Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.

Electronic Supplementary Information

Stannyl radical-mediated synthesis of 6*H*-1,3-oxazin-6-ones from 2-acyloxyazirines or whether free radicals can open the azirine ring?

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1. General information

^{1}H and ^{13}C spectra were recorded on a Bruker AVANCE 400 (400.1 MHz for ^{1}H and 100.6 MHz for ^{13}C) and reported to $CDCl_3$ [$\delta(^{1}H)$=7.28 ppm and $\delta(^{13}C)$=77.00 ppm] or DMSO-d_6 [$\delta(^{1}H)$=2.50 ppm and $\delta(^{13}C)$=39.50 ppm]. Electrospray ionization (ESI), positive or negative mode, mass spectra were measured on a Bruker MaXis mass spectrometer using MeOH for dilution of samples. Single crystal X-ray data were collected by means of Agilent Technologies "Xcalibur" and "SuperNova" diffractometers. IR spectra were recorded on a Shimadzu IR Affinity-1 spectrophotometer in KBr. Melting points were determined on a melting point apparatus SMP30 and are uncorrected. Thin-layer chromatography (TLC) was performed using aluminum sheets precoated with SiO_2 ALUGRAM SIL G/UV254. Macherey-Nagel silica gel was used for column chromatography. All solvents were distilled and dried prior to use. Dichloromethane and chloroform were washed with concentrated H_2SO_4 and H_2O, distilled from P_2O_5, and stored over anhydrous K_2CO_3. Toluene, diethyl ether, and 1,4-dioxane were distilled and stored over sodium metal. MeCN was distilled from P_2O_5 and redistilled from K_2CO_3.

5-Methoxy-3-(4-(trifluoromethyl)phenyl)isoxazole,[1] 2-bromo-2*H*-azirines **1a,f,i**,[2] **1b,h**,[3] **1c,d**,[4] **1e**,[5] 2-acyloxy-2*H*-azirines **2a**,**3a,b,i,j,n–q,u,v,zd,ze,zj–zl,zo,zs**,[6] and 3-(*p*-tolyl)-2*H*-azirine (**22**)[7] are known compounds and were prepared by the reported procedures.

2. Optimization of the synthesis of 5c

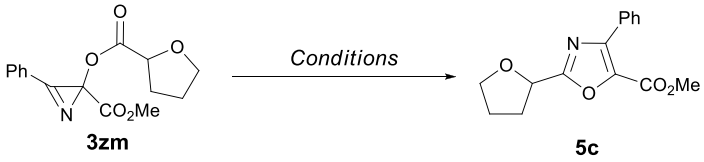
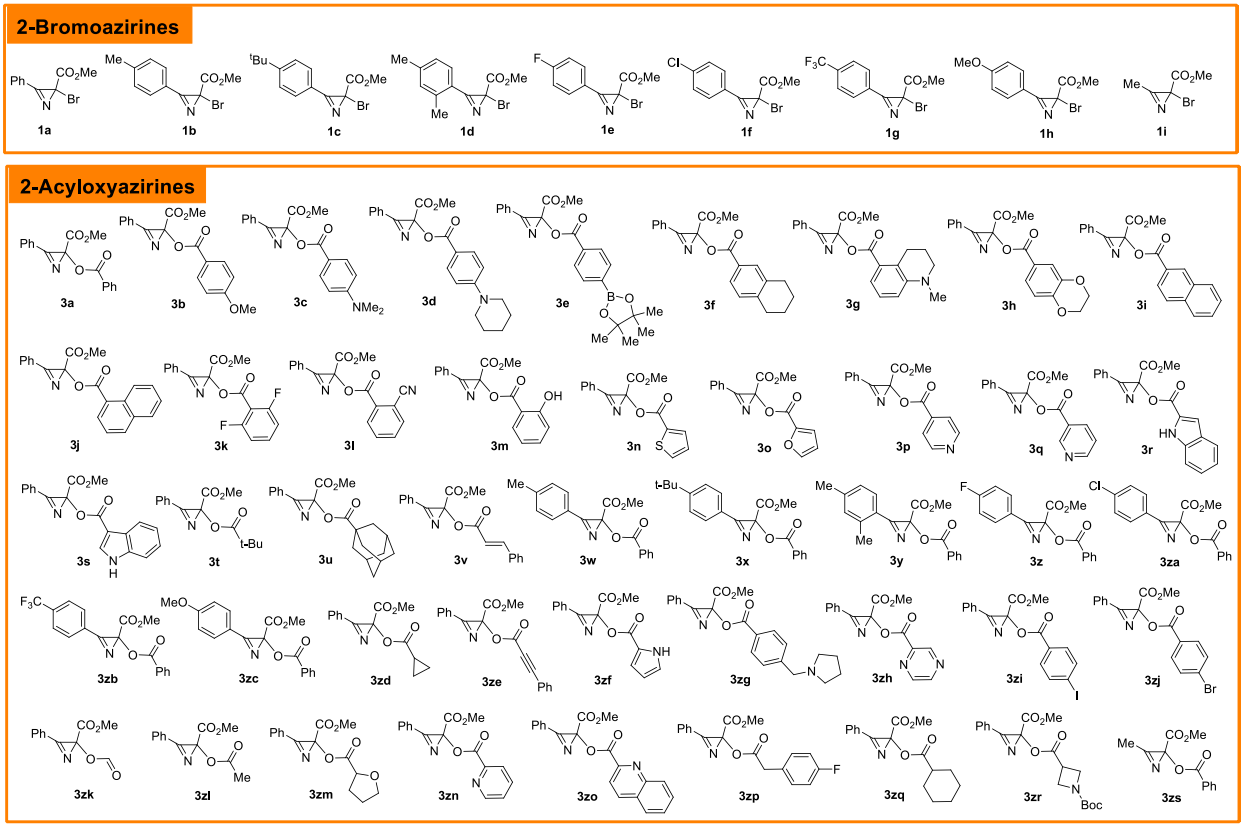


Table S1. Optimization of the synthesis of oxazole 5c

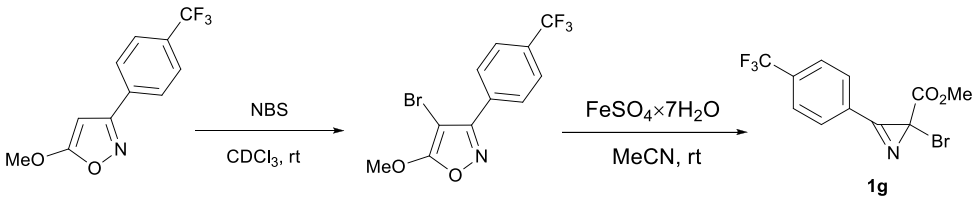
Entry	Reagent (equiv)	Initiator (equiv)	Solvent, °C	Concentration of **3zm**, mol/L	Reaction time, min	Yield of **5c**, %[a]
1	Bu_3SnH (2)	ACHN (0.25)	toluene, 110	0.05	60	13
2	Bu_3SnH (2)	ACHN (0.7)	toluene, 110	0.05	60	34
3	Bu_3SnH (2)	ACHN (1)	toluene, 110	0.05	60	55, 45[b]
4	Bu_3SnH (1)	ACHN (1)	toluene, 110	0.05	60	28
5	Bu_3SnH (2)	AIBN (1)	benzene, 81	0.05	60	7

[a]Yield was determined by ^{1}H NMR spectroscopy using ethylene carbonate as an internal standard. [b]Isolated yield.

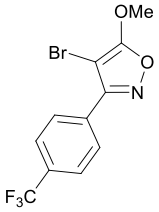
3. Structures of bromoazirines 1 and acyloxyazirines 3



4. Synthesis of azirine 1g

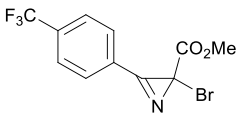


A solution of 5-methoxy-3-[4-(trifluoromethyl)phenyl]isoxazole (486 mg, 2 mmol) and *N*-bromosuccinimide (392 mg, 2.2 mmol) in $CHCl_3$ (25 mL) was stirred at rt for 3 h. The reaction mixture was diluted with 10% $Na_2S_2O_3$ (60 mL) and extracted with CH_2Cl_2 (3×20 mL). The combined organic extracts were dried over anhydrous Na_2SO_4. The solvent was removed under reduced pressure, the product was purified by silica gel flash chromatography (hexane/EtOAc, 5:1) to give 4-bromo-5-methoxy-3-[4-(trifluoromethyl)phenyl]isoxazole (567 mg, 88%).[2]



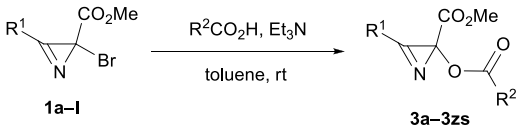
Colorless solid, mp 43–45 °C (from Et_2O/hexane). ^{1}H NMR (400 MHz, $CDCl_3$) δ 4.26 (s, 3H), 7.74–7.80 (m, 2H), 7.97–8.02 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 58.6, 66.7, 123.8 (q, *J* 272.2 Hz), 125.6 (q, *J* 3.8 Hz), 128.1, 128.3, 131.9 (q, *J* 32.6 Hz), 161.4, 169.7. HRMS (ESI-TOF) *m/z* $[M+H]^+$ calcd for $C_{11}H_8{}^{79}BrF_3NO_2^+$: 321.9685; found: 321.9683.

A suspension of 4-bromo-5-methoxy-3-[4-(trifluoromethyl)phenyl]isoxazole (644 mg, 2 mmol) and $FeSO_4 \times 7H_2O$ (239 mg, 1.2 mmol, 60 mol %) in MeCN (15 mL) was stirred at rt for 5 h. The solvent was removed under reduced pressure, and the product was purified by silica gel flash chromatography (hexane/EtOAc, 10:1) to give azirine **1g** (567 mg, 88%).



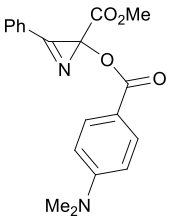
Colorless solid, mp 41–43 °C (from Et_2O/hexane). ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.85 (s, 3H), 7.87–7.99 (m, 2H), 8.07–8.17 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 43.2, 54.8, 123.2, 124.5 (q, *J* 272.7 Hz), 126.7 (q, *J* 3.8 Hz), 131.1, 136.3 (q, *J* 33.3 Hz), 164.5, 166.7. HRMS (ESI-TOF) *m/z* $[M+Na]^+$ calcd for $C_{11}H_7{}^{79}BrF_3NNaO_2^+$: 343.9504; found: 343.9518.

5. Synthesis of 2-acyloxyazirines 3



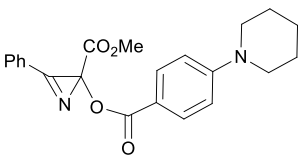
General procedure. To a solution of bromoazirine **1** (1 mmol) and carboxylic acid (1.2 mmol) in toluene (10 mL) Et_3N (202 mg, 2 mmol) was added at ambient temperature, and the reaction mixture was stirred for 3 h. The solvent was removed under reduced pressure and the residue was purified by column chromatography on silica gel (/EtOAc/hexane, from 1:10 to 1:4).[6]

Methyl 2-{[4-(dimethylamino)benzoyl]oxy}-3-phenyl-2*H*-azirine-2-carboxylate (3c)



Compound **3c** (308 mg, 91%) was prepared according to the general procedure from azirine **1a** (254 mg, 1 mmol) and 4-(dimethylamino)benzoic acid (198 mg, 1.2 mmol). Colorless solid, mp 151–152 °C (from Et_2O/hexane). ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.05 (s, 6H), 3.80 (s, 3H), 6.60–6.72 (m, 2H), 7.57–7.65 (m, 2H), 7.65–7.72 (m, 1H), 7.91–8.03 (m, 2H), 8.16–8.28 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 40.0, 53.1, 63.3, 110.6, 115.0, 121.2, 129.3, 131.2, 132.0, 134.4, 153.8, 166.0, 166.1, 168.5. HRMS (ESI-TOF) *m/z* $[M+H]^+$ calcd for $C_{19}H_{19}N_2O_4^+$: 339.1339; found: 339.1337.

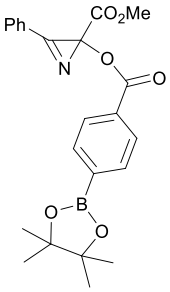
Methyl 3-phenyl-2-{[4-(piperidin-1-yl)benzoyl]oxy}-2*H*-azirine-2-carboxylate (3d)



Compound **3d** (314 mg, 83%) was prepared according to the general procedure from azirine **1a** (254 mg, 1 mmol) and 4-(piperidin-1-yl)benzoic acid (246 mg, 1.2 mmol). Colorless solid, mp 133–134 °C (from Et_2O/hexane). ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.62–1.72 (m, 6H), 3.31–3.45 (m, 4H), 3.80 (s, 3H), 6.79–6.90 (m, 2H), 7.55–7.65 (m, 2H), 7.65–7.74 (m, 1H), 7.90–8.04 (m, 2H), 8.13–8.29 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 24.3, 25.3, 48.5, 53.2,

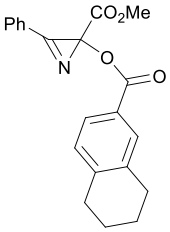
63.4, 113.2, 116.4, 121.2, 129.3, 131.2, 132.0, 134.4, 154.8, 165.9, 166.0, 168.4. HRMS (ESI-TOF) *m/z* $[M+H]^+$ calcd for $C_{22}H_{23}N_2O_4^+$: 379.1652; found: 379.1649.

Methyl 3-phenyl-2-{[4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)benzoyl]oxy}-2*H*-azirine-2-carboxylate (3e)



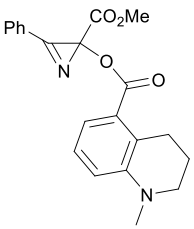
Compound **3e** (316 mg, 75%) was prepared according to the general procedure from azirine **1a** (254 mg, 1 mmol) and 4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)benzoic acid (298 mg, 1.2 mmol). Colorless solid, mp 80–81 °C (from Et_2O/hexane). ^1H NMR (400 MHz, $CDCl_3$) δ 1.37 (s, 12H), 3.81 (s, 3H), 7.58–7.68 (m, 2H), 7.68–7.76 (m, 1H), 7.86–7.94 (m, 2H), 8.04–8.14 (m, 2H), 8.17–8.27 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 24.9, 53.3, 63.9, 84.2, 120.8, 129.1, 129.4, 130.7, 131.3, 134.67, 134.71, 165.5, 166.0, 167.9. HRMS (ESI-TOF) *m/z* $[M+H]^+$ calcd for $C_{23}H_{25}BNO_6^+$: 422.1769; found: 422.1775.

Methyl 3-phenyl-2-[(5,6,7,8-tetrahydronaphthalene-2-carbonyl)oxy]-2*H*-azirine-2-carboxylate (3f)



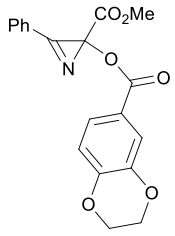
Compound **3f** (280 mg, 80%) was prepared according to the general procedure from azirine **1a** (254 mg, 1 mmol) and 5,6,7,8-tetrahydronaphthalene-2-carboxylic acid (211 mg, 1.2 mmol). Colorless solid, mp 81–82 °C (from Et_2O/hexane). ^1H NMR (400 MHz, $CDCl_3$) 1.78–1.87 (m, 4H), 2.78–2.87 (m, 4H), 3.81 (s, 3H), 7.12–7.17 (m, 1H), 7.59–7.66 (m, 2H), 7.67–7.74 (m, 1H), 7.79–7.85 (m, 2H), 8.18–8.25 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 22.7, 22.8, 29.2, 29.6, 53.2, 63.7, 120.9, 125.7, 127.0, 129.26, 129.33, 131.0, 131.2, 134.6, 137.5, 143.9, 165.7, 166.2, 168.1. HRMS (ESI-TOF) *m/z* $[M+Na]^+$ calcd for $C_{21}H_{19}NNaO_4^+$: 372.1206; found: 372.1217.

2-(Methoxycarbonyl)-3-phenyl-2*H*-azirin-2-yl 1-methyl-1,2,3,4-tetrahydroquinoline-5-carboxylate (3g)



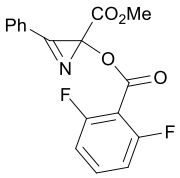
Compound **3g** (302 mg, 83%) was prepared according to the general procedure from azirine **1a** (254 mg, 1 mmol) and 1-methyl-1,2,3,4-tetrahydroquinoline-5-carboxylic acid (229 mg, 1.2 mmol). Colorless solid, mp 126–127 °C (from Et_2O/hexane). ^1H NMR (400 MHz, $CDCl_3$) δ 1.96 (dt, *J* 12.4, 6.1 Hz, 2H), 2.76 (t, *J* 6.3 Hz, 2H), 2.97 (s, 3H), 3.35 (t, *J* 6.3 Hz, 2H), 3.80 (s, 3H), 6.43–6.58 (m, 1H), 7.57–7.64 (m, 2H), 7.64–7.72 (m, 2H), 7.78–7.88 (m, 1H), 8.15–8.31 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 21.7, 27.6, 38.6, 51.5, 53.1, 63.2, 109.2, 114.4, 121.2, 121.4, 129.2, 130.5, 130.6, 131.2, 134.4, 150.5, 166.1, 166.2, 168.5. HRMS (ESI-TOF) *m/z* $[M+H]^+$ calcd for $C_{21}H_{21}N_2O_4^+$: 365.1496; found: 365.1511.

Methyl 2-[(2,3-dihydrobenzo[*b*][1,4]dioxine-6-carbonyl)oxy]-3-phenyl-2*H*-azirine-2-carboxylate (3h)



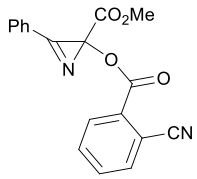
Compound **3h** (346 mg, 98%) was prepared according to the general procedure from azirine **1a** (254 mg, 1 mmol) and 2,3-dihydrobenzo[*b*][1,4]dioxine-6-carboxylic acid (216 mg, 1.2 mmol). Colorless solid, mp 90–91 °C (from Et_2O/hexane). ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.80 (s, 3H), 4.24–4.34 (m, 4H), 6.87–6.93 (m, 1H), 7.59–7.65 (m, 4H), 7.67–7.73 (m, 1H), 8.15–8.24 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 53.2, 63.6, 64.0, 64.6, 117.2, 119.6, 120.9, 121.7, 124.1, 129.3, 131.2, 134.6, 143.2, 148.5, 165.4, 165.5, 168.0. HRMS (ESI-TOF) *m/z* $[M+Na]^+$ calcd for $C_{19}H_{15}NNaO_6^+$: 376.0792; found: 376.0797.

Methyl 2-[(2,6-difluorobenzoyl)oxy]-3-phenyl-2*H*-azirine-2-carboxylate (3k)



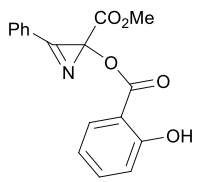
Compound **3k** (232 mg, 70%) was prepared according to the general procedure from azirine **1a** (254 mg, 1 mmol) and 2,6-difluorobenzoic acid (190 mg, 1.2 mmol). Colorless solid, mp 69–70 °C (from Et_2O/hexane). ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.85 (s, 3H), 6.94–7.03 (m, 2H), 7.43–7.53 (m, 1H), 7.60–7.67 (m, 2H), 7.69–7.76 (m, 1H), 8.16–8.24 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 53.4, 64.3, 109.4 (t, *J* 16.7 Hz), 112.2 (dd, *J* 22.4, 3.5 Hz), 120.5, 129.4, 131.3, 133.8 (t, *J* 10.8 Hz), 134.8, 160.9, 161.2 (dd, *J* 259.2, 5.4 Hz), 164.9, 167.4. HRMS (ESI-TOF) *m/z* $[M+Na]^+$ calcd for $C_{17}H_{11}F_2NNaO_4^+$: 354.0548; found: 354.0554.

Methyl 2-[(2-cyanobenzoyl)oxy]-3-phenyl-2*H*-azirine-2-carboxylate (3l)



Compound **3l** (314 mg, 98%) was prepared according to the general procedure from azirine **1a** (254 mg, 1 mmol) and 2-cyanobenzoic acid (177 mg, 1.2 mmol). Colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.82 (s, 3H), 7.62–7.69 (m, 2H), 7.70–7.76 (m, 3H), 7.82–7.88 (m, 1H), 8.19–8.28 (m, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 53.4, 64.5, 113.5, 117.1, 120.4, 129.5, 130.8, 131.4, 131.7, 132.5, 133.4, 134.9, 135.0, 163.2, 165.1, 167.4. HRMS (ESI-TOF) *m/z* $[M+Na]^+$ calcd for $C_{18}H_{12}N_2NaO_4^+$: 343.0689; found: 343.0688.

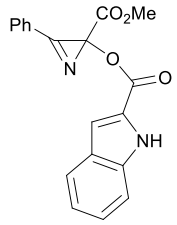
Methyl 2-[(2-hydroxybenzoyl)oxy]-3-phenyl-2*H*-azirine-2-carboxylate (3m)



Compound **3m** (305 mg, 98%) was prepared according to the general procedure from azirine **1a** (254 mg, 1 mmol) and 2-hydroxybenzoic acid (166 mg, 1.2 mmol). Colorless solid, mp 82–83 °C (from Et_2O/hexane). ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.72 (s, 3H), 6.73–6.85 (m, 1H), 6.85–6.95 (m, 1H), 7.33–7.46 (m, 1H), 7.50–7.58 (m, 2H), 7.58–7.68 (m, 1H), 7.76–7.88 (m, 1H), 8.01–8.20 (m, 2H), 10.28 (s,

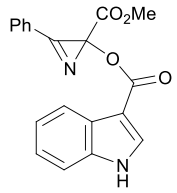
1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 53.4, 64.1, 111.2, 117.6, 119.4, 120.5, 129.4, 130.5, 131.3, 134.9, 136.6, 162.0, 165.0, 167.5, 169.4. HRMS (ESI-TOF) *m/z* $[M+Na]^+$ calcd for $C_{17}H_{13}NNaO_5^+$: 334.0686; found: 334.0689.

2-(Methoxycarbonyl)-3-phenyl-2*H*-azirin-2-yl 1*H*-indole-2-carboxylate (3r)



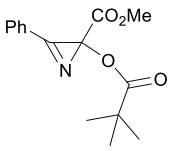
Compound **3r** (261 mg, 78%) was prepared according to the general procedure from azirine **1a** (254 mg, 1 mmol) and 1*H*-indole-2-carboxylic acid (193 mg, 1.2 mmol). Colorless solid, mp 130–131 °C (from Et_2O/hexane). ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.83 (s, 3H), 7.12–7.22 (m, 1H), 7.31–7.40 (m, 2H), 7.41–7.47 (m, 1H), 7.59–7.68 (m, 2H), 7.68–7.77 (m, 2H), 8.17–8.27 (m, 2H), 9.05 (s, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 53.4, 63.8, 110.9, 111.9, 120.7, 121.0, 122.8, 125.5, 126.0, 127.3, 129.4, 131.3, 134.8, 137.3, 160.9, 165.2, 167.9. HRMS (ESI-TOF) *m/z* $[M+H]^+$ calcd for $C_{19}H_{15}N_2O_4^+$: 335.1026; found: 335.1029.

2-(Methoxycarbonyl)-3-phenyl-2*H*-azirin-2-yl 1*H*-indole-3-carboxylate (3s)



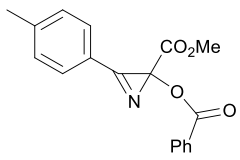
Compound **3s** (241 mg, 72%) was prepared according to the general procedure from azirine **1a** (254 mg, 1 mmol) and 1*H*-indole-3-carboxylic acid (193 mg, 1.2 mmol). Colorless solid, mp 129–130 °C (from Et_2O/hexane). ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.83 (s, 3H), 7.20–7.30 (m, 2H), 7.35–7.46 (m, 1H), 7.57–7.66 (m, 2H), 7.67–7.73 (m, 1H), 7.89–7.95 (m, 1H), 8.15–8.21 (m, 1H), 8.22–8.28 (m, 2H), 9.17 (s, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 53.3, 63.0, 106.6, 111.7, 121.0, 121.3, 122.2, 123.3, 125.8, 139.3, 131.2, 132.5, 134.6, 136.1, 163.8, 165.9, 168.9. HRMS (ESI-TOF) *m/z* $[M+H]^+$ calcd for $C_{19}H_{15}N_2O_4^+$: 335.1026; found: 335.1036.

Methyl 3-phenyl-2-(pivaloyloxy)-2*H*-azirine-2-carboxylate (3t)



Compound **3t** (173 mg, 63%) was prepared according to the general procedure from azirine **1a** (254 mg, 1 mmol) and pivalic acid (123 mg, 1.2 mmol). Colorless solid, mp 56–57 °C (from Et_2O/hexane). ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.27 (s, 9H), 3.78 (s, 3H), 7.58–7.65 (m, 2H), 7.67–7.74 (m, 1H), 8.12–8.19 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 26.9, 38.7, 53.1, 63.3, 120.9, 129.3, 131.1, 134.6, 165.6, 168.0, 177.9. HRMS (ESI-TOF) *m/z* $[M+Na]^+$ calcd for $C_{15}H_{17}NNaO_4^+$: 298.1050; found: 298.1057.

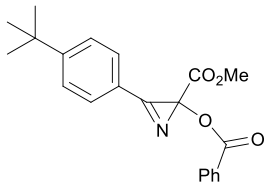
Methyl 2-(benzoyloxy)-3-(*p*-tolyl)-2*H*-azirine-2-carboxylate (3w)



Compound **3w** (294 mg, 95%) was prepared according to the general procedure from azirine **1b** (268 mg, 1 mmol) and benzoic acid (146 mg, 1.2 mmol). Colorless solid, mp 117–118 °C (from Et_2O/hexane). ^{1}H NMR (400

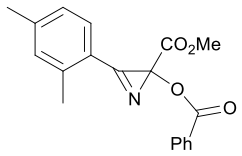
MHz, $CDCl_3$) δ 2.49 (s, 3H), 3.81 (s, 3H), 7.38–7.53 (m, 4H), 7.57–7.65 (m, 1H), 8.01–8.20 (m, 4H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 22.0, 53.2, 63.8, 118.0, 124.4, 128.7, 130.11, 130.12, 131.3, 133.7, 145.9, 164.9, 166.0, 168.1. HRMS (ESI-TOF) *m/z* $[M+Na]^+$ calcd for $C_{18}H_{15}NNaO_4^+$: 332.0893; found: 332.0902.

Methyl 2-(benzoyloxy)-3-[4-(*tert*-butyl)phenyl]-2*H*-azirine-2-carboxylate (3x)



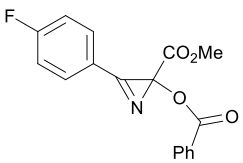
Compound **3x** (341 mg, 97%) was prepared according to the general procedure from azirine **1c** (310 mg, 1 mmol) and benzoic acid (146 mg, 1.2 mmol). Colorless oil. ^1H NMR (400 MHz, $CDCl_3$) δ 1.39 (s, 9H), 3.81 (s, 3H), 7.43–7.51 (s, 2H), 7.57–7.63 (m, 1H), 7.64–7.69 (m, 2H), 8.08–8.19 (m, 4H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 31.0, 35.5, 53.2, 63.7, 117.9, 126.5, 128.4, 128.7, 130.1, 130.2, 133.7, 158.9, 164.9, 166.0, 168.1. HRMS (ESI-TOF) *m/z* $[M+Na]^+$ calcd for $C_{21}H_{21}NNaO_4^+$: 374.1363; found: 374.1369.

Methyl 2-(benzoyloxy)-3-(2,4-dimethylphenyl)-2*H*-azirine-2-carboxylate (3y)



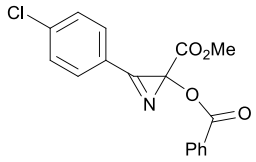
Compound **3y** (304 mg, 94%) was prepared according to the general procedure from azirine **1d** (282 mg, 1 mmol) and benzoic acid (146 mg, 1.2 mmol). Colorless solid, mp 77–78 °C (from Et_2O/hexane). ^1H NMR (400 MHz, $CDCl_3$) δ 2.45 (s, 3H), 2.77 (s, 3H), 3.81 (s, 3H), 7.20–7.29 (m, 2H), 7.42–7.52 (m, 2H), 7.56–7.65 (m, 1H), 8.00–8.08 (m, 1H), 8.09–8.19 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 20.1, 21.9, 53.2, 62.2, 116.7, 1273, 128.4, 128.8, 130.1, 131.9, 133.6, 133.7, 142.6, 145.5, 163.7, 166.0, 168.3. HRMS (ESI-TOF) *m/z* $[M+H]^+$ calcd for $C_{19}H_{18}NO_4^+$: 324.1230; found: 324.1229.

Methyl 2-(benzoyloxy)-3-(4-fluorophenyl)-2*H*-azirine-2-carboxylate (3z)



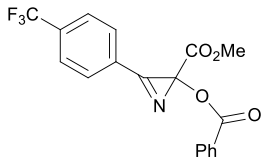
Compound **3z** (310 mg, 99%) was prepared according to the general procedure from azirine **1e** (272 mg, 1 mmol) and benzoic acid (146 mg, 1.2 mmol). Colorless solid, mp 97–98 °C (from Et_2O/hexane). ^1H NMR (400 MHz, $CDCl_3$) δ 3.82 (s, 3H), 7.29–7.37 (m, 2H), 7.44–7.51 (m, 2H), 7.59–7.65 (m, 1H), 8.08–8.15 (m, 2H), 8.22–8.29 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 53.3, 63.8, 117.0 (d, *J* 22.4 Hz), 117.2 (d, *J* 3.2 Hz), 128.49, 128.52, 130.1, 133.9 (d, *J* 6.9 Hz), 134.0, 164.6, 166.0, 166.6 (d, *J* 258.2 Hz), 167.8. HRMS (ESI-TOF) *m/z* $[M+H]^+$ calcd for $C_{17}H_{13}FNO_4^+$: 314.0823; found: 314.0818.

Methyl 2-(benzoyloxy)-3-(4-chlorophenyl)-2*H*-azirine-2-carboxylate (3za)



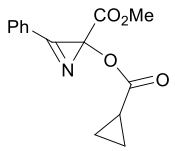
Compound **3za** (303 mg, 92%) was prepared according to the general procedure from azirine **1f** (288 mg, 1 mmol) and benzoic acid (146 mg, 1.2 mmol). Colorless solid, mp 130–131 °C (from Et_2O/hexane). ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.82 (s, 3H), 7.44–7.52 (m, 2H), 7.58–7.66 (m, 3H), 8.08–8.14 (m, 2H), 8.14–8.20 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 53.4, 63.7, 119.3, 128.49, 128.51, 129.9, 130.1, 132.5, 133.9, 141.4, 165.0, 166.0, 167.7. HRMS (ESI-TOF) *m/z* $[M+Na]^+$ calcd for $C_{17}H_{12}{}^{35}ClNNaO_4^+$: 352.0347; found: 352.0341.

Methyl 2-(benzoyloxy)-3-(4-(trifluoromethyl)phenyl)-2*H*-azirine-2-carboxylate (3zb)



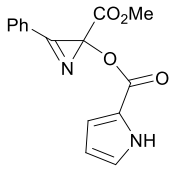
Compound **3zb** (251 mg, 69%) was prepared according to the general procedure from azirine **1g** (322 mg, 1 mmol) and benzoic acid (146 mg, 1.2 mmol). Colorless solid, mp 104–105 °C (from Et_2O/hexane). ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.83 (s, 3H), 7.45–7.52 (m, 2H), 7.60–7.66 (m, 1H), 7.88–7.94 (m, 2H), 8.09–8.15 (m, 2H), 8.33–8.40 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 53.5, 63.6, 123.3 (q, *J* 273 Hz), 124.3, 126.4 (q, *J* 3.6 Hz), 128.4, 128.6, 130.2, 131.6, 134.0, 135.9 (q, *J* 33.3 Hz), 165.7, 165.9, 167.5. HRMS (ESI-TOF) *m/z* $[M+Na]^+$ calcd for $C_{18}H_{12}F_3NNaO_4^+$: 386.0611; found: 386.0603.

Methyl 2-[(cyclopropanecarbonyl)oxy]-3-phenyl-2*H*-azirine-2-carboxylate (3zd)



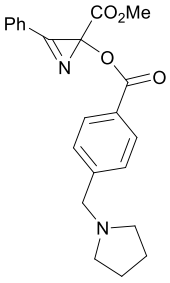
Compound **3zd** (171 mg, 66%) was prepared according to the general procedure from azirine **1a** (254 mg, 1 mmol) and cyclopropanecarboxylic acid (103 mg, 1.2 mmol). Colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 0.91–1.03 (m, 2H), 1.07–1.18 (m, 2H), 1.67–1.76 (m, 1H), 3.78 (s, 3H), 7.57–7.64 (m, 2H), 7.67–7.73 (m, 1H), 8.09–8.15 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 9.15, 9.18, 12.6, 53.2, 63.1, 120.9, 129.3, 131.2, 134.6, 165.4, 168.0, 174.1. HRMS (ESI-TOF) *m/z* $[M+Na]^+$ calcd for $C_{14}H_{13}NNaO_4^+$: 282.0737; found: 282.0731.

2-(Methoxycarbonyl)-3-phenyl-2*H*-azirin-2-yl 1*H*-pyrrole-2-carboxylate (3zf)



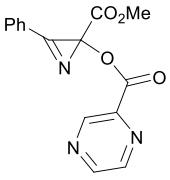
Compound **3zf** (179 mg, 63%) was prepared according to the general procedure from azirine **1a** (254 mg, 1 mmol) and 1*H*-pyrrole-2-carboxylic acid (133 mg, 1.2 mmol). Colorless solid, mp 102–103 °C (from Et_2O/hexane). ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.81 (s, 3H), 6.26–6.35 (m, 1H), 6.98–7.03 (m, 1H), 7.04–7.10 (m, 1H), 7.57–7.66 (m, 2H), 7.68–7.75 (m, 1H), 8.15–8.25 (m, 2H), 9.36 (br s, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 53.3, 63.3, 101.9, 117.4, 120.8, 121.0, 124.2, 129.3, 131.2, 134.6, 159.8, 165.4, 168.1. HRMS (ESI-TOF) *m/z* $[M+Na]^+$ calcd for $C_{15}H_{12}N_2NaO_4^+$: 307.0682; found: 307.0689.

Methyl 3-phenyl-2-((4-(pyrrolidin-1-ylmethyl)benzoyl)oxy)-2*H*-azirine-2-carboxylate (3zg)



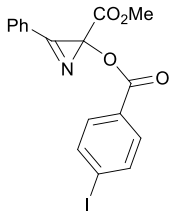
Compound **3zg** (189 mg, 50%) was prepared according to the general procedure from azirine **1a** (254 mg, 1 mmol) and 4-(pyrrolidin-1-ylmethyl)benzoic acid (246 mg, 1.2 mmol). Pink solid, mp 102–103 °C (from Et_2O/hexane). ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.75–1.85 (m, 4H), 2.47–2.56 (m, 2H), 2.68 (s, 2H), 3.81 (s, 3H), 7.41–7.48 (m, 2H), 7.60–7.66 (m, 2H), 7.67–7.74 (m, 1H), 8.03–8.09 (m, 2H), 8.18–8.25 (m, 2H), 8.15–8.25 (m, 2H), 9.36 (br s, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 23.5, 53.3, 54.2, 60.3, 63.7, 120.9, 127.2, 128.7, 129.4, 130.1, 131.3, 134.6, 146.0, 165.6, 165.9, 168.0. HRMS (ESI-TOF) *m/z* $[M+H]^+$ calcd for $C_{22}H_{23}N_2O_4^+$: 379.1652; found: 379.1666.

2-(Methoxycarbonyl)-3-phenyl-2*H*-azirin-2-yl pyrazine-2-carboxylate (3zh)



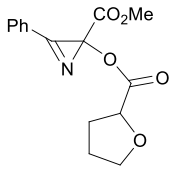
Compound **3zh** (279 mg, 94%) was prepared according to the general procedure from azirine **1a** (254 mg, 1 mmol) and pyrazine-2-carboxylic acid (149 mg, 1.2 mmol). Colorless solid, mp 66–67 °C (from Et_2O/hexane). ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.83 (s, 3H), 7.59–7.67 (m, 2H), 7.69–7.78 (m, 1H), 8.16–8.25 (m, 2H), 8.73–8.84 (m, 2H), 9.34–9.42 (m, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 53.5, 64.7, 120.3, 129.4, 131.4, 134.9, 142.2, 144.7, 146.6, 148.2, 163.3, 164.8, 167.3. HRMS (ESI-TOF) *m/z* $[M+Na]^+$ calcd for $C_{15}H_{11}N_3NaO_4^+$: 320.0642; found: 320.0645.

Methyl 2-[(4-iodobenzoyl)oxy]-3-phenyl-2*H*-azirine-2-carboxylate (3zi)



Compound **3zi** (345 mg, 82%) was prepared according to the general procedure from azirine **1a** (254 mg, 1 mmol) and 4-iodobenzoic acid (298 mg, 1.2 mmol). Colorless solid, mp 122–123 °C (from Et_2O/hexane). ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.81 (s, 3H), 7.60–7.68 (m, 2H), 7.69–7.75 (m, 1H), 7.79–7.88 (m, 4H), 8.17–8.25 (m, 2H), 8.16–8.24 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 53.3, 64.0, 101.8, 120.7, 128.1, 129.4, 131.3, 131.4, 134.8, 137.9, 165.3, 165.5, 167.8. HRMS (ESI-TOF) *m/z* $[M+Na]^+$ calcd for $C_{17}H_{12}INNaO_4^+$: 443.9703; found: 443.9705.

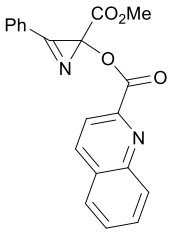
Methyl 3-phenyl-2-[(tetrahydrofuran-2-carbonyl)oxy]-2*H*-azirine-2-carboxylate (3zm)



Compound **3zm** (226 mg, 78%) was prepared as a 1:0.8 diastereomeric mixture according to the general procedure from azirine **1a** (254 mg, 1 mmol) and tetrahydrofuran-2-carboxylic acid (139 mg, 1.2 mmol). Colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.90–2.16 (m, 2.5H), 2.23–2.39 (m, 1.5H), 3.75–3.77 (m, 3H), 3.88–3.98 (m, 1H), 4.00–4.12 (m, 1H), 4.50–4.60 (m, 1H), 7.56–7.63 (m, 2H), 7.66–7.73 (m, 1H), 8.08–8.18 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 25.0, 25.1, 30.09, 30.13, 53.21,

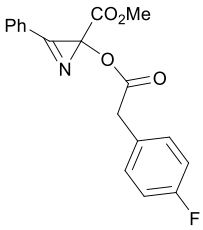
53.24, 63.4, 63.5, 69.5, 69.6, 75.9, 76.4, 120.4, 120.5, 129.3, 131.2, 131.3, 134.7, 134.8, 164.9, 165.2, 167.6, 167.7, 172.8, 172.9. HRMS (ESI-TOF) *m/z* $[M+Na]^+$ calcd for $C_{15}H_{15}NNaO_5^+$: 312.0842; found: 312.0853.

2-(Methoxycarbonyl)-3-phenyl-2*H*-azirin-2-yl quinoline-2-carboxylate (3zo)



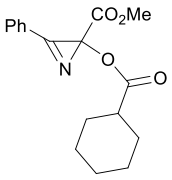
Compound **3zo** (326 mg, 94%) was prepared according to the general procedure from azirine **1a** (254 mg, 1 mmol) and quinoline-2-carboxylic acid (208 mg, 1.2 mmol). Colorless solid, mp 138–139 °C (from Et_2O/hexane). ^1H NMR (400 MHz, $CDCl_3$) δ 3.83 (s, 3H), 7.60–7.73 (m, 4H), 7.77–7.84 (m, 1H), 7.87–7.92 (m, 1H), 8.22–8.30 (m, 3H), 8.30–8.36 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 53.4, 64.6, 120.6, 121.3, 127.5, 128.9, 129.4, 129.5, 130.4, 130.9, 131.4, 134.7, 137.3, 146.5, 147.8, 164.5, 165.2, 167.7. HRMS (ESI-TOF) *m/z* $[M+H]^+$ calcd for $C_{20}H_{15}N_2O_4^+$: 347.1026; found: 347.1032.

Methyl 2-[2-(4-fluorophenyl)acetoxy]-3-phenyl-2*H*-azirine-2-carboxylate (3zp)



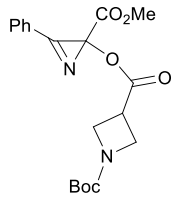
Compound **3zp** (229 mg, 70%) was prepared according to the general procedure from azirine **1a** (254 mg, 1 mmol) and 2-(4-fluorophenyl)acetic acid (185 mg, 1.2 mmol). Colorless solid, mp 60–61 °C (from Et_2O/hexane). ^1H NMR (400 MHz, $CDCl_3$) δ 3.73 (q, *J* 16.0 Hz, 2H), 3.76 (s, 3H), 7.00–7.08 (m, 2H), 7.24–7.32 (m, 2H), 7.56–7.64 (m, 2H), 7.67–7.74 (m, 1H), 8.08–8.16 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 39.7, 53.2, 63.6, 115.5 (d, *J* 21.5 Hz), 120.6, 128.4 (d, *J* 3.2 Hz), 129.3, 131.0 (d, *J* 8.3 Hz), 131.2, 134.7, 160.9, 163.3, 166.4 (d, *J* 253.1 Hz), 170.9. HRMS (ESI-TOF) *m/z* $[M+Na]^+$ calcd for $C_{18}H_{14}FNNaO_4^+$: 350.0799; found: 350.0800.

Methyl 2-[(cyclohexanecarbonyl)oxy]-3-phenyl-2*H*-azirine-2-carboxylate (3zq)



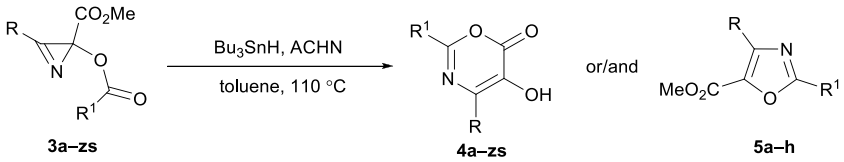
Compound **3zq** (271 mg, 90%) was prepared according to the general procedure from azirine **1a** (254 mg, 1 mmol) and cyclohexanecarboxylic acid (154 mg, 1.2 mmol). Colorless solid, mp 37–38 °C (from Et_2O/hexane). ^1H NMR (400 MHz, $CDCl_3$) δ 1.21–1.36 (m, 3H), 1.47–1.67 (m, 3H), 1.71–1.85 (m, 2H), 1.87–1.97 (m, 1H), 1.98–2.09 (m, 1H), 2.36–2.48 (m, 1H), 3.78 (s, 3H), 7.56–7.66 (m, 2H), 7.66–7.74 (m, 1H), 8.08–8.21 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 25.1, 25.2, 25.7, 28.5, 28.8, 42.6, 53.1, 63.1, 120.9, 129.3, 131.2, 134.6, 165.5, 168.0, 175.3. HRMS (ESI-TOF) *m/z* $[M+Na]^+$ calcd for $C_{17}H_{19}NNaO_4^+$: 324.1206; found: 324.1197.

1-(*tert*-Butyl) 3-(2-(methoxycarbonyl)-3-phenyl-2*H*-azirin-2-yl) azetidine-1,3-dicarboxylate (3zr)



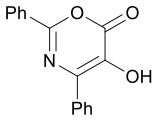
Compound **3zr** (356 mg, 95%) was prepared according to the general procedure from azirine **1a** (254 mg, 1 mmol) and 1-(*tert*-butoxycarbonyl)azetidine-3-carboxylic acid (241 mg, 1.2 mmol). Colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$), *δ*, ppm: 1.45 (s, 9H), 3.40–3.49 (m, 1H), 3.79 (s, 3H), 4.06–4.24 (m, 4H), 7.59–7.67 (m, 2H), 7.69–7.76 (m, 1H), 8.10–8.16 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 28.3, 31.7, 51.3, 53.3, 63.7, 79.9, 120.4, 129.4, 131.2, 134.9, 155.9, 164.9, 167.6, 171.9. HRMS (ESI-TOF) *m/z* $[M+H]^+$ calcd for $C_{19}H_{23}N_2O_6^+$: 375.1551; found: 375.1551.

6. Synthesis of 1,3-oxazin-6-ones 4 and oxazoles 5



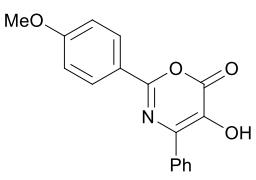
A stirred solution of 2-acyloxy-2*H*-azirine (0.5 mmol), Bu_3SnH (291 mg, 1 mmol) and 1,1'-(diazene-1,2-diyl)dicyclohexanecarbonitrile (ACHN) (122 mg, 0.5 mmol) in anhydrous toluene (10 mL) was heated under reflux for 1 h. The solvent was removed under reduced pressure, and the residue was purified by column chromatography on silica gel ($CHCl_3$–benzene, from 1:100 to 1:0) to give, depending on starting compound, the oxazinone, oxazole or their mixture.

5-Hydroxy-2,4-diphenyl-6*H*-1,3-oxazin-6-one (4a)[8]



Compound **4a** (93 mg, 70%) was prepared according to the general procedure from azirine **3a** (148 mg, 0.5 mmol). Colorless solid, mp 197–199 °C (from Et_2O/hexane). ^{1}H NMR (400 MHz, DMSO-d_6) δ 7.42–7.48 (m, 1H), 7.50–7.65 (m, 5H), 8.10–8.18 (m, 2H), 8.27–8.35 (m, 2H), 10.77 (s, 1H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 127.1, 128.2, 128.7, 128.9, 129.4, 129.9, 131.8, 134.2, 134.7, 135.6, 151.0, 158.6. HRMS (ESI-TOF) *m/z* $[M+H]^+$ calcd for $C_{16}H_{12}NO_3^+$: 266.0812; found: 266.0812.

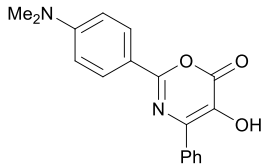
5-Hydroxy-2-(4-methoxyphenyl)-4-phenyl-6*H*-1,3-oxazin-6-one (4b)



Compound **4b** (111 mg, 75%) was prepared according to the general procedure from azirine **3b** (163 mg, 0.5 mmol). Colorless solid, mp 217–218 °C (from Et_2O/hexane). ^{1}H NMR (400 MHz, DMSO-d_6) δ 3.84 (s, 3H), 7.05–7.13 (m, 2H), 7.41–7.48 (m, 1H), 7.48–7.55 (m, 2H), 8.01–8.10

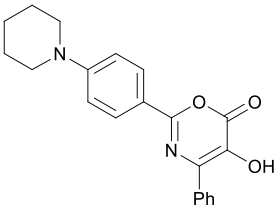
(m, 2H), 8.24–8.34 (m, 2H), 10.56 (bs, 1H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 55.5, 114.4, 122.2, 128.1, 128.7, 129.0, 129.3, 134.3, 134.9, 135.1, 151.2, 158.6, 162.2. HRMS (ESI-TOF) *m/z* $[M+Na]^+$ calcd for $C_{17}H_{13}NO_4^+$: 318.0737; found: 318.0741.

2-[4-(Dimethylamino)phenyl]-5-hydroxy-4-phenyl-6*H*-1,3-oxazin-6-one (4c)



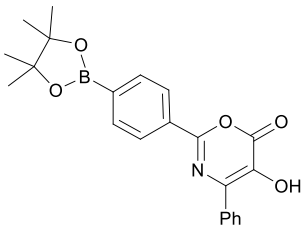
Compound **4c** (139 mg, 90%) was prepared according to the general procedure from azirine **3c** (169 mg, 0.5 mmol). Yellow solid, mp 248–250 °C (from Et_2O/hexane). ^{1}H NMR (400 MHz, DMSO-d_6) δ 3.04 (s, 6H), 6.78–6.86 (m, 2H), 7.4–7.48 (m, 1H), 7.49–7.56 (m, 2H), 7.90–7.99 (m, 2H), 8.24–8.34 (m, 2H), 10.30 (s, 1H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 39.6, 111.3, 116.2, 128.1, 128.6, 128.8, 129.2, 133.8, 134.6, 135.8, 152.40, 152.42, 158.9. HRMS (ESI-TOF) *m/z* $[M+Na]^+$ calcd for $C_{18}H_{16}N_2NaO_3^+$: 331.1053; found: 331.1051.

5-Hydroxy-4-phenyl-2-(4-(piperidin-1-yl)phenyl)-6*H*-1,3-oxazin-6-one (4d)



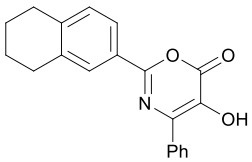
Compound **4d** (153 mg, 99%) was prepared according to the general procedure from azirine **3d** (189 mg, 0.5 mmol). Yellow solid, mp 210–211 °C (from Et_2O/hexane). ^{1}H NMR (400 MHz, DMSO-d_6) δ 1.58–1.65 (m, 6H), 3.35–3.40 (m, 4H), 7.00–7.08 (m, 2H), 7.42–7.48 (m, 1H), 7.49–7.55 (m, 2H), 7.90–7.97 (m, 2H), 8.25–8.33 (m, 2H), 10.37 (s, 1H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 23.9, 24.8, 47.8, 113.8, 117.7, 128.1, 128.6, 128.8, 129.3, 134.1, 134.5, 135.7, 152.1, 153.1, 158.8. HRMS (ESI-TOF) *m/z* $[M+H]^+$ calcd for $C_{18}H_{17}N_2O_3^+$: 309.1234; found: 309.1239.

5-Hydroxy-4-phenyl-2-[4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)phenyl]-6*H*-1,3-oxazin-6-one (4e)



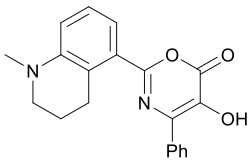
Compound **4e** (145 mg, 74%) was prepared according to the general procedure from azirine **3e** (163 mg, 0.5 mmol). Colorless solid, mp 213–215 °C (from Et_2O/hexane). ^{1}H NMR (400 MHz, DMSO-d_6) δ 1.32 (s, 12H), 7.41–7.48 (m, 1H), 7.49–7.56 (m, 2H), 7.82–7.89 (m, 2H), 8.10–8.17 (m, 2H), 8.26–8.33 (m, 2H), 10.84 (br s, 1H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 24.7, 83.5, 126.3, 128.2, 128.7, 129.3, 132.3, 134.2, 134.7, 134.8, 136.0, 150.7, 158.4. HRMS (ESI-TOF) *m/z* $[M+Na]^+$ calcd for $C_{22}H_{22}BNNaO_5^+$: 414.1483; found: 414.1489.

5-Hydroxy-4-phenyl-2-(5,6,7,8-tetrahydronaphthalen-2-yl)-6*H*-1,3-oxazin-6-one (4f)



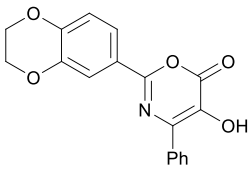
Compound **4f** (126 mg, 79%) was prepared according to the general procedure from azirine **3f** (175 mg, 0.5 mmol). Colorless solid, mp 208–210 °C (from Et_2O/hexane). ^{1}H NMR (400 MHz, DMSO-d_6) δ 1.62–1.86 (m, 4H), 2.66–2.87 (m, 4H), 7.13–7.27 (m, 1H), 7.38–7.59 (m, 3H), 7.68–7.88 (m, 2H), 8.19–8.37 (m, 2H), 10.64 (s, 1H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 22.3, 22.4, 28.7, 28.8, 124.2, 127.0, 127.5, 128.1, 128.7, 129.3, 129.5, 134.3, 134.9, 135.2, 137.3, 141.2, 151.3, 158.6. HRMS (ESI-TOF) *m/z* $[M+H]^+$ calcd for $C_{20}H_{18}NO_3^+$: 320.1281; found: 320.1290.

5-Hydroxy-2-(1-methyl-1,2,3,4-tetrahydroquinolin-5-yl)-4-phenyl-6*H*-1,3-oxazin-6-one (4g)



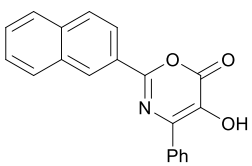
Compound **4g** (150 mg, 90%) was prepared according to the general procedure from azirine **3g** (182 mg, 0.5 mmol). Colorless solid, mp 225–227 °C (from Et_2O/hexane). ^{1}H NMR (400 MHz, DMSO-d_6) δ 1.86–1.96 (m, 2H), 2.75–2.82 (m, 2H), 2.96 (s, 3H), 3.33–3.38 (m, 2H), 6.62–6.71 (m, 2H), 7.41–7.47 (m, 1H), 7.48–7.55 (m, 2H), 7.62–7.69 (m, 1H), 7.74–7.81 (m, 1H), 8.19–8.37 (m, 2H), 10.30 (s, 1H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 21.2, 27.2, 38.3, 50.3, 109.8, 115.7, 121.8, 127.0, 127.3, 128.1, 128.8, 129.2, 133.6, 134.6, 136.0, 149.1, 152.6, 158.9. HRMS (ESI-TOF) *m/z* $[M+H]^+$ calcd for $C_{20}H_{19}N_2O_3^+$: 335.1390; found: 335.1385.

2-(2,3-Dihydrobenzo[*b*][1,4]dioxin-6-yl)-5-hydroxy-4-phenyl-6*H*-1,3-oxazin-6-one (4h)



Compound **4h** (120 mg, 74%) was prepared according to the general procedure from azirine **3h** (177 mg, 0.5 mmol). Colorless solid, mp 239–241 °C (from Et_2O/hexane). ^{1}H NMR (400 MHz, DMSO-d_6) δ 4.23–4.38 (m, 4H), 6.95–7.06 (m, 1H), 7.38–7.55 (m, 4H), 7.56–7.65 (m, 1H), 8.21–8.36 (m, 2H), 10.60 (s, 1H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 64.0, 64.4, 115.8, 117.6, 120.7, 123.0, 128.2, 128.7, 129.3, 134.3, 134.97, 135.02, 143.5, 146.8, 150.8, 158.6. HRMS (ESI-TOF) *m/z* $[M+Na]^+$ calcd for $C_{18}H_{13}NNaO_5^+$: 346.0686; found: 346.0689.

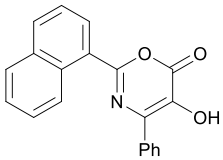
5-Hydroxy-2-(naphthalen-2-yl)-4-phenyl-6*H*-1,3-oxazin-6-one (4i)



Compound **4i** (134 mg, 85%) was prepared according to the general procedure from azirine **3i** (173 mg, 0.5 mmol). Colorless solid, mp 207–209 °C (from Et_2O/hexane). ^{1}H NMR (400 MHz, DMSO-d_6) δ 7.41–7.49 (m, 1H), 7.50–7.57 (m, 2H), 7.57–7.66 (m, 2H), 7.94–8.01 (m, 1H), 8.01–8.10 (m, 1H), 8.11–8.19 (m, 1H), 8.20–8.26 (m, 1H), 8.30–8.40 (m, 2H), 8.62–8.70 (m, 1H), 10.81 (s, 1H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 123.5, 127.0, 127.2, 127.6, 127.7, 128.1,

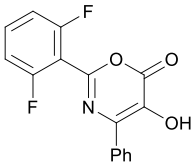
128.2, 128.6, 128.8, 129.1, 129.3, 132.4, 134.3 (2C), 134.9, 135.7, 151.1, 158.6. HRMS (ESI-TOF) *m/z* $[M+H]^+$ calcd for $C_{20}H_{14}NO_3^+$: 316.0968; found: 316.0967.

5-Hydroxy-2-(naphthalen-1-yl)-4-phenyl-6*H*-1,3-oxazin-6-one (4j)



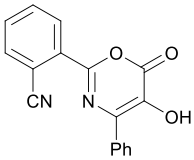
Compound **4j** (110 mg, 70%) was prepared according to the general procedure from azirine **3j** (173 mg, 0.5 mmol). Colorless solid, mp 173–175 °C (from Et_2O/hexane). ^1H NMR (400 MHz, DMSO-d_6) δ 7.43–7.50 (m, 1H), 7.52–7.57 (m, 2H), 7.62–7.73 (m, 3H), 8.06–8.11 (m, 1H), 8.14–8.23 (m, 2H), 8.27–8.33 (m, 2H), 8.90–9.03 (m, 1H), 10.86 (s, 1H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 125.1, 125.4, 126.4, 127.0, 127.6, 128.3, 128.6, 128.7, 129.0, 129.3, 129.8, 132.1, 133.5, 134.4, 134.7, 135.8, 151.6, 159.0. HRMS (ESI-TOF) *m/z* $[M–H]^–$ calcd for $C_{20}H_{12}NO_3^–$: 314.0823; found: 314.0808.

2-(2,6-Difluorophenyl)-5-hydroxy-4-phenyl-6*H*-1,3-oxazin-6-one (4k)



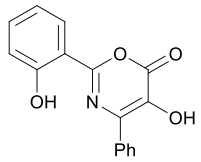
Compound **4k** (63 mg, 42%) was prepared according to the general procedure from azirine **3k** (166 mg, 0.5 mmol). Colorless solid, mp 183–185 °C (from Et_2O/hexane). ^1H NMR (400 MHz, DMSO-d_6) δ 7.29–7.38 (m, 2H), 7.41–7.47 (m, 1H), 7.47–7.54 (m, 2H), 7.65–7.76 (m, 1H), 8.11–8.30 (m, 2H), 10.11 (br s, 1H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 109.3 (t, *J* 16 Hz), 112.7 (dd, *J* 22.4, 3.5 Hz), 128.3, 128.6, 129.5, 133.7, 133.9 (t, *J* 10.6 Hz), 134.5, 136.2, 143.8, 158.3, 159.9 (dd, *J* 254.9, 5.2 Hz). HRMS (ESI-TOF) *m/z* $[M+H]^+$ calcd for $C_{16}H_9F_2NO_3^+$: 302.0623; found: 302.0619.

2-(5-Hydroxy-6-oxo-4-phenyl-6*H*-1,3-oxazin-2-yl)benzonitrile (4l)



Compound **4l** (45 mg, 31%) was prepared according to the general procedure from azirine **3l** (160 mg, 0.5 mmol). Colorless solid, mp 222–224 °C (from Et_2O/hexane). ^1H NMR (400 MHz, DMSO-d_6) δ 7.43–7.57 (m, 3H), 7.76–7.85 (m, 1H), 7.88–7.96 (m, 1H), 8.05–8.12 (m, 1H), 8.15–8.24 (m, 1H), 8.37–8.52 (m, 2H), 11.12 (s, 1H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 115.1, 123.4, 133.4, 134.3, 134.4, 134.7, 136.9, 137.1, 138.7, 139.3, 139.7, 141.0, 141.9, 153.3, 163.4. HRMS (ESI-TOF) *m/z* $[M–H]^–$ calcd for $C_{17}H_9N_2O_3^–$: 289.0619; found: 289.0616.

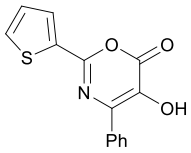
5-Hydroxy-2-(2-hydroxyphenyl)-4-phenyl-6*H*-1,3-oxazin-6-one (4m)



Compound **4m** (20 mg, 14%) was prepared according to the general procedure from azirine **3m** (104 mg, 0.5 mmol). Colorless solid, mp 263–264 °C (from Et_2O/hexane). ^1H NMR (400 MHz, DMSO-d_6) δ 6.95–7.11 (m, 2H), 7.43–7.52 (m, 2H), 7.52–7.60 (m, 2H), 7.78–7.87 (m, 1H), 7.95–8.10 (m, 2H), 10.93 (s, 1H), 12.25 (s, 1H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 112.4, 117.3, 119.5, 127.3, 128.0, 128.5,

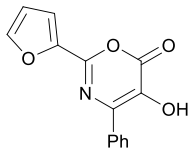
129.6, 133.3, 133.9, 134.1, 135.3, 153.4, 157.4, 158.8. HRMS (ESI-TOF) *m/z* $[M+H]^+$ calcd for $C_{16}H_{11}NO_4^+$: 308.0580; found: 308.0578.

5-Hydroxy-4-phenyl-2-(thiophen-2-yl)-6*H*-1,3-oxazin-6-one (4n)



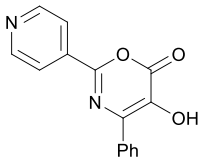
Compound **4n** (113 mg, 83%) was prepared according to the general procedure from azirine **3n** (151 mg, 0.5 mmol). Colorless solid, mp 218–220 °C (from Et_2O/hexane). ^1H NMR (400 MHz, DMSO-d_6) δ 7.24 (dd, 1H, *J* 5.1, 3.8 Hz), 7.40–7.47 (m, 1H), 7.47–7.55 (M, 2H), 7.80 (dd, 1H, *J* 3.8, 1.3 Hz), 7.89 (dd, 1H, *J* 5.1, 1.3 Hz), 8.18–8.27 (m, 2H), 10.70 (s, 1H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 128.2, 128.6, 128.7 129.4, 130.2, 132.2, 133.7, 134.0, 135.05, 135.11, 148.1, 158.1. HRMS (ESI-TOF) *m/z* $[M+H]^+$ calcd for $C_{14}H_{10}NO_3S^+$: 272.0376; found: 272.0375.

2-(Furan-2-yl)-5-hydroxy-4-phenyl-6*H*-1,3-oxazin-6-one (4o)



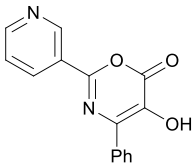
Compound **4o** (75 mg, 59%) was prepared according to the general procedure from azirine **3o** (143 mg, 0.5 mmol). Colorless solid, mp 220–221 °C (from Et_2O/hexane). ^1H NMR (400 MHz, DMSO-d_6) δ 6.76 (dd, 1H, *J* 3.6, 1.8 Hz), 7.31 (d, 1H, *J* 3.6 Hz), 7.41–7.47 (m, 1H), 7.47–7.54 (m, 2H), 8.01 (d, 1H, *J* 1.8 Hz), 8.18–8.29 (m, 2H), 10.73 (s, 1H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 112.7, 115.1, 128.2, 128.7, 129.4, 134.0, 135.1, 135.3, 144.1, 144.3, 145.0, 157.9. HRMS (ESI-TOF) *m/z* $[M+H]^+$ calcd for $C_{14}H_{10}NO_4^+$: 256.0604; found: 256.0606.

5-Hydroxy-4-phenyl-2-(pyridin-4-yl)-6*H*-1,3-oxazin-6-one (4p)



Compound **4p** (91 mg, 68%) was prepared according to the general procedure from azirine **3p** (148 mg, 0.5 mmol). Colorless solid, mp 244–246 °C (from Et_2O/hexane). ^1H NMR (400 MHz, DMSO-d_6) δ 7.42–7.49 (m, 1H), 7.50–7.56 (m, 2H), 7.97–8.04 (m, 2H), 8.26–8.35 (m, 2H), 8.72–8.88 (m, 2H), 11.12 (bs, 1H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 120.6, 128.3, 128.6, 129.4, 134.0, 134.2, 137.0, 137.2, 149.0, 150.6, 158.2. HRMS (ESI-TOF) *m/z* $[M-H]^-$ calcd for $C_{15}H_9N_2O_3^-$: 265.0619; found: 265.0597.

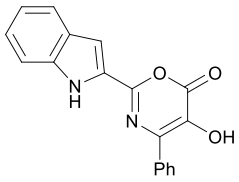
5-Hydroxy-4-phenyl-2-(pyridin-3-yl)-6*H*-1,3-oxazin-6-one (4q)



Compound **4q** (100 mg, 75%) was prepared according to the general procedure from azirine **3q** (148 mg, 0.5 mmol). Colorless solid, mp 202–203 °C (from Et_2O/hexane). ^1H NMR (400 MHz, DMSO-d_6) δ 7.42–7.48 (m, 1H), 7.50–7.57 (m, 2H), 7.97–7.64 (m, 1H), 8.28–8.36 (m, 2H), 8.40–8.49 (m, 1H), 8.70–8.84

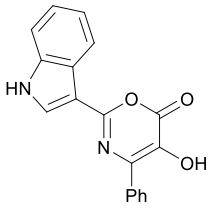
(m, 1H), 9.21–9.33 (m, 1H), 10.94 (s, 1H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 123.9, 126.1, 128.2, 128.7, 129.4, 134.0, 134.5, 134.6, 136.2, 148.0, 149.4, 152.1, 158.3. HRMS (ESI-TOF) *m/z* $[M–H]^-$ calcd for $C_{15}H_9N_2O_3^-$: 265.0619; found: 265.0620.

5-Hydroxy-2-(1*H*-indol-2-yl)-4-phenyl-6*H*-1,3-oxazin-6-one (4r)



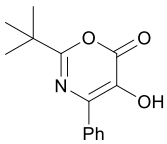
Compound **4r** (56 mg, 37%) was prepared according to the general procedure from azirine **3r** (167 mg, 0.5 mmol). Colorless solid, mp 240–242 °C (from Et_2O/hexane). ^{1}H NMR (400 MHz, DMSO-d_6) δ 7.05–7.13 (m, 1H), 7.18–7.23 (m, 1H), 7.44–7.50 (m, 1H), 7.51–7.58 (m, 3H), 7.64–7.71 (m, 1H), 8.40–8.49 (m, 2H), 10.69 (s, 1H), 11.88 (s, 1H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 105.5, 112.3, 120.1, 121.6, 124.3, 127.4, 128.0, 128.1, 129.0, 129.4, 134.2, 135.05, 135.10, 137.9, 146.9, 158.3. HRMS (ESI-TOF) *m/z* $[M–H]^-$ calcd for $C_{18}H_{11}N_2O_3^-$: 303.0775; found: 303.0769.

5-Hydroxy-2-(1*H*-indol-3-yl)-4-phenyl-6*H*-1,3-oxazin-6-one (4s)



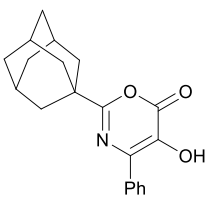
Compound **4s** (68 mg, 45%) was prepared according to the general procedure from azirine **3s** (167 mg, 0.5 mmol). Colorless solid, mp 242–244 °C (from Et_2O/hexane). ^{1}H NMR (400 MHz, DMSO-d_6) δ 7.23–7.30 (m, 2H), 7.44–7.49 (m, 1H), 7.51–7.59 (m, 3H), 8.16–8.23 (m, 1H), 8.31–8.37 (m, 3H), 10.23 (s, 1H), 12.01 (s, 1H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 106.7, 112.4, 120.7, 121.4, 122.7, 124.5, 128.2, 128.7, 129.3, 130.2, 133.4, 134.8, 136.4, 136.8, 151.2, 158.9. HRMS (ESI-TOF) *m/z* $[M+H]^+$ calcd for $C_{18}H_{13}N_2O_3^+$: 305.0921; found: 305.0933.

2-(*tert*-Butyl)-5-hydroxy-4-phenyl-6*H*-1,3-oxazin-6-one (4t)



Compound **4t** (97 mg, 79%) was prepared according to the general procedure from azirine **3t** (177 mg, 0.5 mmol). Colorless solid, mp 165–166 °C (from Et_2O/hexane). ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.43 (s, 9H), 6.55 (s, 1H), 7.42–7.54 (m, 3H), 8.27–8.37 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 27.8, 37.9, 128.3, 129.2, 130.0, 133.4, 133.6, 134.3, 161.2, 162.5. HRMS (ESI-TOF) *m/z* $[M+Na]^+$ calcd for $C_{14}H_{15}NNaO_3^+$: 268.0944; found: 268.0951.

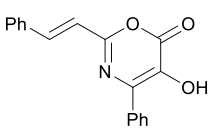
2-(Adamantan-1-yl)-5-hydroxy-4-phenyl-6*H*-1,3-oxazin-6-one (4u)



Compound **4u** (110 mg, 68%) was prepared according to the general procedure from azirine **3u** (177 mg, 0.5 mmol). Colorless solid, mp 219–220 °C (from Et_2O/hexane). ^{1}H NMR (400 MHz, DMSO-d_6) δ 1.67–1.77 (m, 6H), 1.32–2.01 (m, 6H), 2.01–2.09 (m, 3H), 7.37–7.43 (m, 1H), 7.47–7.52 (m, 2H), 8.16–8.25 (m, 2H), 10.44 (s, 1H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 27.3, 35.8, 38.8, 38.9, 128.1, 128.6,

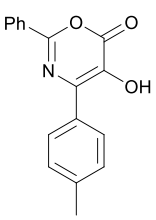
129.2, 134.0, 134.4, 134.7, 159.2, 161.2. HRMS (ESI-TOF) *m/z* $[M+H]^+$ calcd for $C_{20}H_{22}NO_3^+$: 324.1594; found: 324.1594.

(*E*)-5-Hydroxy-4-phenyl-2-styryl-6*H*-1,3-oxazin-6-one (4v)



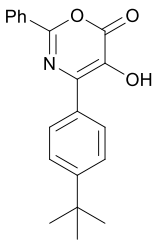
Compound **4v** (102 mg, 70%) was prepared according to the general procedure from azirine **3v** (161 mg, 0.5 mmol). Colorless solid, mp 218–219 °C (from Et_2O/hexane). ^1H NMR (400 MHz, DMSO-d_6) δ 6.96 (d, 1H, *J* 16.2 Hz), 7.40–7.47 (m, 4H), 7.47–7.53 (m, 2H), 7.63 (d, 1H, *J* 16.2 Hz), 8.18–8.27 (m, 2H), 10.72 (s, 1H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 118.8, 127.9, 128.1, 128.7, 128.9, 129.3, 129.9, 134.1, 134.7, 135.37, 135.43, 138.9, 151.8, 158.4. HRMS (ESI-TOF) *m/z* $[M+Na]^+$ calcd for $C_{28}H_{13}NO_3^+$: 314.0788; found: 314.0800.

5-Hydroxy-2-phenyl-4-(*p*-tolyl)-6*H*-1,3-oxazin-6-one (4w)



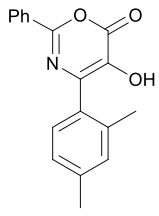
Compound **4w** (70 mg, 50%) was prepared according to the general procedure from azirine **3w** (155 mg, 0.5 mmol). Colorless solid, mp 235–237 °C (from Et_2O/hexane). ^1H NMR (400 MHz, DMSO-d_6) δ 2.38 (s, 3H), 7.30–7.36 (m, 2H), 7.54–7.64 (m, 3H), 8.10–8.16 (m, 2H), 8.20–8.28 (m, 2H), 10.66 (s, 1H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 21.0, 127.1, 127.7, 128.8, 128.9, 129.9, 131.5, 131.8, 134.9, 135.1, 139.1, 150.9, 158.6. HRMS (ESI-TOF) *m/z* $[M+Na]^+$ calcd for $C_{17}H_{13}NNaO_3^+$: 302.0788; found: 302.0791.

4-[4-(*tert*-Butyl)phenyl]-5-hydroxy-2-phenyl-6*H*-1,3-oxazin-6-one (4x)



Compound **4x** (56 mg, 35%) was prepared according to the general procedure from azirine **3x** (176 mg, 0.5 mmol). Colorless solid, mp 165–166 °C (from Et_2O/hexane). ^1H NMR (400 MHz, DMSO-d_6) δ 1.33 (s, 9H), 7.52–7.63 (m, 5H), 8.10–8.16 (m, 2H), 8.20–8.26 (m, 2H), 10.64 (s, 1H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 30.9, 34.5, 125.0, 127.1, 128.6, 128.9, 129.9, 131.4, 131.8, 135.08, 135.14, 151.0, 152.1, 158.5. HRMS (ESI-TOF) *m/z* $[M+Na]^+$ calcd for $C_{20}H_{19}NNaO_3^+$: 344.1257; found: 344.1273.

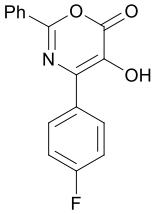
4-(2,4-Dimethylphenyl)-5-hydroxy-2-phenyl-6*H*-1,3-oxazin-6-one (4y)



Compound **4y** (28 mg, 19%) was prepared according to the general procedure azirine **3y** (161 mg, 0.5 mmol). Colorless solid, mp 185–187 °C (from Et_2O/hexane). ^1H NMR (400 MHz, DMSO-d_6) δ 2.29 (s, 3H), 2.33 (s, 3H), 7.06–7.15 (m, 2H), 7.30–7.36 (m, 1H), 7.50–7.65 (m, 3H), 7.98–8.07 (m, 2H),

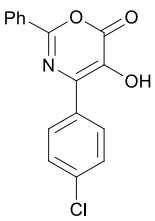
10.21 (s, 1H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 19.6, 20.8, 125.9, 127.0, 128.3, 129.3, 129.9, 130.8, 131.3, 131.8, 135.5, 136.2, 138.1, 139.6, 151.4, 158.0. HRMS (ESI-TOF) *m/z* $[M+Na]^+$ calcd for $C_{18}H_{15}NNaO_3^+$: 316.0944; found: 316.0948.

4-(4-Fluorophenyl)-5-hydroxy-2-phenyl-6*H*-1,3-oxazin-6-one (4z)



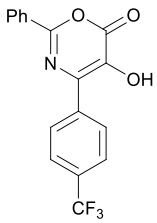
Compound **4z** (130 mg, 92%) was prepared according to the general procedure from azirine **3z** (157 mg, 0.5 mmol). Colorless solid, mp 240–241 °C (from Et_2O/hexane). ^{1}H NMR (400 MHz, DMSO-d_6) δ 7.29–7.39 (m, 2H), 7.51–7.65 (m, 3H), 8.07–8.16 (m, 2H), 8.32–8.43 (m, 2H), 10.85 (s, 1H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 115.2 (d, *J* 21.2 Hz), 127.1, 128.9, 129.8, 130.7 (d, *J* 3.0 Hz), 131.1 (d, *J* 8.5 Hz), 131.9, 133.8, 135.4, 151.1, 158.5, 162.4 (d, *J* 248.1 Hz). HRMS (ESI-TOF) *m/z* $[M+H]^+$ calcd for $C_{16}H_{11}FNO_3^+$: 284.0717; found: 284.0725.

4-(4-Chlorophenyl)-5-hydroxy-2-phenyl-6*H*-1,3-oxazin-6-one (4za)[8]



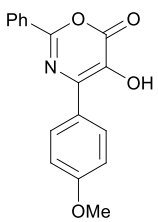
Compound **4za** (106 mg, 71%) was prepared according to the general procedure from azirine **3za** (165 mg, 0.5 mmol). Colorless solid, mp 248–250 °C (from Et_2O/hexane). ^{1}H NMR (400 MHz, DMSO-d_6) δ 7.54–7.63 (m, 5H), 8.09–8.16 (m, 2H), 8.31–8.38 (m, 2H), 11.01 (s, 1H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 127.1, 128.3, 128.9, 129.8, 130.4, 131.9, 133.1, 133.4, 133.9, 136.0, 151.0, 158.4. HRMS (ESI-TOF) *m/z* $[M+H]^+$ calcd for $C_{16}H_{11}{}^{35}ClNO_3^+$: 300.0422; found: 300.0423.

5-Hydroxy-2-phenyl-4-[4-(trifluoromethyl)phenyl]-6*H*-1,3-oxazin-6-one (4zb)



Compound **4zb** (163 mg, 98%) was prepared according to the general procedure from azirine **3zb** (182 mg, 0.5 mmol). Colorless solid, mp 233–235 °C (from Et_2O/hexane). ^{1}H NMR (400 MHz, DMSO-d_6) δ 7.51–7.65 (m, 3H), 7.80–7.90 (m, 2H), 8.44–8.54 (m, 2H), 10.22 (br s, 1H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 124.1 (q, *J* 271.7 Hz), 125.0 (q, *J* 3.0 Hz), 127.1, 128.9, 129.0 (q, *J* 33.0 Hz), 129.2, 129.8, 131.9, 132.7, 137.1, 138.2, 151.0, 158.4. HRMS (ESI-TOF) *m/z* $[M+H]^+$ calcd for $C_{17}H_{11}F_3NO_3^+$: 334.0686; found: 334.0687.

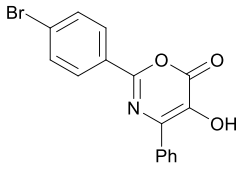
5-Hydroxy-4-(4-methoxyphenyl)-2-phenyl-6*H*-1,3-oxazin-6-one (4zc)



Compound **4zc** (111 mg, 75%) was prepared according to the general procedure from azirine **3zc** (163 mg, 0.5 mmol). Colorless solid, mp 227–229 °C (from Et_2O/hexane). ^{1}H NMR (400 MHz, DMSO-d_6) δ 3.83 (s, 3H), 7.04–7.13 (m, 2H), 7.52–7.64 (m, 3H), 8.07–8.18 (m, 2H), 8.27–8.37 (m, 2H), 10.55 (s, 1H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 55.2, 113.7, 126.6, 127.1, 128.9, 130.0, 130.5,

131.8, 134.2, 135.0, 151.0, 158.5, 160.1. HRMS (ESI-TOF) *m/z* $[M+H]^+$ calcd for $C_{17}H_{14}NO_4^+$: 296.0917; found: 296.0920.

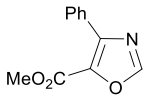
2-(4-Bromophenyl)-5-hydroxy-4-phenyl-6*H*-1,3-oxazin-6-one (4zj)



Compound **4zj** (86 mg, 50%) was prepared according to the general procedure from azirine **3zj** (187 mg, 0.5 mmol). Oxazine **4a** (27 mg, 20%) was isolated as a byproduct.

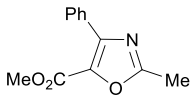
Compound **4zj**: colorless solid, mp 214–215 °C (from Et_2O/hexane). ^1H NMR (400 MHz, DMSO-d_6) δ 7.42–7.48 (m, 1H), 7.49–7.54 (m, 2H), 7.72–7.81 (m, 2H), 7.99–8.08 (m, 2H), 8.26–8.32 (m, 2H), 10.84 (s, 1H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 125.6, 128.2, 128.7, 129.0, 129.2, 129.4, 132.0, 134.1, 134.6, 135.9, 150.2, 158.4. HRMS (ESI-TOF) *m/z* $[M–H]^-$ calcd for $C_{16}H_9{}^{81}BrNO_3^-$: 343.9750; found: 343.9741.

Methyl 4-phenyloxazole-5-carboxylate (5a)



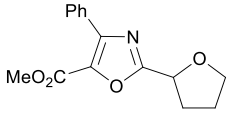
Compound **5a** (38 mg, 37%) was prepared according to the general procedure from azirine **3zk** (110 mg, 0.5 mmol). Colorless oil. ^1H NMR (400 MHz, $CDCl_3$) δ 3.97 (s, 3H), 7.45–7.51 (m, 3H), 8.02 (s, 1H), 8.08–8.13 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 52.2, 128.2, 129.2, 129.8, 136.5, 146.2, 151.6 (2C), 158.7. HRMS (ESI-TOF) *m/z* $[M+Na]^+$ calcd for $C_{11}H_9NNaO_3^+$: 266.0475; found: 226.0474.

Methyl 2-methyl-4-phenyloxazole-5-carboxylate (5b)[9]



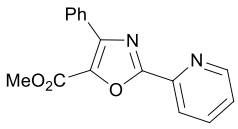
Compound **5b** (33 mg, 30%) was prepared according to the general procedure from azirine **3zl** (117 mg, 0.5 mmol). Colorless solid, mp 52–54 °C (from Et_2O/hexane). ^1H NMR (400 MHz, $CDCl_3$) δ 2.60 (s, 3H), 3.93 (s, 3H), 7.41–7.49 (m, 3H), 7.98–8.11 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 14.2, 52.1, 128.1, 129.2, 129.6, 130.2, 136.2, 147.2, 158.9, 163.0. HRMS (ESI-TOF) *m/z* $[M+H]^+$ calcd for $C_{12}H_{12}NO_3^+$: 218.0812; found: 218.0819.

Methyl 4-phenyl-2-(tetrahydrofuran-2-yl)oxazole-5-carboxylate (5c)



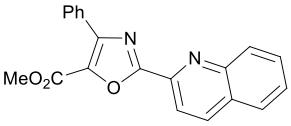
Compound **5c** (61 mg, 45%) was prepared according to the general procedure from azirine **3zm** (145 mg, 0.5 mmol). Colorless solid, mp 56–57 °C (from Et_2O/hexane). ^1H NMR (400 MHz, $CDCl_3$) δ 2.01–2.13 (m, 1H), 2.14–2.26 (m, 1H), 2.34–2.44 (m, 2H), 3.93 (s, 3H), 3.96–4.06 (m, 1H), 4.09–4.19 (m, 1H), 5.10–5.18 (m, 1H), 7.41–7.51 (m, 3H), 8.03–8.13 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 25.7, 30.7, 52.1, 59.3, 73.4, 128.1, 129.3, 129.6, 130.0, 136.4, 146.9, 158.9, 165.4. HRMS (ESI-TOF) *m/z* $[M+Na]^+$ calcd for $C_{15}H_{15}NNaO_4^+$: 296.0893; found: 296.0895.

Methyl 4-phenyl-2-(pyridin-2-yl)oxazole-5-carboxylate (5d)



Compound **5d** (27 mg, 19%) was prepared according to the general procedure from azirine **3zn** (148 mg, 0.5 mmol). Colorless solid, mp 133–134 °C (from Et_2O/hexane). ^1H NMR (400 MHz, $CDCl_3$) δ 3.98 (s, 3H), 7.44–7.53 (m, 4H), 7.85–7.94 (m, 1H), 8.18–8.28 (m, 2H), 8.28–8.37 (m, 1H), 8.80–8.89 (m, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 52.2, 123.3, 125.6, 128.1, 129.4, 129.8, 129.9, 136.9, 137.0, 145.2, 148.2, 150.5, 158.9, 160.5. HRMS (ESI-TOF) *m/z* $[M+H]^+$ calcd for $C_{16}H_{13}N_2O_3^+$: 281.0921; found: 281.0931.

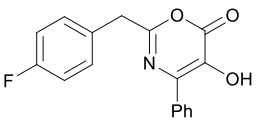
Methyl 4-phenyl-2-(quinolin-2-yl)oxazole-5-carboxylate (5e)



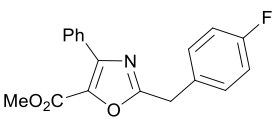
Compound **5e** (31 mg, 19%) was prepared according to the general procedure from azirine **3zo** (173 mg, 0.5 mmol). Colorless solid, mp 162–163 °C (from Et_2O/hexane). ^1H NMR (400 MHz, $CDCl_3$) δ 4.02 (s, 3H), 7.46–7.56 (m, 3H), 7.63–7.69 (m, 1H), 7.79–7.85 (m, 1H), 7.87–7.93 (m, 1H), 8.24–8.30 (m, 2H), 8.33–8.38 (m, 2H), 8.39–8.45 (m, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 52.3, 120.0, 127.6, 128.2 (3C), 128.7, 129.4, 129.87, 129.91, 130.3, 130.5, 137.3, 144.9, 148.1, 148.3, 159.0, 160.7. HRMS (ESI-TOF) *m/z* $[M+Na]^+$ calcd for $C_{20}H_{14}N_2NaO_3^+$: 353.0897; found: 353.0880.

2-(4-Fluorobenzyl)-5-hydroxy-4-phenyl-6*H*-1,3-oxazin-6-one (4zp) and methyl 2-(4-fluorobenzyl)-4-phenyloxazole-5-carboxylate (5f)

Compounds **4zp** (13 mg, 9%) and **5f** (39 mg, 25%) were prepared according to the general procedure from azirine **3zp** (164 mg, 0.5 mmol) and separated by column chromatography on silica gel (EtOAc/hexane, from 1:20 to 1:1).



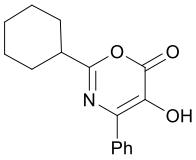
Compound **4zp**: colorless solid, mp 193–194 °C (from Et_2O/hexane). ^1H NMR (400 MHz, $CDCl_3$) δ 3.97 (s, 2H), 6.46 (s, 1H), 6.97–7.16 (m, 2H), 7.30–7.42 (m, 2H), 7.42–7.57 (m, 3H), 8.17–8.33 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 40.1, 115.7 (d, *J* 21.6 Hz), 128.4, 129.1, 129.8 (d, *J* 3.4 Hz), 130.2, 130.8 (d, *J* 8.2 Hz), 133.1, 133.7, 134.8, 151.1, 160.7, 162.2 (d, *J* 246.1 Hz). HRMS (ESI-TOF) *m/z* $[M+H]^+$ calcd for $C_{17}H_{13}FNO_3^+$: 298.0874; found: 298.0883.



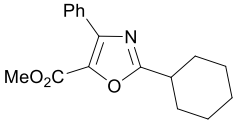
Compound **5f**: colorless solid, mp 58–59 °C (from Et_2O/hexane). ^1H NMR (400 MHz, $CDCl_3$) δ 3.92 (s, 3H), 4.20 (s, 2H), 7.00–7.11 (m, 2H), 7.34–7.41 (m, 2H), 7.43–7.51 (m, 3H), 8.01–8.11 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 33.9, 52.1, 115.7 (d, *J* 21.6 Hz), 128.2, 129.3, 129.7 (d, *J* 3.4 Hz), 130.09, 130.12, 130.5 (d, *J* 8.2 Hz), 136.5, 147.2, 158.9, 162.1 (d, *J* 245.9 Hz), 164.1. HRMS (ESI-TOF) *m/z* $[M+H]^+$ calcd for $C_{18}H_{15}FNO_3^+$: 312.1031; found: 312.1033.

2-Cyclohexyl-5-hydroxy-4-phenyl-6*H*-1,3-oxazin-6-one (4zq) and methyl 2-cyclohexyl-4-phenyloxazole-5-carboxylate (5g)

Compounds **4zq** (46 mg, 34%) and **5g** (36 mg, 25%) were prepared according to the general procedure from azirine **3zq** (151 mg, 0.5 mmol) and separated by column chromatography on silica gel (EtOAc/hexane, from 1:20 to 1:1).



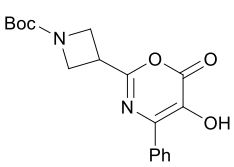
Compound **4zq**: colorless solid, mp 149–150 °C (from Et_2O/hexane). ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.31–1.46 (m, 3H), 1.58–1.67 (m, 2H), 1.72–1.79 (m, 1H), 1.85–1.95 (m, 2H), 2.07–2.15 (m, 2H), 2.60–2.73 (m, 1H), 6.32 (s, 1H), 7.42–7.55 (m, 3H), 8.23–8.36 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 25.5, 25.7, 29.9, 42.7, 128.3, 129.1, 130.0, 133.5, 133.6, 134.6, 160.1, 161.2. HRMS (ESI-TOF) *m/z* $[M+H]^+$ calcd for $C_{16}H_{18}NO_3^+$: 272.1281; found: 272.1290.



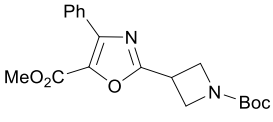
Compound **5g**: colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.32–1.48 (m, 3H), 1.66–1.78 (m, 3H), 2.11–2.19 (m, 2H), 2.87–2.98 (m, 1H), 3.92 (s, 3H), 7.39–7.50 (m, 3H), 8.02–8.11 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 25.5, 25.76, 30.4, 37.7, 52.0, 128.1, 129.3, 129.5, 130.5, 135.6, 147.0, 159.1, 169.6. HRMS (ESI-TOF) *m/z* $[M+Na]^+$ calcd for $C_{17}H_{19}NNaO_3^+$: 308.1257; found: 308.1260.

***tert*-Butyl 3-(5-hydroxy-6-oxo-4-phenyl-6*H*-1,3-oxazin-2-yl)azetidine-1-carboxylate (4zr) and methyl 2-(1-(*tert*-butoxycarbonyl)azetidin-3-yl)-4-phenyloxazole-5-carboxylate (5h)**

Compounds **4zr** (34 mg, 20%) and **5h** (27 mg, yield 15%, 91% purity by ^{1}H NMR) were prepared according to the general procedure from 1-*tert*-butyl 3-(2-(methoxycarbonyl)-3-phenyl-2*H*-azirin-2-yl) azetidine-1,3-dicarboxylate **3zr** (187 mg, 0.5 mmol) and separated by column chromatography on silica gel (EtOAc/hexane, from 1:20 to 1:1).



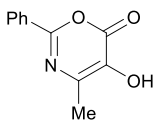
Compound **4zr**: colorless solid, mp 143–144 °C (from Et_2O/hexane). ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.49 (s, 9H), 3.69–3.79 (m, 1H), 4.24–4.37 (m, 4H), 6.78 (bs, 1H), 7.45–7.53 (m, 3H), 8.25–8.33 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 28.4, 32.1, 52.3, 80.1, 128.4, 129.1, 130.3, 133.0, 134.0, 134.6, 155.6, 156.1, 160.3. HRMS (ESI-TOF) *m/z* $[M–H]^–$ calcd for $C_{18}H_{19}N_2O_5^+$: 343.1299; found: 343.1293.



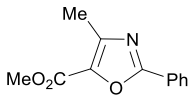
Compound **5h**: colorless solid, mp 97–100 °C (from Et_2O/hexane). ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.48 (s, 9H), 3.94 (s, 3H), 3.96–4.03 (m, 1H), 4.35 (d, *J* 7.5 Hz, 1H), 7.41–7.52 (m, 3H), 8.02–8.12 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 27.1, 28.3, 52.2, 53.1, 80.0, 128.2, 129.2, 129.8, 129.9, 136.6, 147.1, 155.9, 158.7, 164.9. HRMS (ESI-TOF) *m/z* $[M+H]^+$ calcd for $C_{19}H_{22}N_2NaO_5^+$: 381.1421; found: 381.1426.

5-Hydroxy-4-methyl-2-phenyl-6*H*-1,3-oxazin-6-one (4zs) and methyl 4-methyl-2-phenyloxazole-5-carboxylate (5i)[10]

Compounds **4zs** (12 mg, 12%) and **5i** (9 mg, 8%) were prepared according to the general procedure from azirine **3zs** (117 mg, 0.5 mmol) and separated by column chromatography on silica gel (EtOAc/hexane, from 1:20 to 1:1).



Compound **4zs**: colorless solid, mp 201–202 °C (from Et_2O/hexane). ^1H NMR (400 MHz, $CDCl_3$) δ 2.35 (s, 3H), 5.72 (s, 1H), 7.46–7.52 (m, 2H), 7.53–7.58 (m, 1H), 8.12–8.20 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 17.1, 127.7, 128.8, 129.7, 132.2, 134.7, 140.5, 152.9, 158.7. HRMS (ESI-TOF) *m/z* $[M+H]^+$ calcd for $C_{11}H_{10}NO_3^+$: 204.0655; found: 204.0659.



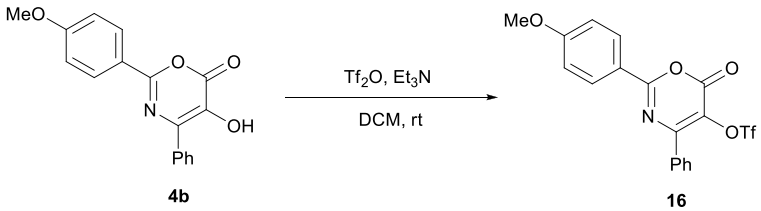
Compound **5i**: colorless solid, mp 58–59 °C (Et_2O–hexane). ^1H NMR (400 MHz, $CDCl_3$) δ 2.56 (s, 3H), 3.96 (s, 3H), 7.45–7.56 (m, 3H), 8.10–8.19 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 13.4, 51.9, 126.4, 127.2, 128.8, 131.5, 137.2, 147.3, 159.2, 162.3. HRMS (ESI-TOF) *m/z* $[M+H]^+$ calcd for $C_{12}H_{12}NO_3^+$: 218.0819; found: 218.0812.

7. Gram scale synthesis of 4b

A stirred solution of methyl 2-[(4-methoxybenzoyl)oxy]-3-phenyl-2*H*-azirine-2-carboxylate **3b** (2.60 g, 8 mmol), Bu_3SnH (4.65 g, 16 mmol) and 1,1'-(diazene-1,2-diyl)dicyclohexanecarbonitrile (1.95 g, 8 mmol) in anhydrous toluene (160 mL) was heated under reflux for 2 h. The solvent was removed under reduced pressure, and the residue was diluted with hexane (50 mL). The mixture was stirred at 0 °C for 1 h. The precipitate of [1,1'-bi(cyclohexane)]-1,1'-dicarbonitrile was filtered out, 15% HCl solution (15 mL) and Et_2O (10 mL) were added to the filtrate and the reaction mixture was stirred at rt for 24 h. The precipitate was filtered off and recrystallized from Et_2O/hexane mixture. The yield of 5-hydroxy-2-(4-methoxyphenyl)-4-phenyl-6*H*-1,3-oxazin-6-one (**4b**) was 1.53 g (65%).

8. Synthesis of oxazines 16−21

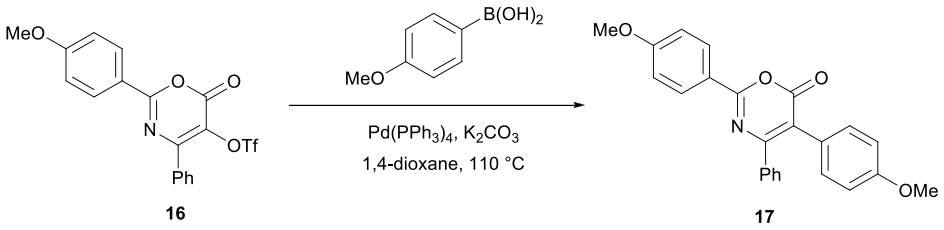
2-(4-Methoxyphenyl)-6-oxo-4-phenyl-6*H*-1,3-oxazin-5-yl trifluoromethanesulfonate (16)



4b **16**

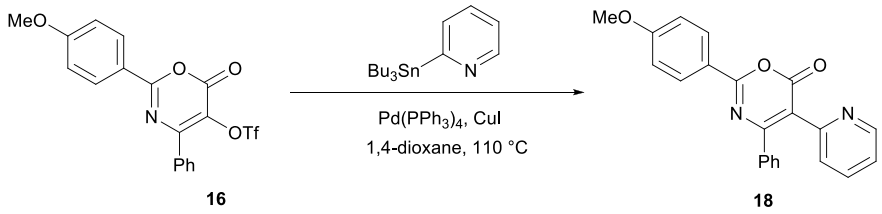
To a stirred solution of 5-hydroxy-2-(4-methoxyphenyl)-4-phenyl-6*H*-1,3-oxazin-6-one (**4b**) (295 mg, 1 mmol) and Et_3N (303 mg, 3 mmol) in DCM (5 mL) Tf_2O (564 mg, 2 mmol) was added dropwise at rt, and the reaction mixture was stirred for 30 min. The solvent was removed under reduced pressure, and the residue was purified by column chromatography on silica gel (hexane/EtOAc, 10:1) to give compound **16** (346 mg, 81%). Colorless solid, mp 132–133 °C (from Et_2O/hexane). ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.94 (s, 3H), 7.00–7.08 (m, 2H), 7.53–7.64 (m, 3H), 7.97–8.05 (m, 2H), 8.24–8.32 (m, 2H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 55.6, 114.5, 118.2 (q, *J* 321.2 Hz), 121.0, 127.2, 128.8, 129.6, 131.4, 131.7, 132.3, 154.3, 155.4, 160.5, 164.6. HRMS (ESI-TOF) *m/z* $[M+Na]^+$ calcd for $C_{18}H_{12}F_3NNaO_6S^+$: 450.0230; found: 450.0245.

2,5-Bis(4-methoxyphenyl)-4-phenyl-6*H*-1,3-oxazin-6-one (17)



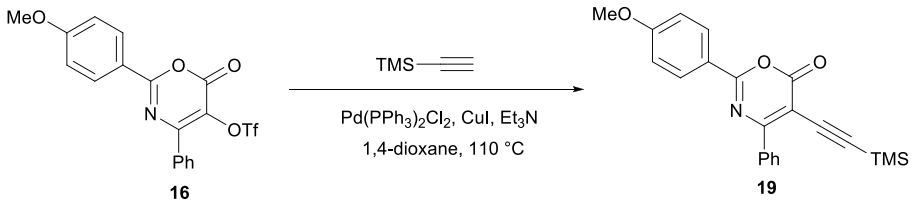
A mixture of triflate **16** (43 mg, 0.1 mmol), $Pd(PPh_3)_4$ (12 mg, 0.01 mmol 10 mol%), (4-methoxyphenyl)boronic acid (23 mg, 0.15 mmol), K_2CO_3 (41 mg, 0.3 mmol) and dioxane (2 mL) was stirred in a screw-capped tube under argon atmosphere at 110 °C for 17 h. The solvent was removed under reduced pressure, and the residue was purified by column chromatography on silica gel (hexane/EtOAc, from 100:1 to 5:1) to give compound **17** (31 mg, 91%). Yellow solid, mp 180–181 °C (from Et_2O/hexane). ^1H NMR (400 MHz, $CDCl_3$) δ 3.83 (s, 3H), 3.92 (s, 3H), 6.83–6.91 (m, 2H), 6.99–7.06 (m, 2H), 7.21–7.26 (m, 2H), 7.27–7.36 (m, 3H), 7.49–7.57 (m, 2H), 8.27–8.36 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 55.2, 55.5, 113.9, 114.2, 116.9, 122.4, 124.9, 127.9, 129.6, 130.0, 130.5, 131.9, 136.7, 158.6, 159.4, 160.7, 160.9, 163.7. HRMS (ESI-TOF) *m/z* $[M+H]^+$ calcd for $C_{24}H_{20}NO_4^+$: 386.1387; found: 386.1388.

2-(4-Methoxyphenyl)-4-phenyl-5-(pyridin-2-yl)-6*H*-1,3-oxazin-6-one (18)



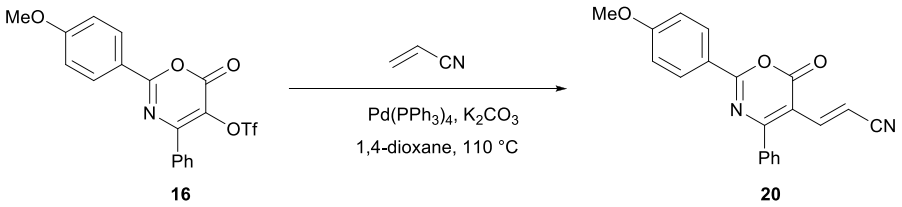
A mixture of triflate **16** (43 mg, 0.1 mmol), $Pd(PPh_3)_4$ (12 mg, 0.01 mmol 10 mol %), CuI (2 mg, 0.01 mmol 10 mol %), 2-(tributylstannyl)pyridine (55 mg, 0.15 mmol) and dioxane (2 mL) was stirred in a screw-capped tube under argon atmosphere at 110 °C for 1 h. The solvent was removed under reduced pressure, and the residue was purified by column chromatography on silica gel (hexane/EtOAc, from 10:1 to 2:1) to give compound **18** (25 mg, 70%). Colorless solid, mp 174–175 °C (from Et_2O/hexane). ^1H NMR (400 MHz, $CDCl_3$) δ 3.93 (s, 3H), 6.95–7.12 (m, 2H), 7.22–7.30 (m, 3H), 7.32–7.38 (m, 1H), 7.38–7.43 (m, 1H), 7.43–7.53 (m, 2H), 7.62–7.79 (m, 1H), 8.25–8.45 (m, 2H), 8.54–8.73 (m, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 55.6, 114.3, 116.6, 122.2, 122.8, 126.2, 127.9, 129.9, 130.1, 130.9, 136.3, 136.4, 149.8, 152.8, 160.2, 161.0, 161.9, 164.0. HRMS (ESI-TOF) *m/z* $[M+H]^+$ calcd for $C_{22}H_{17}N_2O_3^+$: 357.1234; found: 357.1236.

2-(4-Methoxyphenyl)-4-phenyl-5-[(trimethylsilyl)ethynyl]-6*H*-1,3-oxazin-6-one (19)



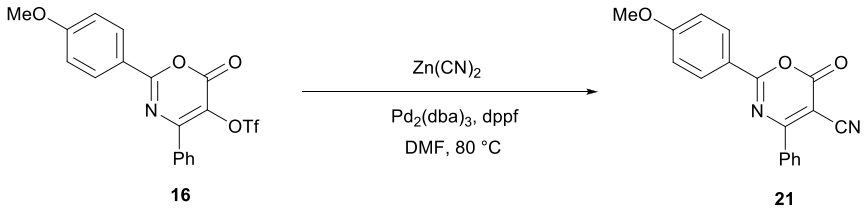
A mixture of triflate **16** (43 mg, 0.1 mmol), $Pd(PPh_3)_2Cl_2$ (7 mg, 0.01 mmol 10 mol %), CuI (2 mg, 0.01 mmol 10 mol %), trimethylsilylacetylene (15 mg, 0.15 mmol), Et_3N (30 mg, 0.3 mmol) and dioxane (2 mL) was stirred in a screw-capped tube under argon atmosphere at 50 °C for 1 h. The solvent was removed under reduced pressure, and the residue was purified by column chromatography on silica gel (hexane/EtOAc from 100:1 to 10:1) to give compound **19** (33 mg, 88%). Yellow solid, mp 138–139 °C (from Et_2O/hexane). ^{1}H NMR (400 MHz, $CDCl_3$) δ 0.27 (s, 9H), 3.92 (s, 3H), 6.96–7.06 (m, 2H), 7.46–7.59 (m, 3H), 8.25–8.33 (m, 2H), 8.34–8.42 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ -0.4, 55.6, 97.7, 100.8, 106.9, 114.3, 121.9, 127.9, 129.7, 131.1, 131.5, 135.5, 159.6, 160.5, 163.5, 164.1. HRMS (ESI-TOF) *m/z* $[M+Na]^+$ calcd for $C_{22}H_{21}NNaO_3Si^+$: 398.1183; found: 398.1188.

(*E*)-3-[2-(4-methoxyphenyl)-6-oxo-4-phenyl-6*H*-1,3-oxazin-5-yl]acrylonitrile (20)



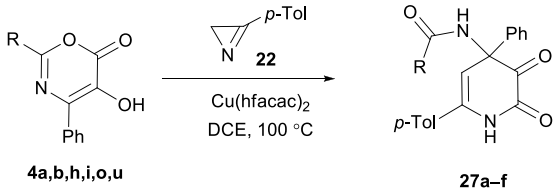
A mixture of triflate **16** (43 mg, 0.1 mmol), $Pd(PPh_3)_4$ (12 mg, 0.01 mmol 10 mol %), acrylonitrile (8 mg, 0.15 mmol), K_2CO_3 (41 mg, 0.3 mmol) and dioxane (2 mL) was stirred in a screw-capped tube under argon atmosphere at 110 °C for 20 h. The solvent was removed under reduced pressure, and the residue was purified by column chromatography on silica gel (hexane/EtOAc, from 10:1 to 4:1) to give compound **20** (10 mg, 30%). Colorless solid, mp 216–217 °C (from Et_2O/hexane). ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.94 (s, 3H), 6.91 (d, *J* 16.3 Hz, 1H), 7.00–7.06 (m, 2H), 7.26 (d, *J* 16.3 Hz, 1H), 7.55–7.63 (m, 3H), 7.65–7.70 (m, 2H), 8.28–8.34 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 55.7, 101.6, 109.9, 114.5, 118.8, 121.3, 128.8, 130.0, 131.5, 131.6, 135.3, 141.7, 158.1, 162.2, 164.8, 165.4. HRMS (ESI-TOF) *m/z* $[M+Na]^+$ calcd for $C_{20}H_{14}N_2NaO_3^+$: 353.0897; found: 353.0900.

2-(4-Methoxyphenyl)-6-oxo-4-phenyl-6*H*-1,3-oxazine-5-carbonitrile (21)



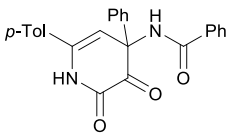
A mixture of triflate **16** (43 mg, 0.1 mmol), $Pd_2(dba)_3$ (10 mg, 0.01 mmol 10 mol %), $Zn(CN)_2$ (24 mg, 0.2 mmol), 1,1'-bis(diphenylphosphino)ferrocene (dppf) (17 mg, 0.03 mmol 30 mol %) and DMF (2 mL) was stirred in a screw-capped tube under argon atmosphere at 80 °C for 45 min. The solvent was removed under reduced pressure, and the residue was purified by column chromatography on silica gel (hexane/EtOAc, from 10:1 to 4:1) to give compound **21** (14 mg, 46%). White solid, mp 185–186 °C (from Et_2O/hexane). ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.96 (s, 3H), 7.02–7.09 (m, 2H), 7.56–7.63 (m, 2H), 7.65–7.63 (m, 2H), 7.65–7.71 (m, 1H), 8.25–8.31 (m, 2H), 8.32–8.38 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 55.8, 89.8, 114.3, 114.8, 120.7, 128.9, 129.5, 132.3, 133.5, 133.6, 157.1, 164.3, 165.6, 169.5. HRMS (ESI-TOF) *m/z* $[M+Na]^+$ calcd for $C_{18}H_{12}N_2NaO_3^+$: 327.0740; found: 327.0741.

9. Synthesis of pyridine-2,3-diones 27



General procedure. Oxazine **4** (0.2 mmol), $Cu(hfacac)_2$ (5 mg, 0.01 mmol), 3-(*p*-tolyl)-2*H*-azirine (**22**) (42 mg, 0.32 mmol) and 1,2-dichloroethane (DCE) (3.0 mL) were placed in a screw cap tube, and the mixture was heated at 100 °C for 30–90 min until full consumption of the oxazine (control by TLC). The solvent was removed under reduced pressure, and the residue was purified by column chromatography on silica gel (hexane/EtOAc, from 2:1 to 1:2) followed by recrystallization from hexane/Et_2O mixture to give compound **27**.

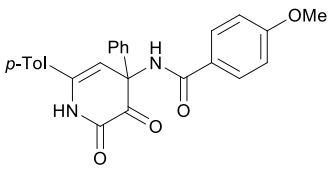
***N*-[6-(4-Methylphenyl)-2,3-dioxo-4-phenyl-1,2,3,4-tetrahydropyridin-4-yl]benzamide (27a)**



Compound **27a** (59 mg, 74%) was prepared according to the general procedure from oxazine **4a** (53 mg, 0.2 mmol). Yellow solid, mp 184–185 °C (from Et_2O/hexane). ^{1}H NMR (400 MHz, DMSO-d_6) δ 2.35 (s, 3H), 5.50 (d, *J* 2.3 Hz, 1H), 7.28 (d, *J* 8.1 Hz, 2H), 7.41–7.44 (m, 1H), 7.47–7.51 (m, 4H), 7.56–7.59 (m, 3H), 7.67–7.69 (m, 2H), 7.97–7.99 (m, 2H), 9.74 (s, 1H), 10.64 (d, *J* 2.0 Hz, 1H). ^{13}C NMR

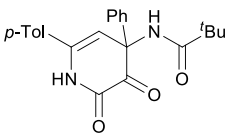
(100 MHz, DMSO-d_6) δ 20.8, 64.9, 107.0, 126.0, 127.5, 128.0, 128.3, 128.7, 128.8, 129.1, 131.0, 132.0 (2C), 136.1, 136.2, 138.8, 155.9, 166.9, 186.0.^{15}N NMR from HMBC ^{1}H-^{15}N spectrum (400 MHz, DMSO-d_6) δ 135.3, 136.0. ν_{max}, cm^{-1}: 3247, 1744, 1690, 1631, 1521, 1487, 1464, 1351, 1308, 1294. HRMS (ESI-TOF) *m/z* [M+Na]$^+$ calcd for $C_{25}H_{20}N_2NaO_3^+$: 419.1366; found: 419.1366.

_N_-(6-(4-Methylphenyl)-2,3-dioxo-4-phenyl-1,2,3,4-tetrahydropyridin-4-yl)-4-methoxybenzamide (27b)



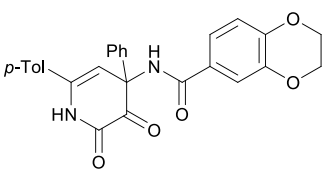
Compound **27b** (60 mg, 71%) was prepared according to the general procedure from oxazine **4b** (59 mg, 0.2 mmol). Yellow solid, mp 198–200 °C (from Et_2O/hexane). ^{1}H NMR (400 MHz, $CDCl_3$–DMSO-d_6 mixture) δ 2.35 (s, 3H), 3.78 (s, 3H), 5.47 (s, 1H), 6.97 (d, *J* 8.4 Hz, 2H), 7.22 (d, *J* 7.6 Hz, 2H), 7.40–7.44 (m, 2H), 7.51–7.59 (m, 5H), 7.95 (d, *J* 7.4 Hz, 2H), 9.50 (s, 1H), 10.50 (s, 1H). ^{13}C NMR (100 MHz, $CDCl_3$–DMSO-d_6 mixture) δ 20.7, 55.0, 64.3, 107.1, 113.8, 125.7, 127.4, 127.8, 127.9, 128.7, 128.8, 131.0, 131.5, 132.1, 135.8, 138.5, 156.0, 159.6, 166.6, 186.0. HRMS (ESI-TOF) *m/z* [M+Na]$^+$ calcd for $C_{26}H_{22}N_2NaO_4^+$: 449.1472; found: 449.1468.

_N_-(6-(4-Methylphenyl)-2,3-dioxo-4-phenyl-1,2,3,4-tetrahydropyridin-4-yl)pivalamide (27c)



Compound **27c** (62 mg, 82%) was prepared according to the general procedure from oxazine **4u** (49 mg, 0.2 mmol). Yellow solid, mp 195–197 °C (from Et_2O/hexane). ^{1}H NMR (400 MHz, $CDCl_3$–DMSO-d_6 mixture) δ 1.17 (s, 9H), 5.43 (s, 1H), 7.19 (d, *J* 7.9 Hz, 2H), 7.30–7.36 (m, 3H), 7.47 (d, *J* 7.9 Hz, 2H), 7.56 (d, *J* 7.3 Hz, 2H), 7.67 (s, 1H), 9.86 (s, 1H). ^{13}C NMR (100 MHz, $CDCl_3$/DMSO-d_6 mixture) δ 20.4, 26.5, 37.3, 64.1, 105.7, 125.2, 126.5, 128.1, 128.2, 128.5, 130.5, 135.6, 135.8, 138.5, 155.5, 177.4, 185.7. HRMS (ESI-TOF) *m/z* [M+Na]$^+$ calcd for $C_{23}H_{24}N_2NaO_3^+$: 399.1679; found: 399.1678.

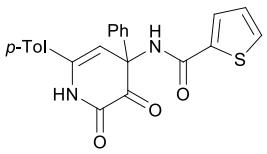
_N_-[6-(4-Methylphenyl)-2,3-dioxo-4-phenyl-1,2,3,4-tetrahydropyridin-4-yl]-2,3-dihydrobenzo[*b*][1,4]dioxine-6-carboxamide (27d)



Compound **27d** (77 mg, 85%) was prepared according to the general procedure from oxazine **4h** (65 mg, 0.2 mmol). Yellow solid, mp 140–142 °C (from Et_2O/hexane). ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.39 (s, 3H), 4.24–4.26 (m, 4H), 5.85 (s, 1H), 6.87 (d, *J* 8.4 Hz, 1H), 7.24 (d, *J* 7.8 Hz, 2H), 7.31–7.41 (m, 5H), 7.48 (d, *J* 7.8 Hz, 2H), 7.64 (d, *J* 7.1 Hz, 2H), 8.36 (s, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 21.2, 64.1, 64.5, 66.0, 106.4, 116.8, 117.3, 120.8, 125.3, 125.7,

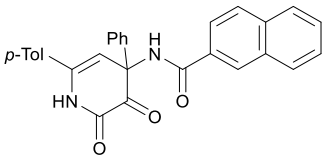
127.1, 129.37, 129.40, 129.7, 130.7, 135.1, 135.9, 140.0, 143.3, 147.0, 156.0, 165.8, 186.9. HRMS (ESI-TOF) *m/z* $[M+Na]^+$ calcd for $C_{27}H_{22}N_2NaO_5^+$: 477.1421; found: 477.1417.

_N_-[6-(4-Methylphenyl)-2,3-dioxo-4-phenyl-1,2,3,4-tetrahydropyridin-4-yl]thiophene-2-carboxamide (27e)



Compound **27e** (67 mg, 83%) was prepared according to the general procedure from oxazine **4o** (54 mg, 0.2 mmol). Yellow solid, mp 144–145 °C (from Et_2O/hexane). ^1H NMR (400 MHz, $CDCl_3$–DMSO-d_6 mixture) δ 2.51 (s, 3H), 5.45 (d, *J* 1.8 Hz, 1H), 7.06–7.09 (m, 1H), 7.21 (d, *J* 7.9 Hz, 2H), 7.37–7.43 (m, 3H), 7.53 (d, *J* 8.0 Hz, 2H), 7.59 (d, *J* 4.8 Hz, 1H), 7.67 (d, *J* 7.2 Hz, 2H), 7.97–7.98 (m, 1H), 9.58 (s, 1H), 10.47 (s, 1H). ^{13}C NMR (100 MHz, $CDCl_3$/DMSO-d_6 mixture) δ 20.7, 64.7, 106.5, 125.7, 127.4, 127.5, 128.4, 128.5, 128.8, 129.7, 130.8, 131.0, 135.8, 136.1, 137.0, 138.6, 155.7, 161.6, 185.9. HRMS (ESI-TOF) *m/z* $[M+Na]^+$ calcd for $C_{23}H_{18}N_2NaO_3S^+$: 425.0930; found: 425.0951.

_N_-[6-(4-Methylphenyl)-2,3-dioxo-4-phenyl-1,2,3,4-tetrahydropyridin-4-yl]-2-naphthamide (27f)



Compound **27f** (68 mg, 76%) was prepared according to the general procedure from oxazine **4i** (63 mg, 0.2 mmol). Yellow solid, mp 142–144 °C (from Et_2O/hexane). ^1H NMR (400 MHz, $CDCl_3$) δ 2.38 (s, 3H), 5.92 (s, 1H), 7.23–7.25 (m, 2H), 7.39–7.41 (m, 3H), 7.49–7.59 (m, 4H), 7.69–7.71 (m, 3H), 7.85–7.91 (m, 4H), 8.36–8.38 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 21.2, 66.1, 106.2, 123.5, 125.3, 126.8, 127.2, 127.7, 127.9, 128.2, 128.5, 129.0, 129.4 (2C), 129.6, 129.7, 130.7, 132.4, 134.9, 135.1, 136.0, 140.0, 156.0, 166.6, 186.8. HRMS (ESI-TOF) *m/z* $[M+Na]^+$ calcd for $C_{29}H_{22}N_2NaO_3^+$: 469.1523; found: 469.1523.

10. X-ray data

Compound 4a (1939718)

Single crystal of compound **4a** was grown by slow evaporation of hexane-diethyl ether solution at 4 °C. A suitable crystal was selected and studied on a SuperNova (single source at offset/far, HyPix3000) diffractometer. The crystal was kept at 100(3) K during data collection. Using Olex2,[11] the structure was solved with the ShelXS[12] structure solution program using Direct Methods and refined with the ShelXL[13] refinement package using Least Squares minimization.

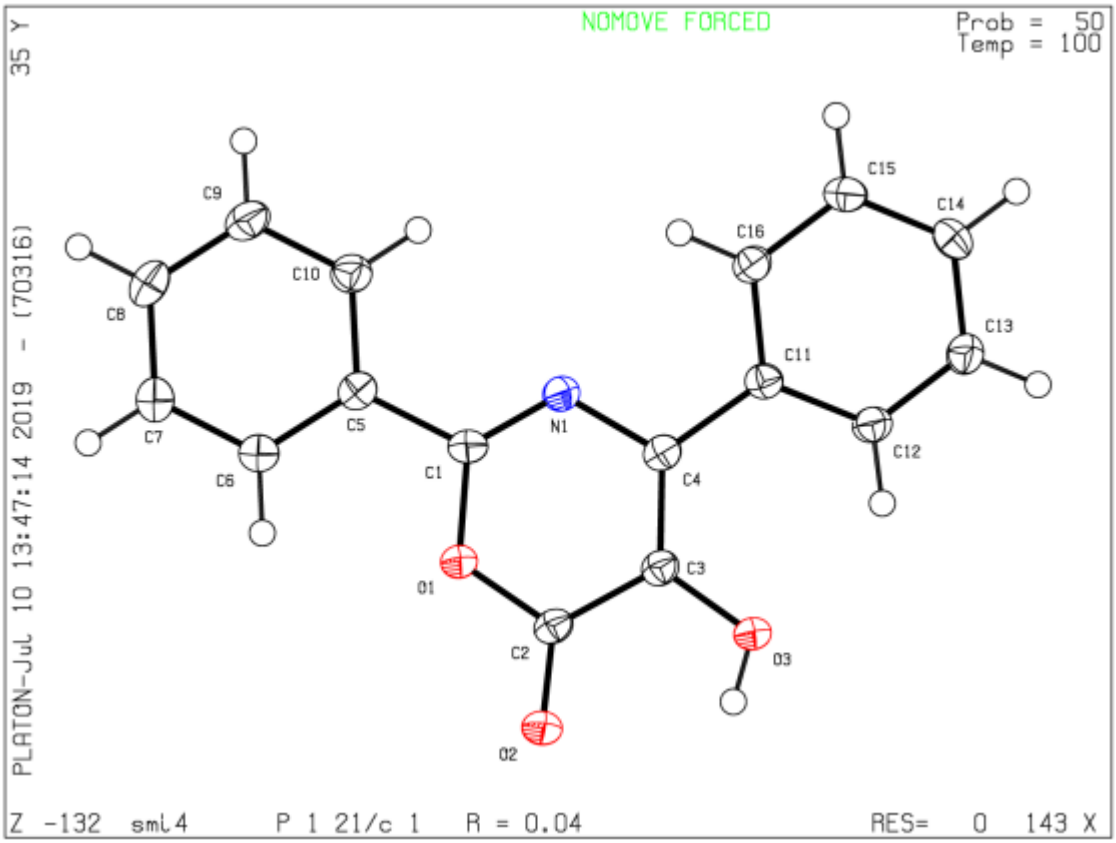


Table S2. Crystal data and structure refinement for 4a.

Empirical formula	$C_{16}H_{11}NO_3$
Formula weight	265.26
Temperature/K	100(3)
Crystal system	monoclinic
Space group	$P2_1/c$
a/Å	5.6374(2)
b/Å	26.9520(7)
c/Å	8.3501(3)
α/°	90
β/°	106.991(4)
γ/°	90
Volume/Å^3	1213.33(7)
Z	4
ρ_{calc}g/cm^3	1.452
μ/mm^{-1}	0.834

F(000)	552.0
Crystal size/mm^3	0.25 × 0.18 × 0.15
Radiation	CuKα (λ = 1.54184)
2Θ range for data collection/°	6.558 to 143.54
Index ranges	-5 ≤ h ≤ 6, -33 ≤ k ≤ 33, -10 ≤ l ≤ 10
Reflections collected	13070
Independent reflections	2368 [R_{int} = 0.0331, R_{sigma} = 0.0217]
Data/restraints/parameters	2368/0/182
Goodness-of-fit on F^2	1.047
Final R indexes [I>=2σ (I)]	R_1 = 0.0371, wR_2 = 0.0994
Final R indexes [all data]	R_1 = 0.0403, wR_2 = 0.1023
Largest diff. peak/hole / e Å^{-3}	0.14/-0.26

Compound 4u (1941719)

Single crystal of compound **4u** was grown by slow evaporation of hexane-diethyl ether solution at 4 °C. A suitable crystal was selected and studied on a SuperNova (Dual, Cu at zero, Atlas) diffractometer. The crystal was kept at 100(2) K during data collection. Using Olex2,[11] the structure was solved with the ShelXS[12] structure solution program using Direct Methods and refined with the ShelXL[13] refinement package using Least Squares minimization.

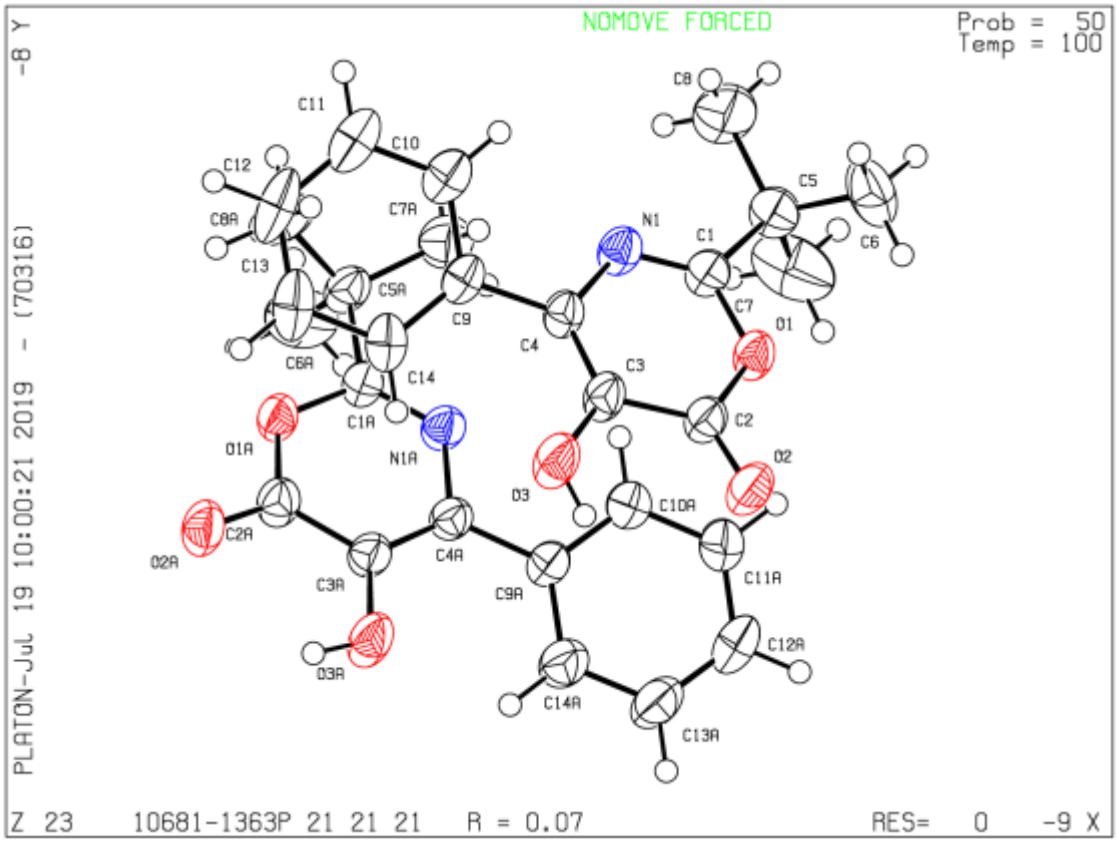


Table S3. Crystal data and structure refinement for 4u.

Empirical formula	$C_{14}H_{15}NO_3$
Formula weight	245.27
Temperature/K	100(2)

Crystal system	orthorhombic
Space group	$P2_12_12_1$
a/Å	10.5893(5)
b/Å	11.4528(9)
c/Å	21.4631(15)
α/°	90
β/°	90
γ/°	90
Volume/Å^3	2603.0(3)
Z	8
ρ_{calc}g/cm^3	1.252
μ/mm^{-1}	0.723
F(000)	1040.0
Crystal size/mm^3	0.5 × 0.2 × 0.2
Radiation	CuKα (λ = 1.54184)
2Θ range for data collection/°	8.238 to 143.998
Index ranges	$-8 \leq h \leq 13$, $-13 \leq k \leq 14$, $-25 \leq l \leq 26$
Reflections collected	13744
Independent reflections	4988 [R_{int} = 0.1063, R_{sigma} = 0.0745]
Data/restraints/parameters	4988/0/334
Goodness-of-fit on F^2	1.058
Final R indexes [I>=2σ (I)]	R_1 = 0.0722, wR_2 = 0.1897
Final R indexes [all data]	R_1 = 0.0880, wR_2 = 0.2183
Largest diff. peak/hole / e Å^{-3}	0.26/-0.36
Flack parameter	0.2(4)

Compound 5c (1939720)

Single crystal of compound **5c** was grown by slow evaporation of hexane-diethyl ether solution at 4 °C. A suitable crystal was selected and studied on a Xcalibur (Eos) diffractometer. The crystal was kept at 100(2) K during data collection. Using Olex2,[11] the structure was solved with the ShelXS[12] structure solution program using Direct Methods and refined with the ShelXL[13] refinement package using Least Squares minimization.

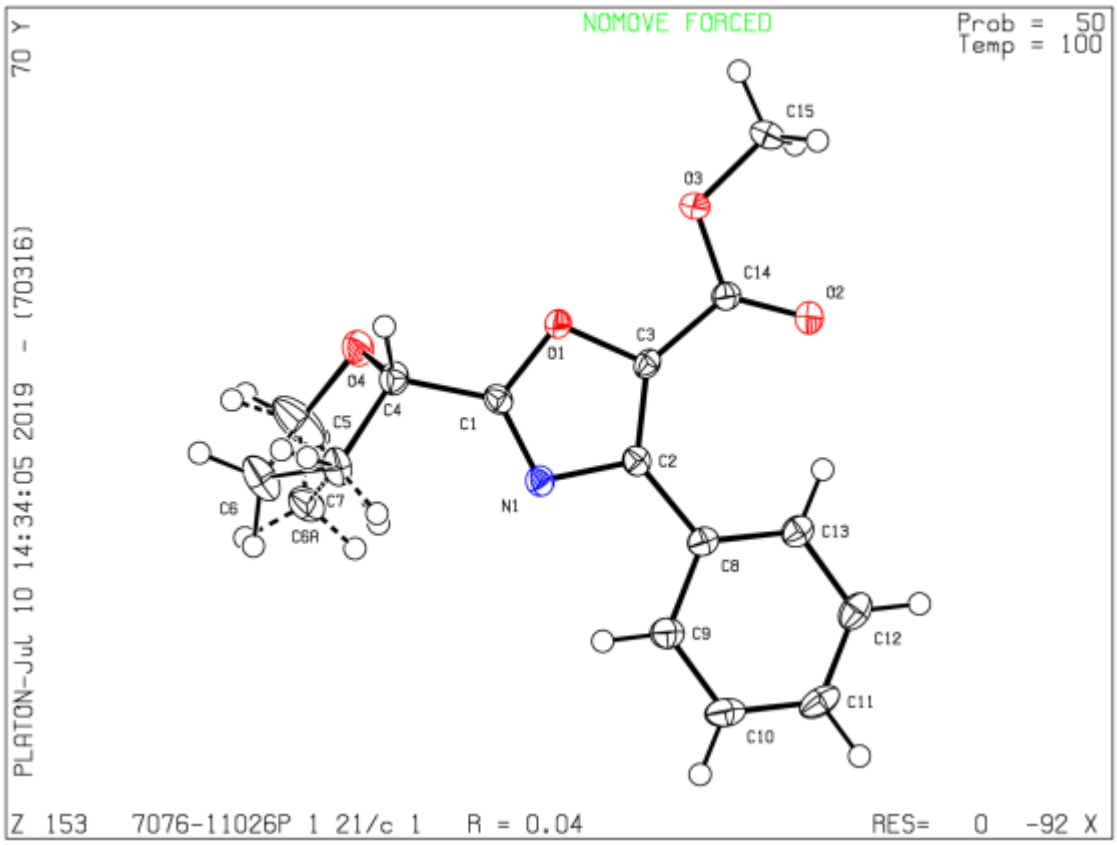


Table S4. Crystal data and structure refinement for 5c.

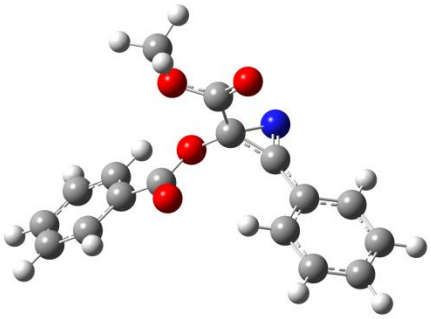
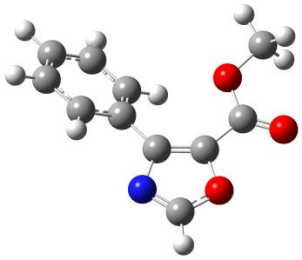
Empirical formula	$C_{15}H_{15}NO_4$
Formula weight	273.28
Temperature/K	100(2)
Crystal system	monoclinic
Space group	$P2_1/c$
a/Å	7.8451(3)
b/Å	17.0778(6)
c/Å	9.7116(4)
α/°	90
β/°	93.581(3)
γ/°	90
Volume/Å^3	1298.59(8)
Z	4
ρ_{calc}g/cm^3	1.398
μ/mm^{-1}	0.102
F(000)	576.0
Crystal size/mm^3	0.5 × 0.4 × 0.2
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	5.724 to 54.998
Index ranges	$-10 \le h \le 10$, $-22 \le k \le 22$, $-11 \le l \le 12$
Reflections collected	14318
Independent reflections	2988 [R_{int} = 0.0268, R_{sigma} = 0.0220]
Data/restraints/parameters	2988/0/191
Goodness-of-fit on F^2	1.030

Final R indexes [I>=2σ (I)]	R_1 = 0.0389, wR_2 = 0.0944
Final R indexes [all data]	R_1 = 0.0468, wR_2 = 0.0997
Largest diff. peak/hole / e Å^{-3}	0.44/-0.34

11. Calculation details

All calculations were performed by using the Gaussian 09 suite of quantum chemical programs.[13] Geometry optimizations of compounds **3a**, **5a**, **6–11**, **13–15**, Me_3Sn radical, $Me_3SnOSnMe$, Me_3SnOMe_3, and transition states TS1–TS9 were performed at the DFT B3LYP level using LANL2DZ basis set for tin atoms and 6-31+G(d,p) basis set for other atoms (PCM solvation model for toluene). Careful verification of the unique imaginary frequencies for transition states was carried out to check whether the frequency indeed pertains to the desired reaction coordinate.

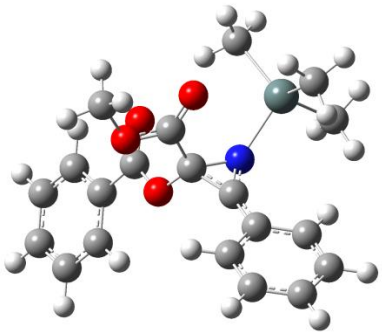
Table S5. Energies (au) and Cartesian coordinates of stationary points for **3a**, **5a**, **6–8**, *E*-**9**, *Z*-**9**, *E*-$\mathbf{9}^{pyr}$, *E*-$\mathbf{9}^{fur}$, **10**, **11, 13–15**, Me_3Sn radical, Me_3SnOMe, $Me_3SnOSnMe_3$, and transition states TS1–TS9 (B3LYP/6-31+G(d,p)/LANL2DZ, a.u., PCM for toluene, 383 K).

Azirine **3a**	Oxazole **5a**
Zero-point correction = 0.264897	Zero-point correction = 0.182244
Thermal correction to Energy = 0.294895	Thermal correction to Energy = 0.201957
Thermal correction to Enthalpy = 0.296108	Thermal correction to Enthalpy = 0.203170
Thermal correction to Gibbs Free Energy = 0.192660	Thermal correction to Gibbs Free Energy = 0.125455
E_0 = -1011.048885, E = -1011.018887,	E_0 = -704.868318, E = -704.848605,
H = -1011.017673, G -1011.121121.	H = -704.847391, G = -704.925106.
Imaginary frequency = 0.	Imaginary frequency = 0.
	
C -2.41215079 -0.97110676 0.05255796	C 0.38739310 -0.81104428 -0.10502911
C -1.40915379 -0.06755776 0.56838496	N 0.41009106 -2.20475436 -0.05802911
C -0.19161779 0.69038224 0.38666196	C -0.93318238 -0.41105946 -0.18942743
N -1.04672479 0.56503124 1.60991996	C 1.65997460 -0.06989085 -0.05830909
O 1.07015021 0.05639724 0.51186196	C -1.70034330 0.82947006 -0.37455318
C -0.19173279 2.02698024 -0.30825904	O -1.71075720 -1.55102018 -0.17209995
O 1.04045521 2.45324924 -0.60754004	O -2.91747081 0.86820710 -0.42253990
O -1.21599179 2.63836724 -0.54368704	O -0.90563887 1.90680746 -0.50391300
C 1.12370721 3.72480524 -1.29021704	C -1.57850627 3.16592241 -0.72241106
C -3.47848279 -1.37210776 0.87918396	C -0.83560265 -2.56526745 -0.09629339
C -4.44741379 -2.23735776 0.37877196	C 2.79329229 -0.64146426 -0.66512632
C -4.35593979 -2.70457476 -0.93908104	C 4.02504818 0.01139259 -0.62253242
C -3.29507279 -2.30768376 -1.75943204	C 4.14894234 1.23552000 0.04191010
C -2.31995079 -1.43943776 -1.26882504	C 3.03207889 1.80047776 0.66475332
C 1.57802521 -0.54508076 -0.60120004	C 1.79579117 1.15512877 0.61579122
C 2.91706621 -1.14299776 -0.35986404	H -2.15616193 3.12934629 -1.64839837
O 0.97947521 -0.57851576 -1.66127304	H -0.78224938 3.90523832 -0.79451887
C 3.54482121 -1.80618076 -1.42612504	H -2.24294082 3.39080013 0.11448173
C 4.80108121 -2.38276276 -1.24670604	H 2.69875141 -1.59747073 -1.16878473

C	5.43728721 -2.30021776 -0.00298404	H	4.88851084 -0.43790330 -1.10420542
C	4.81471621 -1.63993176 1.06118096	H	5.10929994 1.74129550 0.08042209
C	3.55725521 -1.06082576 0.88708996	H	3.12387215 2.74261357 1.19723753
H	2.18743921 3.89664324 -1.44594804	H	0.93847905 1.59638297 1.10912270
H	0.68954821 4.51235824 -0.67123904	H	-1.24150257 -3.56611745 -0.07041478
H	0.59557421 3.67228224 -2.24440104		
H	-3.53792179 -1.00092476 1.89758196		
H	-5.27365879 -2.54846876 1.01039596		
H	-5.11439679 -3.37928376 -1.32514404		
H	-3.22858179 -2.67333676 -2.77928104		
H	-1.48412379 -1.12584576 -1.88568904		
H	3.03769621 -1.85991476 -2.38349104		
H	5.28405121 -2.89507776 -2.07319504		
H	6.41637721 -2.74937376 0.13612796		
H	5.30856721 -1.57560576 2.02592596		
H	3.07154321 -0.54698876 1.70827796		

Radical **6**

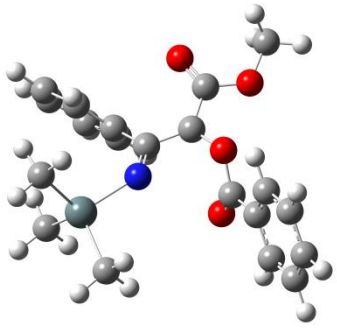
Zero-point correction = 0.372625
Thermal correction to Energy = 0.372625
Thermal correction to Enthalpy = 0.418537
Thermal correction to Gibbs Free Energy = 0.278294
E_0 = -1134.051644, E = -1134.006945,
H = -1134.005732, G = -1134.145976.
Imaginary frequency = 0.

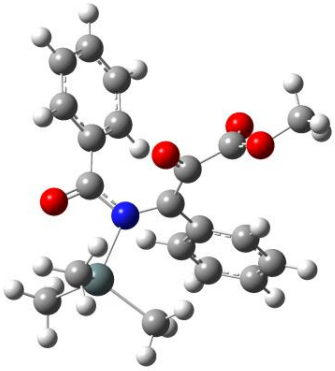
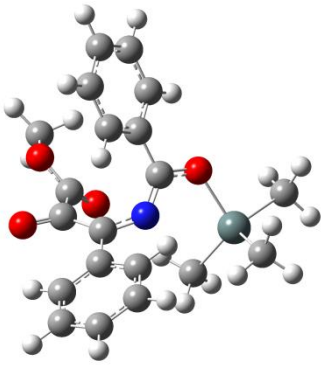


C	-0.79998277 1.53414655 -0.38941383	C	-0.76631799 0.60089655 0.17972141
N	-0.62320677 0.23206855 -0.75602683	N	-0.35798999 -0.61512145 0.33417041
C	0.27764523 0.81221955 0.24494717	C	0.24579801 1.65399655 0.24316541
C	-1.62078877 2.66259055 -0.49350383	C	-2.19123299 0.99576655 -0.10065559
C	0.14088723 0.33490055 1.67395317	C	-0.01689499 3.08299455 0.49306041
O	1.60555723 1.11610855 -0.16850883	O	1.55906201 1.30135955 0.25561641
O	-0.75593377 -0.40763545 2.03432417	O	-1.10006899 3.53349455 0.83882541
O	1.06453223 0.86125655 2.48238917	O	1.08479001 3.84207055 0.31396841
C	1.00064523 0.46264655 3.87112617	C	0.91815301 5.25224755 0.56255241
C	2.50098923 0.09266255 -0.15251483	C	2.09181701 0.53397755 -0.76907459
C	3.84317923 0.49834855 -0.64642283	C	3.38192501 -0.08293545 -0.37748259
O	2.20950123 -1.02633645 0.23353717	O	1.57142901 0.46183355 -1.85960259
Sn	-1.83203277 -1.50307445 -0.70928983	Sn	-1.39402799 -2.39475245 0.19561541
C	-0.63112777 -3.10651445 0.02418217	C	0.16932701 -3.77563645 -0.28266359
C	-3.63360477 -1.09817145 0.37558917	C	-2.20507899 -2.81516945 2.13968541
C	-2.23886077 -1.70998745 -2.80481383	C	-2.89656399 -2.37803445 -1.33940259
C	4.86525723 -0.46441245 -0.64527483	C	4.09839401 -0.78501645 -1.36029559
C	6.14031423 -0.12905045 -1.09861183	C	5.31525101 -1.38545045 -1.04124259
C	6.40147223 1.16783555 -1.55619883	C	5.82326001 -1.28873445 0.25961041
C	5.38478123 2.12883755 -1.55988083	C	5.11152901 -0.59050445 1.24092841
C	4.10663823 1.79855955 -1.10687683	C	3.89280901 0.01238655 0.92699741
C	-1.34273177 3.84204655 0.26306517	C	-3.19171099 0.75978455 0.85253341
C	-2.15209977 4.96253455 0.14447617	C	-4.52582299 1.05779155 0.56507941
C	-3.25756277 4.96509755 -0.72533383	C	-4.87425199 1.58202955 -0.68398659
C	-3.53815977 3.81567155 -1.48208783	C	-3.88033999 1.81557755 -1.63985659
C	-2.74274277 2.68149255 -1.37712183	C	-2.54433999 1.53051555 -1.34809459
H	0.04337023 0.76053455 4.30398617	H	0.16954601 5.67182155 -0.11380959

Radical **7**

Zero-point correction = 0.372463
Thermal correction to Energy = 0.417351
Thermal correction to Enthalpy = 0.418565
Thermal correction to Gibbs Free Energy = 0.277344
E_0 = -1134.066614, E = -1134.021725,
H = -1134.020512, G = -1134.161733.
Imaginary frequency = 0.



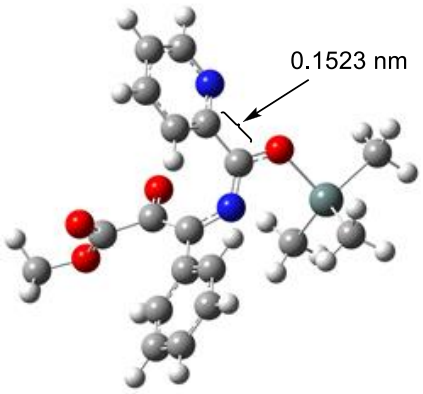
H 1.82418223 0.98415055 4.35641317 H 1.12394323 -0.61912145 3.95451717 H -0.76630277 -3.99623145 -0.59803883 H 0.42096123 -2.81199645 0.00642417 H -0.90803977 -3.34343445 1.05435517 H -4.02027777 -0.10564445 0.12720517 H -3.44072477 -1.13957945 1.44969117 H -4.39669077 -1.83997845 0.11786517 H -2.86111877 -2.59161245 -2.99067783 H -2.76552877 -0.83231545 -3.19173883 H -1.30437977 -1.82320145 -3.36239183 H 4.64515023 -1.46474245 -0.28763183 H 6.92905123 -0.87544045 -1.09618983 H 7.39508223 1.42831855 -1.90973683 H 5.58688423 3.13439955 -1.91642083 H 3.31486823 2.53876455 -1.10977783 H -0.48804777 3.85041855 0.93362517 H -1.92493177 5.84855555 0.73153417 H -3.88475977 5.84682755 -0.81328683 H -4.38676177 3.81013655 -2.16127783 H -2.96207777 1.80419055 -1.97858483	H 1.89622701 5.69385655 0.37554541 H 0.60828301 5.42213955 1.59647141 H 0.65279201 -3.49353345 -1.22266759 H 0.92830801 -3.77844245 0.50532141 H -0.22603499 -4.79104145 -0.38822959 H -2.44420399 -3.88001245 2.22537941 H -3.11869099 -2.24128645 2.31774841 H -1.47692999 -2.56285545 2.91642841 H -3.33426999 -3.37701745 -1.43751559 H -3.69163199 -1.66668845 -1.10296759 H -2.45463299 -2.09930745 -2.30035259 H 3.69042901 -0.85055845 -2.36335359 H 5.86699001 -1.92777045 -1.80318059 H 6.77161201 -1.75679945 0.50783841 H 5.50503001 -0.51672845 2.25031741 H 3.33676401 0.55210355 1.68463341 H -2.92141699 0.36500555 1.82797941 H -5.29119499 0.88499555 1.31654541 H -5.91208099 1.81021155 -0.90946159 H -4.14476799 2.21973655 -2.61302059 H -1.77440199 1.71276955 -2.09309059
Radical **8** Zero-point correction = 0.373296 Thermal correction to Energy = 0.418079 Thermal correction to Enthalpy = 0.419292 Thermal correction to Gibbs Free Energy = 0.279598 E_0 = -1134.097964, E = -1134.053181, H = -1134.051967, G = -1134.191662. Imaginary frequency = 0.	Radical *E*-**9** Zero-point correction = 0.373067 Thermal correction to Energy = 0.418052 Thermal correction to Enthalpy = 0.419265 Thermal correction to Gibbs Free Energy = 0.276914 E_0 = -1134.102651, E = -1134.057666, H = -1134.056453, G = -1134.198804. Imaginary frequency = 0.
	
C -0.35674509 -0.96105103 -0.12052006 N 0.65334591 -0.02919203 0.05279594 C -1.38211609 -0.69399103 -1.11819606 C -0.26872209 -2.21480303 0.62364894 C -2.70898509 -1.45860303 -1.06040406 O -1.28612509 0.21195597 -1.96003706 O -3.41303409 -1.48992803 -0.06936406 O -3.03061409 -1.98958903 -2.24599506 C -4.33609309 -2.60495503 -2.33925606 C 0.47514591 1.33761697 0.09525794 C -0.79742009 1.97889797 0.53599794 O 1.48152191 2.03072897 -0.15097906 Sn 2.75738391 -0.25855203 -0.46446206 C 3.92389691 0.41917597 1.19268394 C 2.92591991 -2.39505203 -0.65206006 C 3.14512591 0.59475997 -2.38552406 C -1.08309309 3.26643297 0.05382394 C -2.23401109 3.93341697 0.47061994 C -3.09980609 3.33024397 1.39069594	C -1.36533526 -1.06728586 -0.19094195 N -0.05322726 -0.86547886 0.09493905 C -1.96586526 -0.31434986 -1.28073195 C -2.05222126 -2.15615086 0.51872005 C -3.48674726 -0.28577086 -1.44239995 O -1.31722626 0.43269114 -2.03563095 O -4.23841926 0.12860314 -0.57991095 O -3.87165426 -0.66223886 -2.67006695 C -5.27832026 -0.51873986 -2.97056195 C 0.60903774 0.26397714 0.12963505 C 0.06961374 1.59473414 0.51608805 O 1.90379574 0.22355914 -0.08513895 Sn 2.73316974 -1.57382186 -0.61539995 C 2.66715774 -2.84233586 1.10157005 C 1.78007074 -2.29282086 -2.38405095 C 4.70320474 -0.83306286 -0.98765595 C 0.78613874 2.75221514 0.16686105 C 0.30774074 4.01145114 0.52830305 C -0.87965826 4.12831114 1.25874505

C	-2.80996509	2.05738797	1.88929994
C	-1.66613209	1.37951297	1.46090194
C	0.30475191	-2.21991503	1.91605594
C	0.39381991	-3.39759603	2.65389494
C	-0.07178409	-4.60316203	2.11534694
C	-0.62462309	-4.61936003	0.82938194
C	-0.72119009	-3.44287403	0.09009994
H	-4.42596909	-3.41679403	-1.61382106
H	-4.40128409	-2.98577703	-3.35731606
H	-5.11319209	-1.86022103	-2.15434106
H	4.83311191	-0.18241103	1.28810794
H	4.19793591	1.46839397	1.06175694
H	3.35024291	0.32544697	2.11968194
H	3.94520991	-2.63030603	-0.97944006
H	2.23279191	-2.78713103	-1.40210306
H	2.73995891	-2.91005503	0.29347194
H	3.87877991	-0.00983603	-2.92782706
H	2.22073591	0.62968897	-2.96918606
H	3.52123691	1.61430397	-2.27582606
H	-0.39928609	3.72697697	-0.65093606
H	-2.45563609	4.92262297	0.08085994
H	-3.99447609	3.85166297	1.71895694
H	-3.47353009	1.58763197	2.60896894
H	-1.45103609	0.39566497	1.86254494
H	0.65864991	-1.28571103	2.34019794
H	0.82316191	-3.37645203	3.65133494
H	0.00106891	-5.52209903	2.68938894
H	-0.96863709	-5.55431703	0.39701194
H	-1.11092309	-3.48590103	-0.92209006

C	-1.58810926	2.97940414	1.62444005
C	-1.11879126	1.71870814	1.25454205
C	-1.68125926	-2.45677086	1.84726105
C	-2.30677526	-3.48386286	2.55109805
C	-3.30892426	-4.24782786	1.94129505
C	-3.67027826	-3.97919586	0.61690605
C	-3.04773526	-2.95008286	-0.08913295
H	-5.87769926	-1.10838386	-2.27295395
H	-5.39370126	-0.88799886	-3.98860495
H	-5.56938026	0.53197514	-2.90537295
H	3.45593074	-3.59889286	1.04075705
H	2.82701674	-2.24996886	2.00739705
H	1.69834174	-3.34084486	1.17427605
H	2.49871874	-2.83978186	-3.00221895
H	1.38772974	-1.45322386	-2.96450495
H	0.95015174	-2.95560886	-2.12896895
H	5.37909874	-1.64962986	-1.26112795
H	4.69114074	-0.10744986	-1.80617295
H	5.10063074	-0.34144786	-0.09482895
H	1.70685974	2.65336414	-0.39657495
H	0.86097274	4.90082514	0.24090705
H	-1.25018926	5.10908714	1.54302105
H	-2.50664926	3.06255214	2.19737405
H	-1.67383026	0.83555514	1.55028205
H	-0.90280126	-1.86782486	2.32161805
H	-2.01400426	-3.68890786	3.57699105
H	-3.79566026	-5.04954186	2.48901805
H	-4.42999426	-4.58165686	0.12718505
H	-3.31309626	-2.79189186	-1.12939695

Radical *E*-**9**^{pyr}

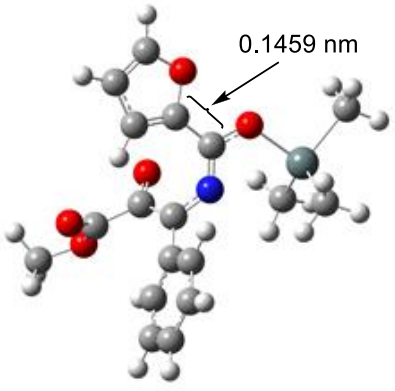
Zero-point correction = 0.361163
Thermal correction to Energy = 0.405840
Thermal correction to Enthalpy = 0.407054
Thermal correction to Gibbs Free Energy = 0.265224
E_0 = -1150.146490, -1150.101812,
H = -1150.100599, G = -1150.242428.
Imaginary frequency = 0.



C	2.03766360	-0.44388277	0.17455216
N	0.72251960	-0.25027777	-0.10958484
C	2.66004660	0.36701123	1.20888216
C	2.71008660	-1.57151677	-0.48598784
C	4.18310460	0.39207923	1.35133916
O	2.02955160	1.16651623	1.92350416
O	4.92417460	0.77275623	0.46436816
O	4.58124160	0.05865523	2.58642616

Radical *E*-**9**^{fur}

Zero-point correction = 0.342926
Thermal correction to Energy = 0.386333
Thermal correction to Enthalpy = 0.387546
Thermal correction to Gibbs Free Energy = 0.249005
E_0 = -1131.906474, E = -1131.863067,
H = -1131.861853, G = -1132.000395.
Imaginary frequency = 0.

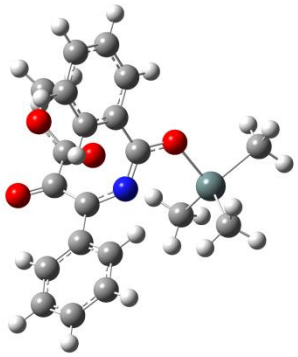


C	2.03766360	-0.44388277	0.17455216
N	0.72251960	-0.25027777	-0.10958484
C	2.66004660	0.36701123	1.20888216
C	2.71008660	-1.57151677	-0.48598784
C	4.18310460	0.39207923	1.35133916
O	2.02955160	1.16651623	1.92350416
O	4.92417460	0.77275623	0.46436816
O	4.58124160	0.05865523	2.58642616

C	5.99185060	0.20767823	2.86667716
C	0.07325260	0.88270723	-0.19551384
C	0.67169060	2.19779323	-0.60693484
O	-1.22127940	0.88499523	-0.03471784
Sn	-2.14976940	-0.83130877	0.58465916
C	-2.07528040	-2.21443977	-1.04161584
C	-1.25007440	-1.45453377	2.41598516
C	-4.10033440	-0.00372177	0.84751616
N	0.05041260	3.29912623	-0.15503284
C	0.54961360	4.48652423	-0.51127484
C	1.66452660	4.63976023	-1.34276284
C	2.29074360	3.49177423	-1.82574484
C	1.78936360	2.24501723	-1.45074484
C	2.31221360	-1.94626077	-1.78785284
C	2.92535060	-3.00957877	-2.44718184
C	3.94141960	-3.73778677	-1.81702684
C	4.32890560	-3.39645877	-0.51699284
C	3.71899560	-2.33076477	0.14425016
H	6.58155860	-0.40824477	2.18377516
H	6.11680160	-0.12604277	3.89574316
H	6.28502960	1.25453823	2.76173816
H	-2.85899040	-2.97000877	-0.92712884
H	-2.24054540	-1.68764677	-1.98619484
H	-1.10356240	-2.71110977	-1.08032984
H	-1.99098140	-1.95354677	3.04828816
H	-0.86170740	-0.58481977	2.95321916
H	-0.42337440	-2.14177777	2.22308716
H	-4.80596840	-0.77376877	1.17534916
H	-4.07930140	0.79015823	1.59943316
H	-4.46362040	0.42053723	-0.09295084
H	0.03266760	5.35895123	-0.11709484
H	2.02229960	5.63114623	-1.60214284
H	3.15428460	3.55975623	-2.48021384
H	2.25292660	1.33448723	-1.81182184
H	1.52118360	-1.38707577	-2.27707984
H	2.61131760	-3.27147077	-3.45363384
H	4.41857960	-4.56795777	-2.32961484
H	5.09901560	-3.97093477	-0.01023184
H	4.00471960	-2.11698977	1.16892416

Radical *Z*-**9**

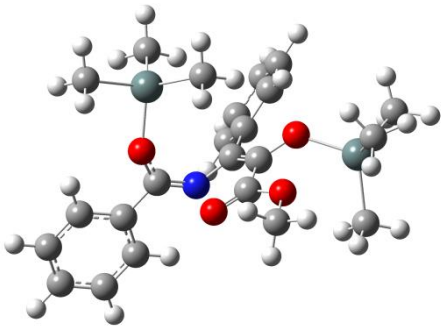
Zero-point correction = 0.373553
Thermal correction to Energy = 0.418185
Thermal correction to Enthalpy = 0.419399
Thermal correction to Gibbs Free Energy = 0.280139
E_0 = -1134.103055, E = -1134.058424,
H = -1134.057210, G = -1134.196470.
Imaginary frequency = 0.



C	2.11361830	-1.22690331	1.03878264
N	0.89468130	-0.85039131	0.56079164
C	2.86366830	-0.36576031	1.94283464

Intermediate **10**

Zero-point correction = 0.482856
Thermal correction to Energy = 0.540692
Thermal correction to Enthalpy = 0.541906
Thermal correction to Gibbs Free Energy = 0.369302
E_0 = -1257.169320, E = 1257.111484,
H = -1257.110271, G = -1257.282874.
Imaginary frequency = 0.



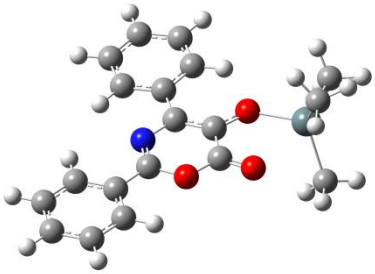
C	-0.15167198	1.51733608	1.67810179
C	0.07269202	0.36142708	0.76005379
C	-0.87855798	-0.07660592	-0.14151121

C	2.58444430	-2.56934431	0.66511564
C	2.16538430	0.85807169	2.56031464
O	4.03060030	-0.58050331	2.31407564
O	1.05903730	0.83764369	3.07224564
O	2.97487630	1.92254969	2.56460464
C	2.48491230	3.09743069	3.24414364
C	0.50231630	0.28439069	0.05578564
C	1.36820030	1.31800469	-0.58246536
O	-0.78569870	0.54579569	0.02397264
Sn	-2.12073170	-0.81843831	0.76452864
C	-2.12876570	-2.43192931	-0.63592636
C	-1.67576970	-1.31884131	2.78847564
C	-3.85291970	0.41828469	0.56834664
C	0.88799330	2.63429469	-0.69925336
C	1.67096330	3.61859269	-1.30282936
C	2.93161230	3.29630569	-1.81634736
C	3.40508930	1.98345069	-1.72555236
C	2.63078630	0.99892669	-1.11129736
C	1.97775230	-3.21948631	-0.43561936
C	2.37188130	-4.49662931	-0.82659036
C	3.37898930	-5.16857831	-0.12383336
C	3.98465030	-4.54391631	0.97166364
C	3.60069230	-3.26183931	1.36390164
H	1.55474130	3.44142669	2.78597464
H	3.26980430	3.84372069	3.12959264
H	2.31322530	2.87652669	4.30015364
H	-3.08018170	-2.97055431	-0.57907936
H	-2.01197870	-2.04751931	-1.65356136
H	-1.31653270	-3.13123431	-0.42601636
H	-2.58217870	-1.25491931	3.39806064
H	-0.92462570	-0.62899031	3.18005264
H	-1.27788170	-2.33544931	2.84535864
H	-4.75652270	-0.13577731	0.84210464
H	-3.77485970	1.29198869	1.22214864
H	-3.96017870	0.76536369	-0.46348236
H	-0.09483270	2.87353869	-0.30925936
H	1.29578430	4.63521869	-1.37682136
H	3.53924730	4.06200469	-2.28996736
H	4.37700330	1.72367069	-2.13388136
H	3.00424430	-0.01778131	-1.05994836
H	1.19384930	-2.70643431	-0.98190636
H	1.89342130	-4.96900631	-1.68003636
H	3.68622730	-6.16590931	-0.42552836
H	4.76319430	-5.05829531	1.52802764
H	4.08430430	-2.79165431	2.20873464

N	1.23639702	-0.35214692	1.03085179
O	-2.06404398	0.57126108	-0.29089221
C	-0.67115598	-1.28517692	-0.97245721
O	-1.83824798	-1.64321992	-1.59766021
O	0.35219002	-1.93299692	-1.12274521
C	-1.76869698	-2.82515392	-2.41483721
Sn	-3.91793298	-0.15308492	-0.16981721
C	-4.72518198	-0.30110192	-2.14559721
C	-3.90633598	-1.94784792	0.99624379
C	-4.87319198	1.45923308	0.86938179
C	-1.00659798	2.59782308	1.37474179
C	-1.14024398	3.67388408	2.25549679
C	-0.43755398	3.69888308	3.46369079
C	0.41575902	2.63606208	3.77744379
C	0.56366002	1.56652208	2.89421979
C	2.30563202	-0.39634892	0.32050579
C	3.42850702	-1.27365192	0.78519279
O	2.55997602	0.24453908	-0.81368521
C	4.64708802	-1.30173392	0.09088779
C	5.69497602	-2.11620492	0.52921179
C	5.53658002	-2.91432892	1.66548279
C	4.32099602	-2.89528592	2.36042079
C	3.27477102	-2.08359792	1.92267079
H	-2.76746398	-2.95188892	-2.83243721
H	-1.48976298	-3.69317192	-1.81239921
H	-1.03547898	-2.69273392	-3.21390921
H	-5.75906398	0.05767208	-2.16113321
H	-4.13259098	0.31719508	-2.82644921
H	-4.70645998	-1.33106592	-2.51061421
H	-4.84748598	-2.04416992	1.54636379
H	-3.08779298	-1.91491292	1.72185279
H	-3.77457098	-2.82989792	0.36498479
H	-4.73660498	2.39777208	0.32324979
H	-5.94823698	1.27272208	0.96485679
H	-4.45098498	1.57906808	1.87109079
H	-1.56047598	2.59208208	0.44654779
H	-1.79868098	4.49757308	1.99233179
H	-0.55028798	4.53503408	4.14824479
H	0.97137902	2.63991708	4.71134779
H	1.23315902	0.75004708	3.13845779
H	4.76360702	-0.68631792	-0.79359521
H	6.63313702	-2.12857892	-0.01883321
H	6.35049502	-3.54847992	2.00614779
H	4.18811002	-3.51710292	3.24150579
H	2.32716302	-2.06709592	2.44953879
Sn	2.19030902	1.93476408	-1.80902821
C	0.31031702	1.82117508	-2.81444921
C	2.40346702	3.53283208	-0.40817521
C	3.81443102	1.83279708	-3.19131121
H	-0.52969198	1.85950808	-2.11849921
H	0.23142802	2.65887208	-3.51569921
H	0.25239202	0.88907508	-3.38375521
H	3.38075402	3.47040408	0.07906679
H	1.62514902	3.49882208	0.35717679
H	2.33834202	4.49264108	-0.93099621
H	3.77626002	2.66789908	-3.89822221
H	4.77154702	1.87141508	-2.66320621
H	3.76777302	0.89848608	-3.75833521

Intermediate **11**

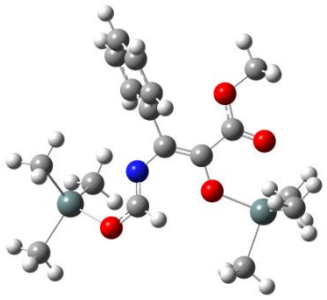
Zero-point correction = 0.332376
Thermal correction to Energy = 0.371003
Thermal correction to Enthalpy = 0.372216
Thermal correction to Gibbs Free Energy = 0.247655
E_0 = -1019.039190, E = -1019.000564,
H = -1018.999350, G = -1019.123911.
Imaginary frequency = 0.



C	0.14566417	2.25901679	-0.09726150
C	-0.09215883	0.79835179	-0.09547950
C	0.89420117	-0.18240221	-0.09464450
N	-1.42326183	0.41171079	-0.09683850
O	2.20207117	0.03831579	-0.09399550
C	0.48314717	-1.57736021	-0.09673650
O	1.28110417	-2.51260621	-0.09913450
Sn	3.72827317	-1.32005721	-0.10077650
C	3.80574417	-2.40389821	1.73811550
C	3.79951617	-2.39370921	-1.94590250
C	5.24100217	0.20296579	-0.09855550
C	1.43811817	2.82528579	-0.05183950
C	1.60753617	4.21139379	-0.05144850
C	0.50240917	5.06513679	-0.09856650
C	-0.78412783	4.51692879	-0.14540550
C	-0.96098683	3.13481979	-0.14375350
C	-1.76649283	-0.82584921	-0.09617950
C	-3.16394383	-1.28916721	-0.09455450
O	-0.85377483	-1.85205421	-0.09644650
C	-3.47951483	-2.65951521	-0.10323350
C	-4.81368583	-3.07017521	-0.10167450
C	-5.84328083	-2.12459921	-0.09117750
C	-5.53300883	-0.75910121	-0.08201750
C	-4.20396683	-0.34174321	-0.08368850
H	4.84638817	-2.57260921	2.03258450
H	3.31571117	-1.82608021	2.52795750
H	3.29477517	-3.36377521	1.64075450
H	4.83916217	-2.56126121	-2.24452150
H	3.30731917	-1.81135921	-2.73104750
H	3.28844217	-3.35389221	-1.85217150
H	6.24055117	-0.24514921	-0.10470250
H	5.14757917	0.84146779	-0.98249150
H	5.15467117	0.83240979	0.79260350
H	2.30163517	2.17657679	-0.01653450
H	2.61213217	4.62359979	-0.01443350
H	0.64016017	6.14275579	-0.09896550
H	-1.65311983	5.16808879	-0.18300350
H	-1.95891483	2.71581479	-0.17906250
H	-2.68517883	-3.39701421	-0.11129950
H	-5.04747483	-4.13066321	-0.10860850
H	-6.88017683	-2.44792621	-0.08983950
H	-6.32850183	-0.01979521	-0.07329550

Intermediate **13**

Zero-point correction = 0,402101
Thermal correction to Energy = 0.453380
Thermal correction to Enthalpy = 0.454594
Thermal correction to Gibbs Free Energy = 0.297147
E_0 = -1026.194212, E = -1026.142933,
H = -1026.141720, G = -1026.299166.
Imaginary frequency = 0.



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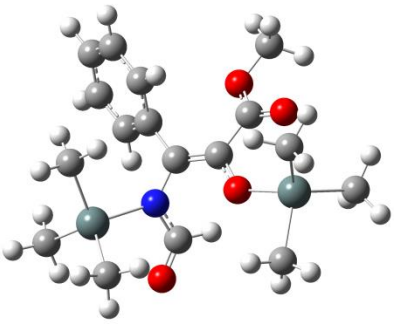
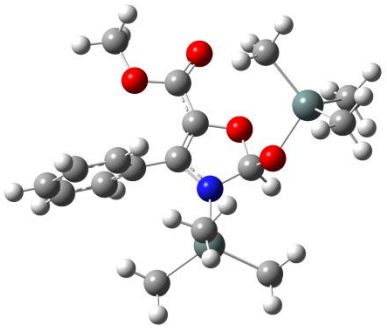
C	-2.75162812	0.19340637	-0.17344068
N	-0.38170012	-0.35853663	-0.35301668
O	-3.11607812	-1.09471963	-0.34291168
C	-3.86636012	1.07293337	0.23272932
O	-3.60275412	2.35687037	0.48263932
O	-5.00422912	0.60029637	0.36292532
C	-4.71546312	3.17664337	0.89726432
Sn	-4.92169512	-1.95093563	-0.05648468
C	-5.55031412	-1.96208863	1.99059232
C	-6.35249412	-1.39490063	-1.54929968
C	-4.19547512	-3.91942663	-0.54260768
C	-1.21830512	2.85093837	-1.29832468
C	-0.69355412	4.14577537	-1.30764568
C	0.12859188	4.57852037	-0.26236868
C	0.42863288	3.70367837	0.78751632
C	-0.08970912	2.40658237	0.78973632
C	-0.44703012	-1.50958963	-0.93344268
O	0.57764388	-2.33867963	-0.89211668
H	-4.29920412	4.17533637	1.02256932
H	-5.12768312	2.80895537	1.83973432
H	-5.49505412	3.17533437	0.13217632
H	-4.68253012	-1.83028863	2.64499232
H	-6.25695112	-1.15194463	2.18441432
H	-6.02089212	-2.91940263	2.23664732
H	-6.91860012	-2.27146963	-1.88009168
H	-5.83392512	-0.97473463	-2.41716768
H	-7.04416012	-0.64248663	-1.16354068
H	-5.00227912	-4.65758163	-0.47162768
H	-3.79904312	-3.94625363	-1.56275768
H	-3.39619012	-4.21951963	0.14231732
H	-1.85449512	2.51663037	-2.11311268
H	-0.92289412	4.81431537	-2.13308568
H	0.53625688	5.58558337	-0.26839068
H	1.06799288	4.03062737	1.60317632
H	0.14911788	1.72646937	1.60192232
Sn	2.24106488	-1.71511163	0.11387532
C	3.05992188	-0.00432463	-0.86712368
C	1.76274088	-1.50599163	2.18645232
C	3.42708588	-3.46206463	-0.23294768
H	4.12122188	0.09909937	-0.61933068
H	2.96916988	-0.12039463	-1.95126168

H -3.95520483 0.71339979 -0.07558050	H 2.52851188 0.90104637 -0.56740068 H 1.04253088 -2.27593863 2.47880232 H 1.32506788 -0.52601063 2.38724532 H 2.66394288 -1.62741163 2.79602832 H 4.41354588 -3.36056863 0.23126432 H 2.93865488 -4.34666663 0.18643632 H 3.56709788 -3.62229763 -1.30613368 H -1.30083812 -1.86670863 -1.50727068
Intermediate **14** Zero-point correction = 0.402514 Thermal correction to Energy = 0.453658 Thermal correction to Enthalpy = 0.454871 Thermal correction to Gibbs Free Energy = 0.300181 E_0 = -1026.196017, E = -1026.144873, H = -1026.143659, G = -1026.298350. Imaginary frequency = 0.  C -1.73959528 1.46121968 -0.32606510 C -0.81969428 0.31871668 -0.55785110 C 0.54697172 0.33178268 -0.41203710 N -1.45156928 -0.89867532 -0.92633410 O 1.24725872 -0.81426332 -0.44291510 C 1.39950872 1.54509168 -0.28089410 O 0.84330172 2.71868468 -0.58158710 O 2.58753672 1.43398268 0.03063890 C 1.68479872 3.88550468 -0.45761310 Sn 3.18635472 -1.16988432 -0.01398110 C 4.49846072 -0.42690732 -1.53232310 C 3.64952972 -0.71382732 2.02503890 C 3.00280572 -3.29817932 -0.23108910 C -1.68396228 2.23692268 0.84555790 C -2.58930328 3.27659968 1.05925390 C -3.57868028 3.55592768 0.10964190 C -3.65777228 2.78051668 -1.05158110 C -2.75334228 1.73740368 -1.26167810 C -1.03006928 -1.56875132 -2.03080410 O -1.51513728 -2.65448232 -2.36888010 H 1.04736872 4.72456968 -0.73258610 H 2.53869472 3.80937668 -1.13429810 H 2.03982172 3.98960568 0.57021390 H 4.95877472 0.51436468 -1.22382810 H 5.28245072 -1.16053732 -1.74463510 H 3.93577572 -0.25181932 -2.45483310 H 4.11651472 0.27025368 2.10587890 H 4.32466672 -1.46974232 2.43853190 H 2.73179072 -0.71296732 2.62193690 H 2.64120672 -3.55559132 -1.23127810 H 3.97152372 -3.78672332 -0.07875910 H 2.29640872 -3.70188732 0.50075090 H -0.93542928 2.01059368 1.59914390	Oxazoline **15** Zero-point correction = 0.404013 Thermal correction to Energy = 0.454353 Thermal correction to Enthalpy = 0.455566 Thermal correction to Gibbs Free Energy = 0.300039 E_0 = -1026.177989, E = -1026.127649, H = -1026.126436, G = -1026.281963. Imaginary frequency = 0.  C -1.92616586 0.77384454 -0.02162540 C -0.57860886 0.53712354 -0.59948540 C 0.37871814 1.45283154 -0.94154740 N -0.13048586 -0.73475846 -0.88583540 O 1.48309714 0.78621054 -1.48446840 C 0.46661014 2.89314954 -0.86326040 O -0.66812986 3.46587154 -0.37652540 O 1.45152914 3.54738654 -1.19453440 C -0.64620986 4.89813954 -0.26434340 Sn 3.86471914 -0.26774746 0.20399060 C 3.52357614 1.52775754 1.31033760 C 4.69074314 -1.81898546 1.42498560 C 4.96202214 0.01099254 -1.61241740 C -2.12983686 0.68669754 1.36377860 C -3.40138386 0.89505054 1.90555260 C -4.48150486 1.18783654 1.06730560 C -4.28431286 1.27603254 -0.31467140 C -3.01389586 1.06894454 -0.85694840 C 1.28316714 -0.61654546 -1.25474940 O 2.10145014 -1.09527346 -0.24325840 H -1.62830086 5.17135954 0.12208160 H -0.47718086 5.36044854 -1.24036640 H 0.13817214 5.22069354 0.42568960 H 3.16268214 2.31713354 0.64643460 H 2.77682514 1.35171854 2.09059360 H 4.45011914 1.86129154 1.78892360 H 4.03773914 -2.02049946 2.27949260 H 5.67570514 -1.53088846 1.80645660 H 4.80105314 -2.74253946 0.84894860 H 4.48825814 0.78080354 -2.22678040 H 5.98756514 0.32372254 -1.39092740 H 5.00324914 -0.92210446 -2.18248540 H -1.28782086 0.47478054 2.01650160 H -3.54570086 0.83389754 2.98052660

H	-2.53263928	3.85992568	1.97420390	H	-5.46954386	1.35067354	1.48840960
H	-4.28651828	4.36244268	0.27862890	H	-5.11888886	1.50658354	-0.97070740
H	-4.42416828	2.98620768	-1.79372010	H	-2.85846986	1.14356154	-1.92914440
H	-2.82133128	1.13662568	-2.16367610	Sn	-0.90066786	-2.60153646	-0.36037040
Sn	-2.89742728	-2.00981732	0.16195990	C	-0.66752986	-2.91105546	1.74538660
C	-3.12390128	-0.91441832	1.99266990	C	-2.95138386	-2.63784746	-0.96797740
C	-4.70464228	-2.01669532	-0.97918610	C	0.28671714	-3.94404246	-1.52625940
C	-2.09283528	-3.94178432	0.59967890	H	-0.86323986	-3.95927646	1.99344960
H	-2.15255928	-0.74894232	2.46865690	H	0.35492414	-2.66569646	2.04373560
H	-3.60005728	0.05592868	1.83272490	H	-1.36298486	-2.28632346	2.31203960
H	-3.74428628	-1.49717032	2.68216290	H	-3.04211286	-2.35888846	-2.02167640
H	-5.50650628	-2.50070432	-0.41237310	H	-3.55310986	-1.94697146	-0.37273540
H	-4.55748328	-2.55987532	-1.91559810	H	-3.35332986	-3.64869046	-0.84261840
H	-5.01347528	-0.99255832	-1.20712210	H	-0.06854786	-4.97064646	-1.39252240
H	-2.59038528	-4.36586632	1.47793590	H	0.21928814	-3.69620146	-2.58986040
H	-2.22801828	-4.61104032	-0.25228910	H	1.33436114	-3.89551746	-1.21899740
H	-1.02249128	-3.86252032	0.81025990	H	1.50641414	-1.13597946	-2.19617340
H	-0.25223428	-1.06841032	-2.62876410				

Me_3Sn radical

Zero-point correction = 0.106662
Thermal correction to Energy = 0.119237
Thermal correction to Enthalpy = 0.120450
Thermal correction to Gibbs Free Energy = 0.058614
E_0 = -122.993294, E = -122.980719,
H = -122.979505, G = -123.041342.
Imaginary frequency = 0.

Sn	0.06862775	-0.03760152	-0.28268791
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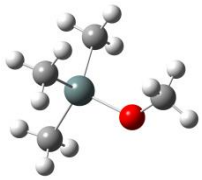
H	-1.12584125	1.56216948	1.59205209
H	-0.75409225	2.55754448	0.16540309
H	-2.18019825	1.49808948	0.16083009
C	2.08417675	0.19711848	0.49608709
H	2.52614175	1.13817648	0.15639109
H	2.05072675	0.20196748	1.59215209
H	2.72523675	-0.62704052	0.17027309
C	-0.73610025	-1.90072252	0.49580209
H	-1.76641125	-2.04976352	0.16029009
H	-0.13485325	-2.75253552	0.16522809
H	-0.72618625	-1.86985052	1.59191309

Me_3SnOMe

Zero-point correction = 0.148881
Thermal correction to Energy = 0.166753
Thermal correction to Enthalpy = 0.167967
Thermal correction to Gibbs Free Energy = 0.092607
E_0 = -238.145603, E = -238.127730,
H = -238.126516, G = -238.201876.
Imaginary frequency = 0.



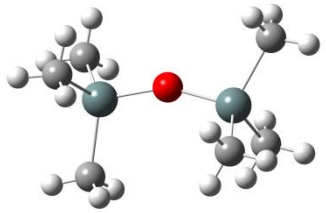
O	1.02282036	-0.17226726	-0.72865259
C	2.28371536	-0.17173026	-0.08541959
H	2.43456136	0.72108474	0.54259741
H	3.06752636	-0.17395226	-0.85294759
H	2.43343636	-1.06195926	0.54653841
Sn	-0.69759564	-0.17179326	0.22613141
C	-0.78372164	1.60251074	1.43089941
C	-2.11008964	-0.17306526	-1.37404359
C	-0.78302864	-1.94441926	1.43337541
H	-1.75029364	1.67234774	1.94036441
H	0.00265036	1.59809574	2.19181841
H	-0.65756864	2.49278874	0.80767141
H	-3.13593764	-0.17866926	-0.99291659
H	-1.96821064	-1.05790126	-2.00119959
H	-1.97597664	0.71652674	-1.99614559
H	-1.74894964	-2.01313626	1.94421841
H	-0.65809364	-2.83560326	0.81119441
H	0.00434036	-1.93933526	2.19325741

$Me_3SnOSnMe_3$

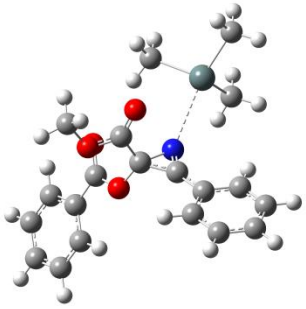
Zero-point correction = 0.218980
Thermal correction to Energy = 0.246786
Thermal correction to Enthalpy = 0.247999
Thermal correction to Gibbs Free Energy = 0.147583
E_0 = -321.342662, E = -321.314856,
H = -321.313643, G = -321.414059.
Imaginary frequency = 1.

TS1

Zero-point correction = 0.371633
Thermal correction to Energy = 0.416129
Thermal correction to Enthalpy = 0.417342
Thermal correction to Gibbs Free Energy = 0.274372
E_0 = -1134.020749, E = -1133.976253,
H = -1133.975040, G = -1134.118010.
Imaginary frequency = 1.



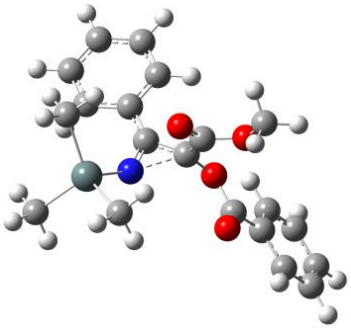
Sn	1.88256700	0.00003000	-0.02421100
C	2.27049900	1.63087500	1.32027300
C	2.37447700	-1.88565400	0.87972400
C	2.88901300	0.26268500	-1.89810500
O	-0.00014700	-0.01213000	-0.43717700
H	1.93725800	2.57568000	0.87964100
H	1.74095900	1.48557100	2.26714200
H	3.34107300	1.71144300	1.53628700
H	1.83606200	-2.01276700	1.82413100
H	3.44792700	-1.95289600	1.08562300
H	2.10018800	-2.70905900	0.21294200
H	2.56876100	1.19424600	-2.37454800
H	3.97431100	0.30073300	-1.75834000
H	2.65601400	-0.56655400	-2.57295200
Sn	-1.88274900	-0.00129900	-0.02256900
C	-2.13158600	-0.40626700	2.07402300
C	-2.62628400	1.94500300	-0.53691800
C	-2.77515700	-1.52997600	-1.23326100
H	-3.19311000	-0.42183400	2.34285800
H	-1.69922700	-1.37804800	2.33230200
H	-1.63828200	0.36292800	2.67662200
H	-2.39791900	2.17087400	-1.58307000
H	-2.16154600	2.71202500	0.09029900
H	-3.71146900	1.99981900	-0.40091100
H	-3.85694400	-1.57801800	-1.07081500
H	-2.59372400	-1.32639800	-2.29302700
H	-2.34584600	-2.50725100	-0.99217800



C	0.05587335	1.92956383	0.25414939
N	-0.10710365	0.72065383	-0.13333161
C	0.94821935	0.99542383	0.90146339
C	-0.43428565	3.27222883	0.09807339
C	0.70278035	0.53303683	2.31636339
O	2.29340135	0.99044483	0.45995539
O	-0.40554265	0.28908283	2.75265339
O	1.83163635	0.48866083	3.03647639
C	1.69195035	0.05368883	4.40731739
C	2.88722635	-0.23257117	0.30159539
C	4.27957635	-0.12251517	-0.20877361
O	2.31658335	-1.27475217	0.55544839
Sn	-2.45850265	-1.03176517	-0.10789661
C	-2.47338665	-1.08821317	-2.28029961
C	-1.27370165	-2.69822217	0.59786739
C	-4.51513165	-1.35634917	0.56170239
C	5.00232835	-1.31038317	-0.40412561
C	6.30994335	-1.26122417	-0.88513761
C	6.90321335	-0.02687917	-1.17459361
C	6.18585735	1.15855683	-0.98164861
C	4.87663035	1.11473283	-0.49996061
C	0.13909635	4.32613683	0.83483339
C	-0.35184265	5.62179583	0.68776939
C	-1.41598565	5.87298083	-0.18736061
C	-1.99034665	4.82628783	-0.92004361
C	-1.50338265	3.52816983	-0.78459161
H	1.03197735	0.73133383	4.95330439
H	2.69960835	0.07874683	4.81952839
H	1.28632935	-0.95968317	4.43850739
H	-2.82305065	-2.07029817	-2.62119061
H	-3.13925265	-0.32336917	-2.69193461
H	-1.46539865	-0.92271817	-2.67112061
H	-1.39206365	-2.81896117	1.67868639
H	-0.21540765	-2.53322717	0.38055939
H	-1.60092565	-3.62048717	0.10287839
H	-4.86709265	-2.32682317	0.18987639
H	-4.56796865	-1.35982517	1.65430939
H	-5.17898465	-0.57388517	0.18218339
H	4.52631135	-2.25821217	-0.17623061
H	6.86582235	-2.18186817	-1.03541961
H	7.92188735	0.01067783	-1.55003961
H	6.64556535	2.11615483	-1.20731961
H	4.31694735	2.03087783	-0.35128161
H	0.96156435	4.12002883	1.51326139
H	0.09076035	6.43528083	1.25439939
H	-1.79728865	6.88373683	-0.29894661
H	-2.81539665	5.02551883	-1.59718661
H	-1.93642465	2.71090183	-1.35283861

TS2

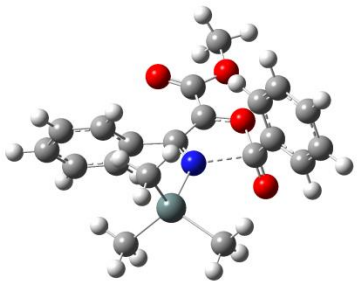
Zero-point correction = 0.370673
Thermal correction to Energy = 0.415215
Thermal correction to Enthalpy = 0.416429
Thermal correction to Gibbs Free Energy = 0.276117
E_0 = -1134.028937, E = -1133.984395,
H = -1133.983182, G = -1134.123494.
Imaginary frequency = 1.



C	-0.87674378	0.85007543	-0.37265068
N	-1.22535278	-0.31015257	-0.87148268
C	0.15761922	0.10383343	0.29864032
C	-1.39865078	2.18931143	-0.33897568
C	-0.11087178	-0.60435657	1.56602732
O	1.46190422	0.27108943	-0.12782568
O	-1.20927078	-1.00657157	1.93529732
O	1.00364722	-0.68760857	2.32509832
C	0.85726722	-1.35838057	3.59105932
C	2.25276422	-0.83453757	-0.35843168
C	3.61757922	-0.44928257	-0.80023668
O	1.85271222	-1.97166857	-0.22324268
Sn	-2.93576578	-1.53577357	-0.87998268
C	-2.21196578	-3.46412657	-0.32613668
C	-4.44792778	-0.74794657	0.42036932
C	-3.53542078	-1.50144157	-2.94276668
C	4.53283322	-1.48023557	-1.06970468
C	5.82701622	-1.17456057	-1.48797368
C	6.21626122	0.16134943	-1.64051068
C	5.30744322	1.19087043	-1.37329768
C	4.01053922	0.89067043	-0.95419268
C	-0.83757878	3.15599743	0.52681132
C	-1.33373278	4.45604243	0.54607932
C	-2.39842778	4.82089043	-0.29107768
C	-2.95736278	3.87144943	-1.15662168
C	-2.46111478	2.57020843	-1.19016068
H	0.13110622	-0.83654157	4.21881832
H	1.84705222	-1.33256657	4.04586732
H	0.53231622	-2.39017857	3.43735132
H	-2.97264378	-4.22677557	-0.52082768
H	-1.31647278	-3.70619557	-0.90518768
H	-1.95625078	-3.47707157	0.73563132
H	-4.75492378	0.25188043	0.10159932
H	-4.05927578	-0.69199557	1.43974432
H	-5.32622278	-1.40211357	0.40902032
H	-4.32041778	-2.24398257	-3.12069268
H	-3.92178578	-0.51854757	-3.22789768
H	-2.68336078	-1.73948157	-3.58617868
H	4.21472322	-2.51010557	-0.94710668
H	6.53128622	-1.97475257	-1.69519968
H	7.22486822	0.39896843	-1.96658268
H	5.60852422	2.22744743	-1.49209968
H	3.30432622	1.68629643	-0.74750468

TS3

Zero-point correction = 0.372003
Thermal correction to Energy = 0.415893
Thermal correction to Enthalpy = 0.417107
Thermal correction to Gibbs Free Energy = 0.279431
E_0 = -1134.060870, E = -1134.016979,
H = -1134.015766, G = -1134.153441.
Imaginary frequency = 1.

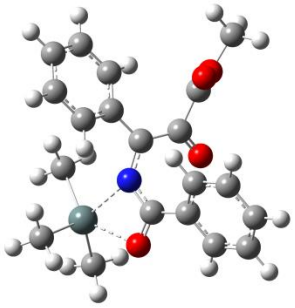


C	-0.65833706	0.63559916	-0.16277009
N	0.49203494	0.05264016	-0.30890709
C	-0.59401006	2.06887816	-0.36789009
C	-1.93719006	-0.07647884	0.15305491
C	-1.67750306	3.04259916	-0.15290309
O	0.59137794	2.55119016	-0.72194009
O	-2.76109406	2.76526316	0.34423091
O	-1.33067406	4.28148016	-0.55323009
C	-2.33012506	5.30331316	-0.36675909
C	1.64142394	1.58060416	-1.14157709
C	2.81067094	1.65470616	-0.20459909
O	1.71943394	1.34060216	-2.33064509
Sn	1.01002194	-1.96940484	-0.31228509
C	2.79734994	-2.05595184	-1.47799309
C	1.37904694	-2.47705784	1.73716791
C	-0.54622206	-3.13792784	-1.20799809
C	4.08433194	1.39070016	-0.72569809
C	5.20968594	1.45576116	0.09968591
C	5.06915694	1.78543616	1.45104991
C	3.79855694	2.05419516	1.97367491
C	2.67392094	1.99074016	1.14995891
C	-2.11669406	-0.66655384	1.41185591
C	-3.28512106	-1.37896584	1.69587291
C	-4.27697206	-1.51581984	0.72060491
C	-4.09963706	-0.93065084	-0.53788209
C	-2.93797606	-0.21045784	-0.82012009
H	-3.23061906	5.06349716	-0.93733909
H	-1.87358506	6.22036816	-0.73700509
H	-2.58527706	5.39853216	0.69140491
H	2.65639894	-1.53874684	-2.43049609
H	3.63129994	-1.58745984	-0.94963409
H	3.05480394	-3.10063384	-1.68000709
H	1.85466994	-3.46100584	1.79984291
H	0.44781294	-2.50693584	2.30897491
H	2.04825094	-1.74136884	2.19273891
H	-0.22226306	-4.18208784	-1.26956509
H	-1.46841206	-3.08952284	-0.62486909
H	-0.75352006	-2.78147484	-2.22092909
H	4.17909294	1.14329916	-1.77763609
H	6.19390494	1.25420216	-0.31339609
H	5.94375694	1.83854116	2.09324791
H	3.68518494	2.31748716	3.02139391
H	1.69247394	2.20526616	1.55888191

H	-0.02288978	2.87084543	1.18666532	H	-1.35217406	-0.55136084	2.17497691
H	-0.89636378	5.18857543	1.21855432	H	-3.42051306	-1.82220984	2.67830291
H	-2.78442778	5.83571743	-0.27190768	H	-5.18445306	-2.07076084	0.94028291
H	-3.77564278	4.15206343	-1.81393668	H	-4.86747806	-1.03279084	-1.29930709
H	-2.87399878	1.84641743	-1.88670468	H	-2.80633706	0.24811116	-1.79602509

TS4

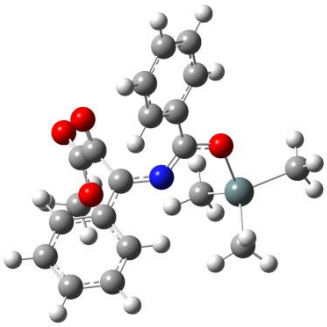
Zero-point correction = 0.373100
Thermal correction to Energy = 0.416737
Thermal correction to Enthalpy = 0.417951
Thermal correction to Gibbs Free Energy = 0.282153
E_0 = -1134.095603, E = -1134.051965,
H = -1134.050752, G = -1134.186550.
Imaginary frequency = 1.



C	-0.85824015	-0.35261390	-0.06873741
N	0.37716585	0.21654610	0.12054359
C	-1.74698615	0.22422710	-1.06715141
C	-1.14502715	-1.59905090	0.64054259
C	-3.24040615	-0.11344090	-1.03143741
O	-1.38209315	1.08568410	-1.88274641
O	-3.93285415	0.06356010	-0.04691141
O	-3.69356015	-0.51897790	-2.22313341
C	-5.12175115	-0.72014090	-2.33074541
C	0.68286685	1.52695610	0.13244559
C	-0.20931415	2.63777710	0.54034859
O	1.90749385	1.76686710	-0.13524941
Sn	2.58255985	-0.38105490	-0.45004641
C	3.51143785	-0.60314890	1.46309459
C	1.88034585	-2.25733290	-1.24863741
C	3.87297885	0.41135510	-1.97323441
C	0.11584785	3.94018710	0.12526559
C	-0.68009115	5.01800110	0.51038159
C	-1.79527015	4.80850410	1.32952459
C	-2.11273915	3.51680210	1.76044859
C	-1.32670415	2.43323210	1.36615259
C	-0.58884015	-1.81327090	1.92201059
C	-0.84046115	-2.99041190	2.62261859
C	-1.64175015	-3.98952590	2.05708259
C	-2.18490715	-3.80109690	0.78088259
C	-1.93880215	-2.62359290	0.07799859
H	-5.45453215	-1.46919390	-1.60865941
H	-5.28667415	-1.06421690	-3.35060541
H	-5.64553315	0.22112010	-2.15070441
H	4.42986985	-1.19127290	1.36592659
H	3.76790085	0.37617010	1.87581459
H	2.84645085	-1.11841390	2.16141059
H	2.74333885	-2.84246890	-1.58522541
H	1.22789485	-2.08680790	-2.11067641
H	1.32923985	-2.83551790	-0.50321141
H	4.58080785	-0.35553190	-2.30540241
H	3.28555685	0.73295910	-2.83889141
H	4.42786685	1.27433610	-1.59559341

TS5

Zero-point correction = 0.371936
Thermal correction to Energy = 0.416083
Thermal correction to Enthalpy = 0.417297
Thermal correction to Gibbs Free Energy = 0.278070
E_0 = -1134.,082016, E = -1134.037868,
H = -1134.036655, G = -1134.175882.
Imaginary frequency = 1.



C	2.17039476	-0.30677964	0.14738550
N	0.81012676	-0.32854664	-0.08301450
C	2.61878976	0.18996536	1.49810450
C	3.08797076	-0.97398164	-0.72748450
C	2.66594576	-0.82203264	2.68789450
O	2.91272976	1.34071136	1.74656350
O	2.86205676	-0.47933564	3.83316350
O	2.47939276	-2.08242664	2.28141850
C	2.55360776	-3.10158264	3.30537450
C	-0.04129924	0.65476636	-0.00891950
C	0.24943276	2.11669036	-0.03134950
O	-1.33190924	0.36255836	0.01954950
Sn	-1.93558024	-1.57876764	-0.02630150
C	-1.38738724	-2.43942964	-1.90367150
C	-1.21638524	-2.56972064	1.72283550
C	-4.03626724	-1.19675564	0.08193550
C	-0.66058724	3.01171136	0.55652250
C	-0.42716924	4.38663436	0.50898450
C	0.69996276	4.88382236	-0.15298250
C	1.59679476	3.99900036	-0.76090150
C	1.37889876	2.62322936	-0.69438450
C	2.64182076	-1.56167864	-1.94278150
C	3.53705776	-2.19043364	-2.80120050
C	4.90334276	-2.25579264	-2.48891250
C	5.36285276	-1.67476664	-1.29785150
C	4.47770776	-1.04216164	-0.43152250
H	3.53237176	-3.07326264	3.78906250
H	2.40618576	-4.04580964	2.78381650
H	1.77111976	-2.94101164	4.05007350
H	-2.16715424	-3.13141764	-2.23703450
H	-1.27877124	-1.65406064	-2.65746950
H	-0.44258824	-2.98148464	-1.82328250
H	-1.39109724	-1.94579964	2.60457450
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H	-1.74931324	-3.51609764	1.86056650
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H	-0.41514815 -3.12906490 3.61240659	H	1.58697576 -1.51263164 -2.18934850
H	-1.83506615 -4.90869290 2.60220759	H	3.17123676 -2.63347064 -3.72379450
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		H	4.86417276 -0.58287064 0.47440450

TS6

Zero-point correction = 0.482463
Thermal correction to Energy = 0.539774
Thermal correction to Enthalpy = 0.540987
Thermal correction to Gibbs Free Energy = 0.375593
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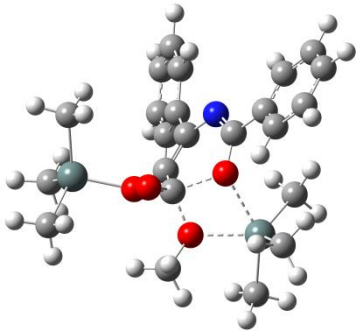
Imaginary frequency = 1.



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O	0.07184354 -1.31835384 1.85291786	O	2.93010847 1.12655501 -0.00190207
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TS7

Zero-point correction = 0.402359
Thermal correction to Energy = 0.452231
Thermal correction to Enthalpy = 0.453444
Thermal correction to Gibbs Free Energy = 0.302671
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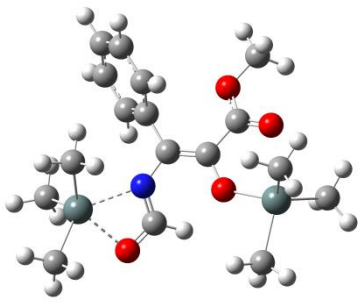
Imaginary frequency = 1.



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TS8

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Thermal correction to Energy = 0.452069
Thermal correction to Enthalpy = 0.453282
Thermal correction to Gibbs Free Energy = 0.301268
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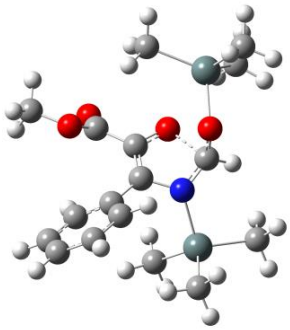

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O	0.12905938	2.83226870	-0.47499767
O	0.70817538	1.97150070	-2.48483567
C	0.29499138	4.15822870	-1.01271567
Sn	3.09487638	-0.95854930	0.47577733
C	3.33603238	1.15882070	0.34689233
C	4.12345638	-1.66116830	2.22699433
C	3.62227538	-2.15197630	-1.21616767
C	-2.39384062	0.80443470	2.05553933

TS9

Zero-point correction = 0.403258
Thermal correction to Energy = 0.452555
Thermal correction to Enthalpy = 0.453768
Thermal correction to Gibbs Free Energy = 0.304469
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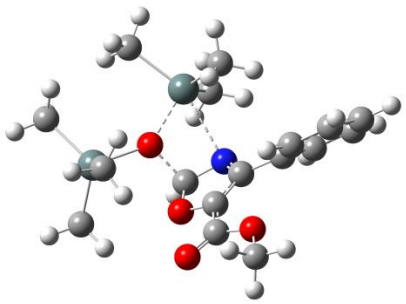
Imaginary frequency = 1.



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O	-0.34477199	1.40447516	-1.22387928
C	-2.08447999	2.73373416	-0.25086428
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C	-3.90612999	4.04212416	0.51655672
Sn	2.40906501	0.95106316	0.16256672
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C	4.11702101	-0.11802284	0.88202972
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C	-3.42472262	1.55782170	2.61998433	C	-5.25705299	-0.62627984	1.32487172
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H	0.37680338	-2.75534730	-0.21353167	H	0.48473901	-0.03930484	-2.42110028

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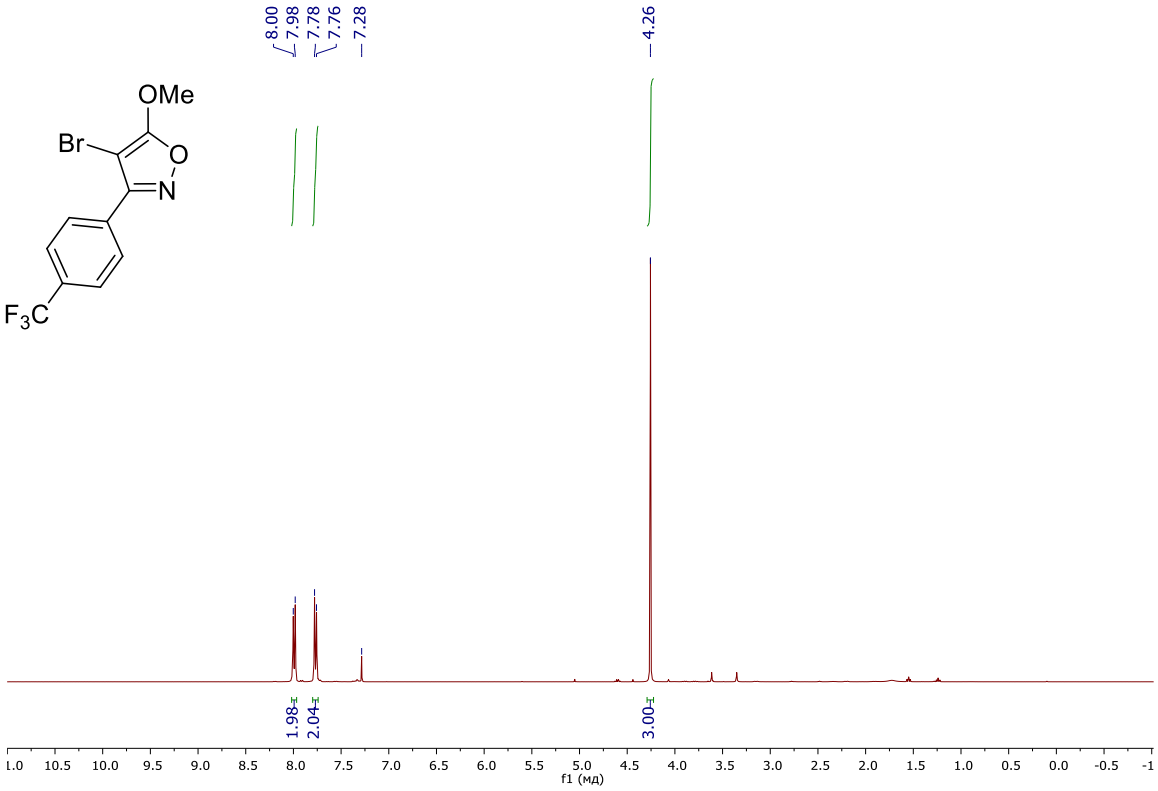
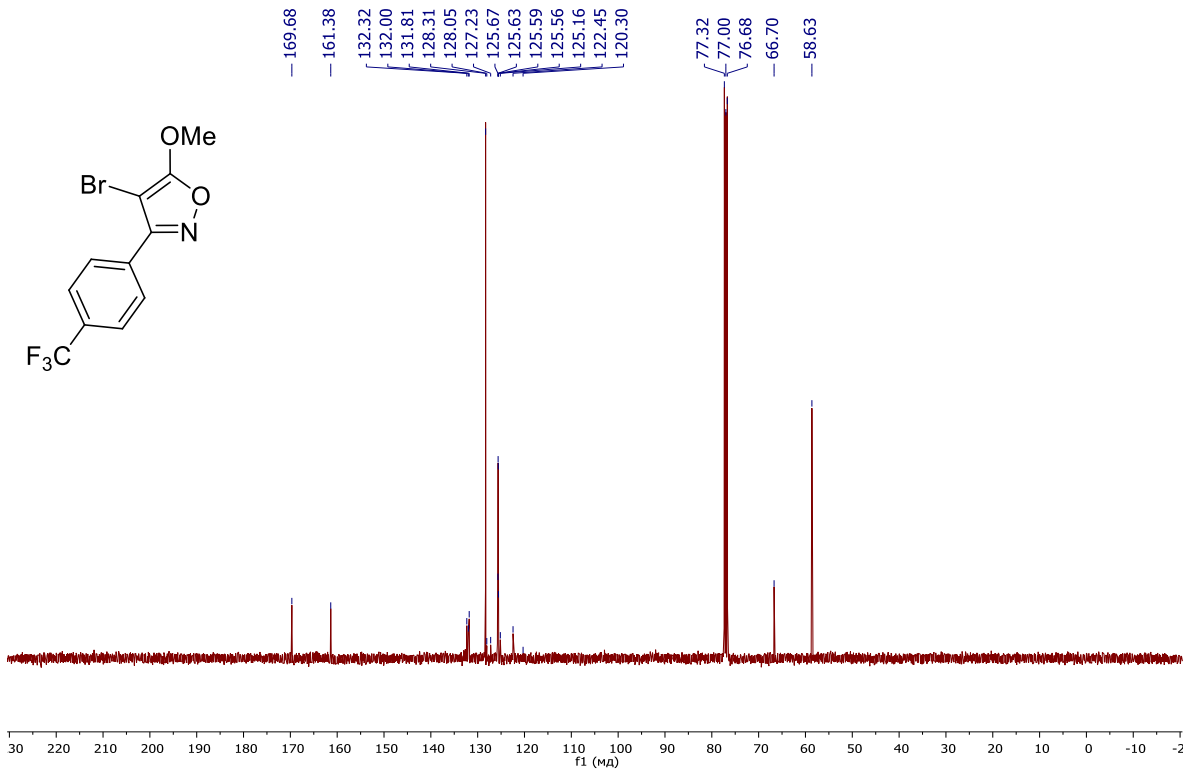
13. NMR spectra of new compounds

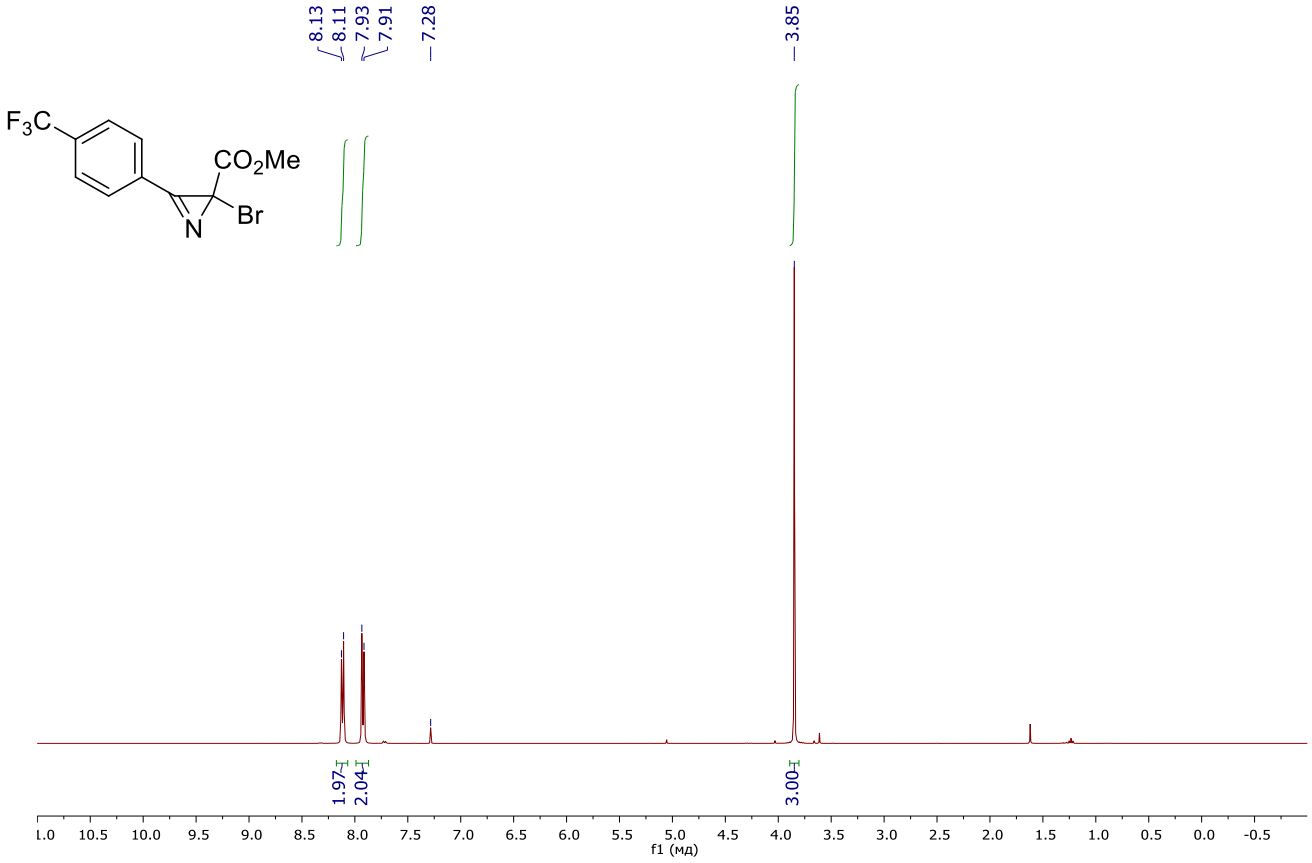
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of 4-bromo-5-methoxy-3-(4-(trifluoromethyl)phenyl)-isoxazole



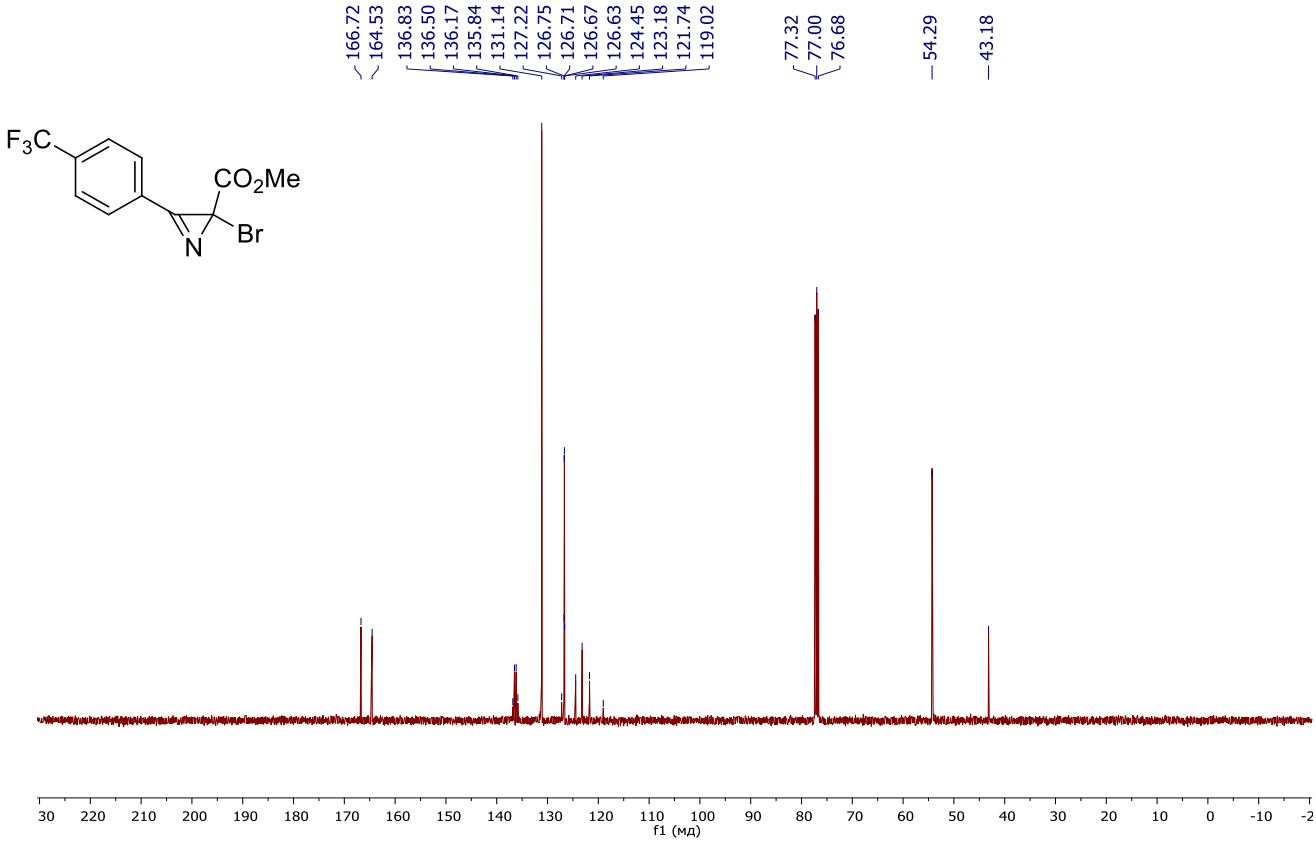
^{13}C NMR (100 MHz, $CDCl_3$) spectrum of 4-bromo-5-methoxy-3-(4-(trifluoromethyl)phenyl)-isoxazole



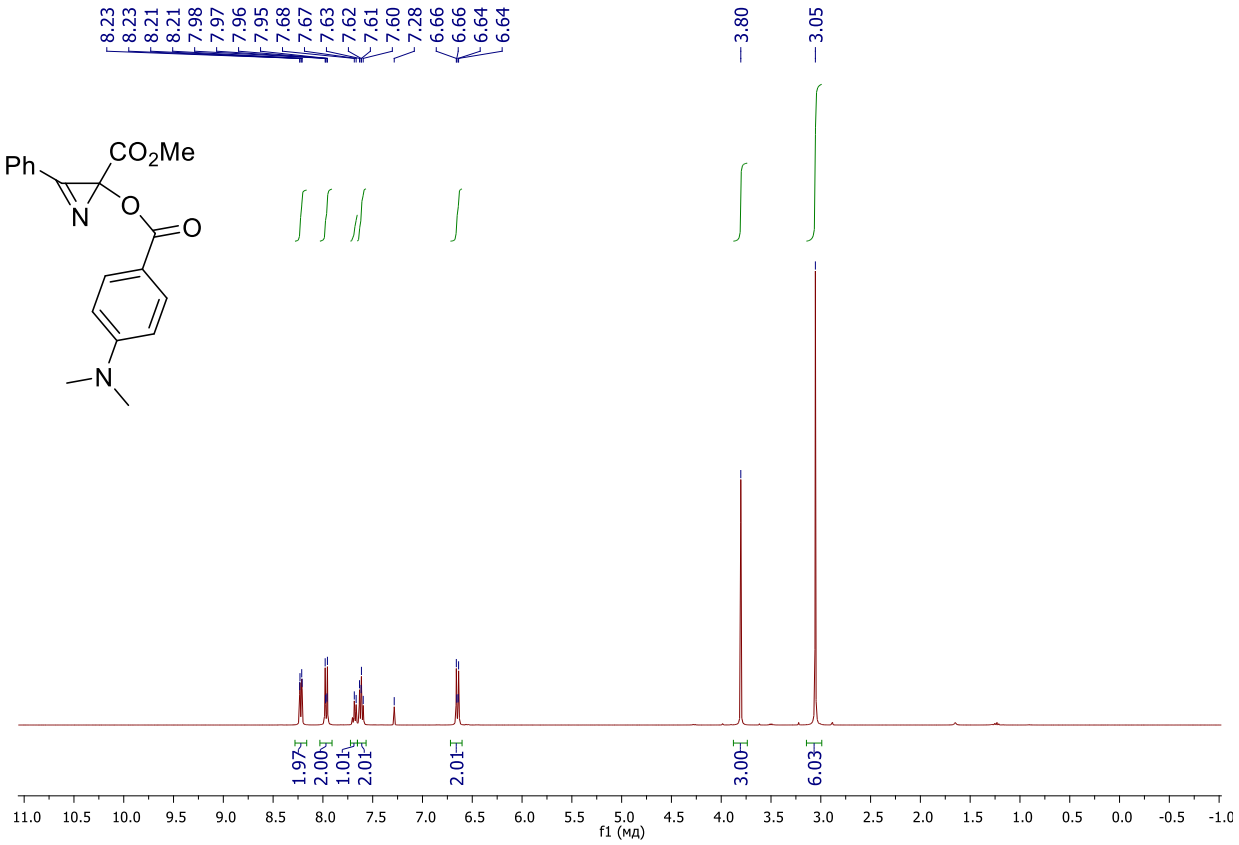
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of **28g**



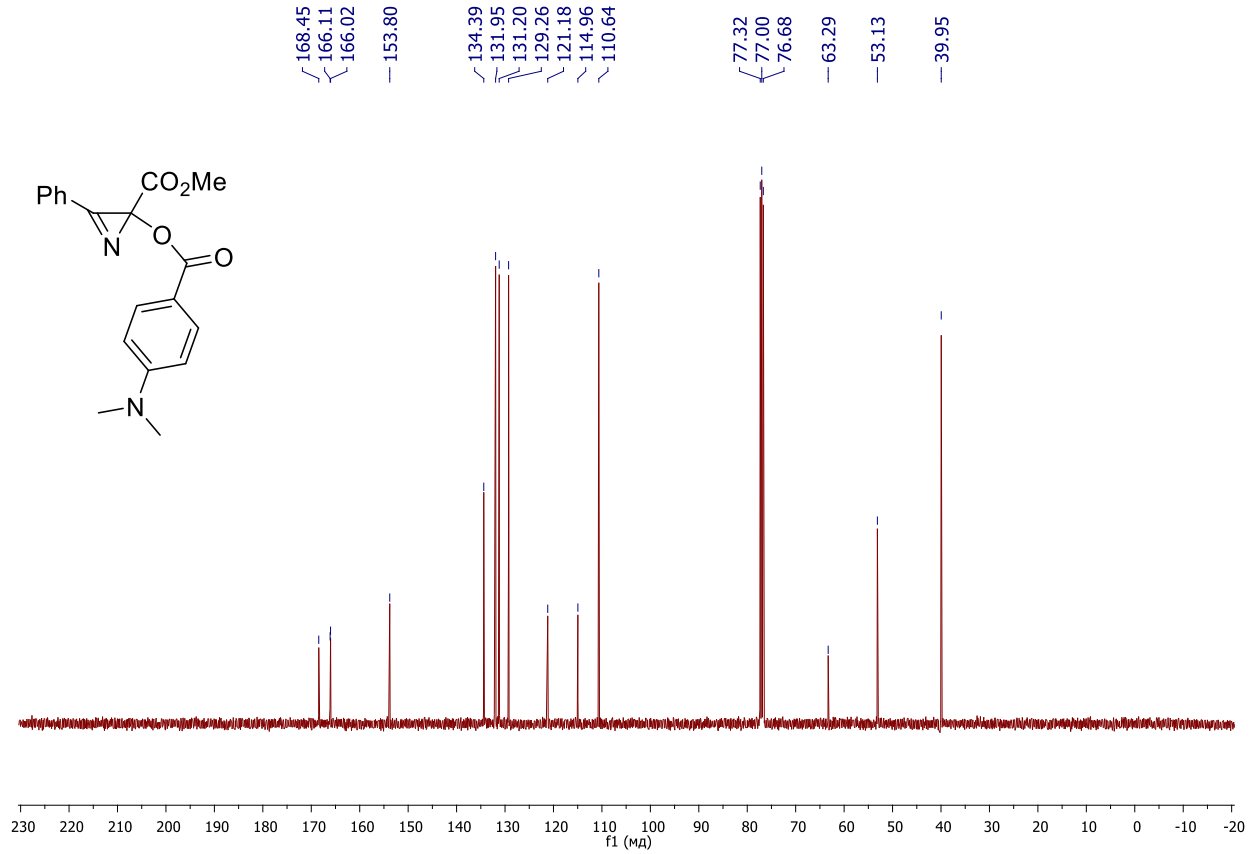
^{13}C NMR (100 MHz, $CDCl_3$) spectrum of **28g**



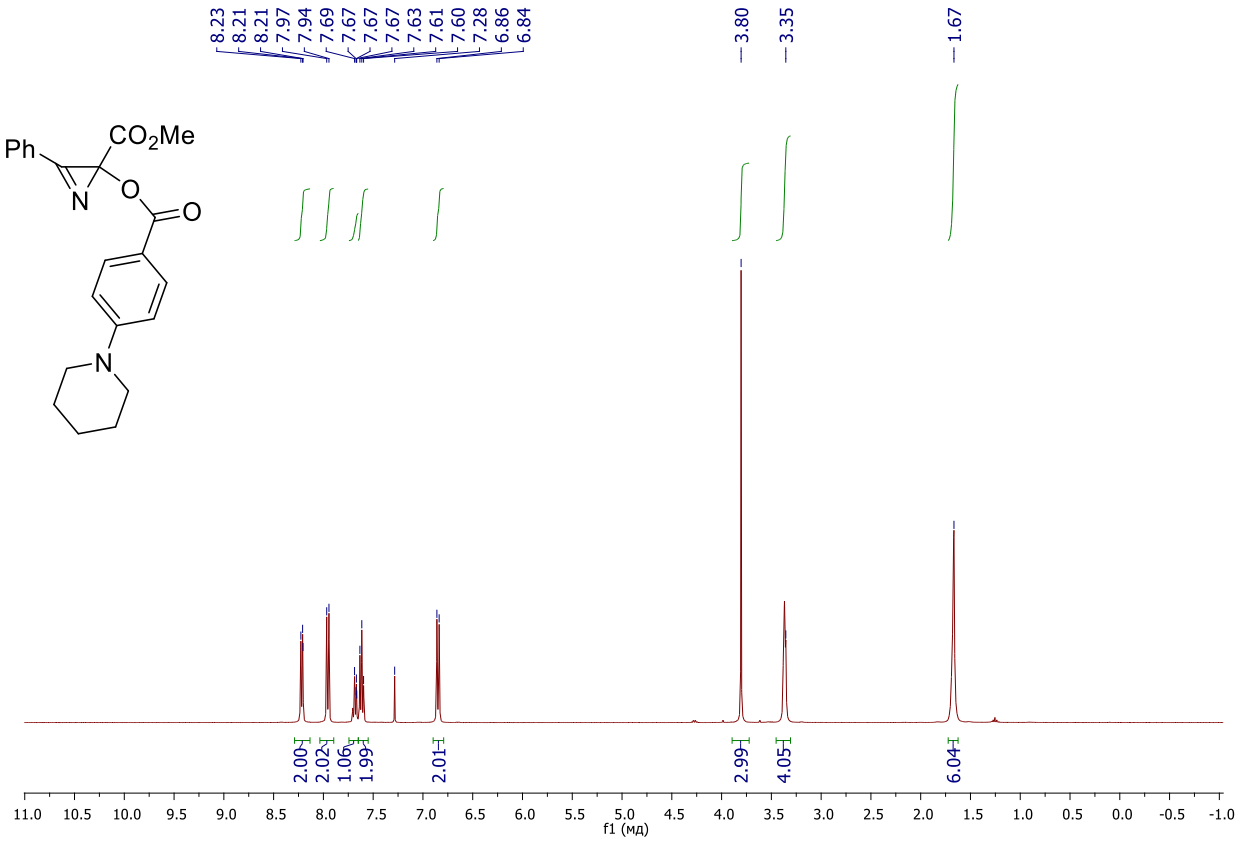
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of **3c**



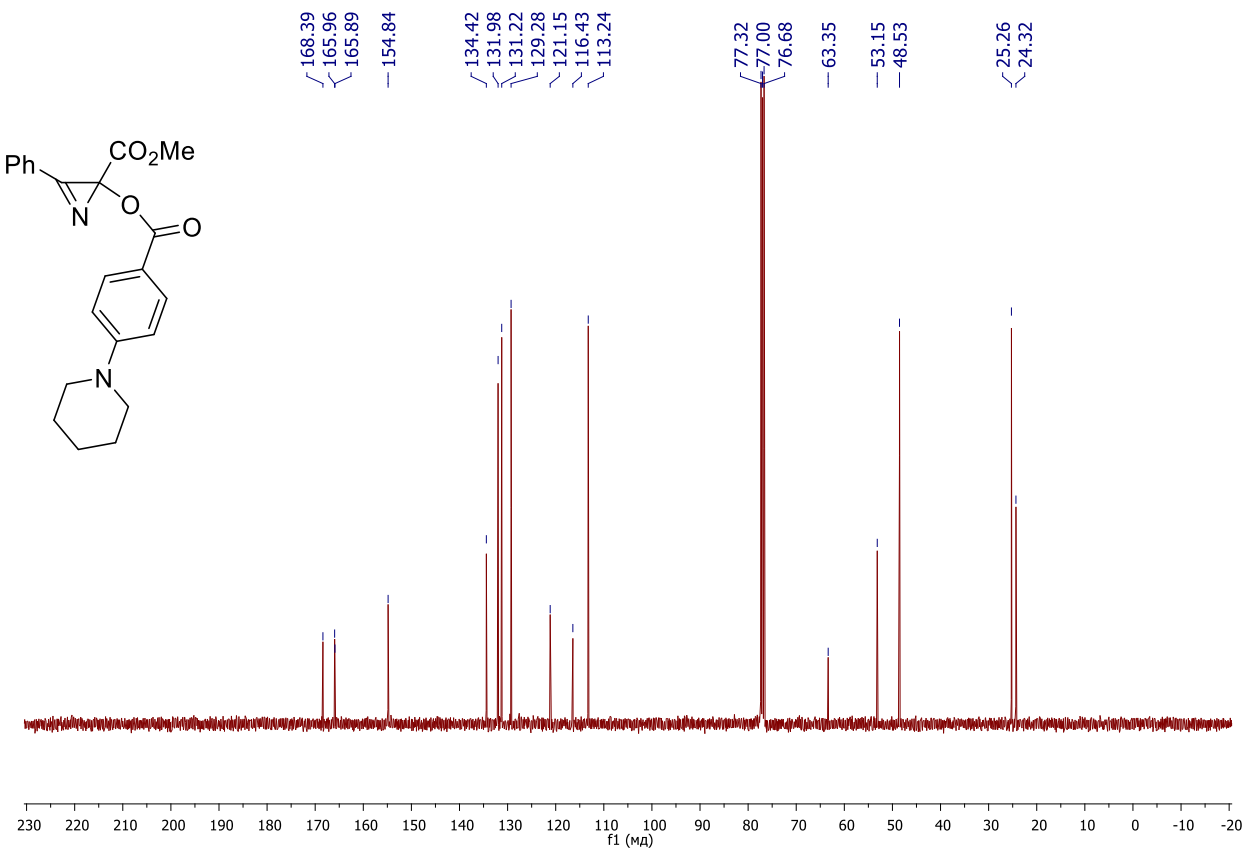
^{13}C NMR (100 MHz, $CDCl_3$) spectrum of **3c**



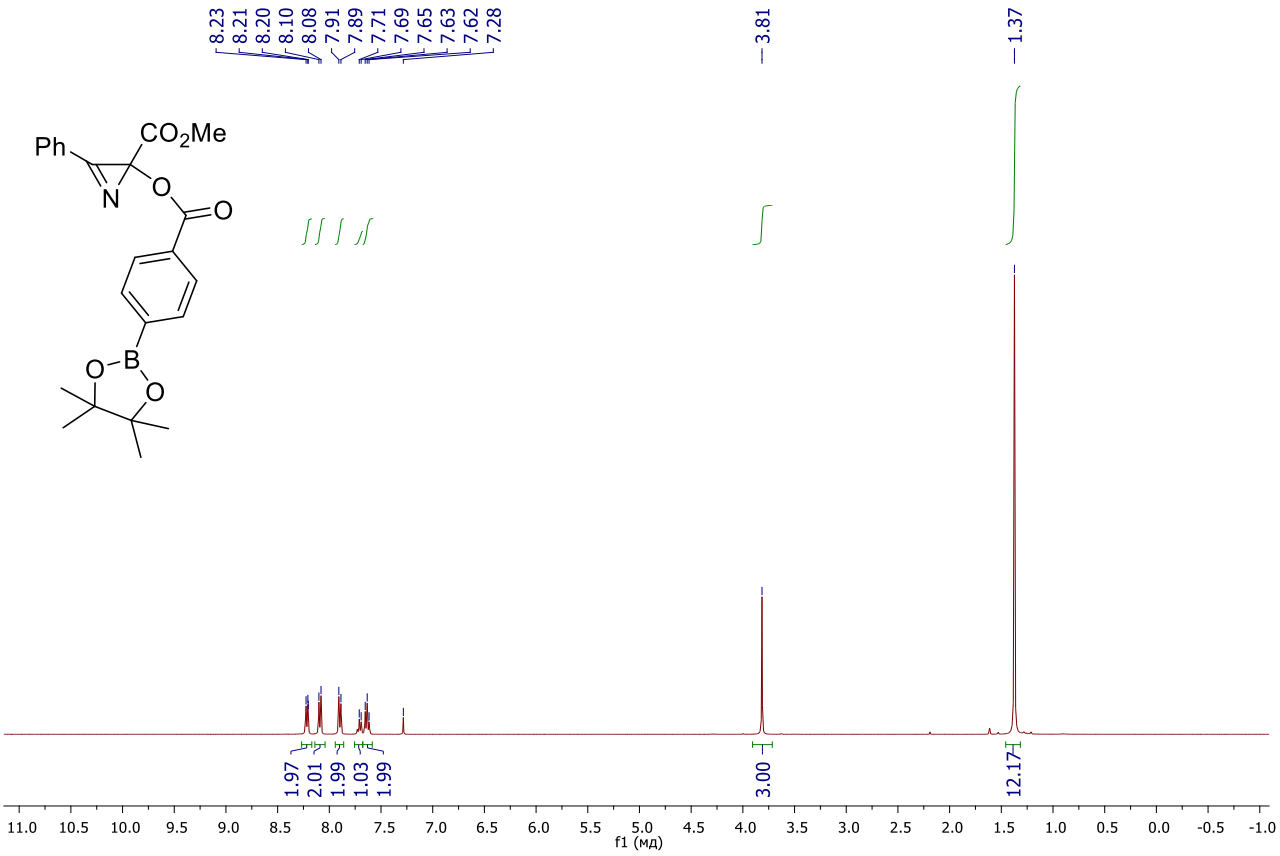
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of **3d**



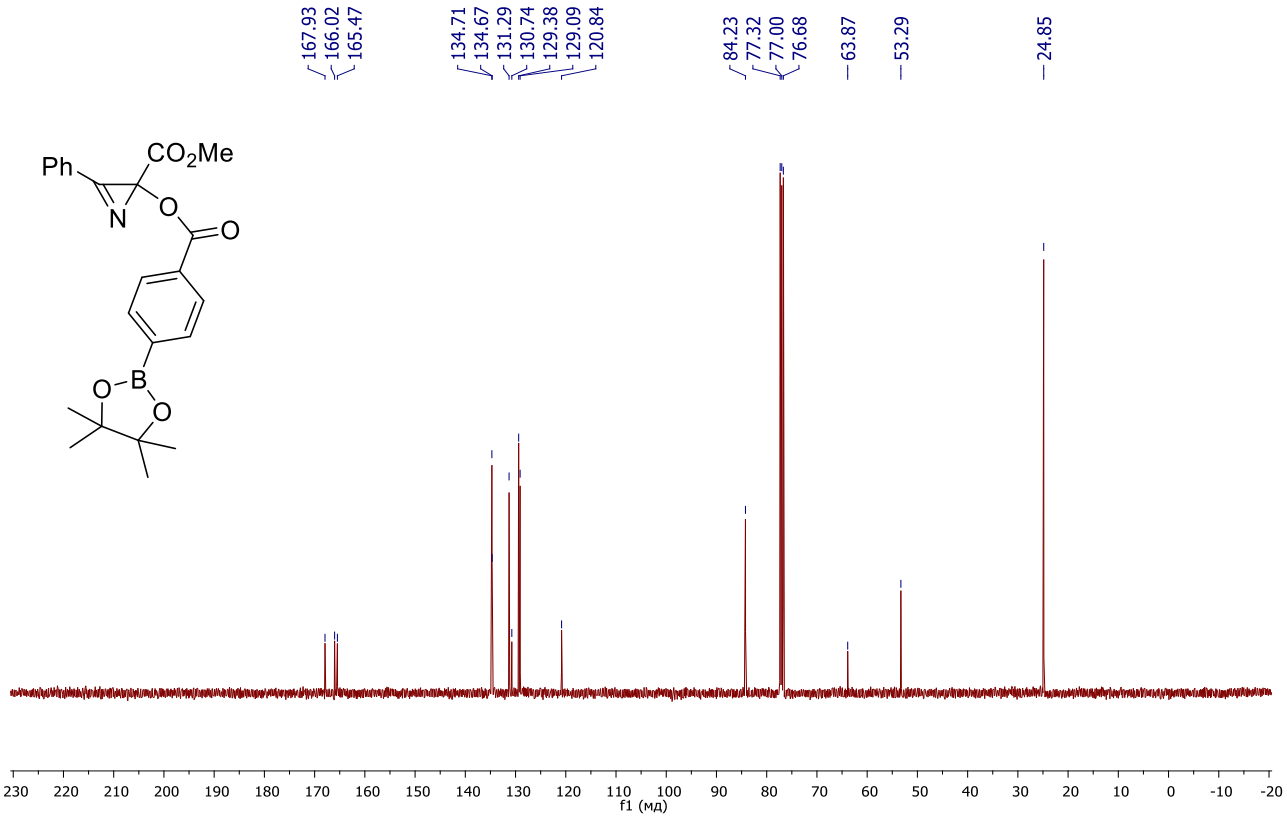
^{13}C NMR (100 MHz, $CDCl_3$) spectrum of **3d**



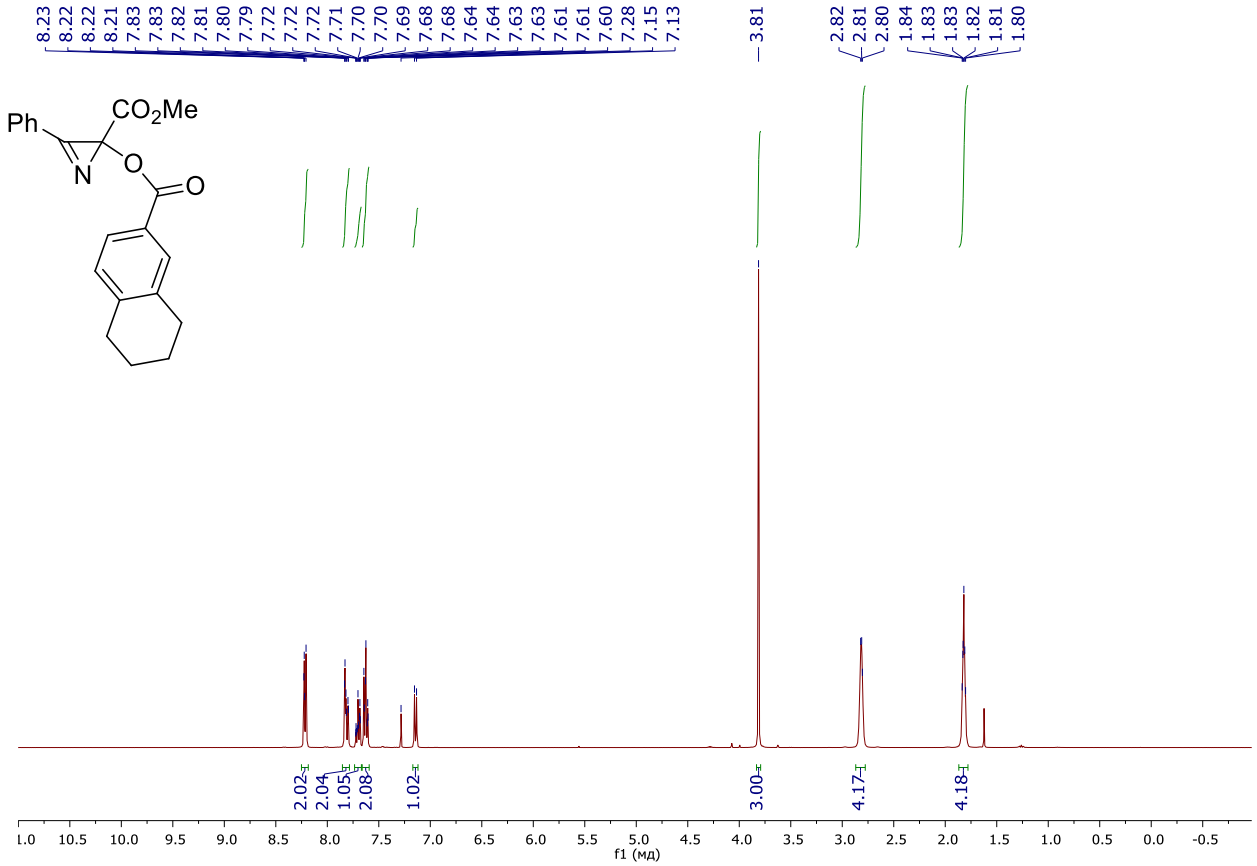
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of **3e**



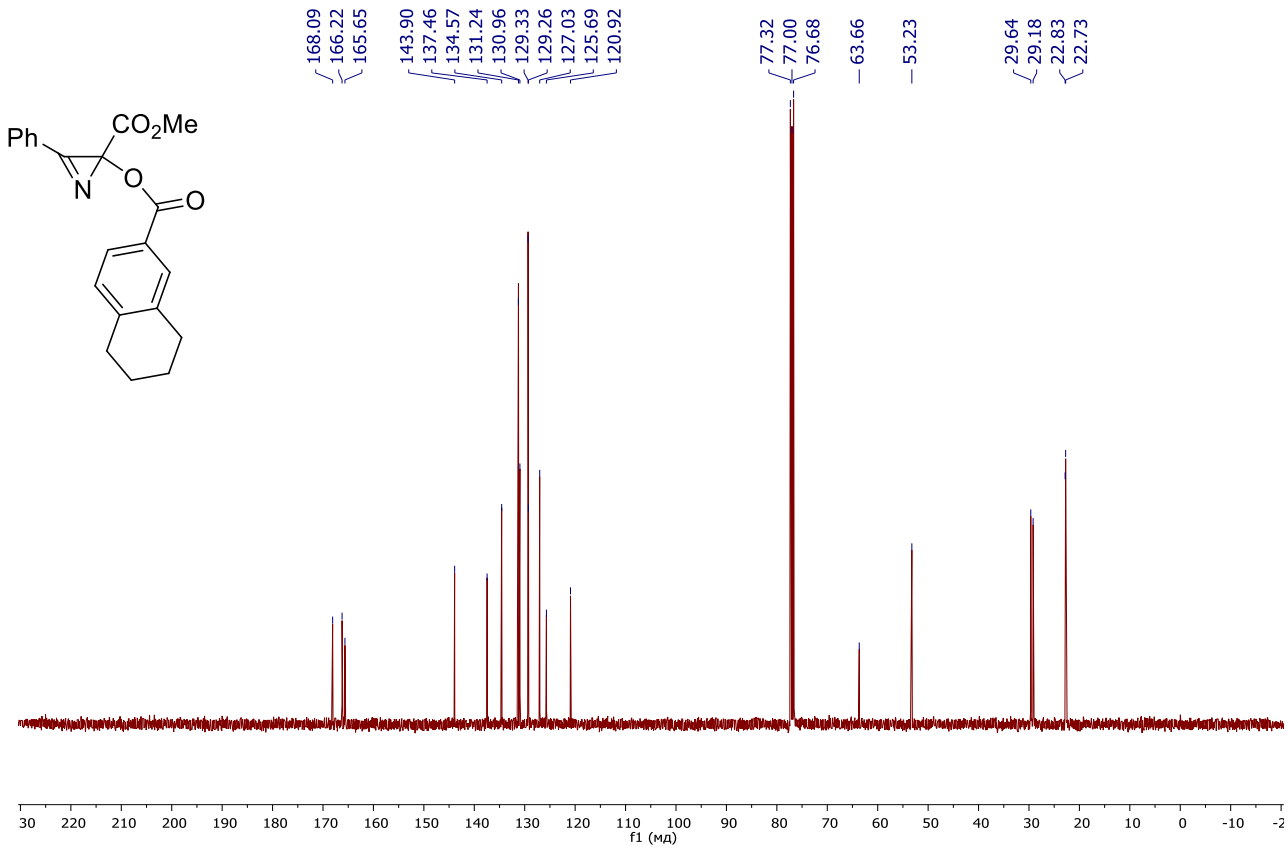
^{13}C NMR (100 MHz, $CDCl_3$) spectrum of **3e**



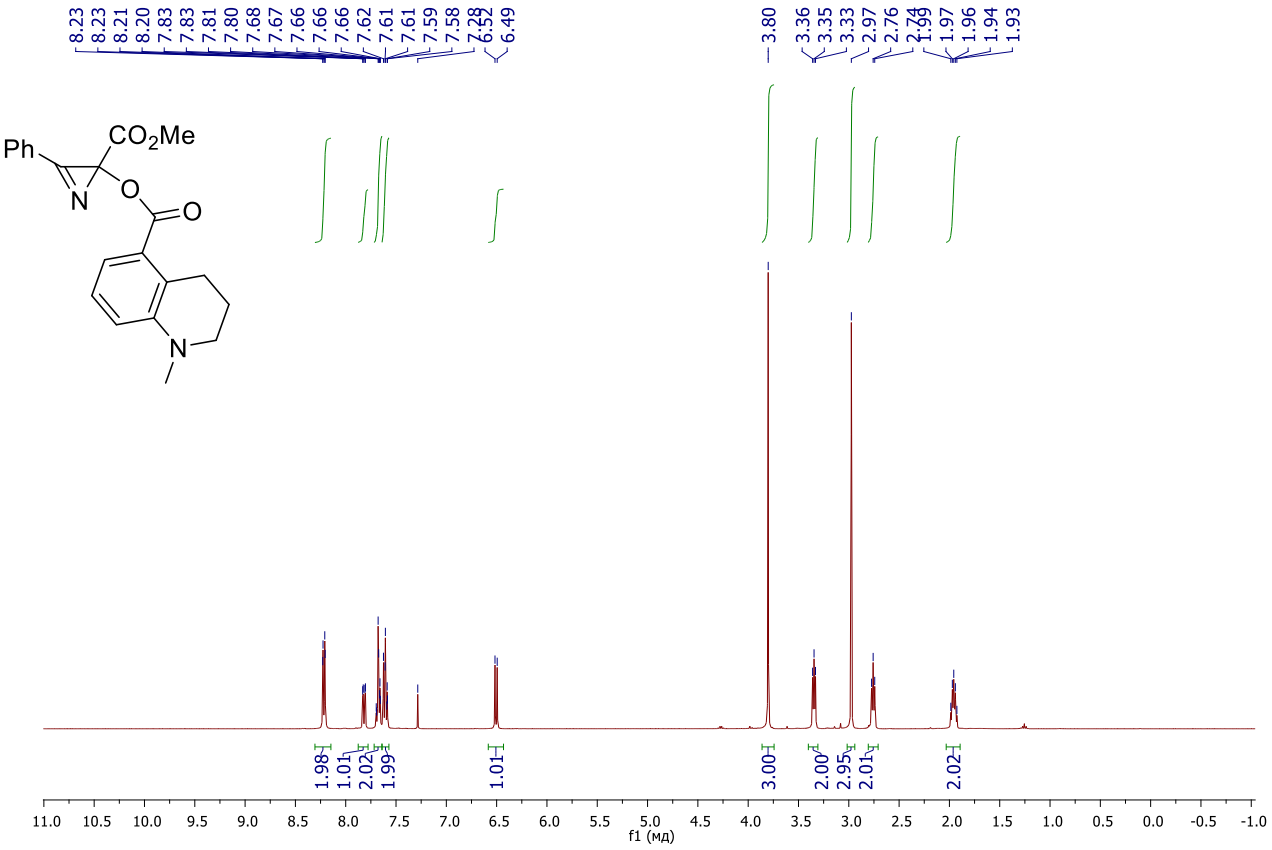
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of **3f**



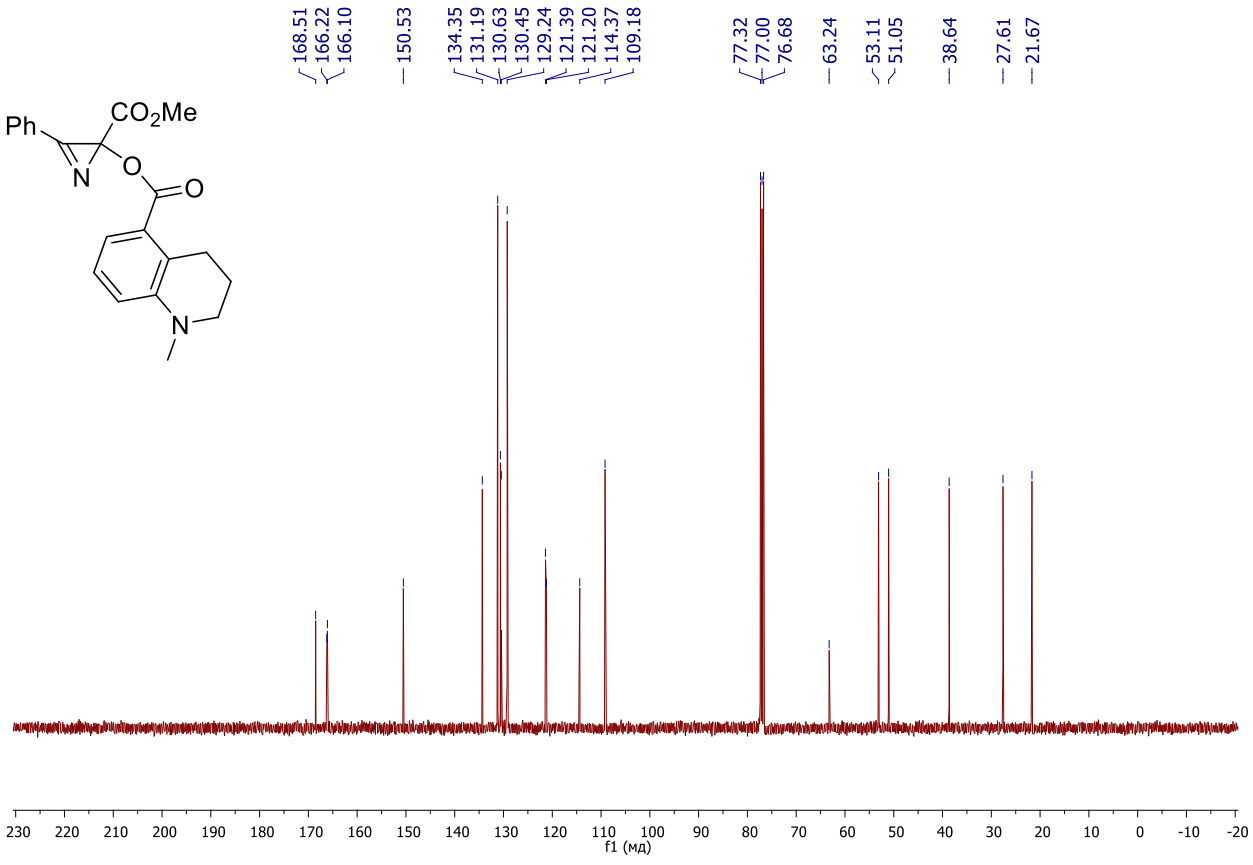
^{13}C NMR (100 MHz, $CDCl_3$) spectrum of **3f**



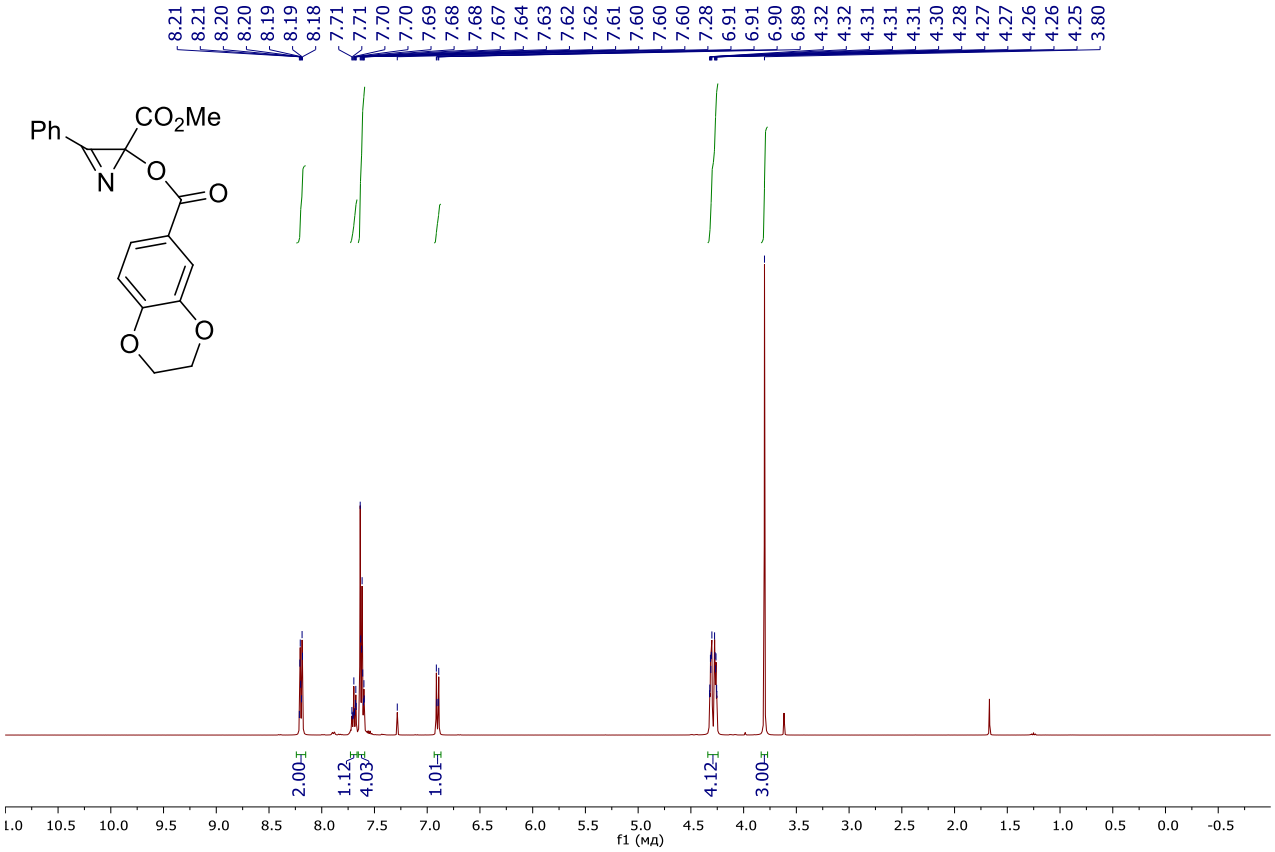
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of **3g**



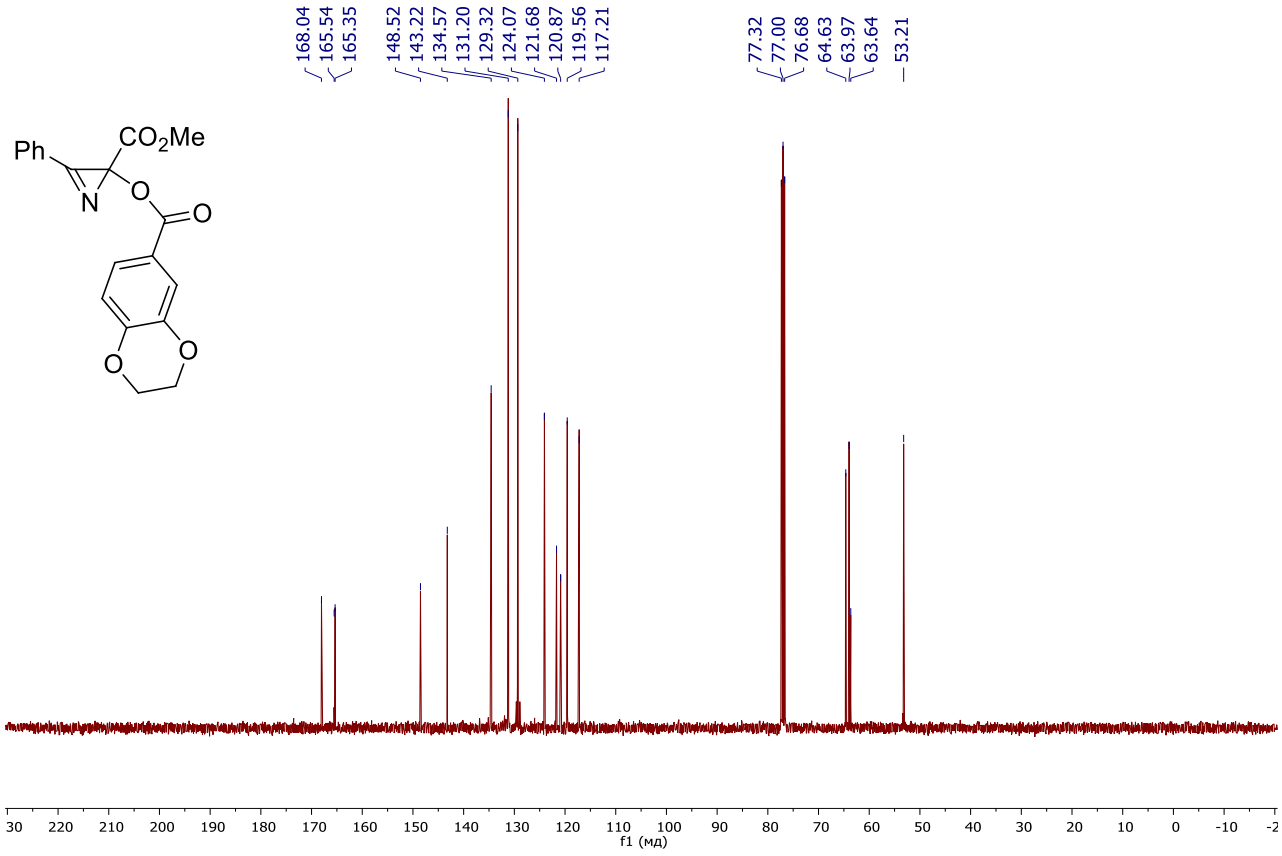
^{13}C NMR (100 MHz, $CDCl_3$) spectrum of **3g**



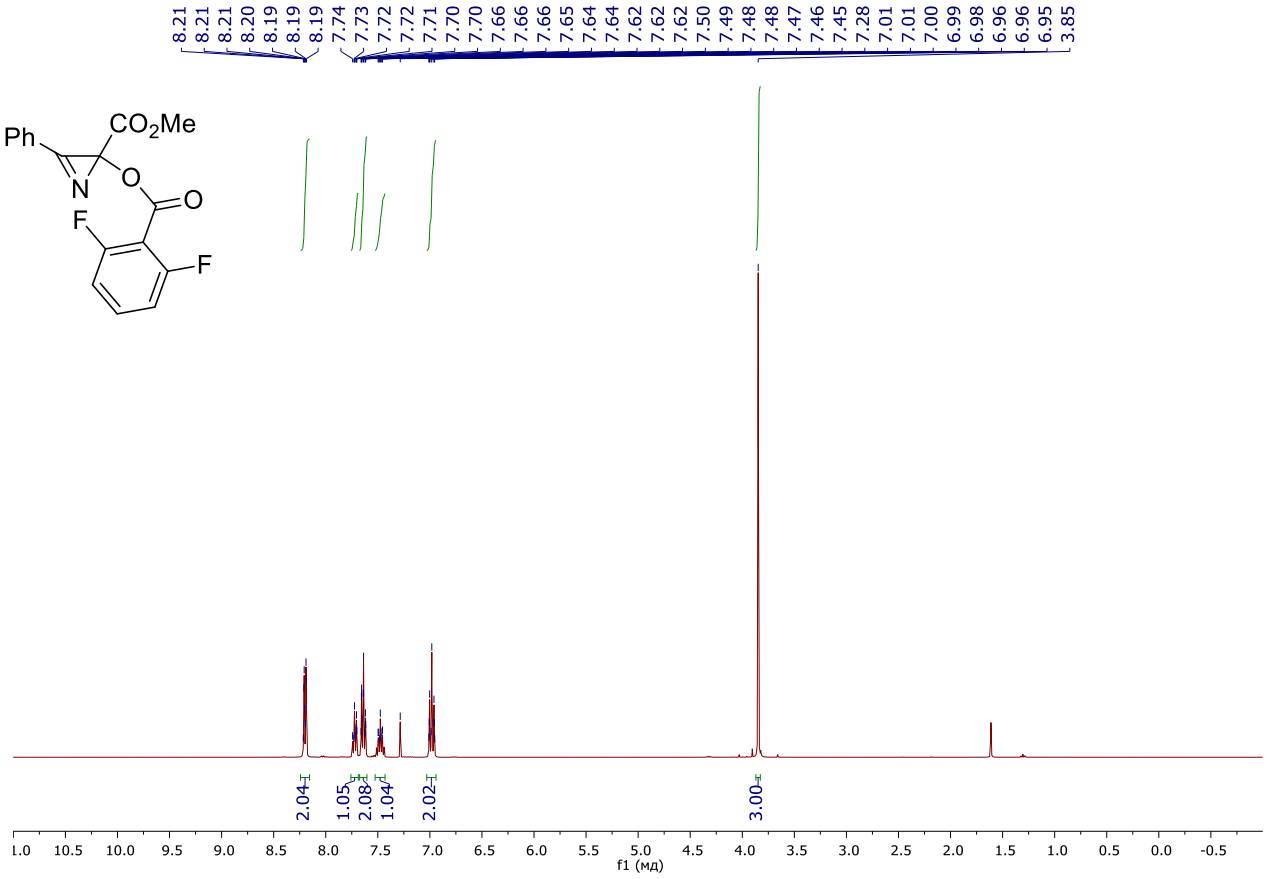
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of **3h**



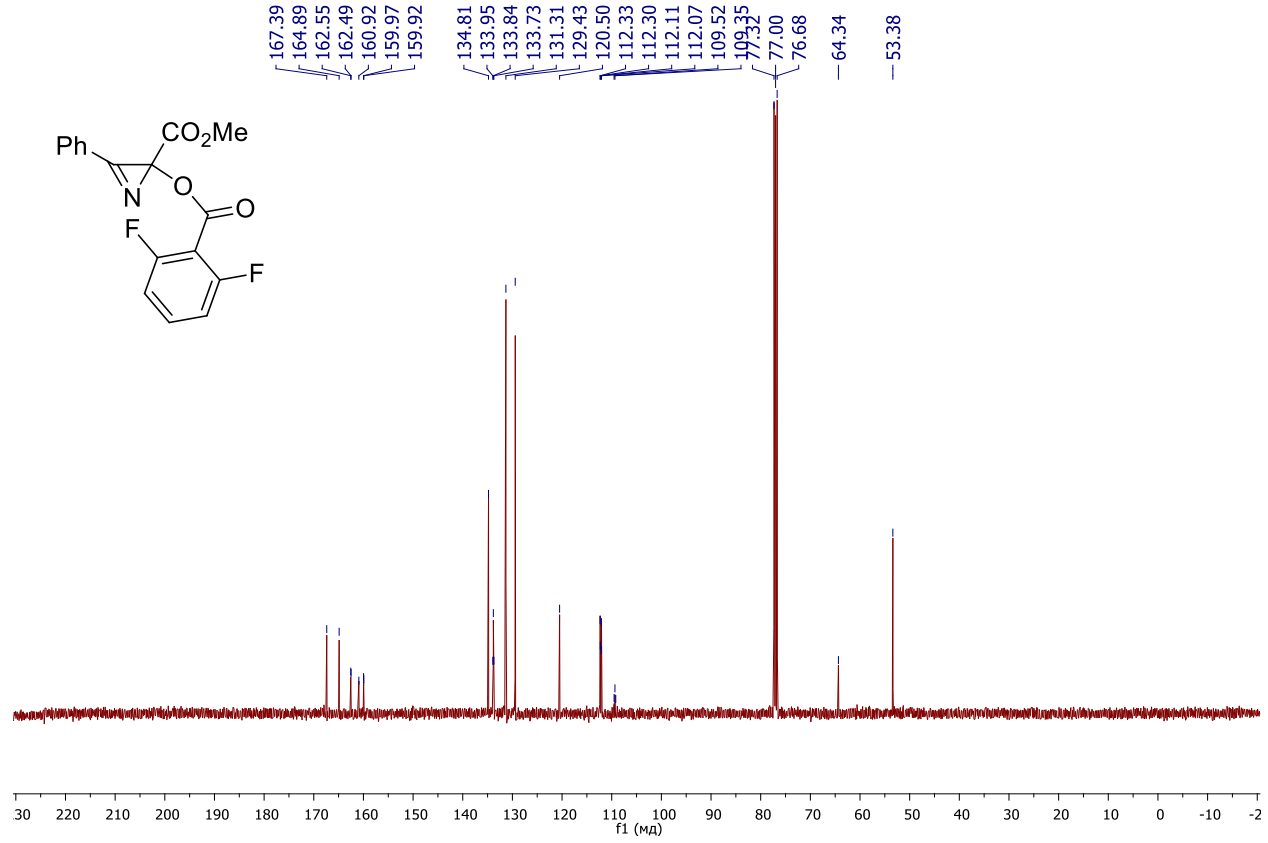
^{13}C NMR (100 MHz, $CDCl_3$) spectrum of **3h**



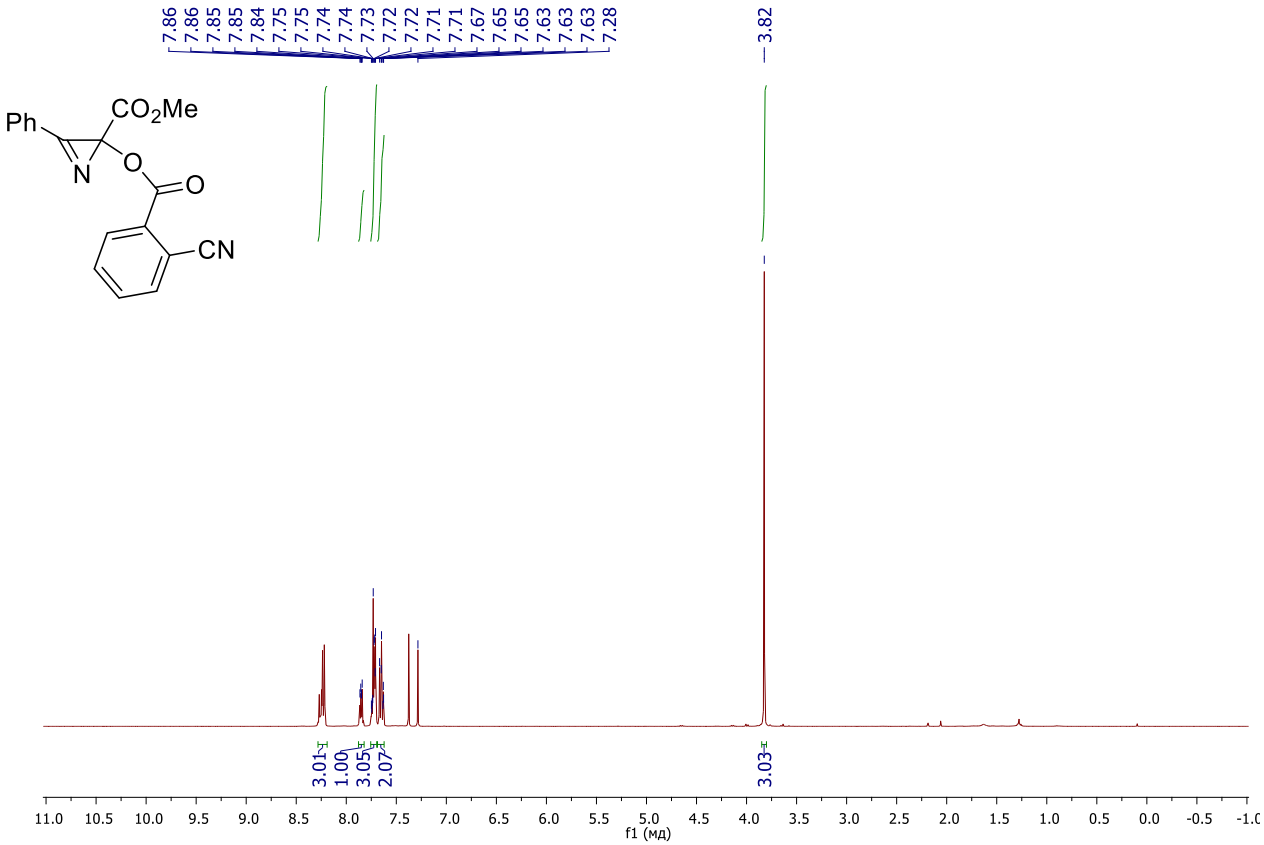
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of **3k**



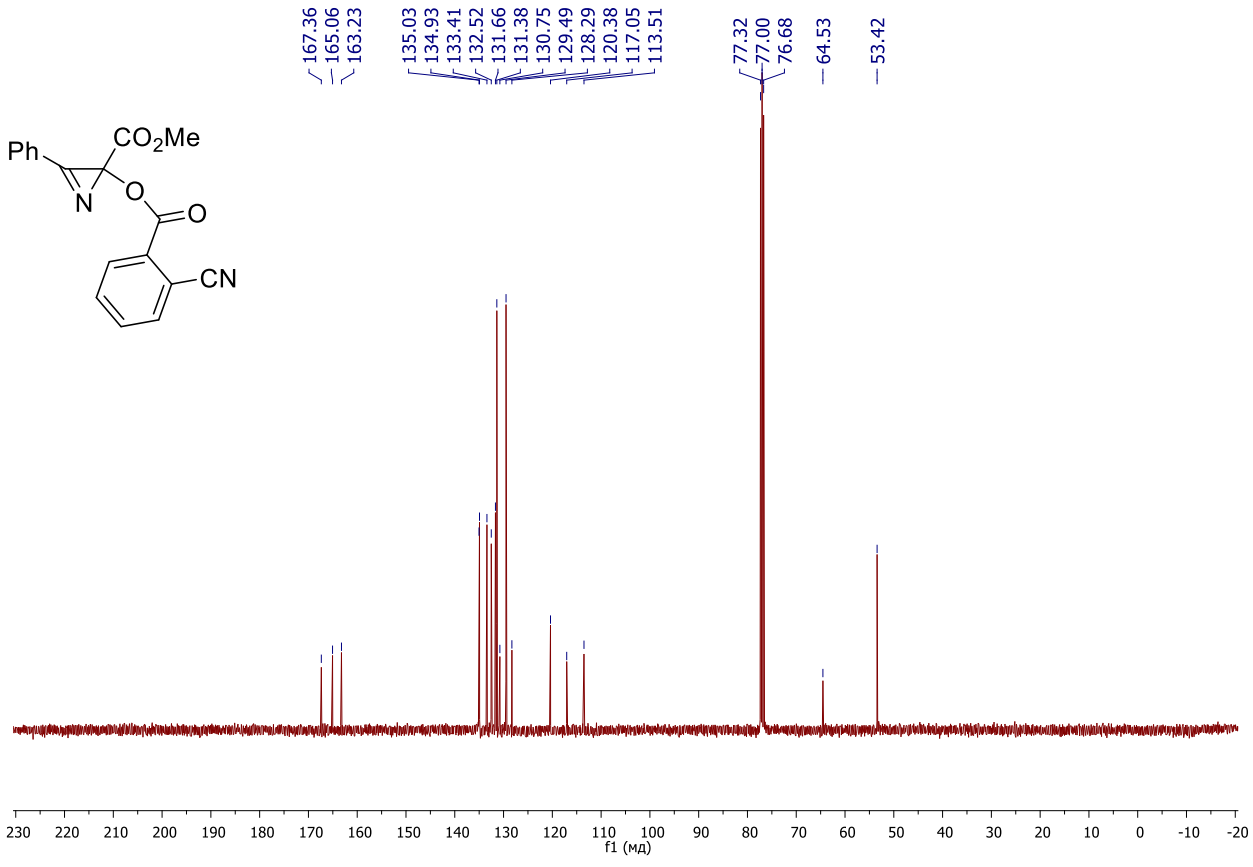
^{13}C NMR (100 MHz, $CDCl_3$) spectrum of **3k**



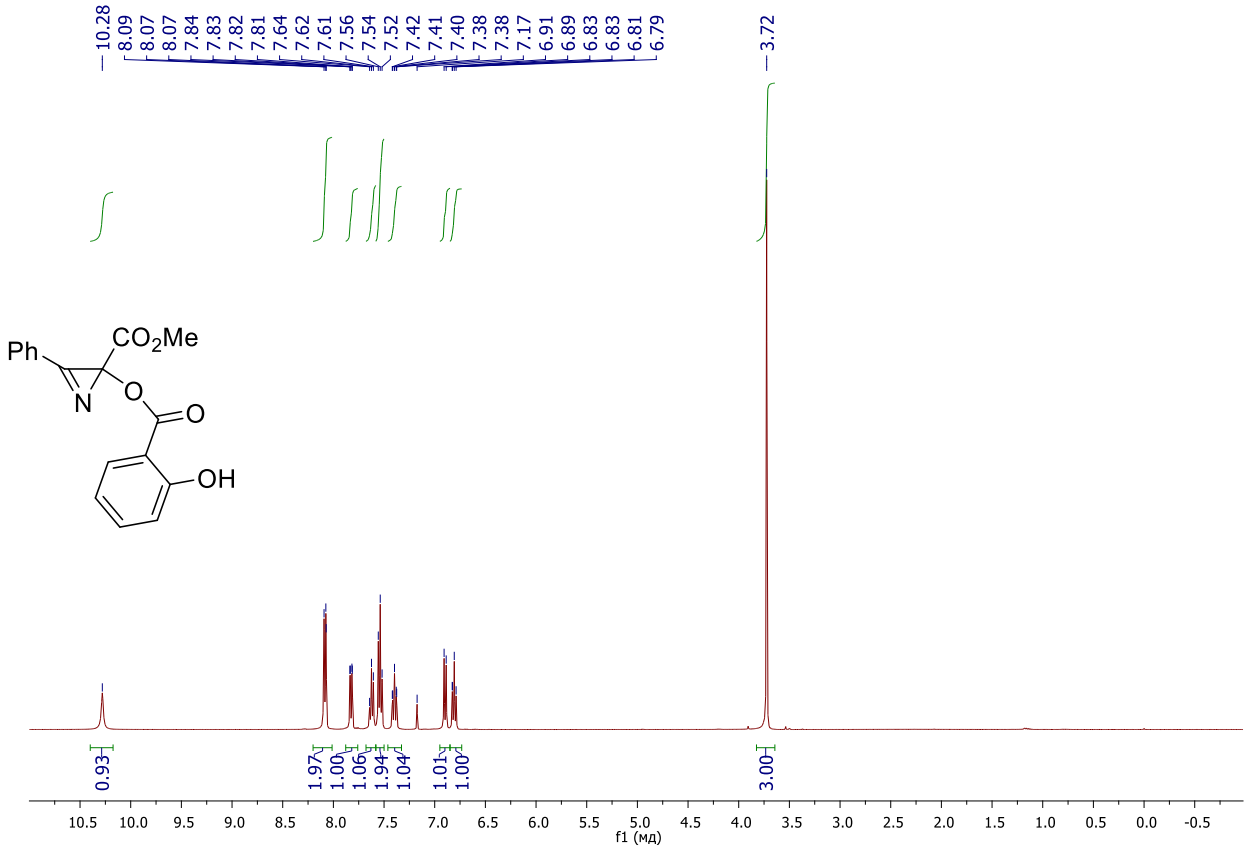
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of **3l**



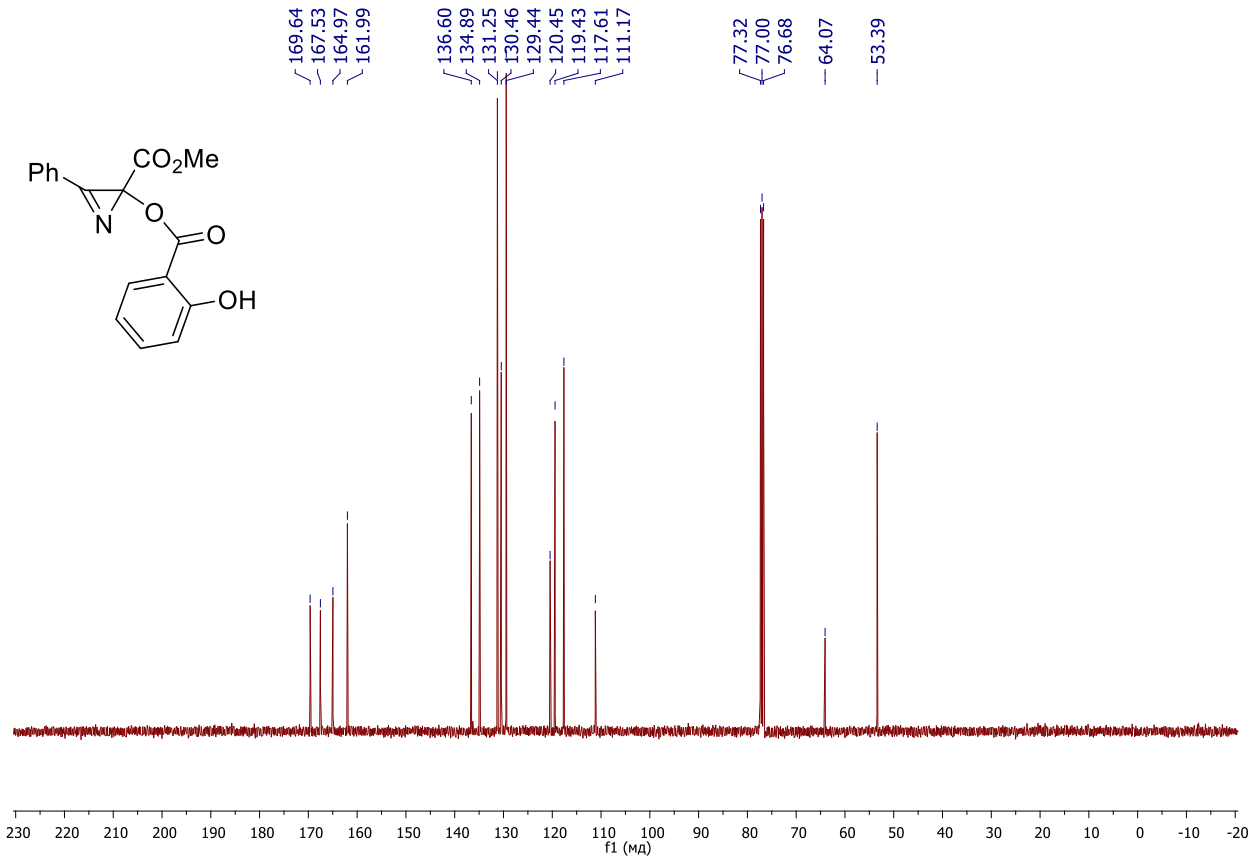
^{13}C NMR (100 MHz, $CDCl_3$) spectrum of **3l**



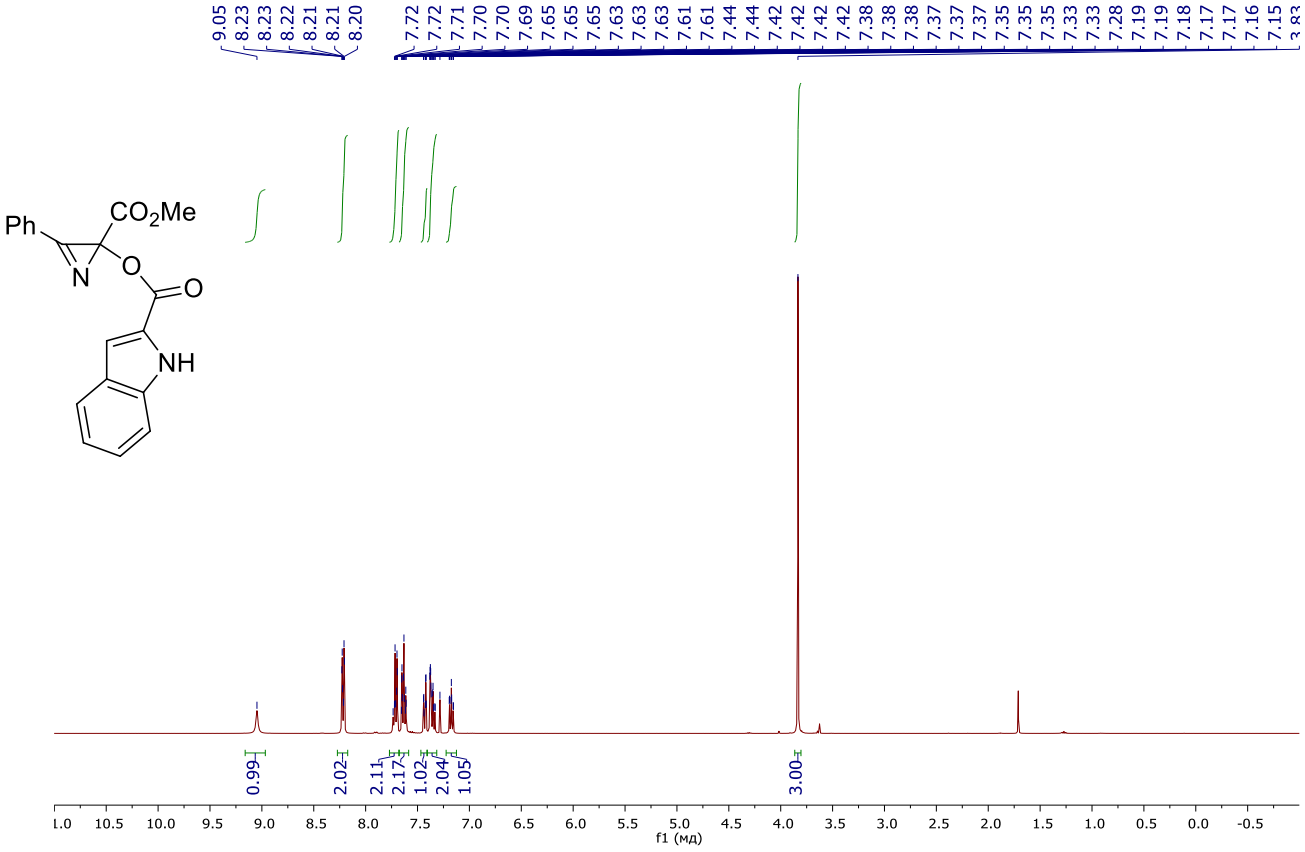
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of **3m**



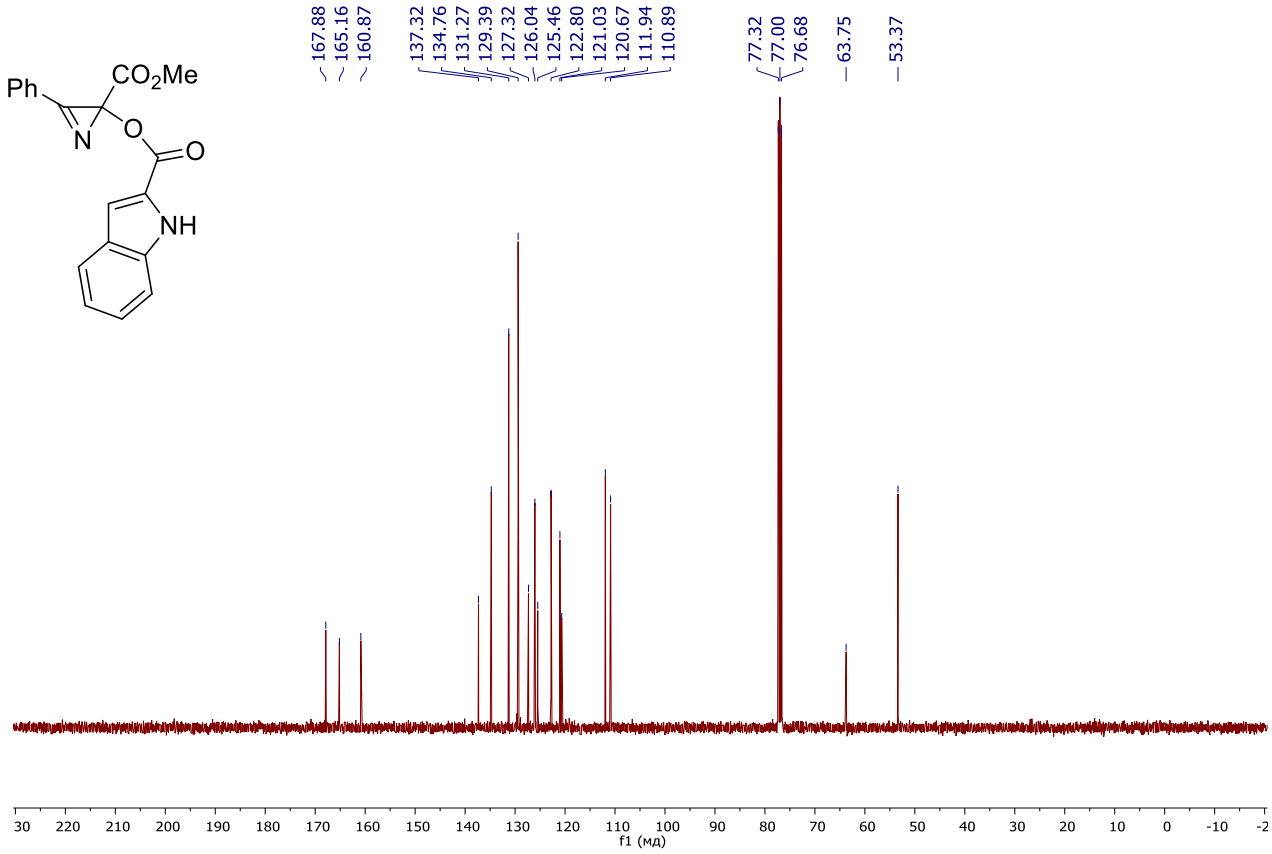
^{13}C NMR (100 MHz, $CDCl_3$) spectrum of **3m**



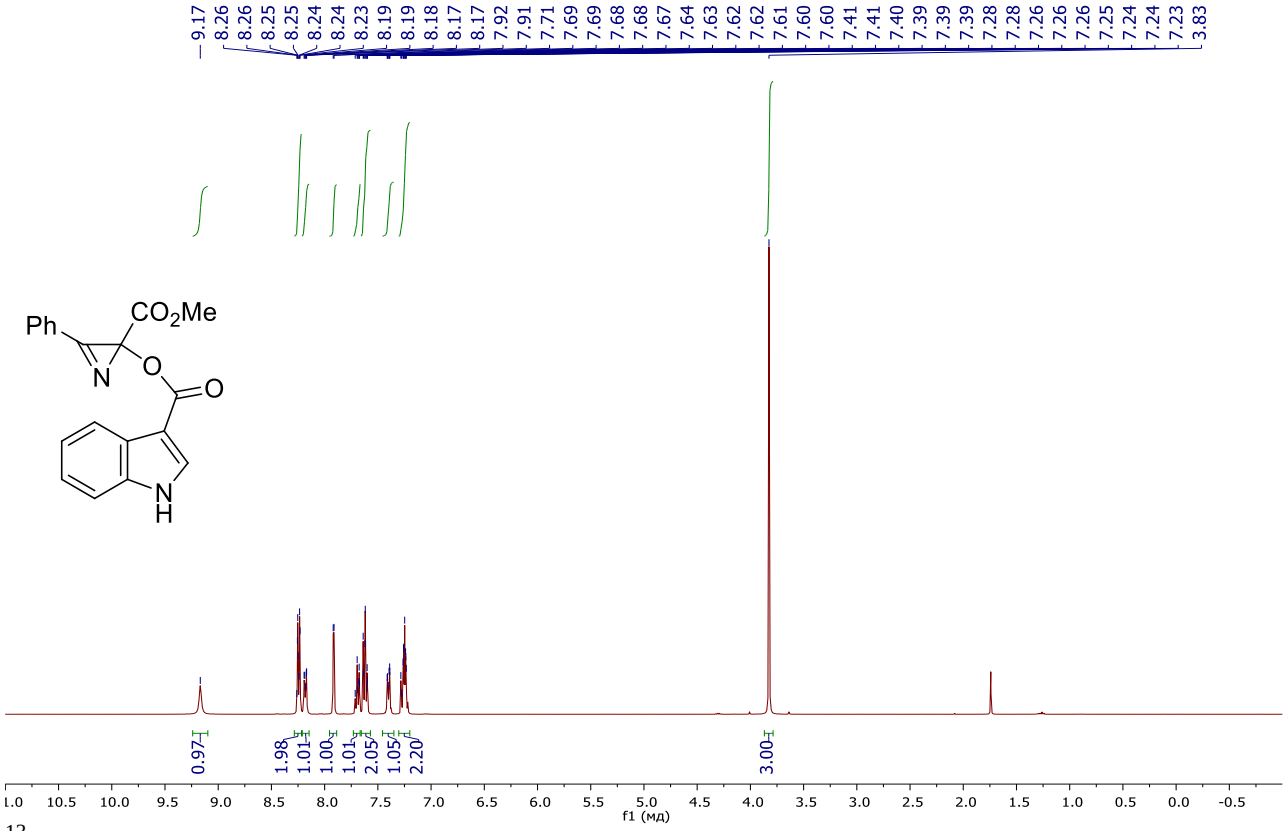
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of **3r**



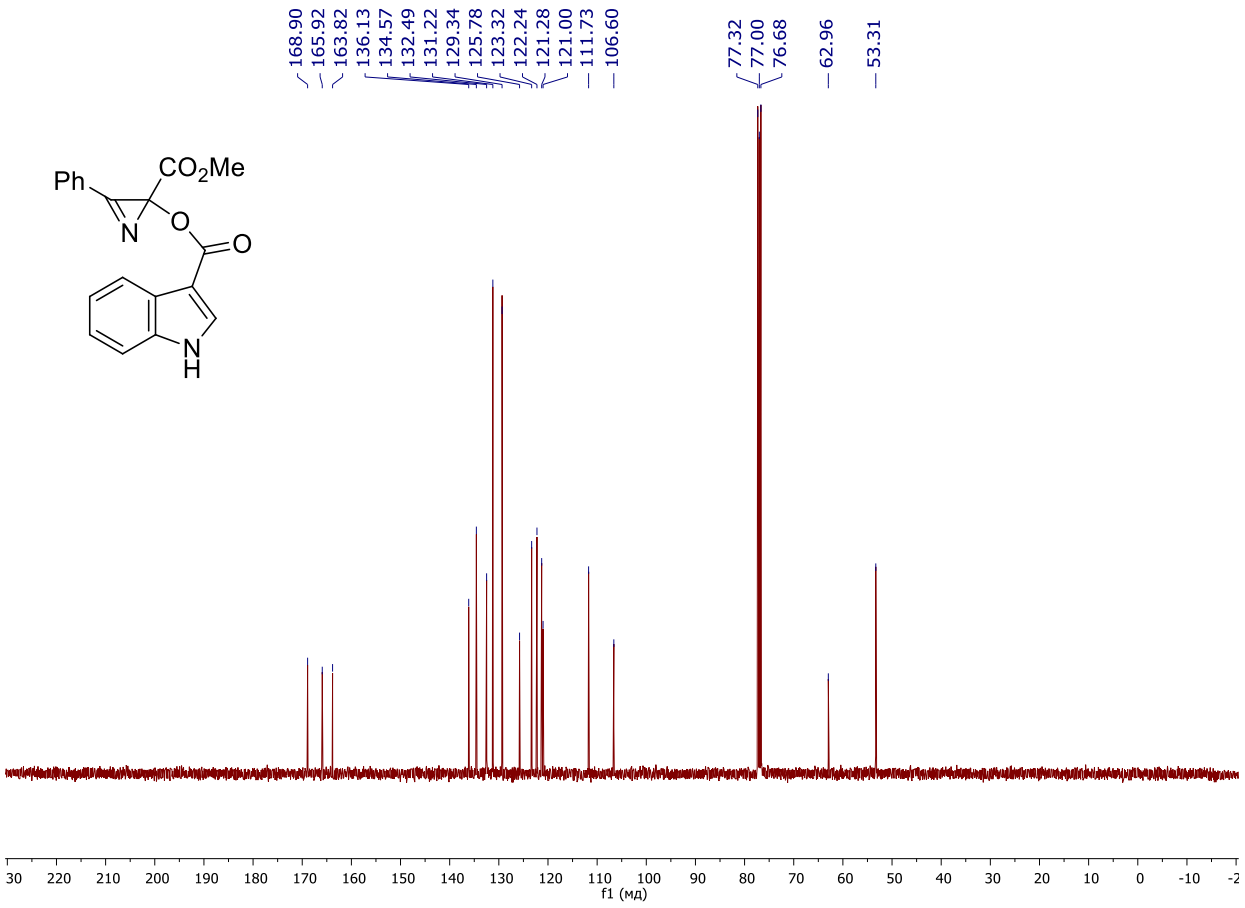
^{13}C NMR (100 MHz, $CDCl_3$) spectrum of **3r**



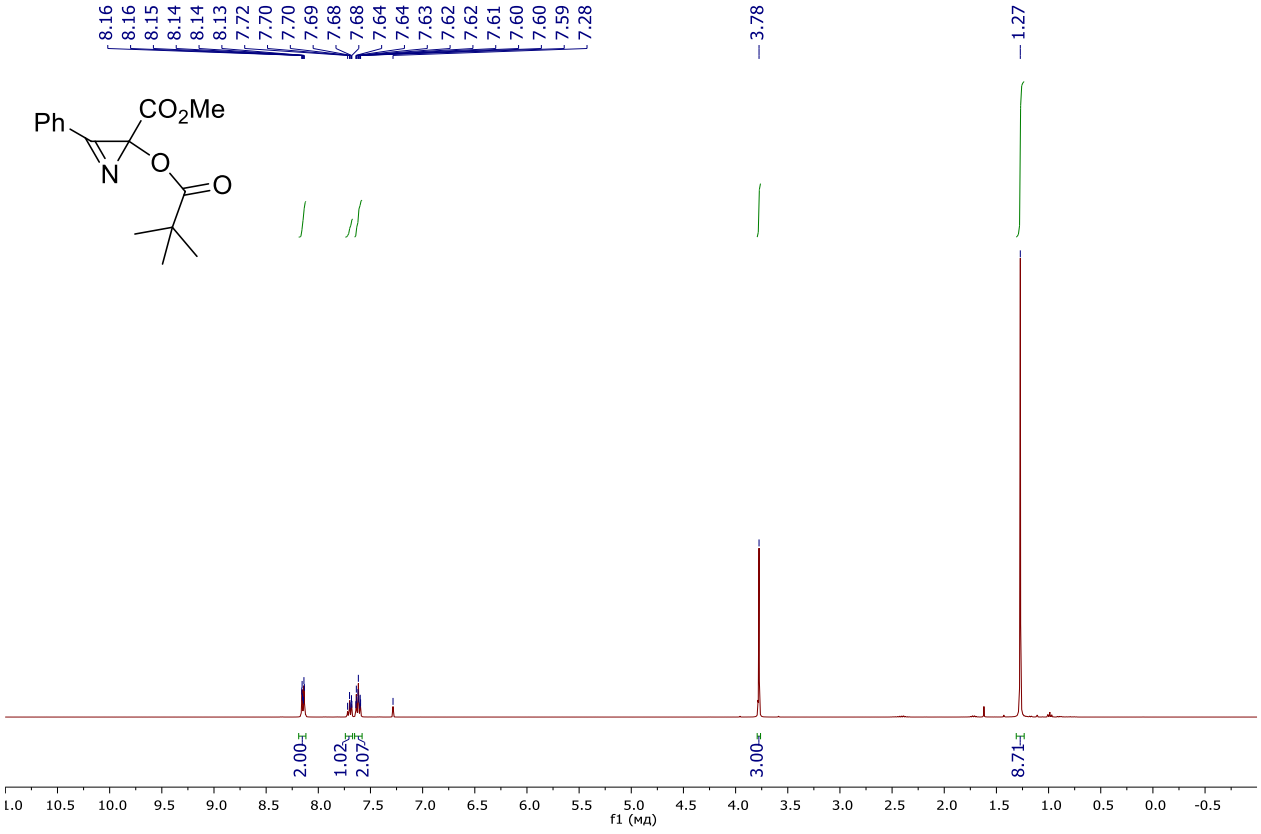
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of **3s**



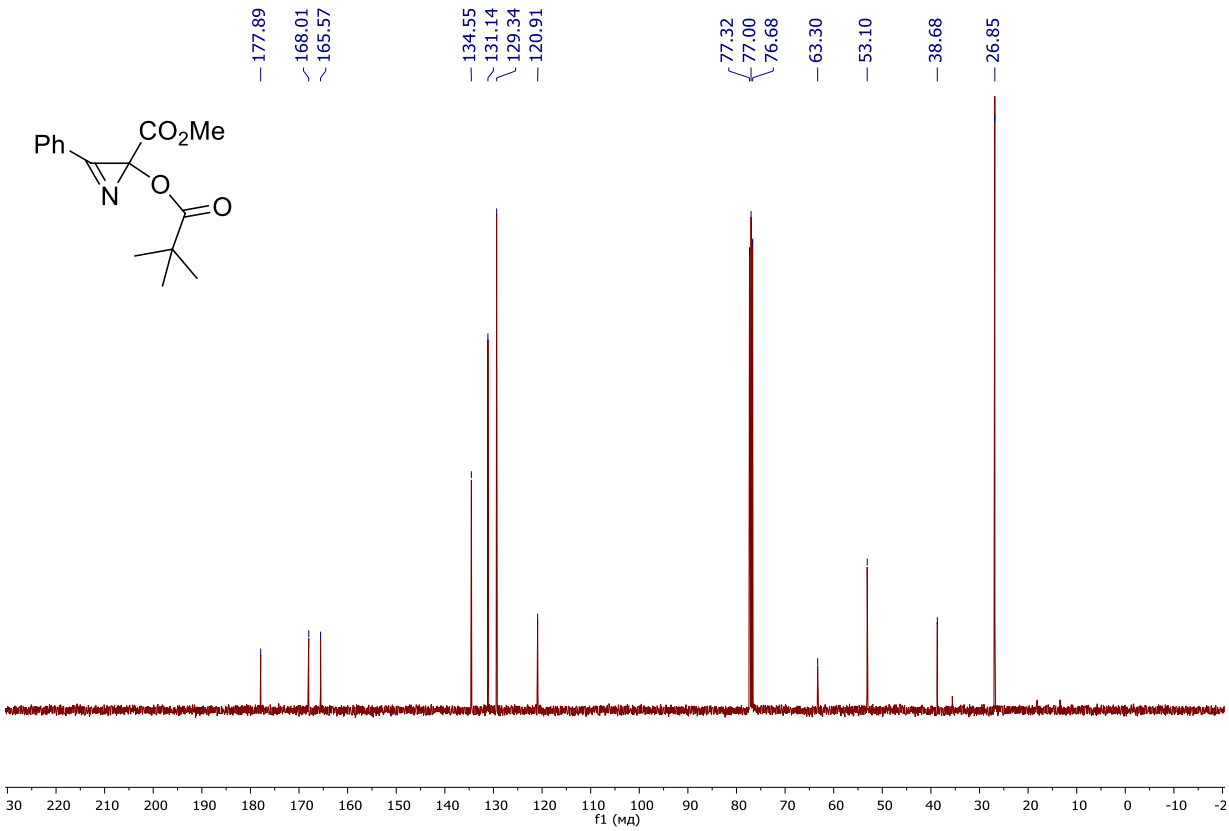
^{13}C NMR (100 MHz, $CDCl_3$) spectrum of **3s**



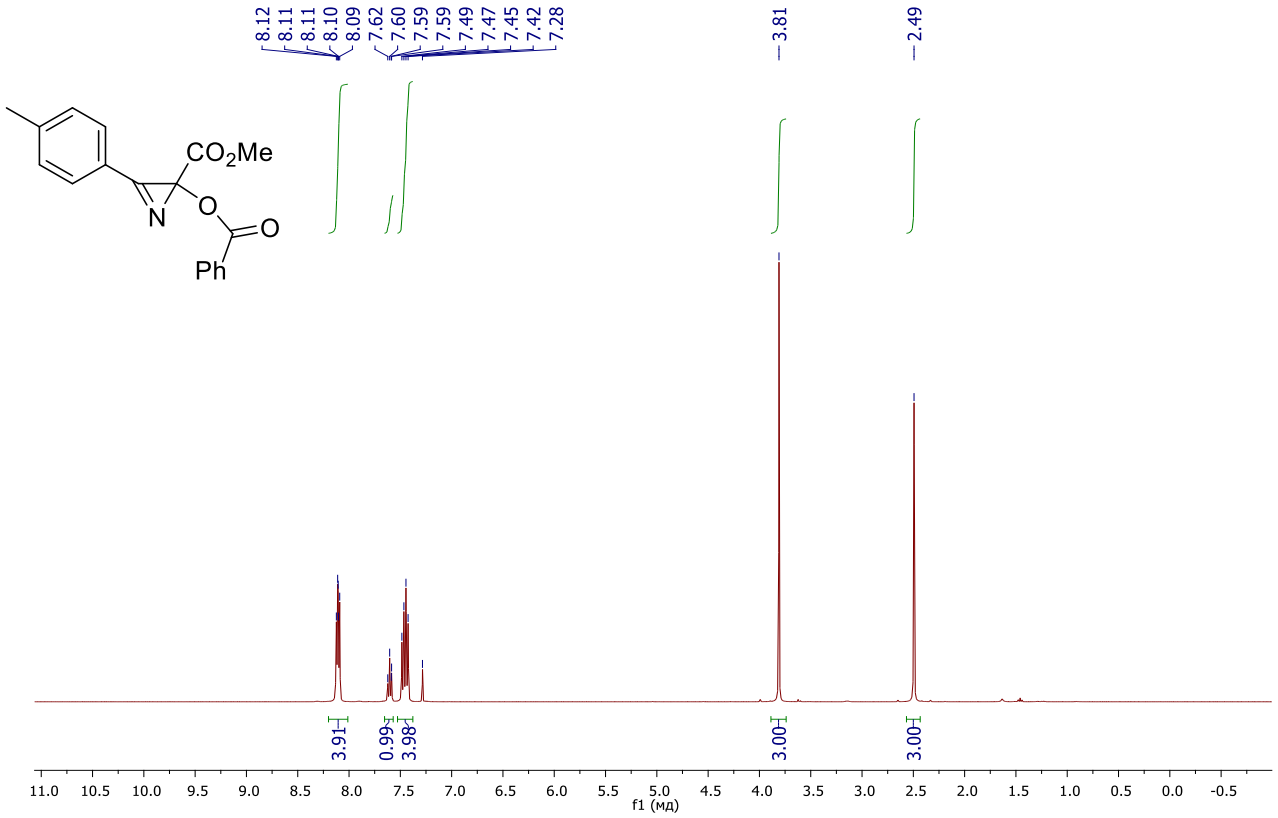
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of **3t**



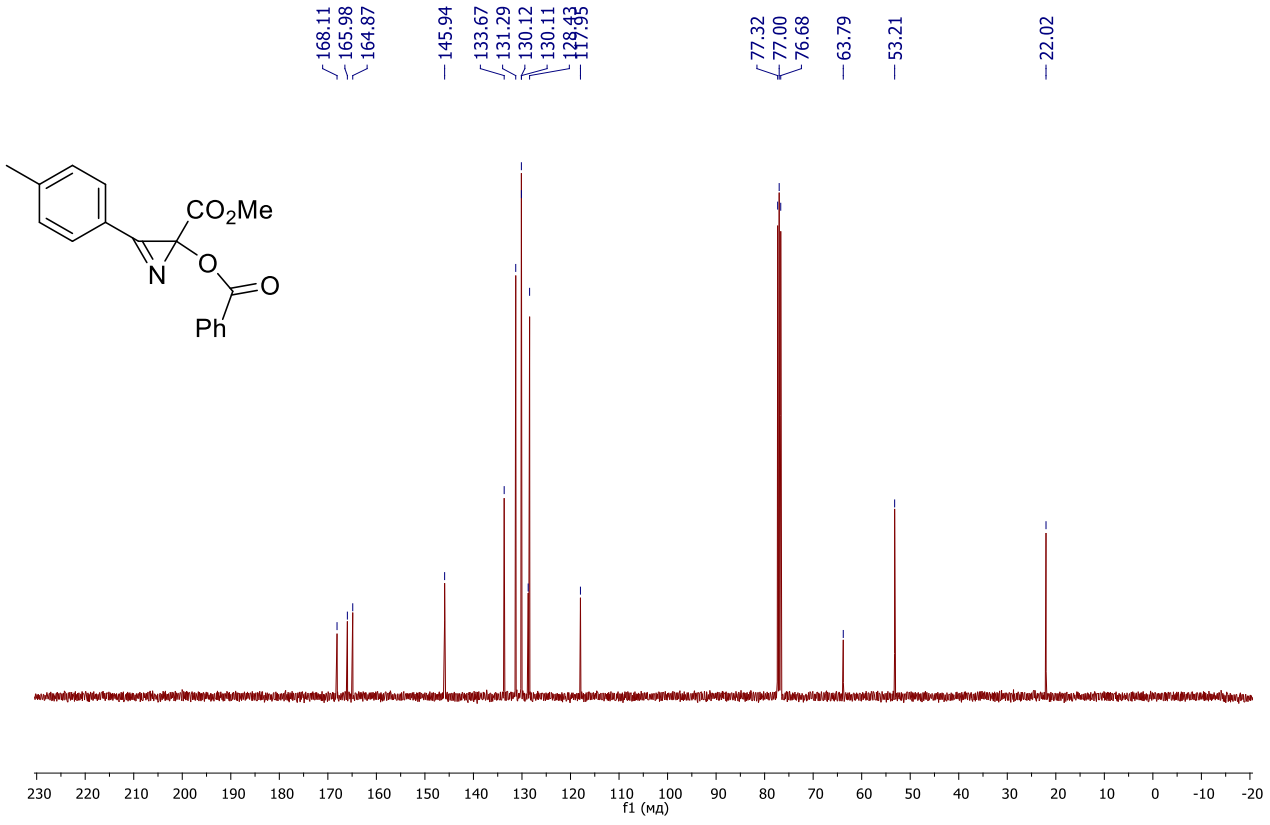
^{13}C NMR (100 MHz, $CDCl_3$) spectrum of **3t**



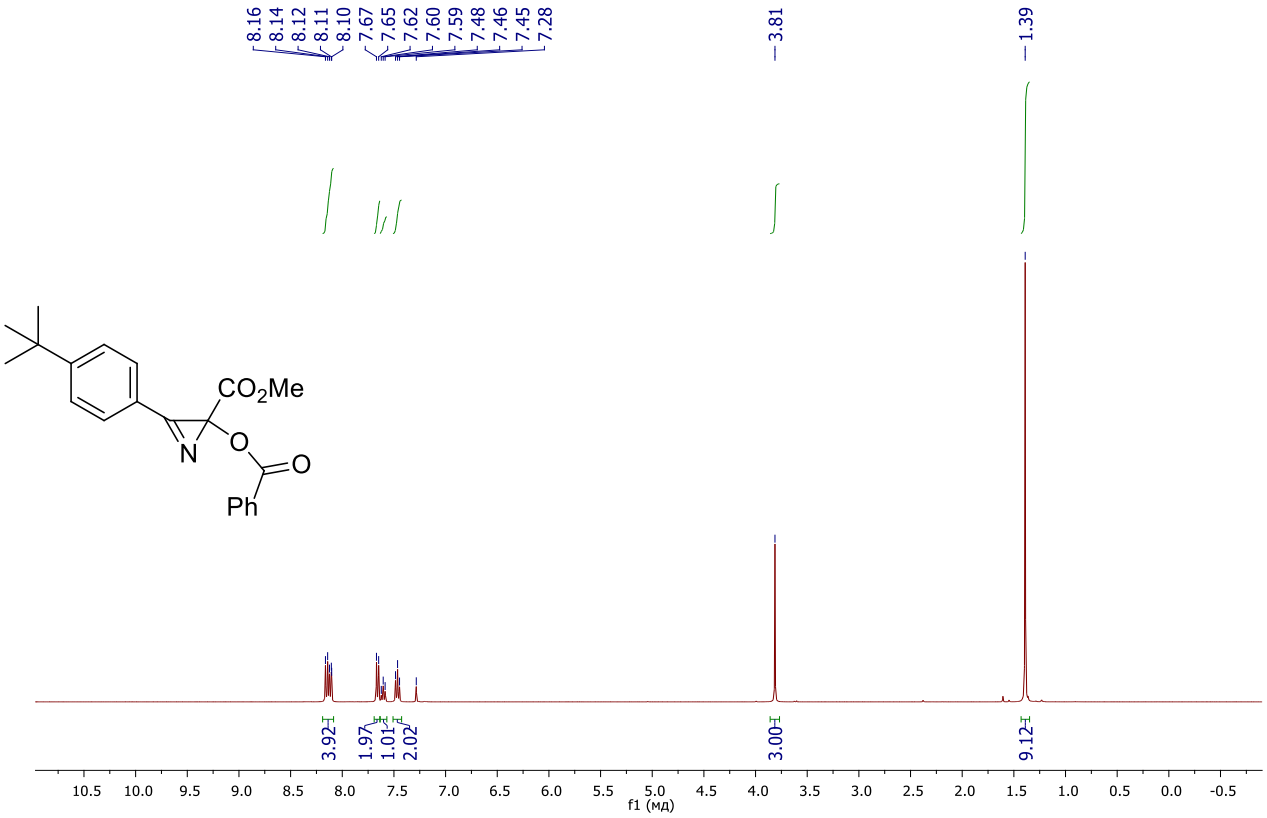
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of **3w**



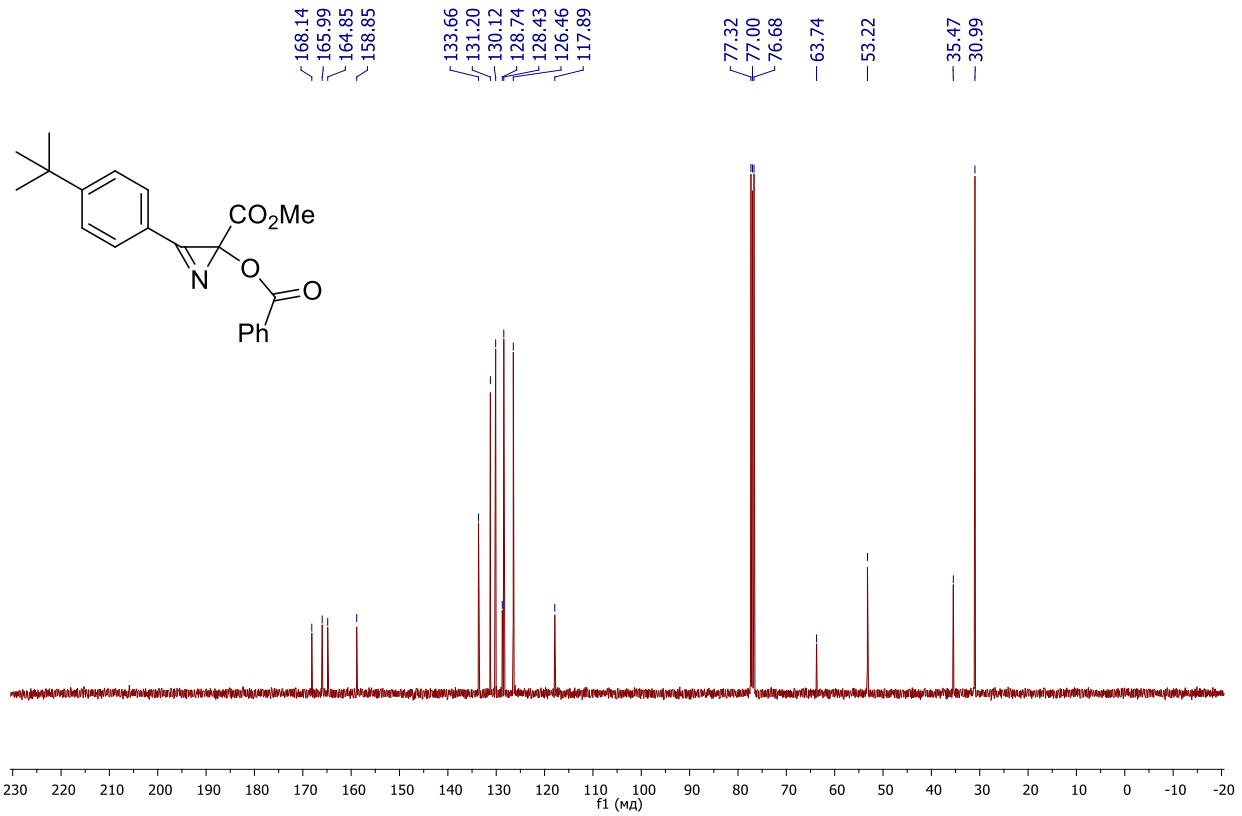
^{13}C NMR (100 MHz, $CDCl_3$) spectrum of **3w**



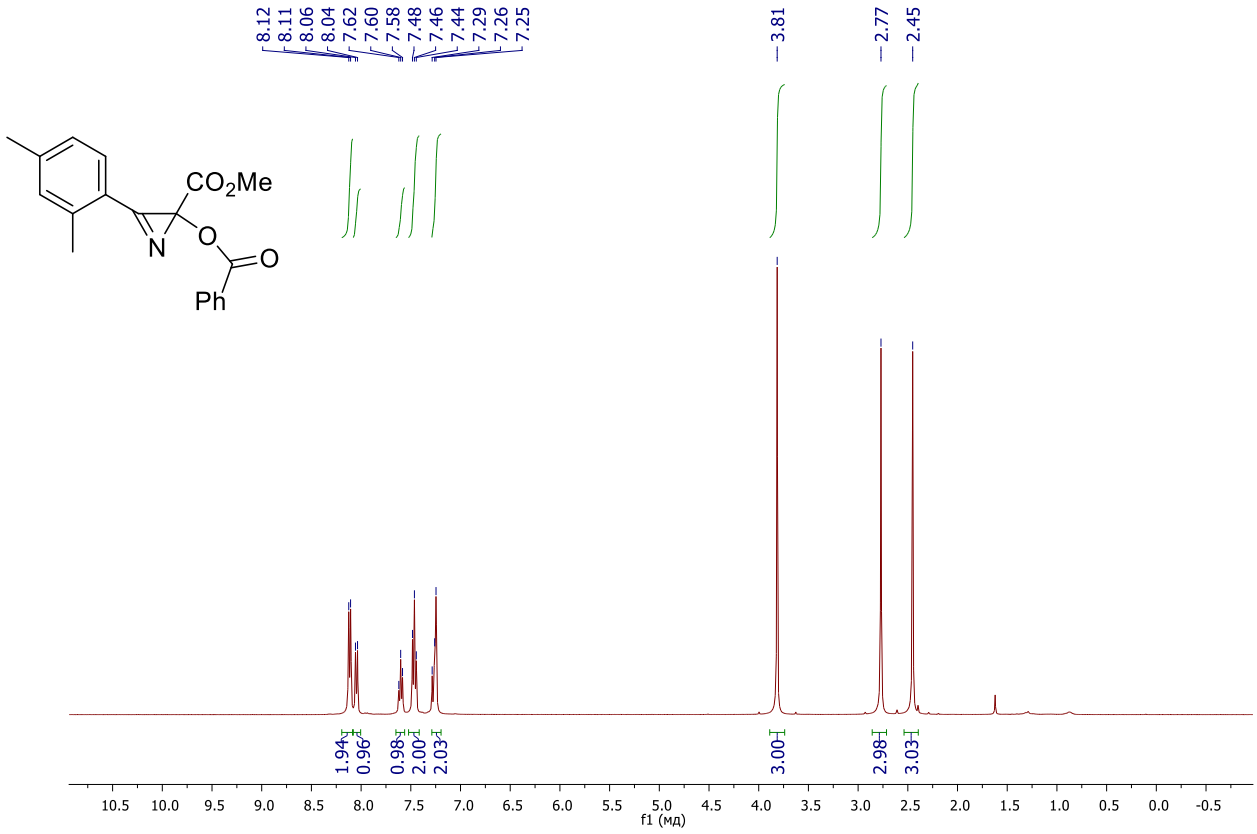
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of **3x**



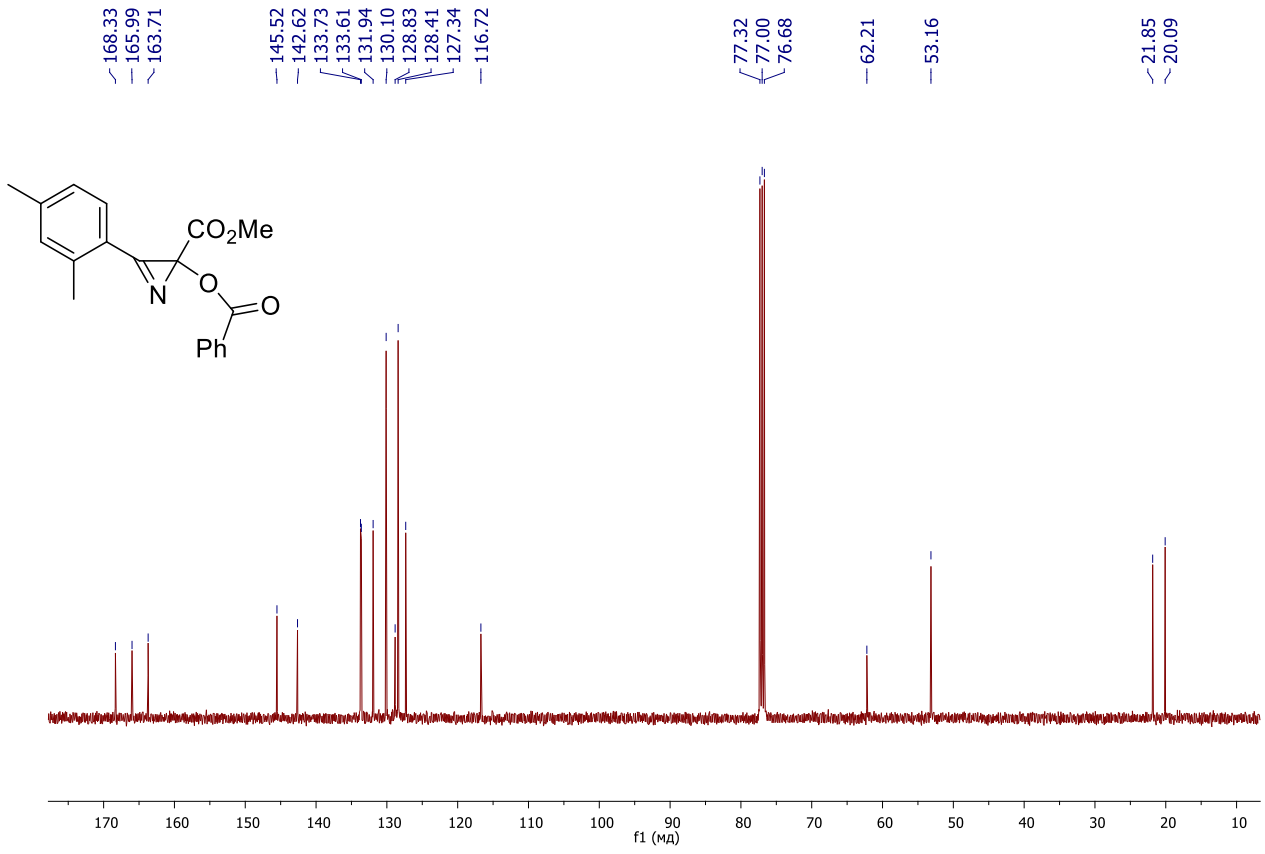
^{13}C NMR (100 MHz, $CDCl_3$) spectrum of **3x**



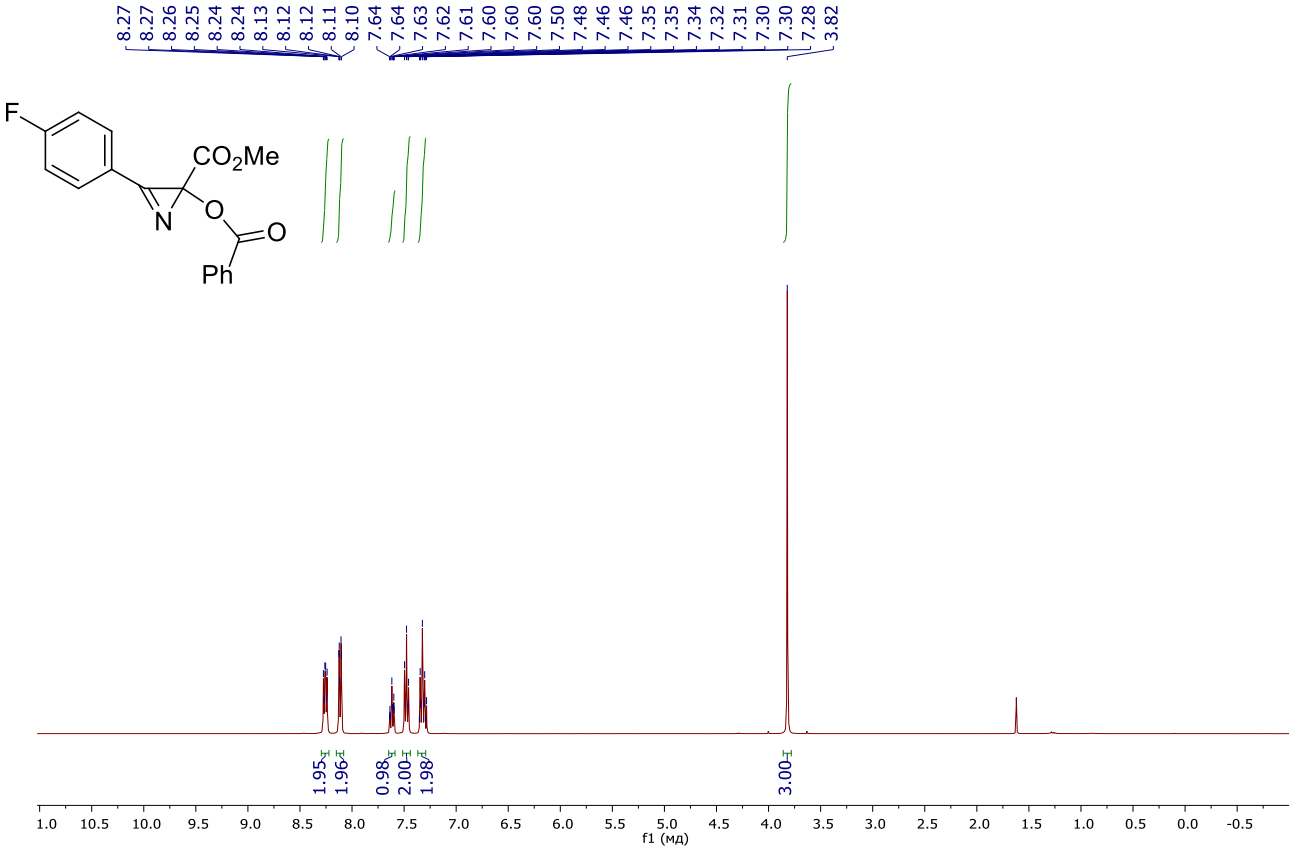
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of **3y**



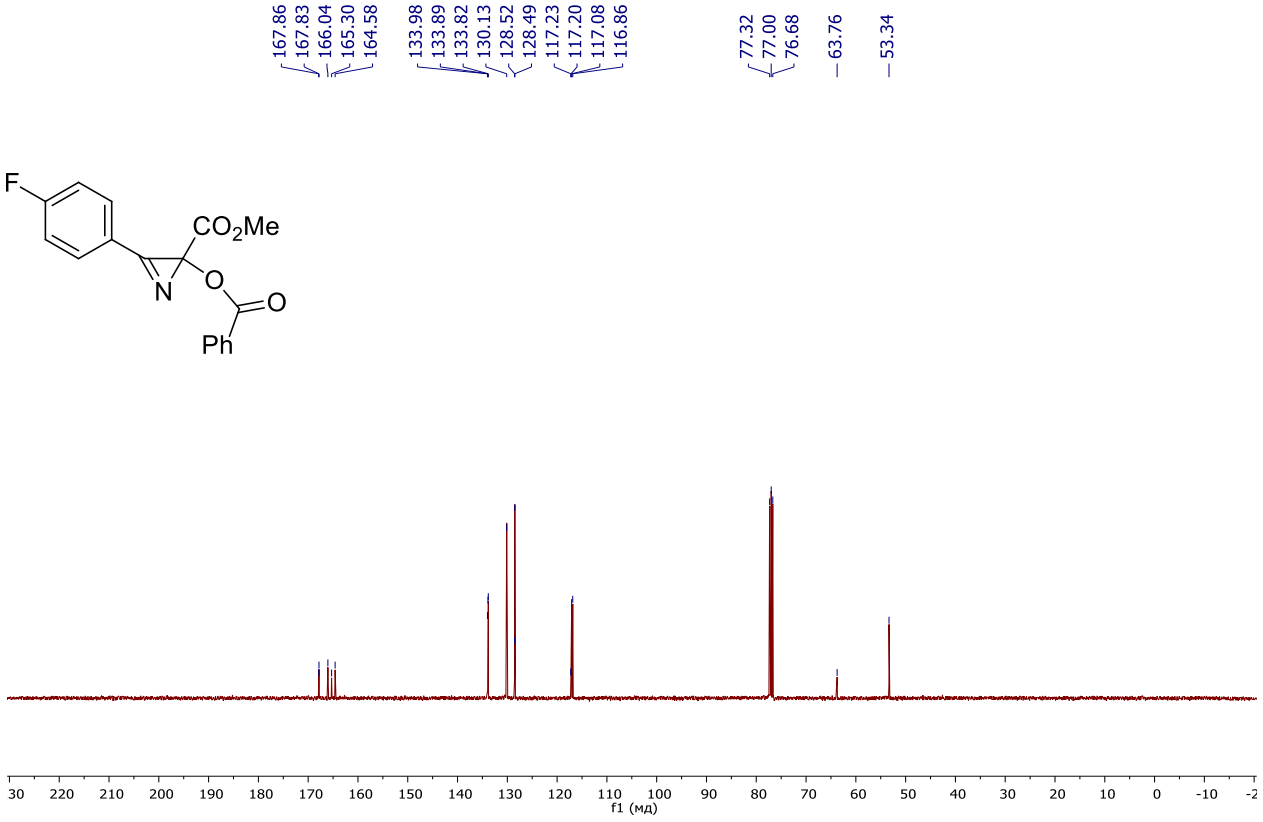
^{13}C NMR (100 MHz, $CDCl_3$) spectrum of **3y**



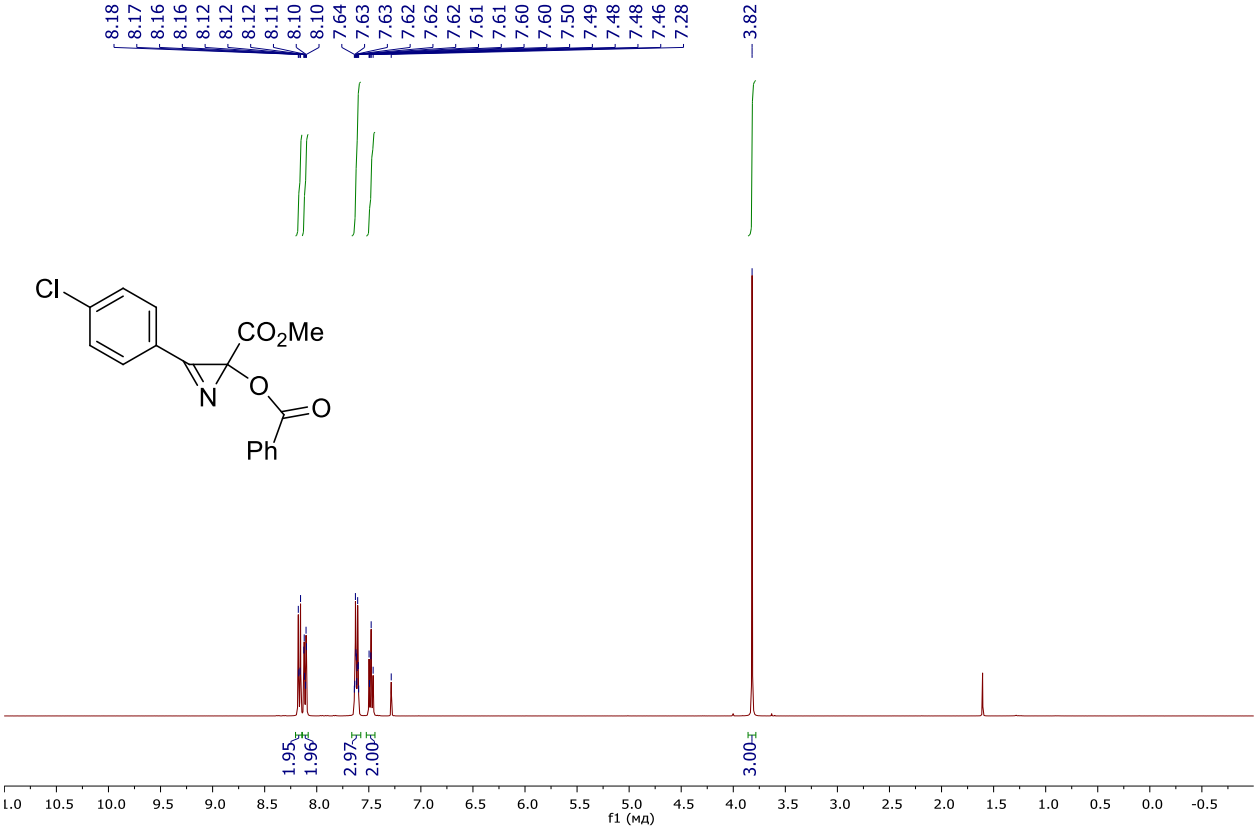
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of **3z**



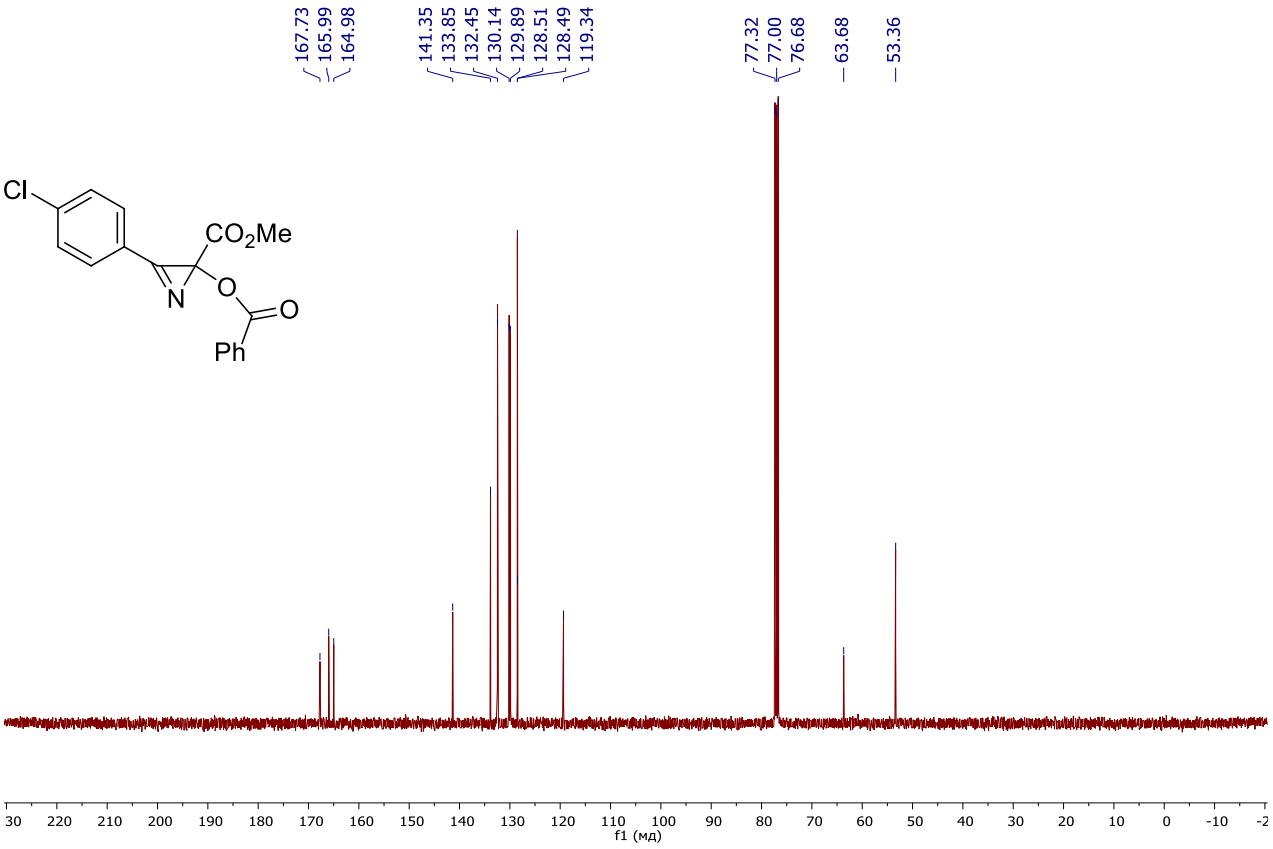
^{13}C NMR (100 MHz, $CDCl_3$) spectrum of **3z**



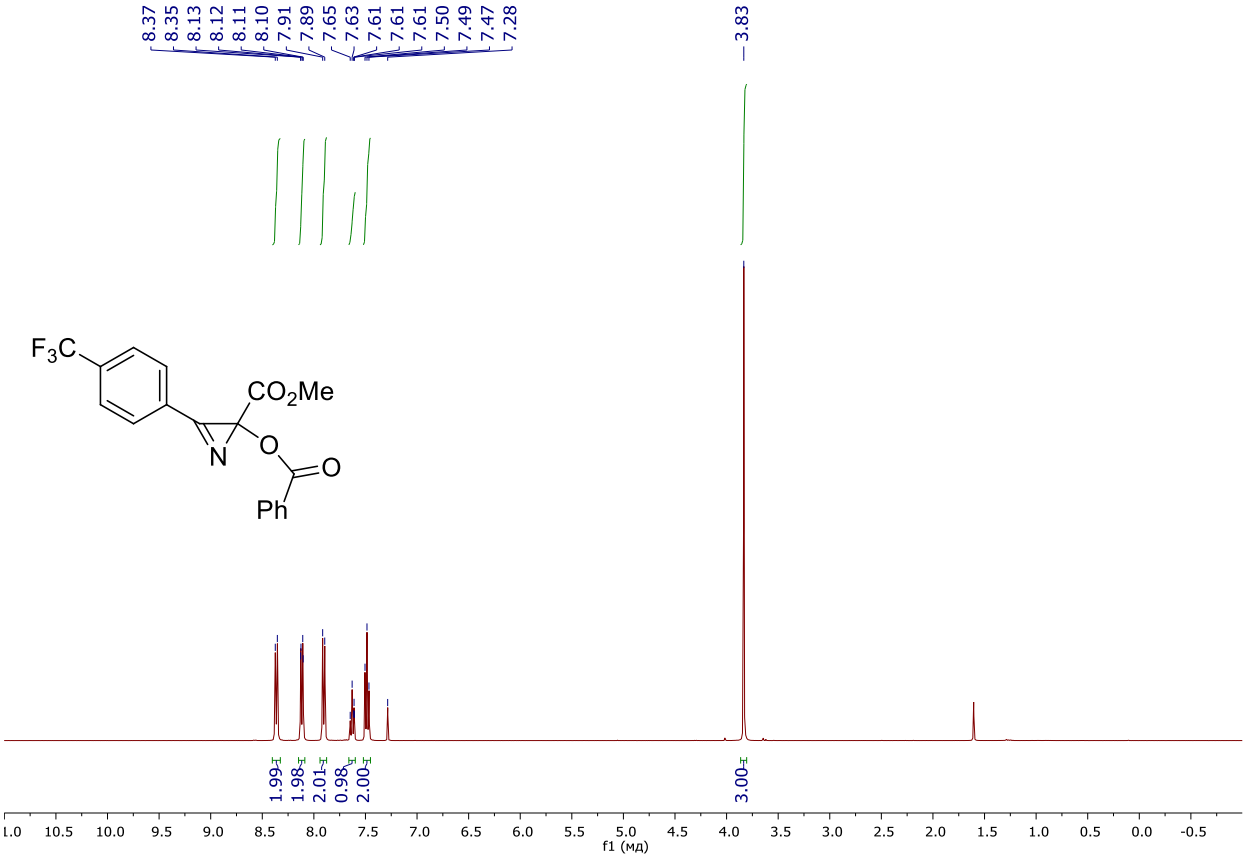
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of **3za**



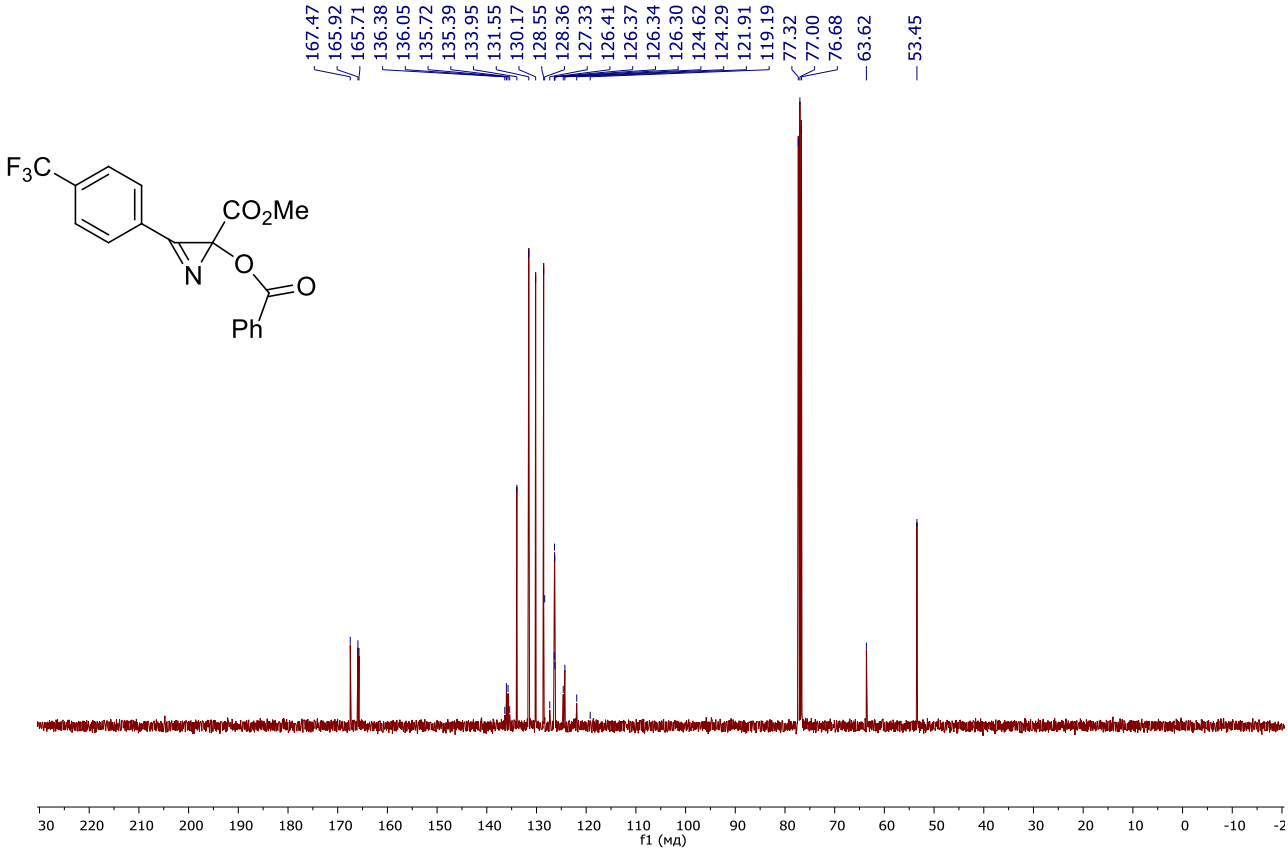
^{13}C NMR (100 MHz, $CDCl_3$) spectrum of **3za**



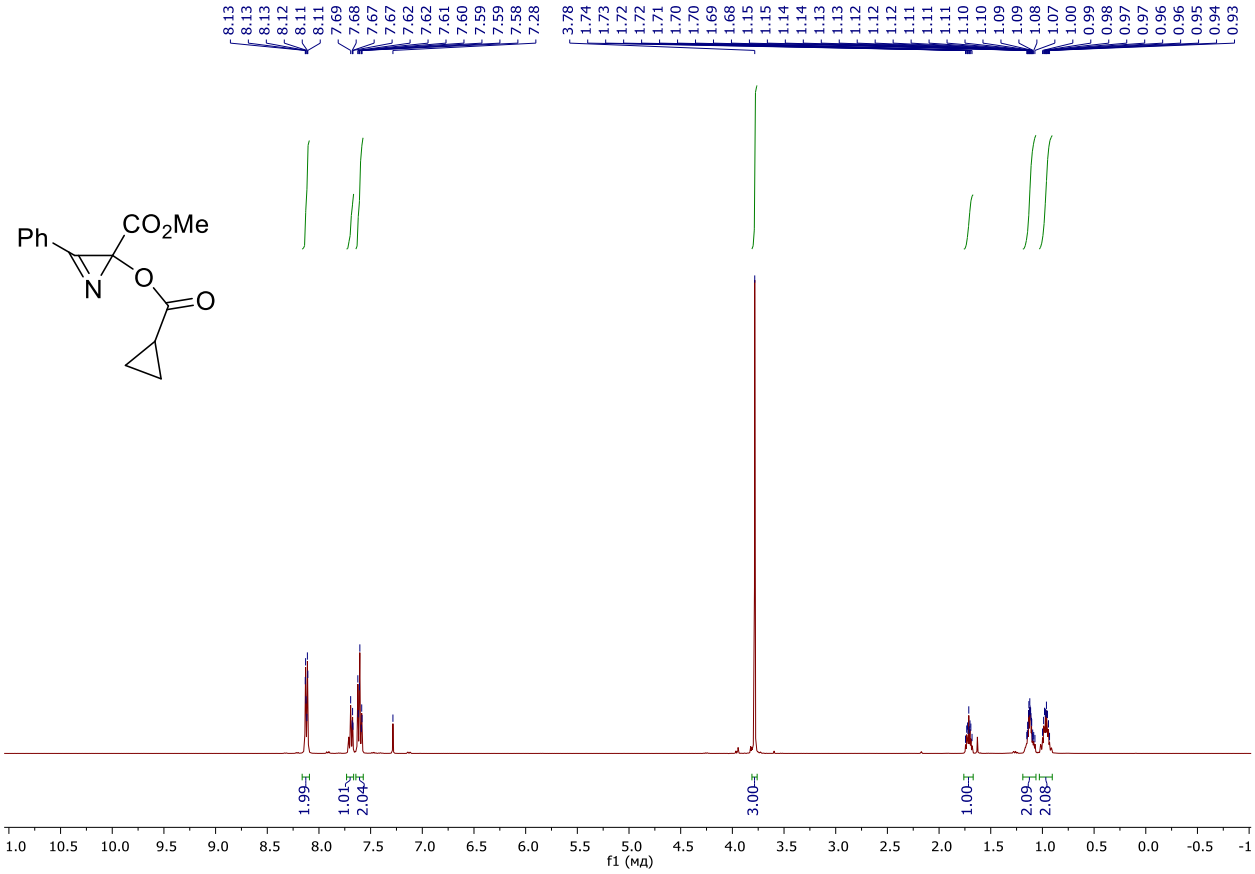
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of **3zb**



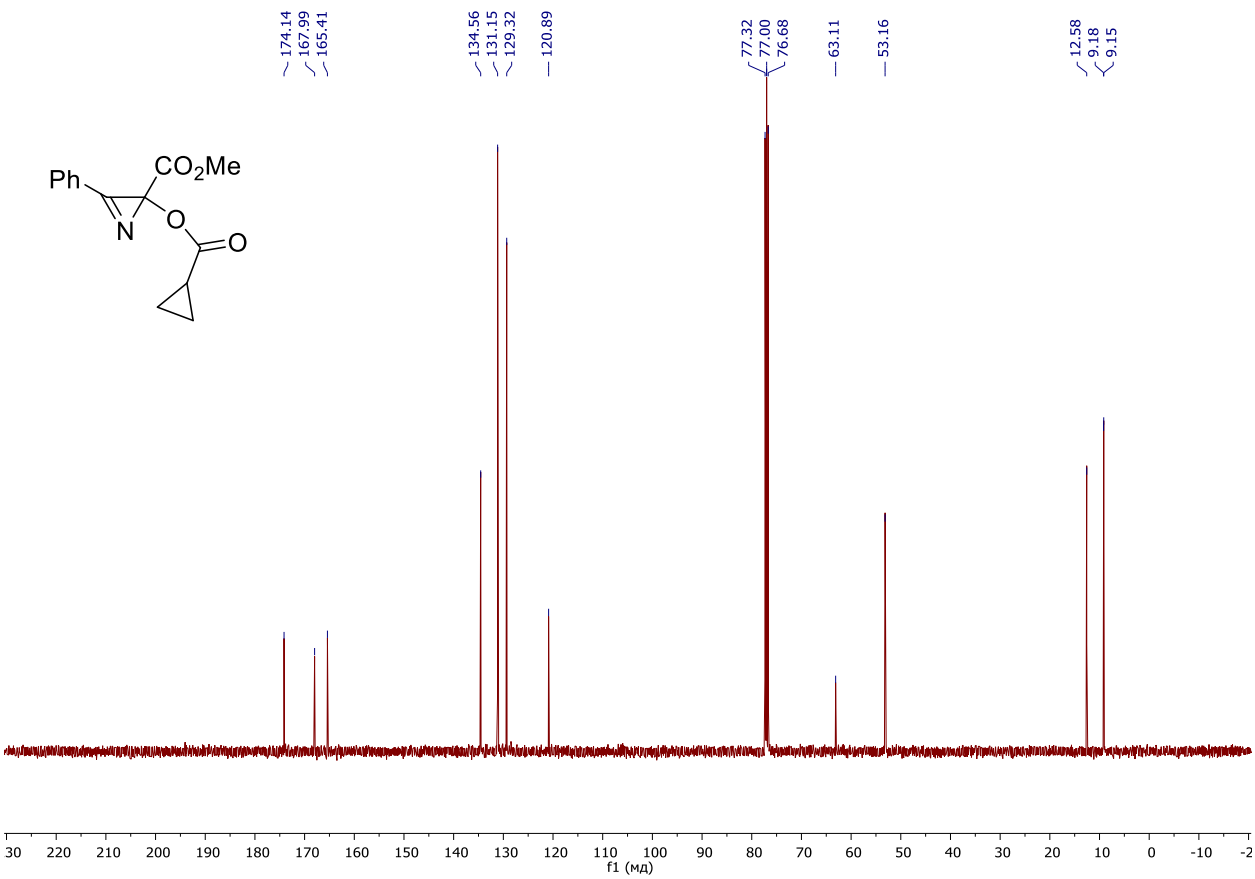
^{13}C NMR (100 MHz, $CDCl_3$) spectrum of **3zb**



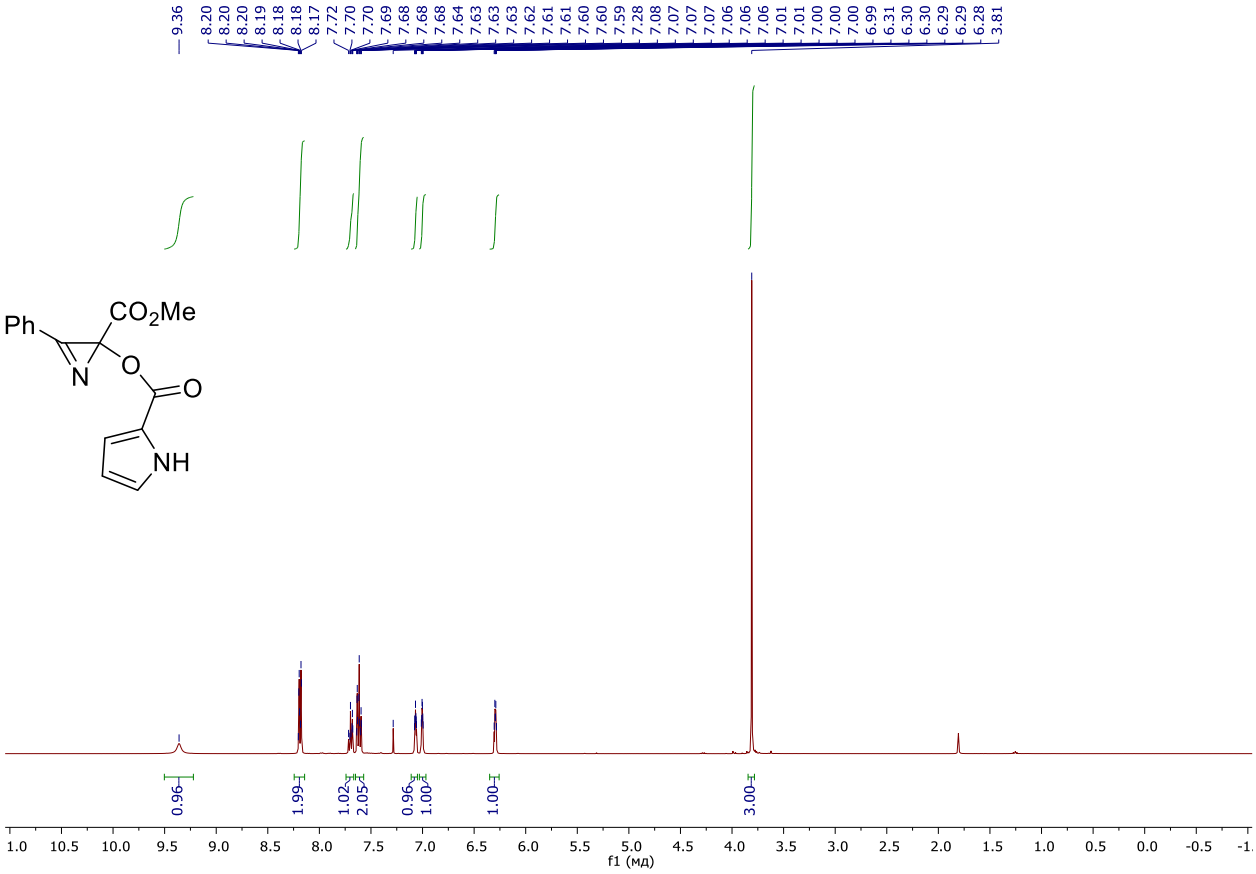
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of **3zd**



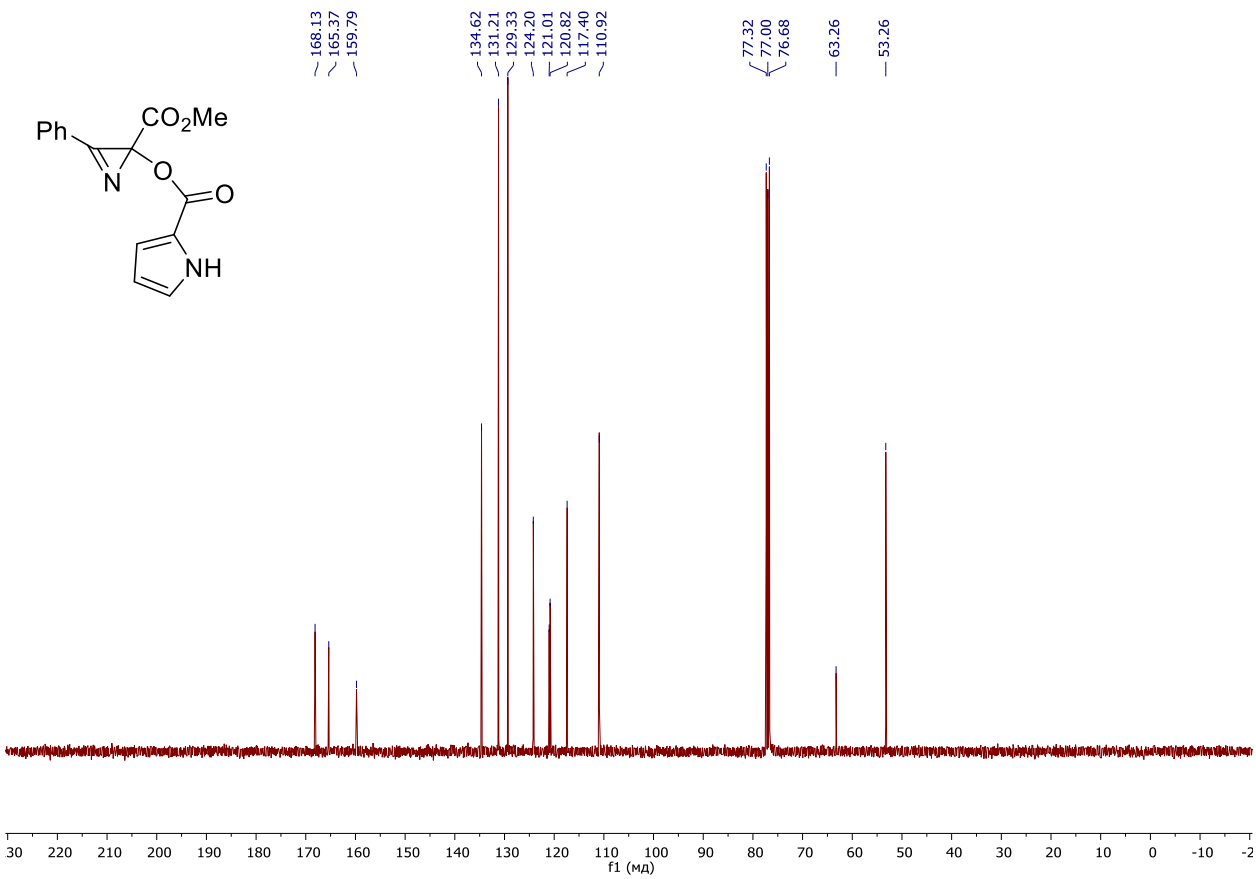
^{13}C NMR (100 MHz, $CDCl_3$) spectrum of **3zd**



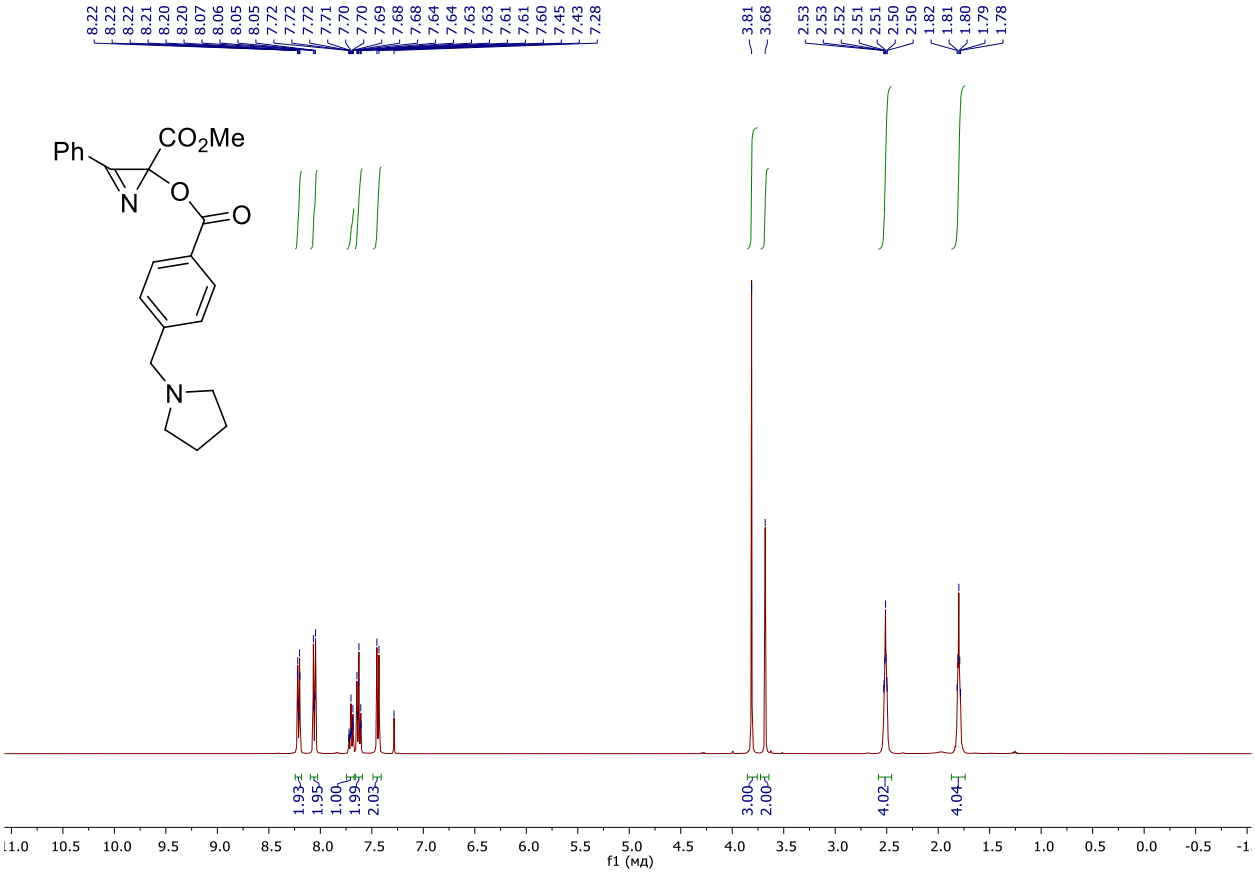
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of **3zf**



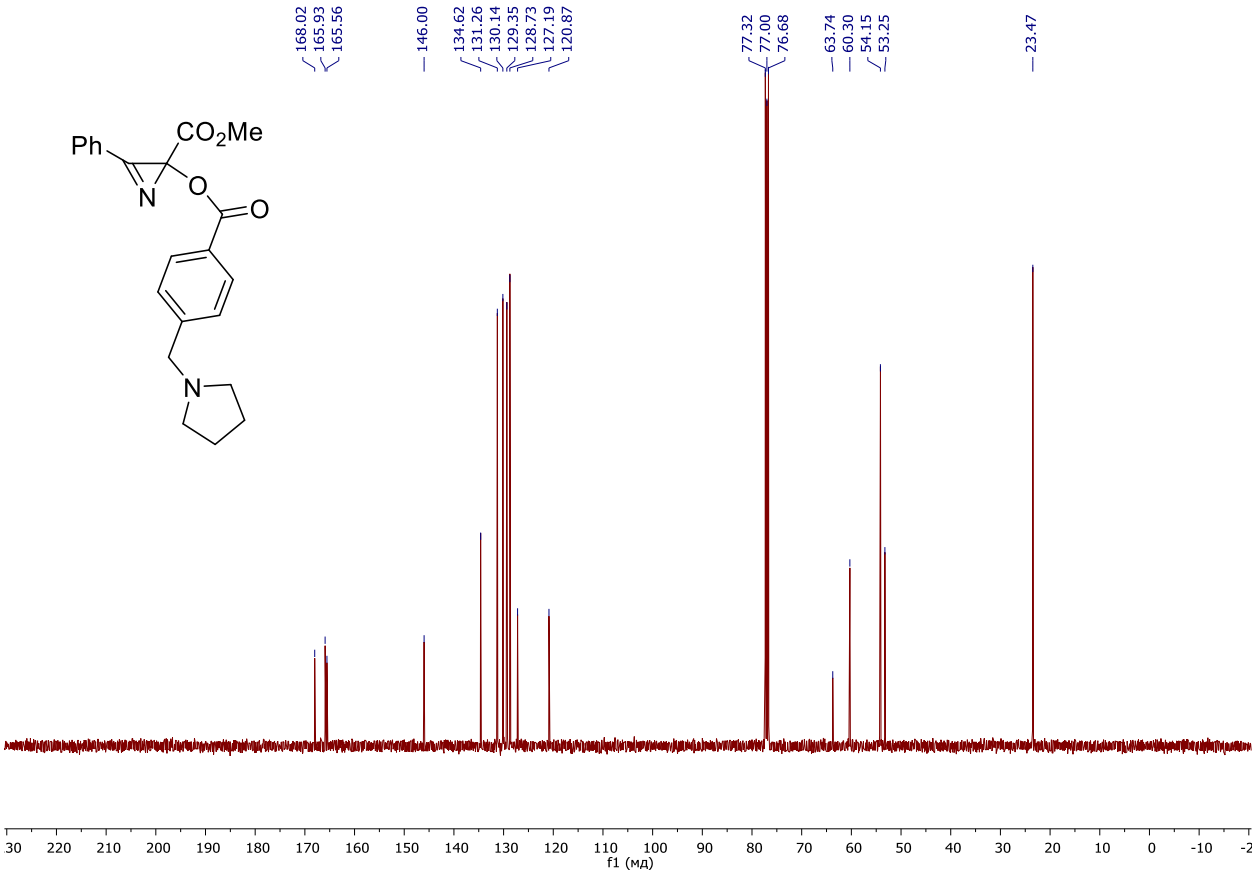
^{13}C NMR (100 MHz, $CDCl_3$) spectrum of **3zf**



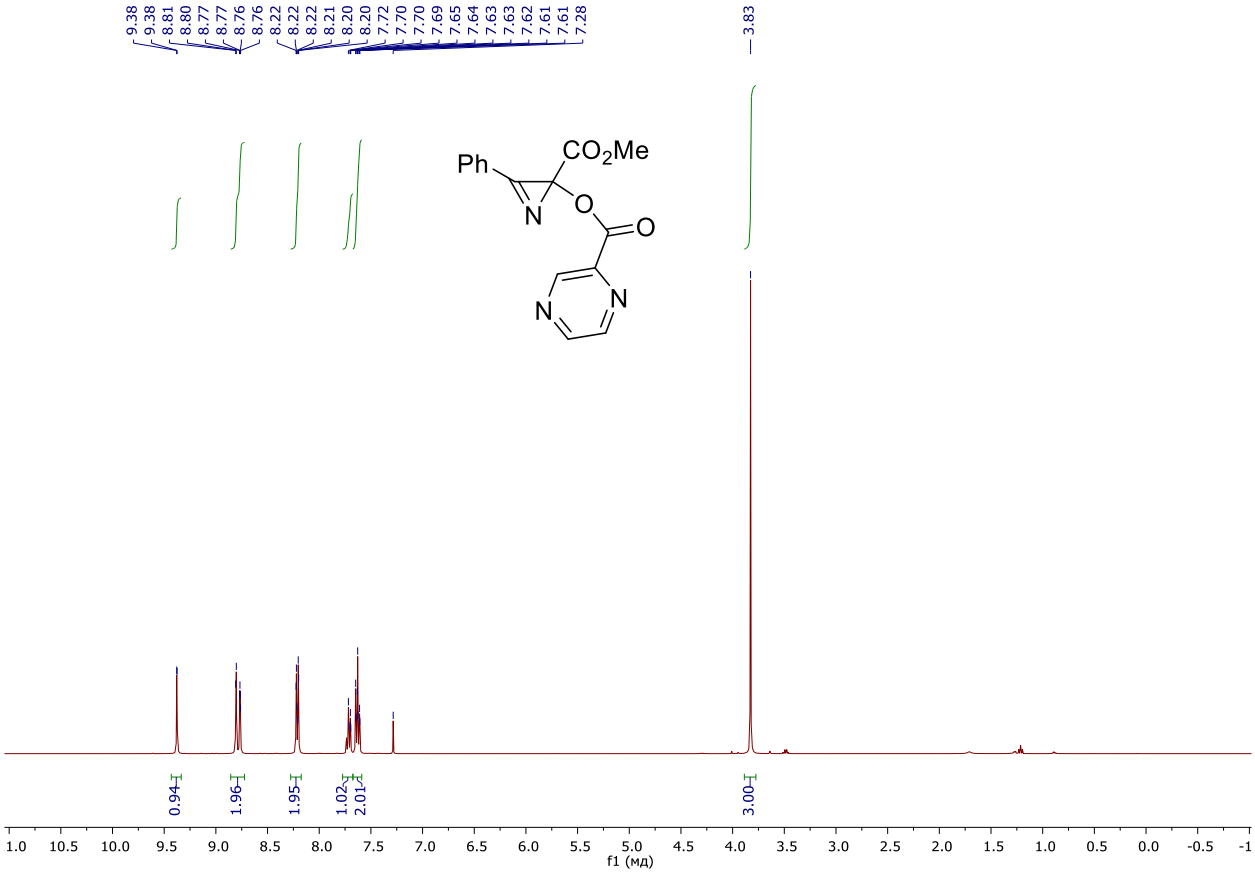
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of **3zg**



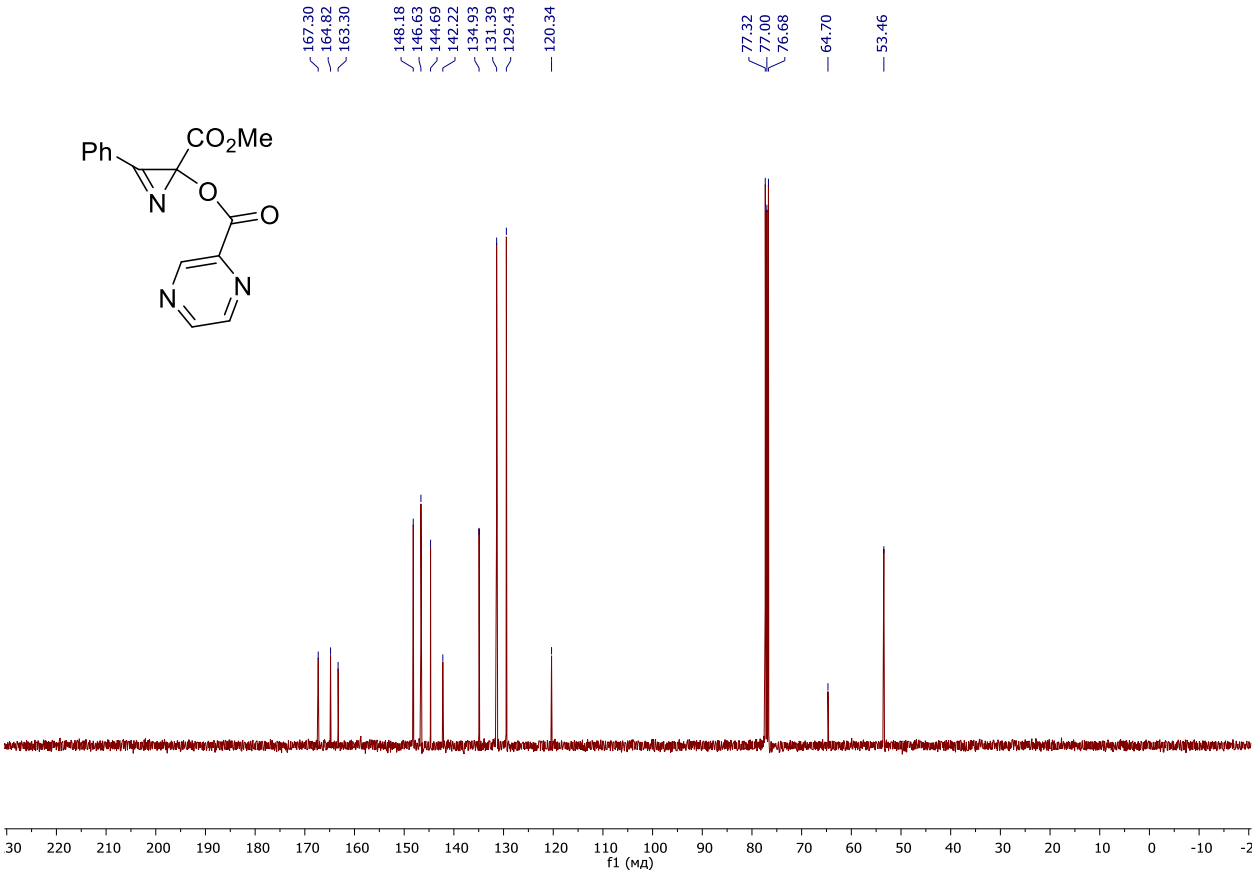
^{13}C NMR (100 MHz, $CDCl_3$) spectrum of **3zg**



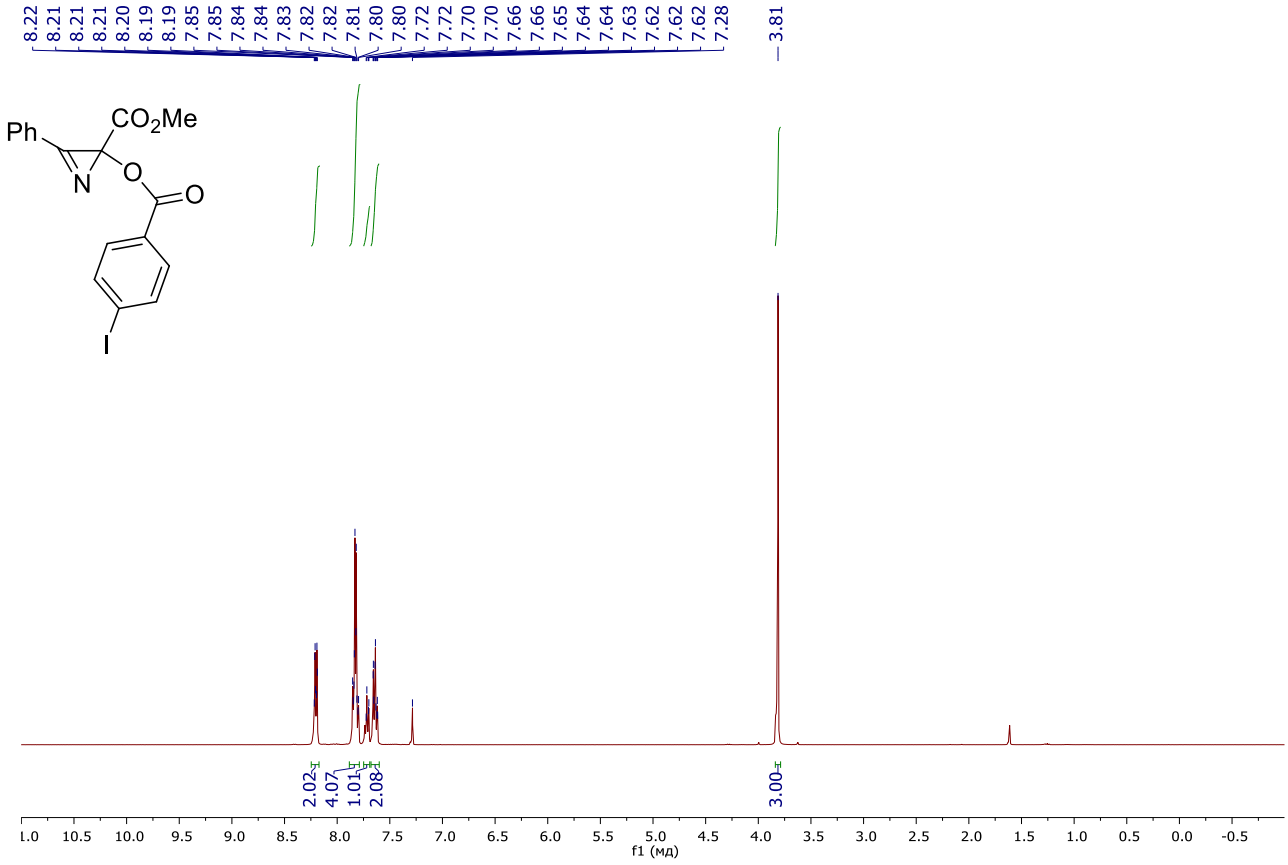
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of **3zh**



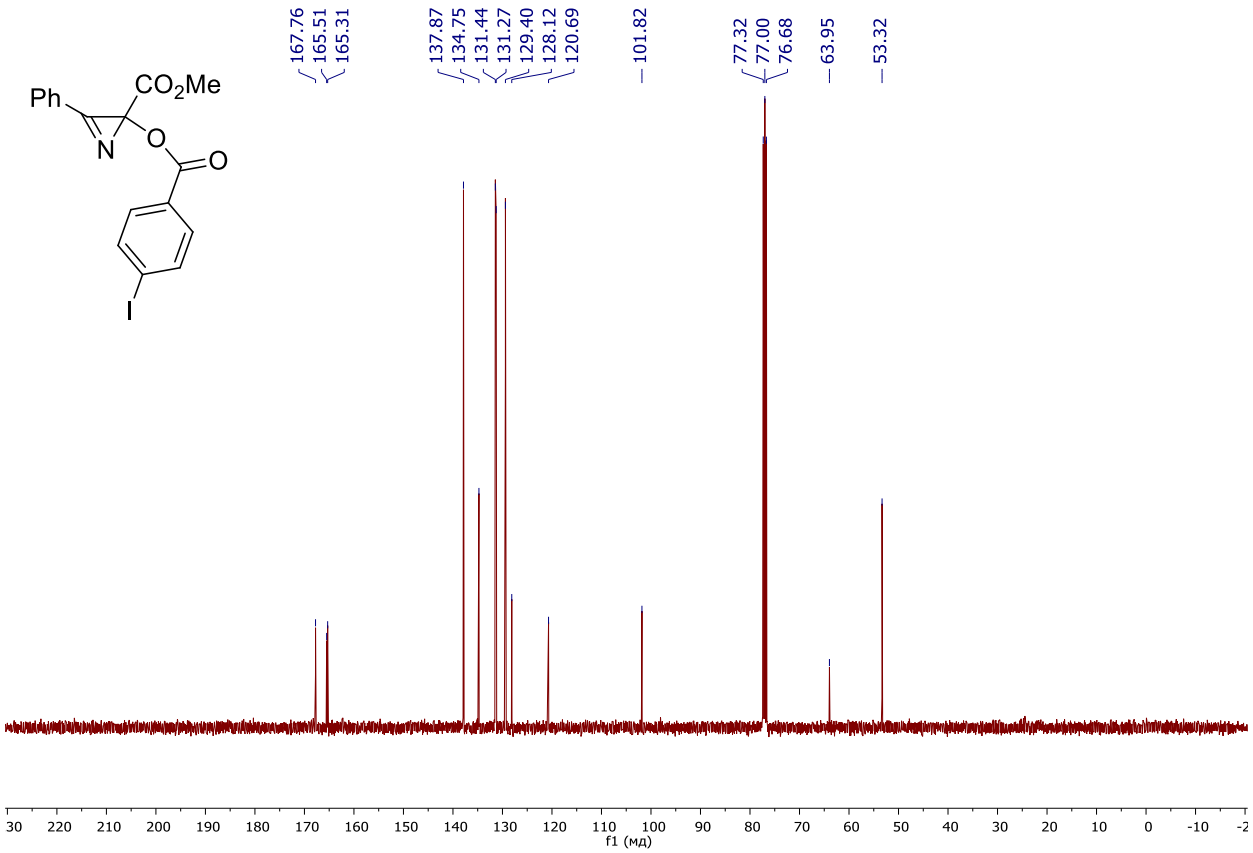
^{13}C NMR (100 MHz, $CDCl_3$) spectrum of **3zh**



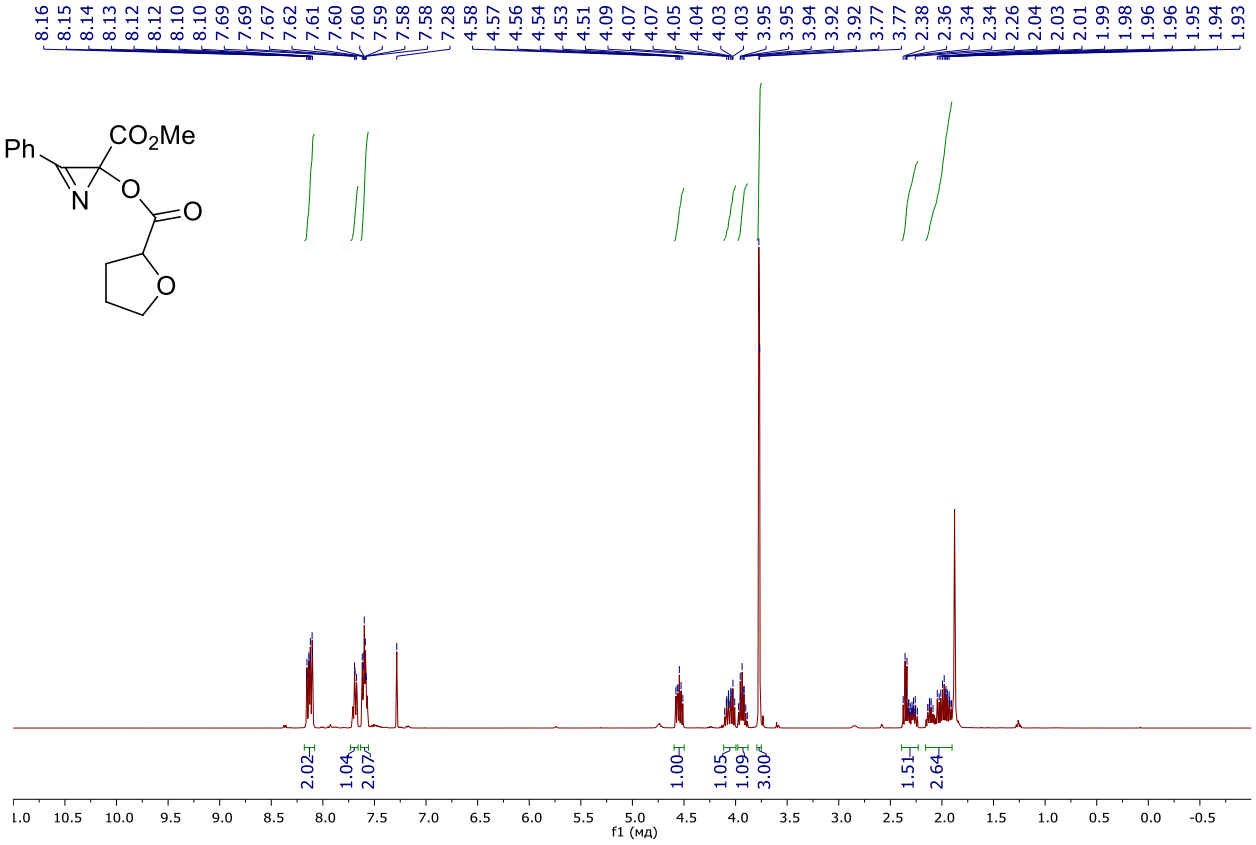
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of **3zi**



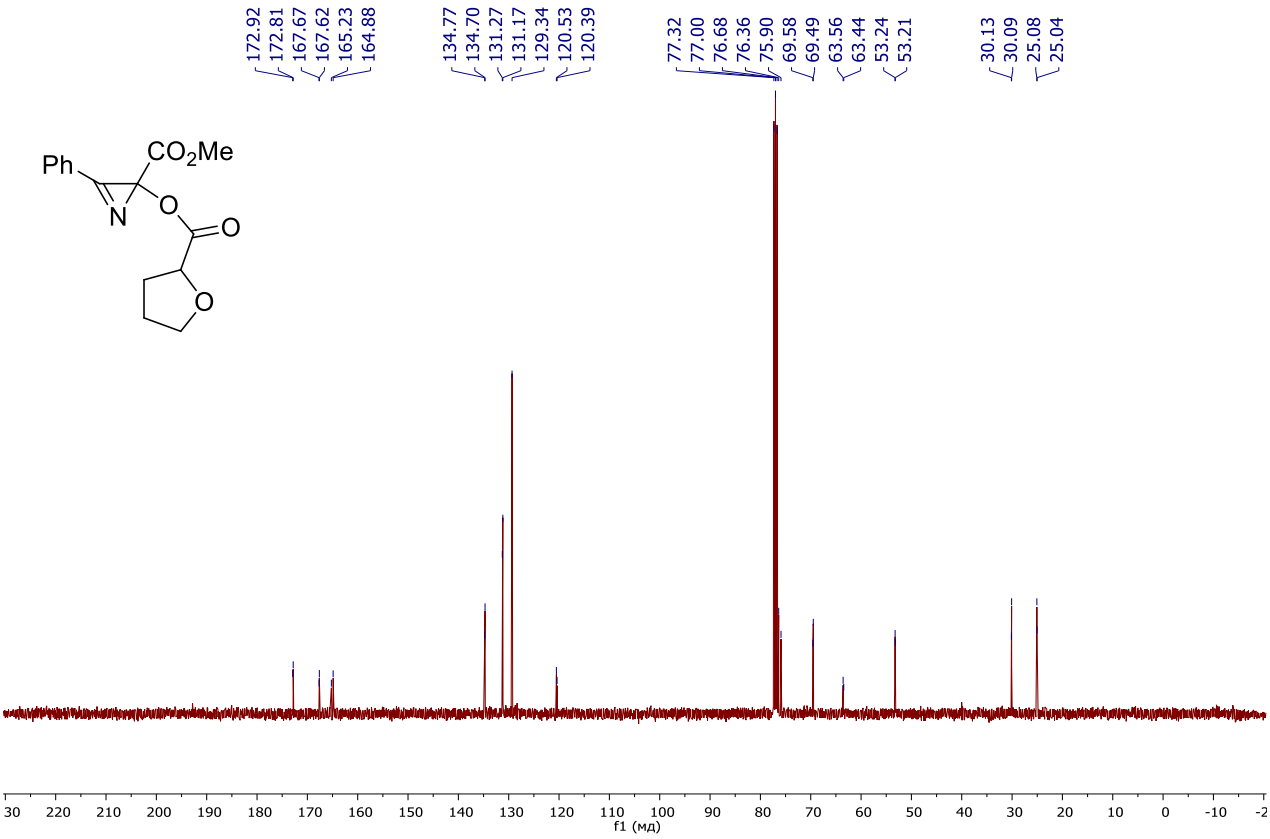
^{13}C NMR (100 MHz, $CDCl_3$) spectrum of **3zi**



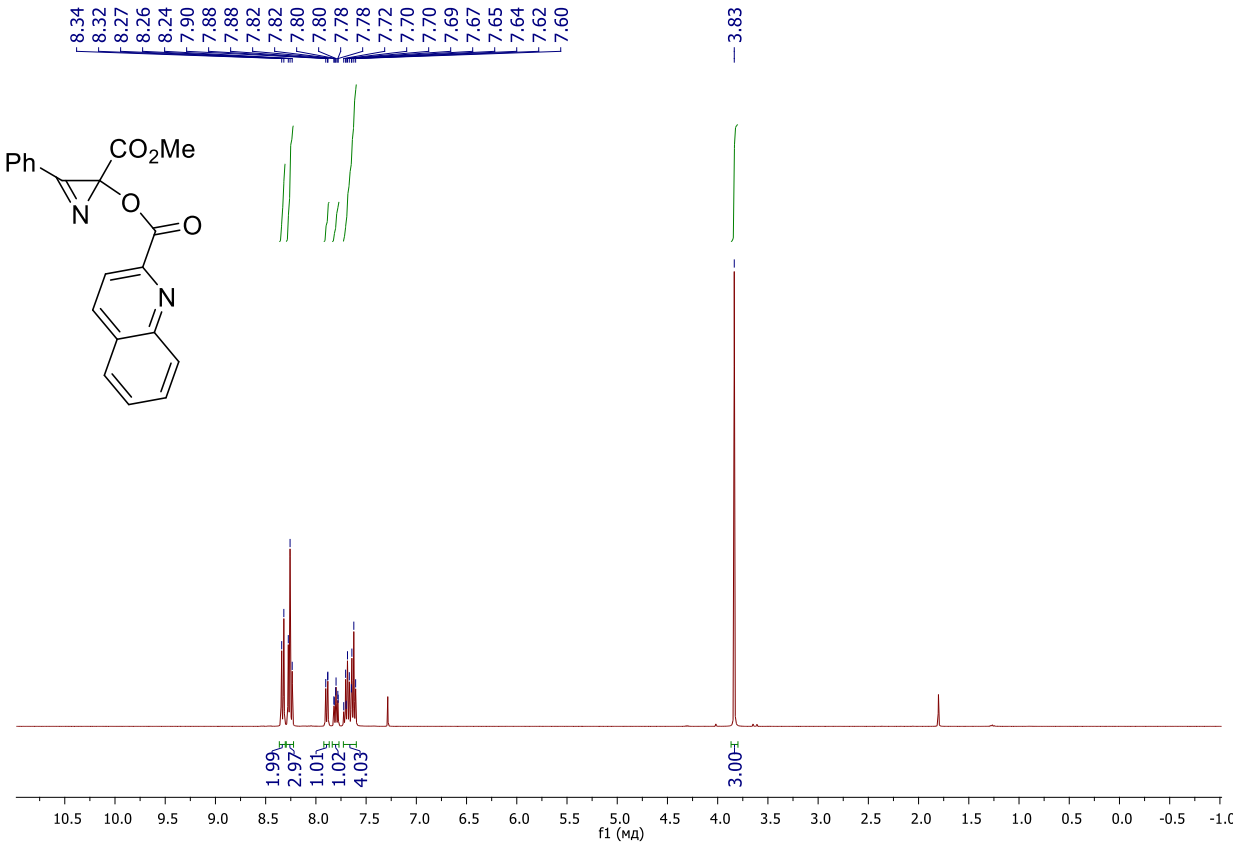
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of **3zm**



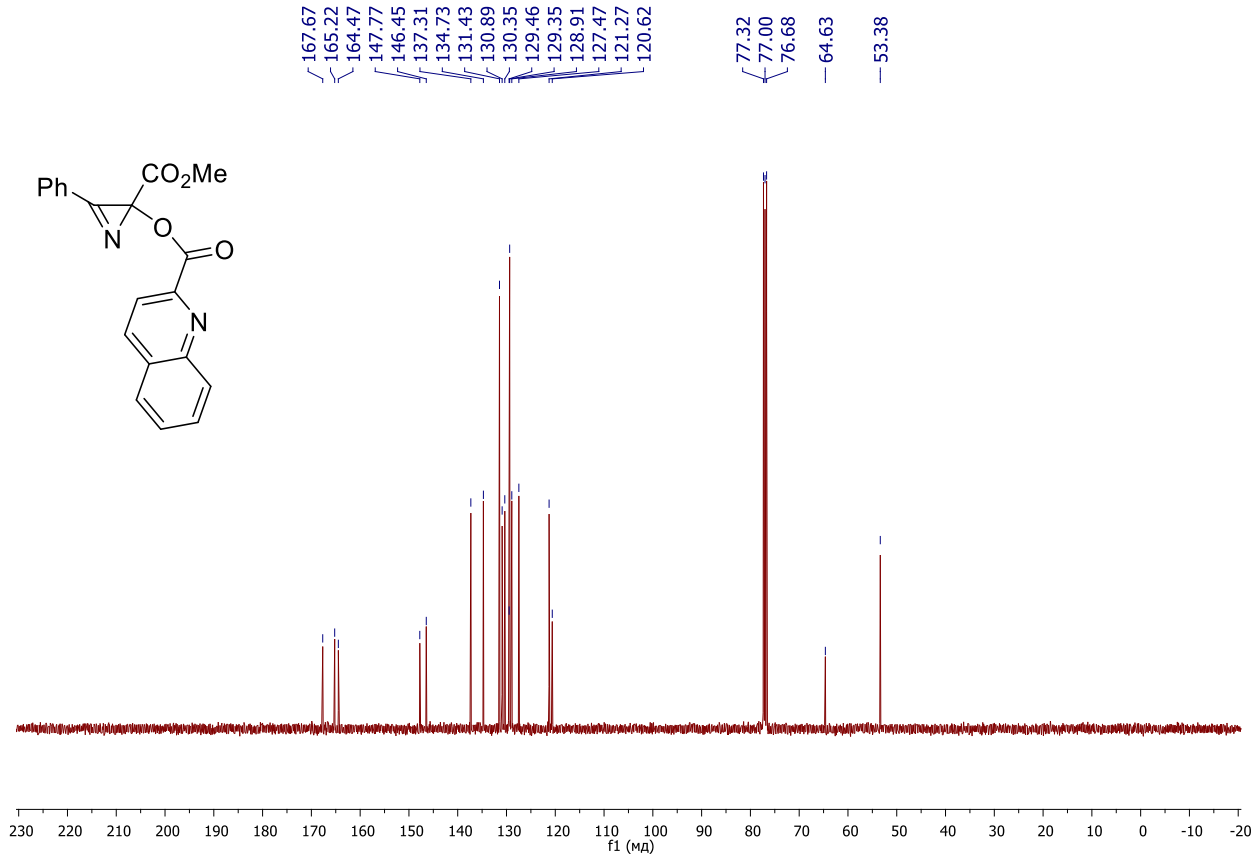
^{13}C NMR (100 MHz, $CDCl_3$) spectrum of **3zm**



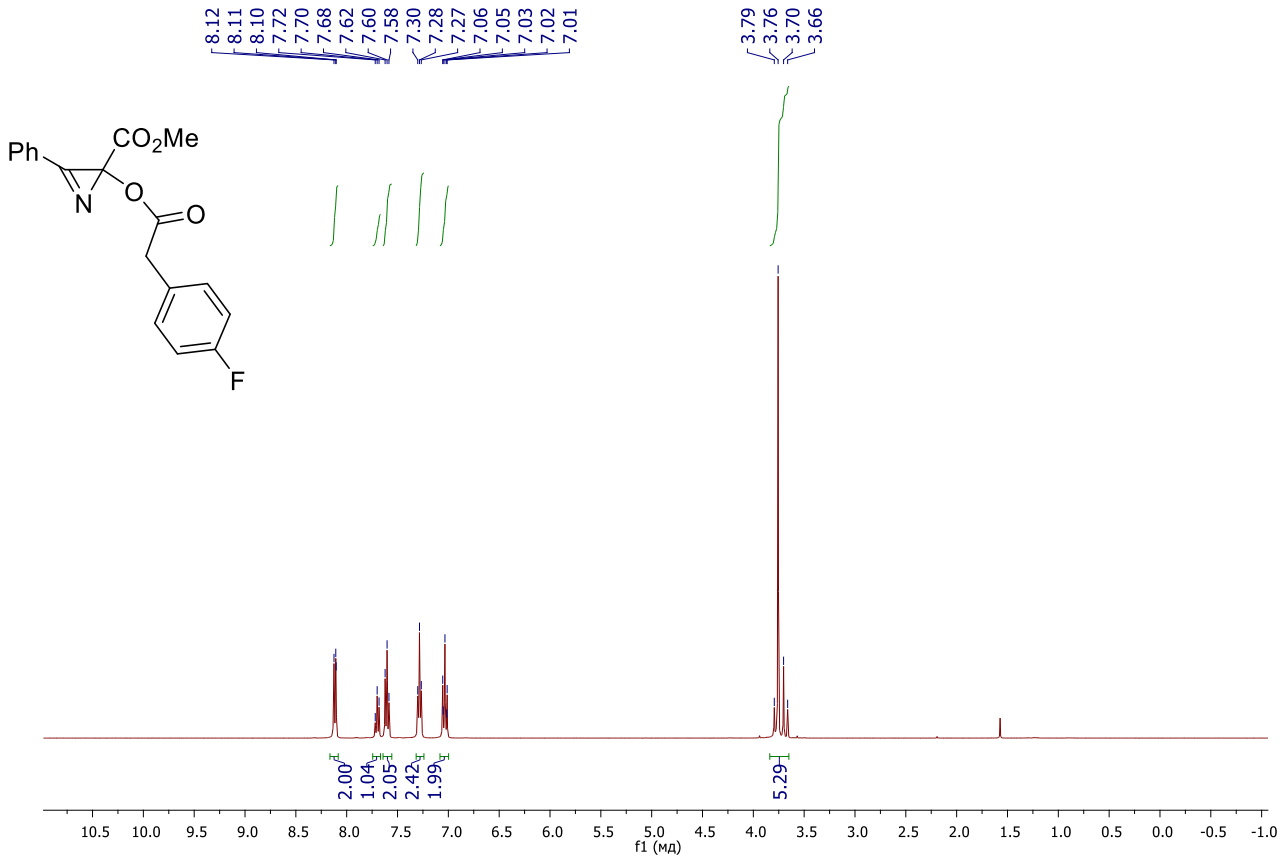
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of **3zo**



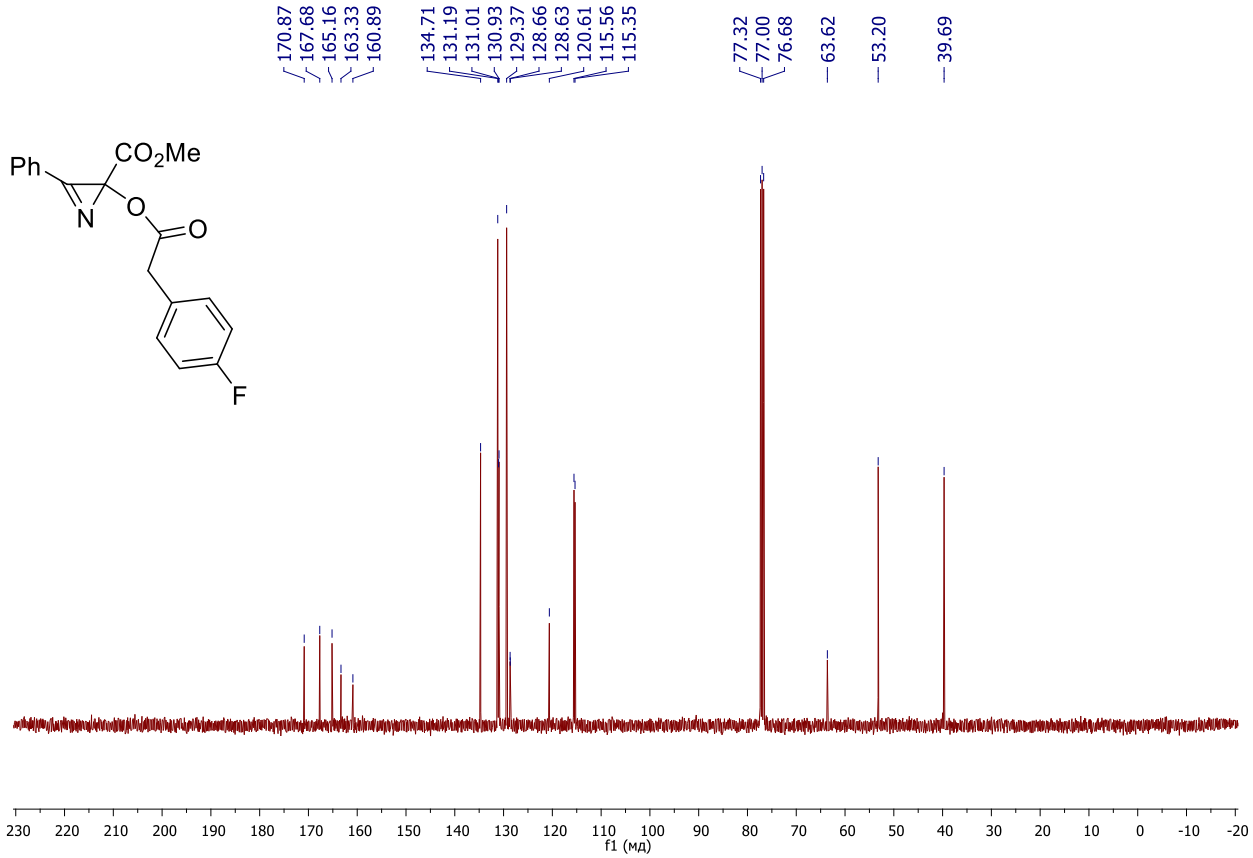
^{13}C ^{13}C NMR (100 MHz, $CDCl_3$) spectrum of **3zo**



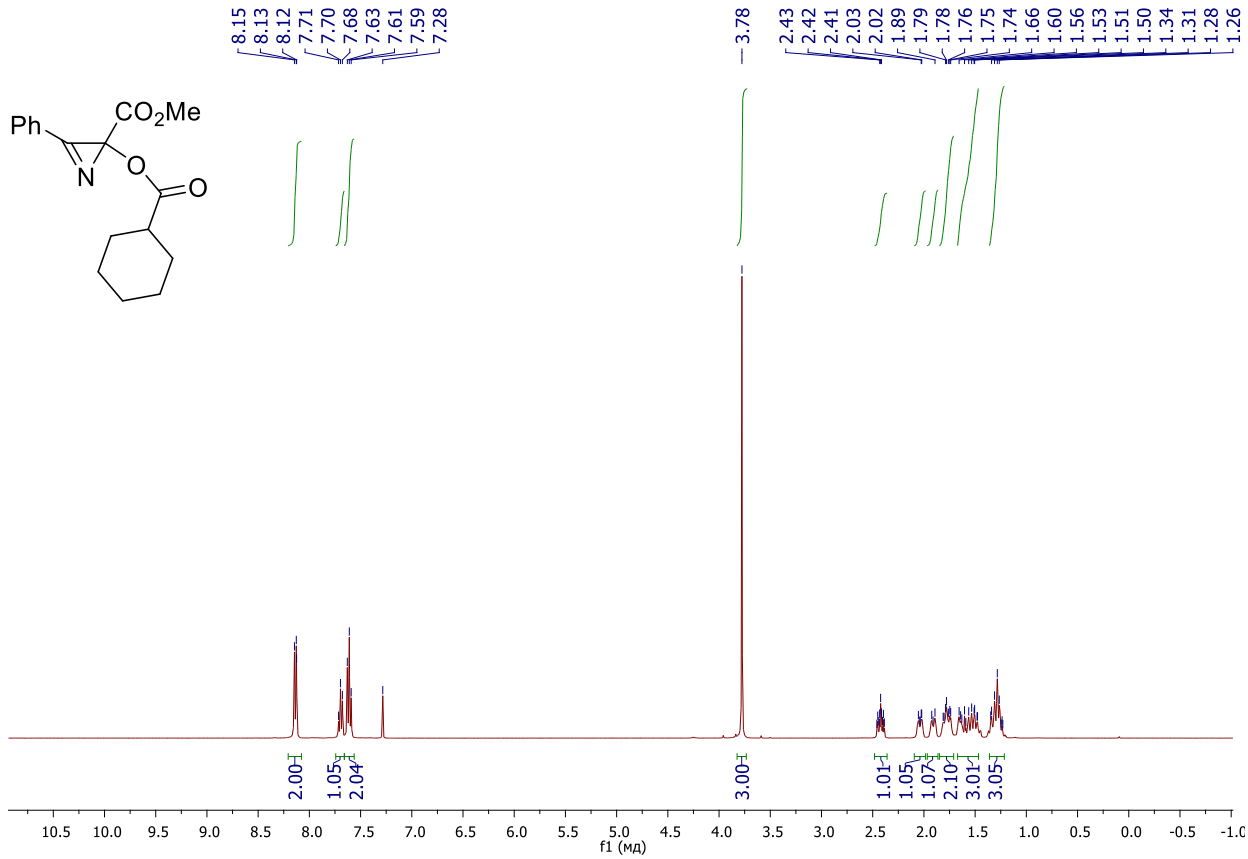
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of **3zp**



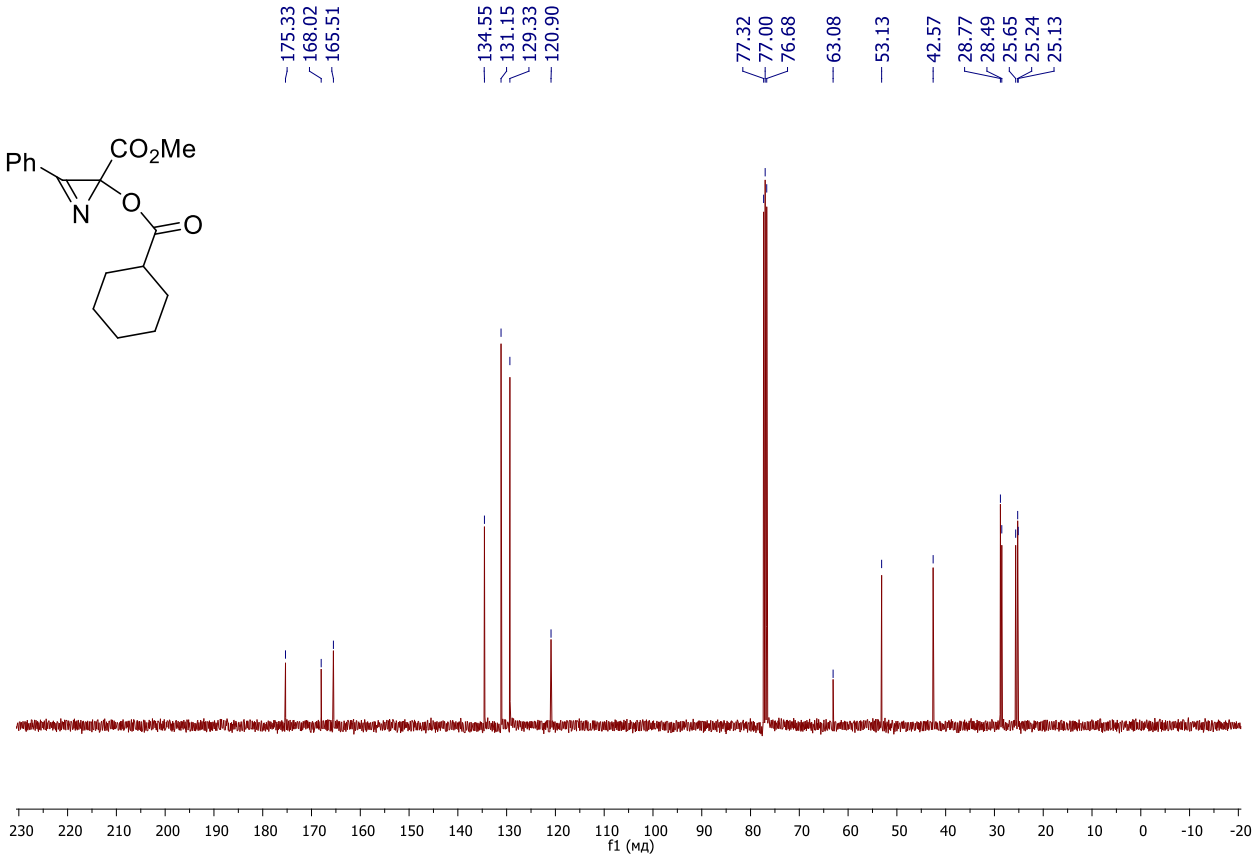
^{13}C NMR (100 MHz, $CDCl_3$) spectrum of **3zp**



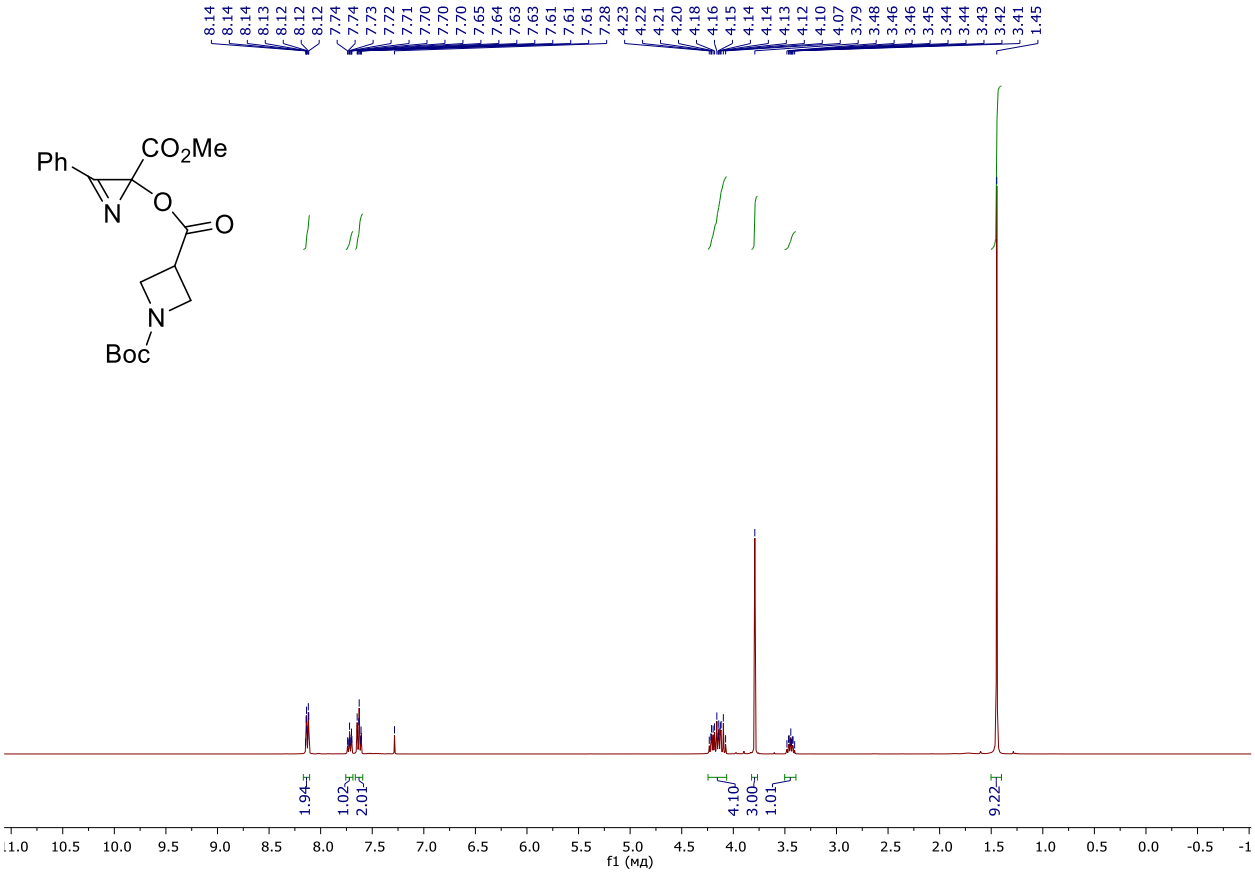
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of **3zq**



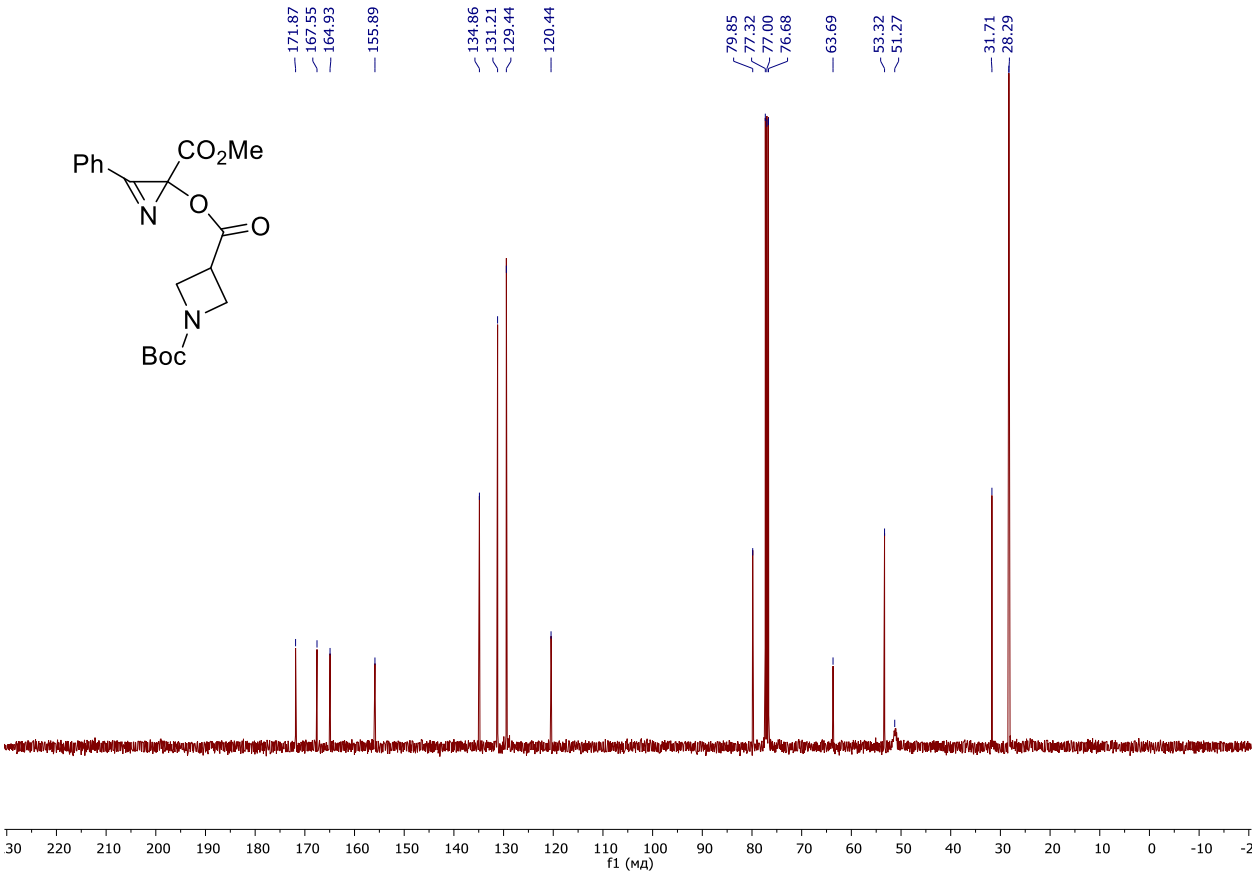
^{13}C NMR (100 MHz, $CDCl_3$) spectrum of **3zq**



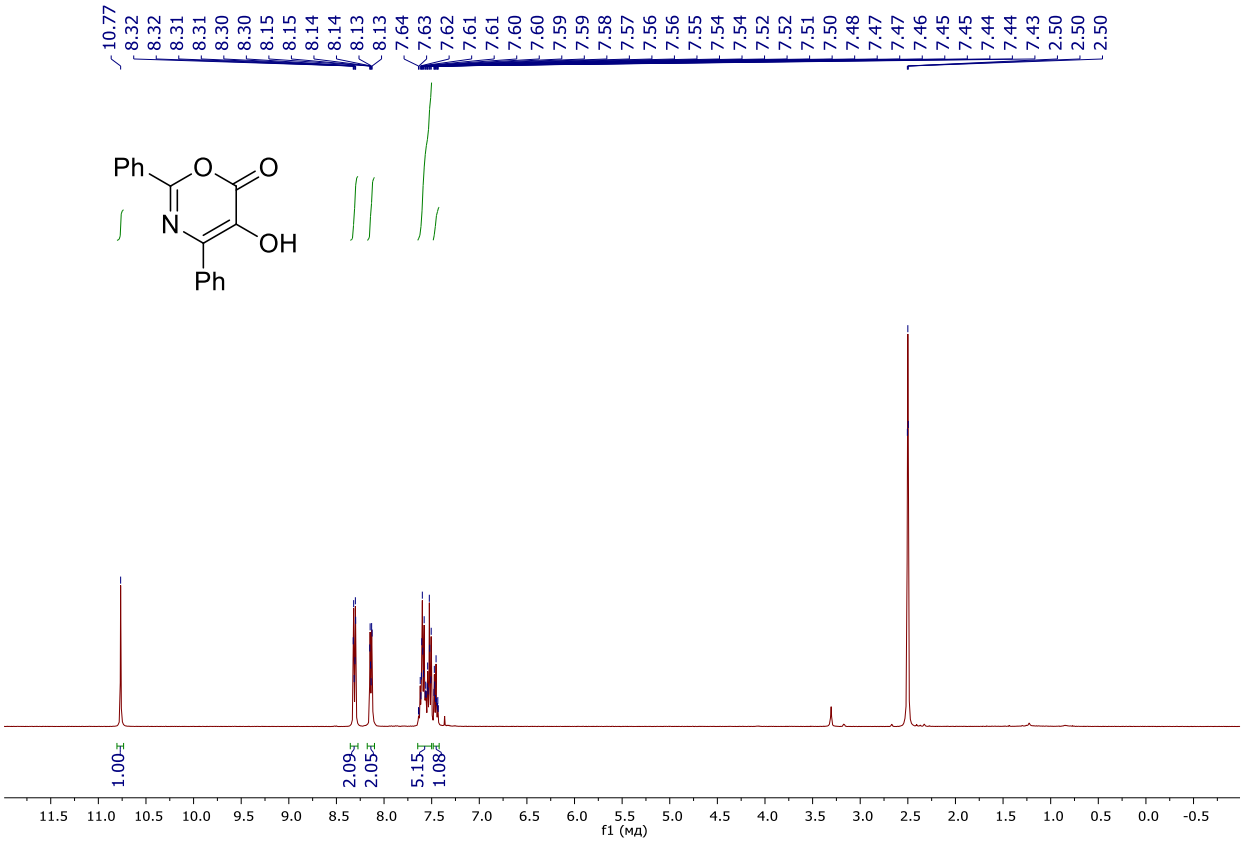
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of **3zr**



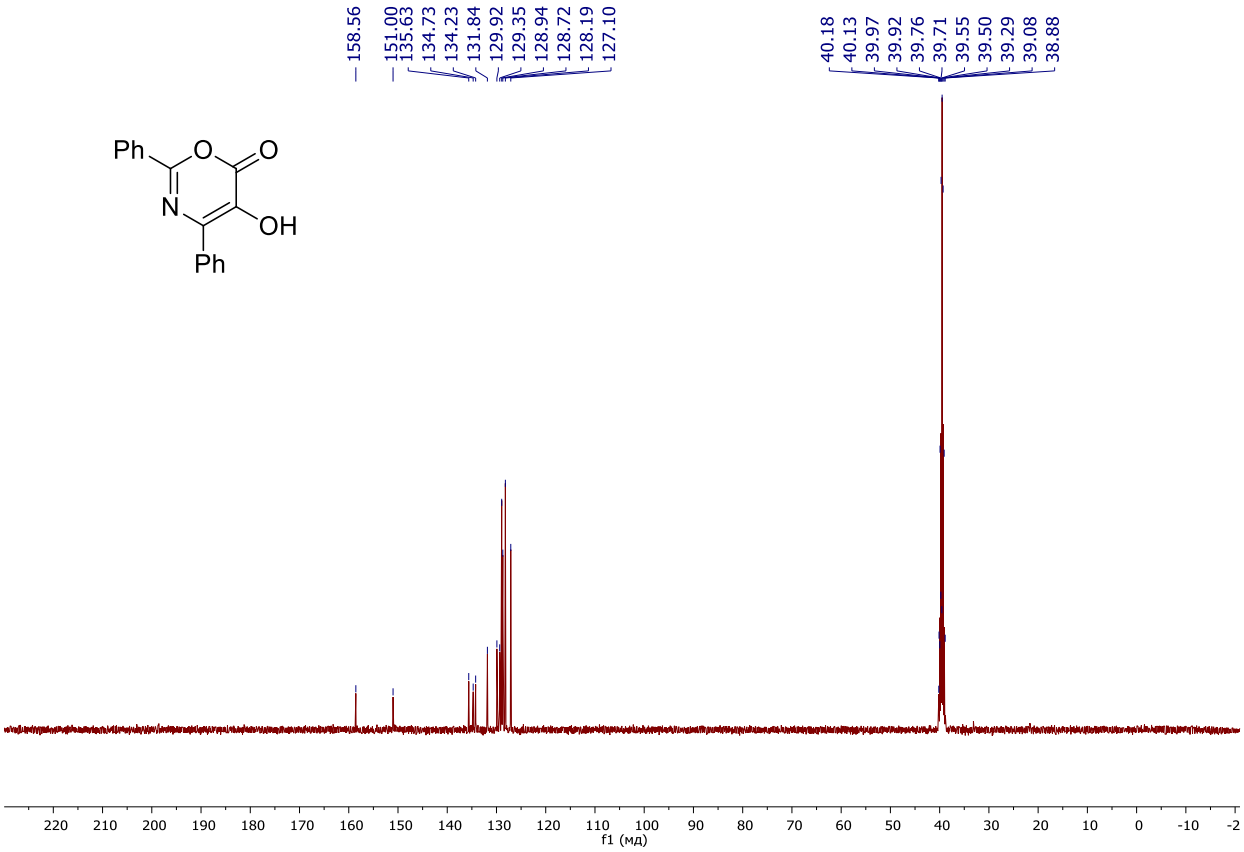
^{13}C NMR (100 MHz, $CDCl_3$) spectrum of **3zr**



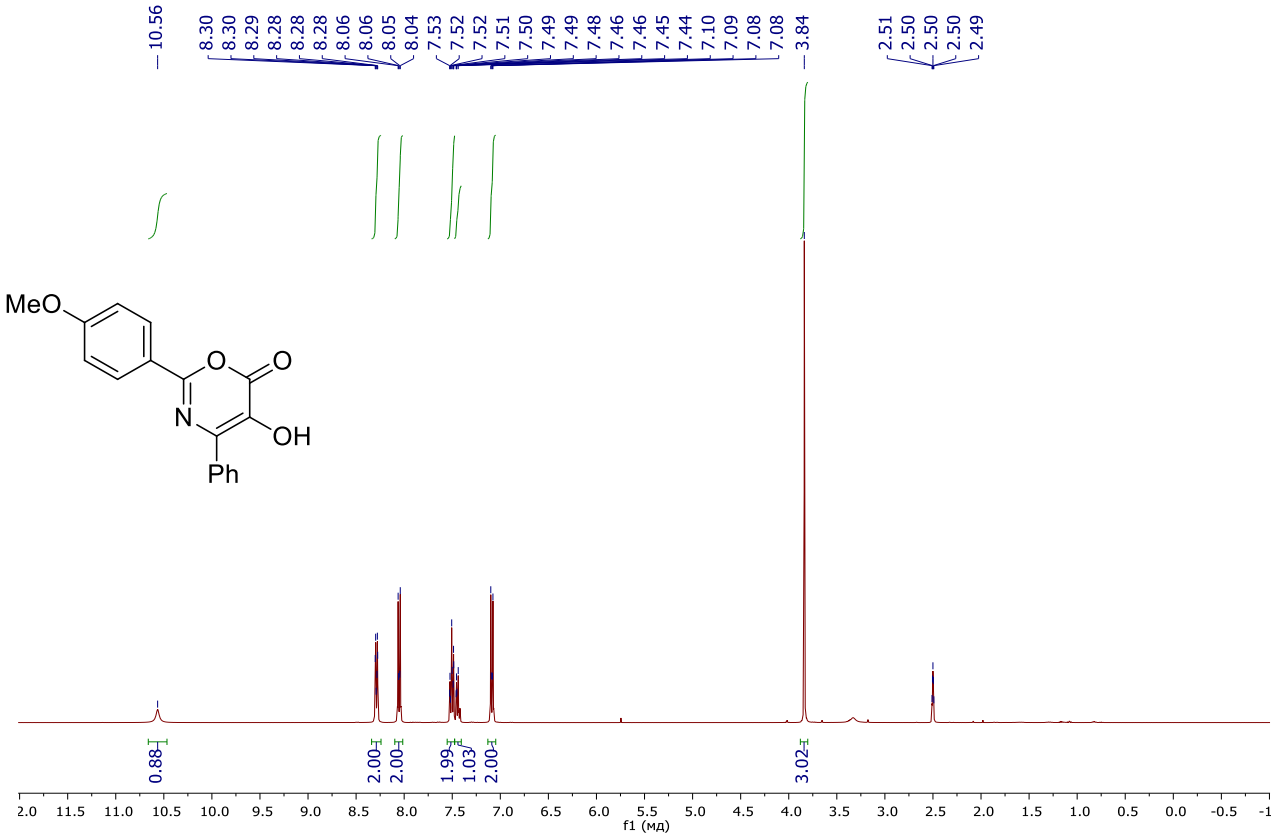
^{1}H NMR (400 MHz, DMSO-d_6) spectrum of **4a**



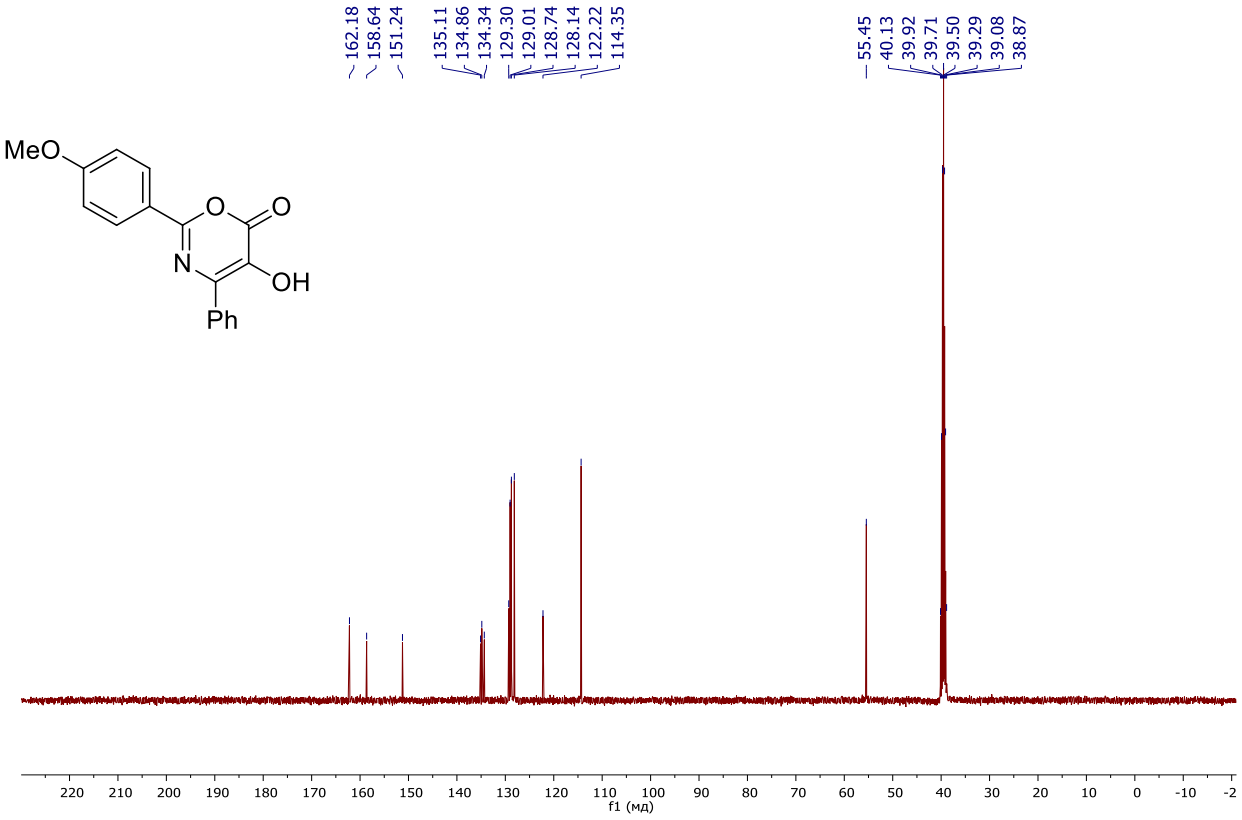
^{13}C NMR (100 MHz, DMSO-d_6) spectrum of **4a**



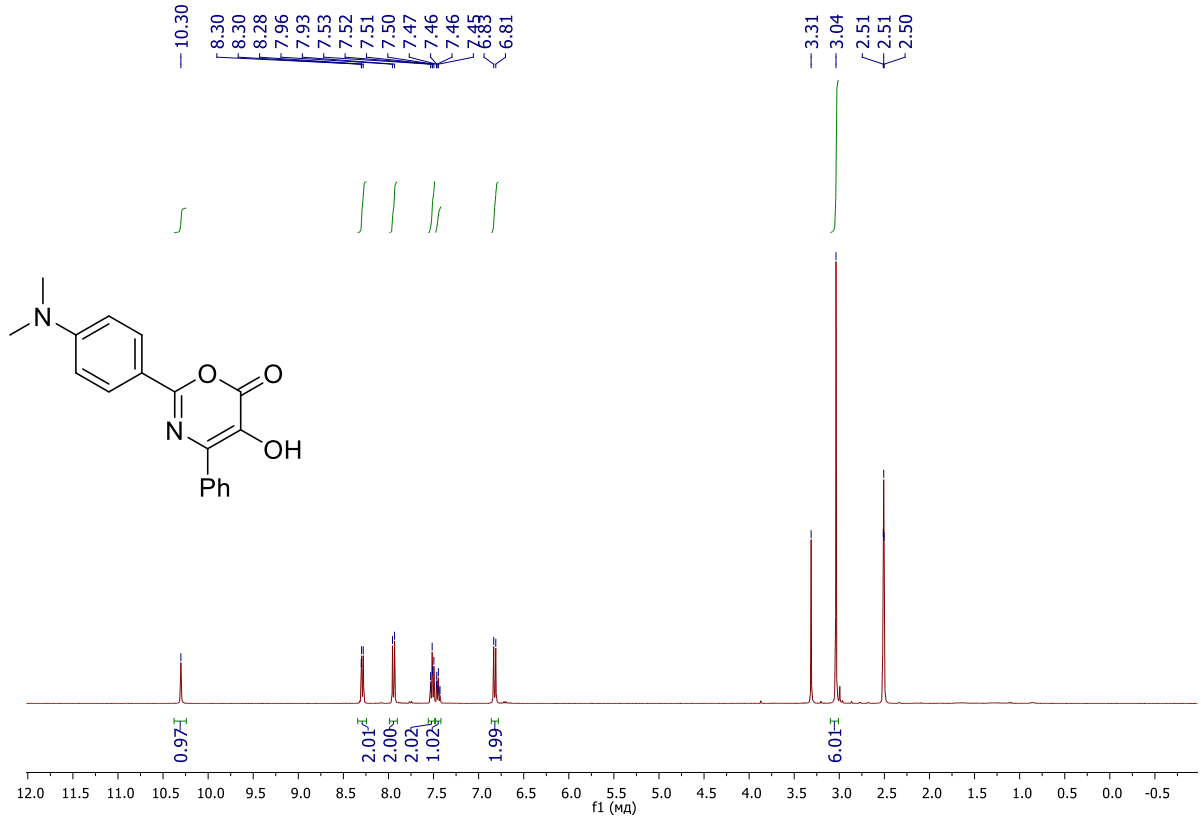
^{1}H NMR (400 MHz, DMSO-d_6) spectrum of **4b**



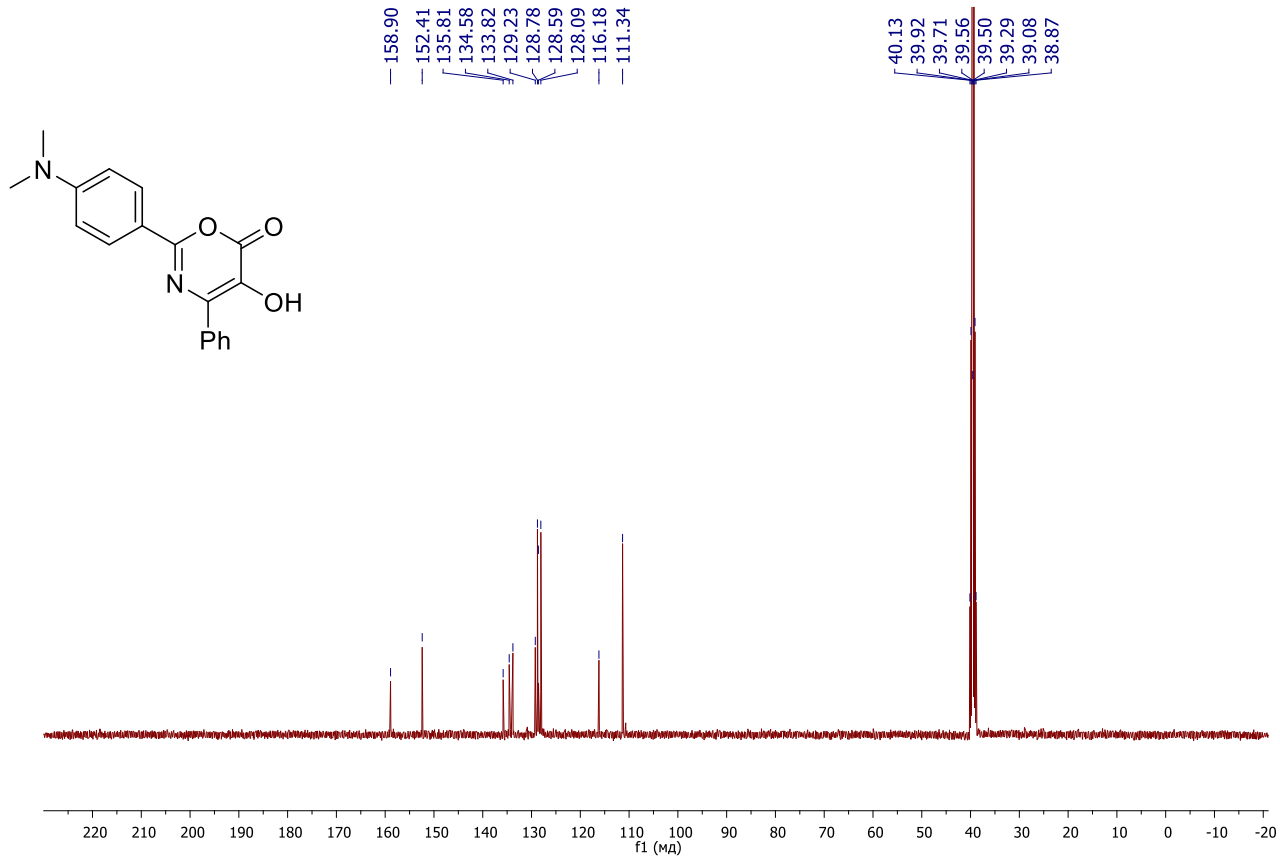
^{13}C NMR (100 MHz, DMSO-d_6) spectrum of **4b**



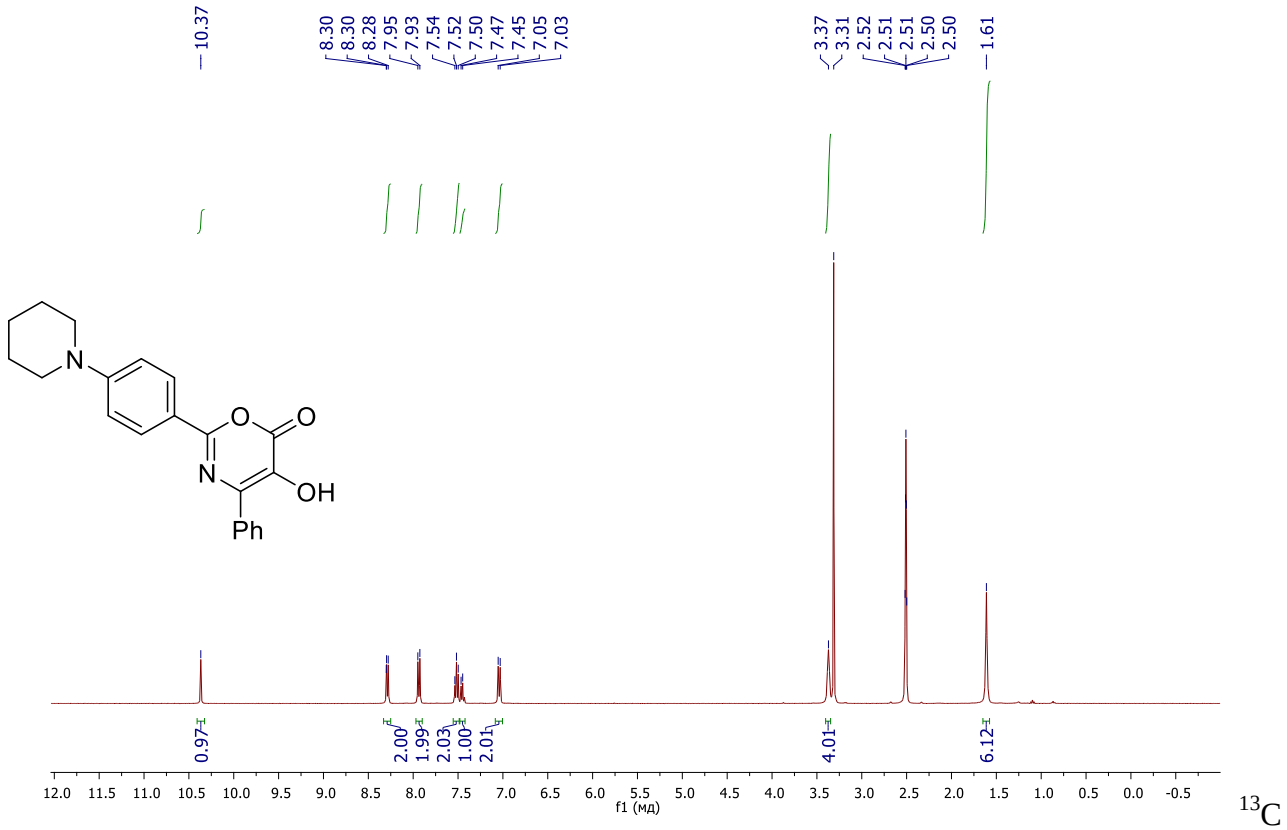
^{1}H NMR (400 MHz, DMSO-d_6) spectrum of **4c**



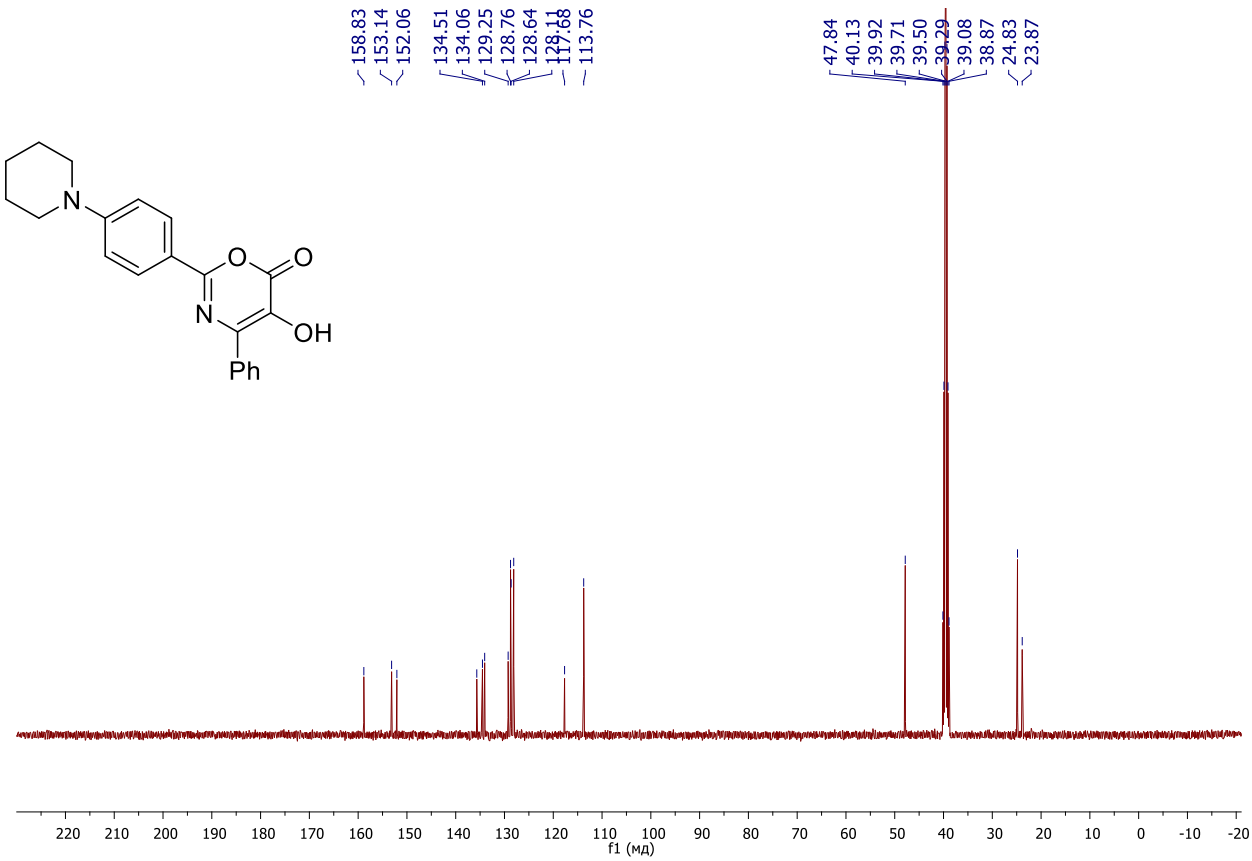
^{13}C NMR (100 MHz, DMSO-d_6) spectrum of **4c**



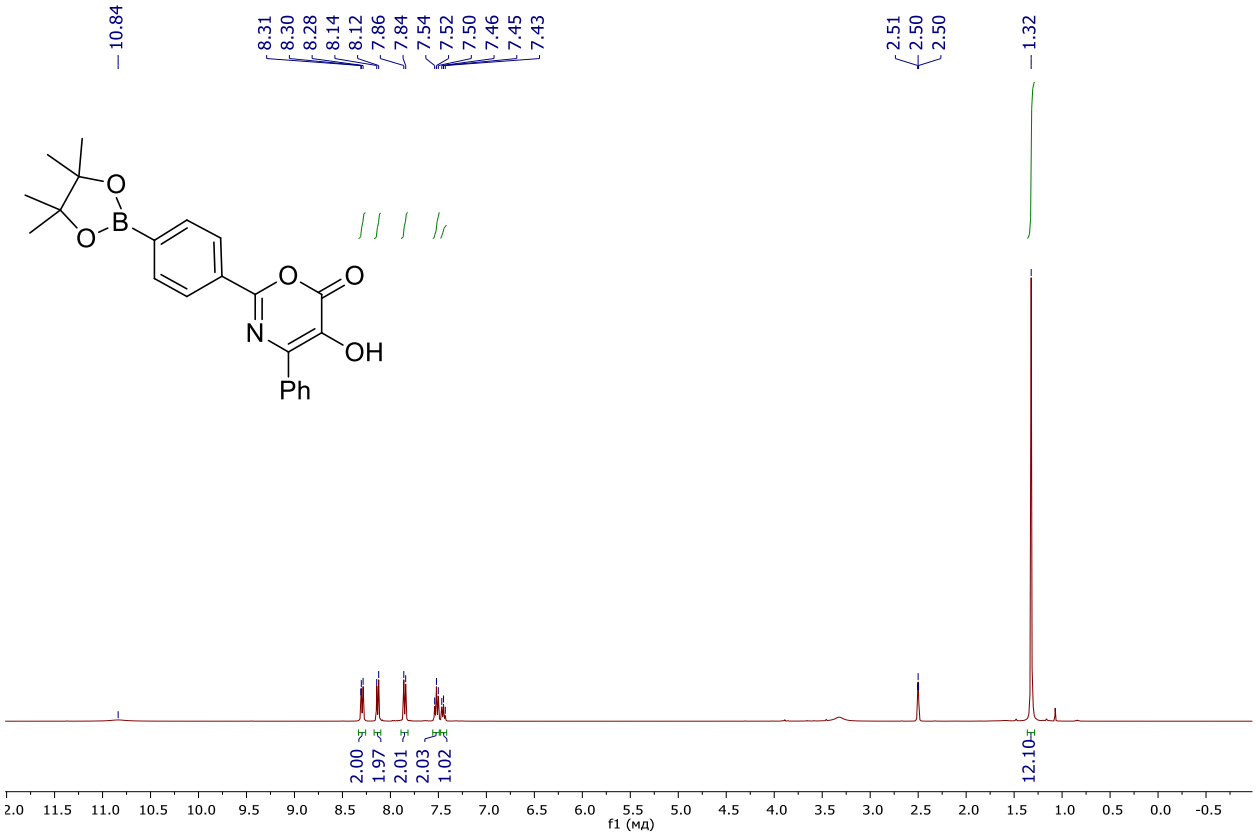
^{1}H NMR (400 MHz, DMSO-d_6) spectrum of **4d**



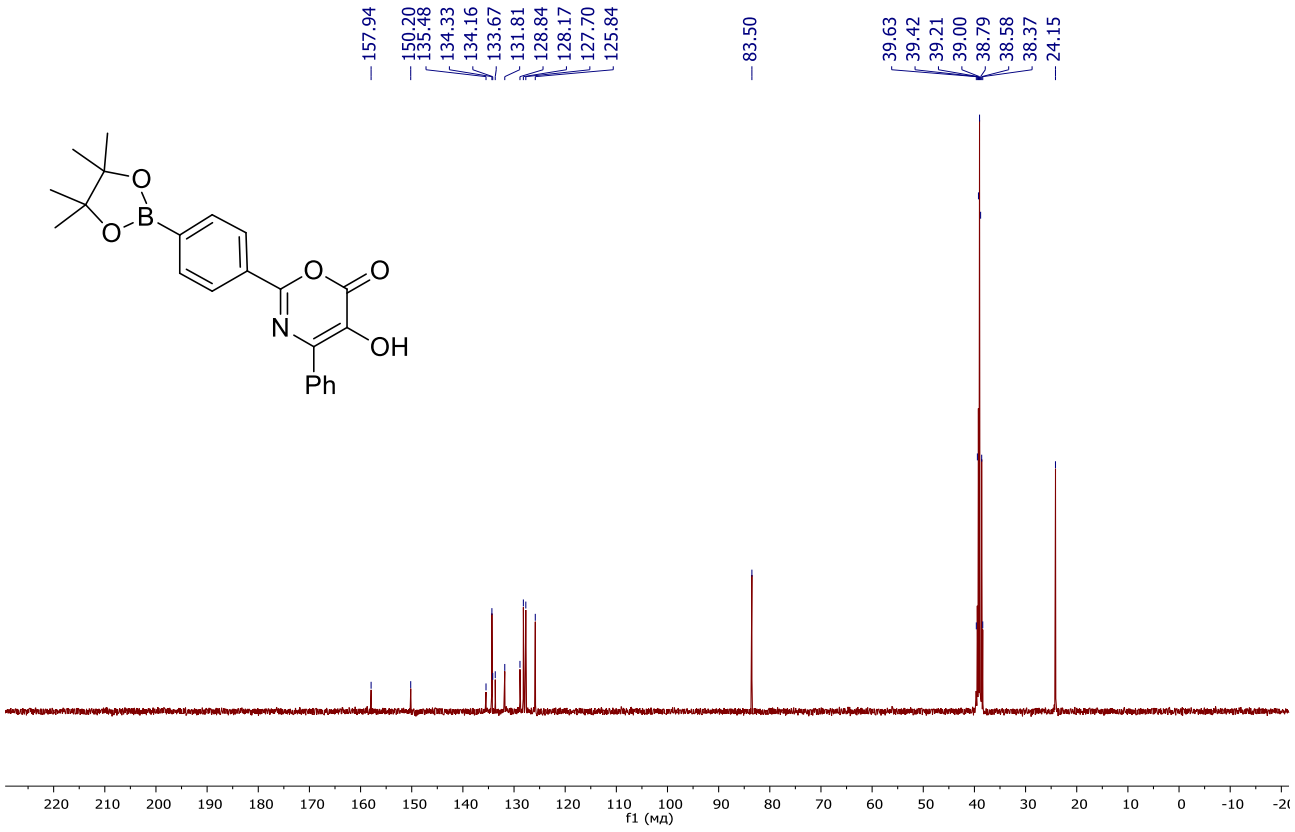
^{13}C NMR (100 MHz, DMSO-d_6) spectrum of **4d**



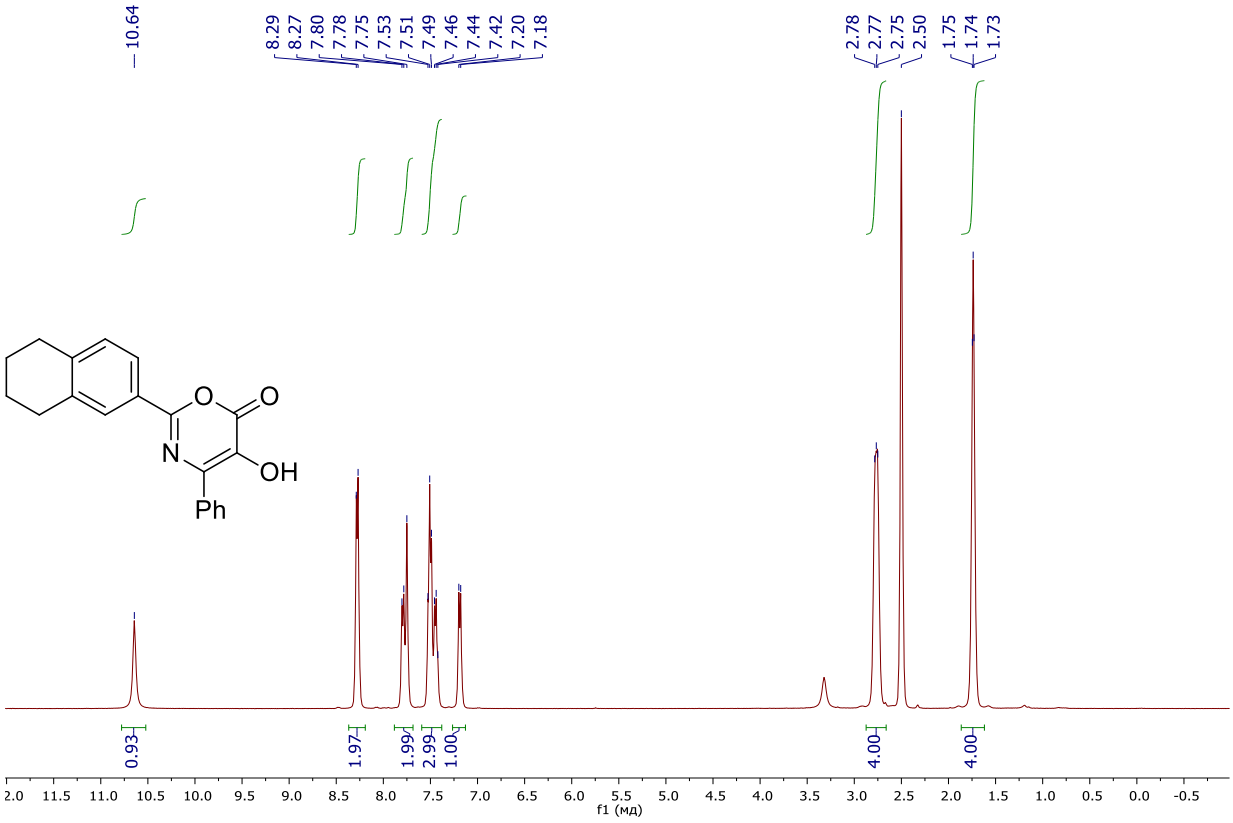
^{1}H NMR (400 MHz, DMSO-d_6) spectrum of **4e**



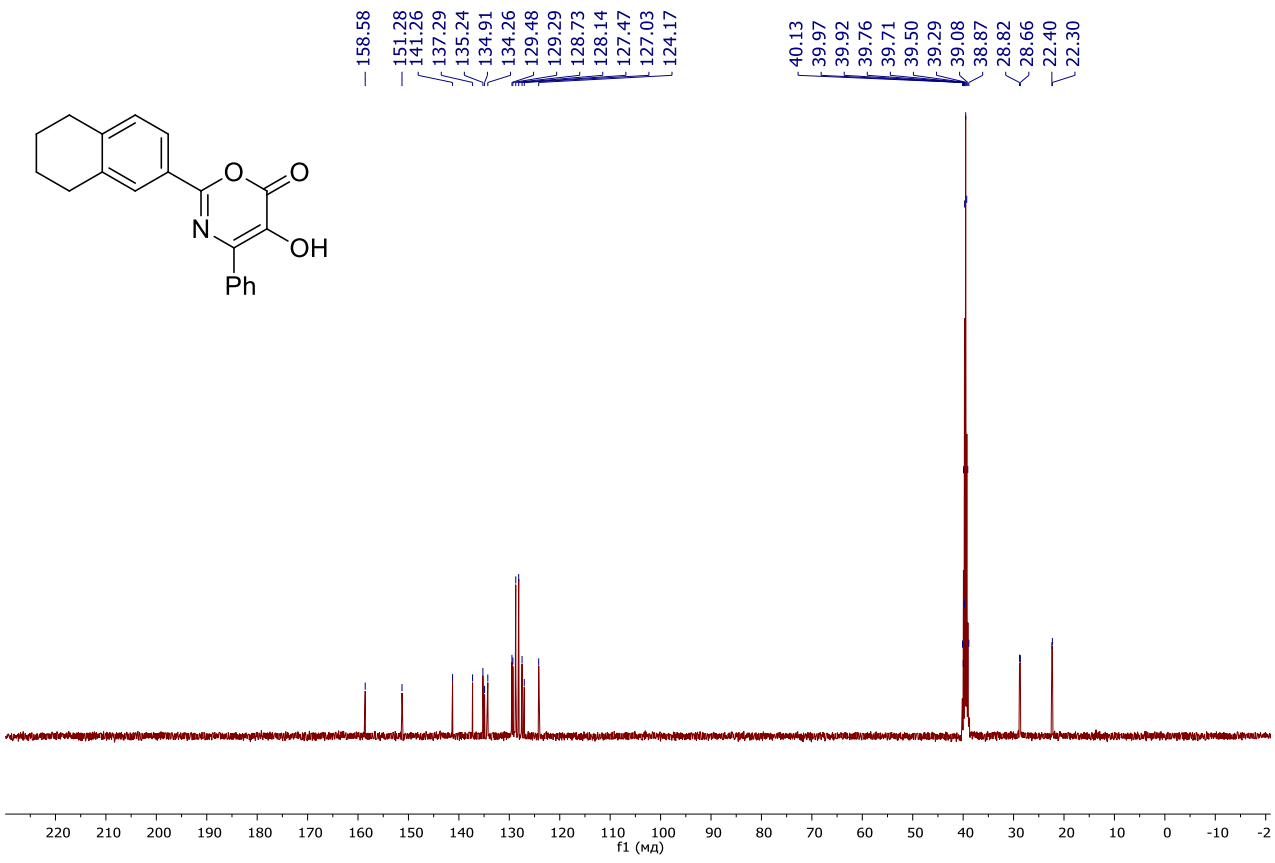
^{13}C NMR (100 MHz, DMSO-d_6) spectrum of **4e**



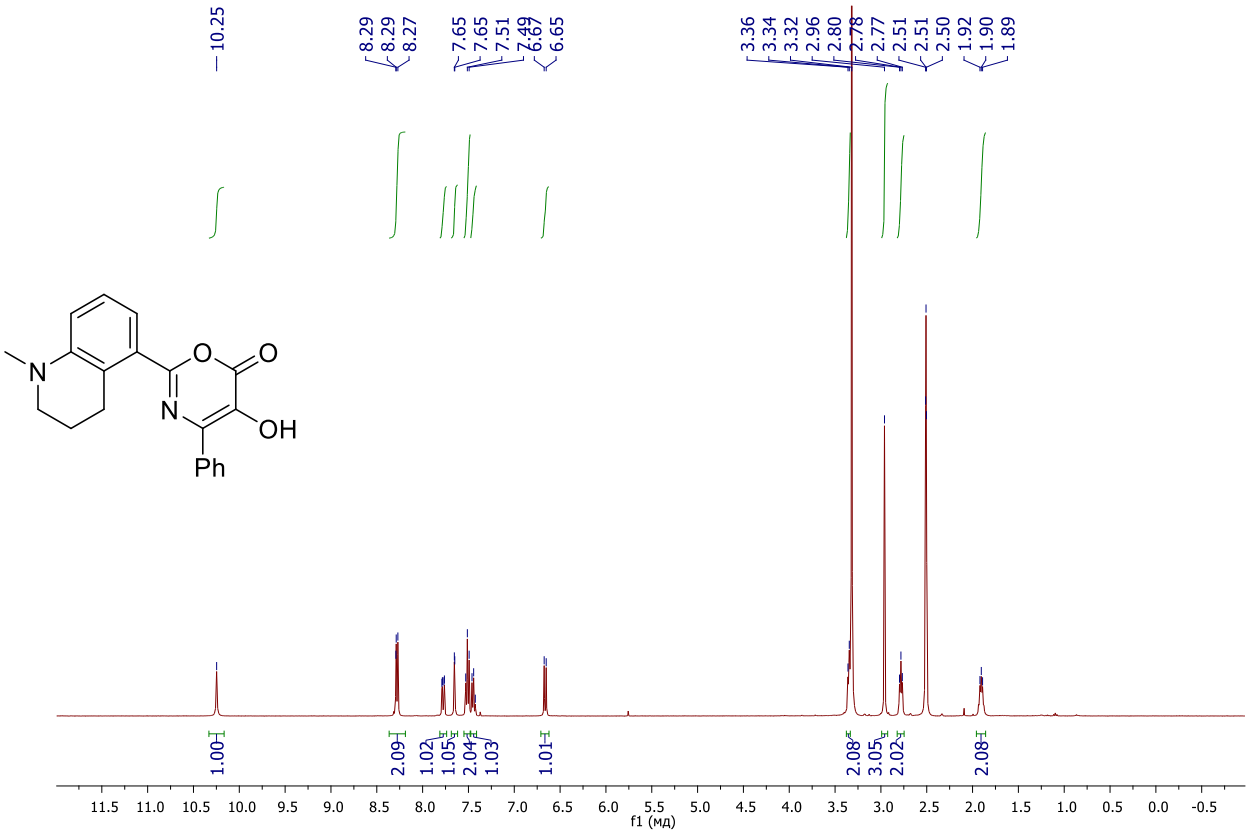
^{1}H NMR (400 MHz, DMSO-d_6) spectrum of **4f**



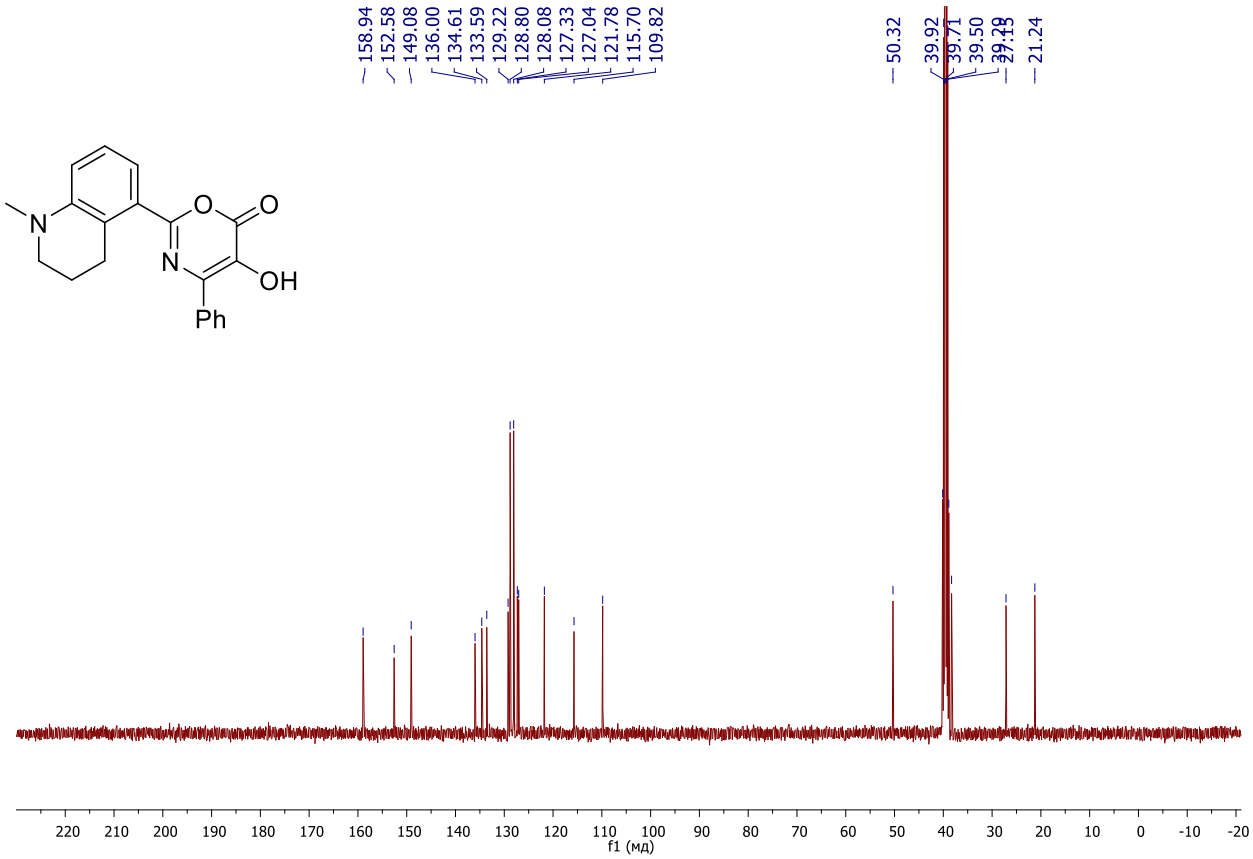
^{13}C NMR (100 MHz, DMSO-d_6) spectrum of **4f**



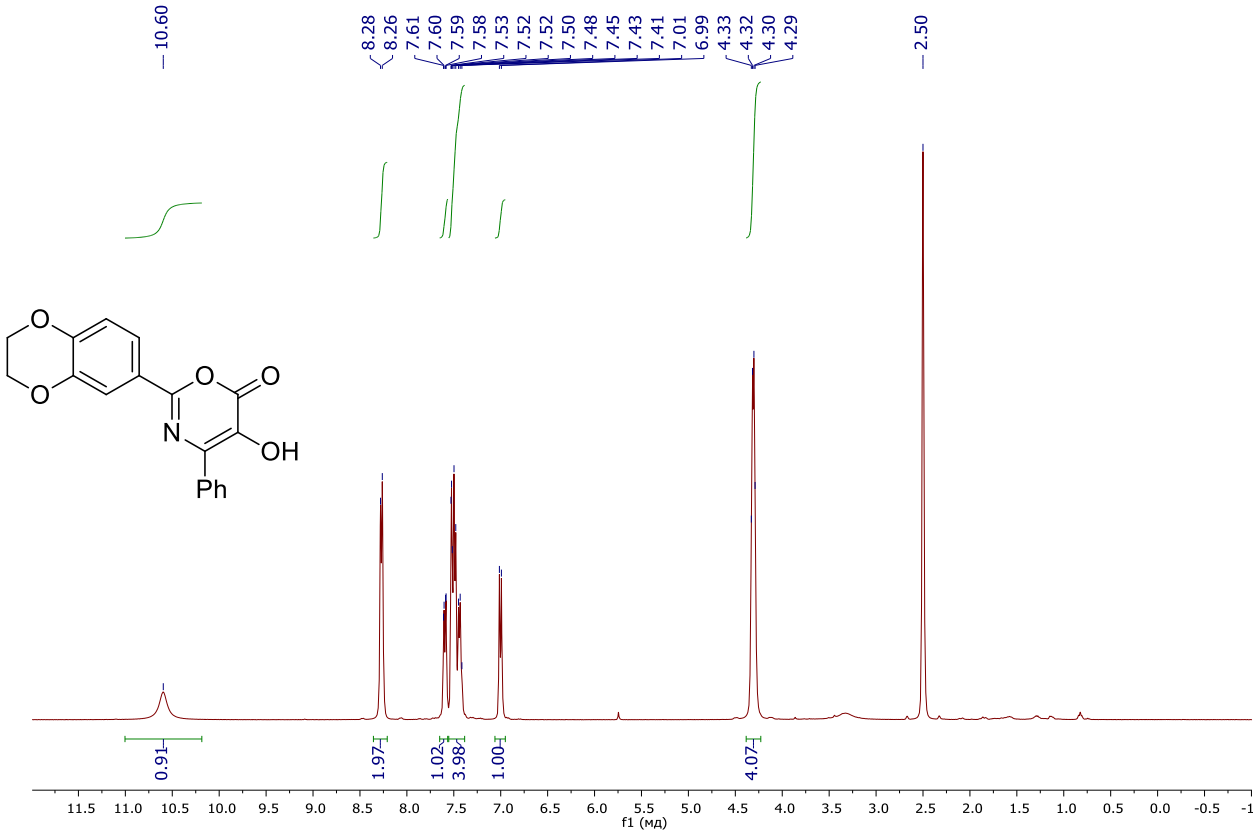
^{1}H NMR (400 MHz, DMSO-d_6) spectrum of **4g**



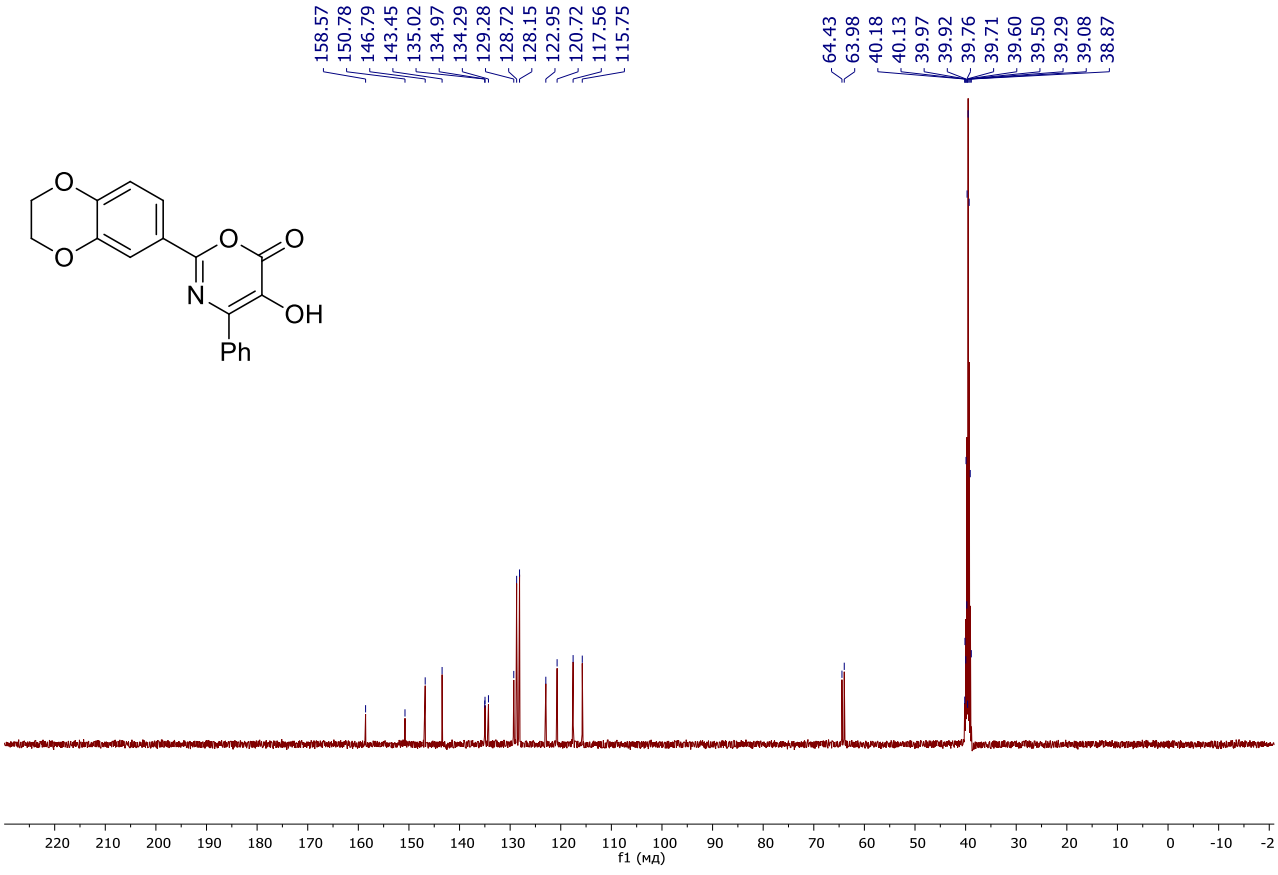
^{13}C NMR (100 MHz, DMSO-d_6) spectrum of **4g**



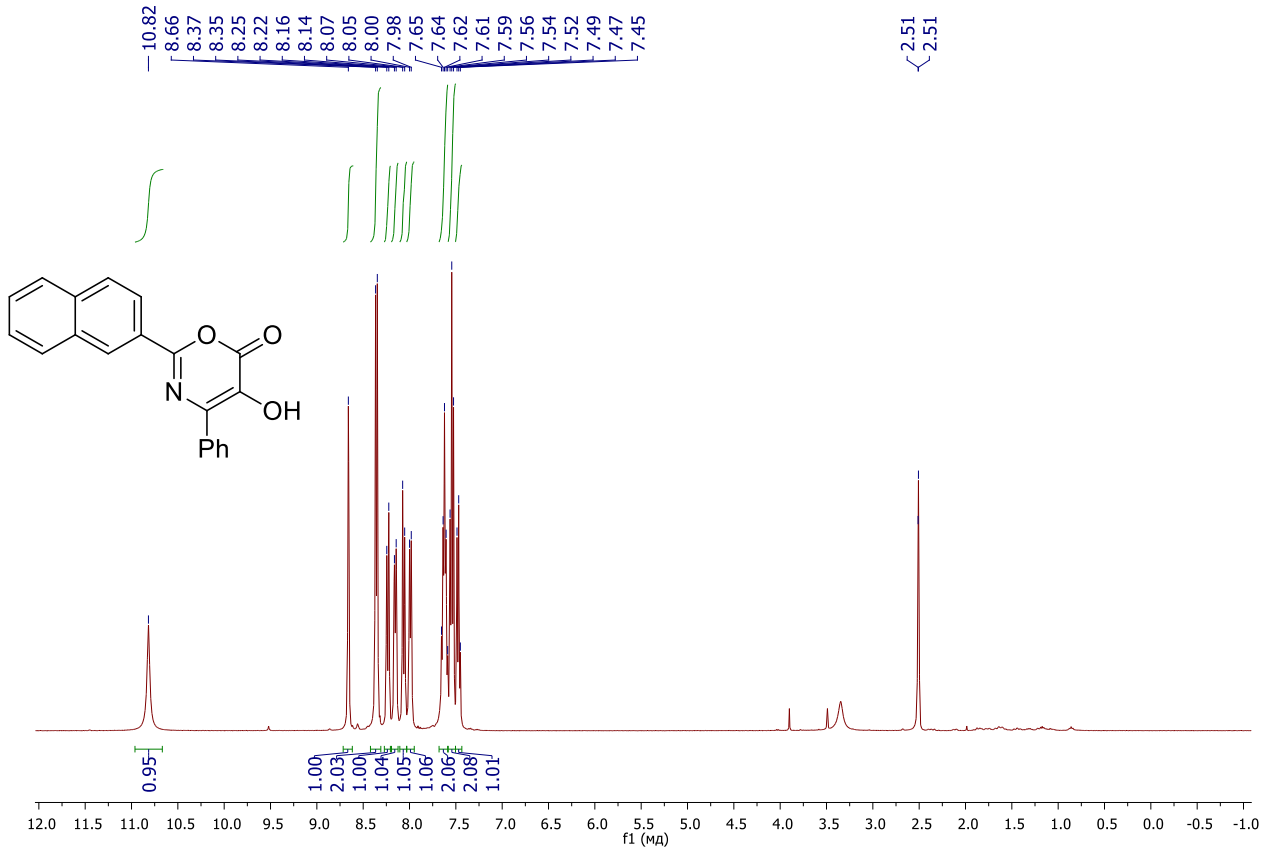
^{1}H NMR (400 MHz, DMSO-d_6) spectrum of **4h**



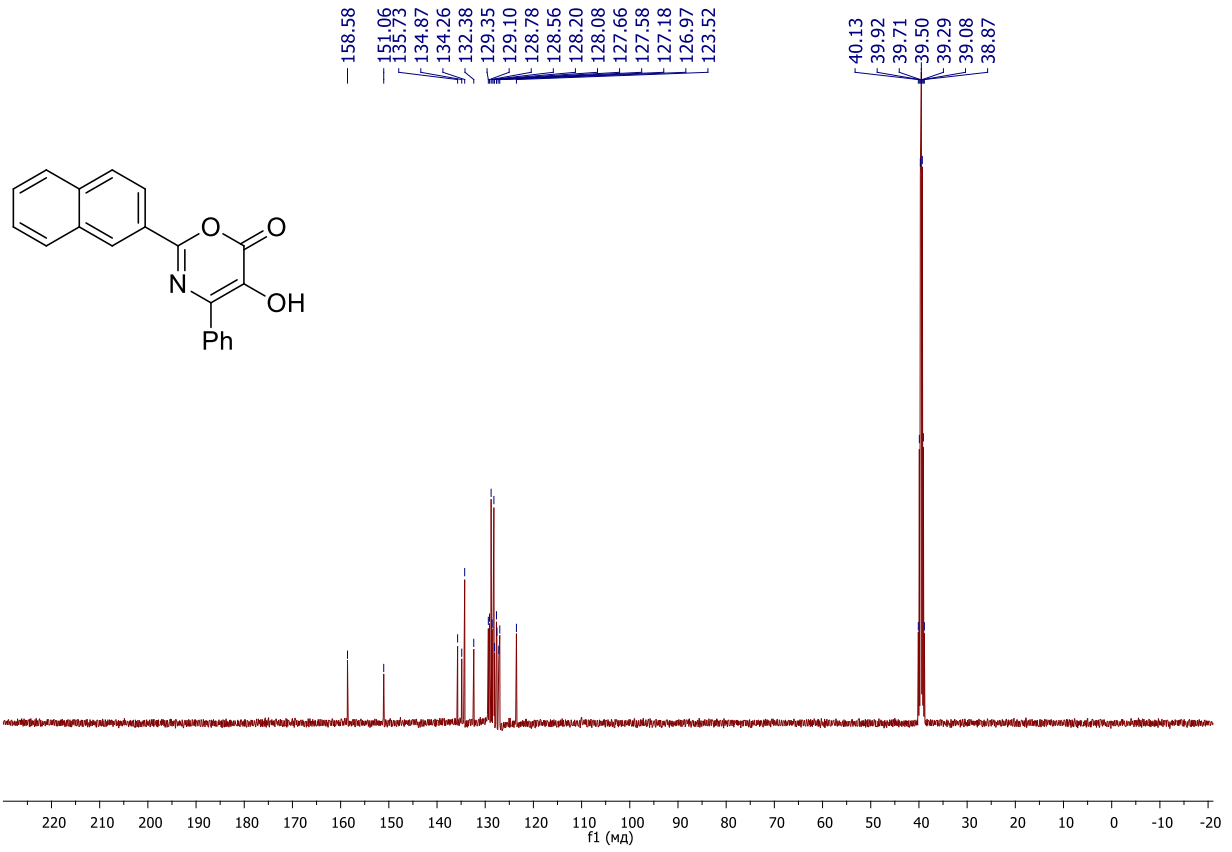
^{13}C NMR (100 MHz, DMSO-d_6) spectrum of **4h**



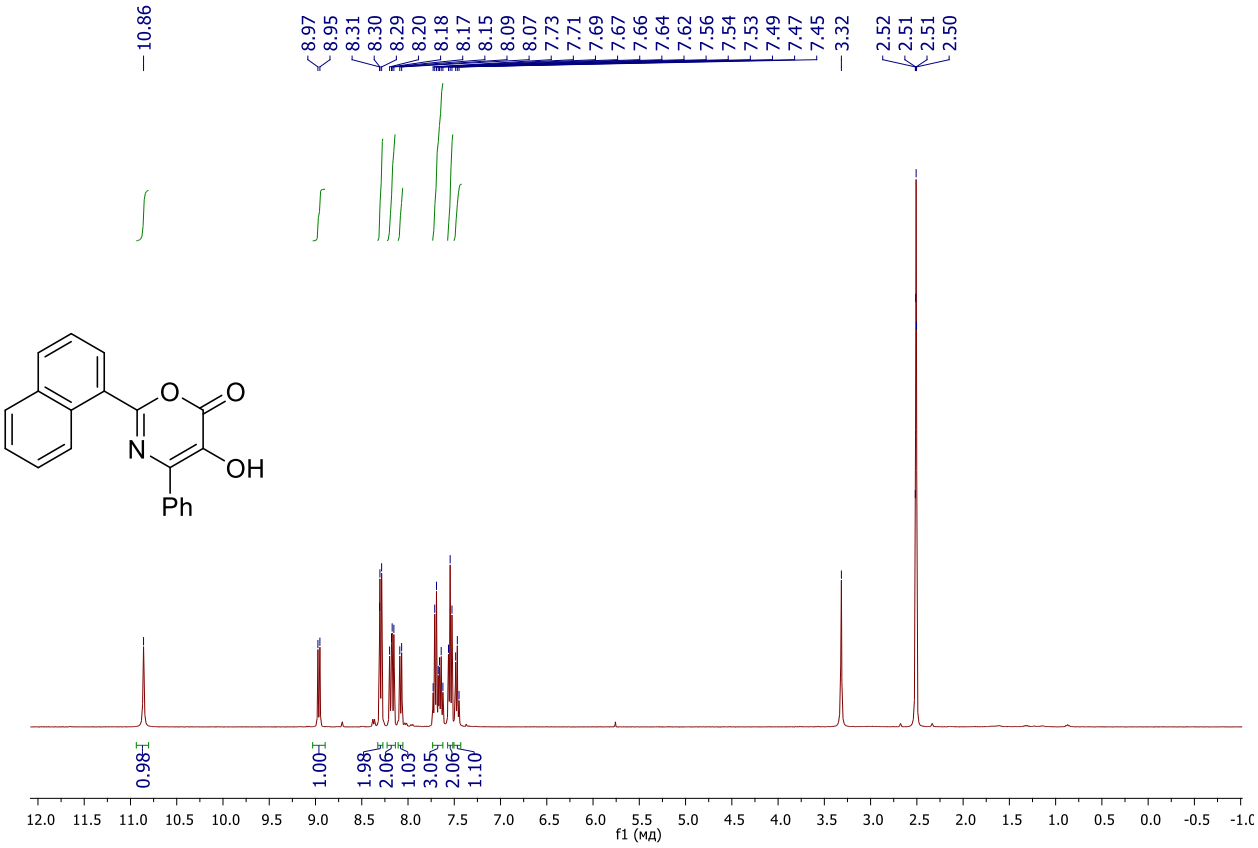
^{1}H NMR (400 MHz, DMSO-d_6) spectrum of **4i**



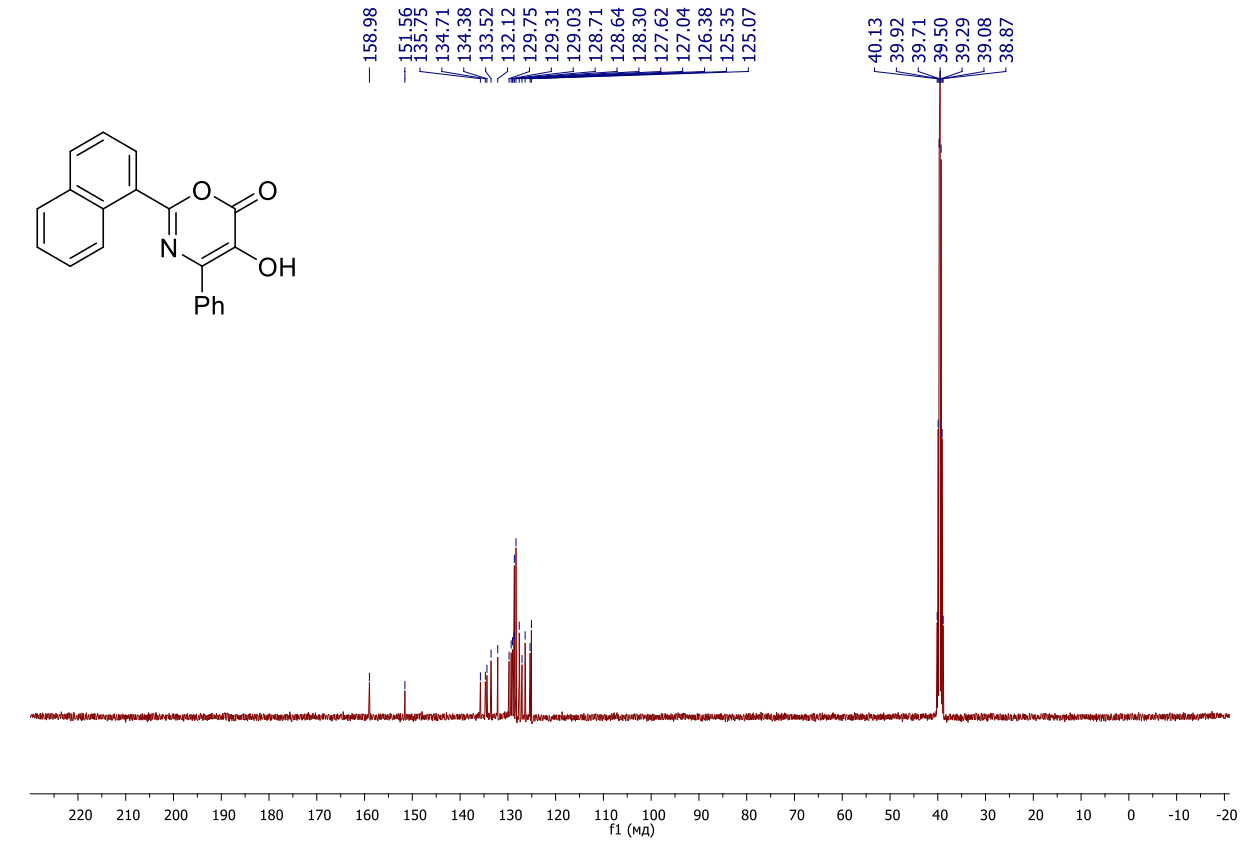
^{13}C NMR (100 MHz, DMSO-d_6) spectrum of **4i**



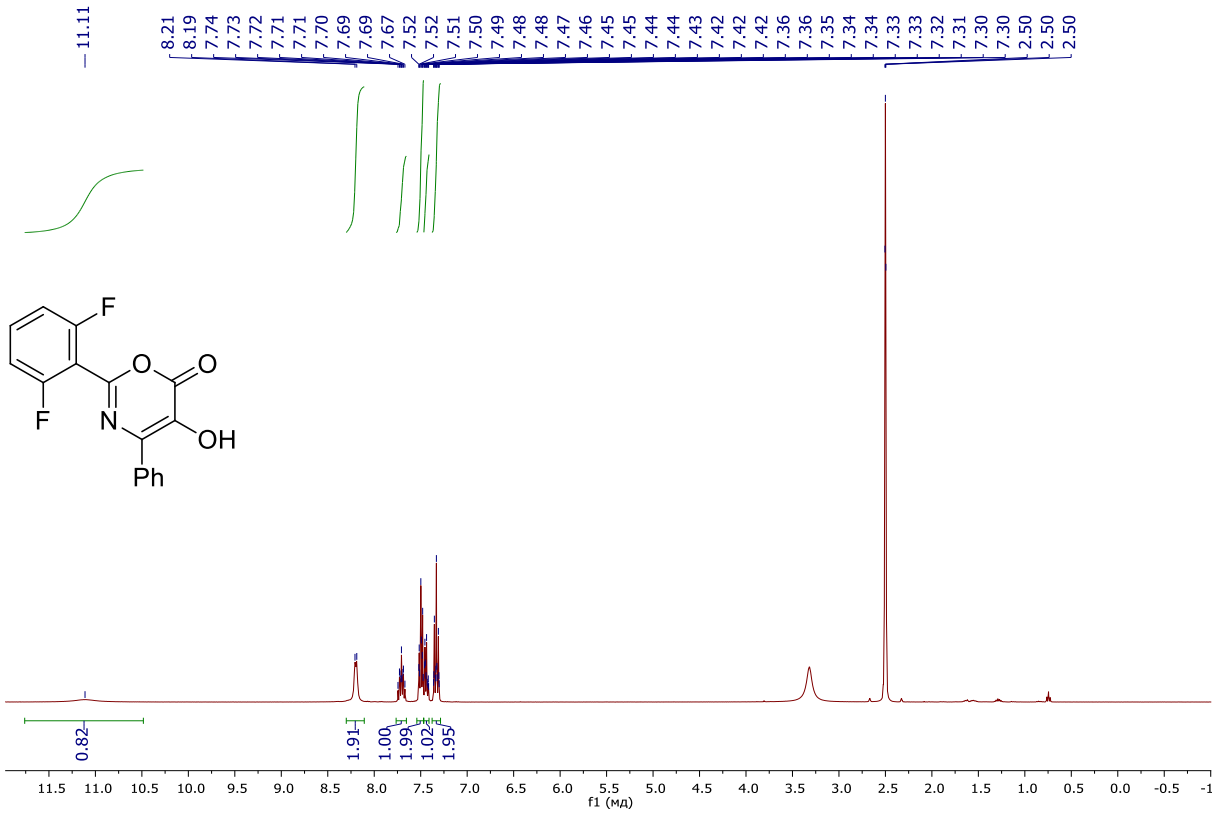
^{1}H NMR (400 MHz, DMSO-d_6) spectrum of **4j**



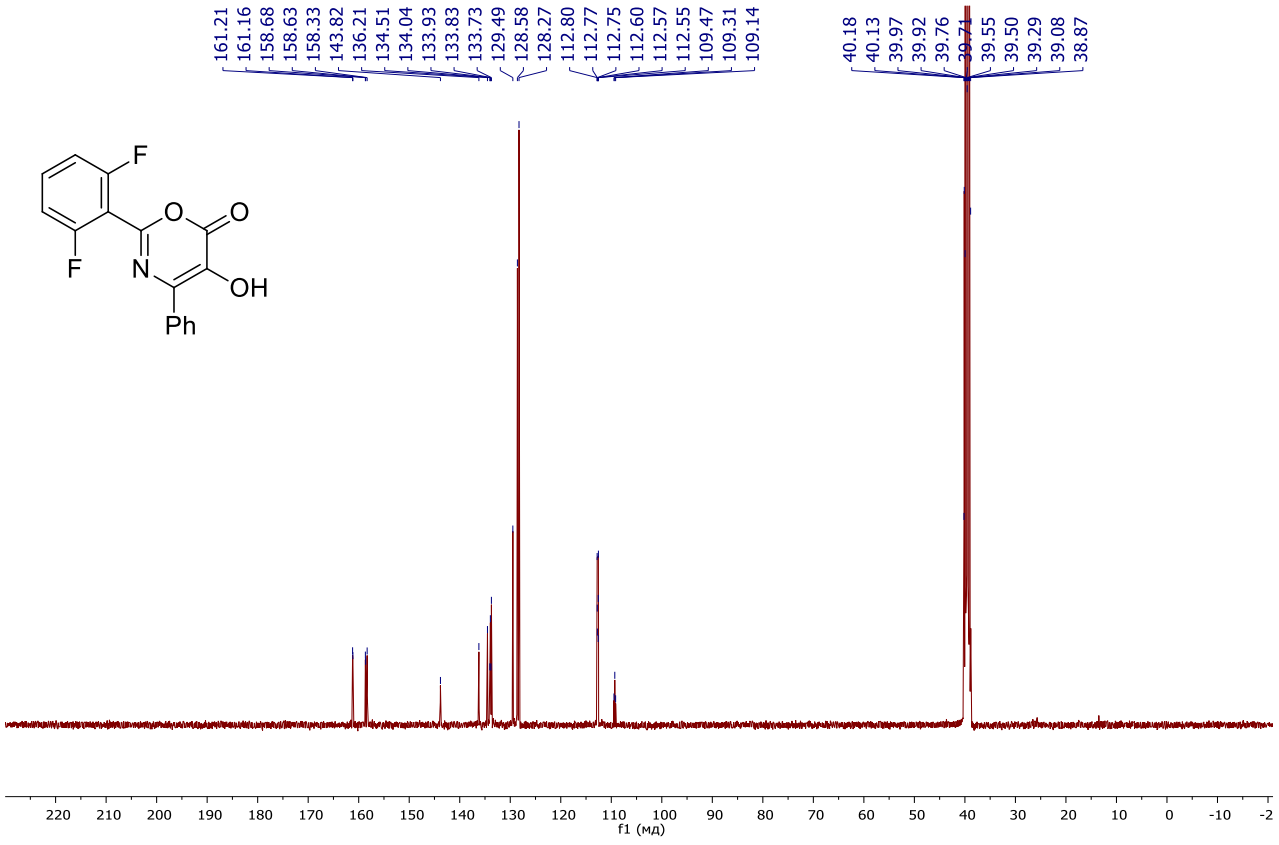
^{13}C NMR (100 MHz, DMSO-d_6) spectrum of **4j**



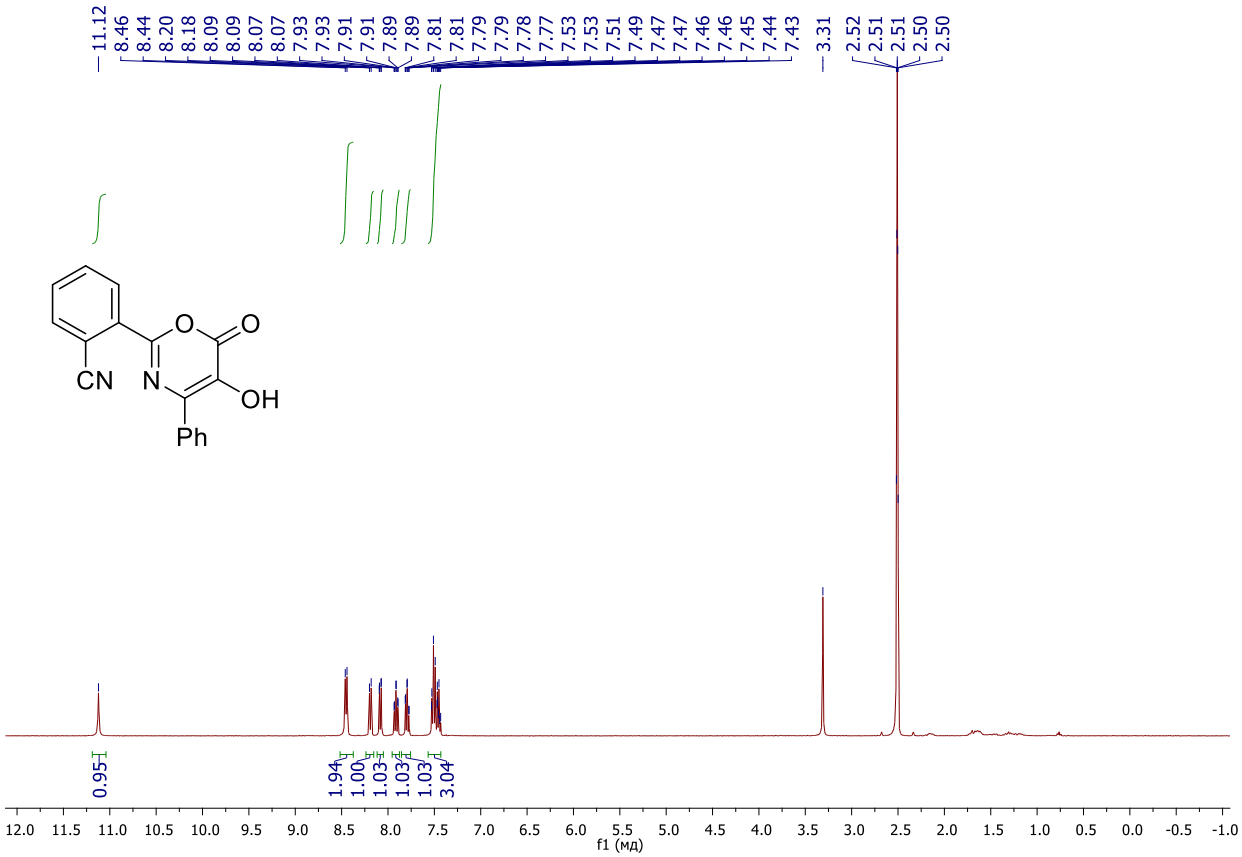
^{1}H NMR (400 MHz, DMSO-d_6) spectrum of **4k**



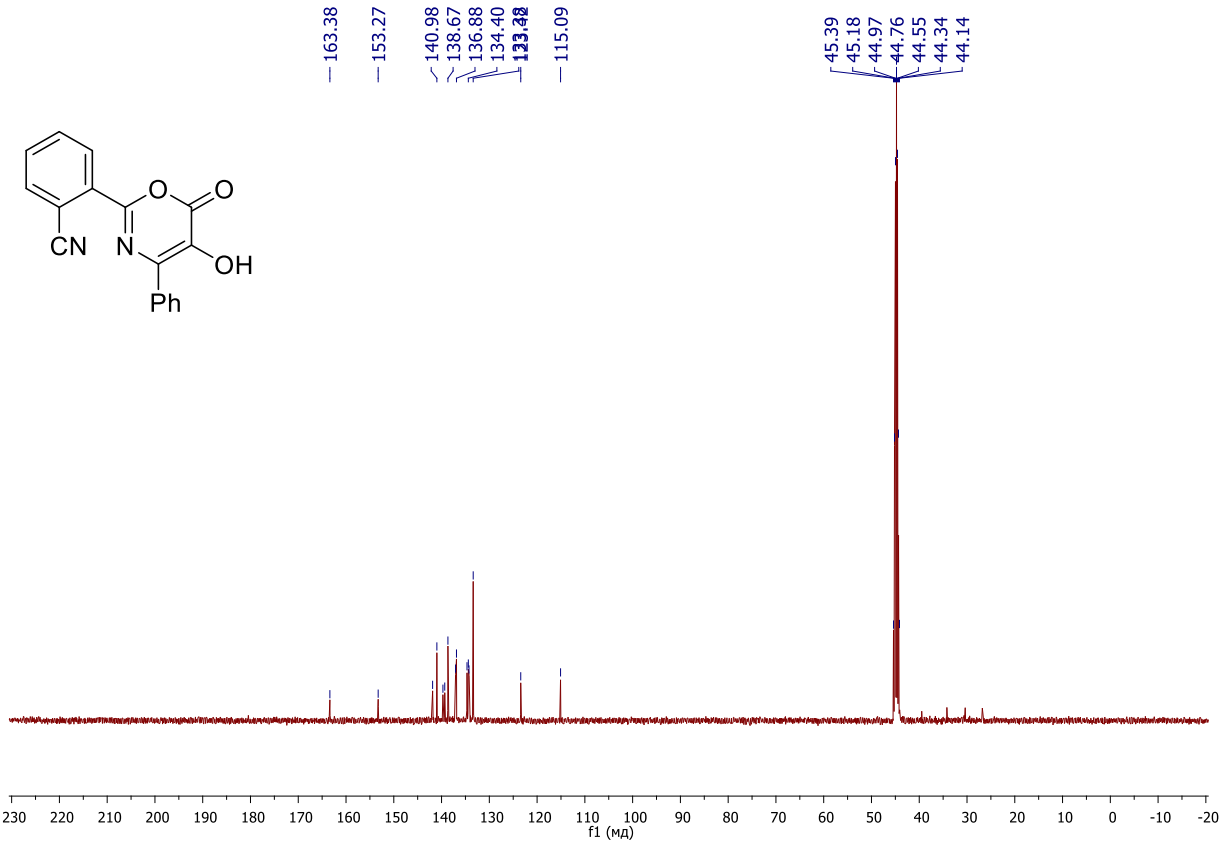
^{13}C NMR (100 MHz, DMSO-d_6) spectrum of **4k**



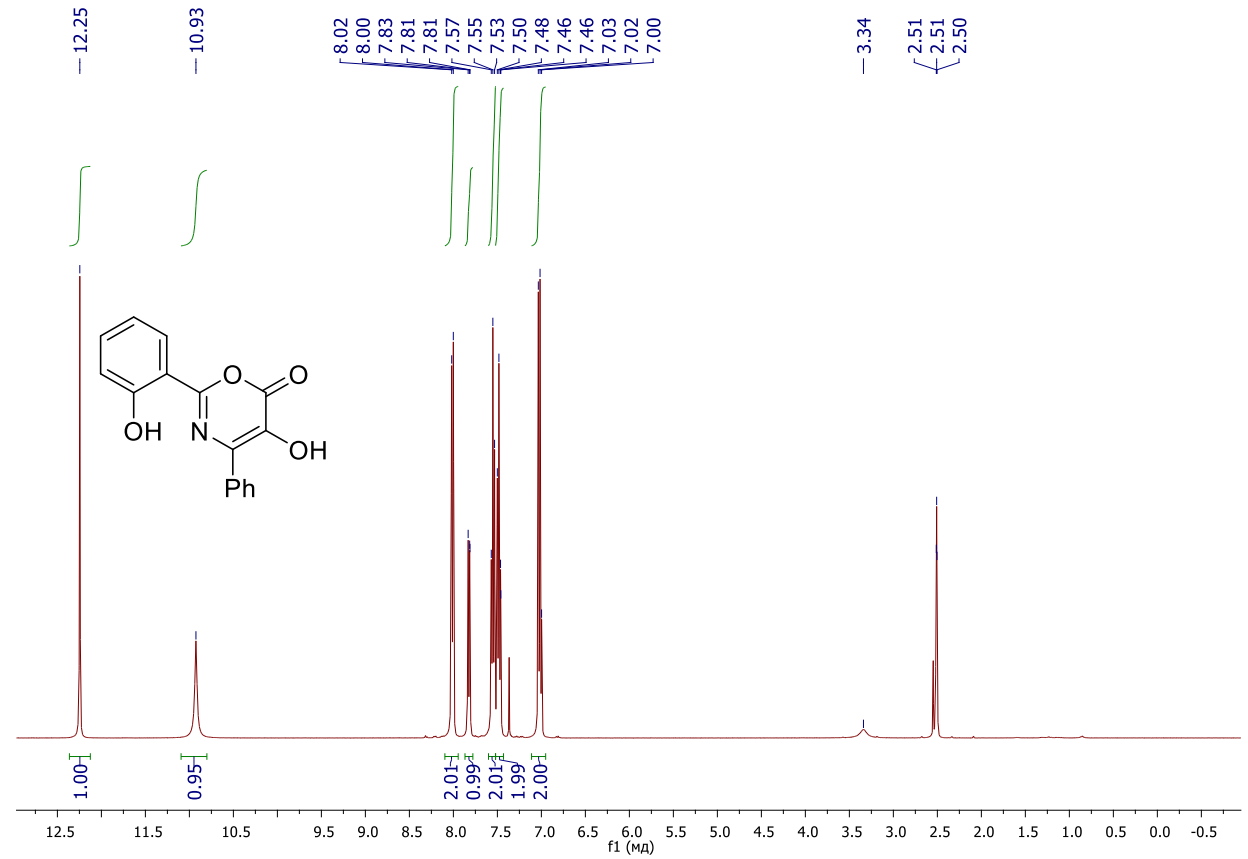
^{1}H NMR (400 MHz, DMSO-d_6) spectrum of **4l**



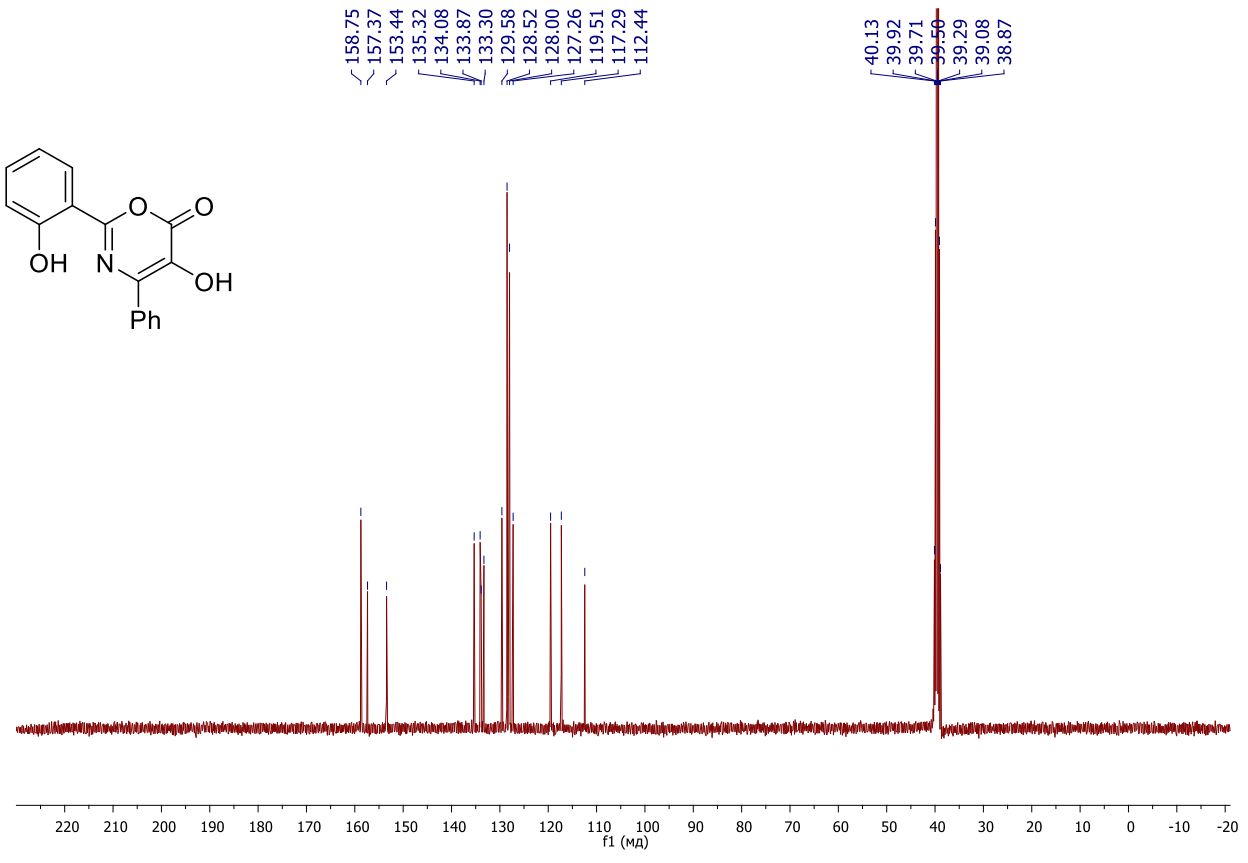
^{13}C NMR (100 MHz, DMSO-d_6) spectrum of **4l**



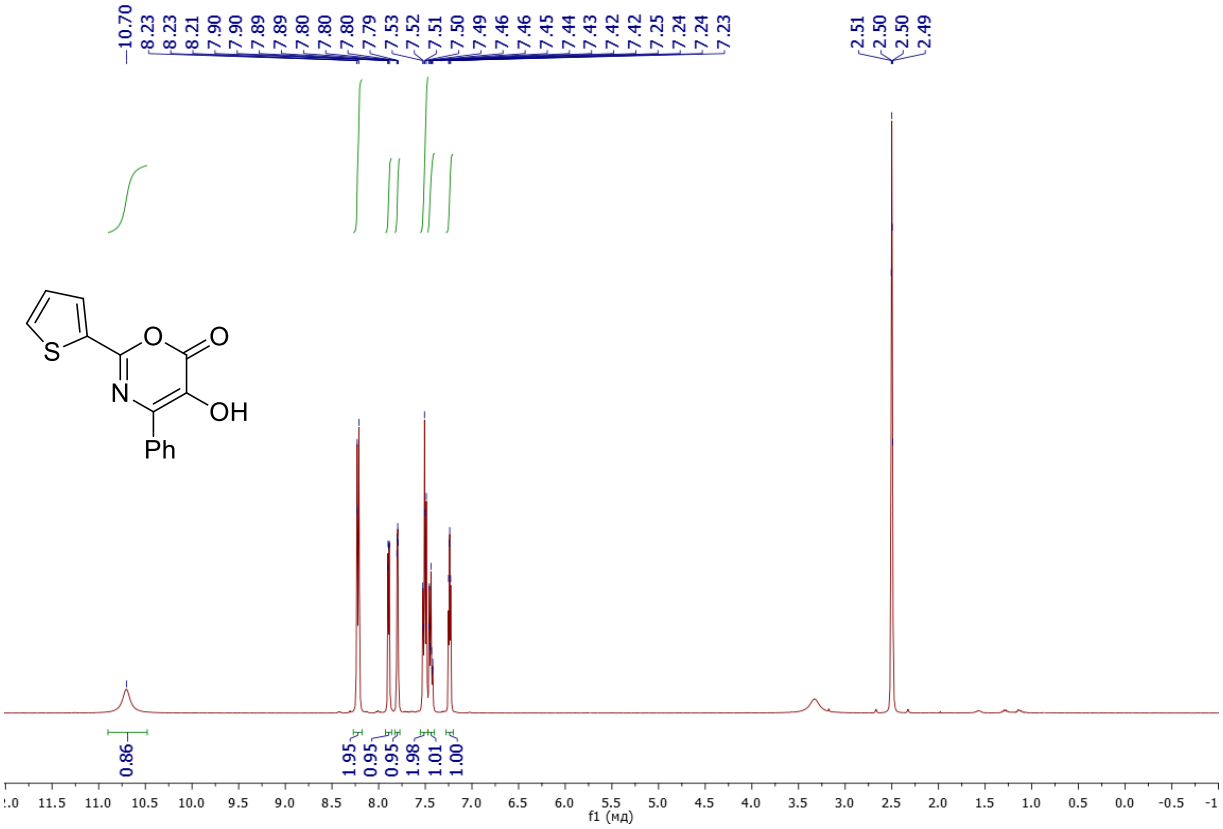
^{1}H NMR (400 MHz, DMSO-d_6) spectrum of **4m**



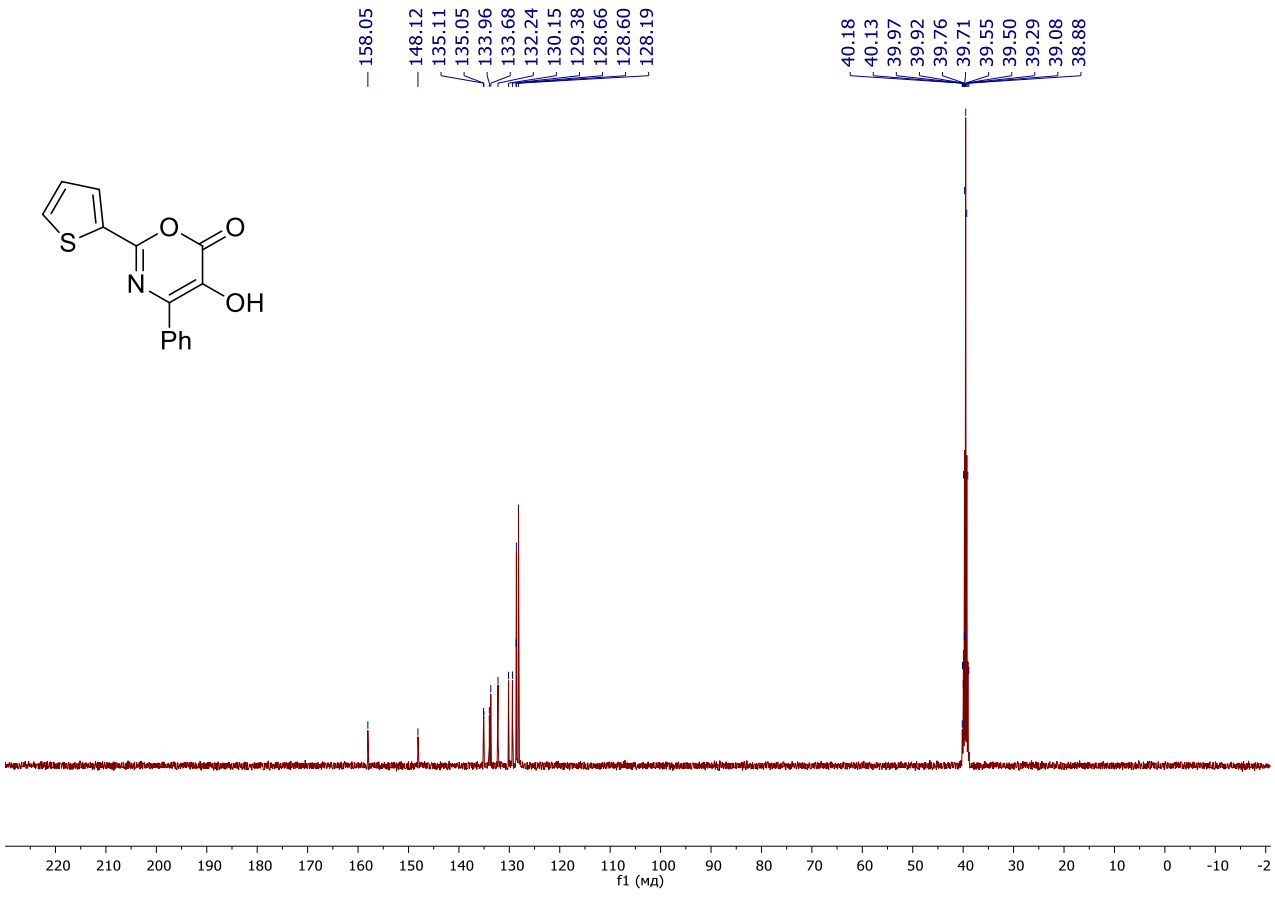
^{13}C NMR (100 MHz, DMSO-d_6) spectrum of **4m**



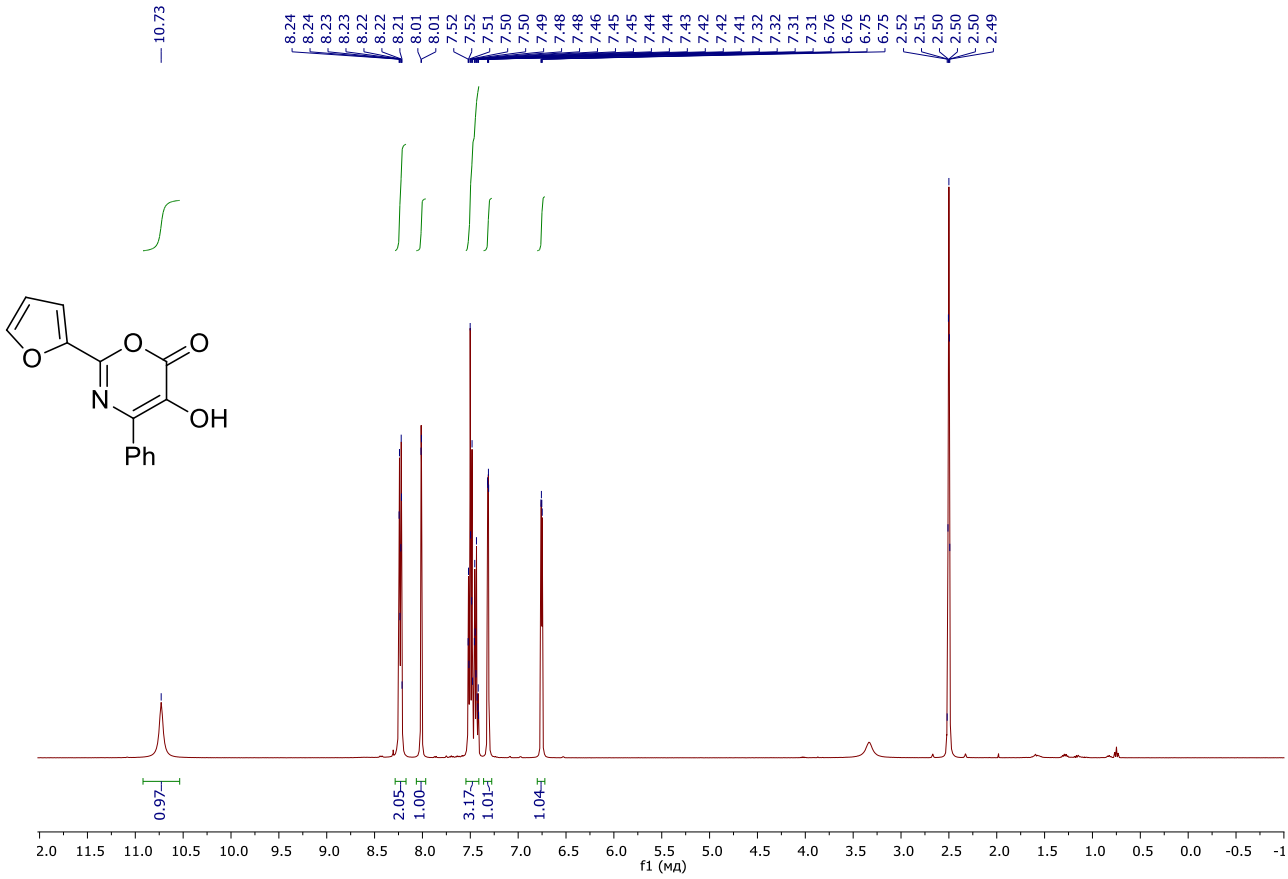
^{1}H NMR (400 MHz, DMSO-d_6) spectrum of **4n**



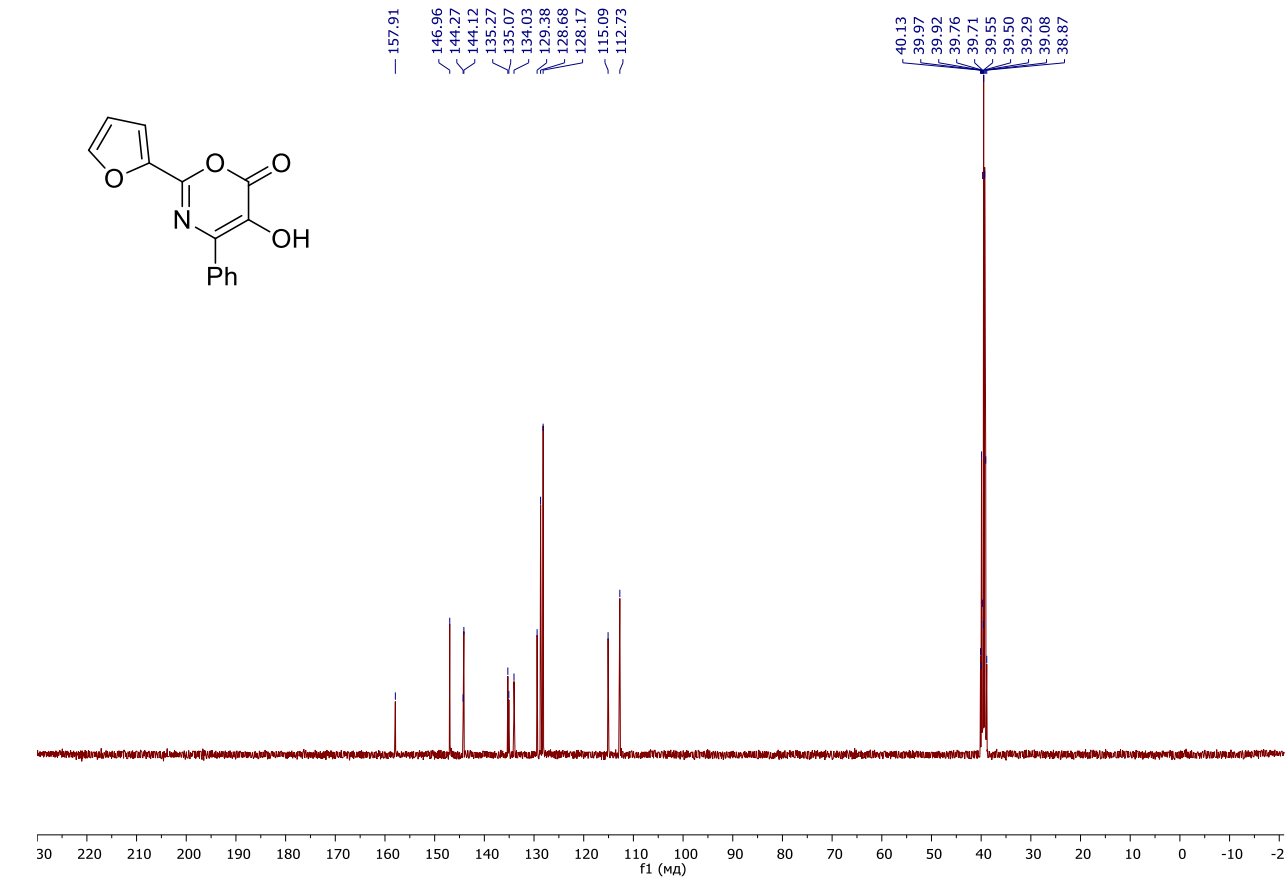
^{13}C NMR (100 MHz, DMSO-d_6) spectrum of **4n**



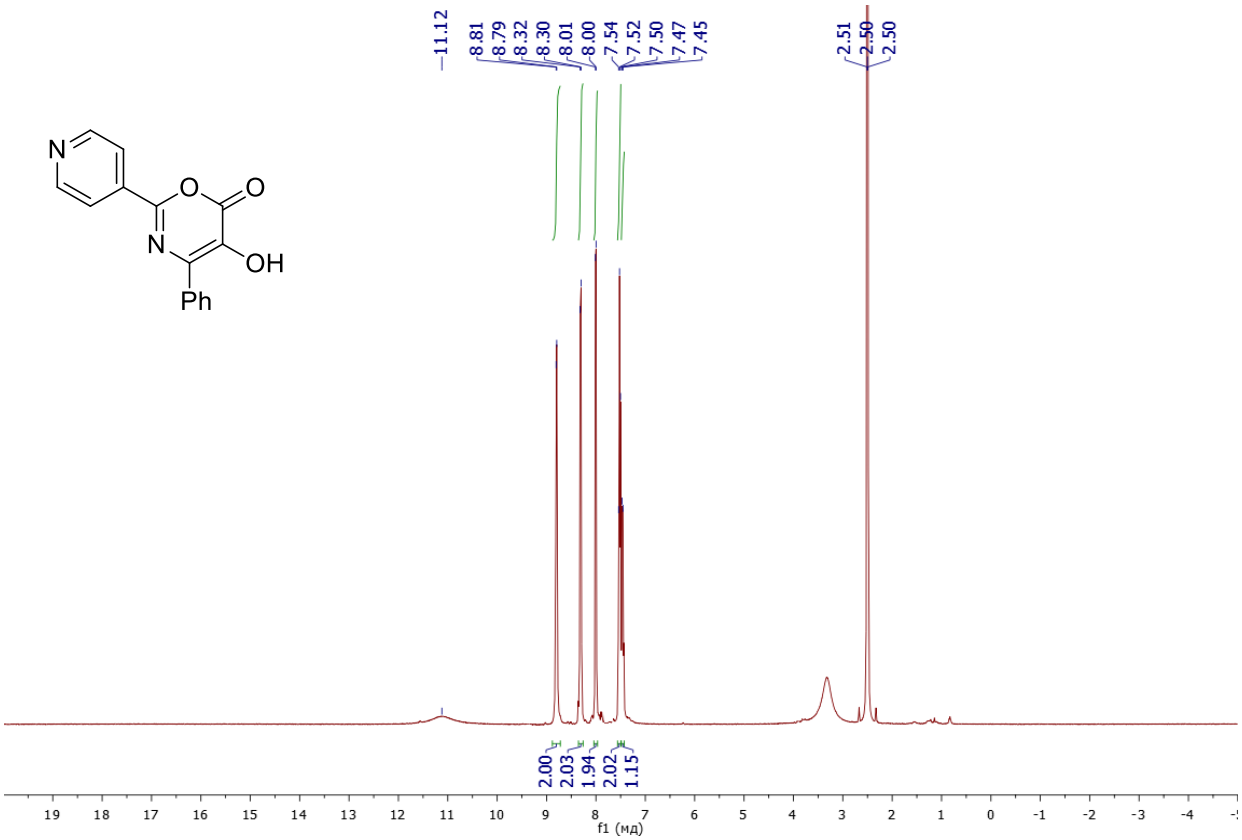
^{1}H NMR (400 MHz, DMSO-d_6) spectrum of **4o**



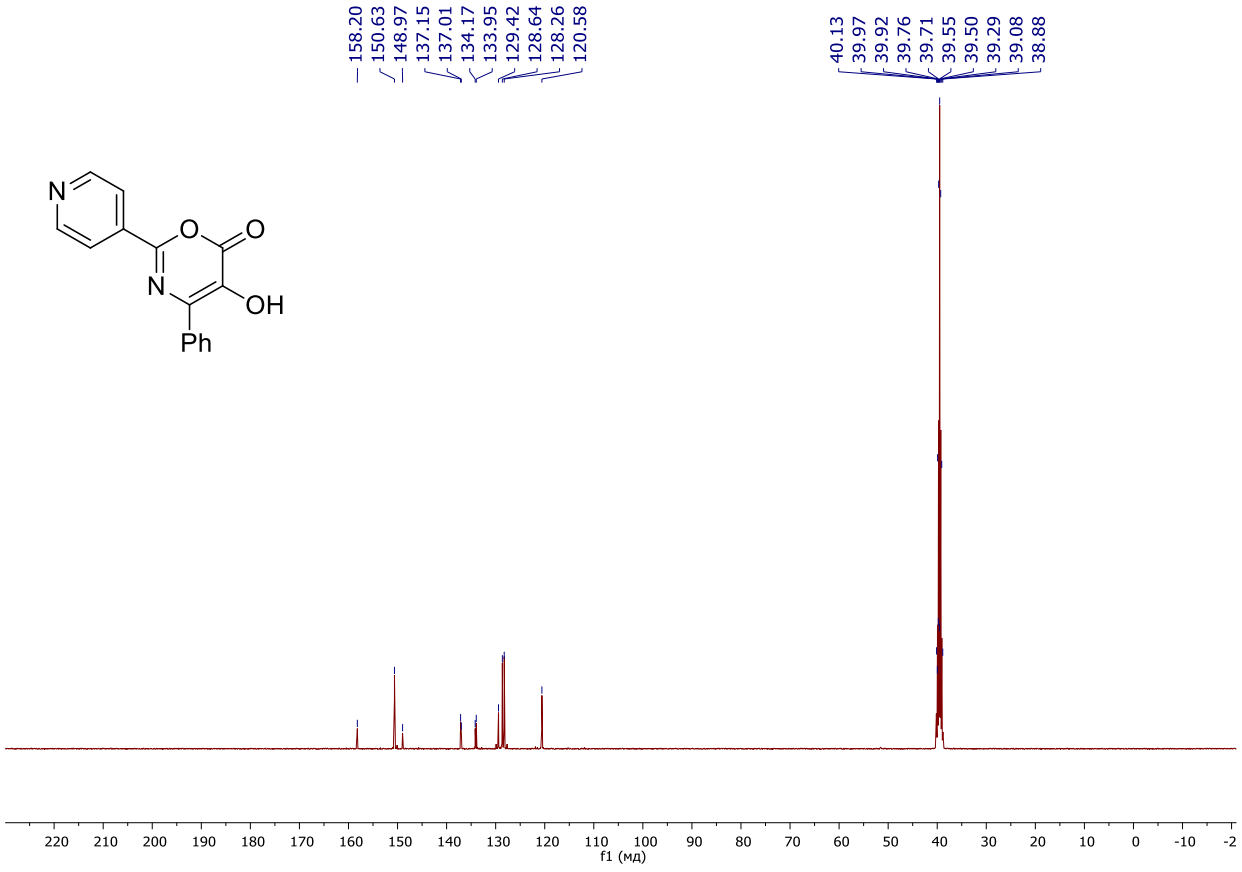
^{13}C NMR (100 MHz, DMSO-d_6) spectrum of **4o**



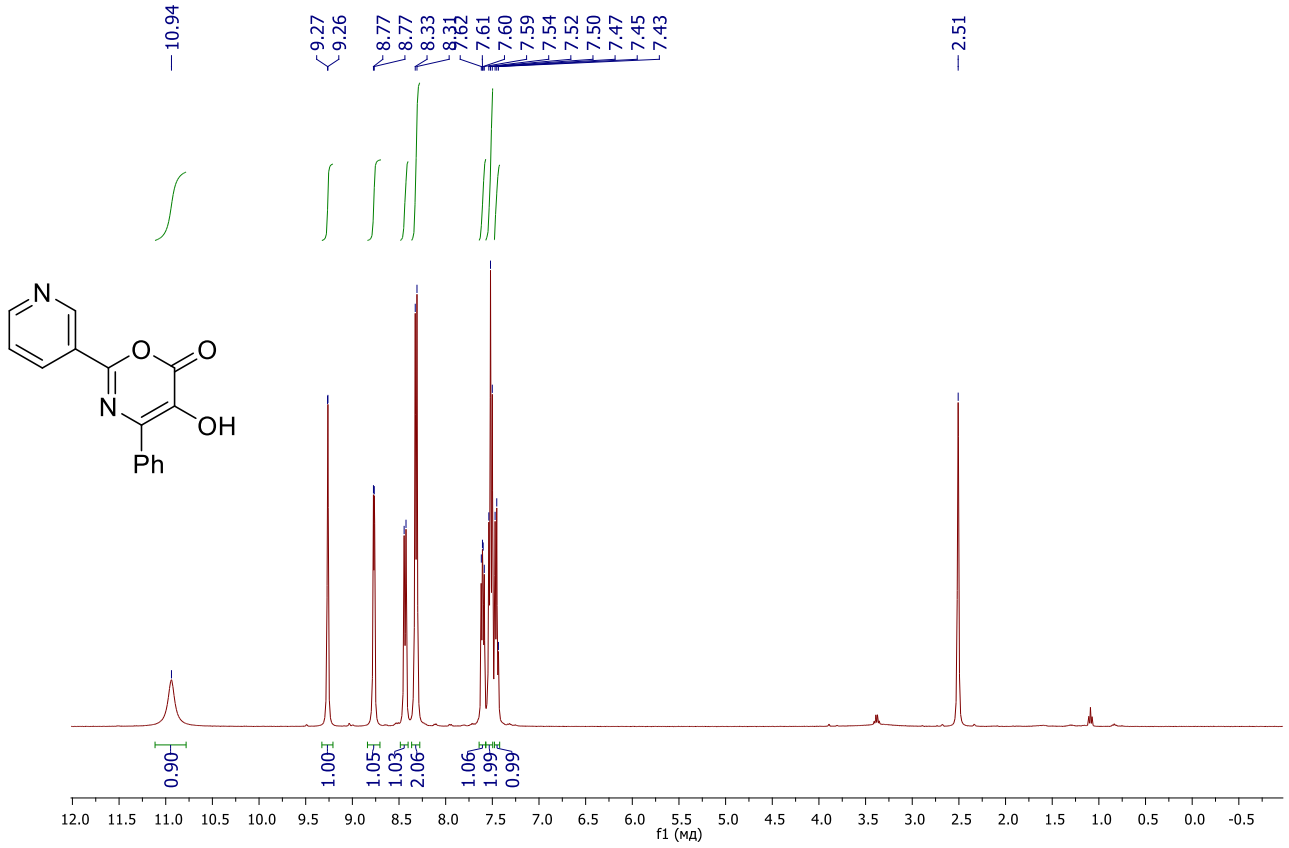
^{1}H NMR (400 MHz, DMSO-d_6) spectrum of **4p**



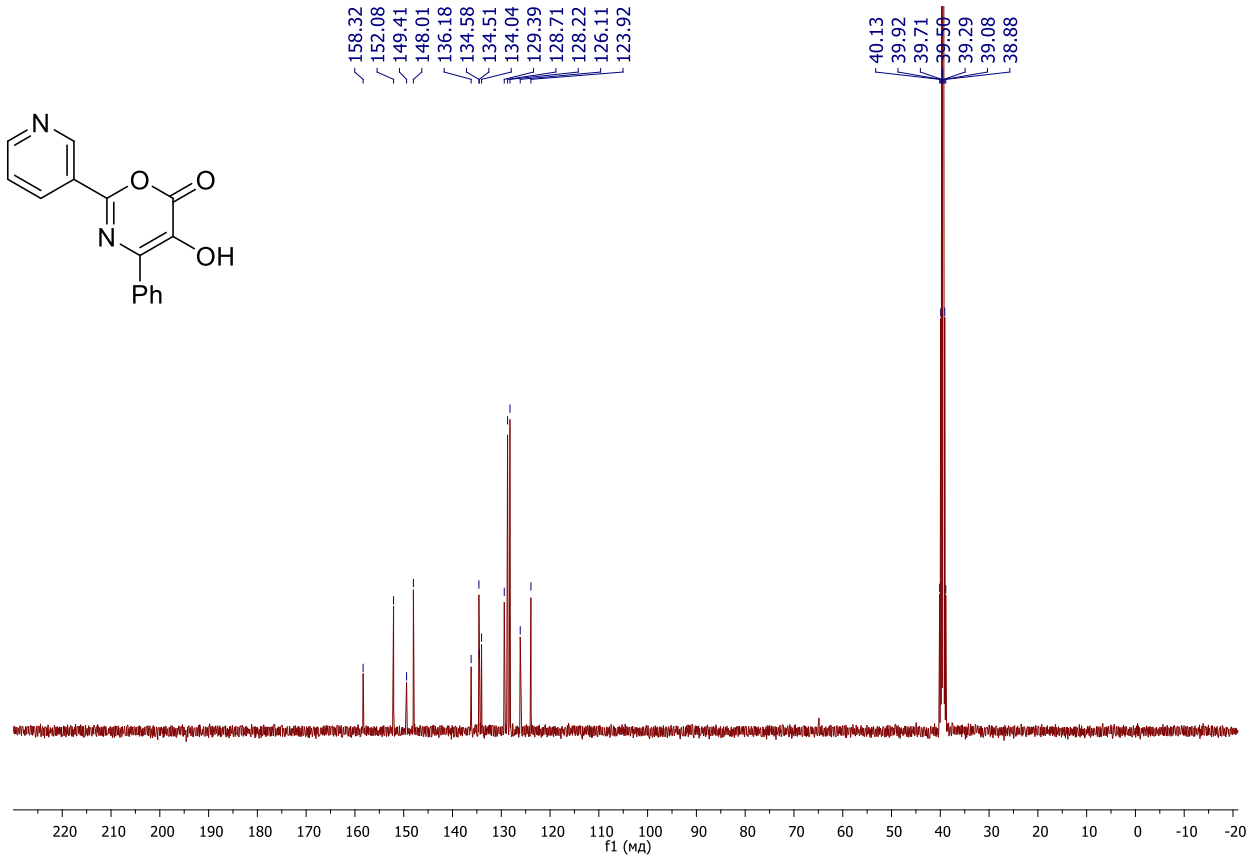
^{13}C NMR (100 MHz, DMSO-d_6) spectrum of **4p**



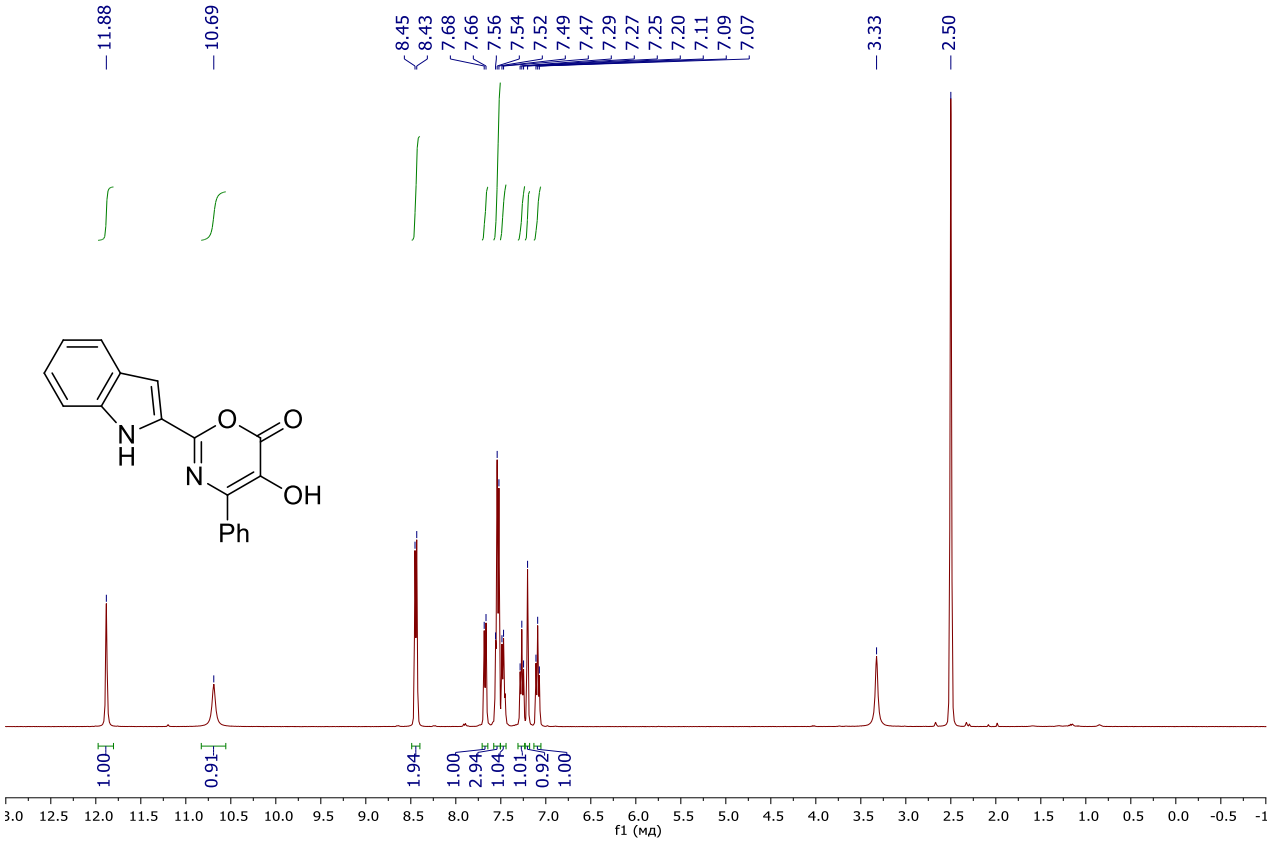
^{1}H NMR (400 MHz, DMSO-d_6) spectrum of **4q**



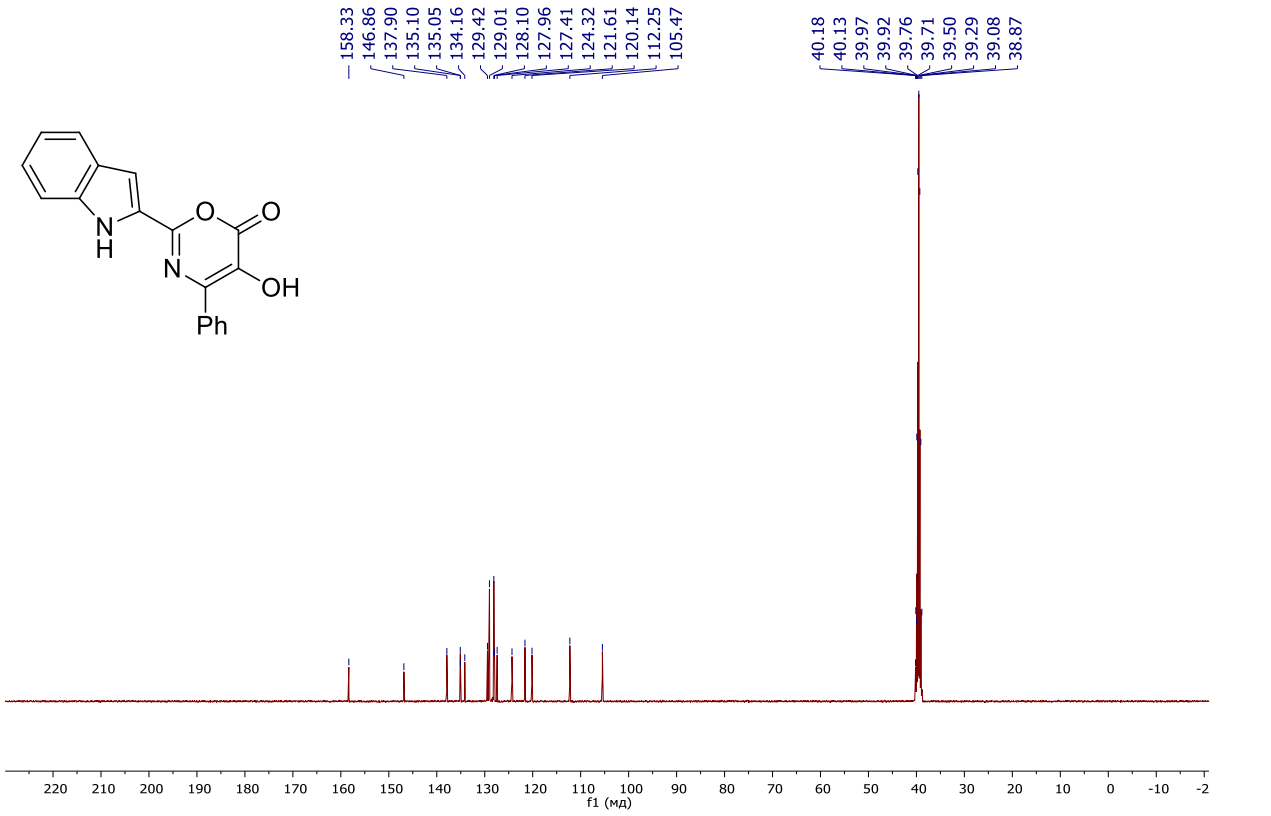
^{13}C NMR (100 MHz, DMSO-d_6) spectrum of **4q**



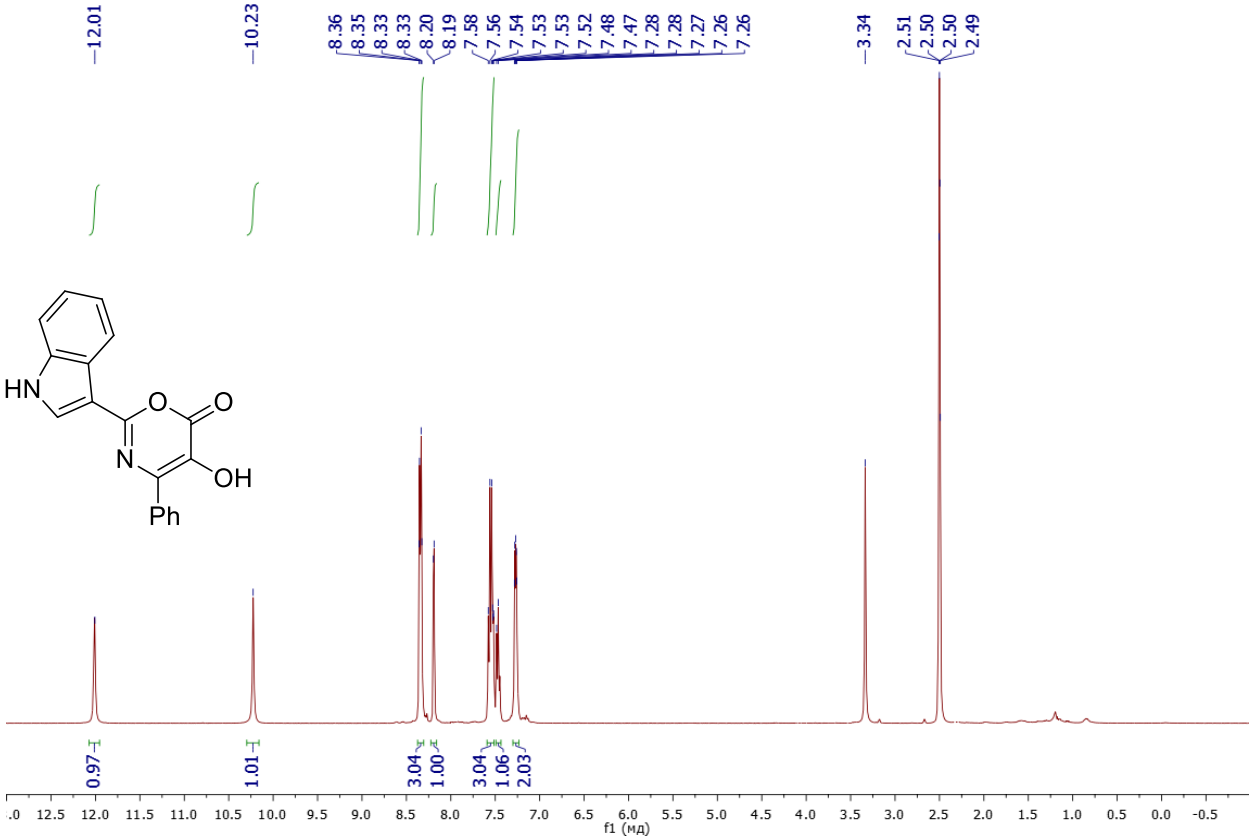
^{1}H NMR (400 MHz, DMSO-d_6) spectrum of **4r**



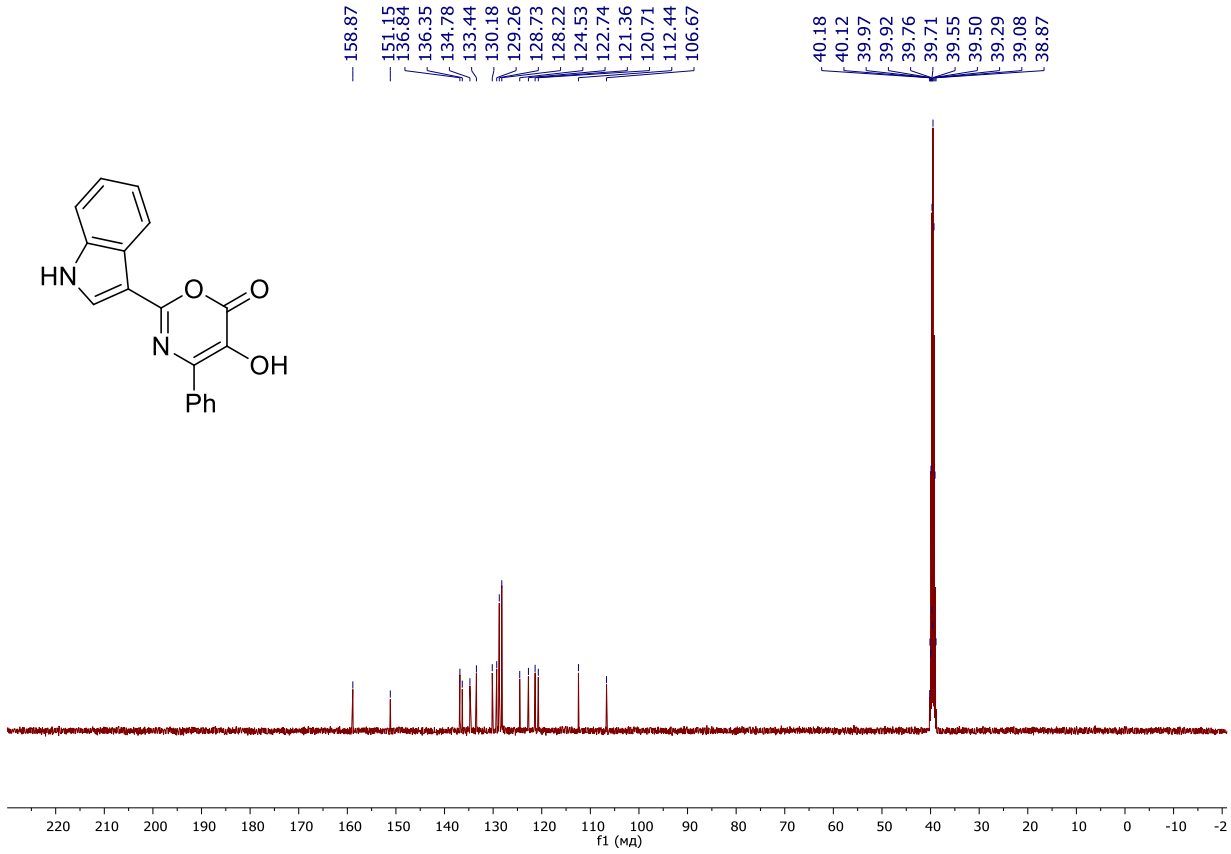
^{13}C NMR (100 MHz, DMSO-d_6) spectrum of **4r**



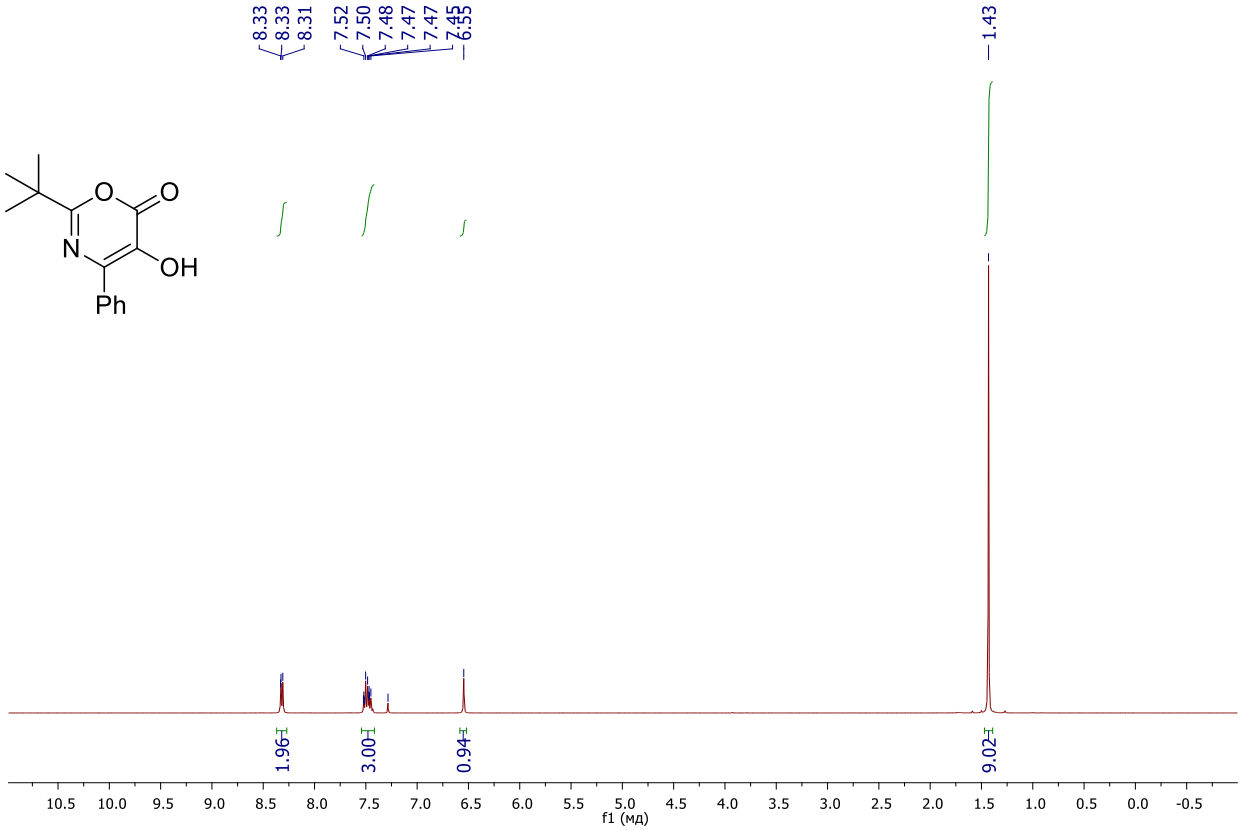
^{1}H NMR (400 MHz, DMSO-d_6) spectrum of **4s**



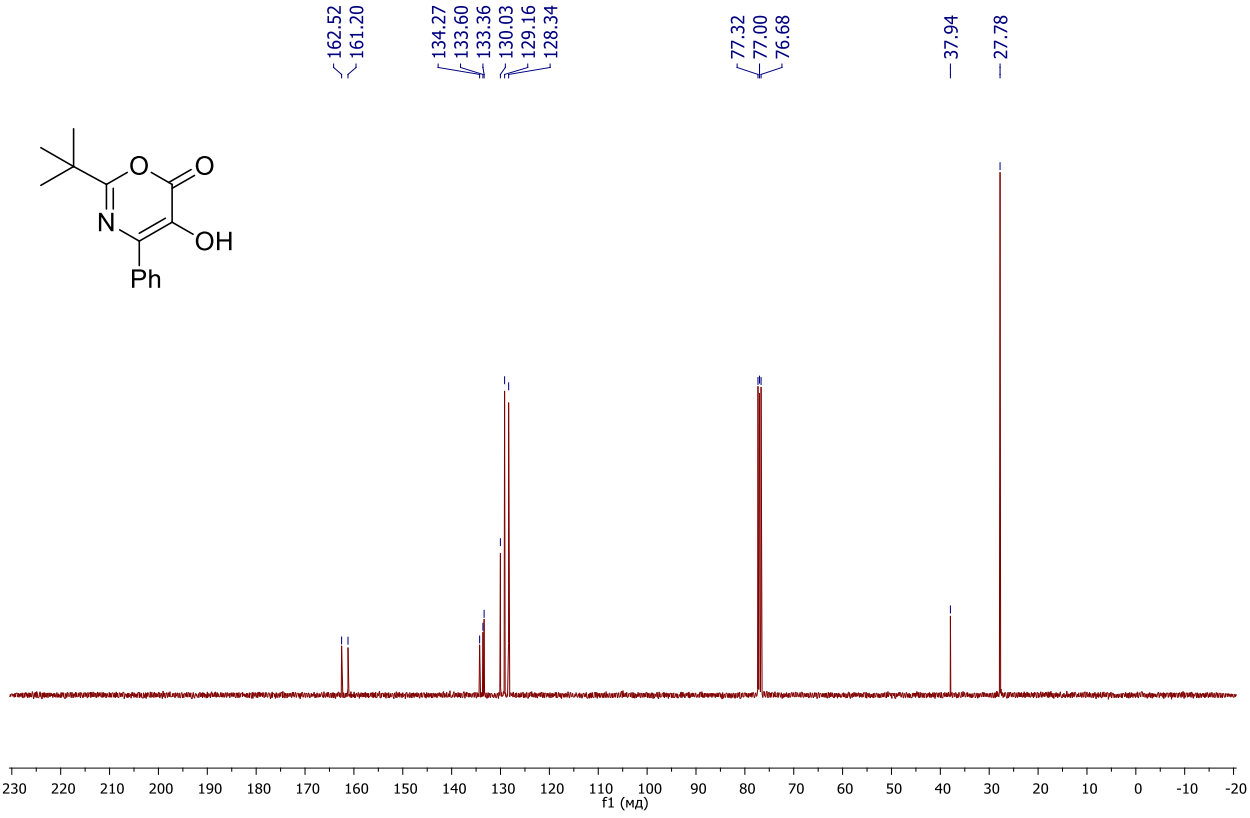
^{13}C NMR (100 MHz, DMSO-d_6) spectrum of **4s**



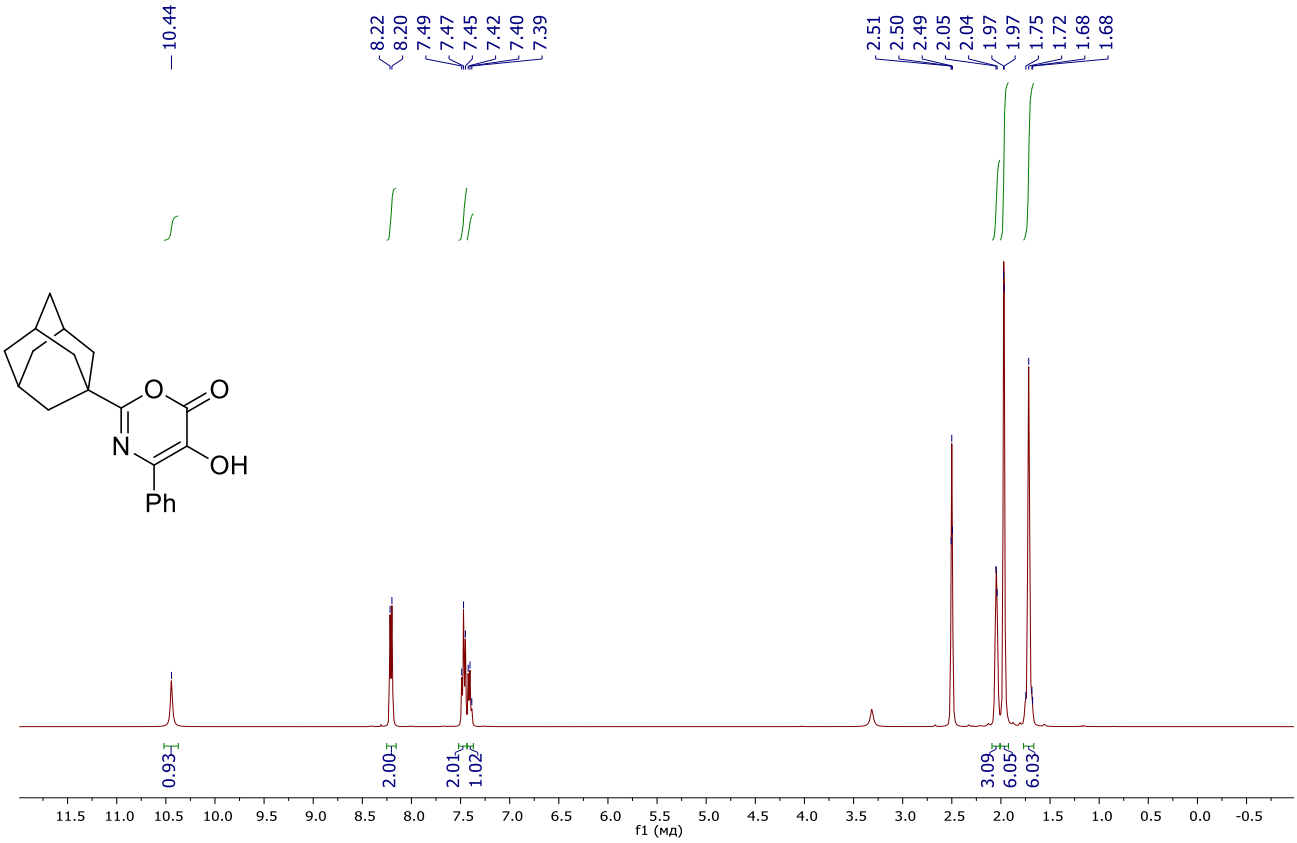
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of **4t**



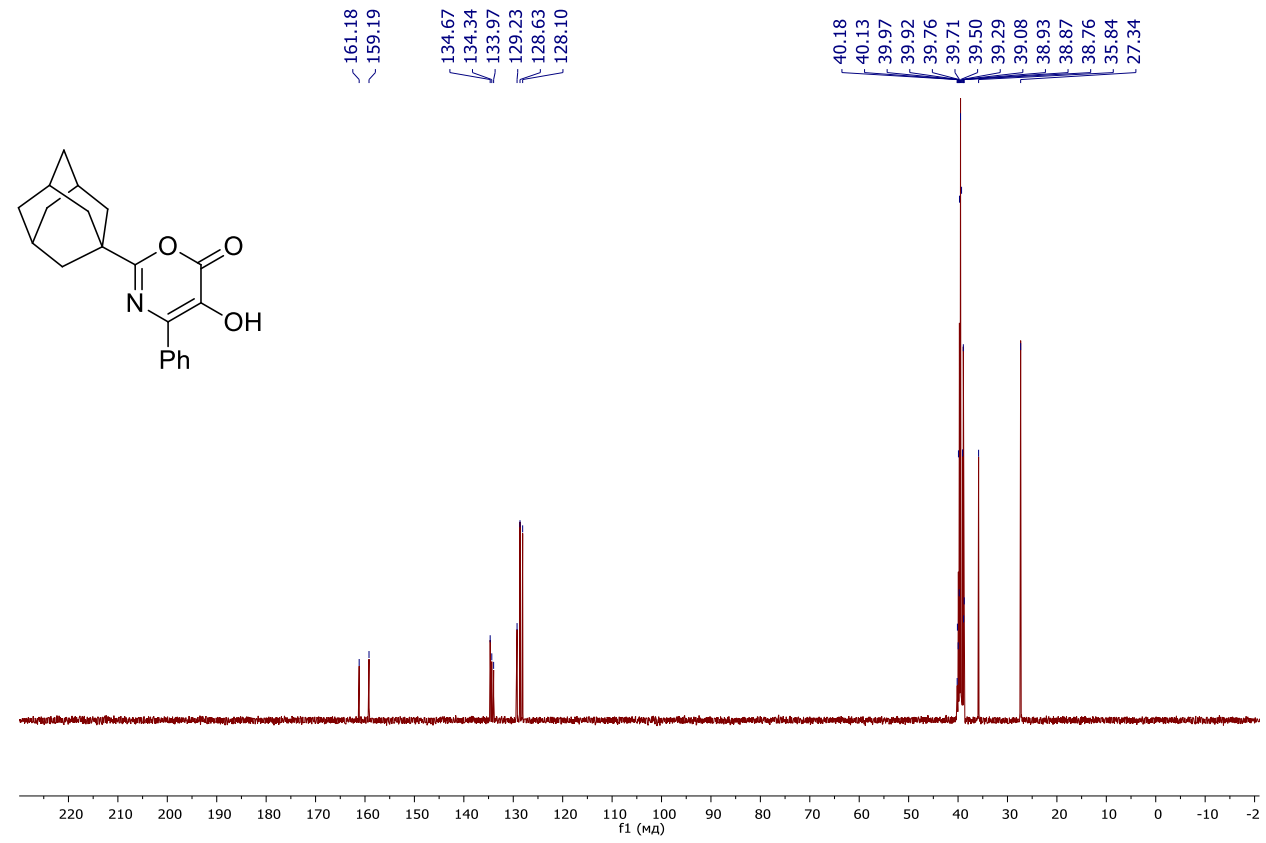
^{13}C NMR (100 MHz, $CDCl_3$) spectrum of **4t**



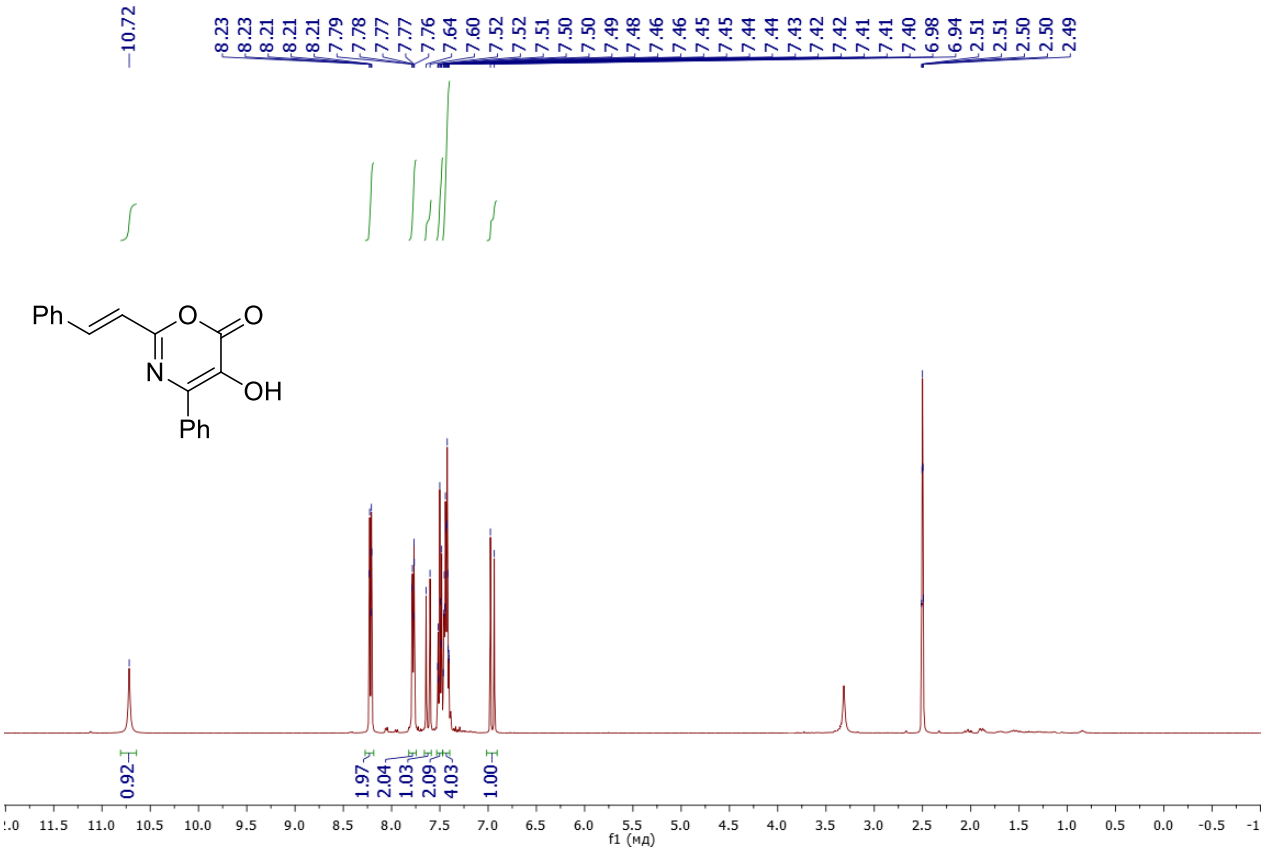
^{1}H NMR (400 MHz, DMSO-d_6) spectrum of **4u**



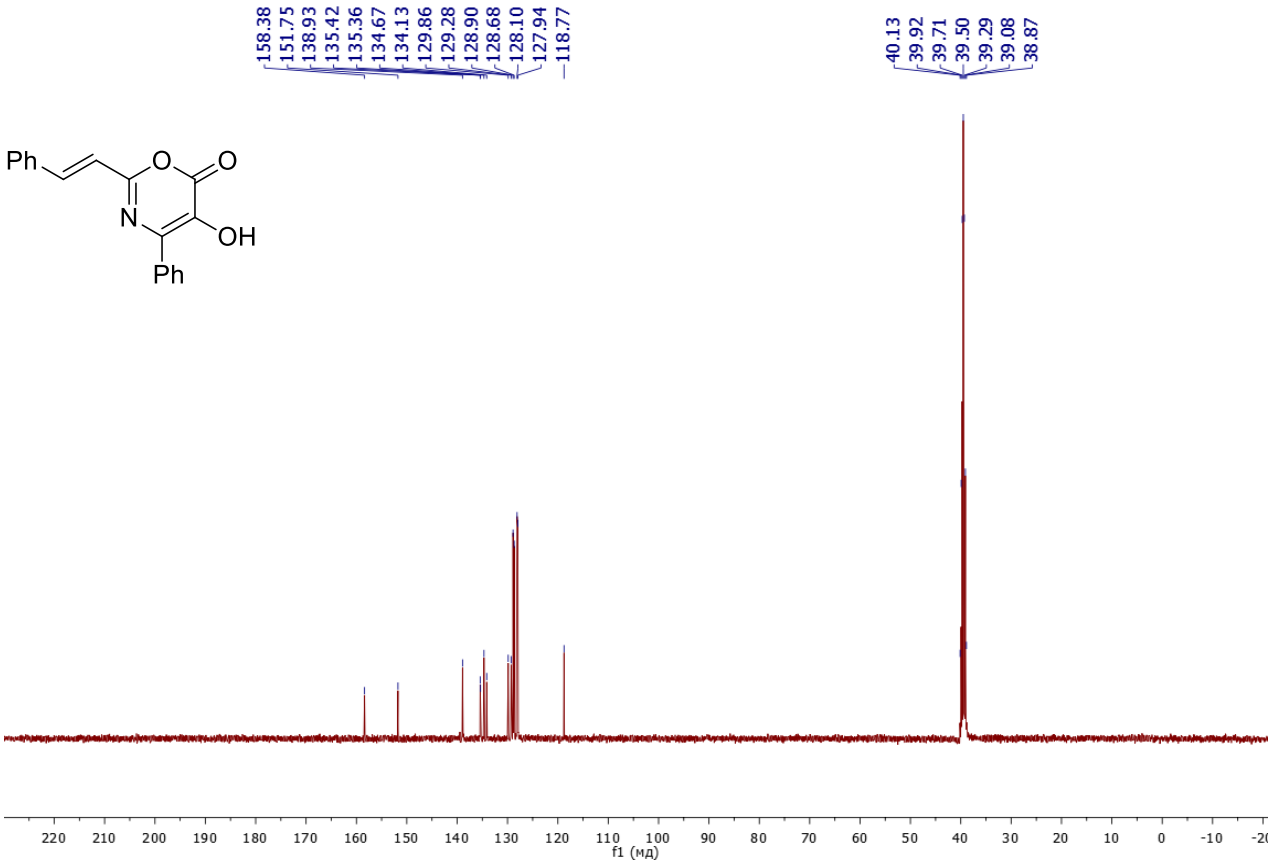
^{13}C NMR (100 MHz, DMSO-d_6) spectrum of **4u**



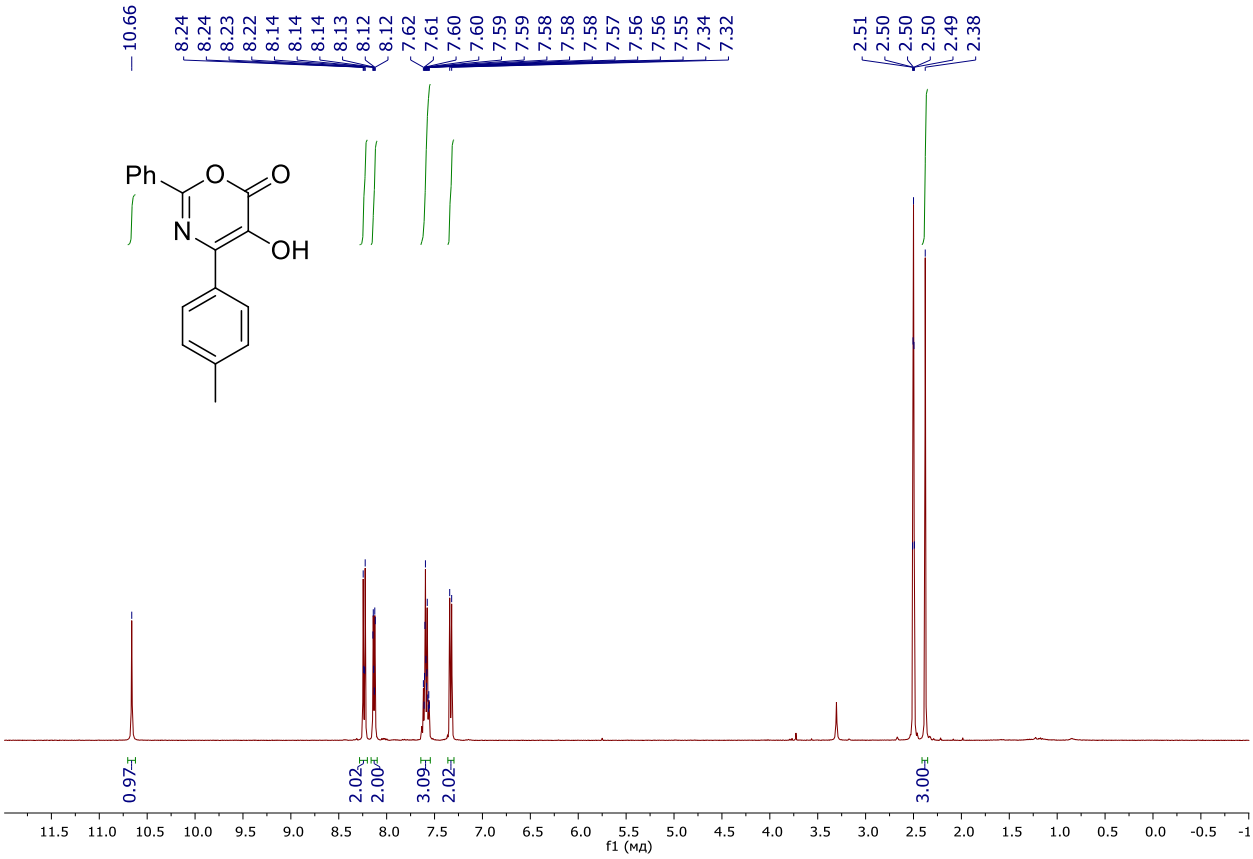
^{1}H NMR (400 MHz, DMSO-d_6) spectrum of **4v**



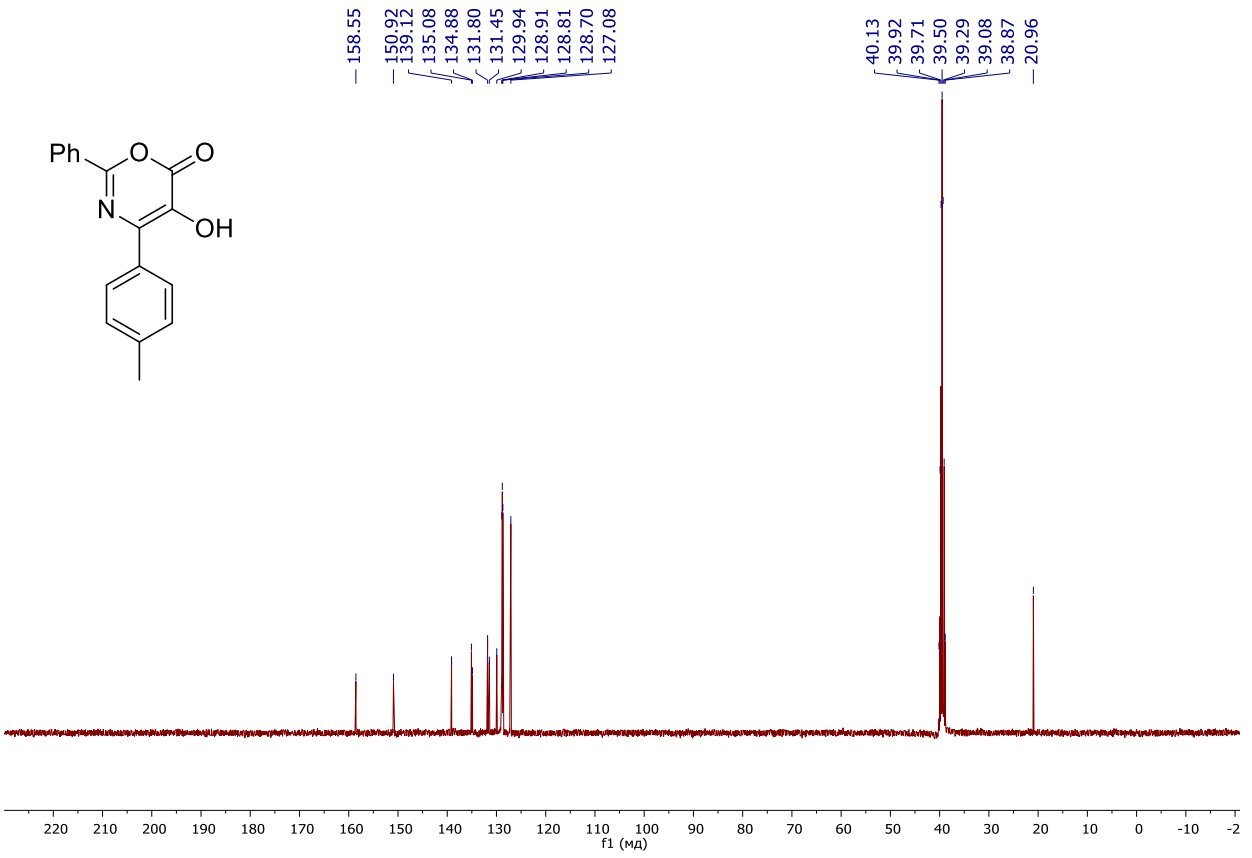
^{13}C NMR (100 MHz, DMSO-d_6) spectrum of **4v**



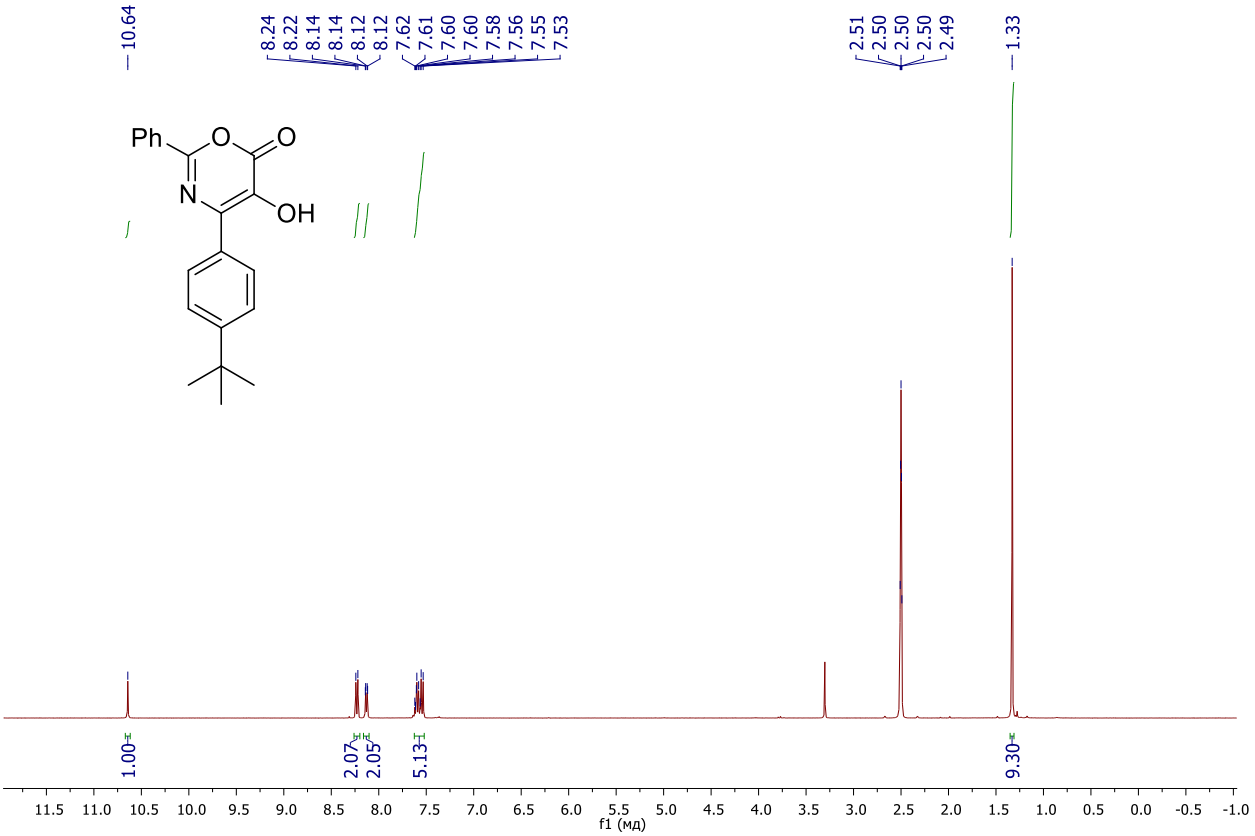
^{1}H NMR (400 MHz, DMSO-d_6) spectrum of **4w**



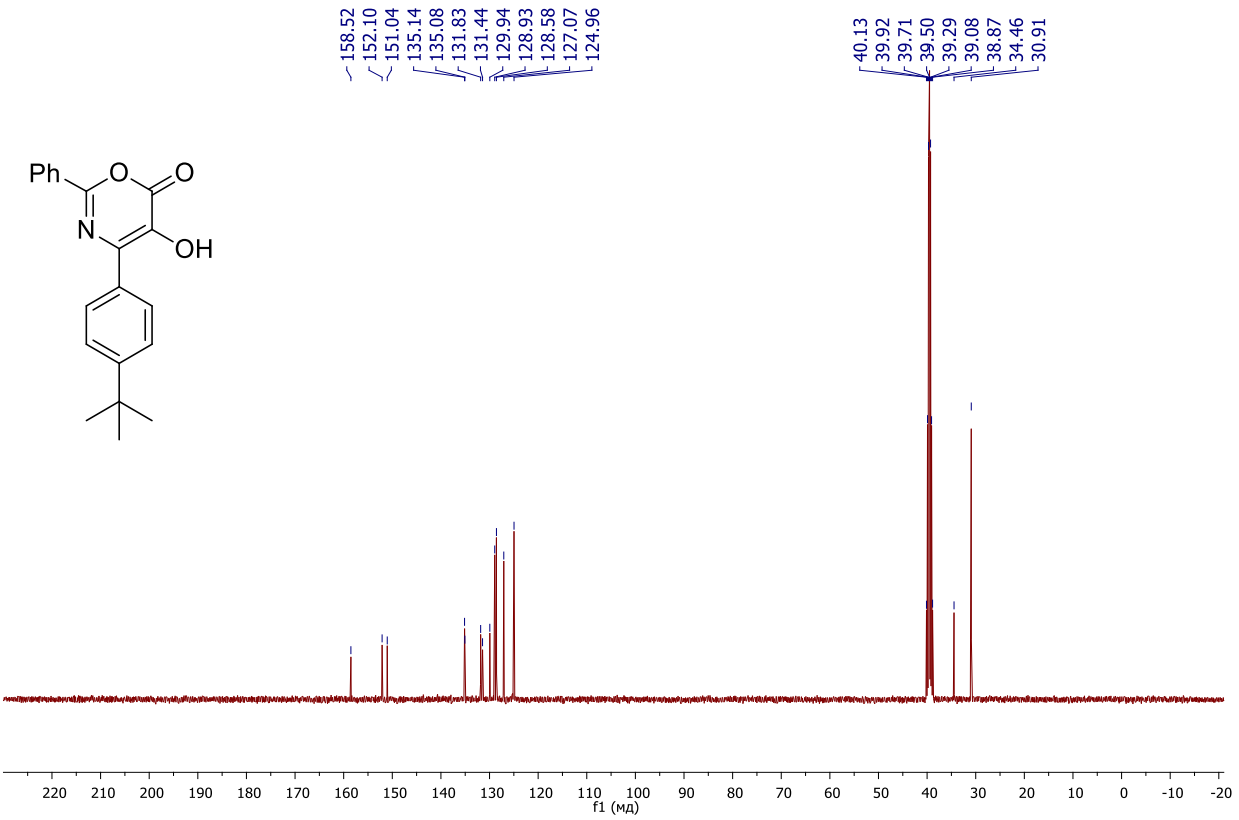
^{13}C NMR (100 MHz, DMSO-d_6) spectrum of **4w**



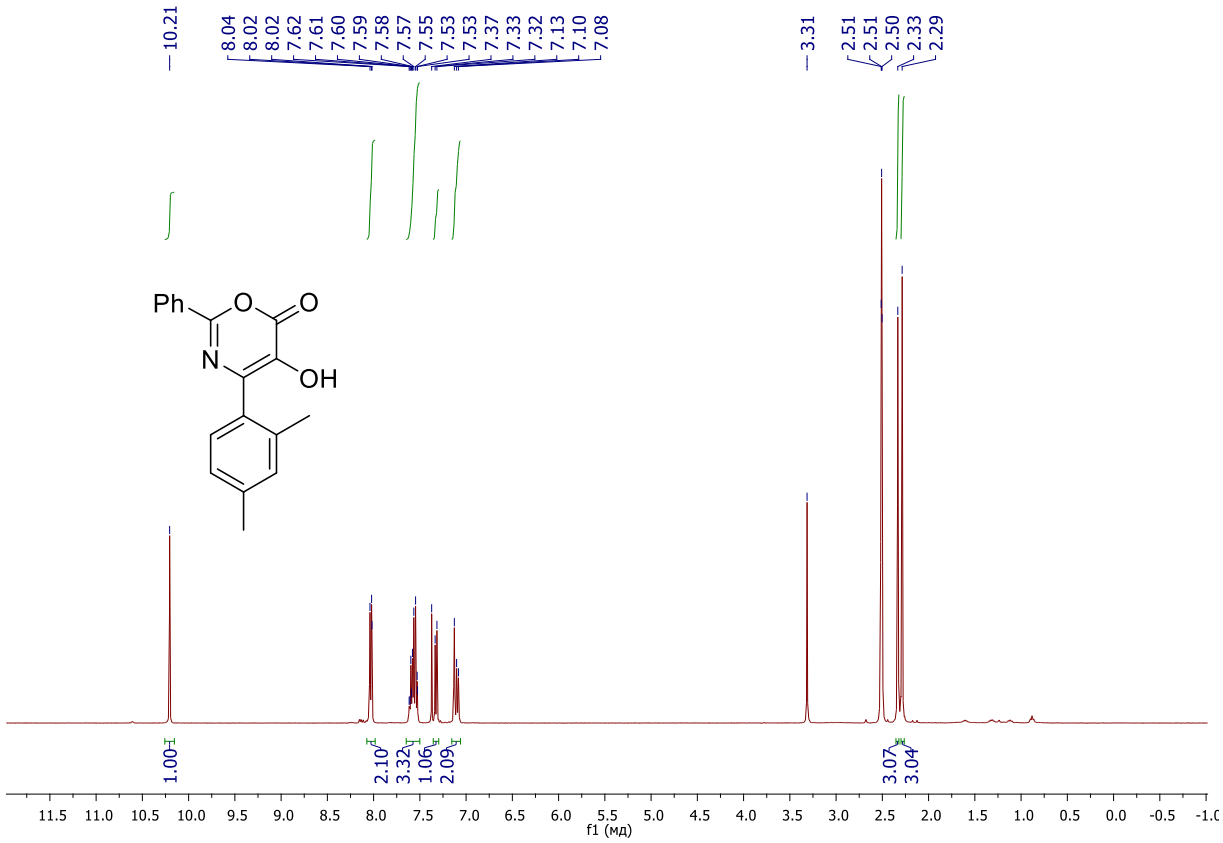
^{1}H NMR (400 MHz, DMSO-d_6) spectrum of **4x**



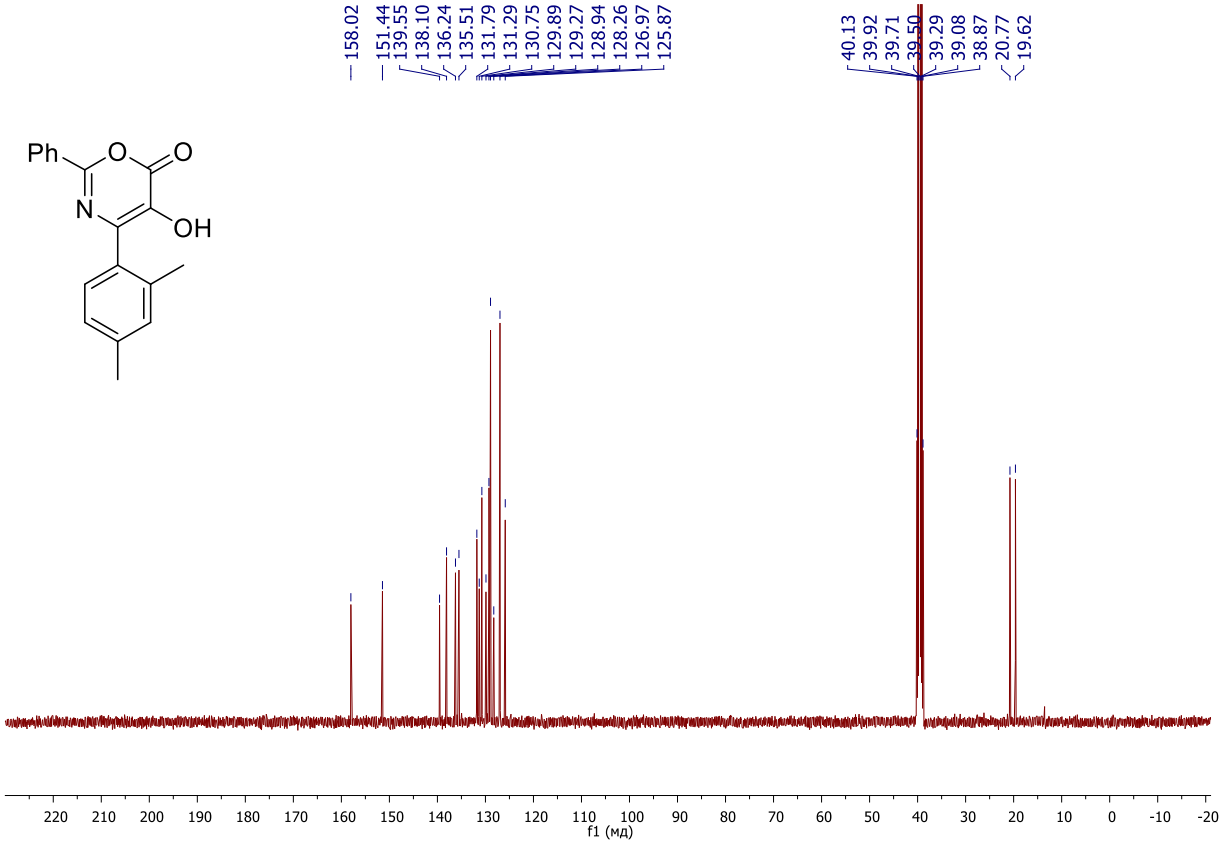
^{13}C NMR (100 MHz, DMSO-d_6) spectrum of **4x**



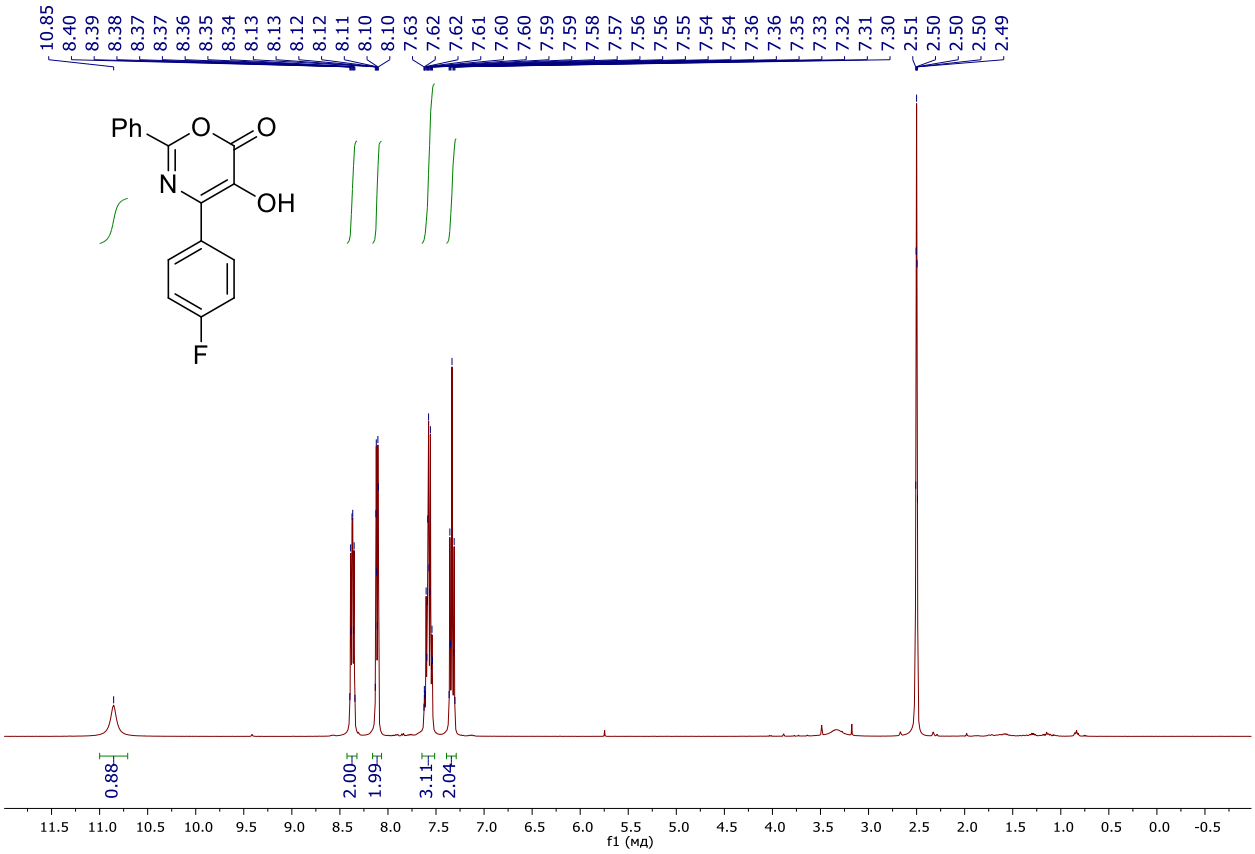
^{1}H NMR (400 MHz, DMSO-d_6) spectrum of **4y**



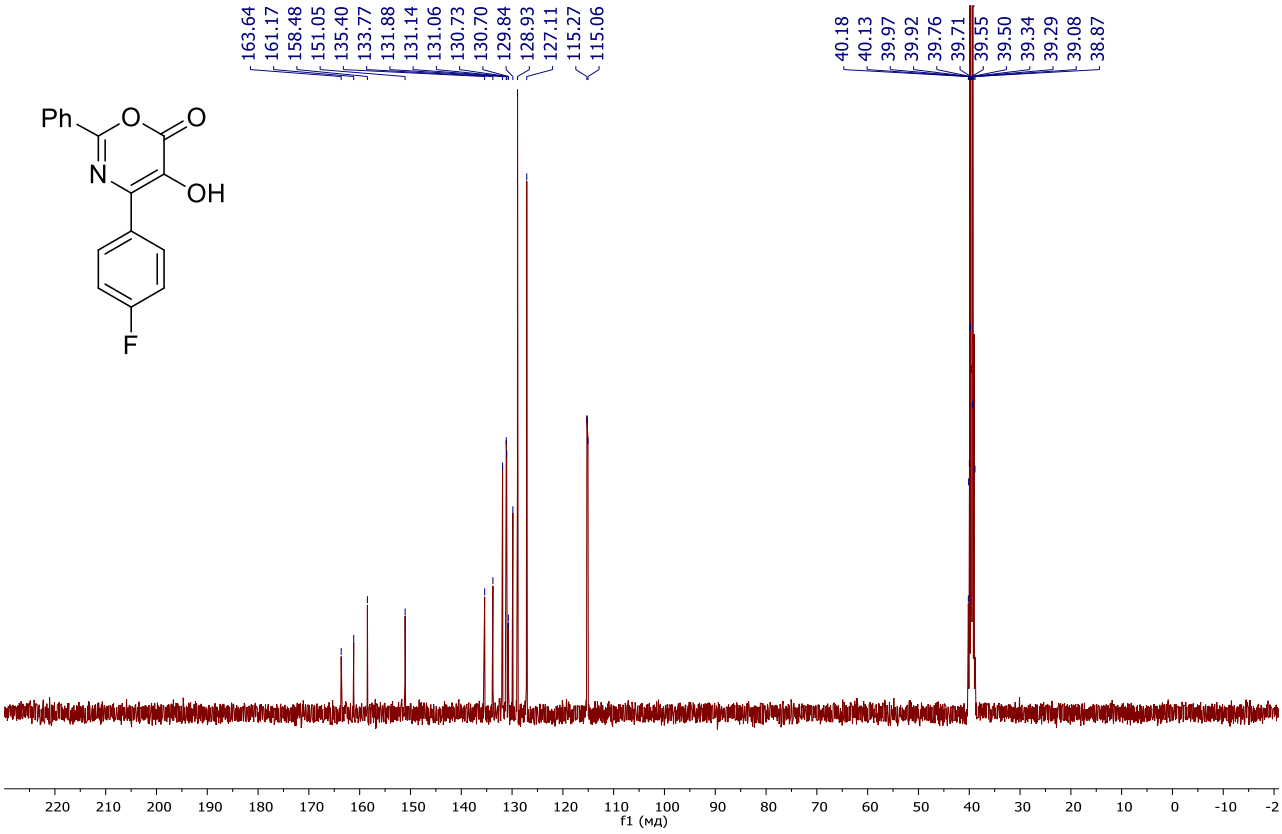
^{13}C NMR (100 MHz, DMSO-d_6) spectrum of **4y**



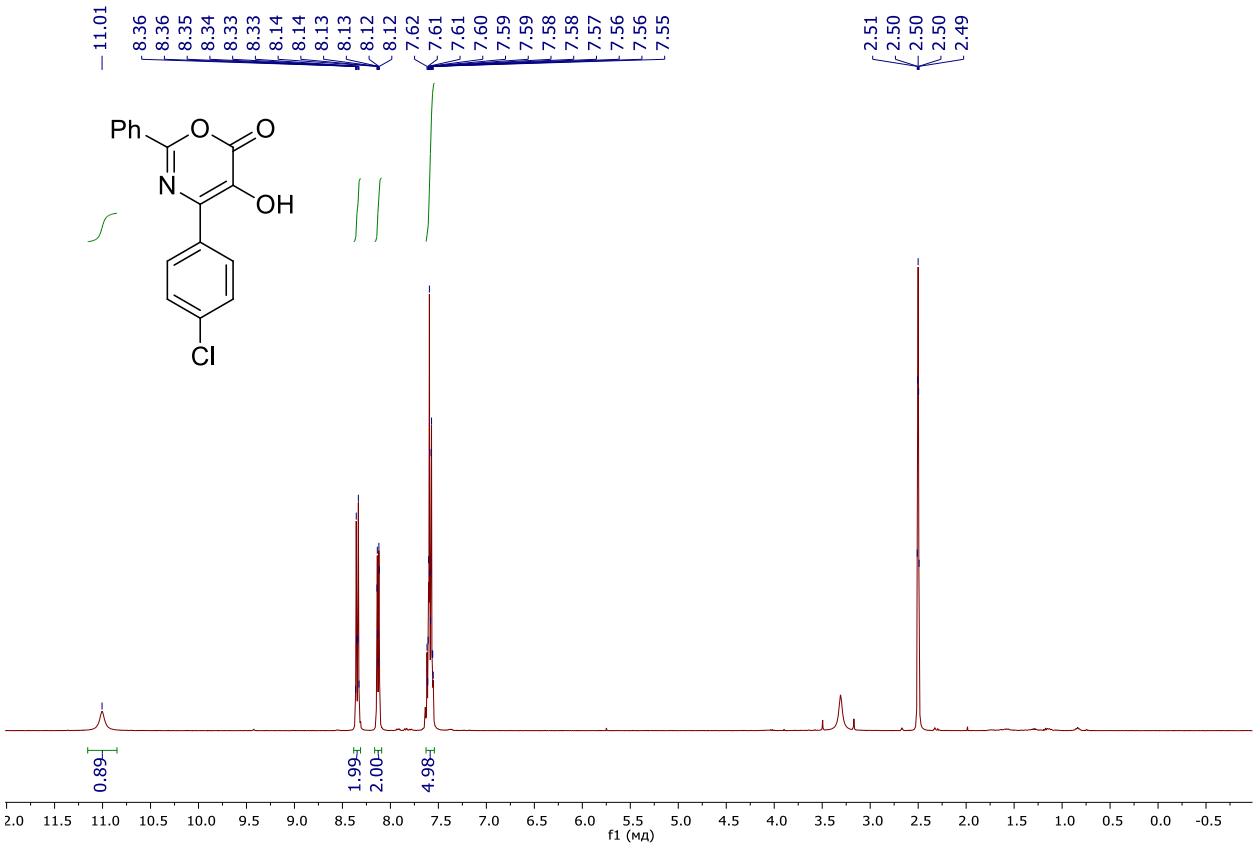
^{1}H NMR (400 MHz, DMSO-d_6) spectrum of **4z**



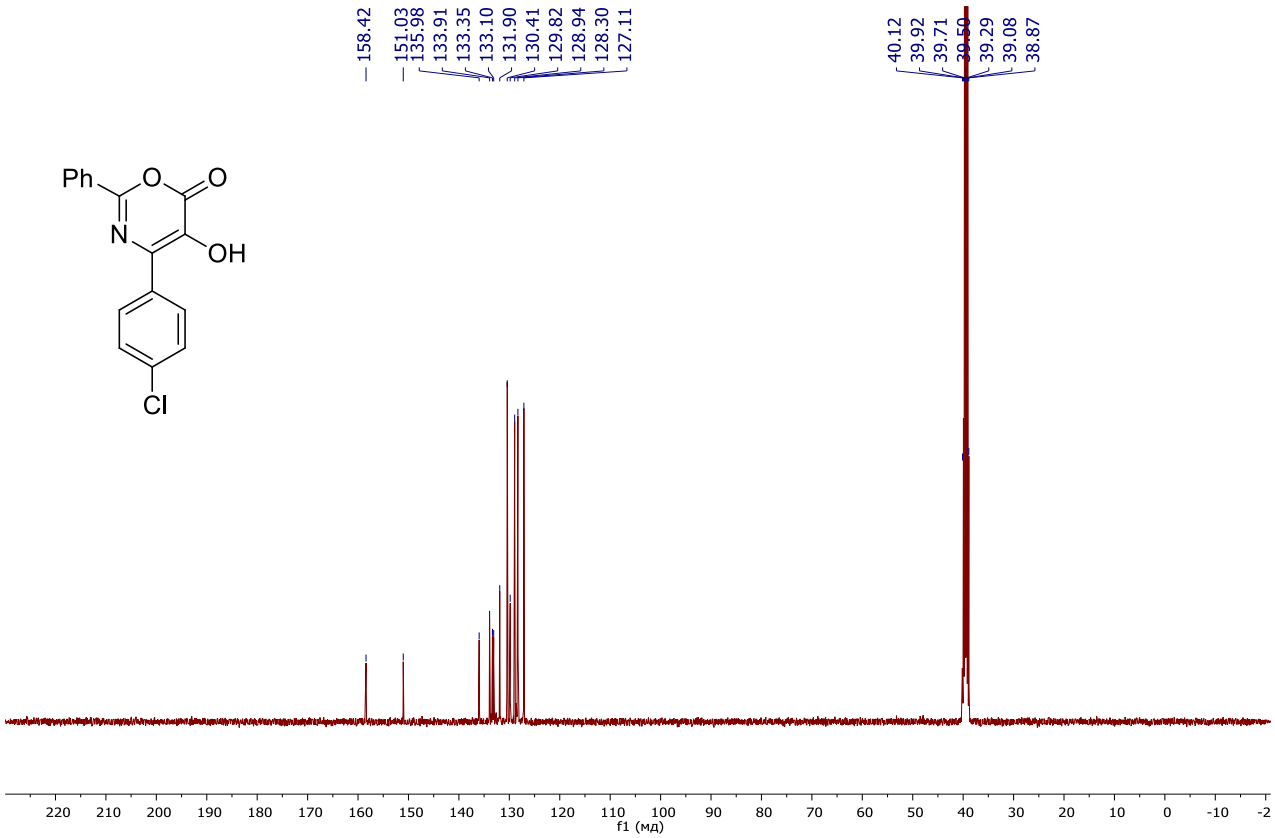
^{13}C NMR (100 MHz, DMSO-d_6) spectrum of **4z**



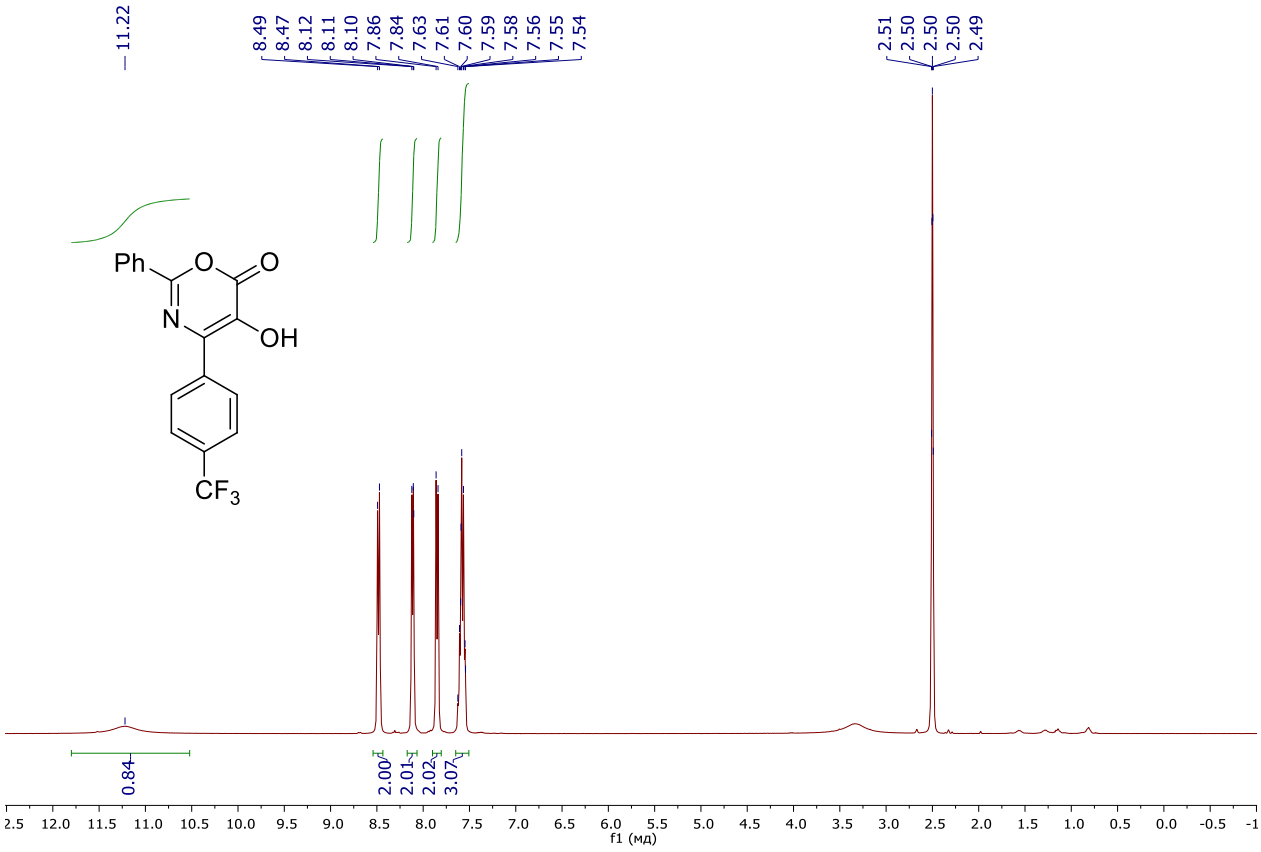
^{1}H NMR (400 MHz, DMSO-d_6) spectrum of **4za**



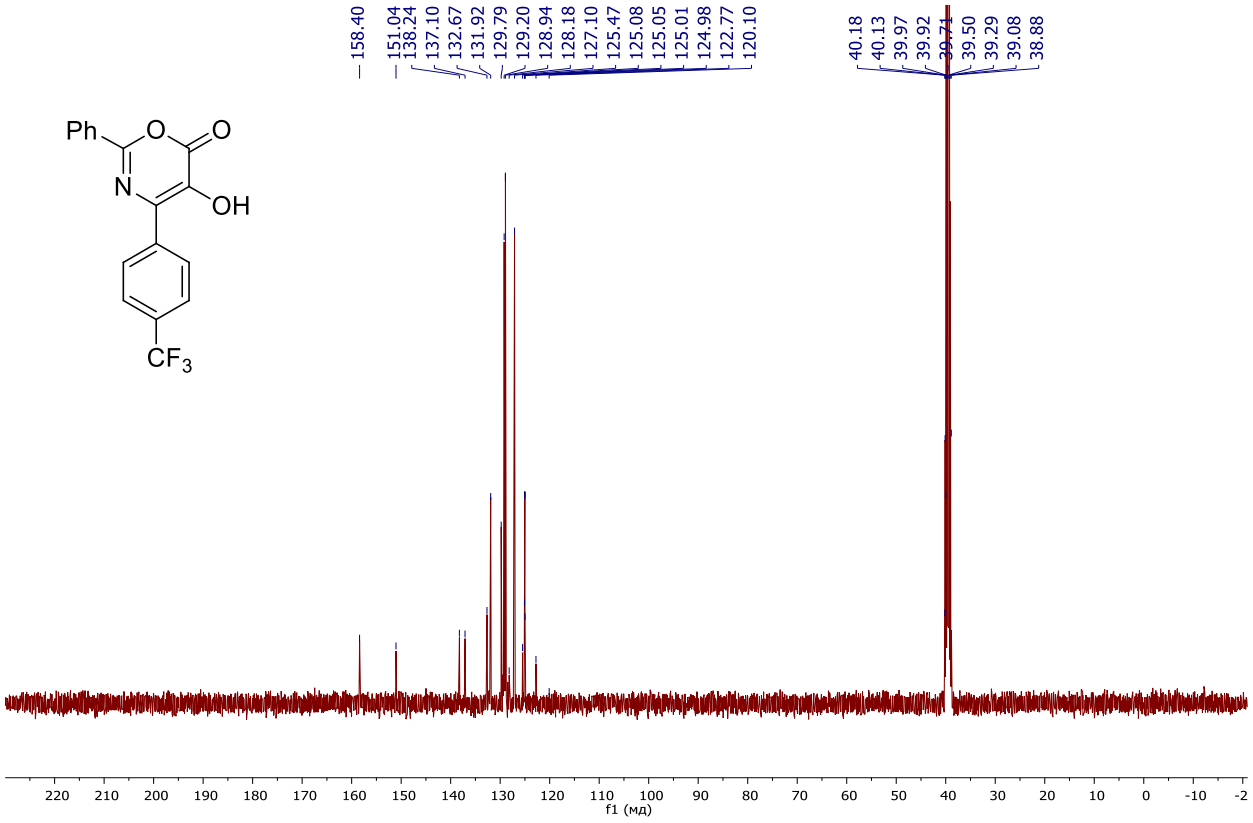
^{13}C NMR (100 MHz, DMSO-d_6) spectrum of **4za**



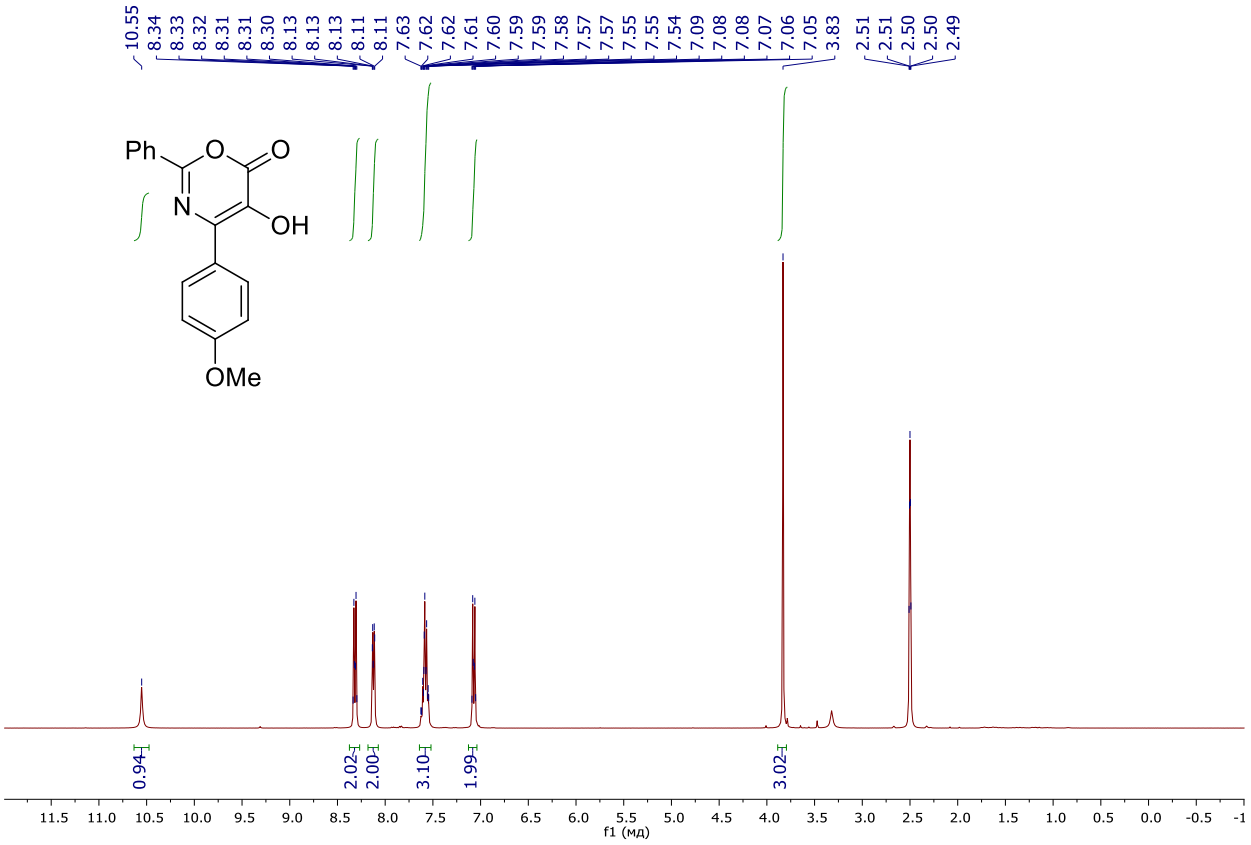
^{1}H NMR (400 MHz, DMSO-d_6) spectrum of **4zb**



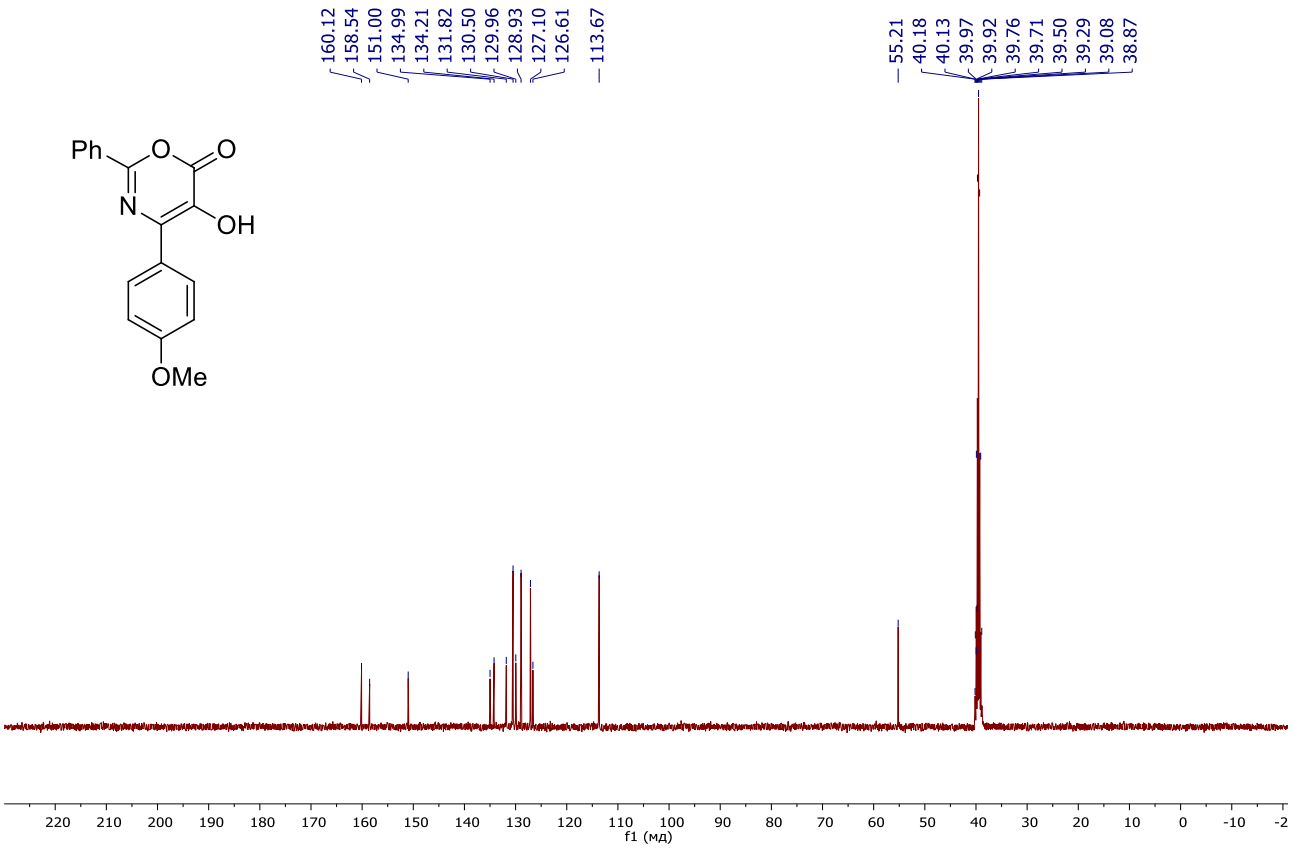
^{13}C NMR (100 MHz, DMSO-d_6) spectrum of **4zb**



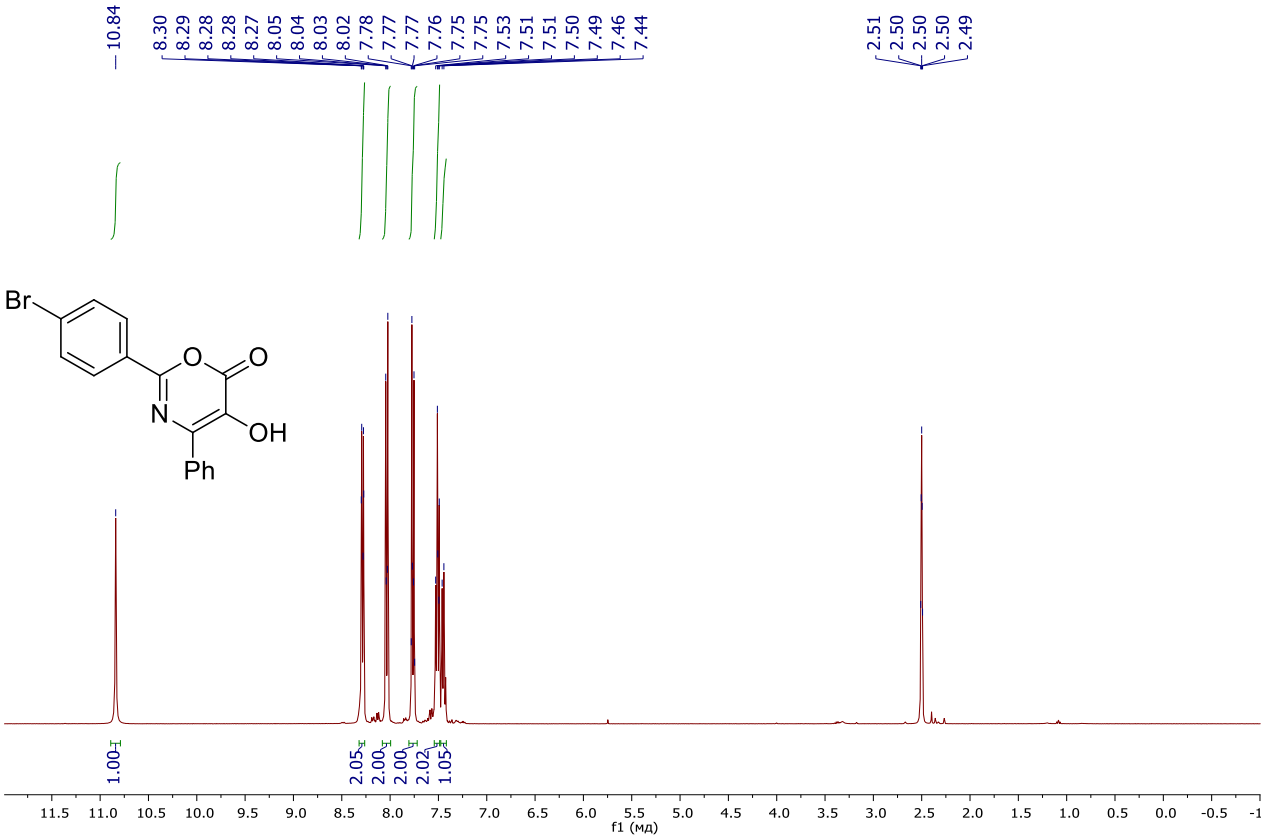
^{1}H NMR (400 MHz, DMSO-d_6) spectrum of **4zc**



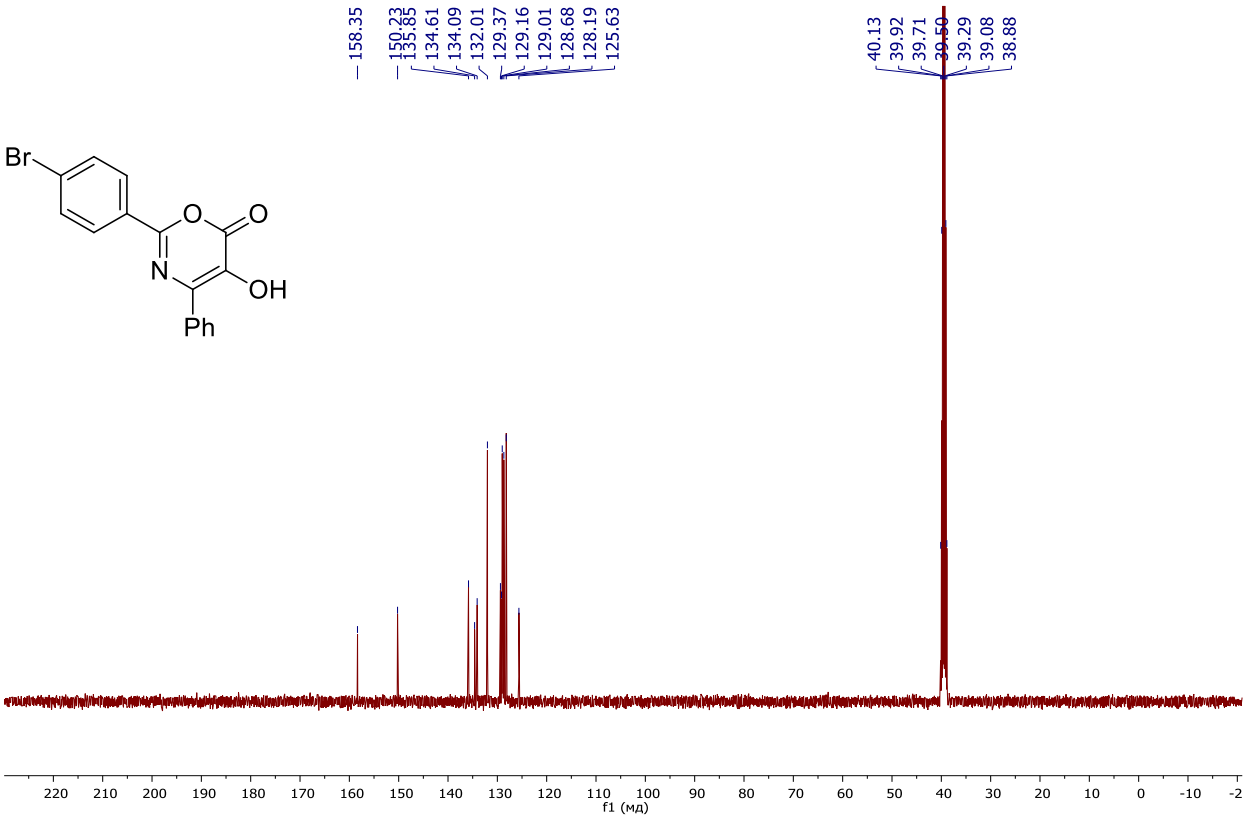
^{13}C NMR (100 MHz, DMSO-d_6) spectrum of **4zc**



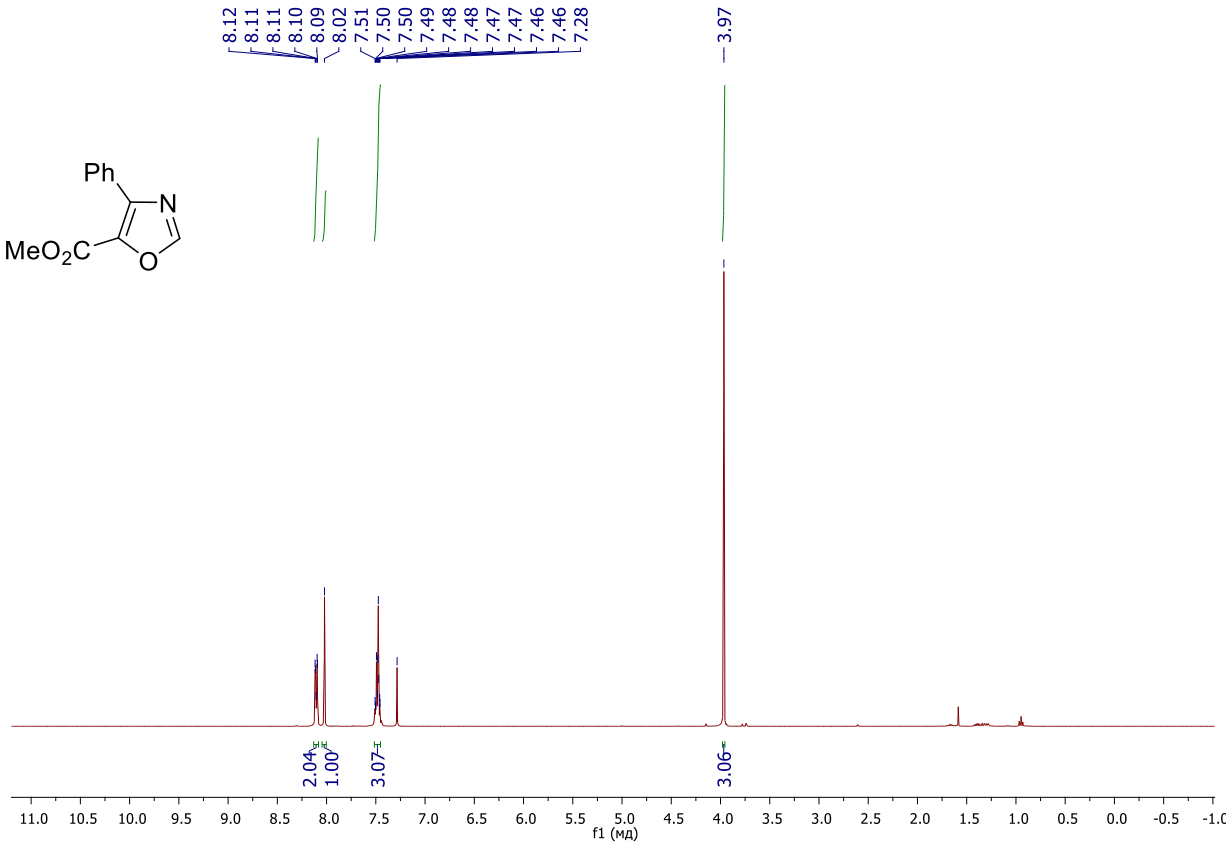
^{1}H NMR (400 MHz, DMSO-d_6) spectrum of **4zj**



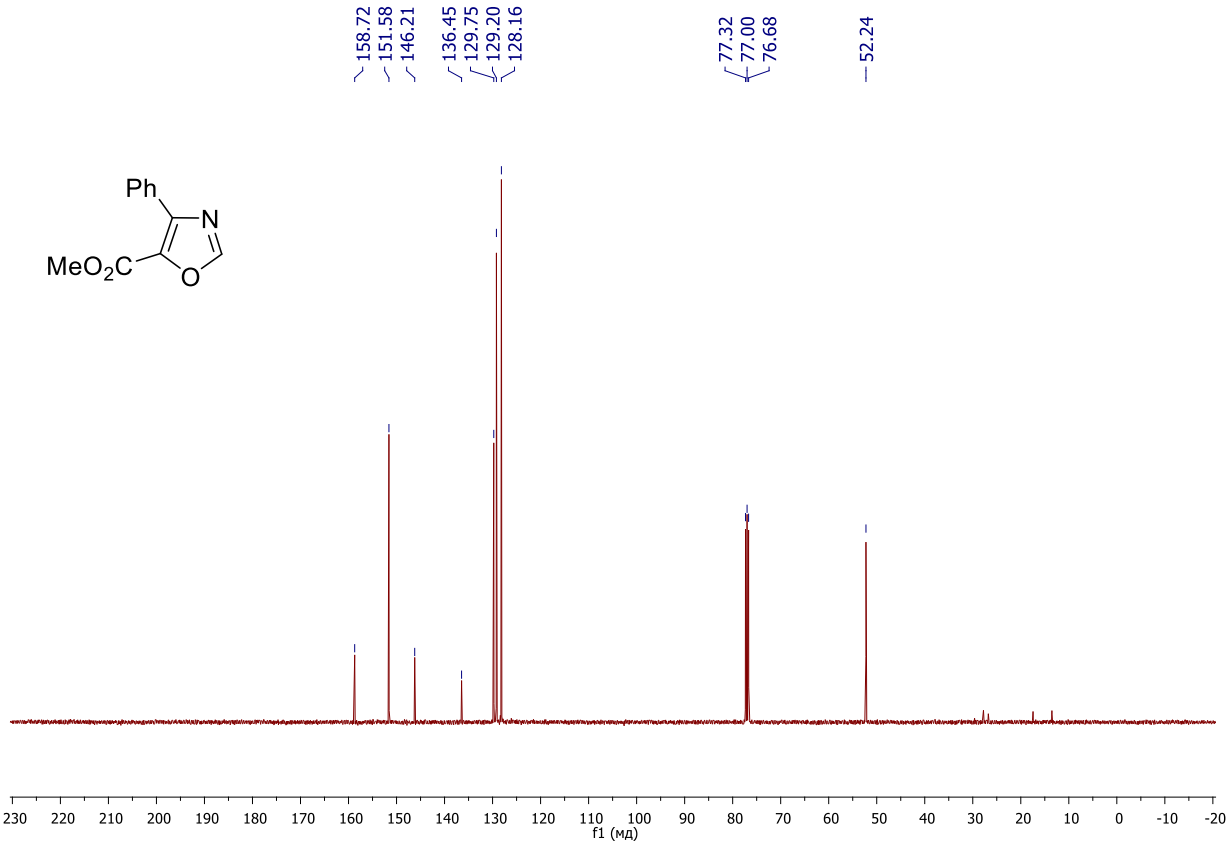
^{13}C NMR (100 MHz, DMSO-d_6) spectrum of **4zj**



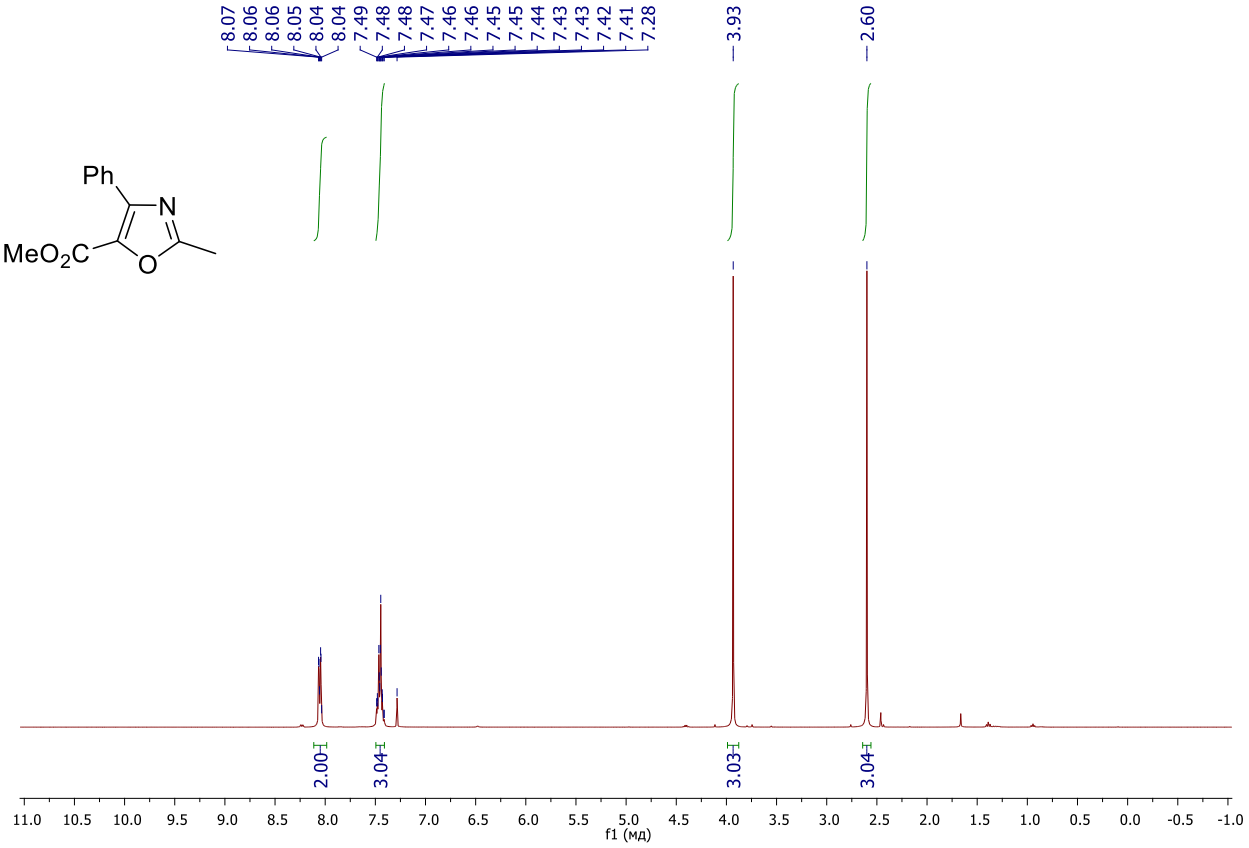
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of **5a**



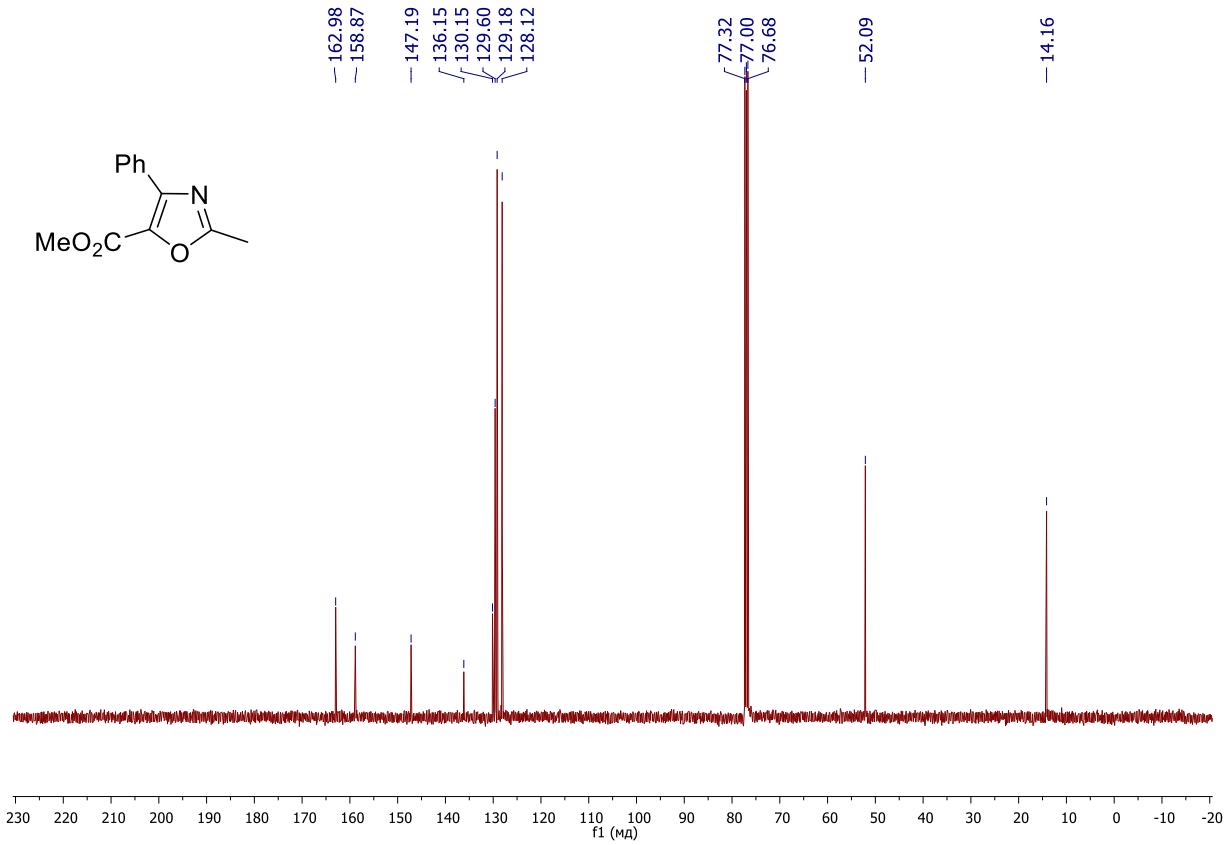
^{13}C NMR (100 MHz, $CDCl_3$) spectrum of **5a**



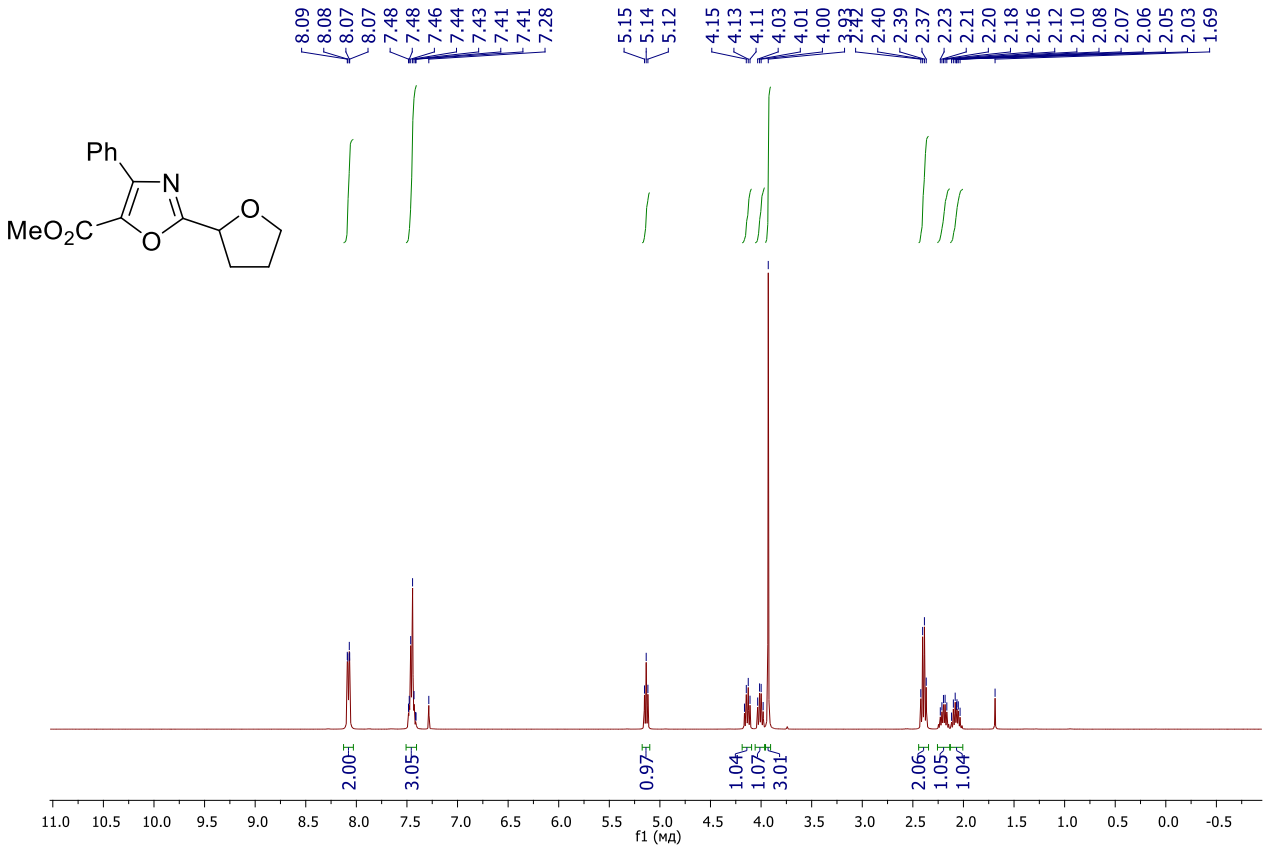
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of **5b**



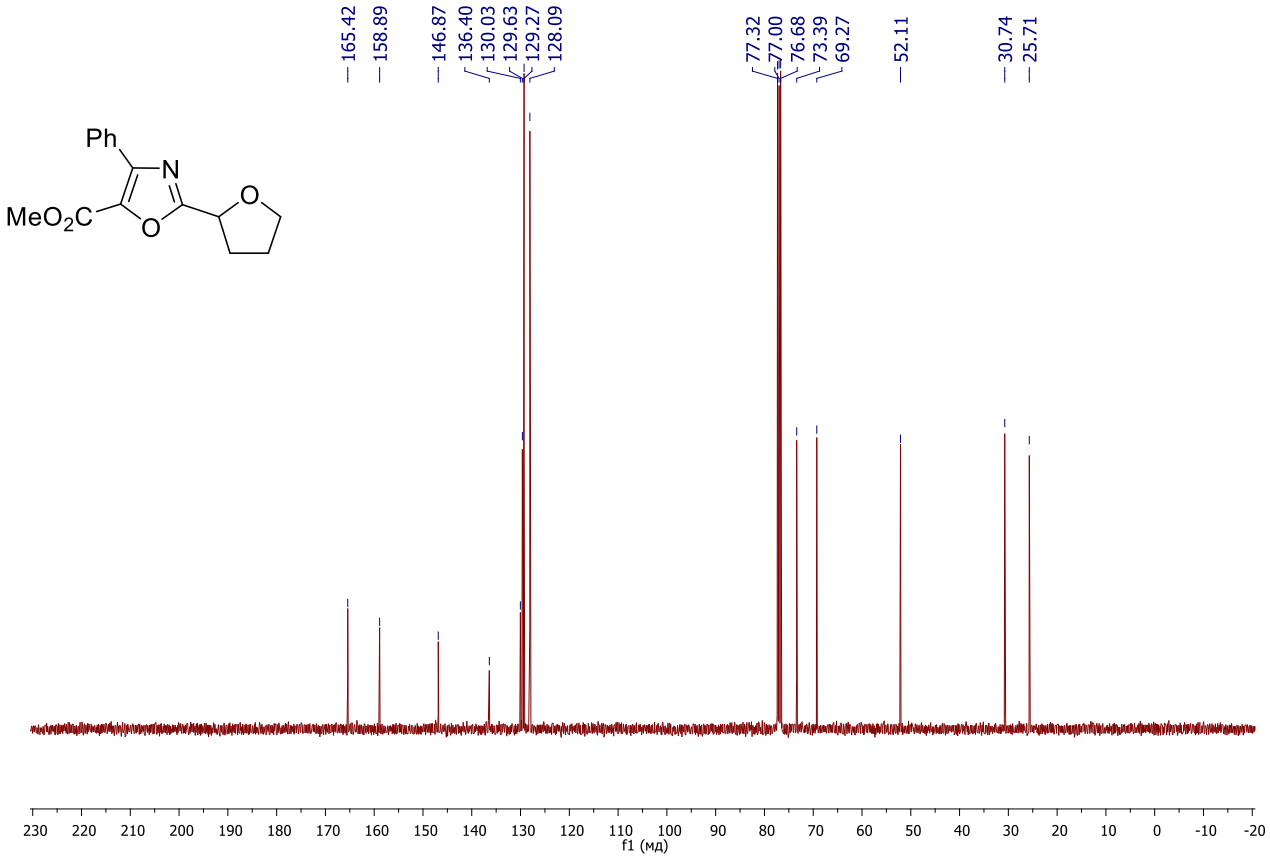
^{13}C NMR (100 MHz, $CDCl_3$) spectrum of **5b**



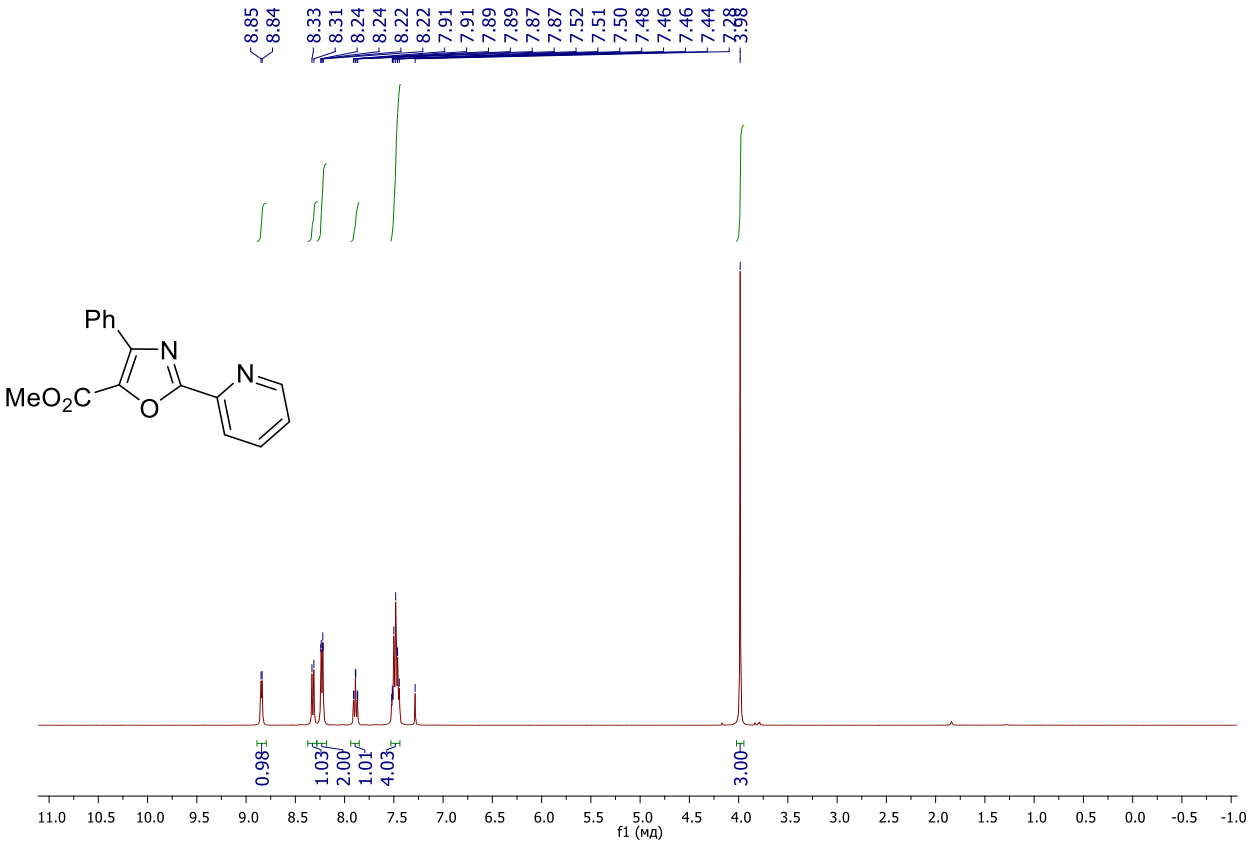
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of **5c**



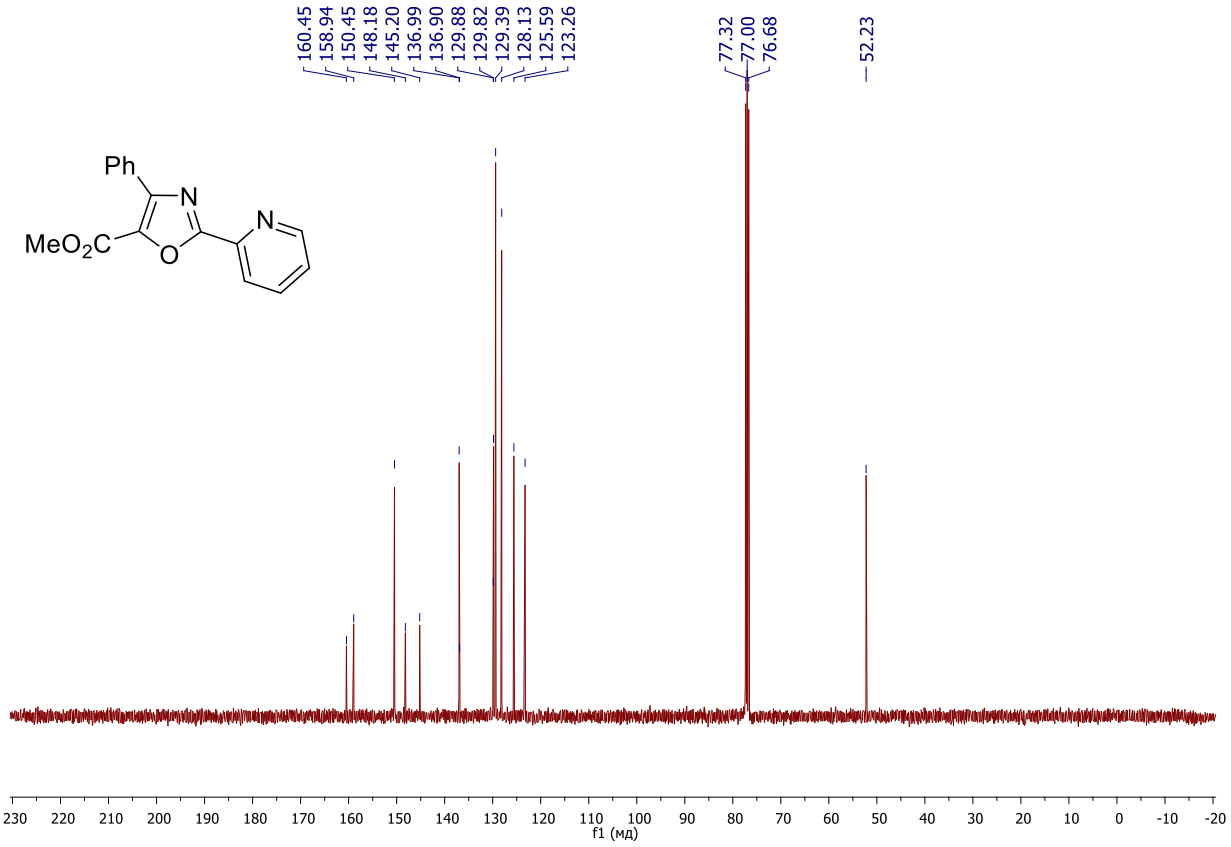
^{13}C NMR (100 MHz, $CDCl_3$) spectrum of **5c**



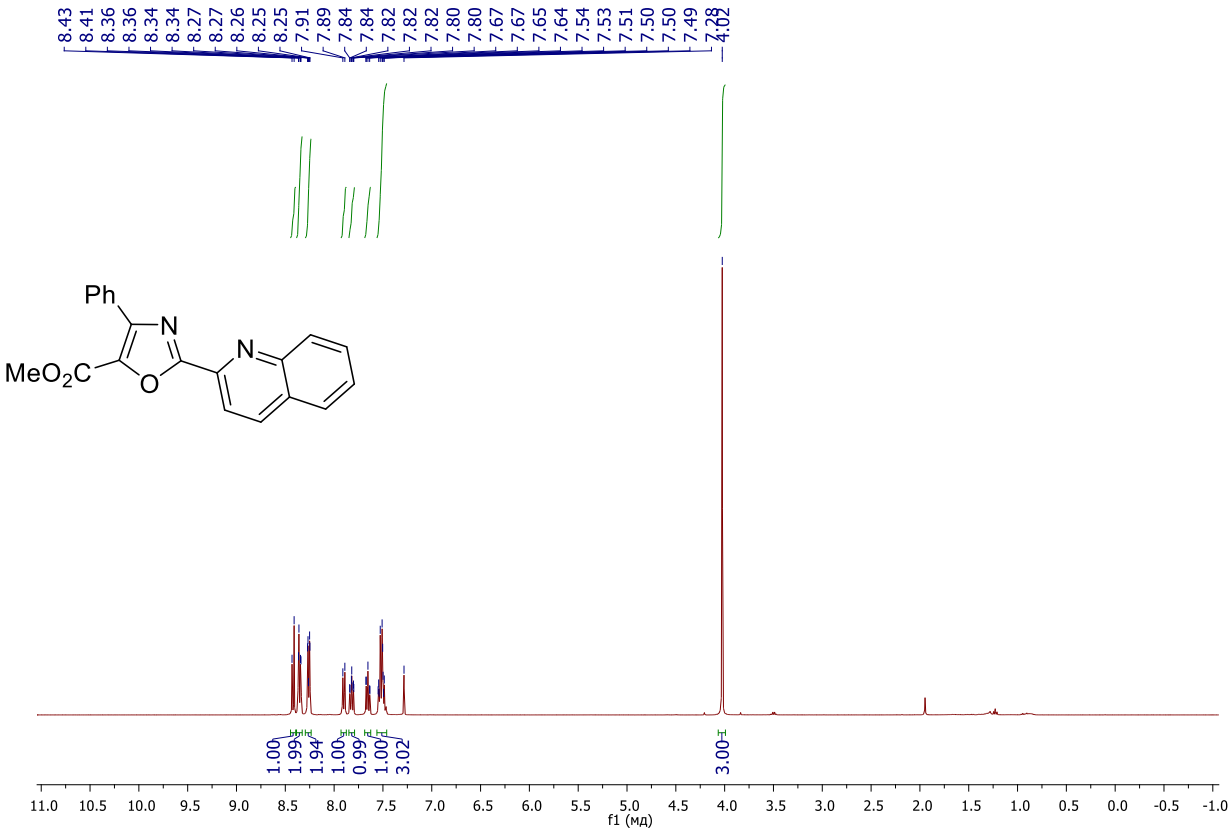
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of **5d**



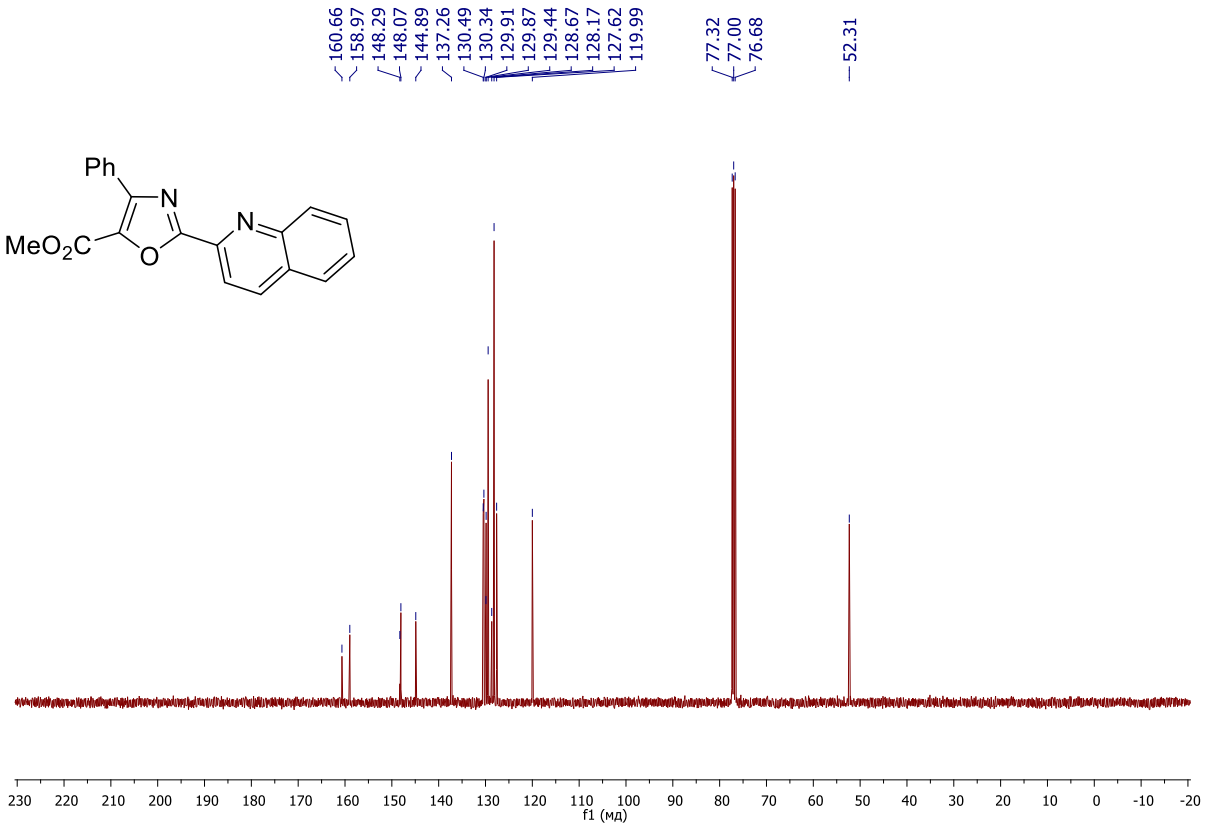
^{13}C NMR (100 MHz, $CDCl_3$) spectrum of **5d**



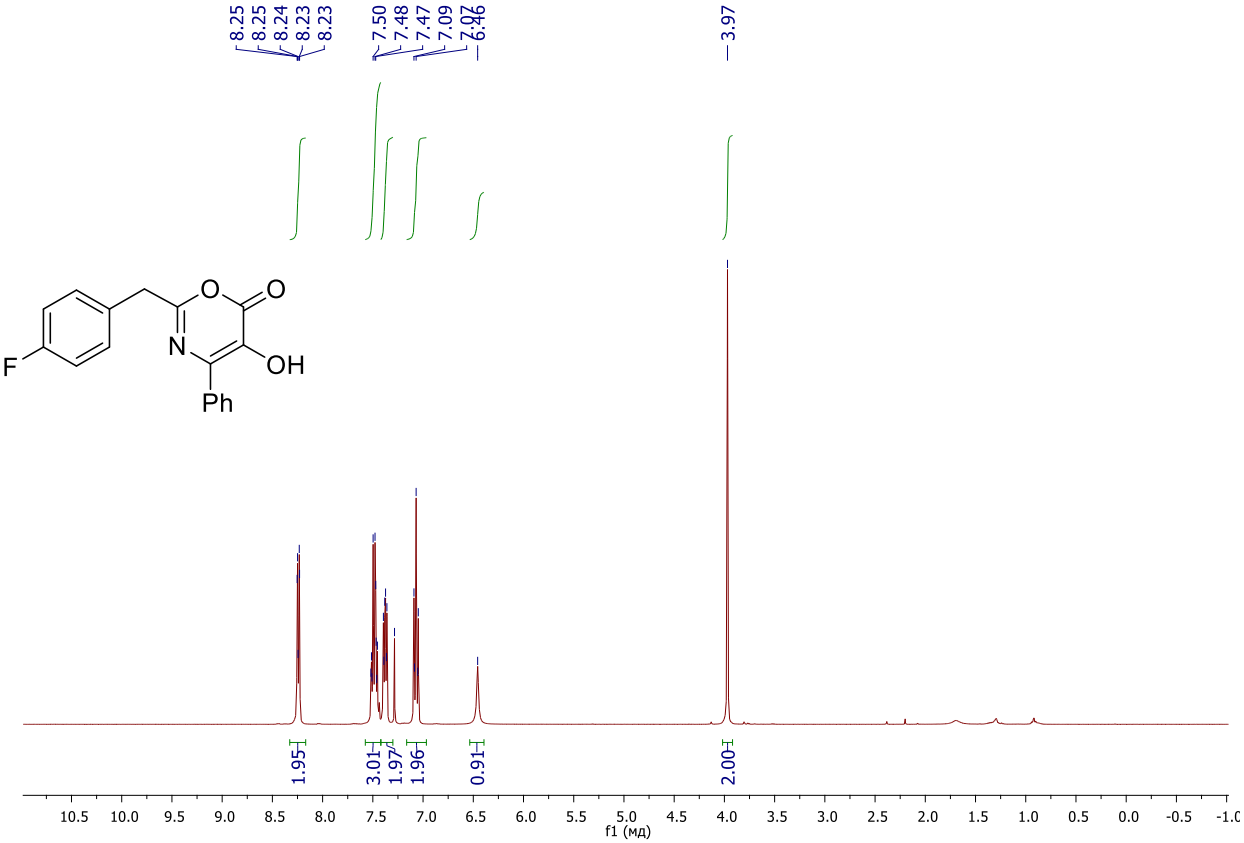
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of **5e**



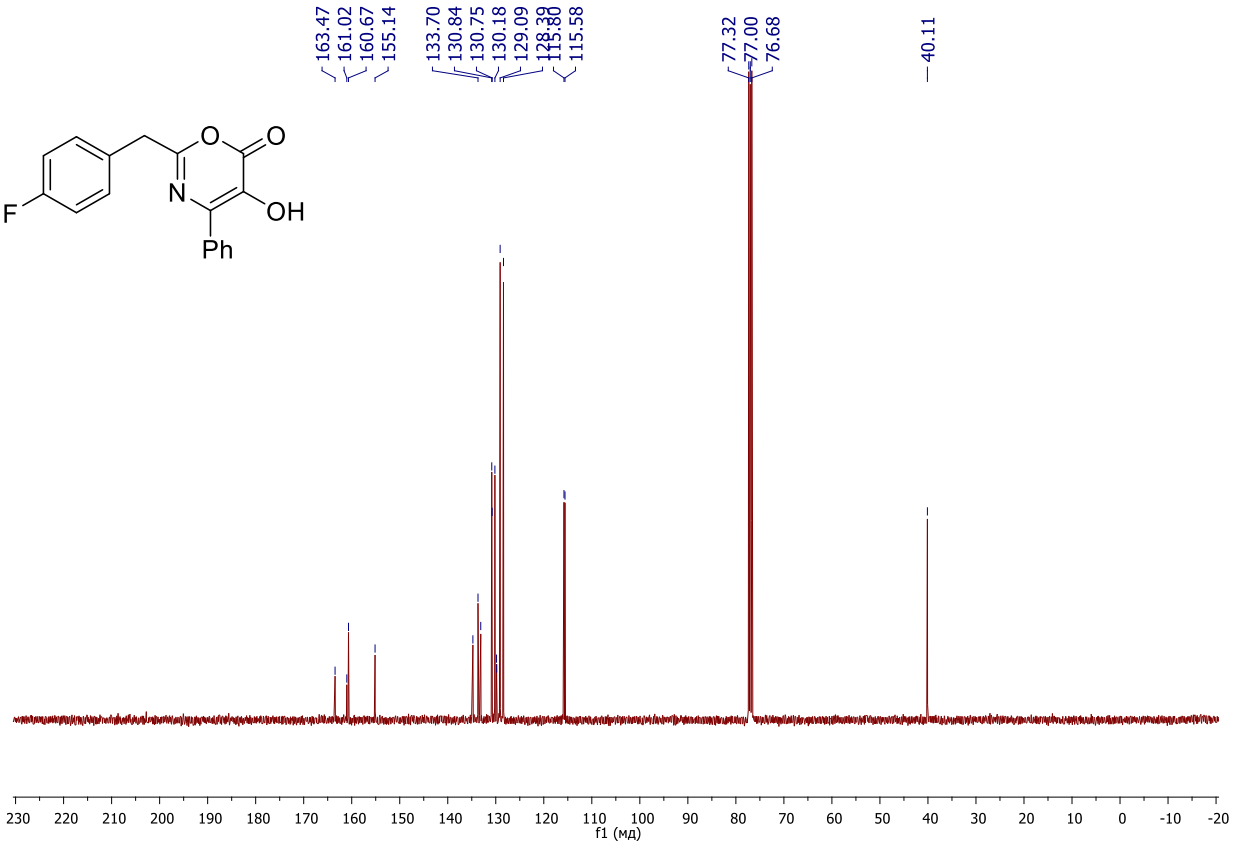
^{13}C NMR (100 MHz, $CDCl_3$) spectrum of **5e**



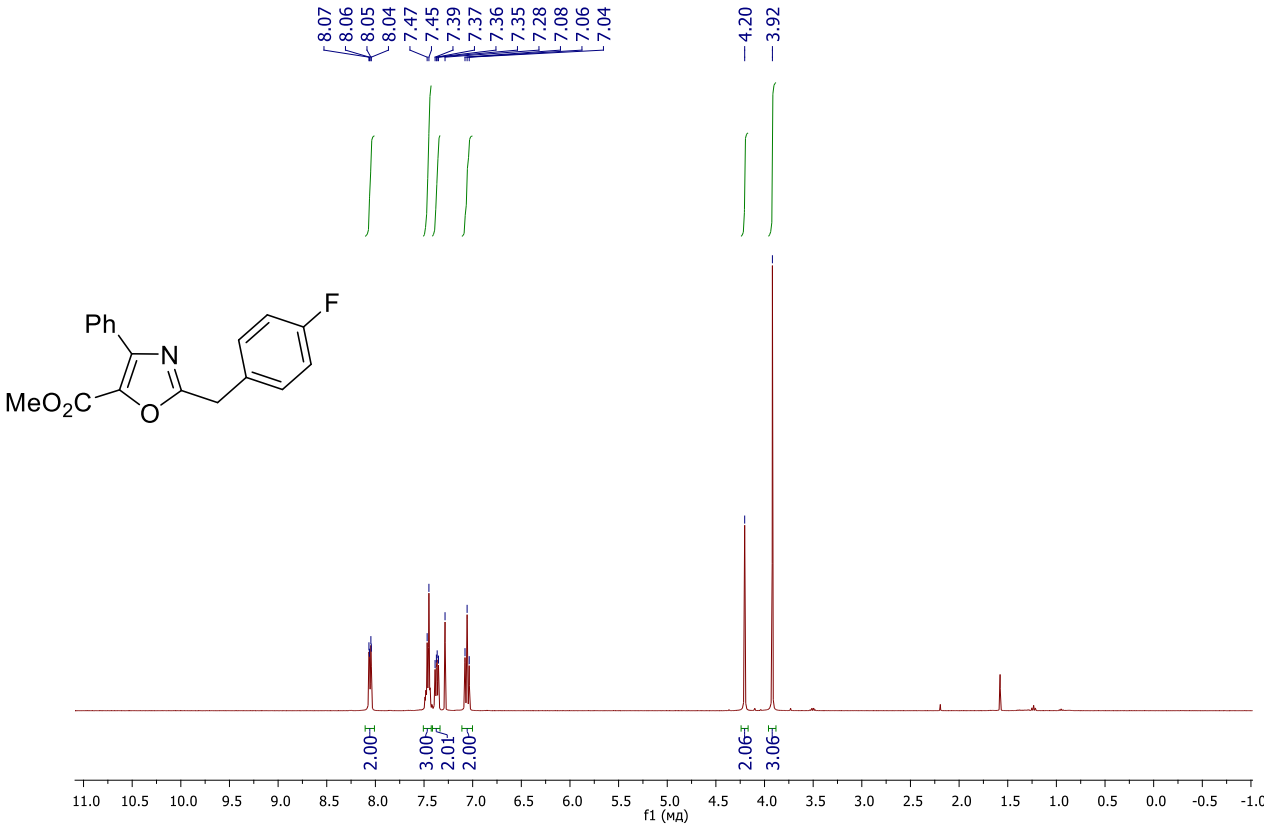
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of **4zp**



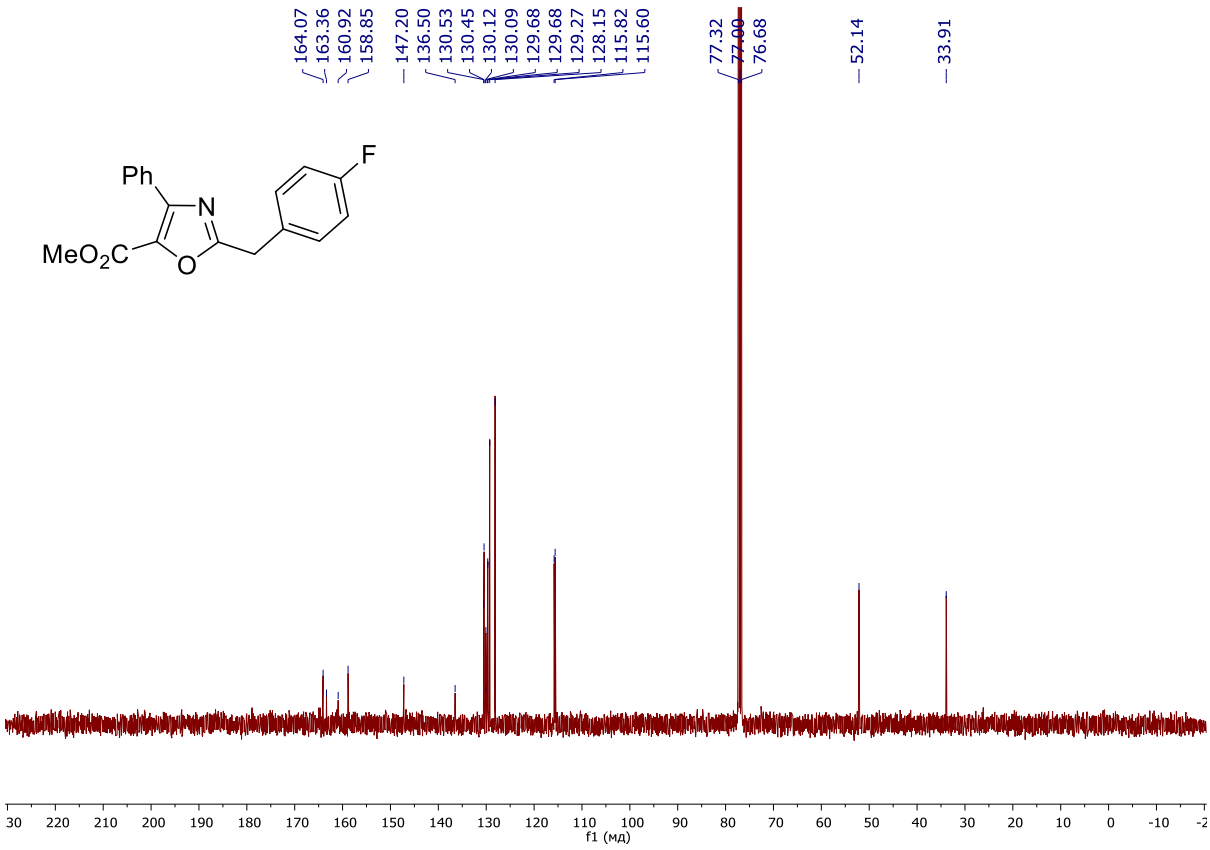
^{13}C NMR (100 MHz, $CDCl_3$) spectrum of **4zp**



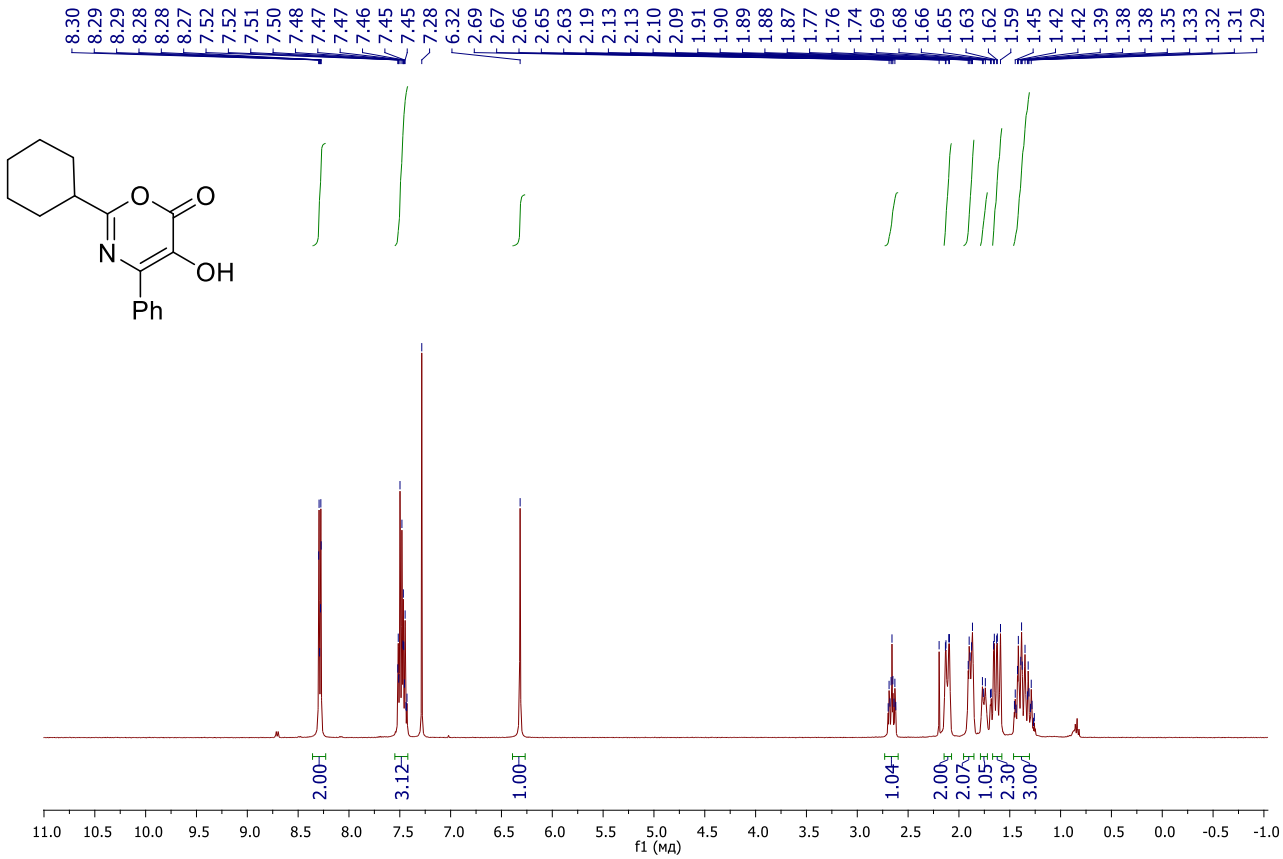
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of **5f**



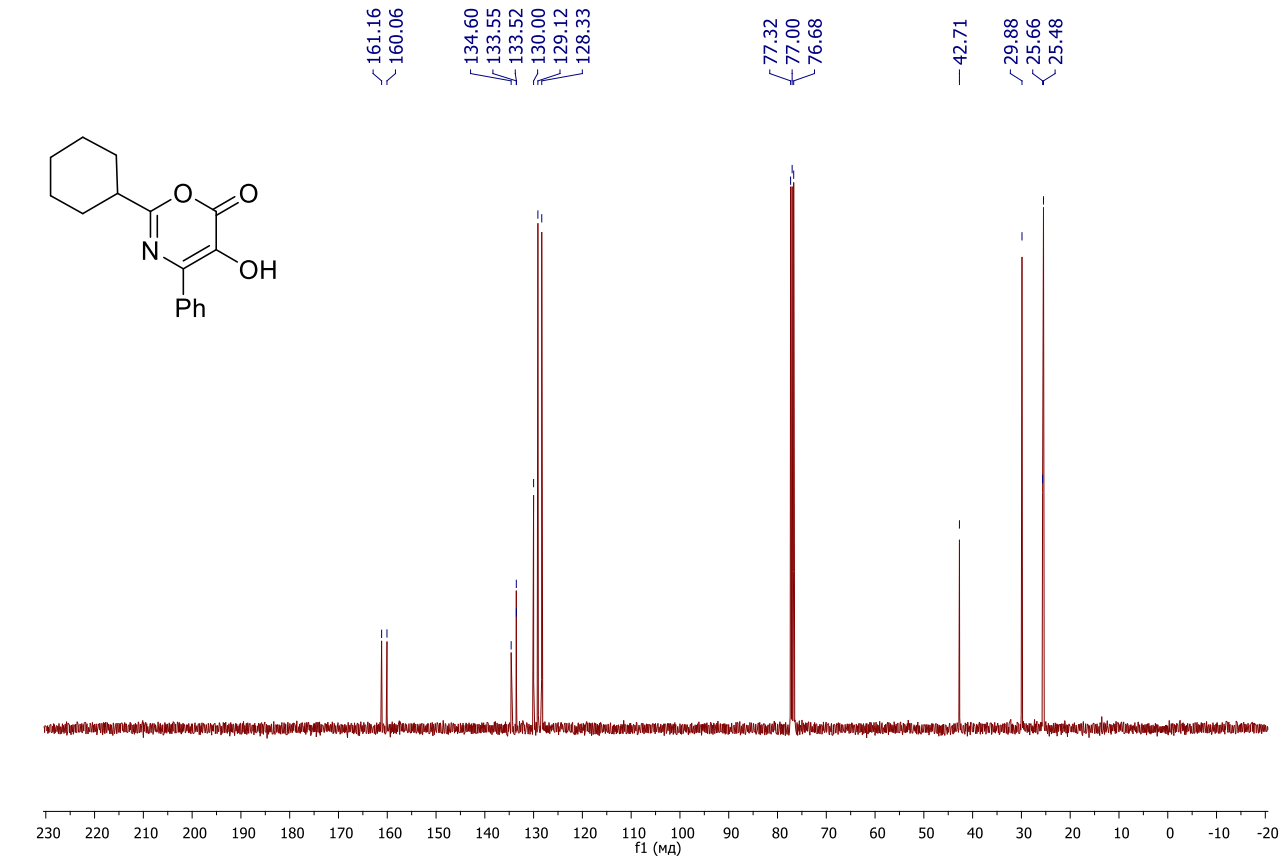
^{13}C NMR (100 MHz, $CDCl_3$) spectrum of **5f**



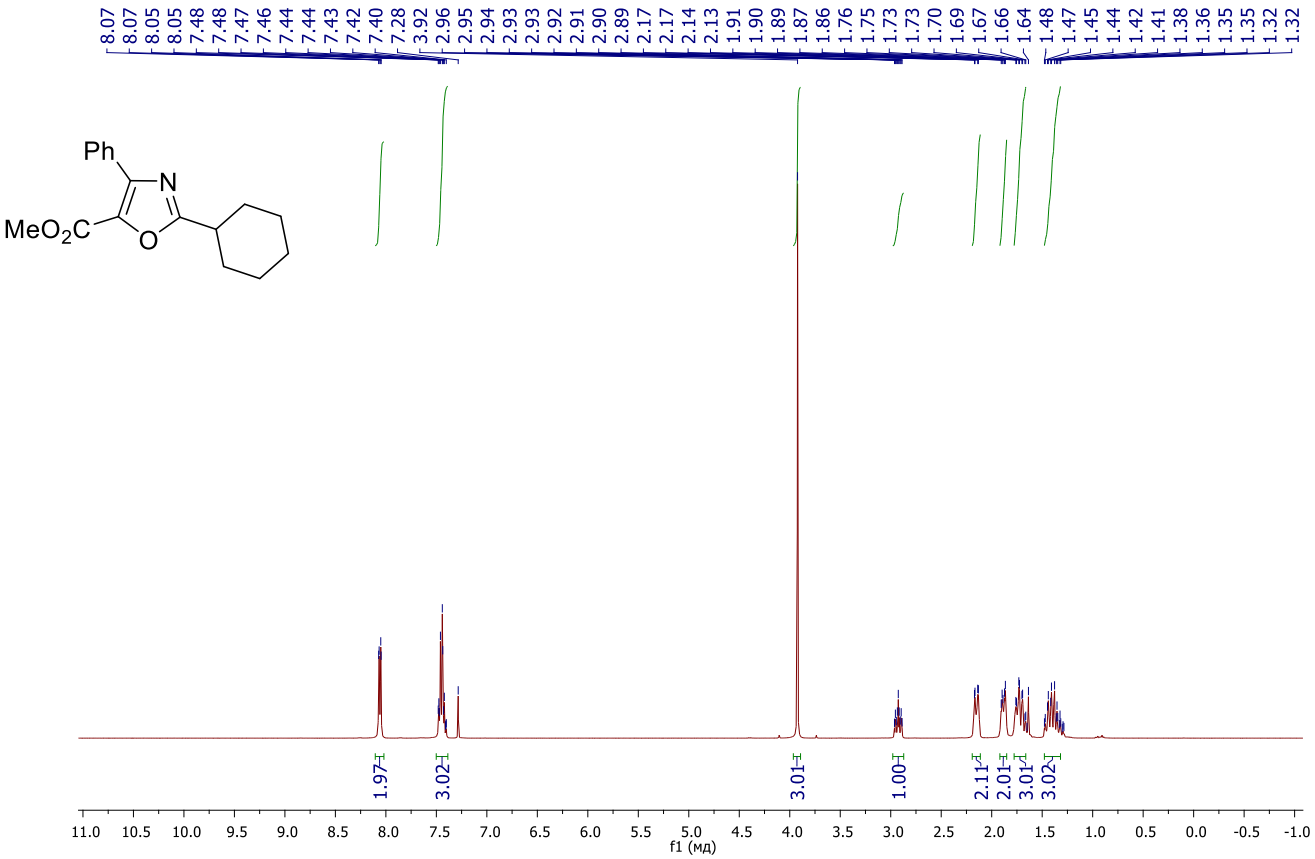
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of **4zq**



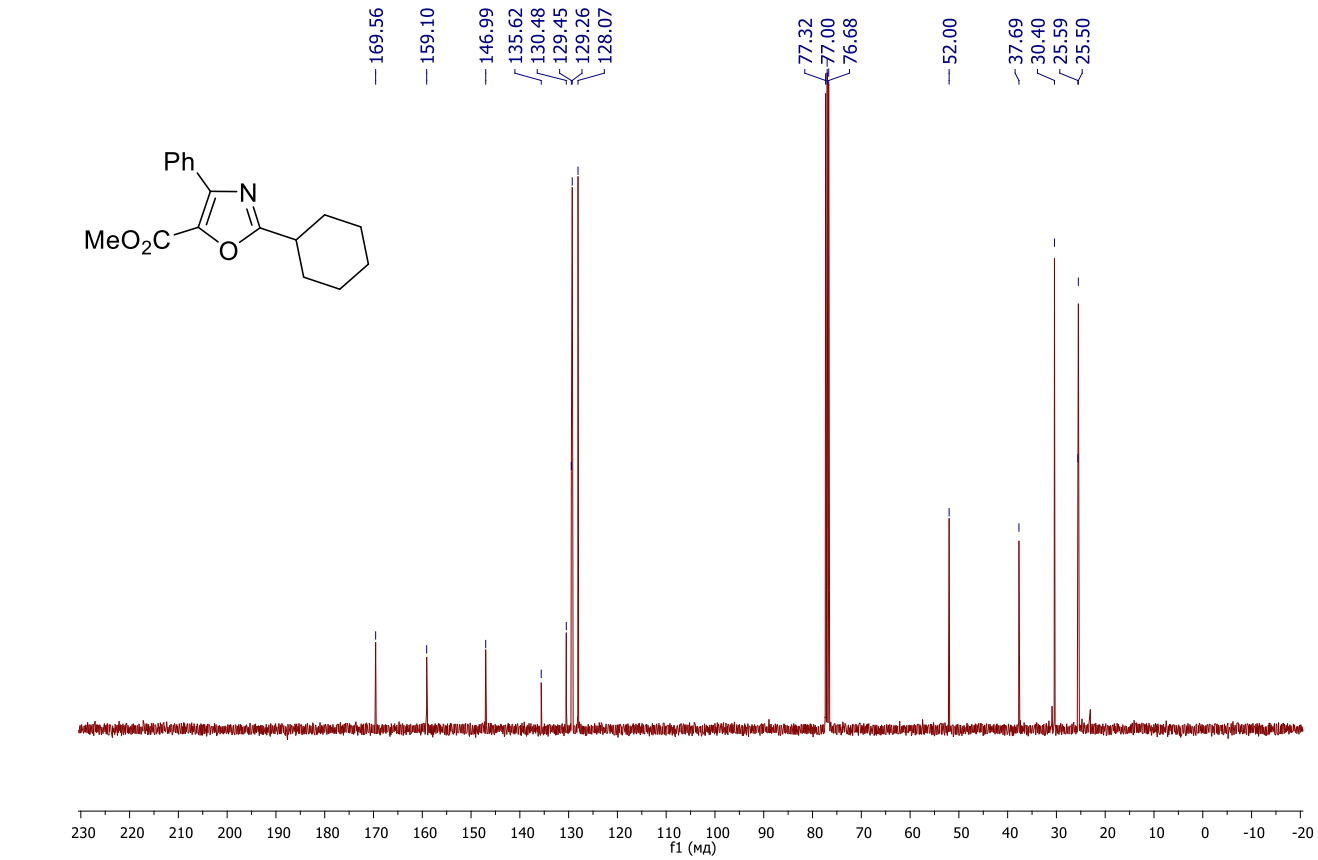
^{13}C NMR (100 MHz, $CDCl_3$) spectrum of **4zq**



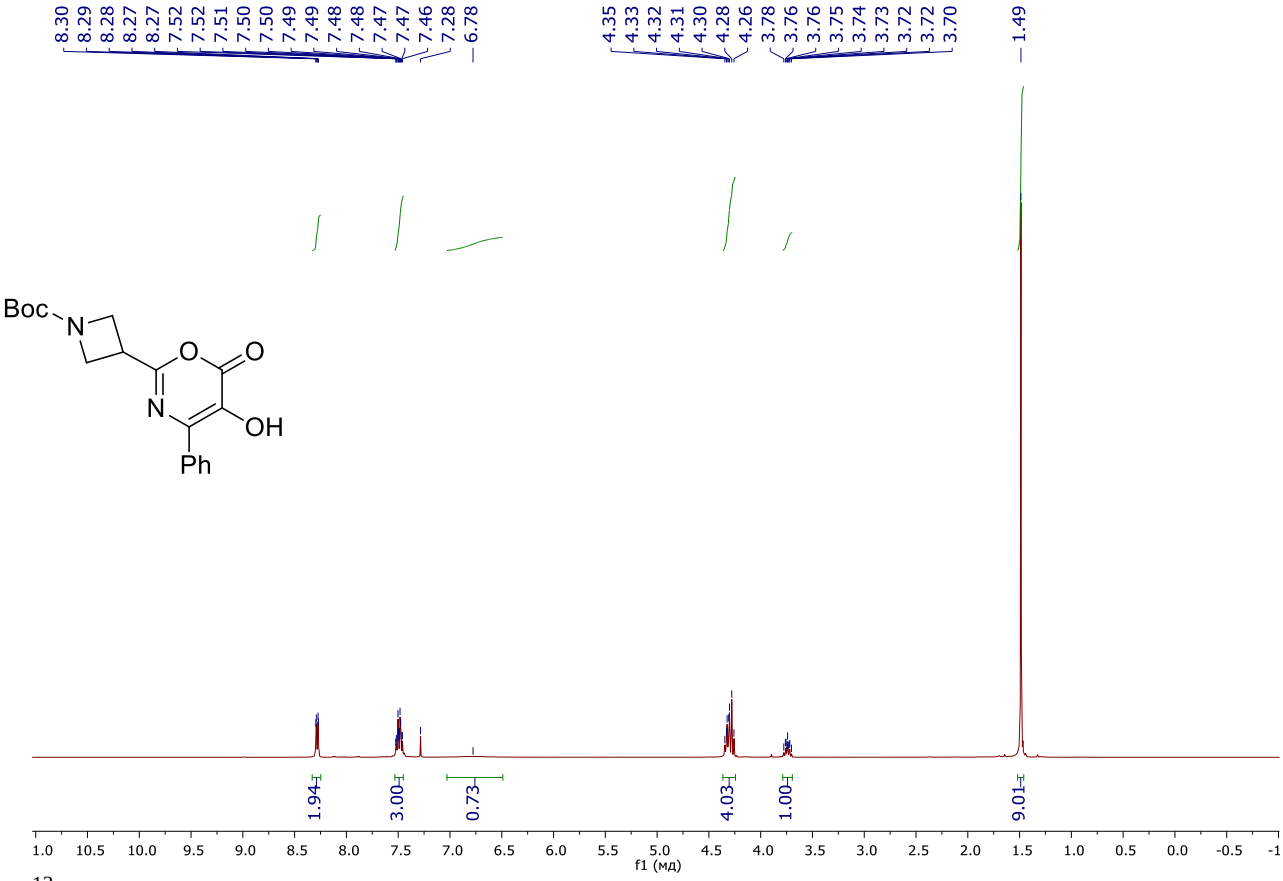
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of **5g**



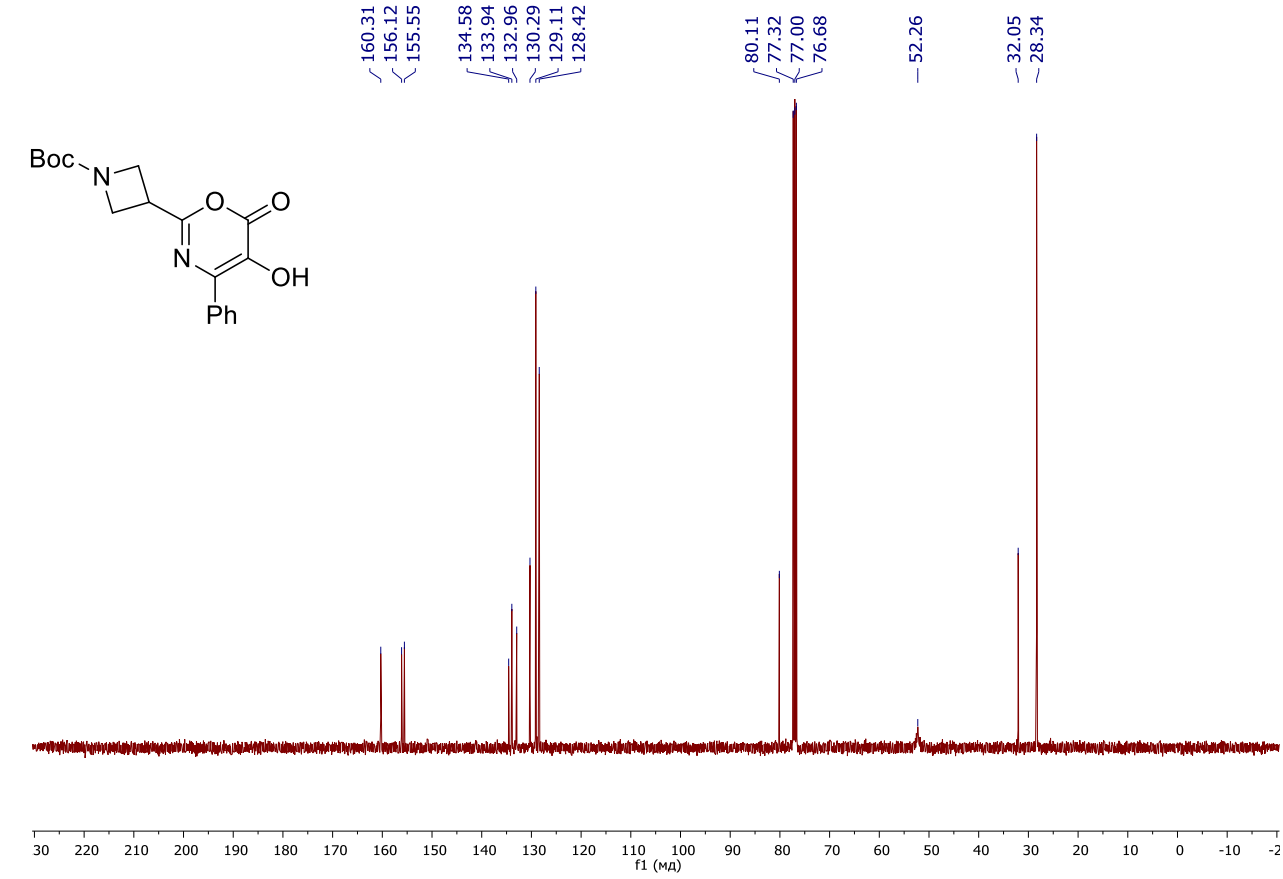
^{13}C NMR (100 MHz, $CDCl_3$) spectrum of **5g**



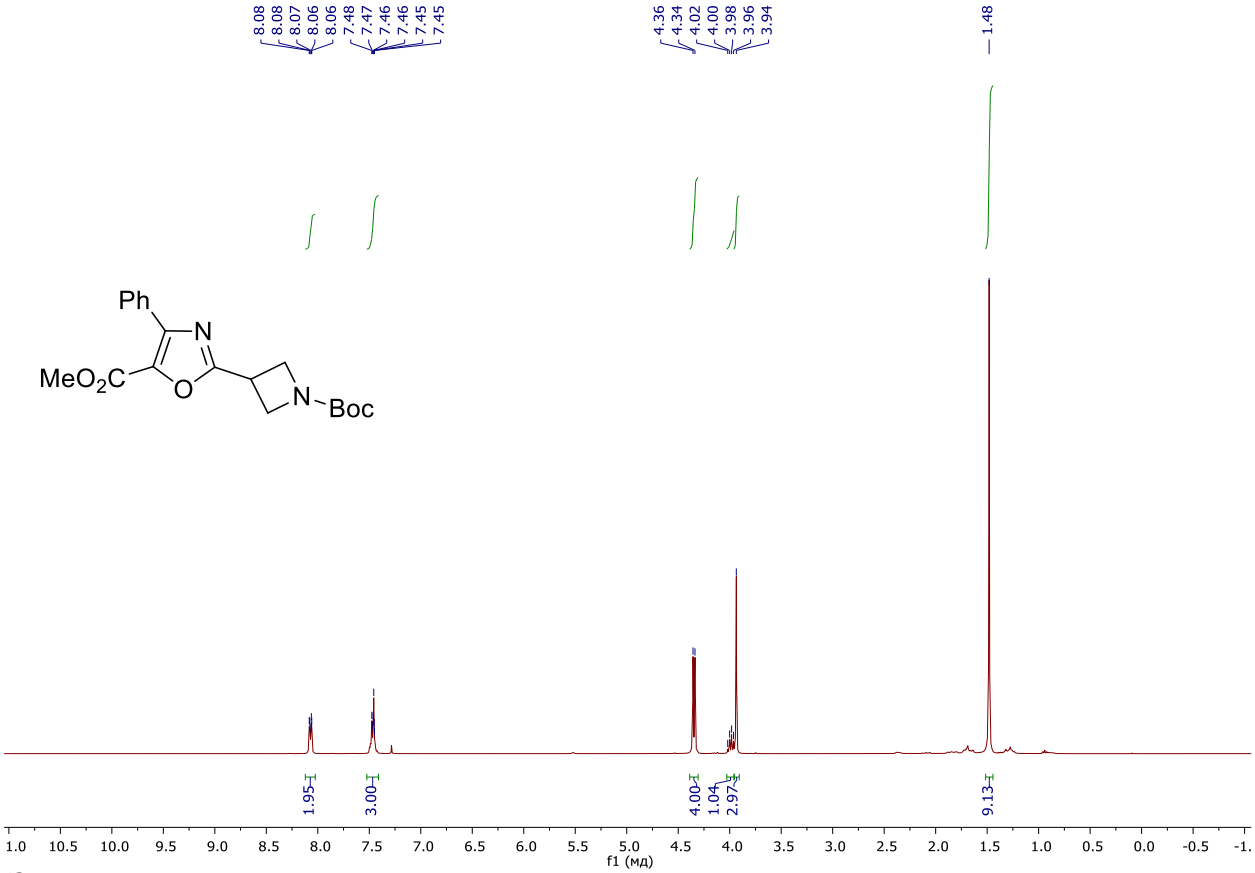
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of **4zr**



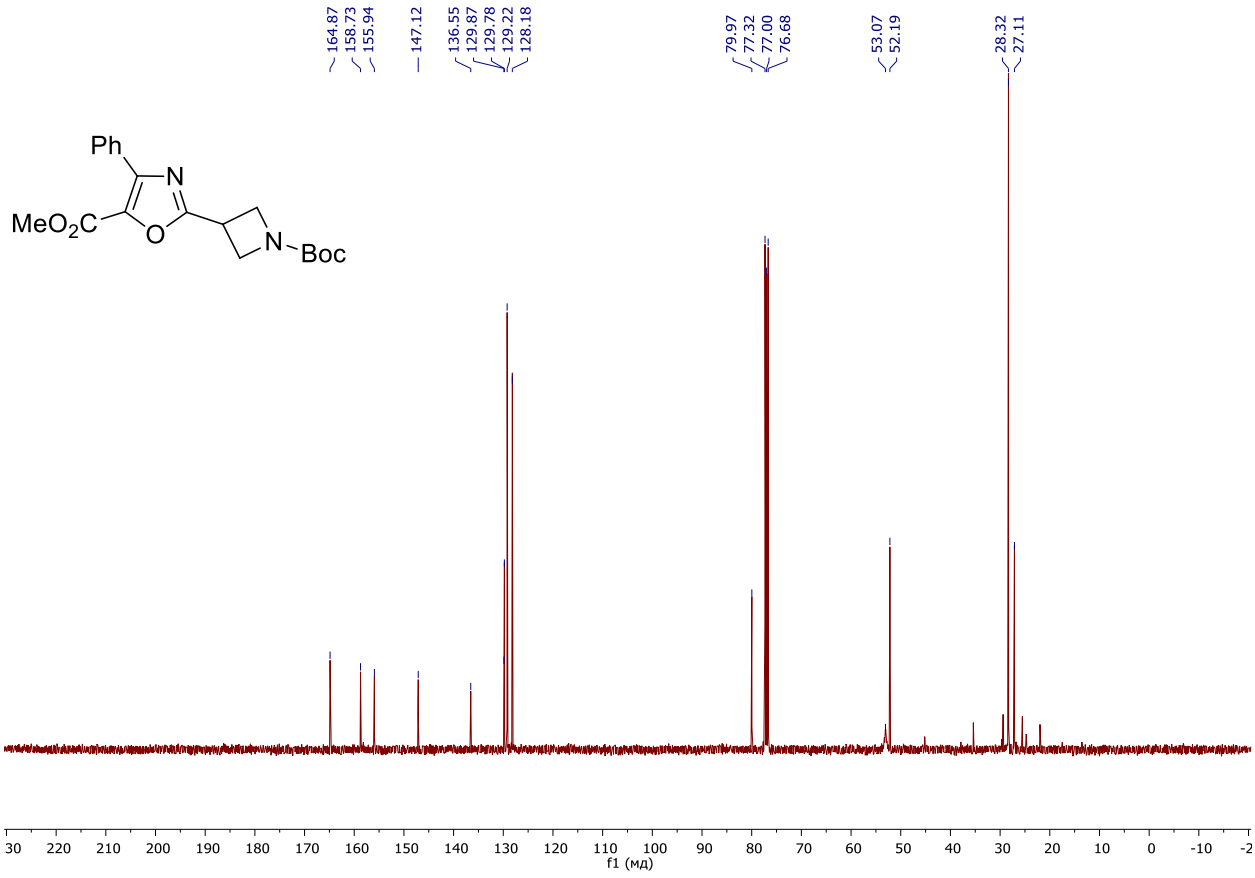
^{13}C NMR (100 MHz, $CDCl_3$) spectrum of **4zr**



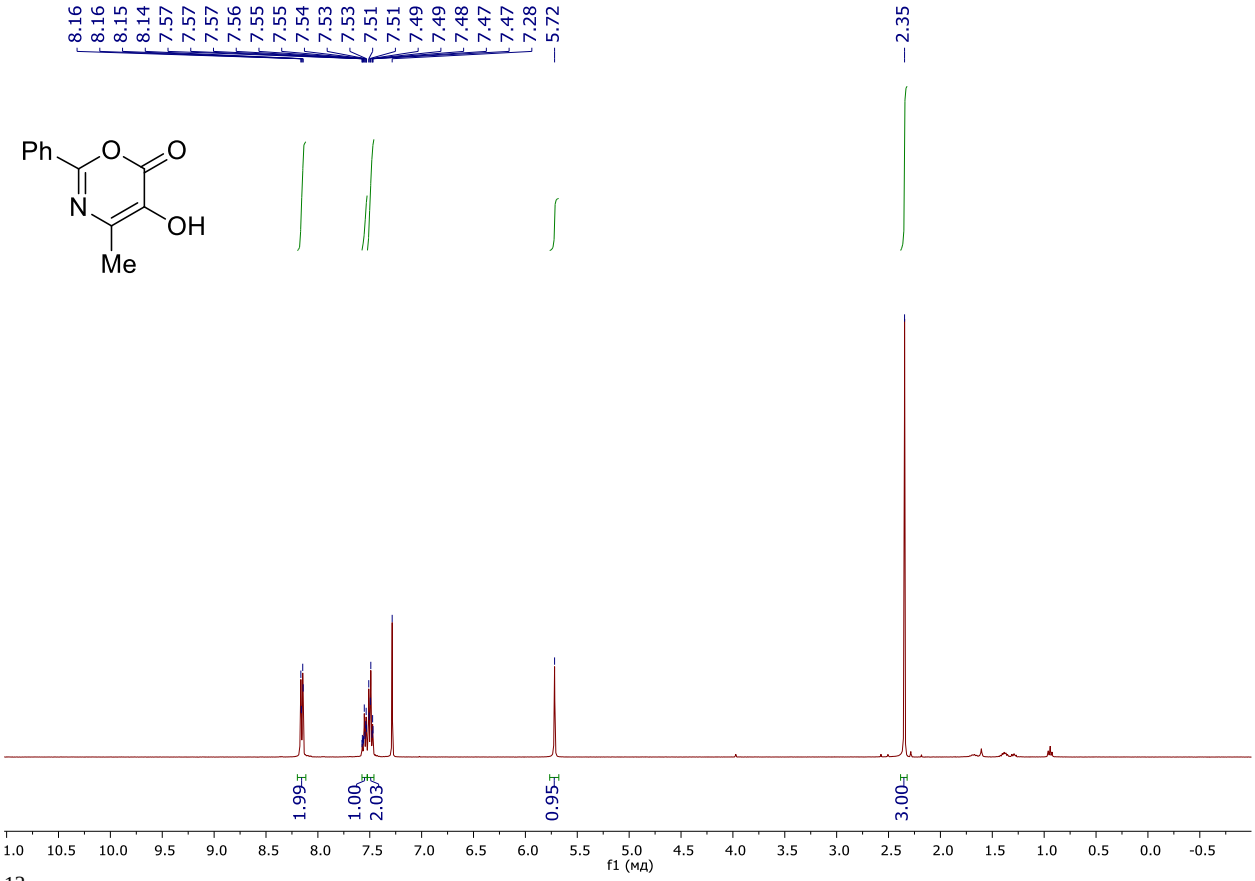
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of **5h**



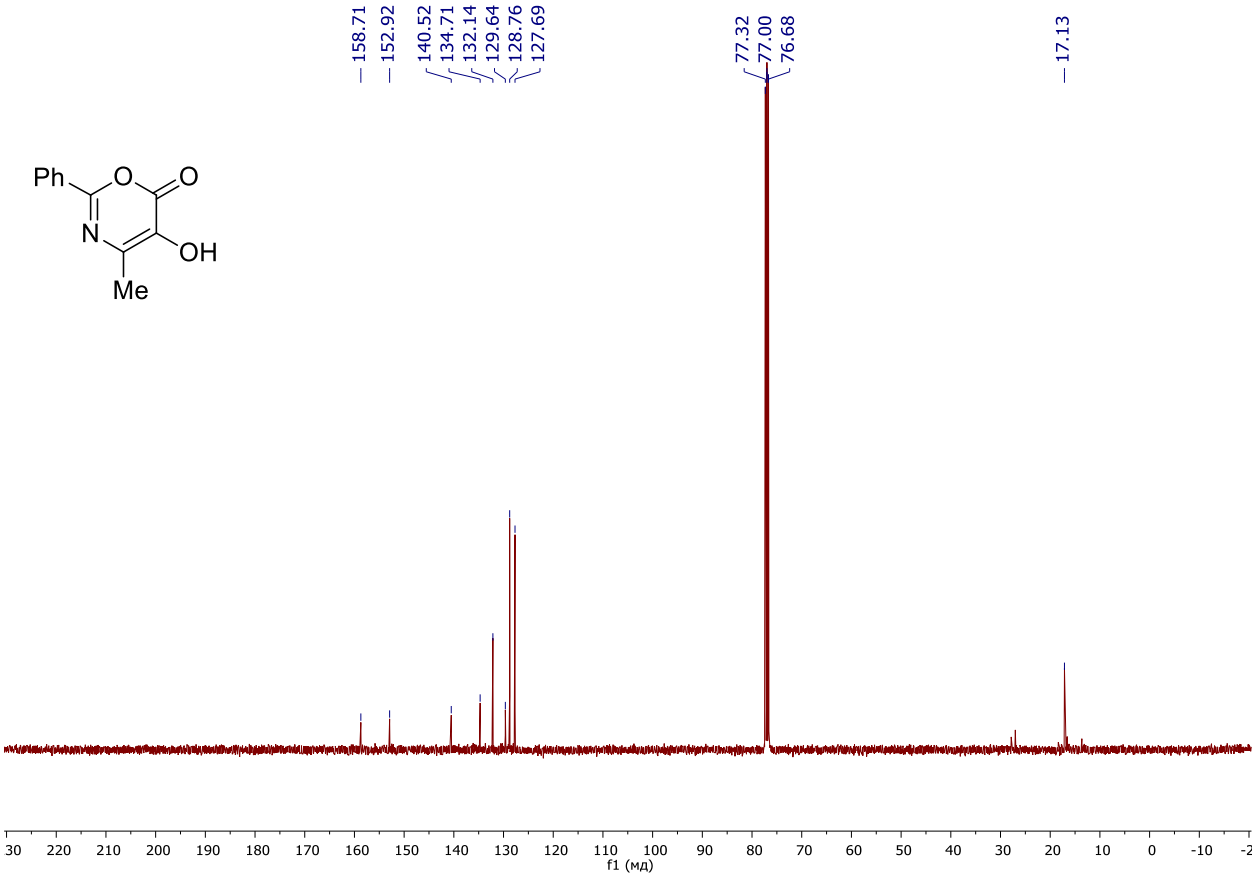
^{13}C NMR (100 MHz, $CDCl_3$) spectrum of **5h**



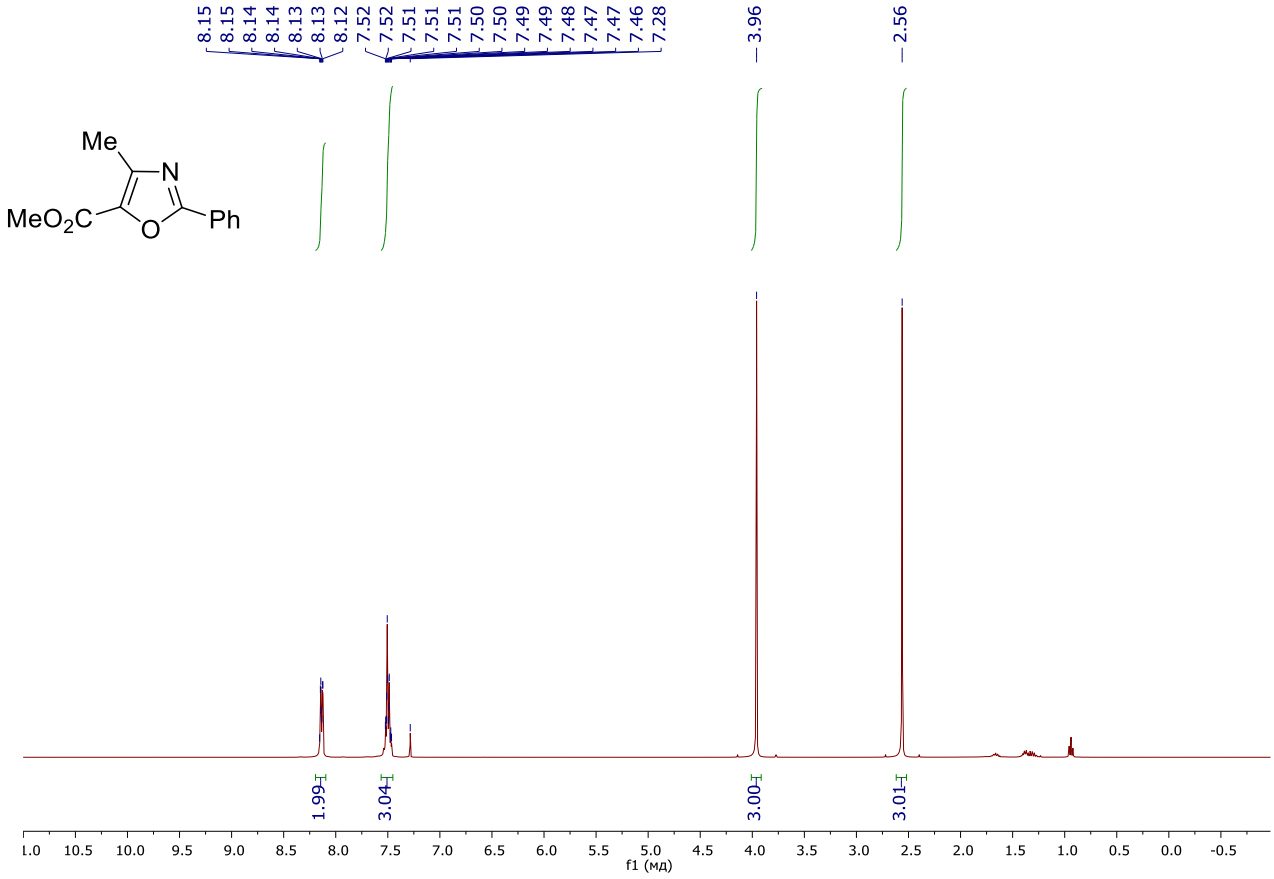
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of **4zs**



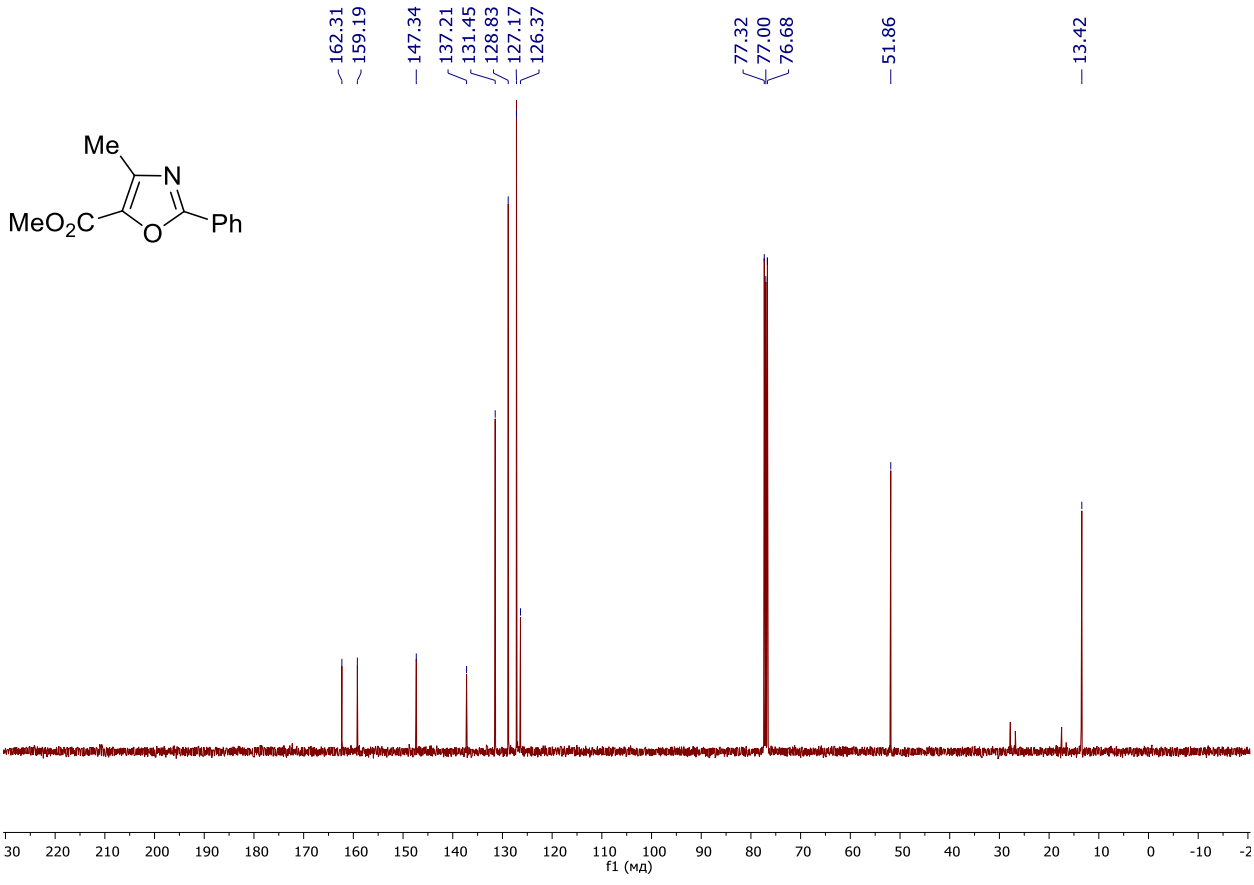
^{13}C NMR (100 MHz, $CDCl_3$) spectrum of **4zs**



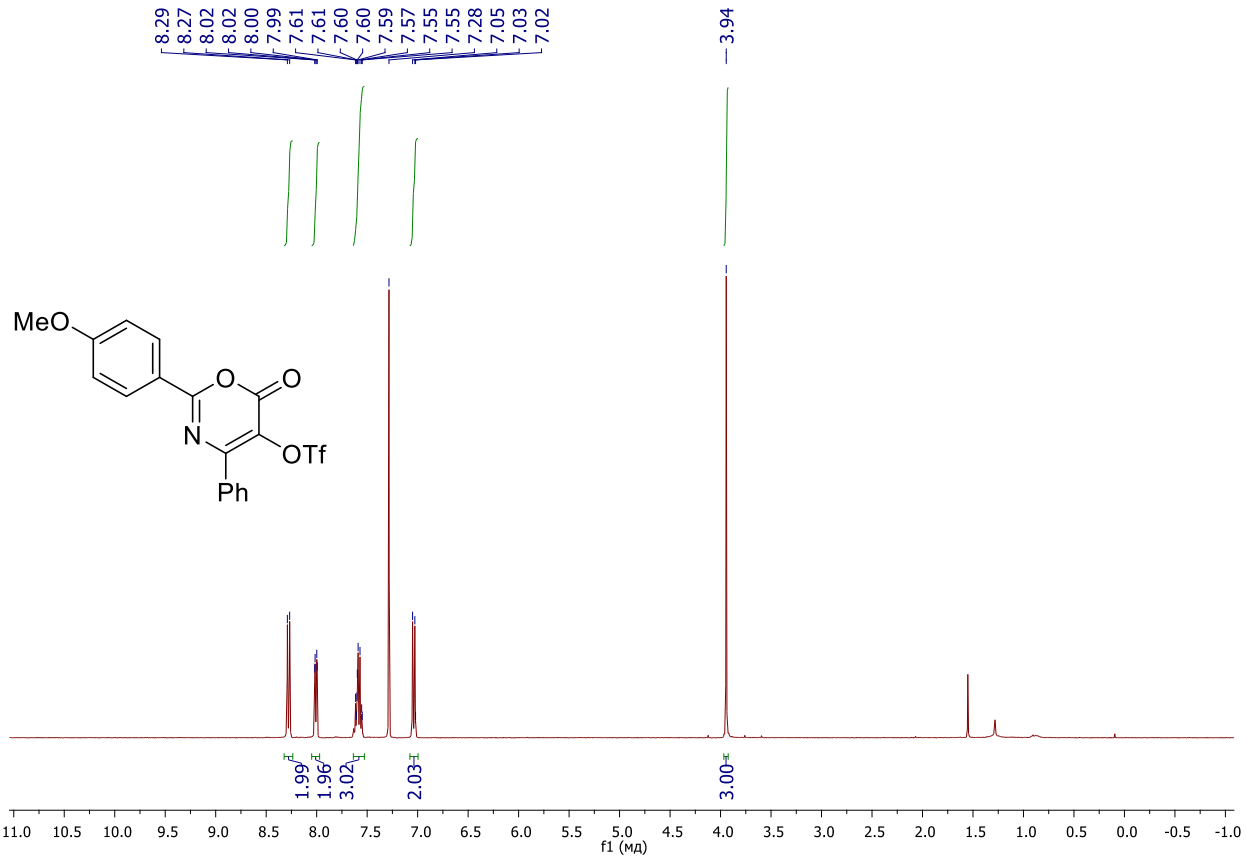
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of **5i**



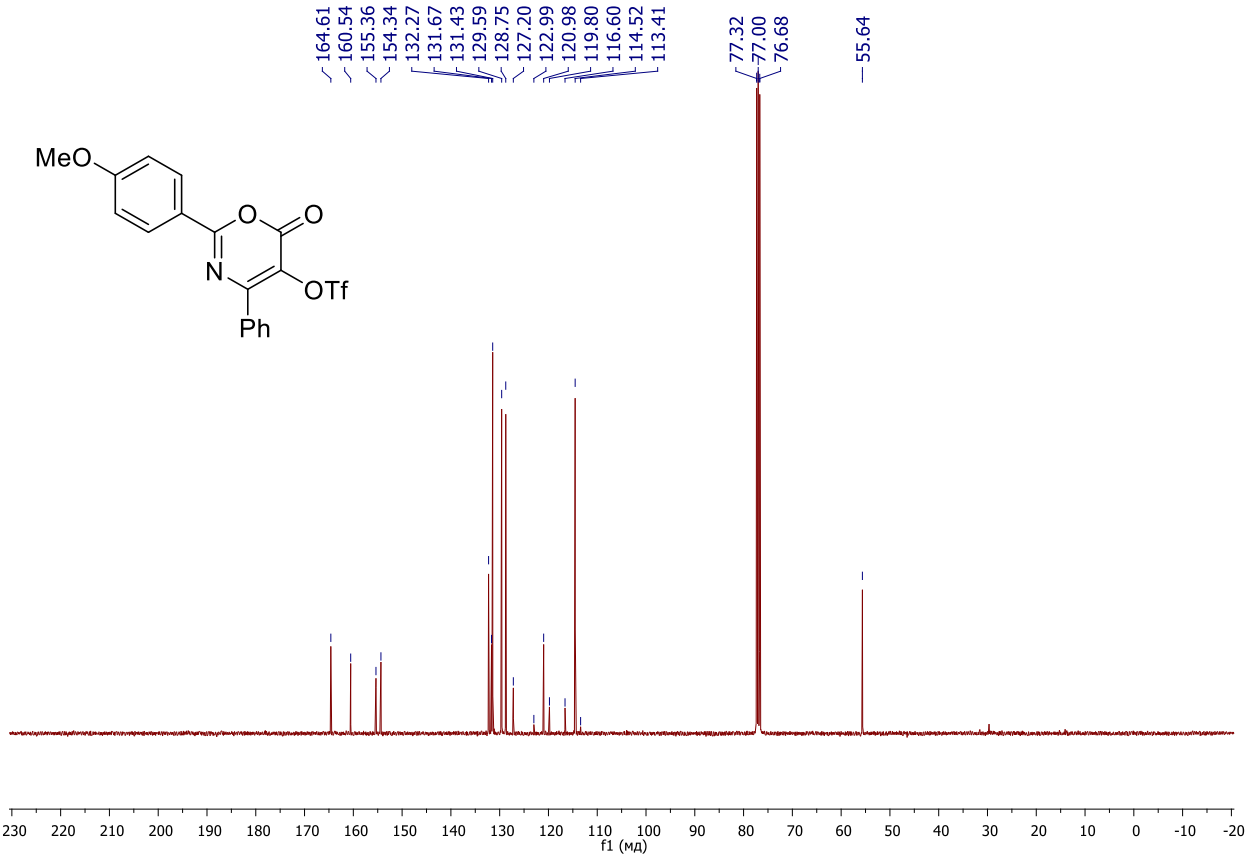
^{13}C NMR (100 MHz, $CDCl_3$) spectrum of **5i**



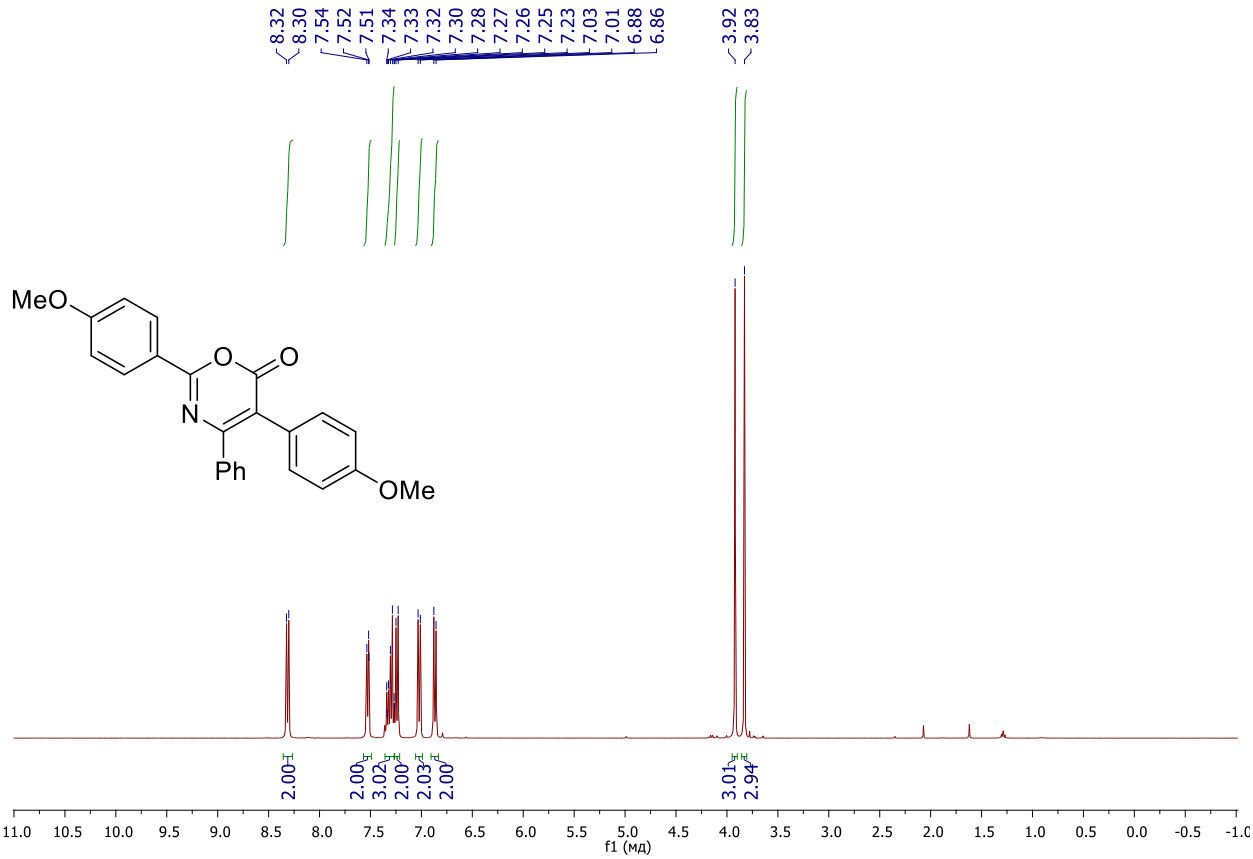
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of **16**



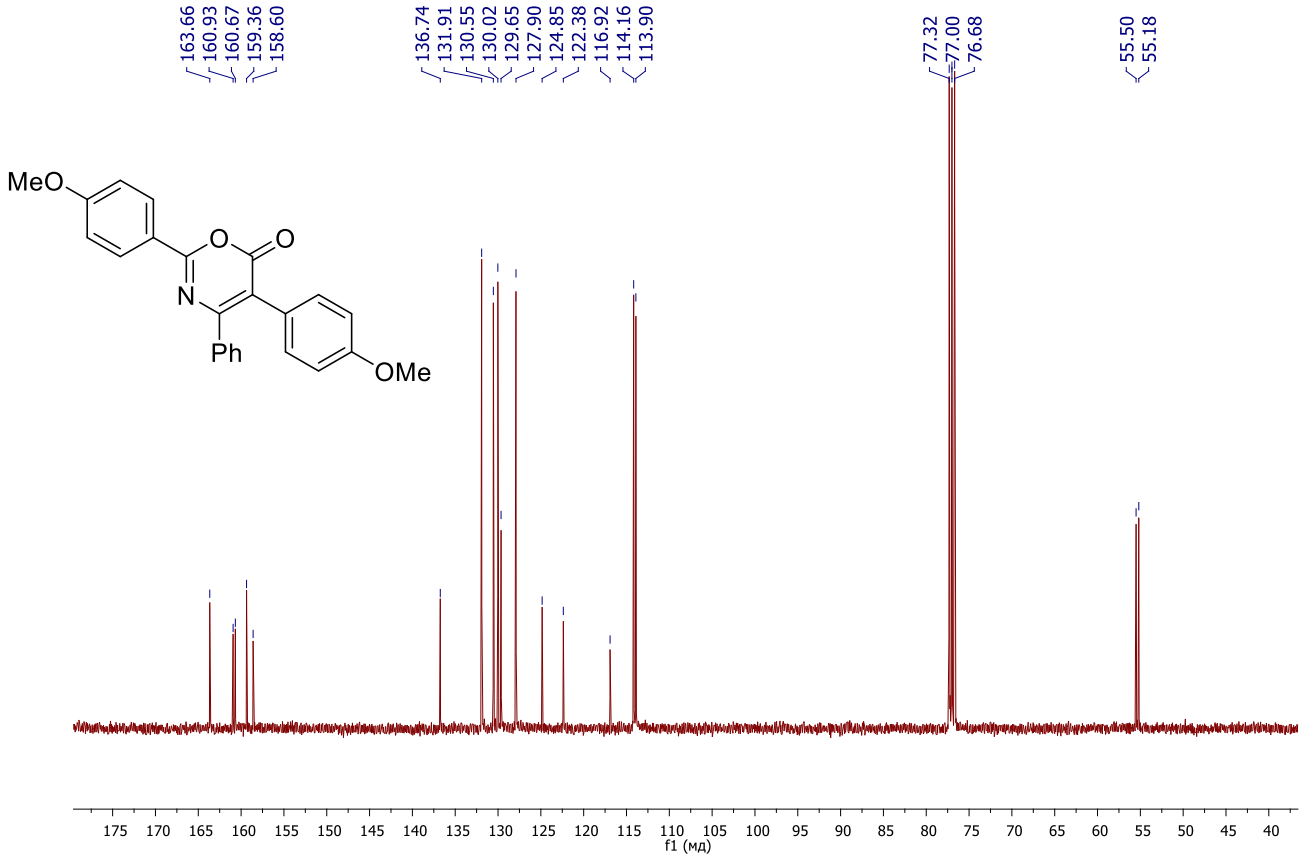
^{13}C NMR (100 MHz, $CDCl_3$) spectrum of **16**



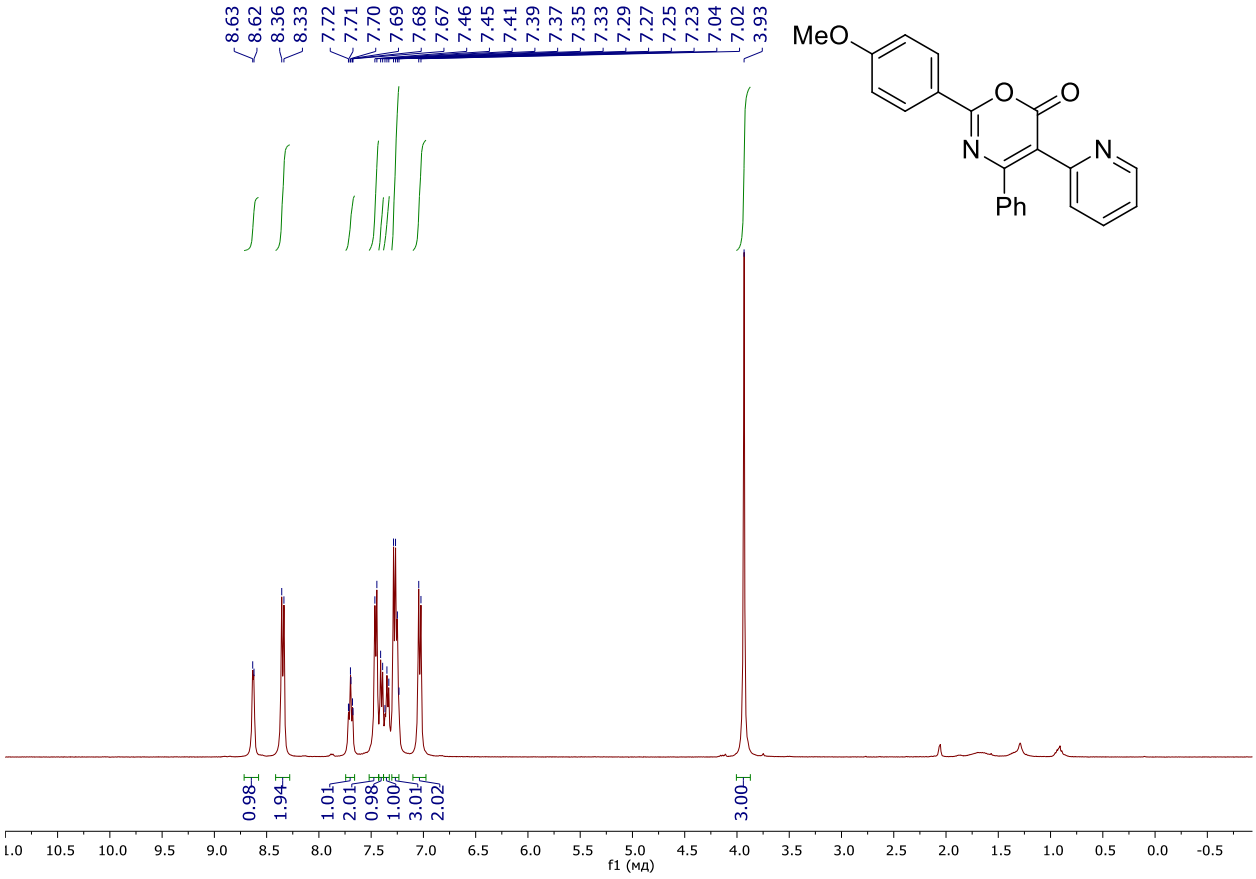
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of **17**



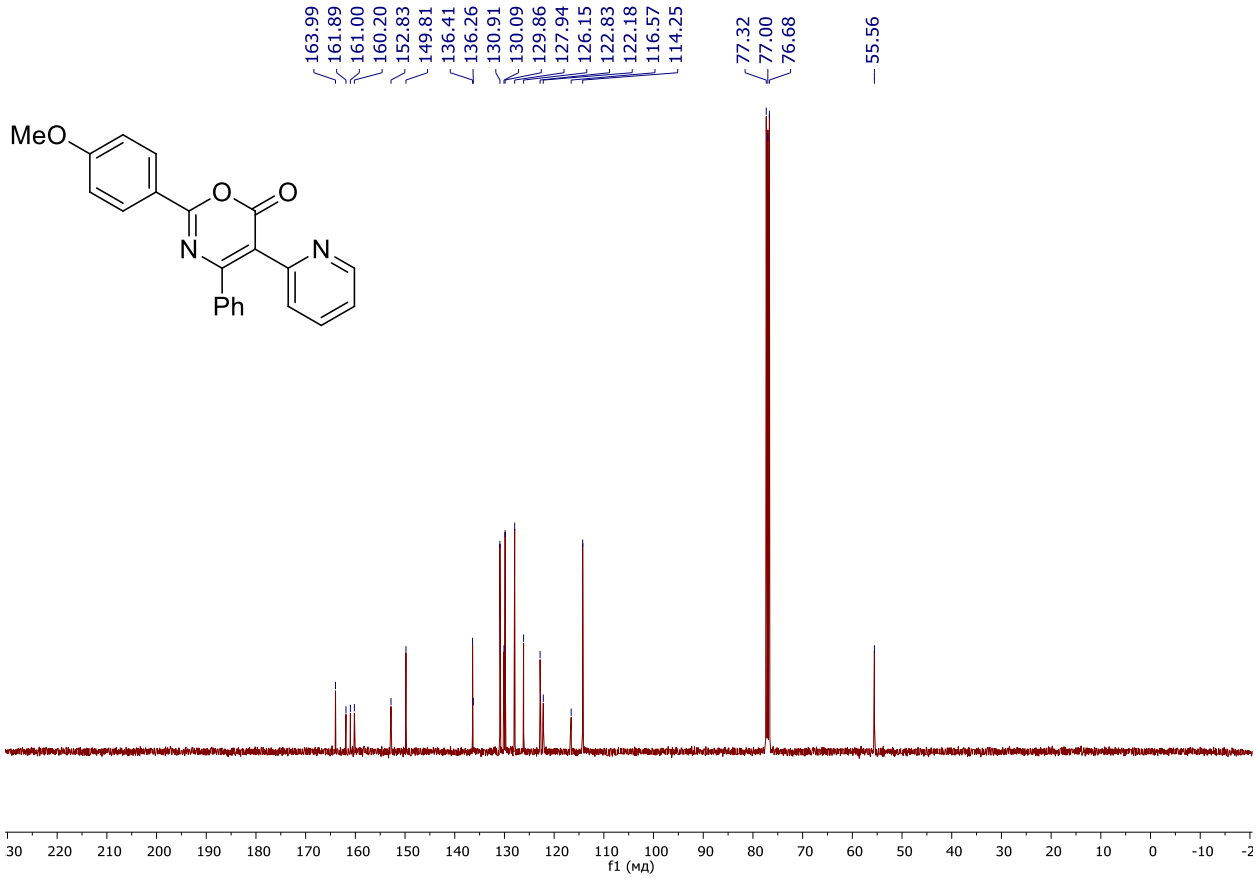
^{13}C NMR (100 MHz, $CDCl_3$) spectrum of **17**



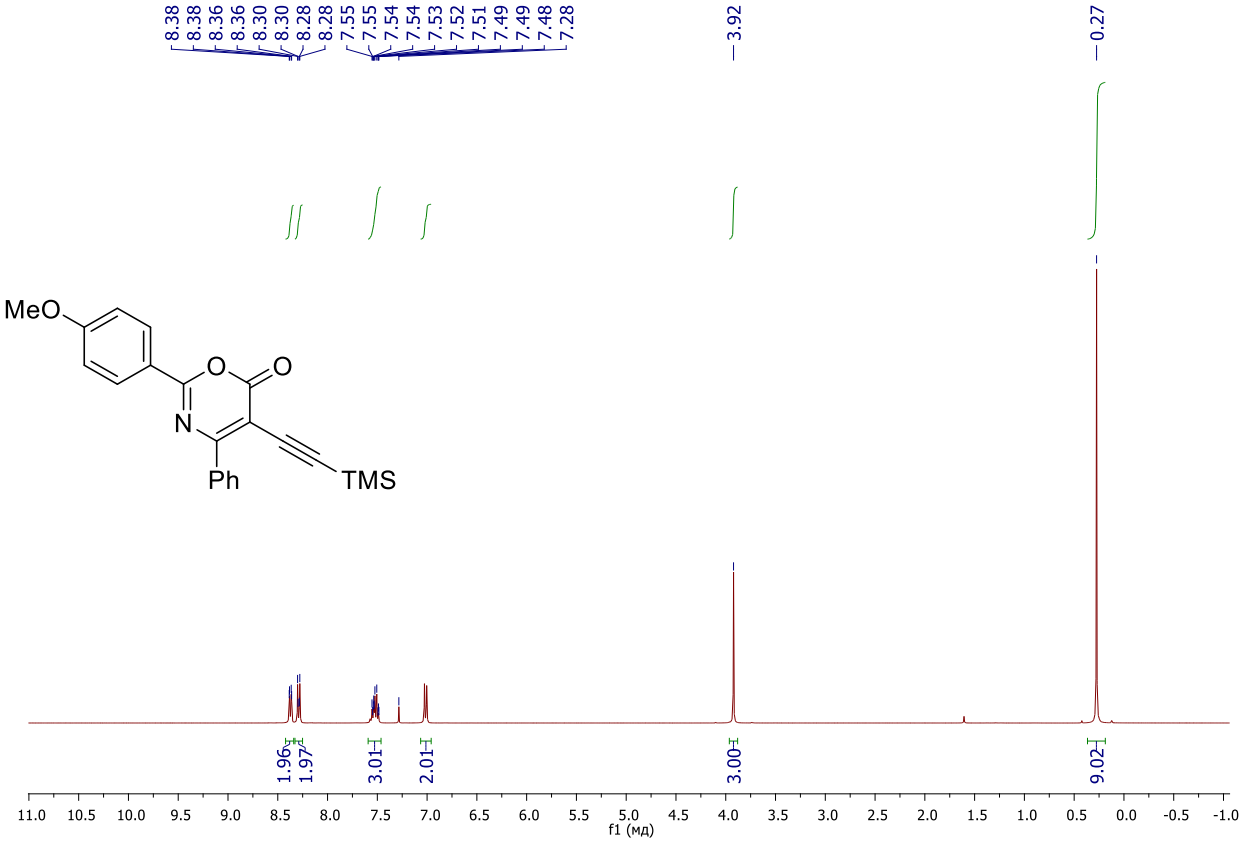
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of **18**



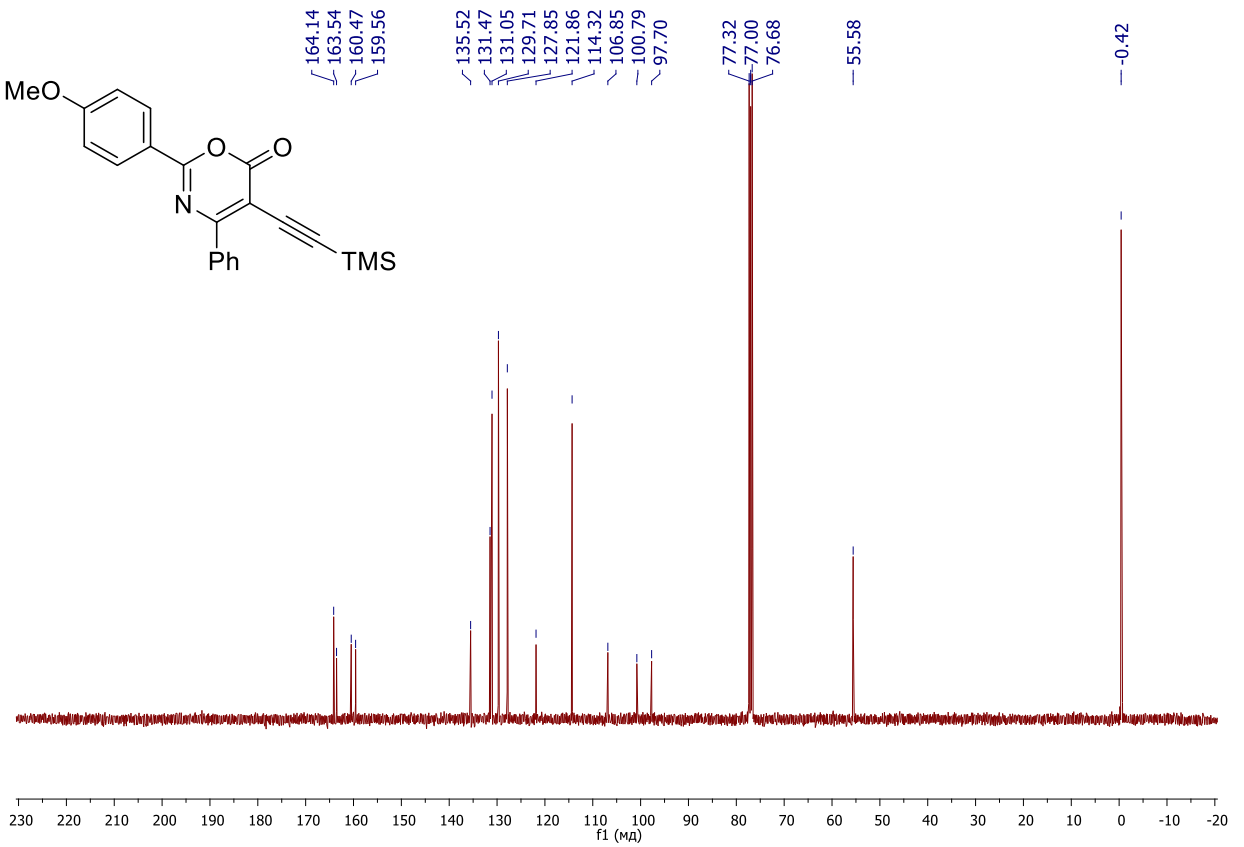
^{13}C NMR (100 MHz, $CDCl_3$) spectrum of **18**



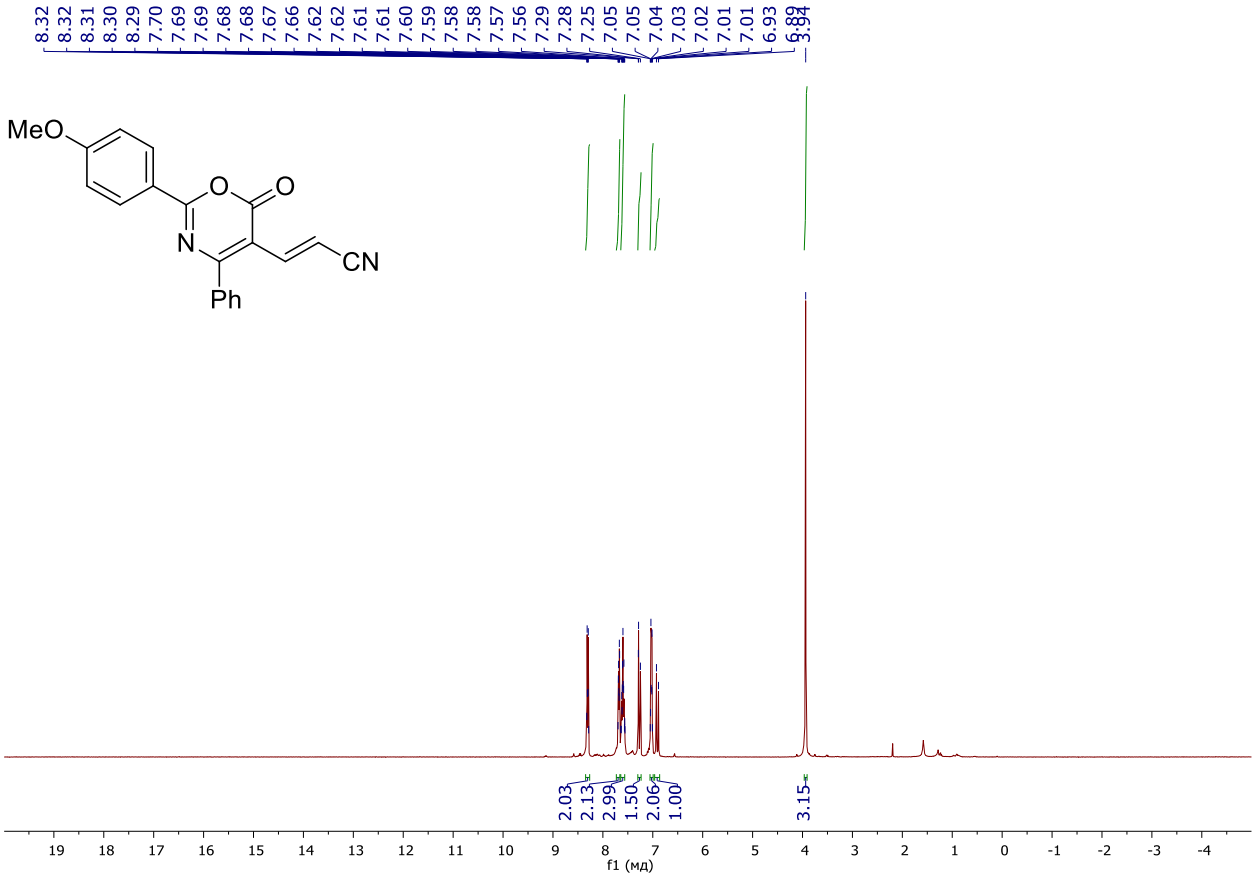
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of **19**



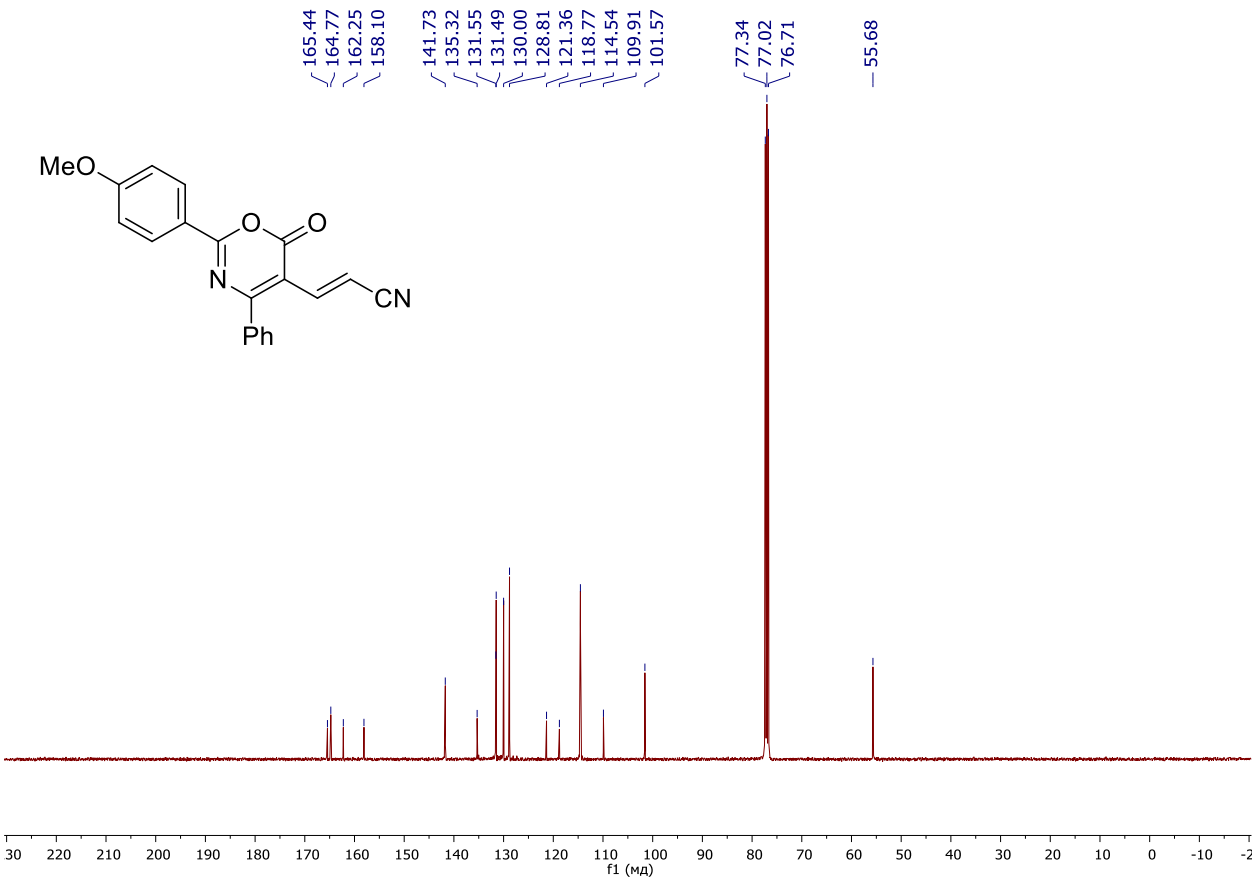
^{13}C NMR (100 MHz, $CDCl_3$) spectrum of **19**



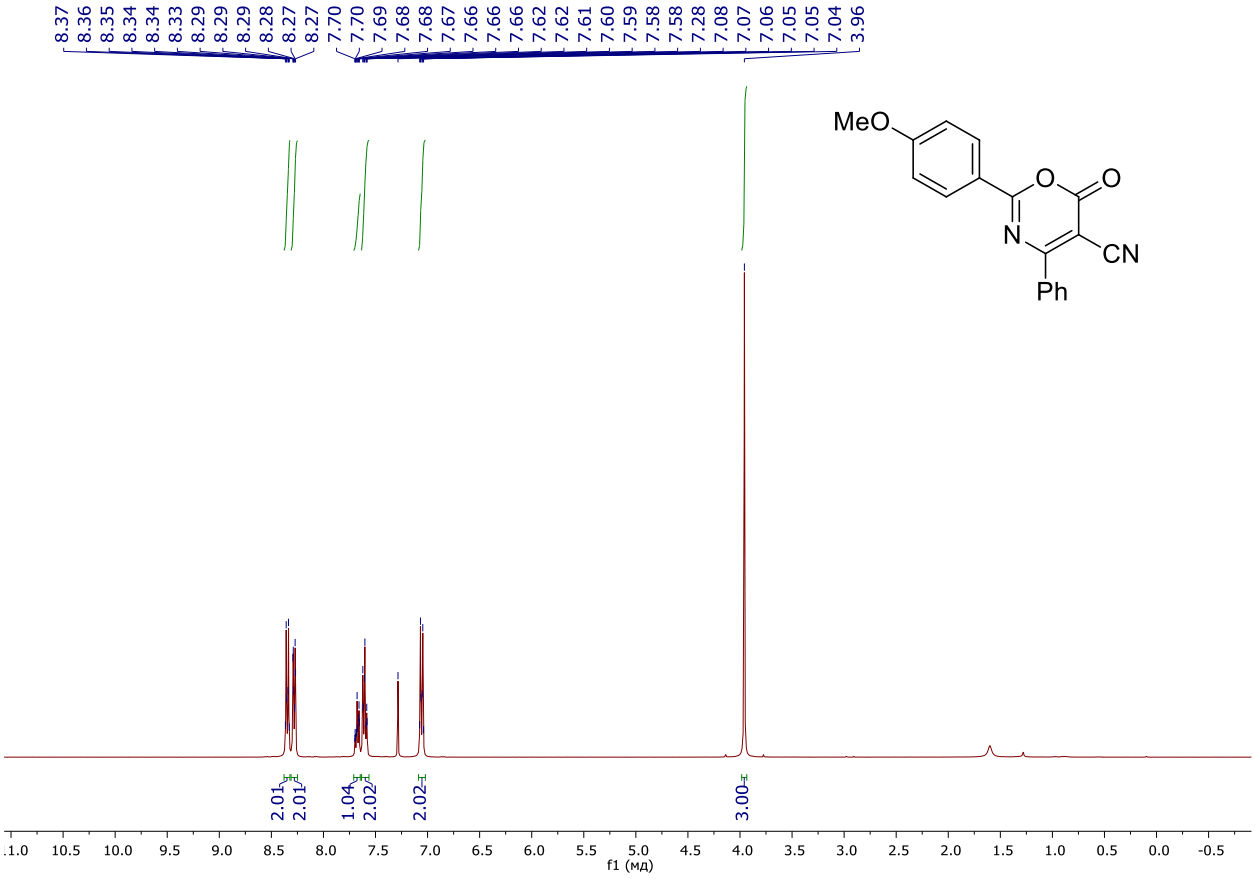
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of **20**



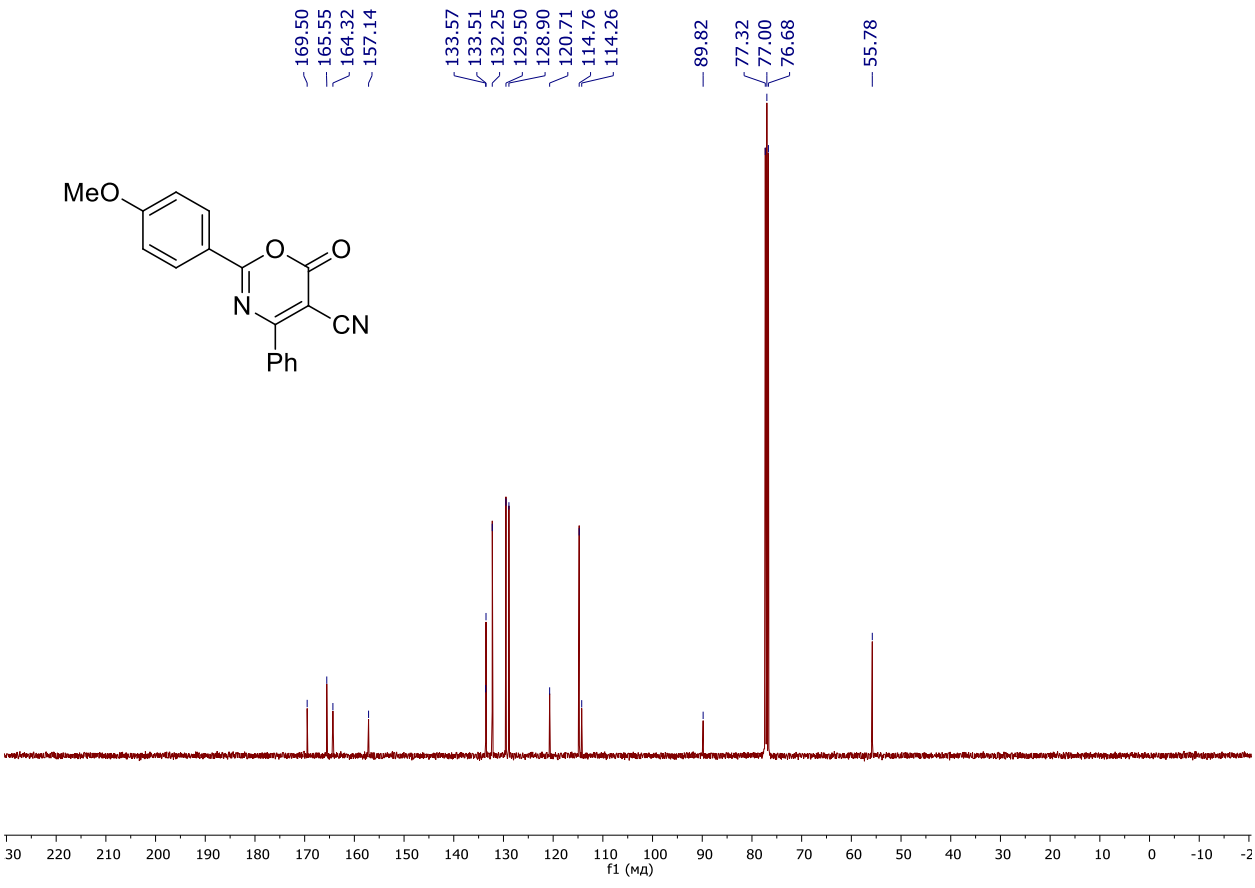
^{13}C NMR (100 MHz, $CDCl_3$) spectrum of **20**



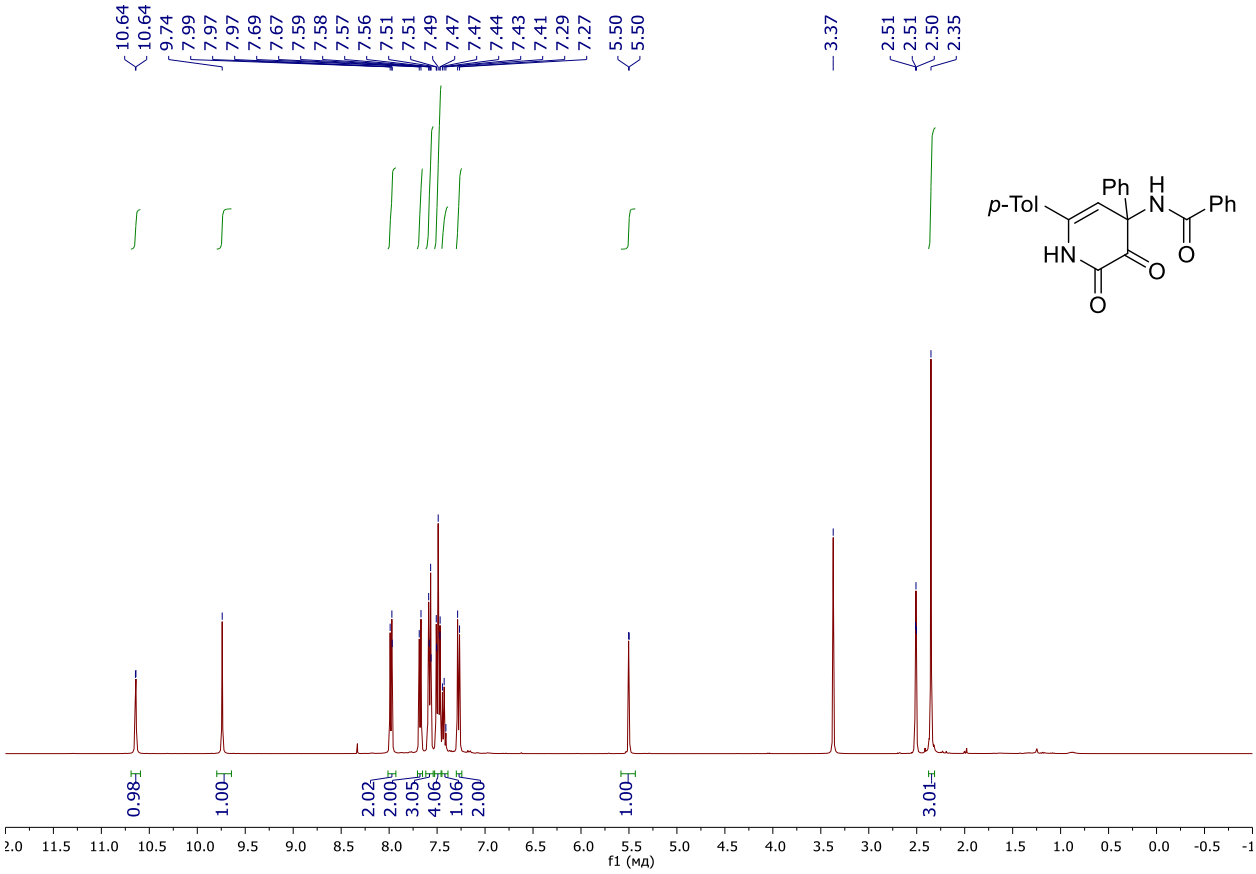
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of **21**



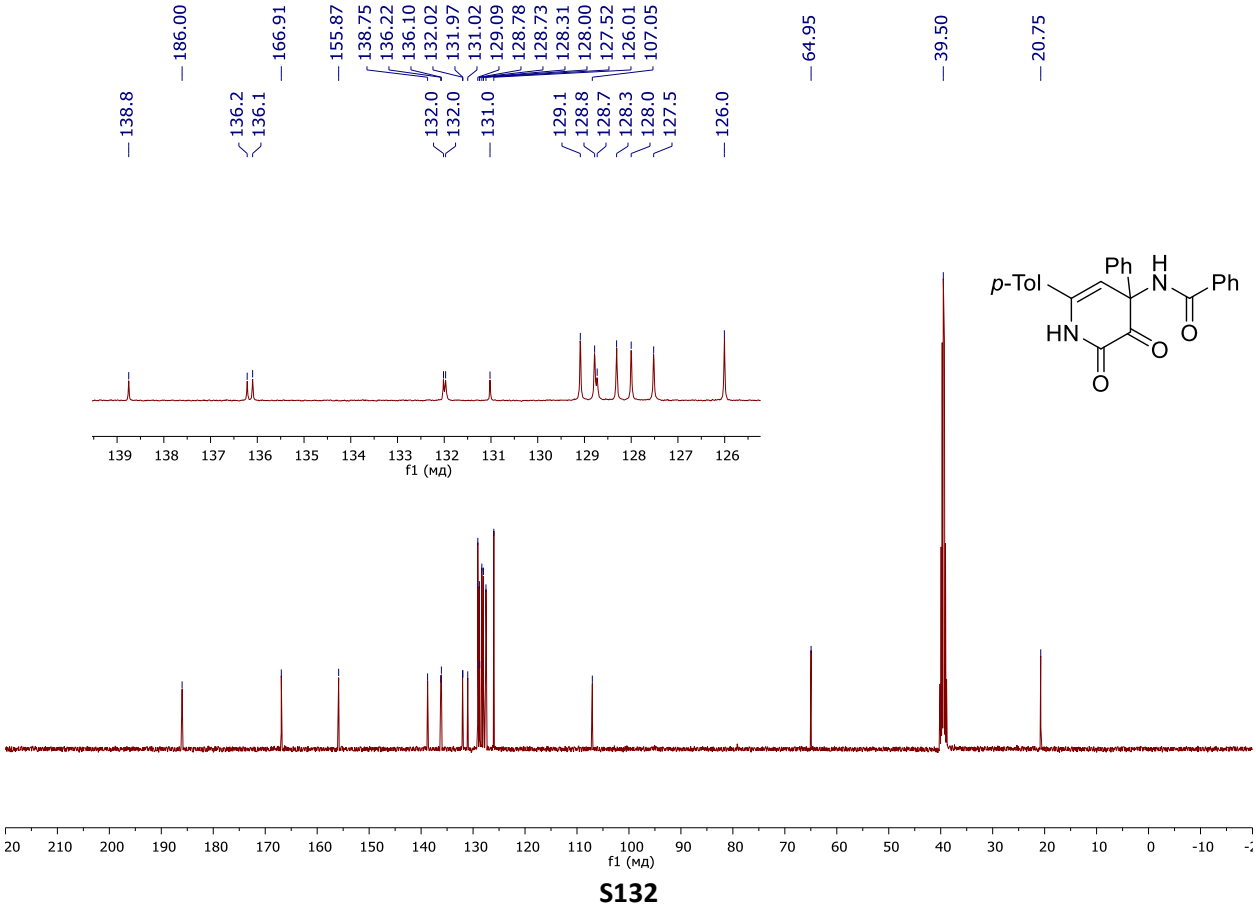
^{13}C NMR (100 MHz, $CDCl_3$) spectrum of **21**



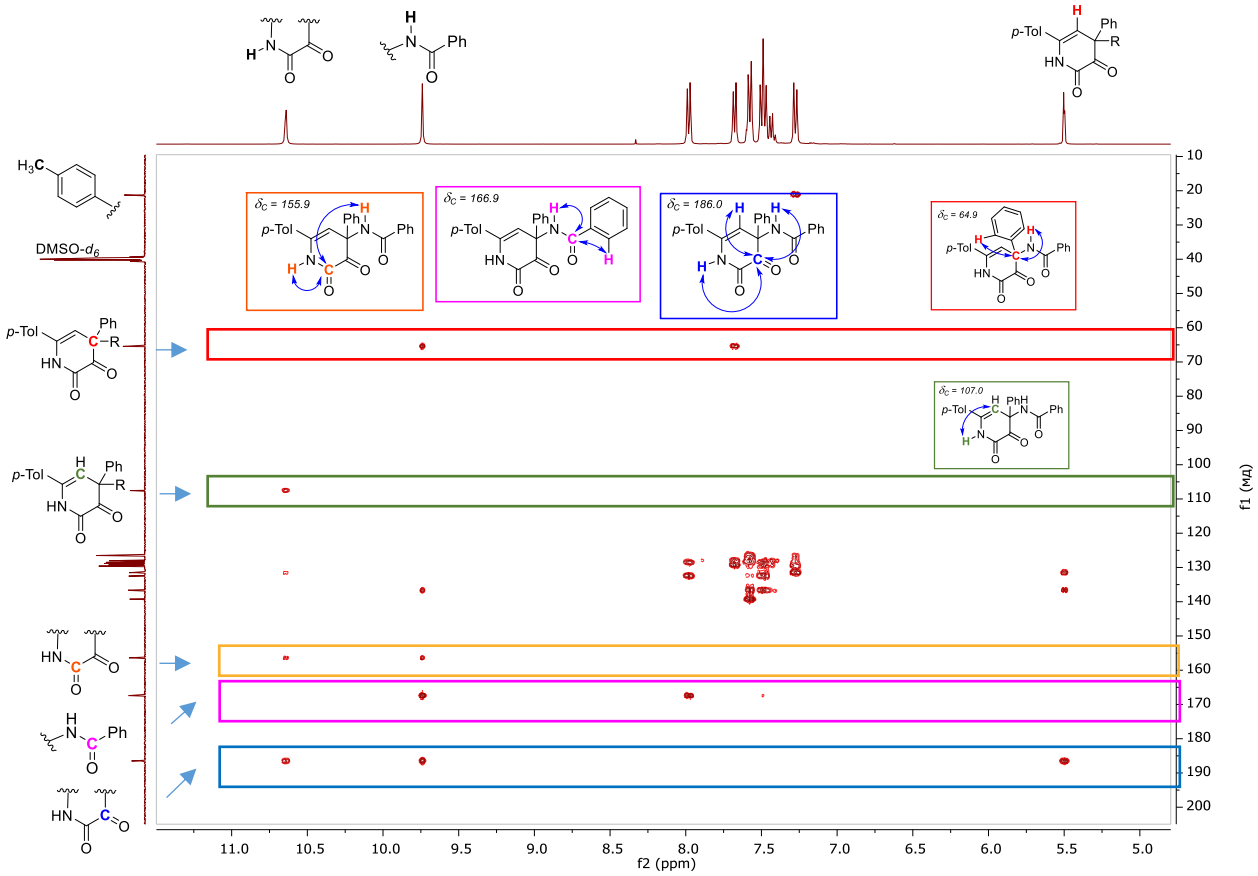
^{1}H NMR (400 MHz, DMSO-d_6) spectrum of **27a**



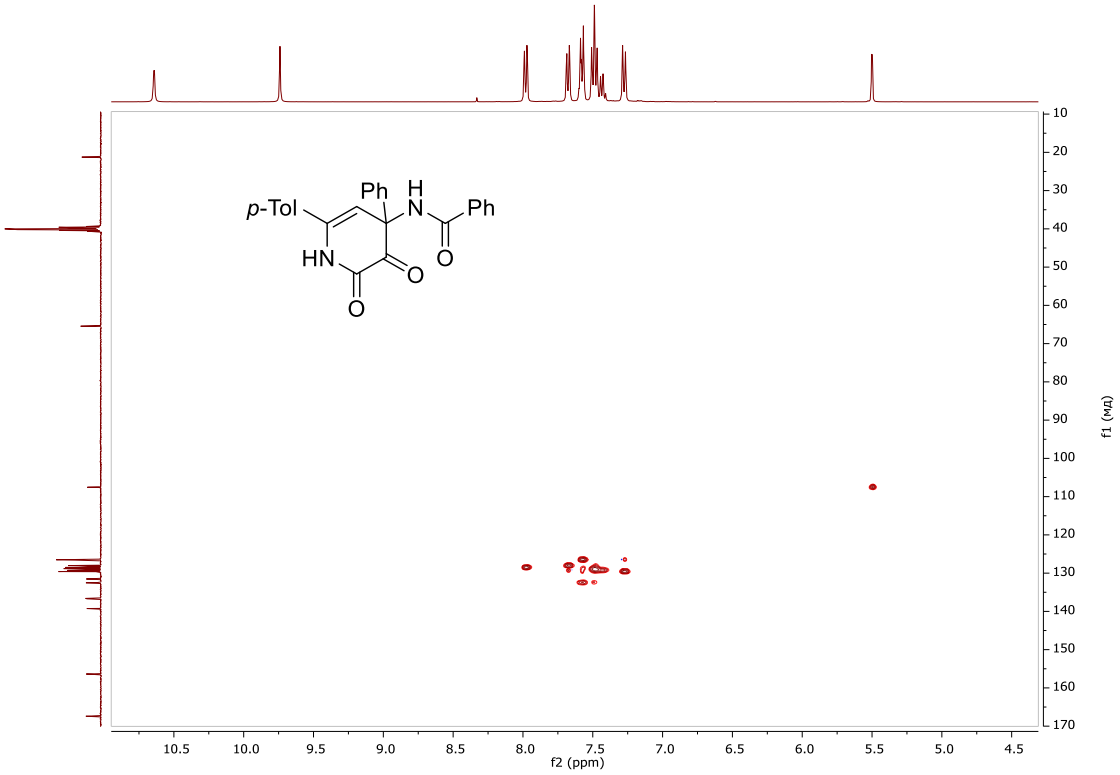
^{13}C NMR (100 MHz, DMSO-d_6) spectrum of **27a**



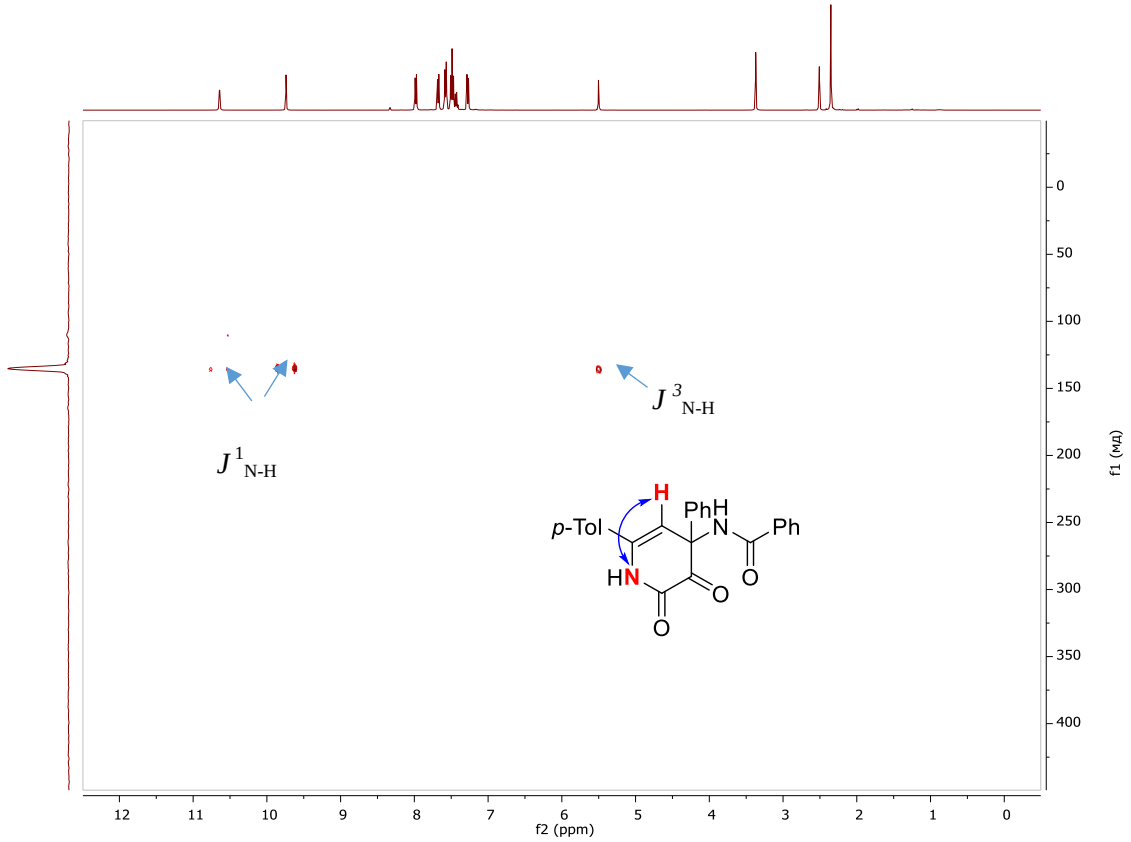
HMBC ^{1}H-^{13}C (400 MHz, DMSO-d_6) spectrum of **27a**



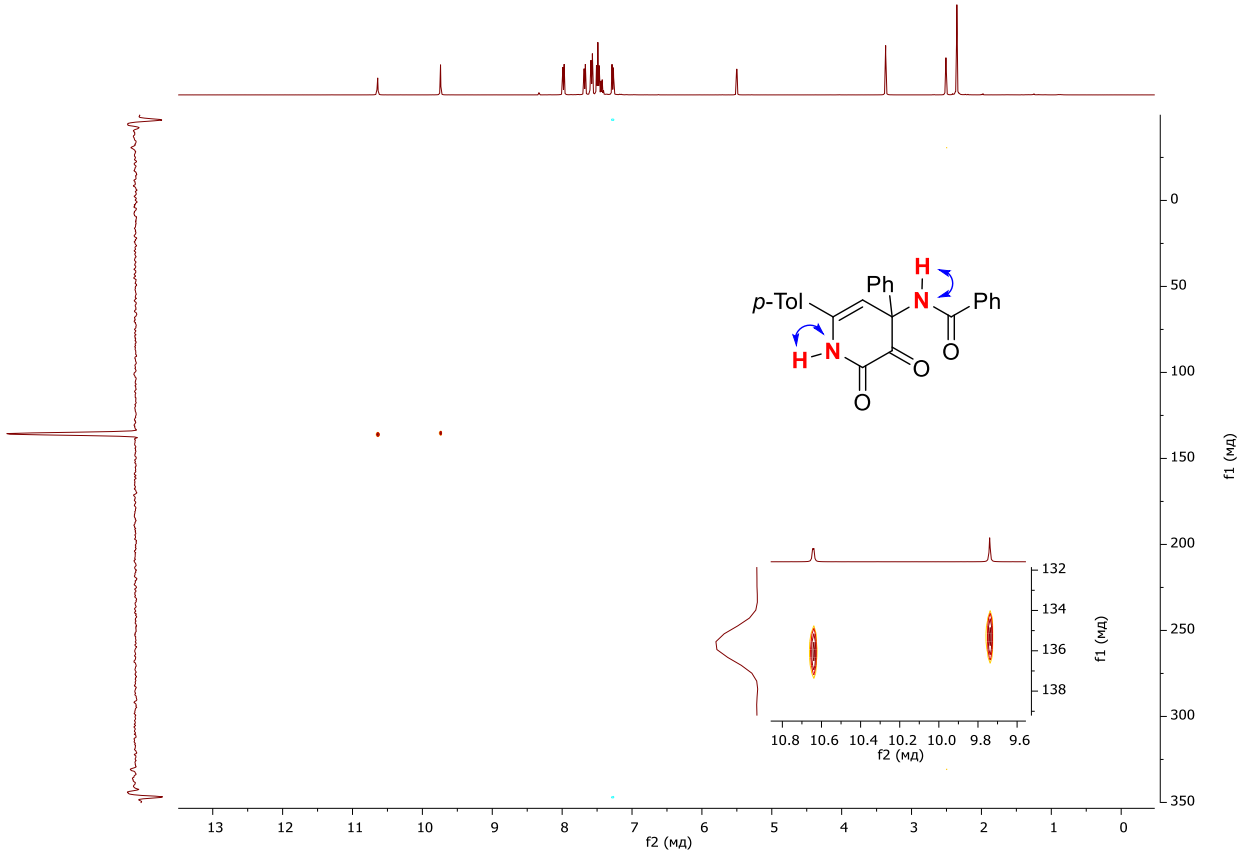
HSQC ^{1}H-^{13}C (400 MHz, DMSO-d_6) spectrum of **27a**



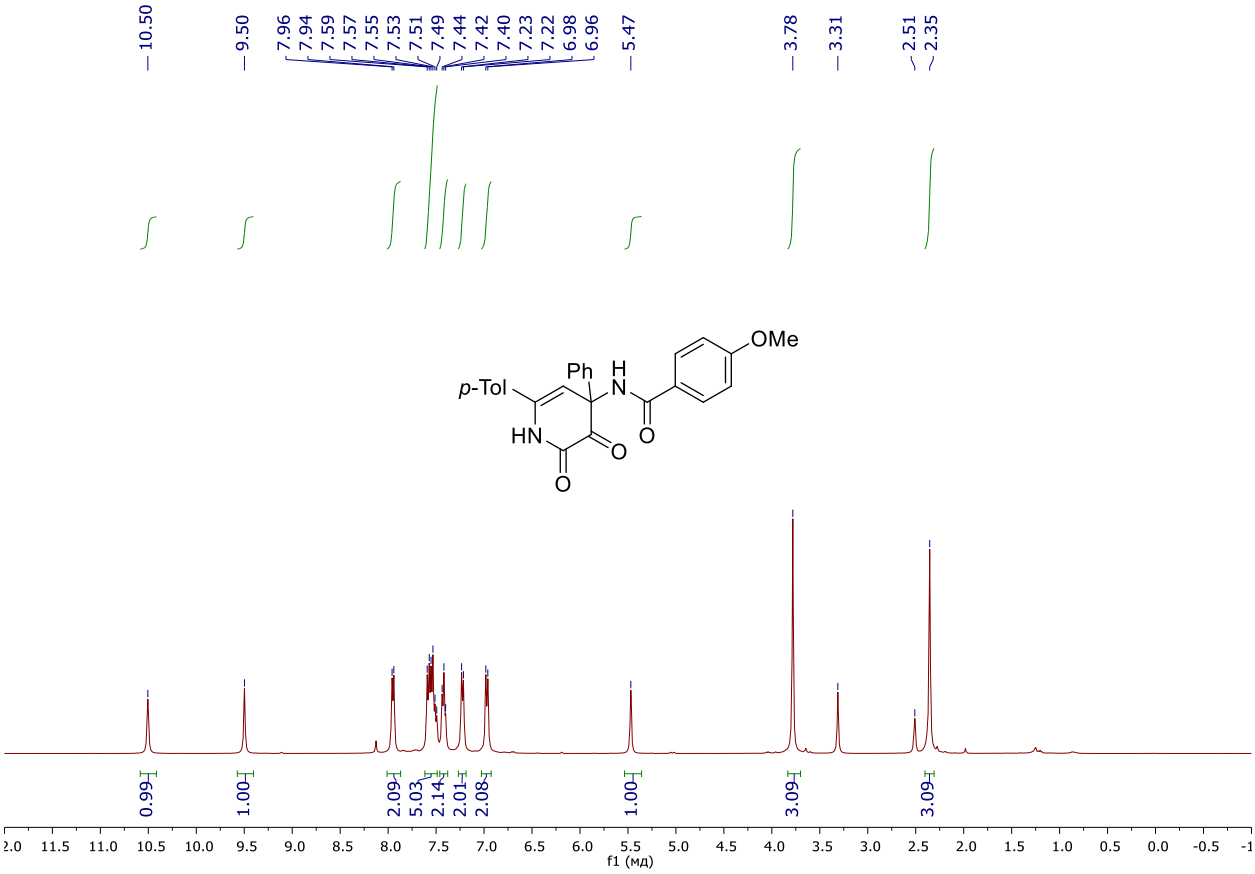
HMBC ^{1}H-^{15}N (400 MHz, DMSO-d_6) spectrum of **27a**



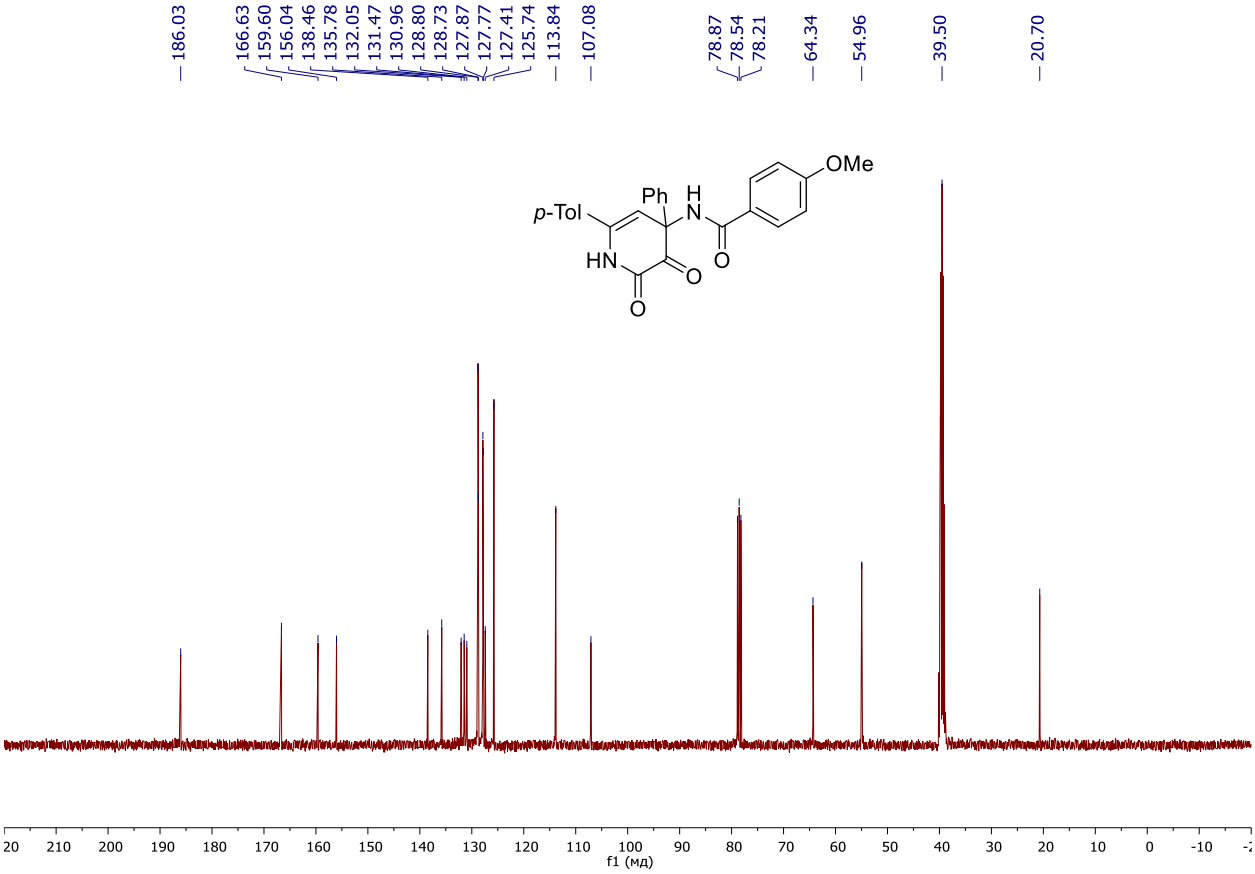
HSQC ^{1}H-^{15}N (400 MHz, DMSO-d_6) spectrum of **27a**



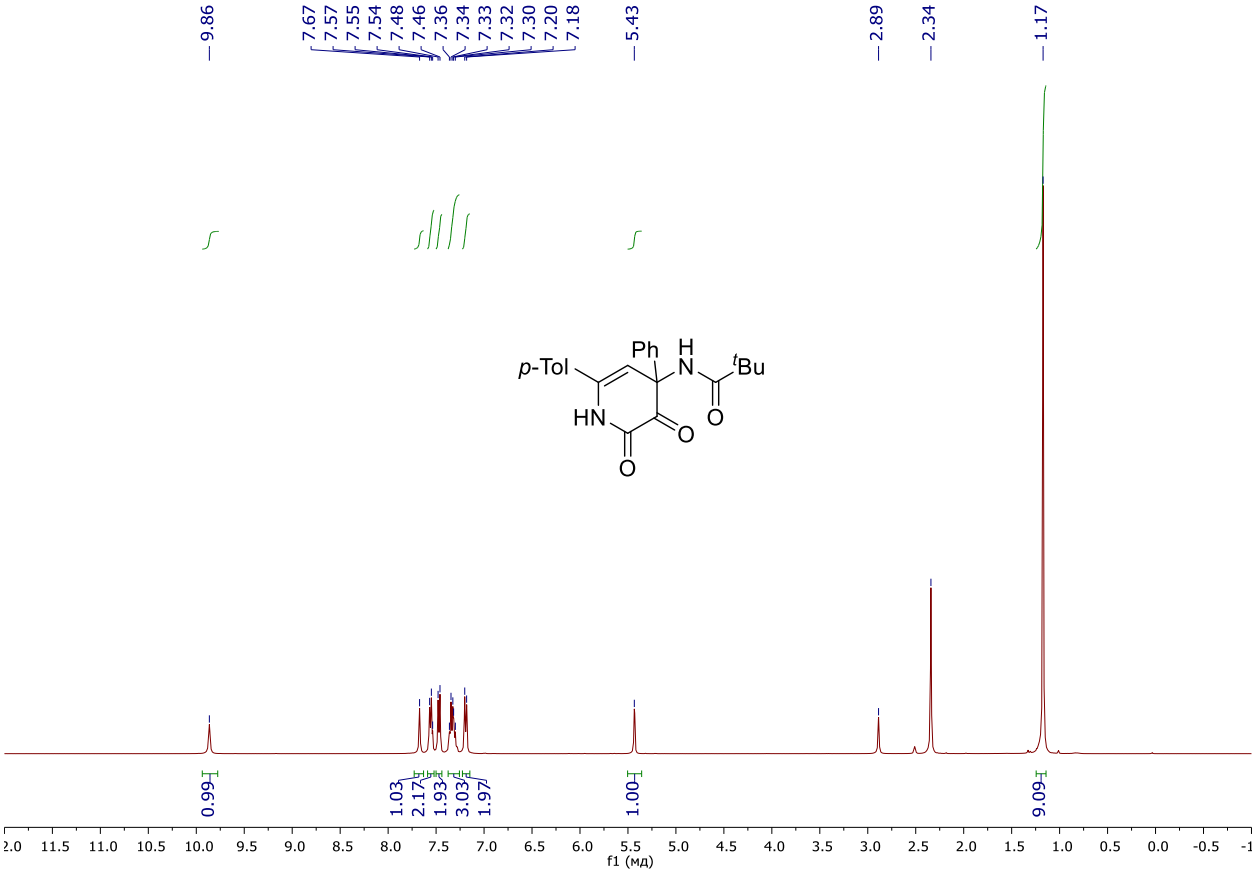
^{1}H NMR (400 MHz, $CDCl_3$–DMSO-d_6 mixture) spectrum of **27b**



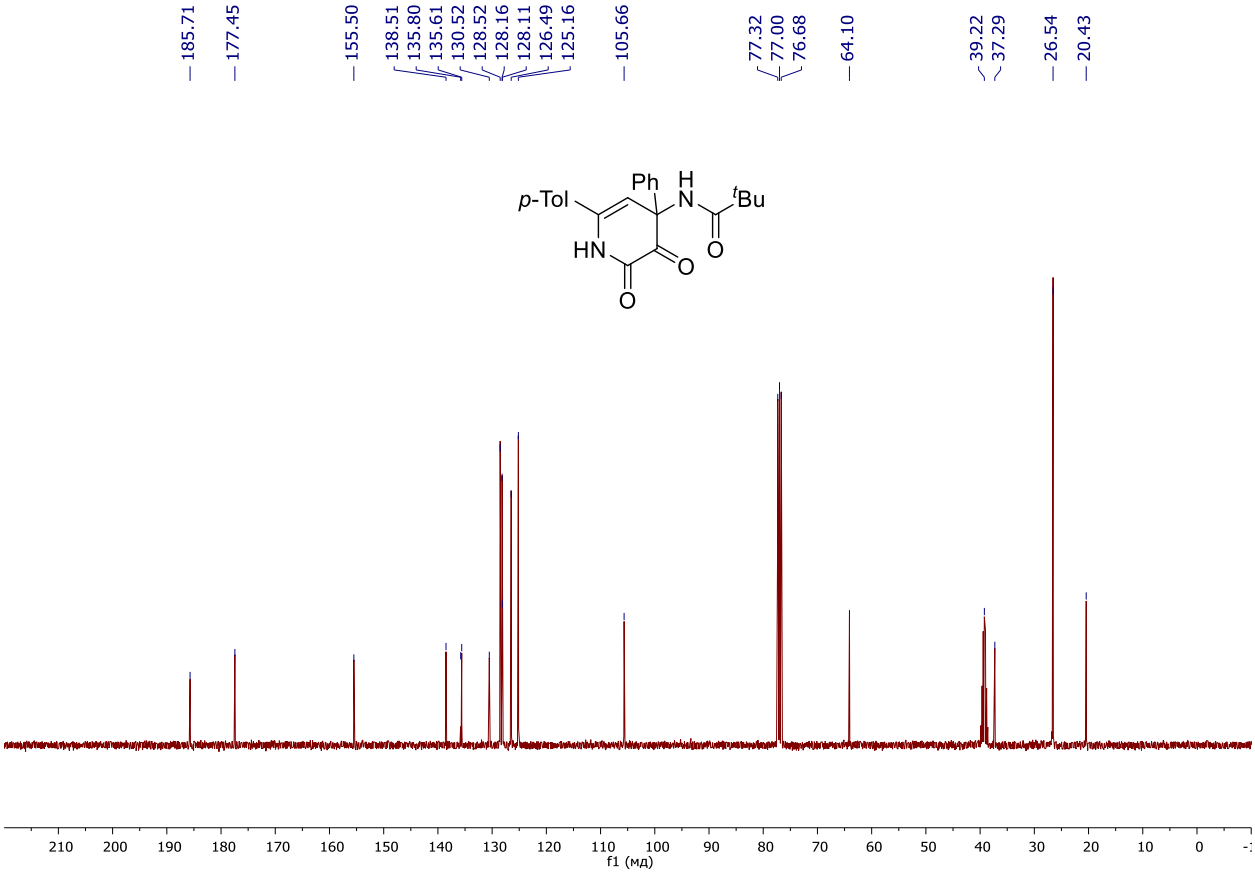
^{13}C NMR (100 MHz, $CDCl_3$–DMSO-d_6 mixture) spectrum of **27b**



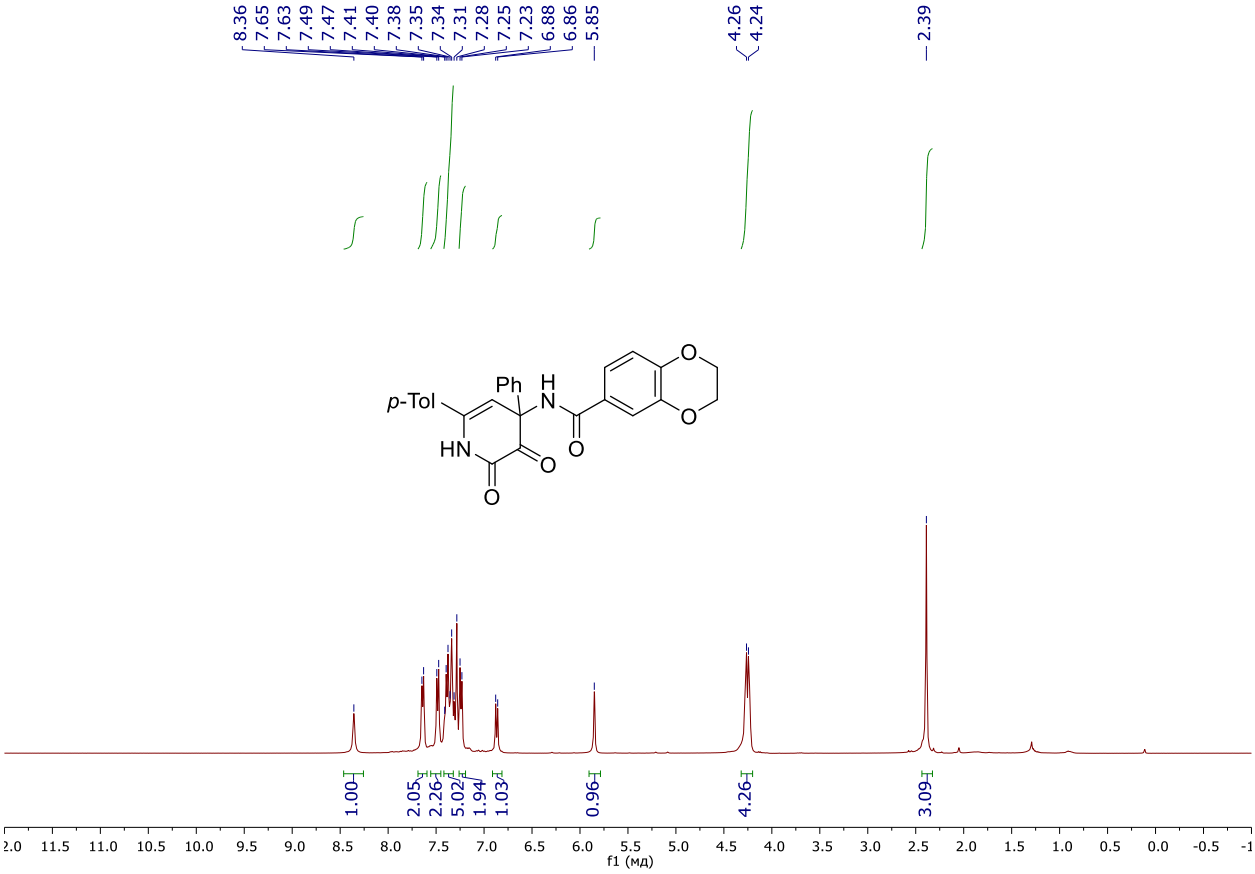
^{1}H NMR (400 MHz, $CDCl_3$–DMSO-d_6 mixture) spectrum of **27c**



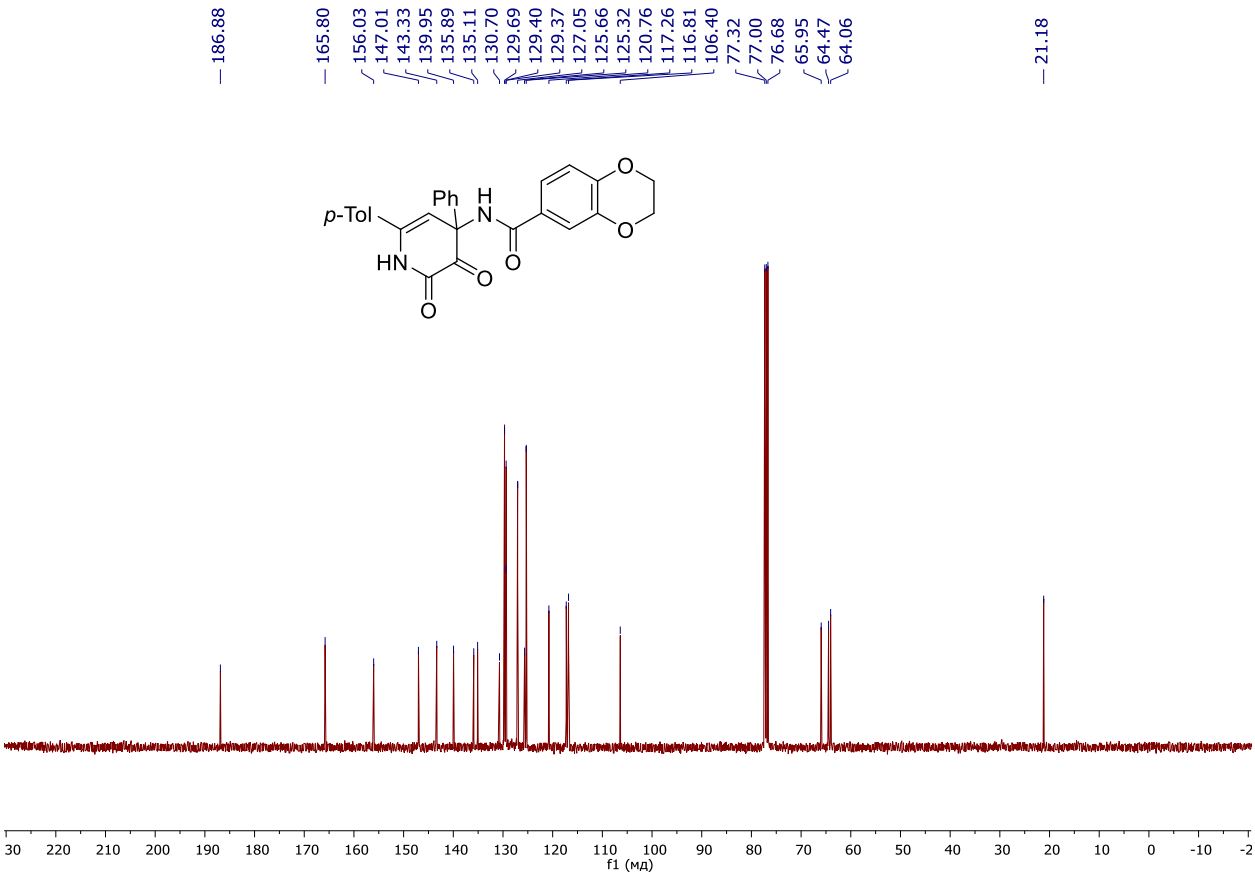
^{13}C NMR (100 MHz, $CDCl_3$–DMSO-d_6 mixture) spectrum of **27c**



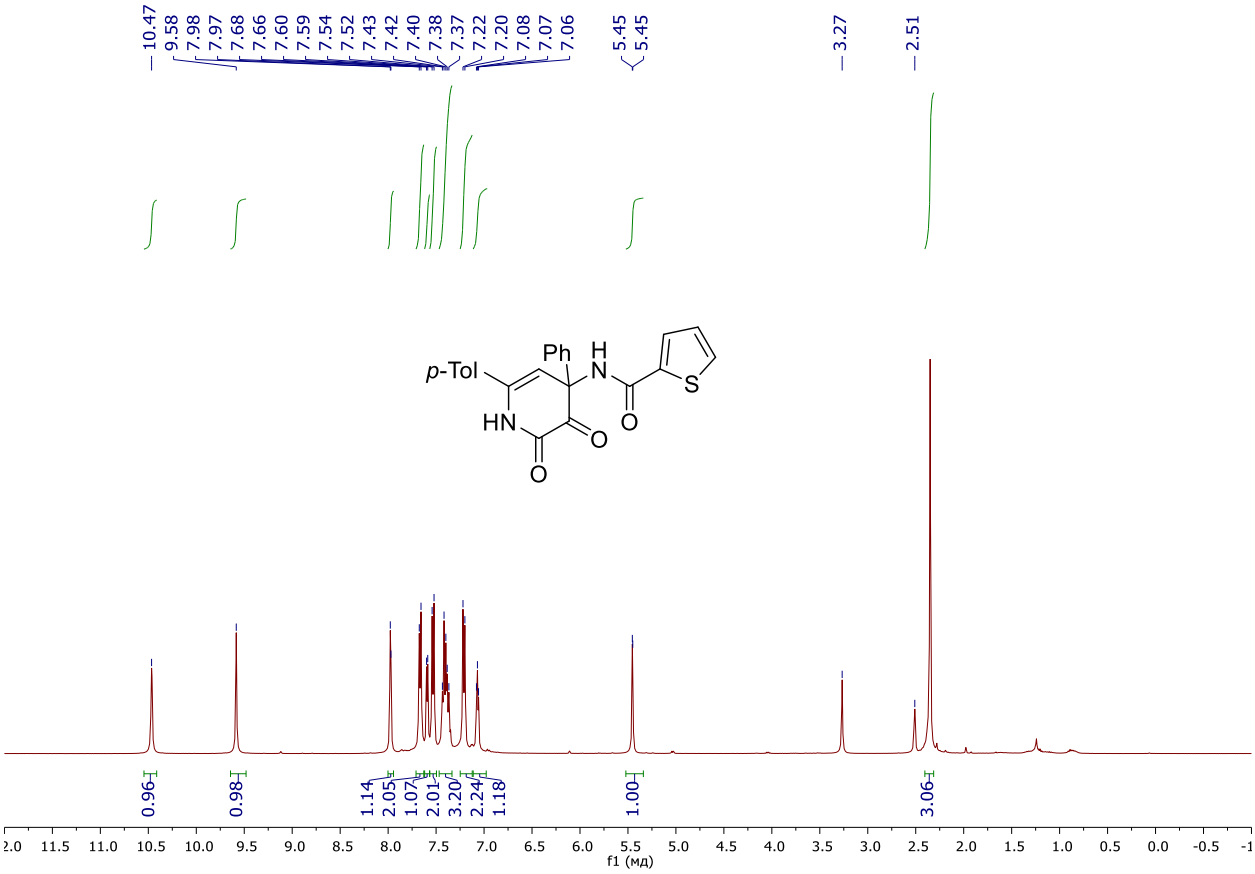
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of **27d**



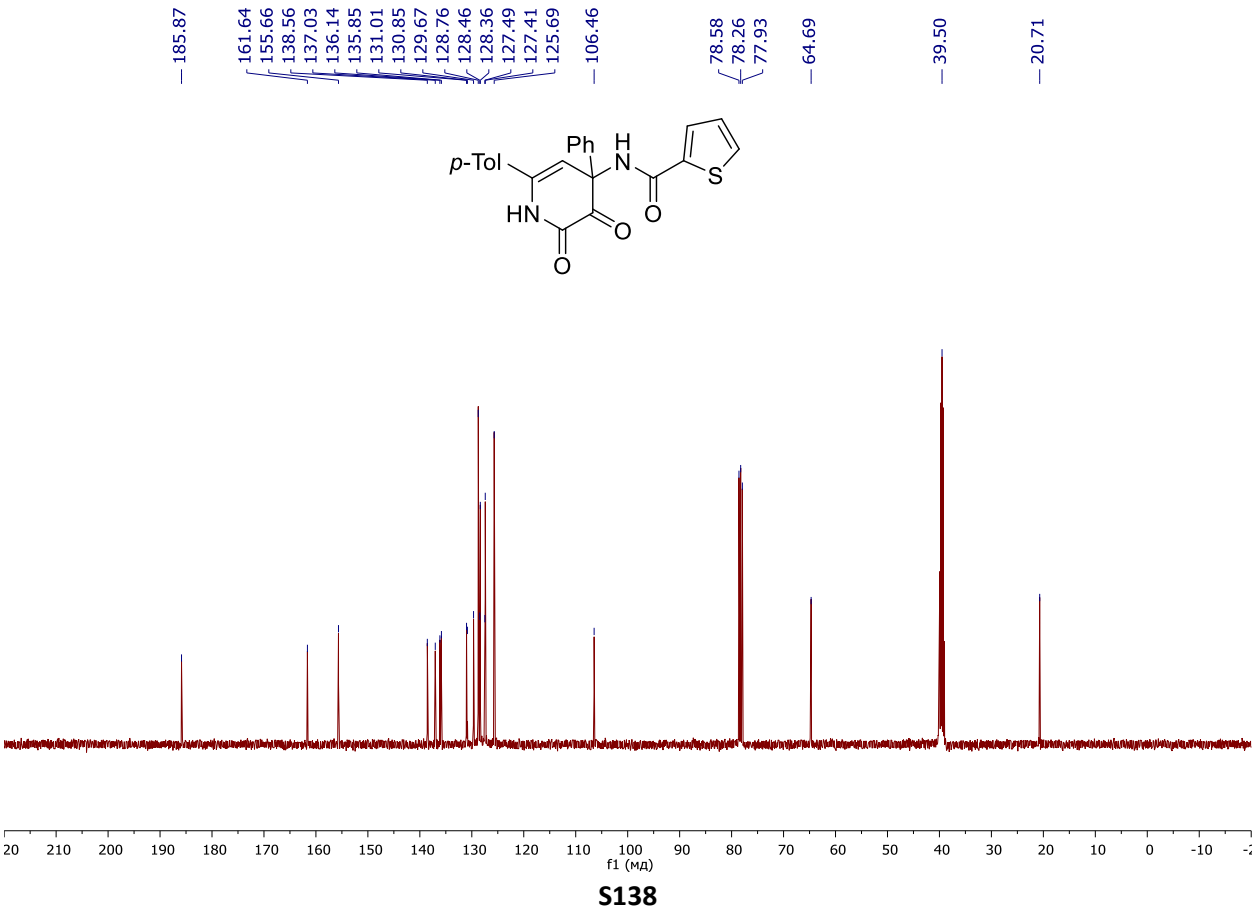
^{13}C NMR (100 MHz, $CDCl_3$) spectrum of **27d**



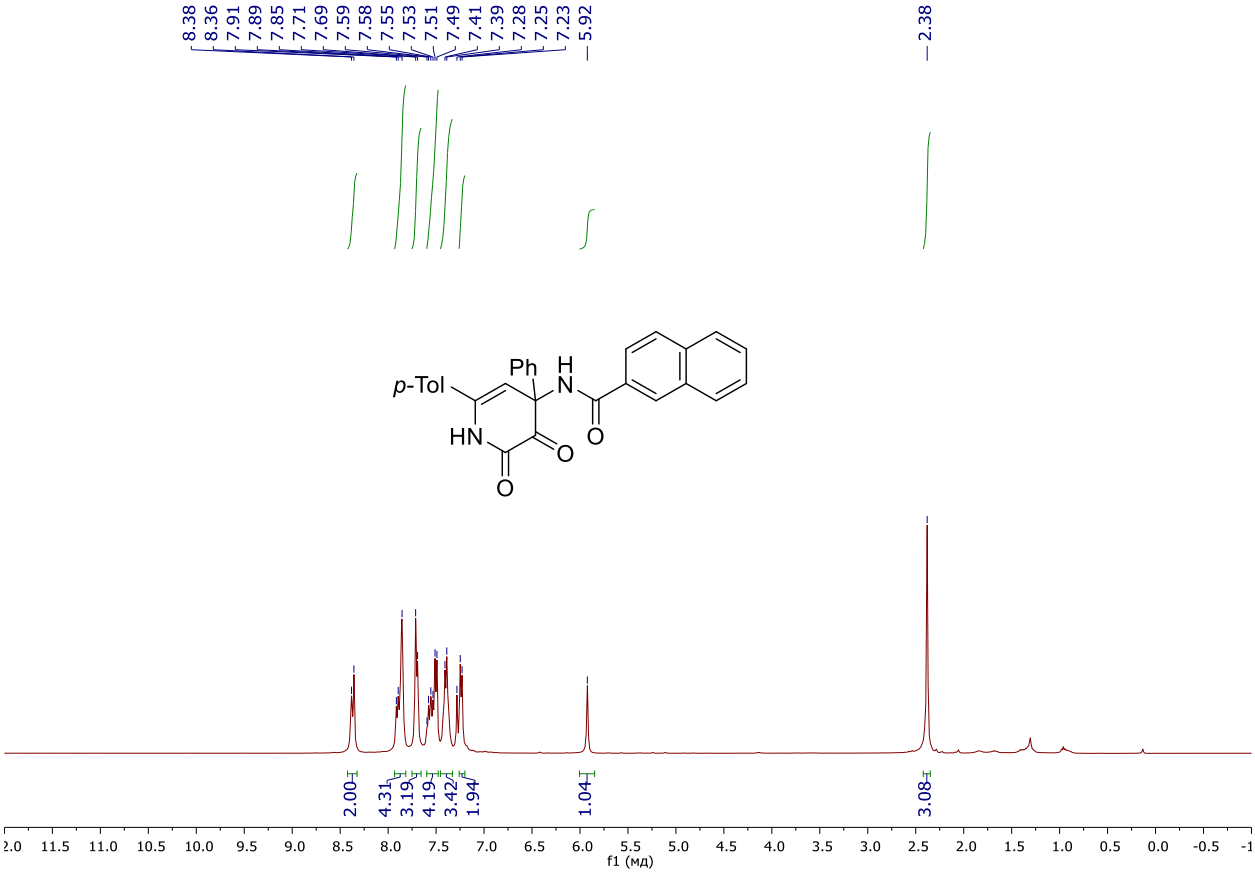
^{1}H NMR (400 MHz, $CDCl_3$–DMSO-d_6 mixture) spectrum of **27e**



^{13}C NMR (100 MHz, $CDCl_3$–DMSO-d_6 mixture) spectrum of **27e**



^{1}H NMR (400 MHz, $CDCl_3$) spectrum of **27f**



^{13}C NMR (100 MHz, $CDCl_3$) spectrum of **27f**