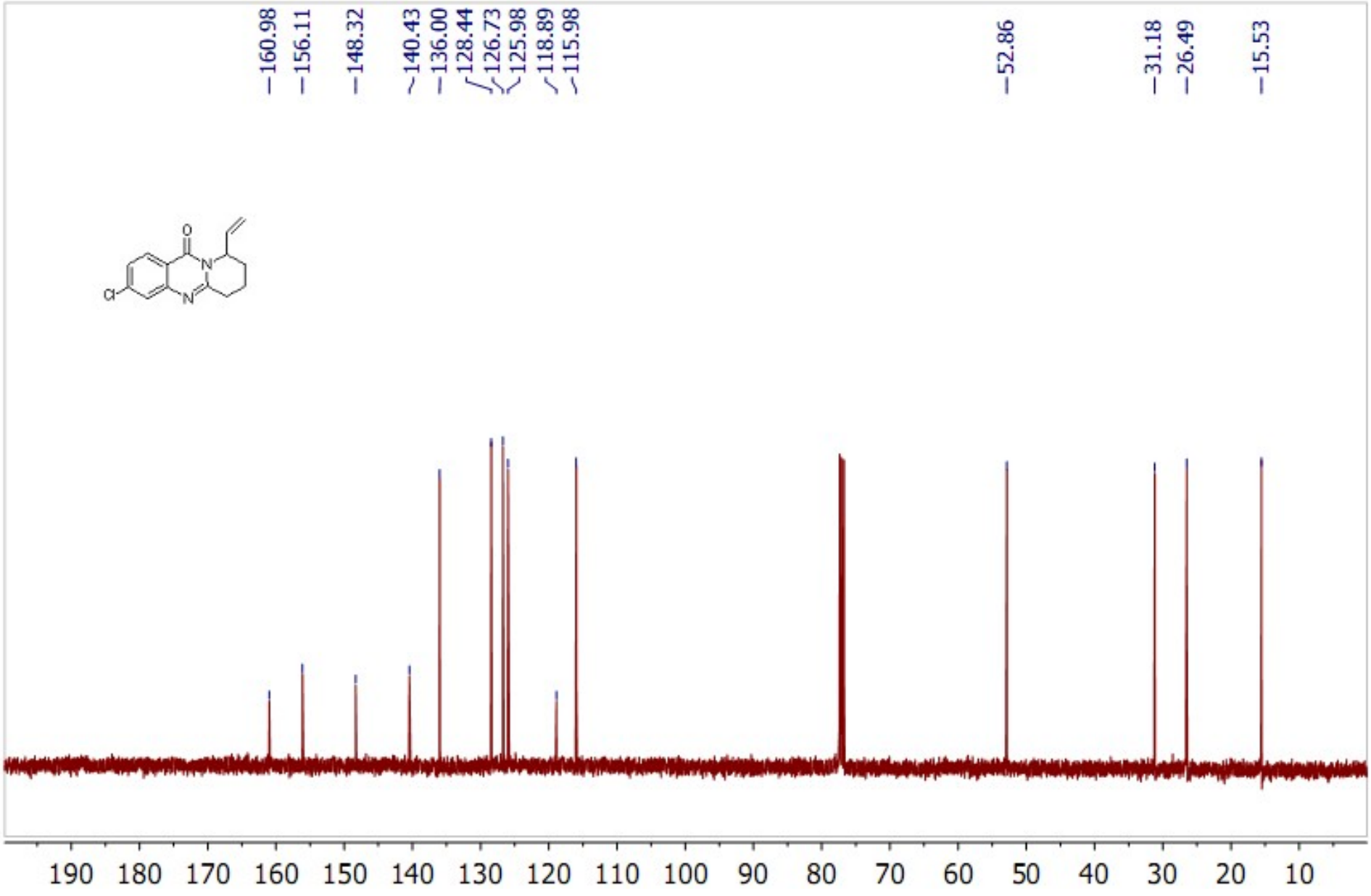
^{13}C NMR spectrum (151 MHz, $CDCl_3$) of compound 12e



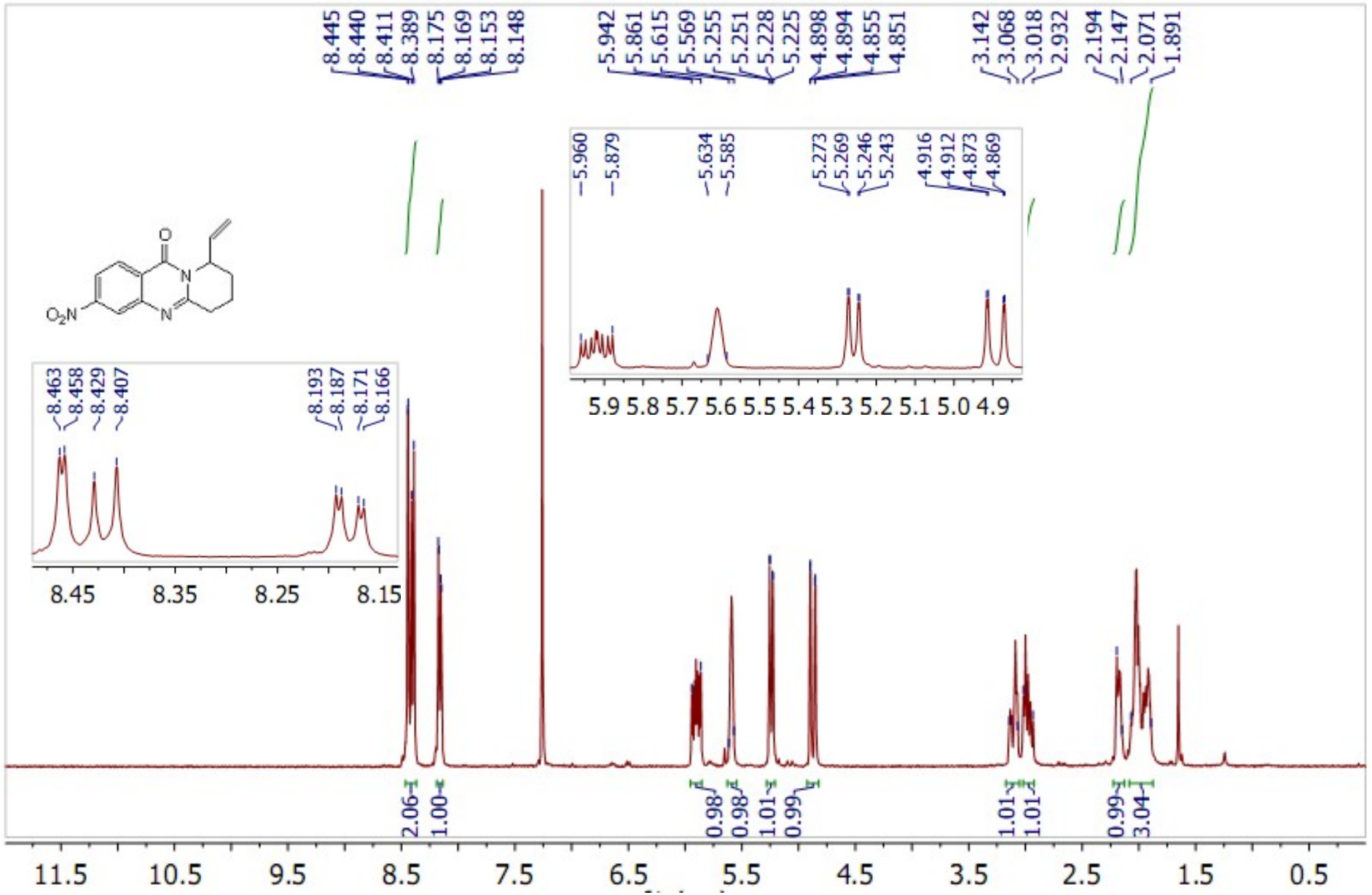
^{1}H NMR spectrum (300 MHz, $CDCl_3$) of compound 12f



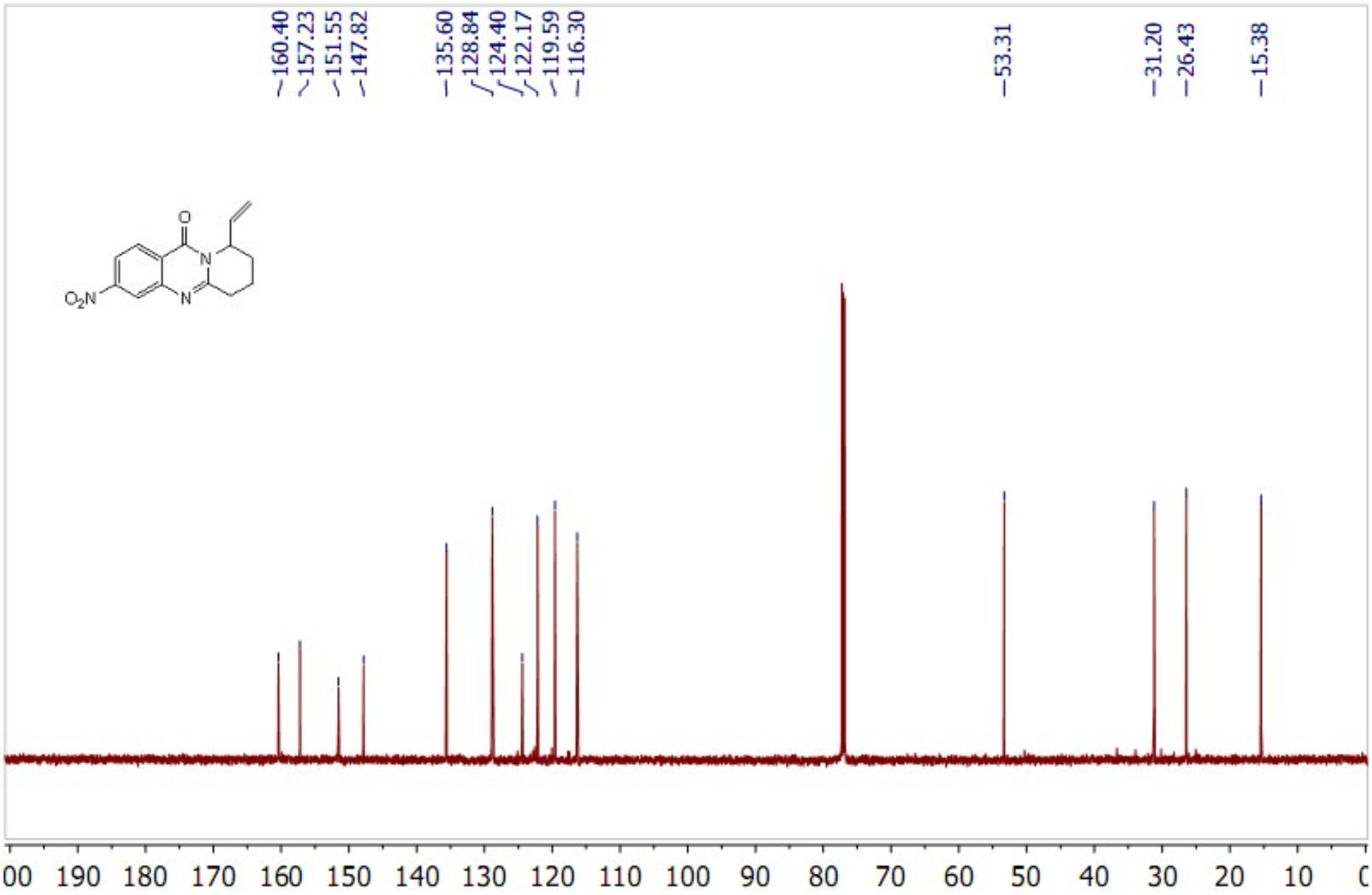
^{13}C NMR spectrum (101 MHz, $CDCl_3$) of compound 12f



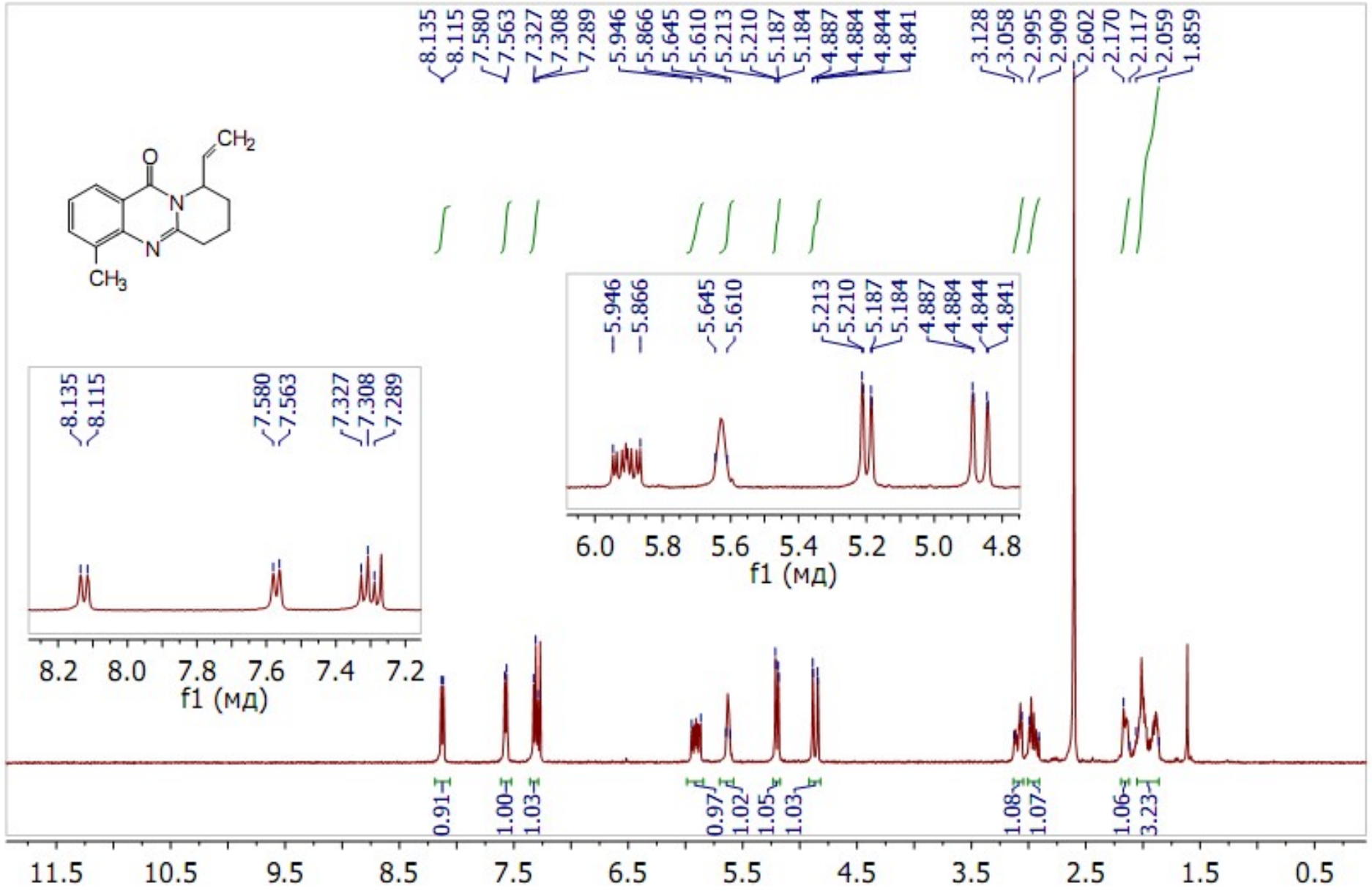
^{1}H NMR spectrum (400 MHz, $CDCl_3$) of compound 12g



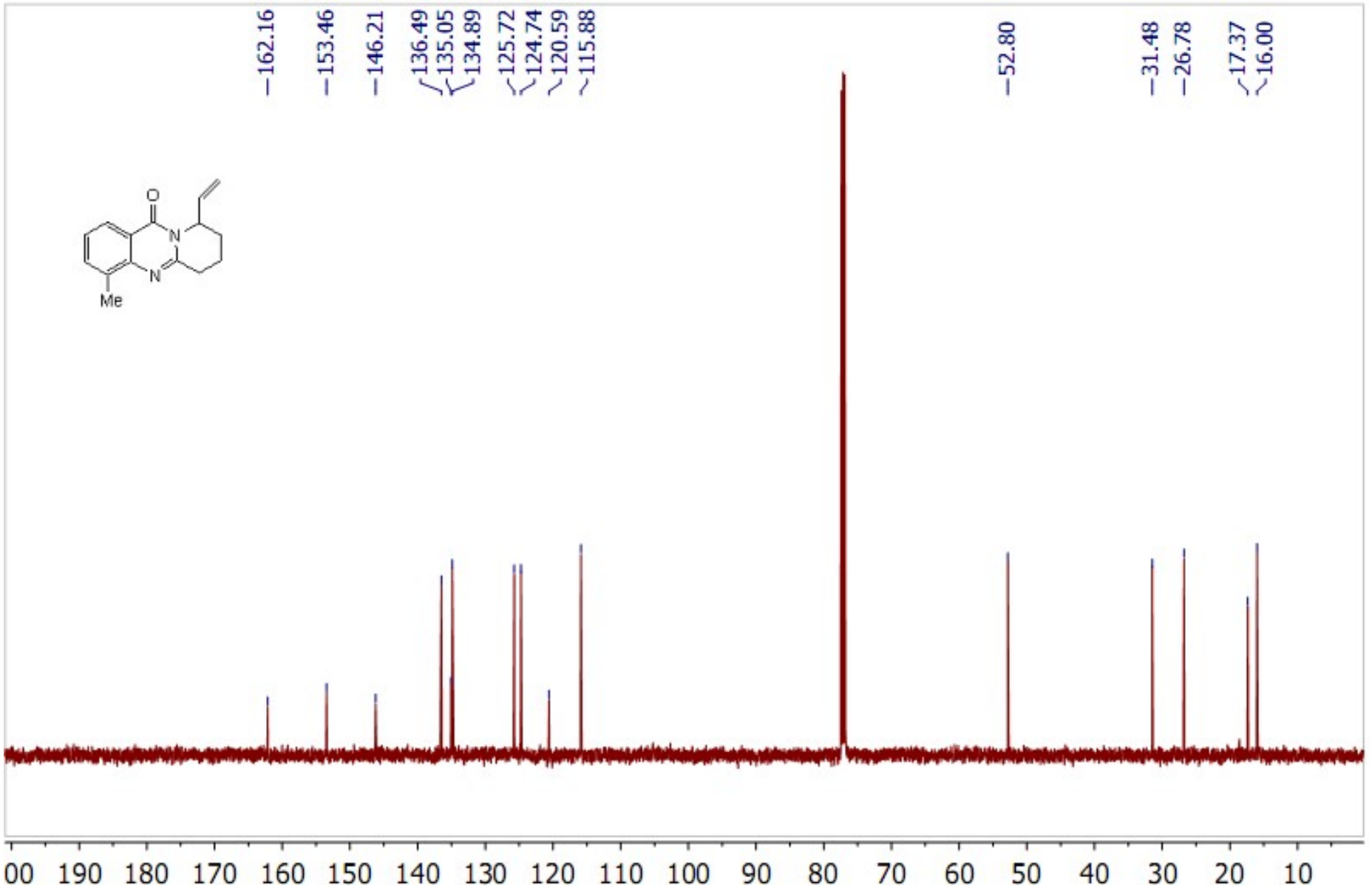
^{13}C NMR spectrum (151 MHz, $CDCl_3$) of compound 12g



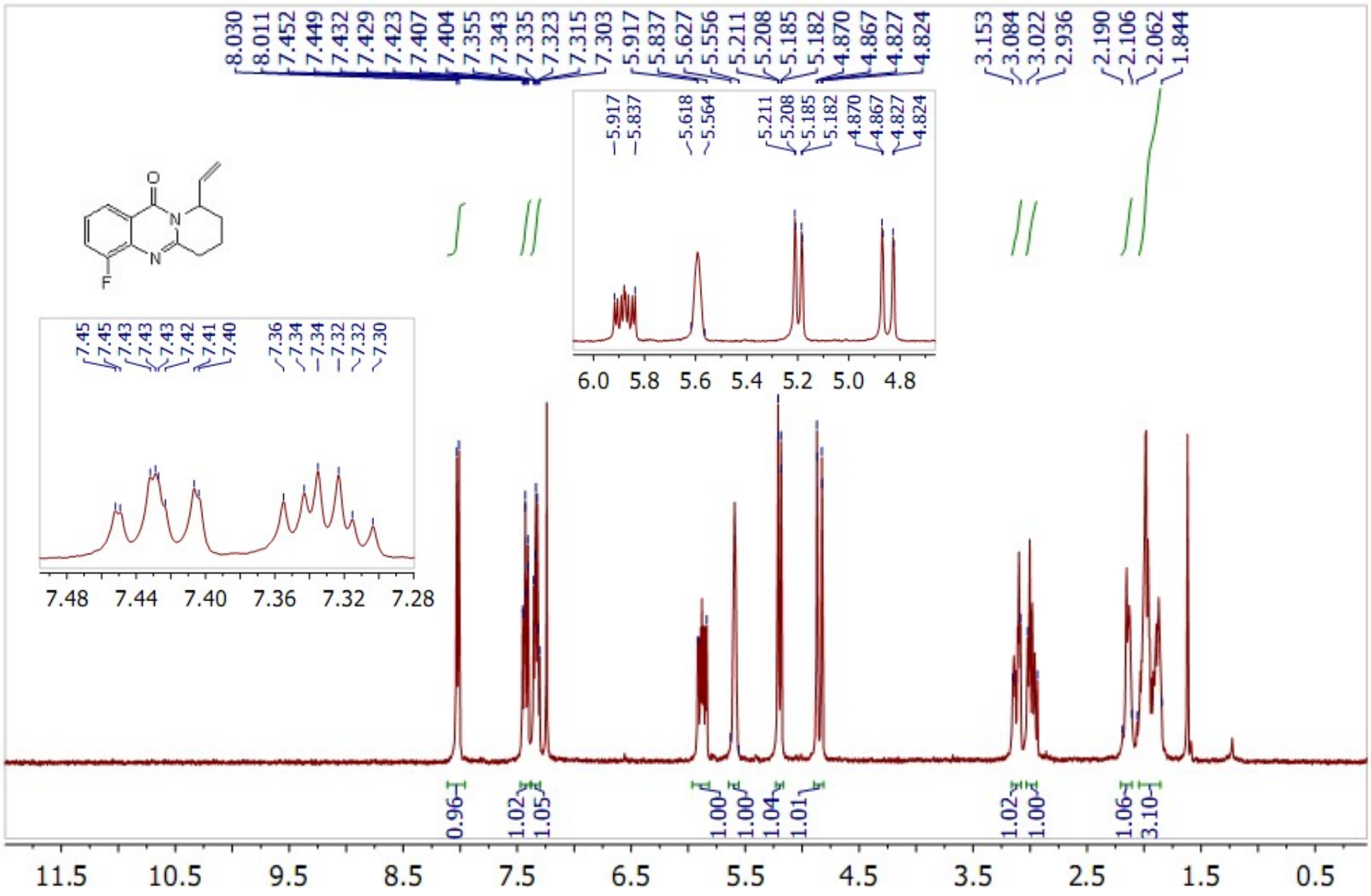
^{1}H NMR spectrum (400 MHz, $CDCl_3$) of compound 12h



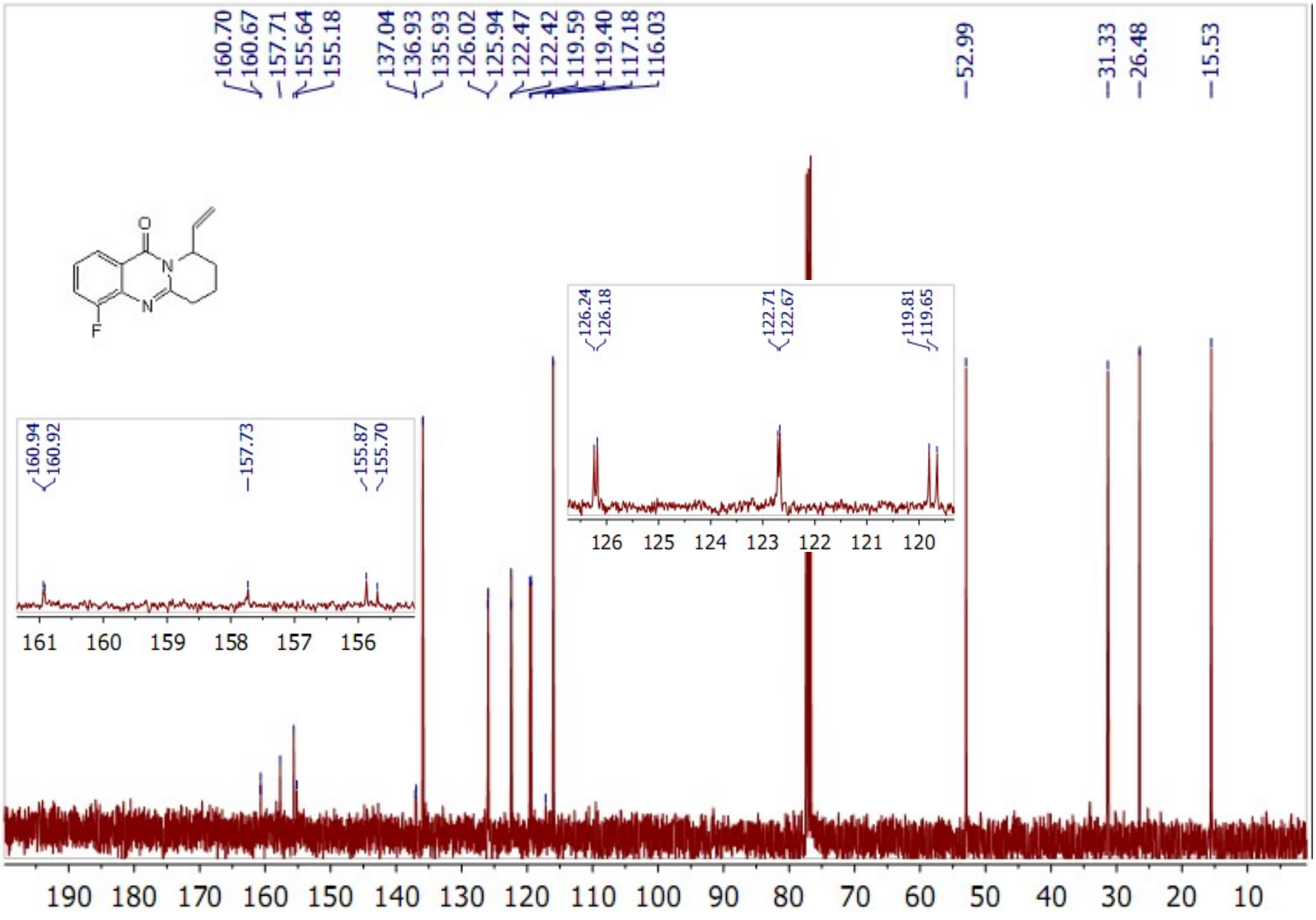
^{13}C NMR spectrum (126 MHz, $CDCl_3$) of compound 12h



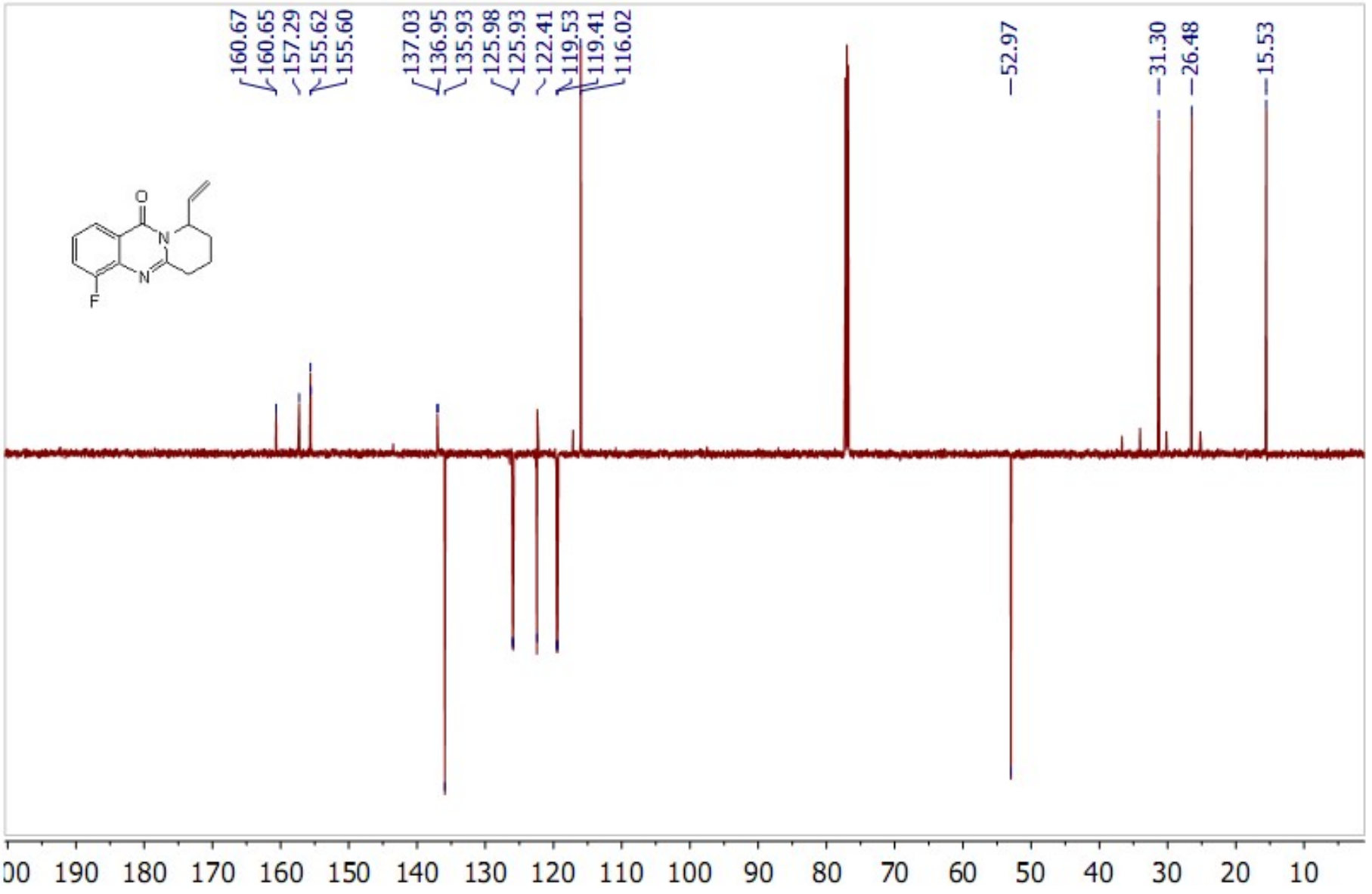
^{1}H NMR spectrum (400 MHz, $CDCl_3$) of compound 12i



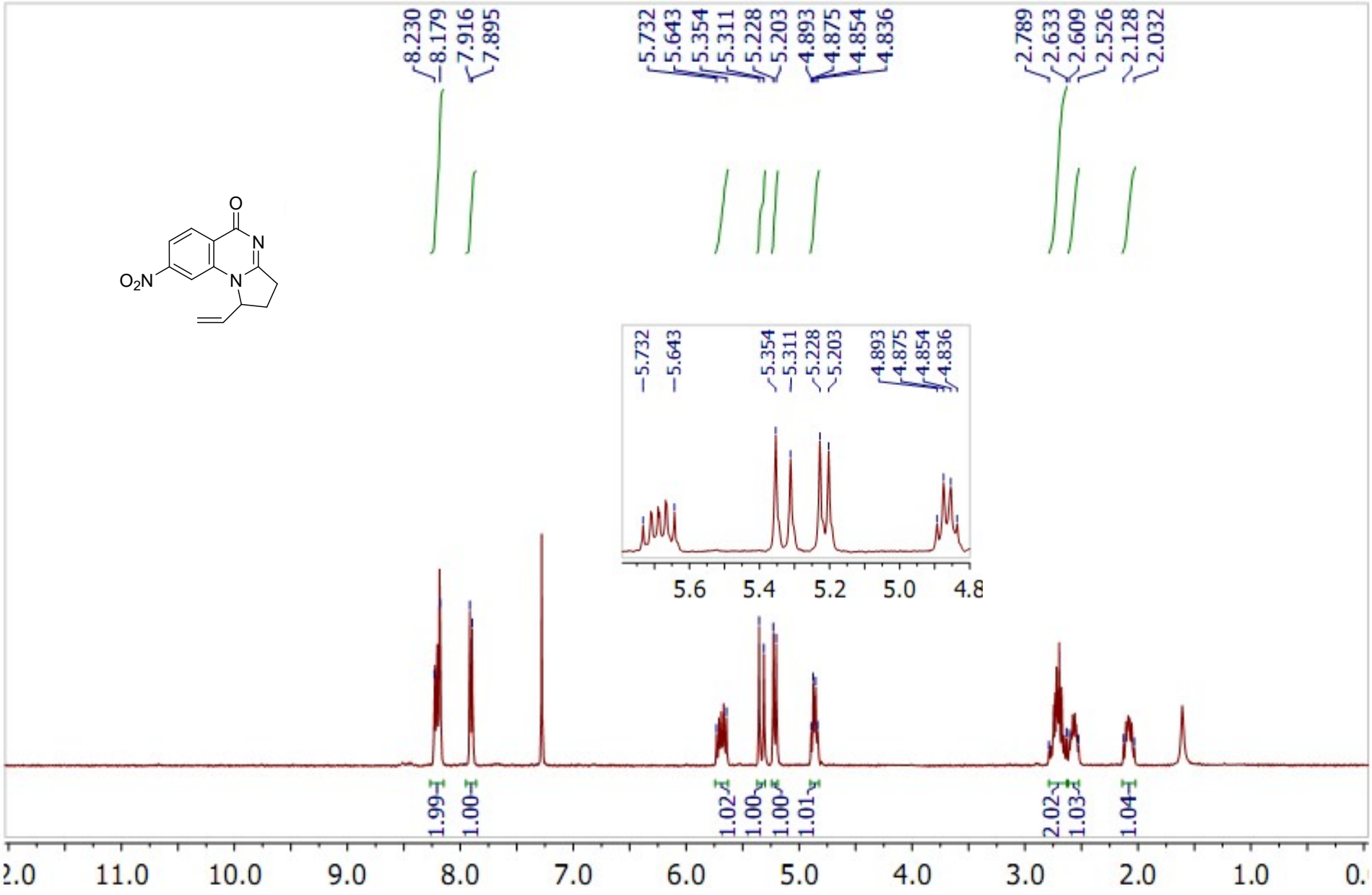
^{13}C NMR spectrum (101 MHz, $CDCl_3$) of compound 12i



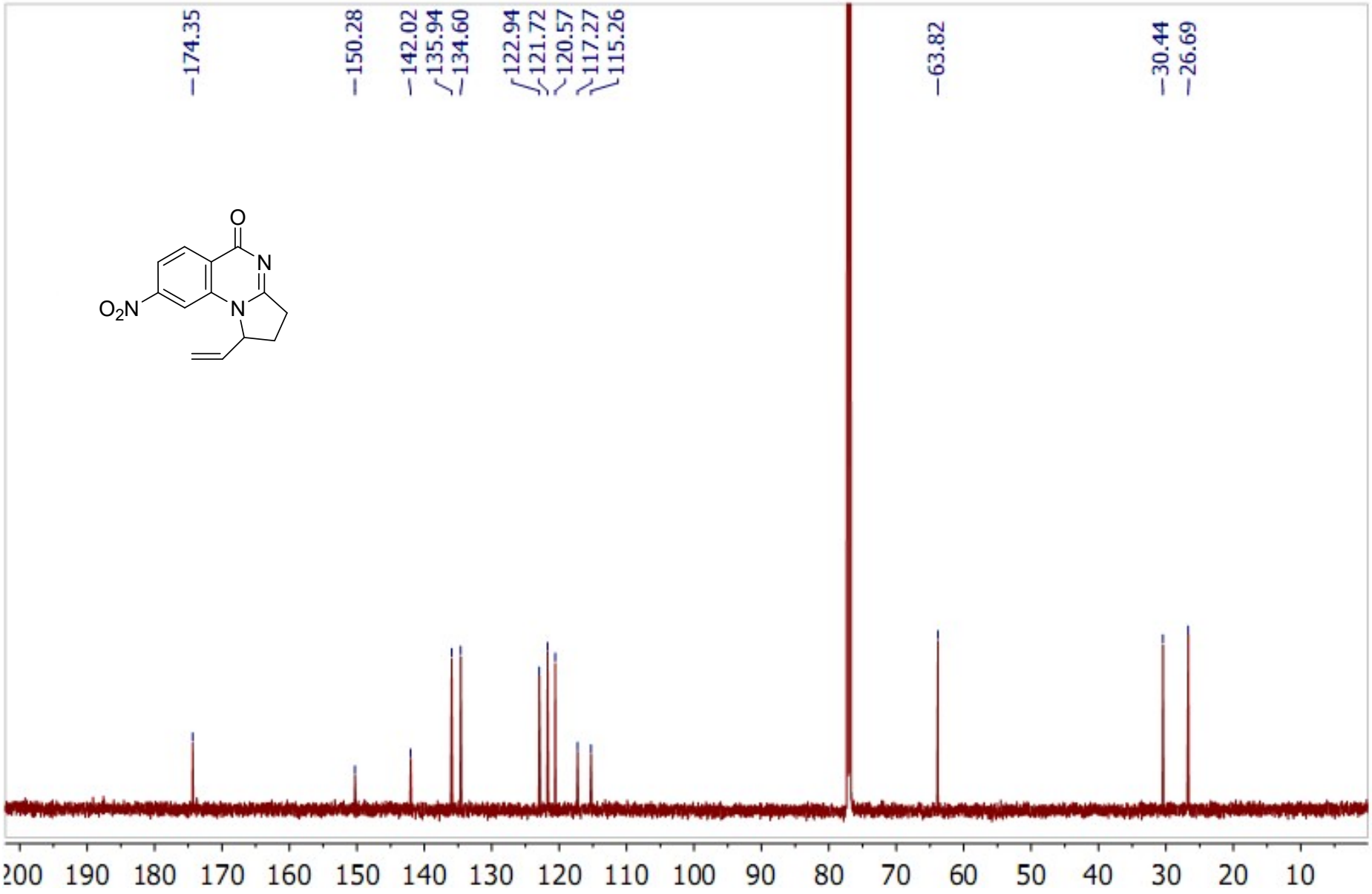
^{13}C/APT NMR spectrum (151 MHz, $CDCl_3$) of compound 12i



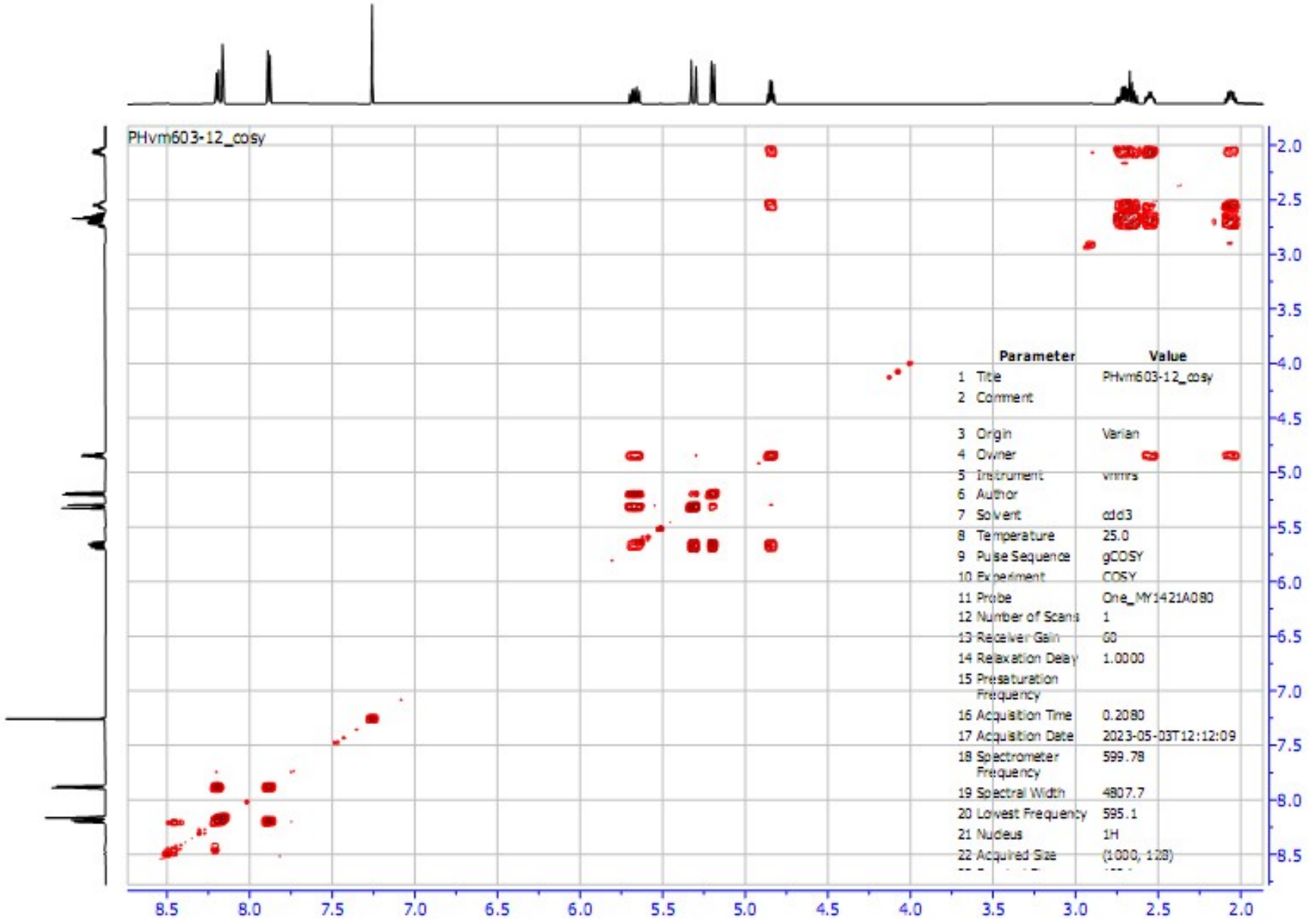
1H NMR spectrum (400 MHz, $CDCl_3$) of compound 13g



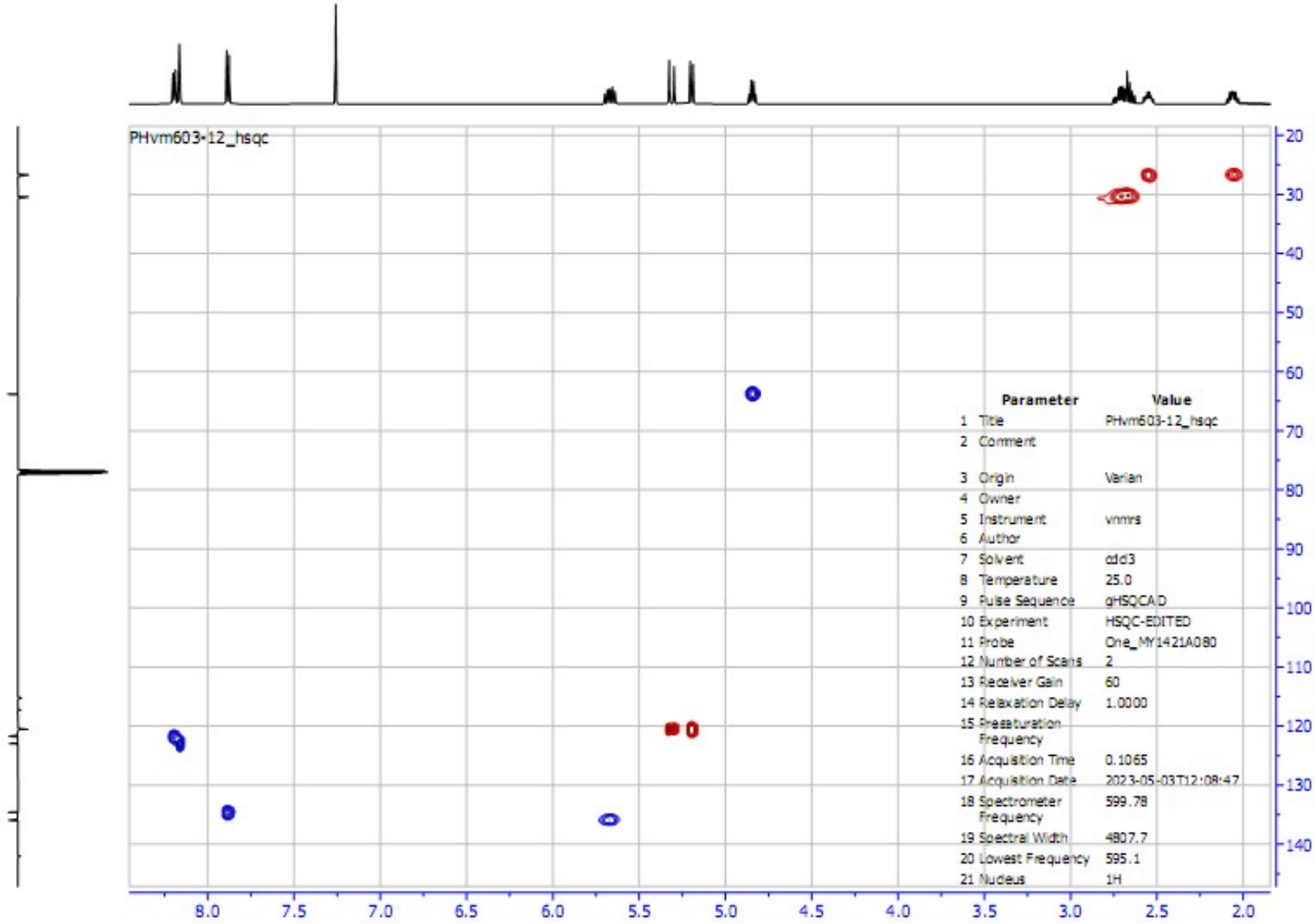
13C NMR spectrum (151 MHz, CDCl3) of compound 13g



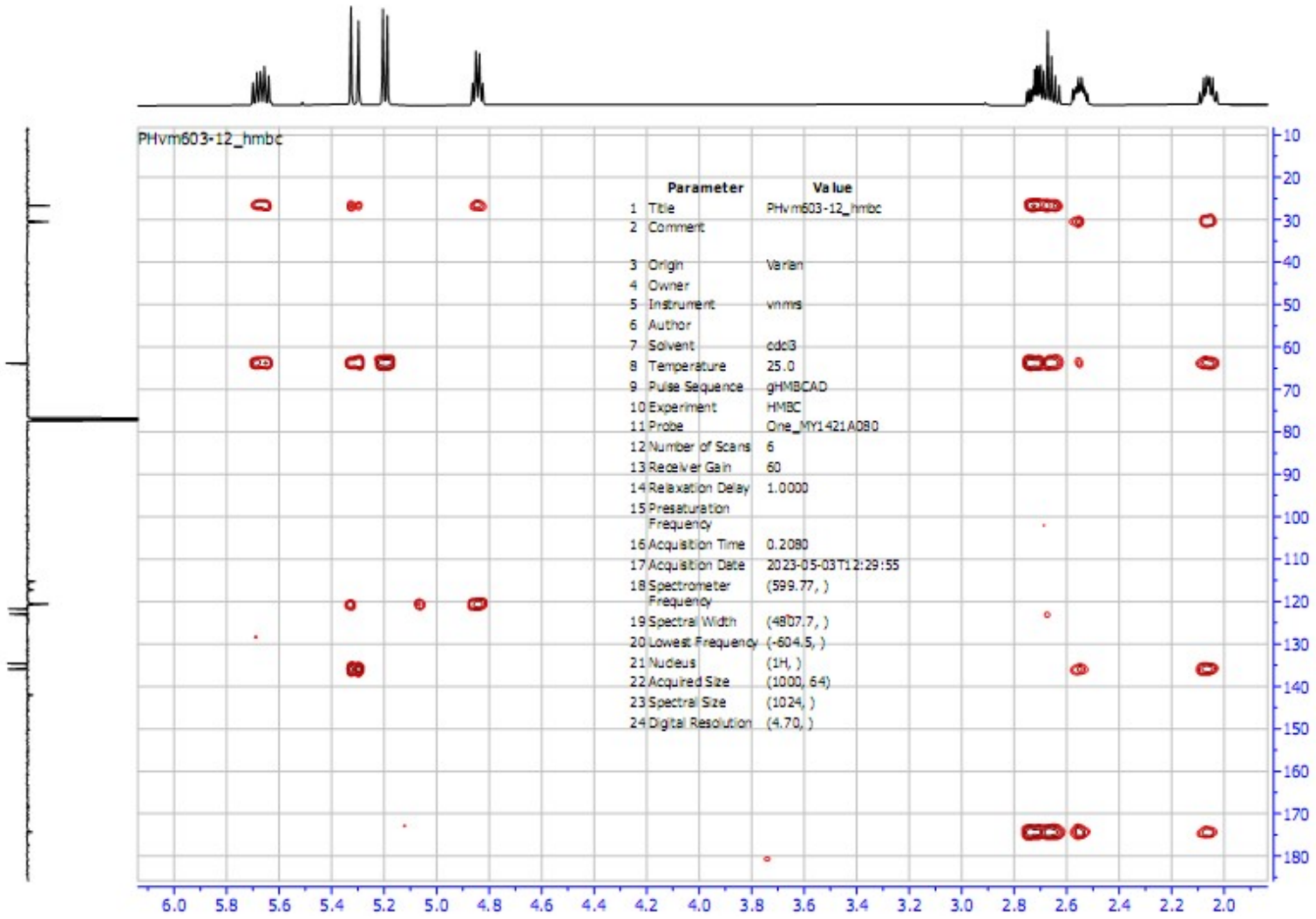
COSY NMR spectrum (151 MHz, CDCl3) of compound 13g



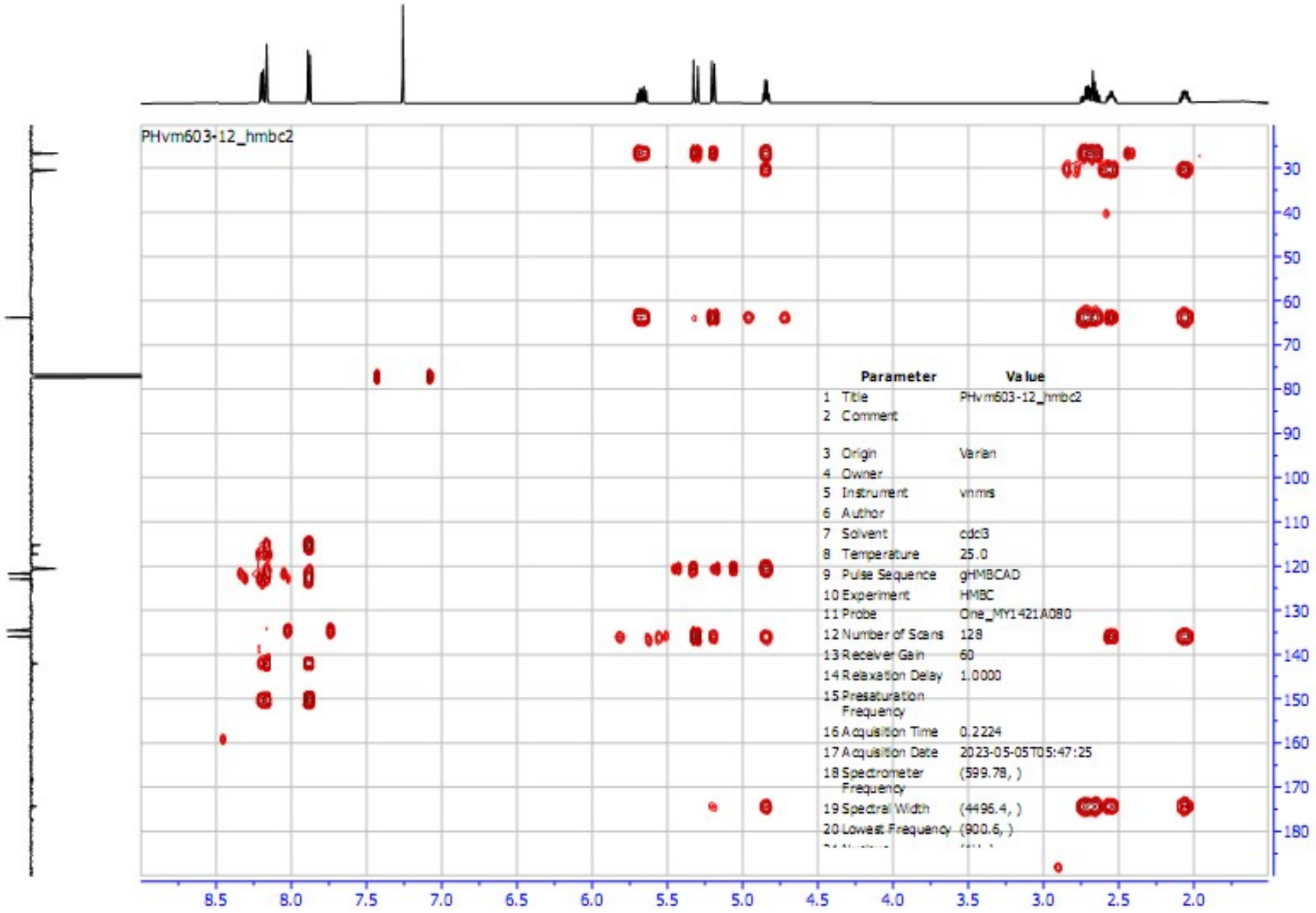
HSQC NMR spectrum (151 MHz, CDCl3) of compound 13g



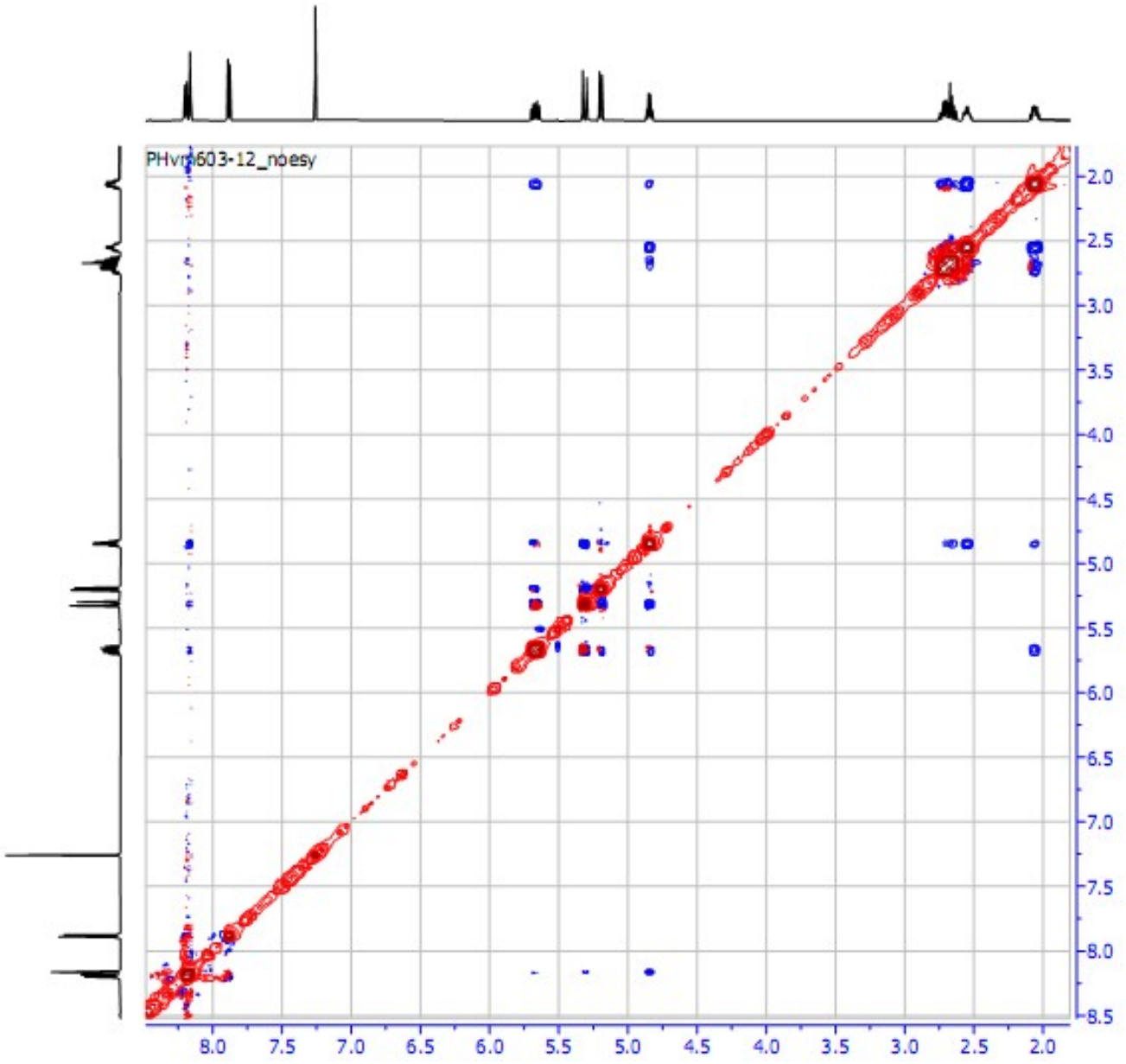
HSBC NMR spectrum (151 MHz, CDCl3) of compound 13g

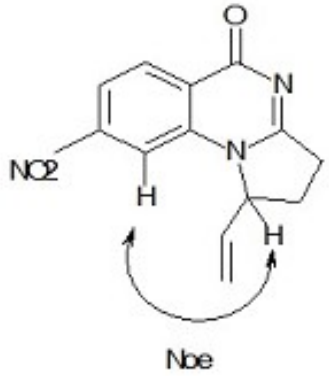


HSBC2 NMR spectrum (151 MHz, CDCl3) of compound 13g



NOESY NMR spectrum (151 MHz, CDCl3) of compound 13g





	Parameter	Value
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2	Comment	
3	Origin	Varian
4	Owner	
5	Instrument	vnmrs
6	Author	
7	Solvent	cdcl3
8	Temperature	25.0
9	Pulse Sequence	NOESY
10	Experiment	NOESY
11	Probe	One_MY1421A080
12	Number of Scans	16
13	Receiver Gain	26
14	Relaxation Delay	1.0000
15	Presaturation Frequency	
16	Acquisition Time	0.2080
17	Acquisition Date	2023-05-05T06:47:03
18	Spectrometer Frequency	599.78
19	Spectral Width	4807.7
20	Lowest Frequency	595.1
21	Nucleus	1H