Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.

Electronic supplementary information

Rhodium-catalyzed migrative annulation and olefination of 2-aroylpyrroles with diazoesters

Daniil M. Strashkov, Kirill V. Zavyalov, Pavel A. Sakharov, Anastasiya V. Agafonova, Nikolai V. Rostovskii, Alexander F. Khlebnikov, and Mikhail S. Novikov*

St. Petersburg State University, Institute of Chemistry, 7/9 Universitetskaya nab., St. Petersburg, 199034, Russia

*E-mail: m.novikov@spbu.ru

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1. General information

Melting points were determined on a melting point apparatus Stuart® SMP30 and are uncorrected. ^{1}H, ^{13}C NMR, and ^{19}F spectra were recorded with a Bruker AVANCE 400 (400 MHz for ^{1}H, 100 MHz for ^{13}C and 376 MHz for ^{19}F) at 298K. Chemical shifts are reported in parts per million (δ, ppm) and are referenced to 7.26 ($CDCl_3$) or 2.50 (DMSO-d_6) for ^{1}H NMR and 77.0 ($CDCl_3$) or 39.52 (DMSO-d_6) for ^{13}C NMR. The following abbreviations were used: s – singlet, d – doublet, t – triplet, q – quartet, b.s – broad singlet, m – multiplet. Single crystal X-ray data were collected by means of Agilent Technologies "Xcalibur" diffractometer. High-resolution mass-spectra with Electrospray ionization (ESI), were measured on a Bruker MaXis HRMS-ESI-QTOF mass spectrometer. Thin-layer chromatography (TLC) was conducted on aluminum sheets precoated with SiO_2 ALUGRAM SIL G/UV254. Column chromatography was performed on a silica gel Kieselgel 60 (0.04−0.063 mm). All solvents were distilled and dried prior to use. 1,2-Dichloroethane was washed thrice with concentrated H_2SO_4, then water, followed by distillation over P_2O_5 and subsequent distillation over anhydrous K_2CO_3. The catalyst $Rh_2(Piv)_4$ was used prepared. Commercial $Rh_2(OAc)_4$, acetophenones were purchased from Sigma-Aldrich, and abcr GmbH, and were used without any purification.

3-Aryl-2*H*-azirine-2-carbaldehydes,[1] except 3-(3-methoxyphenyl)-2*H*-azirine-2-carbaldehyde, phosphorus ylides,[2,3] except 1-(2,5-dimethylphenyl)-2-(triphenyl-λ^5-phosphanylidene)ethan-1-one, (2-benzoylvinyl)-3-phenyl-2*H*-azirine,[4] diazoesters (dimethyl diazomalonate (**3a**),[5] methyl 2-diazo-2-(4-nitrophenyl)acetate (**3b**),[6] methyl 2-diazo-3-oxobutanoate (**3c**),[7] methyl 2-diazo-2-(dimethoxyphosphoryl)acetate (**3d**),[8] methyl 2-diazo-2-tosylacetate (**3e**)[9], and indoles ((1*H*-indol-2-yl)(phenyl)methanone (**2s**), (1*H*-indol-2-yl)(4-bromophenyl)methanone (**2t**),[10] (1*H*-indol-2-yl)(3-nitrophenyl)methanone (**2u**),[11] are known compounds which were prepared according to the literature procedures.

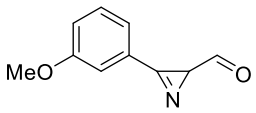
2. ^{1}H NMR analysis of reaction mixtures

Table S-1. Ratio **2a**:**5a**:**6a**:**7a** depending on the amount of reacted diazoester **3a**

Entry	Amount of **3a** (equiv)	**2a** : **5a** : **6a** : **7a** ratio
1	0.5	93:4:3:0
2	1	37:45:6:12
3	1.5	8:73:9:10
4	2.0	0:82:8:10

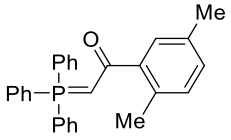
3. Synthesis of starting materials

Synthesis of 3-(3-methoxyphenyl)-2*H*-azirine-2-carbaldehyde



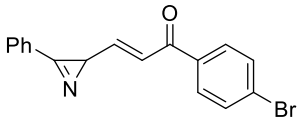
This compound (772 mg, 63%) was prepared according to the literature procedure[1] from 3-chloro-3-(3-methoxyphenyl)acrylaldehyde. Yellow oil. ^{1}H NMR ($CDCl_3$, 400 MHz) δ 8.94 (d, 1H, *J* = 6.6 Hz), 7.53–7.44 (m, 2H), 7.41–7.38 (m, 1H), 7.23–7.18 (m, 1H), 3.88 (s, 3H), 2.87 (d, 1H, *J* = 6.6 Hz). ^{13}C{^{1}H} NMR ($CDCl_3$, 100 MHz) δ 199.9, 160.2, 159.5, 130.6, 123.7, 123.2, 121.1, 114.3, 55.6, 39.2. HRMS (ESI–TOF) calcd for $C_{10}H_9NNaO_2$ $[M+Na]^+$ 198.0525; found 198.0530.

Synthesis of 1-(2,5-dimethylphenyl)-2-(triphenyl-λ^5-phosphanylidene)ethan-1-one



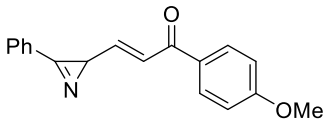
This compound (3.13 g, 51%) was prepared according to the literature procedure.[2] Colorless solid, mp 155–158 °C (from $CDCl_3$). ^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.79–7.71 (6H, m), 7.60–7.53 (3H, m), 7.51–7.44 (6H, m), 7.42 (1H, d, *J* = 1.8 Hz), 7.03 (1H, d, *J* = 7.8 Hz), 6.98 (1H, dd, *J* = 7.8 Hz, *J* = 1.8 Hz), 4.00 (1H, d, *J* = 25.3 Hz), 2.48 (3H, s), 2.30 (3H, s). ^{13}C{^{1}H} NMR ($CDCl_3$, 100 MHz) δ 190.0 (d, *J* = 3.1 Hz), 143.7 (d, *J* = 15.4 Hz), 134.3, 133.1 (d, *J* = 10 Hz), 132.1, 132.0 (d, *J* = 2.3 Hz), 130.3, 128.8 (d, *J* = 12.3 Hz), 128.3 (d, *J* = 11.6 Hz), 127.7, 126.8, 54.2 (d, *J* = 106.3 Hz), 20.9, 19.9. HRMS (ESI–TOF): *m/z* calcd for $C_{28}H_{26}OP$ $[M+H]^+$ 409.1716; found 409.1717.

Synthesis of (*E*)-1-(4-bromophenyl)-3-(3-phenyl-2*H*-azirin-2-yl)prop-2-en-1-one



This compound (1.90 g, 67%) was prepared according to the literature procedure[4] from 2-formyl-3-phenyl-2*H*-azirine (1.27 g, 8.8 mmol) and 1-(4-bromophenyl)-2-(triphenyl-λ^5-phosphanylidene)ethan-1-one (4.01 g, 8.8 mmol). Colorless solid, mp 50–51 °C (from Et_2O). ^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.89–7.85 (2H, m), 7.81–7.77 (2H, m), 7.66–7.54 (5H, m), 7.08 (1H, d, *J* = 16 Hz), 6.90 (1H, dd, *J* = 15.8 Hz, *J* = 7.6 Hz), 3.03 (1H, d, *J* = 7.6 Hz). ^{13}C{^{1}H} NMR ($CDCl_3$, 100 MHz) δ 188.3, 165.0, 150.6, 136.5, 133.8, 131.9, 130.1, 130.0, 129.4, 127.9, 124.9, 123.5, 33.2. HRMS (ESI–TOF): *m/z* calcd for $C_{17}H_{12}{}^{79}BrNNaO$ $[M+Na]^+$ 347.9994; found 347.9998.

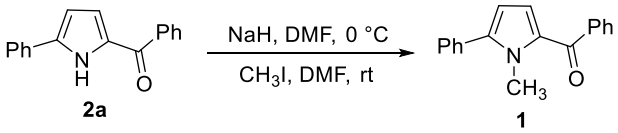
Synthesis of (*E*)-1-(4-methoxyphenyl)-3-(3-phenyl-2*H*-azirin-2-yl)prop-2-en-1-one



This compound (1.43 g, 59%) was prepared according to the literature procedure[4] from 2-formyl-3-phenyl-2*H*-azirine (1.35 g, 9.3 mmol) and 1-(4-methoxyphenyl)-2-(triphenyl-λ^5-phosphanylidene)ethan-1-one (3.30 g, 9.3 mmol). Colorless solid, mp 70–71 °C (from Et_2O). ^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.97–7.93 (2H, m), 7.89–7.85 (2H, m), 7.64–7.60 (1H, m), 7.60–7.54 (2H, m), 7.15 (1H, d, *J* = 15.3 Hz), 6.96–6.92 (2H, m), 6.87 (1H, dd, *J* = 15.3, 7.6 Hz), 3.86 (3H, s), 3.03 (1H, d, *J* = 7.6 Hz). ^{13}C{^{1}H} NMR ($CDCl_3$, 100 MHz) δ 187.7, 165.4, 163.4, 148.7, 133.6, 130.8, 130.6, 130.0, 129.3, 125.3, 123.7, 113.8, 55.4, 33.2. HRMS (ESI–TOF): *m/z* calcd for $C_{18}H_{15}NNaO_2$ $[M+Na]^+$ 300.0995; found 300.0995.

4. Synthesis of pyrroles 1, 2

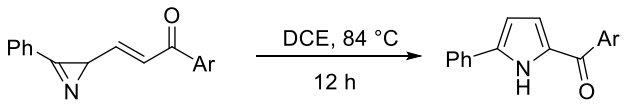
Synthesis of pyrrole 1



A solution of pyrrole **2a** (0.2 g, 0.810 mmol) in anhydrous DMF (10 mL) was dropwise added to a stirred suspension of NaH (0.067 g, 60% in mineral oil, 1.619 mmol, preliminary washed with dry hexane) in anhydrous DMF (5 mL) at 0 °C. After stirring for 30 min at rt, the mixture was cooled in the ice bath, and a solution of MeI (0.144 g, 1.012 mmol) in anhydrous DMF (10 mL) was slowly added. The mixture was stirred for 2 h at rt, and then H_2O (10 mL) was slowly added. The product was extracted with EtOAc (3×20 mL), and the combined organic fractions were washed with water and brine and dried over Na_2SO_4. The solvent was removed under reduced pressure, and the residue was recrystallized from $CHCl_3$ to give (1-methyl-5-phenyl-1*H*-pyrrol-2-yl)(phenyl)methanone (**1**) (0.204 g, 97%). Yellow solid, mp 80–84 °C. ^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.88–7.83 (2H, m), 7.57–7.52 (1H, m), 7.49–7.40 (7H, m), 6.80 (1H, d, *J* = 4.1 Hz), 6.25 (1H, d, *J* = 4.1 Hz), 3.99 (3H, s). ^{13}C{^{1}H} NMR ($CDCl_3$, 100 MHz) δ 186.1, 143.6, 140.2, 131.9, 131.7, 131.3, 129.3, 129.2, 128.6, 128.3, 128.0, 123.0, 109.5, 35.1. HRMS (ESI–TOF): *m/z* calcd for $C_{18}H_{15}NNaO$ $[M+Na]^+$ 284.1046; found 284.1033.

Synthesis of pyrroles 2

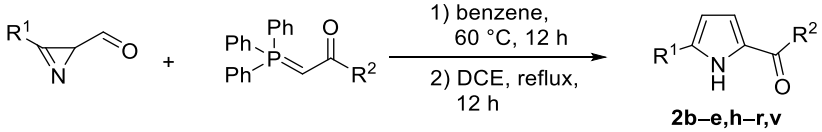
Method A



2a,f,g

A 0.1 M solution of a 2-(2-aroylvinyl)azirine (2–4 mmol) in DCE was heated under reflux for 12 h. The solvent was removed under reduced pressure, and the product was isolated by column chromatography on silica gel.

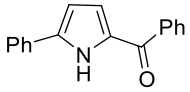
Method B



2b–e,h–r,v

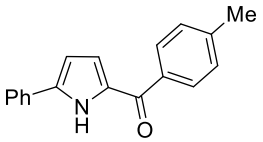
To a 0.1 M solution of an azirinecarbaldehyde in anhydrous benzene a phosphorus ylide was added in the amount indicated below, and the mixture was stirred at 60 °C until the azirine was consumed (*ca*. 12 h) (control by TLC, hexane/EtOAc 5:1). The solvent was evaporated under reduced pressure, DCE was added in a volume equal to that of benzene evaporated, and the mixture was heated under reflux for 12 h. The product was purified by crystallization from DCE followed by recrystallization from the solvent indicated below or by column chromatography on silica gel.

Phenyl(5-phenyl-1*H*-pyrrol-2-yl)methanone (**2a**)



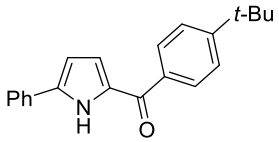
Compound **2a** (490 mg, 98%) was prepared according to method *A* from (*E*)-1-phenyl-3-(3-phenyl-2*H*-azirin-2-yl)prop-2-en-1-one (0.50 g, 2.02 mmol) using hexane/EtOAc (5:1) as eluent for chromatography. Colorless solid, mp 167–168 °C (from Et_2O) (Lit. mp 164–166 °C).[4] ^{1}H NMR ($CDCl_3$, 400 MHz) δ 10.65 (1H, br.s), 7.99–7.91 (2H, m), 7.80–7.71 (2H, m), 7.63–7.56 (1H, m), 7.51 (2H, dd, *J* = 8.2, 6.7 Hz), 7.43–7.29 (3H, m), 6.97 (1H, dd, *J* = 4.0, 2.4 Hz), 6.66 (1H, dd, *J* = 4.0, 2.7 Hz). ^{13}C{^{1}H} NMR ($CDCl_3$, 100 MHz) δ 184.7, 139.5, 138.6, 131.8, 131.0, 129.04, 128.96, 128.3, 128.2, 125.3, 121.5, 108.8. HRMS (ESI-TOF): *m/z* calcd for $C_{17}H_{13}NNaO$ $[M+Na]^+$ 270.0889; found: 270.0894.

(4-Methylphenyl)(5-phenyl-1*H*-pyrrol-2-yl)methanone (2b)



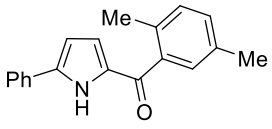
Compound **2b** (433 mg, 14%) was prepared according to method *B* from 3-phenyl-2*H*-azirine-2-carbaldehyde (1.69 g, 11.63 mmol) and 1-(*p*-tolyl)-2-(triphenyl-λ^5-phosphanylidene)ethan-1-one (4.58 g, 11.63 mmol) using hexane/EtOAc (5:1) as eluent for chromatography. Colorless solid, mp 192–193 °C (from $CHCl_3$). ^{1}H NMR (DMSO-d_6, 400 MHz) δ 12.25 (1H, br.s), 7.97–7.93 (2H, m), 7.77–7.73 (2H, m), 7.44–7.39 (2H, m), 7.35–7.30 (3H, m), 6.83 (1H, *J* = 4.0, 2.4 Hz), 6.74 (1H, dd, *J* = 4.0, 2.4 Hz), 2.39 (3H, s). ^{13}C{^{1}H} NMR (DMSO-d_6, 100 MHz) δ 183.2, 141.7, 138.9, 136.0, 131.8, 131.0, 128.9, 128.7, 127.7, 125.5, 120.7, 108.5, 79.2, 21.1. HRMS (ESI–TOF): *m/z* calcd for $C_{18}H_{16}NO$ $[M+H]^+$ 262.1226; found 262.1223.

[4-(*tert*-Butyl)phenyl](5-phenyl-1*H*-pyrrol-2-yl)methanone (2c)



Compound **2c** (367 mg, 70%) was prepared according to method *B* from 3-phenyl-2*H*-azirine-2-carbaldehyde (0.25 g, 1.72 mmol) and 1-(4-*tert*-butylphenyl)-2-(triphenyl-λ^5-phosphanylidene)ethan-1-one (1 g, 2.29 mmol) using sequential recrystallization from EtOH and Et_2O. Colorless solid, mp 169–170 °C (from Et_2O). ^{1}H NMR (DMSO-d_6, 400 MHz) δ 12.23 (1H, br.s), 7.97–7.92 (2H, m), 7.82–7.77 (2H, m), 7.58–7.53 (2H, m), 7.45–7.39 (2H, m), 7.34–7.29 (1H, m), 6.85 (1H, dd, *J* = 4.0, 2.3 Hz), 6.75 (1H, dd, *J* = 4.0, 2.3 Hz), 1.33 (9H, s). ^{13}C{^{1}H} NMR (DMSO-d_6, 100 MHz) δ 183.1, 154.5, 138.8, 136.0, 131.8, 131.0, 128.7, 128.6, 127.7, 125.5, 125.2, 120.7, 108.6, 34.7, 30.9. HRMS (ESI–TOF): *m/z* calcd for $C_{21}H_{21}NNaO$ $[M+Na]^+$ 326.1515; found 326.1520.

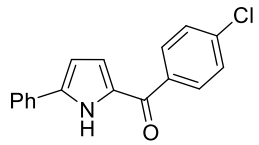
(2,5-Dimethylphenyl)(5-phenyl-1*H*-pyrrol-2-yl)methanone (2d)



Compound **2d** (416 mg, 73%) was prepared according to method *B* from 3-phenyl-2*H*-azirine-2-carbaldehyde (0.30 g, 2.07 mmol) and 1-(2,5-dimethylphenyl)-2-(triphenyl-λ^5-phosphanylidene)-ethan-1-one (2.09 g, 5.13 mmol) using sequential recrystallization from EtOH and Et_2O. Colorless solid, mp 163–165 (from Et_2O). ^{1}H NMR (DMSO-d_6, 400 MHz): δ 12.33 (1H, br.s),

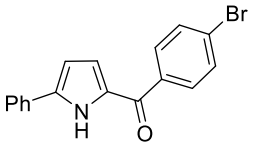
7.97–7.92 (2H, m), 7.45–7.39 (2H, m), 7.35–7.29 (1H, m), 7.26–7.17 (3H, m), 6.71 (1H, dd, J = 3.9, J = 2.4 Hz), 6.49 (1H, dd, J = 3.9 Hz, J = 2.2 Hz), 2.32 (3H, s), 2.26 (3H, s). $^{13}C\{^{1}H\}$ NMR (DMSO-d_6, 100 MHz): δ 185.7, 139.4, 139.0, 134.2, 132.9, 132.3, 131.0, 130.5, 130.2, 128.7, 128.2, 127.8, 125.6, 121.6, 108.6, 20.5, 18.8. HRMS (ESI–TOF): *m/z* calcd for $C_{19}H_{18}NO$ $[M+H]^+$ 276.1383; found 276.1384.

(4-Chlorophenyl)(5-phenyl-1*H*-pyrrol-2-yl)methanone (2e)



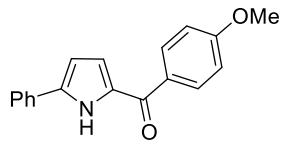
Compound **2e** (246 mg, 45%) was prepared according to method *B* from 3-phenyl-2*H*-azirine-2-carbaldehyde (0.15 g, 1.93 mmol) and 1-(4-chlorophenyl)-2-(triphenyl-λ^5-phosphanylidene)-ethan-1-one (1.75 g, 5.15 mmol) using sequential recrystallization from EtOH and Et_2O. Colorless solid, mp 235–236 °C (from Et_2O). ^{1}H NMR (DMSO-d_6, 400 MHz) δ 12.32 (1H, br.s), 7.98–7.91 (2H, m), 7.87–7.80 (2H, m), 7.63–7.59 (2H, m), 7.46–7.37 (2H, m), 7.35–7.28 (1H, m), 6.86 (1H, dd, J = 3.8, 2.4 Hz), 6.78 (1H, dd, J = 3.9, 2.4 Hz). $^{13}C\{^{1}H\}$ NMR (DMSO-d_6, 100 MHz) δ 182.1, 139.5, 137.4, 136.4, 131.4, 130.8, 130.5, 128.8, 128.5, 127.9, 125.7, 121.4, 108.8. HRMS (ESI–TOF): *m/z* calcd for $C_{17}H_{13}{}^{35}ClNO$ $[M+H]^+$ 282.0680; found 282.0688.

(4-Bromophenyl)(5-phenyl-1*H*-pyrrol-2-yl)methanone (**2f**)



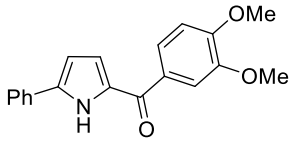
Compound **2f** (737 mg, 74%) was prepared according to method *A* from (*E*)-1-(4-bromophenyl)-3-(3-phenyl-2*H*-azirin-2-yl)prop-2-en-1-one (1 g, 3.08 mmol) using benzene/EtOAc (10:1) as eluent for chromatography. Yellow solid, mp 232–233 °C (from Et_2O). ^{1}H NMR ($CDCl_3$, 400 MHz) δ 9.81 (1H, br.s), 7.82–7.77 (2H, m), 7.67–7.62 (4H, m), 7.48–7.41 (2H, m), 7.39–7.33 (1H, m), 6.91 (1H, dd, J = 3.9, 2.6 Hz), 6.64 (1H, dd, J = 3.9, 2.6 Hz). $^{13}C\{^{1}H\}$ NMR (DMSO-d_6, 100 MHz) δ 182.2, 139.5, 137.7, 131.4, 130.8, 130.6, 128.7, 127.9, 125.6, 125.3, 121.4, 108.8. HRMS (ESI–TOF): *m/z* calcd for $C_{17}H_{13}{}^{79}BrNO$ $[M+H]^+$ 326.0175; found 326.0189.

(4-Methoxyphenyl)(5-phenyl-1*H*-pyrrol-2-yl)methanone (**2g**)



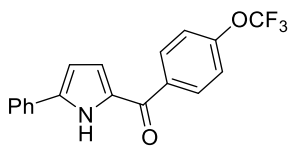
Compound **2g** (890 mg, 89%) was prepared according to method *A* from (*E*)-1-(4-methoxyphenyl)-3-(3-phenyl-2*H*-azirin-2-yl)prop-2-en-1-one (1.0 g, 3.83 mmol) using hexane/EtOAc (5:1) as eluent for chromatography. Colorless solid, mp 167–168 °C (from Et_2O). ^{1}H NMR ($CDCl_3$, 400 MHz) δ 10.56 (1H, br.s), 8.02–7.92 (2H, m), 7.78–7.67 (2H, m), 7.42–7.35 (2H, m), 7.34–7.29 (1H, m), 7.04–6.98 (2H, m), 6.97 (1H, dd, *J* = 3.5, 2.4 Hz), 6.65 (1H, dd, *J* = 3.5, 2.4 Hz), 3.91 (3H, s). ^{13}C{^{1}H} NMR ($CDCl_3$, 100 MHz) δ 183.5, 162.7, 138.8, 131.8, 131.2, 131.13, 131.11, 129.0, 128.0, 125.2, 120.6, 113.6, 108.6, 55.4. HRMS (ESI–TOF): *m/z* calcd for $C_{18}H_{15}NNaO_2$ $[M+Na]^+$ 300.0995; found 300.1004.

(3,4-Dimethoxyphenyl)(5-phenyl-1*H*-pyrrol-2-yl)methanone (2h)



Compound **2h** (103 mg, 16%) was prepared according to method *B* from 3-phenyl-2*H*-azirine-2-carbaldehyde (0.30 g, 2.07 mmol) and 1-(3,4-dimethoxyphenyl)-2-(triphenyl-λ^5-phosphanylidene)ethan-1-one (0.95 g, 2.16 mmol) using petroleum ether/EtOAc (5:1) as eluent for chromatography. Colorless solid, mp 196–198 °C (DMSO/H_2O). ^{1}H NMR (DMSO-d_6, 400 MHz) δ 12.17 (1H, br.s), 7.98–7.87 (2H, m), 7.56–7.47 (1H, m), 7.46–7.36 (3H, m), 7.35–7.24 (1H, m), 7.13–7.04 (1H, m), 6.91–6.84 (1H, m), 6.77–6.70 (1H, m), 3.84 (6H, br.s). ^{13}C{^{1}H} NMR (DMSO-d_6, 100 MHz) δ 182.3, 152.0, 148.4, 138.5, 131.8, 131.1, 128.7, 127.6, 125.5, 122.7, 120.3, 111.7, 110.9, 108.4, 55.7, 55.5. HRMS (ESI–TOF): *m/z* calcd for $C_{19}H_{18}NO_3$ $[M+H]^+$ 308.1281; found 308.1293.

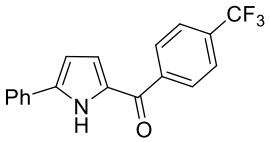
(5-Phenyl-1*H*-pyrrol-2-yl)[4-(trifluoromethoxy)phenyl]methanone (2i)



Compound **2i** (125 mg, 37%) was prepared according to method *B* from 3-phenyl-2*H*-azirine-2-carbaldehyde (0.15 g, 1.04 mmol) and 1-(4-trifluoromethoxyphenyl)-2-(triphenyl-λ^5-phospha-

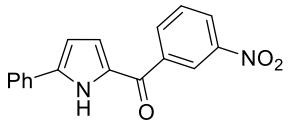
nylidene)ethan-1-one (1.23 g, 2.65 mmol) after the recrystallization from EtOH. Colorless solid, mp 189–191 °C (from EtOH). ^{1}H NMR (DMSO-d_6, 400 MHz) δ 12.35 (1H, br.s), 7.99–7.93 (4H, m), 7.55–7.48 (2H, m), 7.47–7.39 (2H, m), 7.36–7.29 (1H, m), 6.87 (1H, d, *J* = 3.8 Hz), 6.78 (1H, d, *J* = 4.0 Hz). ^{13}C{^{1}H} NMR (DMSO-d_6, 100 MHz) δ 181.8, 150.4 (q, *J* = 1.5 Hz), 139.6, 137.6, 131.4, 130.9 (2C), 128.8, 127.9, 125.7, 121.5, 120.7, 120.0 (q, *J* = 257.2 Hz), 108.9. ^{19}F NMR (DMSO-d_6, 376 MHz) δ -56.6. HRMS (ESI–TOF): *m/z* calcd for $C_{18}H_{13}F_3NO_2$ $[M+H]^+$ 332.0893; found 332.0891.

(5-Phenyl-1*H*-pyrrol-2-yl)[4-(trifluoromethyl)phenyl]methanone (2j)



Compound **2j** (780 mg, 79%) was prepared according to method *B* from 3-phenyl-2*H*-azirine-2-carbaldehyde (0.45 g, 3.1 mmol) and 1-(4-trifluoromethylphenyl)-2-(triphenyl-λ^5-phosphanylidene)ethan-1-one (2.05 g, 4.6 mmol) after recrystallization from EtOH. Colorless solid, mp 209–210 °C (from EtOH). ^{1}H NMR (DMSO-d_6, 400 MHz) δ 12.42 (1H, br.s), 8.04–7.98 (2H, m), 7.98–7.93 (2H, m), 7.93–7.87 (2H, m), 7.47–7.40 (2H, m), 7.37–7.30 (1H, m), 6.88 (1H, dd, *J* = 4.0, 2.4 Hz), 6.80 (1H, dd, *J* = 4.0, 2.4 Hz). ^{13}C{^{1}H} NMR (DMSO-d_6, 100 MHz) δ 182.1, 142.3, 140.0, 131.4, 131.2 (q, *J* = 32.1 Hz), 130.8, 129.3, 128.8, 128.0, 125.7, 125.4 (q, *J* = 3.8 Hz), 123.9 (q, *J* = 274.8 Hz), 122.0, 109.1. ^{19}F NMR (DMSO-d_6, 376 MHz) δ -61.4. HRMS (ESI–TOF): *m/z* calcd for $C_{18}H_{13}F_3NO$ $[M+H]^+$ 316.0944; found 316.0946.

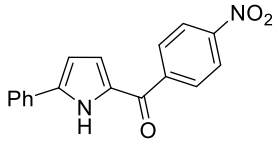
(3-Nitrophenyl)(5-phenyl-1*H*-pyrrol-2-yl)methanone (2k)



Compound **2k** (405 mg, 17%) was prepared from 3-phenyl-2*H*-azirine-2-carbaldehyde (1.20 g, 8.3 mmol) and 1-(3-nitrophenyl)-2-(triphenyl-λ^5-phosphanylidene)ethan-1-one (6.63 g, 9.41 mmol) according to method *B* by heating under reflux in toluene for 9 d and using petroleum ether/EtOAc (4:1) as eluent for chromatography.Yellow solid, mp 205–206 °C (from EtOH). ^{1}H NMR ($CDCl_3$, 400 MHz) δ 10.00 (1H, br.s), 8.79 (1H, d, *J* = 2.0 Hz), 8.46 (dd, *J* = 8.1, 2.0 Hz, 1H), 8.28–8.23 (m, 1H), 7.72 (3H, dd, *J* = 17.2, 8.0 Hz), 7.48 (2H, dd, *J* = 8.3, 6.9 Hz), 7.43–7.35 (1H, m), 6.98 (1H, dd, *J* = 4.1, 2.3 Hz), 6.71 (1H, dd, *J* = 4.1, 2.6 Hz). ^{13}C{^{1}H} NMR ($CDCl_3$, 100 MHz) δ 181.4, 148.1, 140.3, 139.8, 134.5, 130.8, 130.4, 129.6, 129.2, 128.8, 126.2, 125.3,

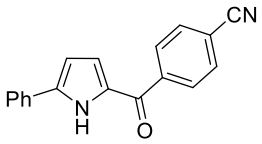
123.8, 121.8, 109.4. HRMS (ESI–TOF): *m/z* calcd for $C_{17}H_{13}N_2O_3$ $[M+H]^+$ 293.0921; found 293.0931.

(4-Nitrophenyl)(5-phenyl-1*H*-pyrrol-2-yl)methanone (2l)



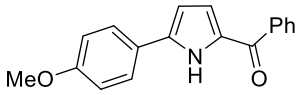
Compound **2l** (285 mg, 35%) was prepared according to method *B* from 3-phenyl-2*H*-azirine-2-carbaldehyde (0.40 g, 2.76 mmol) and 1-(4-nitrophenyl)-2-(triphenyl-λ^5-phosphanylidene)ethan-1-one (3.08 g, 6.53 mmol) after recrystallization from MeOH. Yellow solid, mp 233–234 °C (from MeOH). ^{1}H NMR (DMSO-d_6, 400 MHz) δ 12.46 (1H, br.s), 8.39–8.33 (2H, m), 8.07–8.01 (2H, m), 7.99–7.94 (2H, m), 7.47–7.40 (2H, m), 7.38–7.32 (1H, m), 6.89 (1H, dd, *J* = 4.0, 2.3 Hz), 6.82 (1H, dd, *J* = 4.0, 2.3 Hz). ^{13}C{^{1}H} NMR (DMSO-d_6, 100 MHz) δ 181.5, 148.9, 144.2, 140.4, 131.3, 130.7, 129.8, 128.8, 128.1, 125.8, 123.6, 122.3, 109.2. HRMS (ESI–TOF): *m/z* calcd for $C_{17}H_{12}N_2NaO_3$ $[M+Na]^+$ 315.0740; found 315.0742.

4-(5-Phenyl-1*H*-pyrrole-2-carbonyl)benzonitrile (2m)



Compound **2m** (678 mg, 94%) was prepared according to method *B* from 3-phenyl-2*H*-azirine-2-carbaldehyde (0.39 g, 2.66 mmol) and 4-(2-oxo-3-(triphenyl-λ^5-phosphanylidene)propyl)-benzonitrile (1.96 g, 4.84 mmol) after recrystallization from EtOH. Light yellow solid, mp 232–233 °C (from EtOH). ^{1}H NMR (DMSO-d_6, 400 MHz) δ 12.42 (1H, br.s), 8.04–7.92 (6H, m), 7.47–7.40 (2H, m), 7.37–7.30 (1H, m), 6.86 (1H, d, *J* = 4.0 Hz), 6.79 (1H, d, *J* = 4.0 Hz). ^{13}C{^{1}H} NMR (DMSO-d_6, 100 MHz) δ 181.8, 142.7, 140.4, 132.4, 131.5, 130.9, 129.2, 128.8, 128.0, 125.7, 122.1, 118.4, 113.6, 109.2. HRMS (ESI–TOF): *m/z* calcd for $C_{18}H_{13}N_2O$ $[M+H]^+$ 273.1022; found 273.1016.

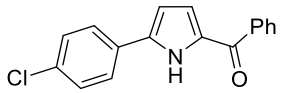
[5-(4-Methoxyphenyl)-1*H*-pyrrol-2-yl)](phenyl)methanone (2n)



Compound **2n** (194 mg, 26%) was prepared according to method *B* from 3-(4-methoxyphenyl)-2*H*-azirine-2-carbaldehyde (0.35 g, 1.98 mmol) and 1-phenyl-2-(triphenyl-λ^5-phosphanylidene)ethan-1-one (1.50 g, 3.95 mmol) after recrystallization from DCE. Yellow solid, mp

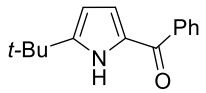
191–192 °C (from DCE). ^{1}H NMR (DMSO-d_6, 400 MHz) δ 12.15 (1H, br.s), 7.93–7.86 (2H, m), 7.84–7.78 (2H, m), 7.63–7.57 (1H, m), 7.56–7.48 (2H, m), 7.03–6.94 (m, 2H), 6.80 (1H, dd, J = 4.1, 2.1 Hz), 6.65 (1H, dd, J = 4.1, 2.1 Hz), 3.80 (3H, s). ^{13}C{^{1}H} NMR (DMSO-d_6, 100 MHz) δ 183.1, 159.1, 139.4, 138.9, 131.4, 131.2, 128.5, 128.3, 127.1, 123.6, 121.4, 114.2, 107.8, 55.2. HRMS (ESI–TOF): *m/z* calcd for $C_{18}H_{15}NNaO_2$ $[M+Na]^+$ 300.0995; found 300.1003.

[5-(4-Chlorophenyl)-1*H*-pyrrol-2-yl](phenyl)methanone (2o)



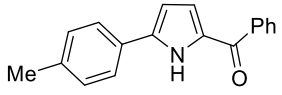
Compound **2o** (194 mg, 19%) was prepared according to method *B* from 3-(4-chlorophenyl)-2*H*-azirine-2-carbaldehyde (0.62 g, 3.41 mmol) and 1-phenyl-2-(triphenyl-λ^5-phosphanylidene)-ethan-1-one (2.87 g, 7.56 mmol) after recrystallization from DCE. Yellow solid, mp 231–232 °C (from DCE). ^{1}H NMR (DMSO-d_6, 400 MHz) δ 12.35 (1H, br.s), 8.01–7.95 (2H, m), 7.86–7.80 (2H, m), 7.66–7.60 (1H, m), 7.58–7.52 (2H, m), 7.51–7.46 (2H, m), 6.84 (1H, dd, J = 4.0, 2.4 Hz), 6.80 (1H, dd, J = 4.0, 2.4 Hz). ^{13}C{^{1}H} NMR (DMSO-d_6, 100 MHz) δ 183.6, 138.6, 137.8, 132.3, 132.0, 131.7, 129.9, 128.8, 128.6, 128.4, 127.3, 121.1, 109.1. HRMS (ESI–TOF): *m/z* calcd for $C_{17}H_{12}{}^{35}ClNNaO$ $[M+Na]^+$ 304.0500; found 304.0506.

[5-(*tert*-Butyl)-1*H*-pyrrol-2-yl](phenyl)methanone (2p)



Compound **2p** (117 mg, 32%) was prepared according to method *B* from 3-(*tert*-butyl)-2*H*-azirine-2-carbaldehyde (0.20 g, 1.6 mmol) and 1-phenyl-2-(triphenyl-λ^5-phosphanylidene)ethan-1-one (0.97 g, 1.6 mmol) using petroleum ether/EtOAc (6:1) as eluent for chromatography. Colorless solid, mp 176–178 °C (from Et_2O). ^{1}H NMR ($CDCl_3$, 400 MHz) δ 9.48 (1H, br.s), 7.90–7.82 (2H, m), 7.57–7.50 (1H, m), 7.50–7.42 (2H, m), 6.79 (1H, dd, J = 3.8, 2.6 Hz), 6.10 (1H, dd, J = 3.8, 2.6 Hz), 1.36 (9H, s). ^{13}C{^{1}H} NMR ($CDCl_3$, 100 MHz) δ 184.2, 150.4, 138.7, 131.5, 129.8, 128.8, 128.2, 120.5, 106.7, 31.9, 30.1. HRMS (ESI–TOF): *m/z* calcd for $C_{15}H_{18}NO$ $[M+H]^+$ 228.1383; found 228.1391.

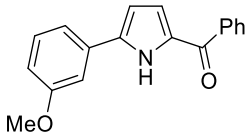
Phenyl[5-(4-methylphenyl)-1*H*-pyrrol-2-yl]methanone (2q)



Compound **2q** (697 mg, 85%) was prepared according to method *B* from 3-(*p*-tolyl)-2*H*-azirine-2-carbaldehyde (0.50 g, 3.155 mmol) and 1-phenyl-2-(triphenyl-λ^5-phosphanylidene)ethan-1-one

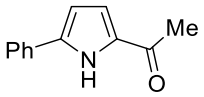
(1.20 g, 6.29 mmol) using petroleum ether/EtOAc (5:1) as eluent for chromatography. Yellow solid, mp 171–173 (from Et_2O). ^1H NMR (DMSO-d_6, 400 MHz) δ 12.21 (1H, br.s), 7.87–7.79 (4H, m), 7.64–7.58 (1H, m), 7.57–7.50 (2H, m), 7.26–7.19 (2H, d, *J* = 8.1 Hz), 6.81 (1H, dd, *J* = 3.9, 2.2 Hz), 6.71 (1H, dd, *J* = 3.9, 2.2 Hz), 2.33 (3H, s). $^{13}C\{^1H\}$ NMR (DMSO-d_6, 100 MHz) δ 183.3, 139.4, 138.8, 137.3, 131.5, 131.4, 129.3, 128.5, 128.4, 128.2, 125.5, 121.2, 108.2, 20.8. HRMS (ESI–TOF): *m/z* calcd for $C_{18}H_{15}NNaO$ $[M+Na]^+$ 284.1046; found 284.1051.

[5-(3-Methoxyphenyl)-1*H*-pyrrol-2-yl](phenyl)methanone (2r)



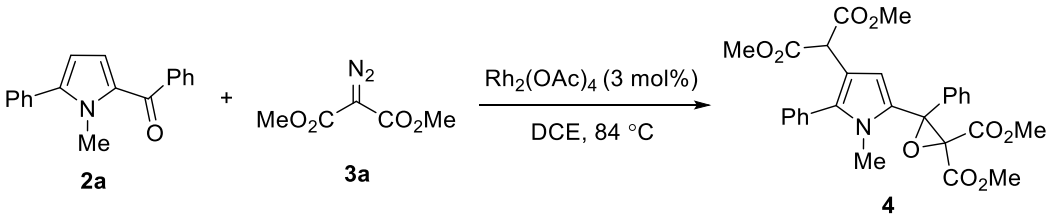
Compound **2r** (390 mg, 70%) was prepared according to method *B* from 3-(3-methoxyphenyl)-2*H*-azirine-2-carbaldehyde (0.63 g, 3.57 mmol) and 1-phenyl-2-(triphenyl-λ^5-phosphanylidene)ethan-1-one (1.36 g, 3.57 mmol) after recrystallization from DCE. Yellow solid, mp 153–154 °C (from DCE). ^1H NMR (DMSO-d_6, 400 MHz) δ 12.33 (1H, br.s), 7.87–7.78 (2H, m), 7.66–7.58 (2H, m), 7.58–7.50 (2H, m), 7.49 (1H, d, *J* = 8.0 Hz), 7.32 (1H, t, *J* = 8.0 Hz), 6.88 (1H, dd, *J* = 8.0, 2.5 Hz), 6.82 (1H, m), 6.78 (1H, m), 3.84 (3H, s). $^{13}C\{^1H\}$ NMR (DMSO-d_6, 100 MHz) δ 183.5, 159.7, 139.1, 138.7, 132.3, 131.7, 131.6, 129.8, 128.6, 128.4, 121.1, 118.1, 114.1, 110.3, 108.9, 55.3. HRMS (ESI–TOF): *m/z* calcd for $C_{18}H_{15}NNaO_2$ $[M+Na]^+$ 300.0995; found 300.1004.

1-(5-Phenyl-1*H*-pyrrol-2-yl)ethan-1-one (2v)



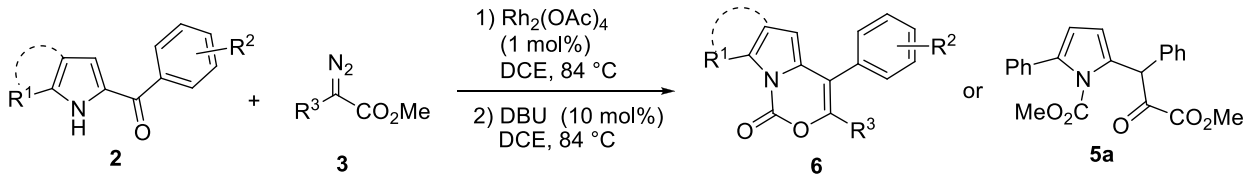
Compound **2v** (290 mg, 57%) was prepared according to method *B* from 3-phenyl-2*H*-azirine-2-carbaldehyde (0.40 g, 2.76 mmol) and 1-(triphenyl-λ^5-phosphanylidene)propan-2-one (1.32 g, 4.14 mmol) using petroleum ether/EtOAc (4:1) as eluent for chromatography. Colorless solid, mp 157–159 °C (from Et_2O) (Lit. mp 163–164 °C[12]). ^1H NMR ($CDCl_3$, 400 MHz) δ 10.38 (1H, br.s), 7.74–7.66 (2H, m), 7.44–7.37 (2H, m), 7.35–7.28 (1H, m), 6.98 (1H, dd, *J* = 4.0 Hz, 2.4 Hz), 6.58 (1H, dd, *J* = 4.0 Hz, 2.4 Hz), 2.47 (3H, s). $^{13}C\{^1H\}$ NMR ($CDCl_3$, 100 MHz) δ 187.7, 138.8, 132.6, 131.0, 128.8, 128.0, 125.2, 118.5, 108.2, 25.2. HRMS (ESI–TOF): *m/z* calcd for $C_{12}H_{11}NNaO$ $[M+Na]^+$ 208.0733; found 208.0740.

5. Synthesis of oxirane 4



A solution of dimethyl diazomalonate **3a** (76 mg, 0.48 mmol) in DCE (2 mL) was added dropwise to a stirred solution of pyrrole **1a** (15 mg, 0.057 mmol) and $Rh_2(OAc)_4$ (4.5 mg, 0.0017 mmol) in DCE (2 mL) at 84 °C. After the reaction was completed (control by TLC, hexane/EtOAc 5:1), the solvent was removed under reduced pressure, and dimethyl 3-[4-di(methoxycarbonyl)methyl-1-methyl-5-phenyl-1*H*-pyrrol-2-yl]-3-phenyloxirane-2,2-dicarboxylate (**4**) (23 mg, 80%) was isolated by column chromatography (eluent hexane/EtOAc 5:1). Yellow oil. ^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.42–7.29 (8H, m), 7.25–7.21 (2H, m), 6.58 (1H, s), 4.42 (1H, s), 3.82 (3H, s), 3.75 (3H, s), 3.69 (3H, s), 3.50 (3H, s), 3.22 (3H, s). ^{13}C{^{1}H} NMR ($CDCl_3$, 100 MHz) δ 169.3, 169.2, 164.3, 163.8, 135.0, 134.9, 130.8, 130.4, 128.8, 128.5, 128.3, 128.2, 127.0, 125.8, 111.9, 110.0, 68.8, 65.8, 53.3, 52.7, 52.6, 52.5, 49.6, 32.6. HRMS (ESI–TOF) calcd for $C_{28}H_{27}NNaO_9$ $[M+Na]^+$ 544.1578; found 544.1585.

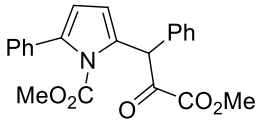
6. Synthesis of pyruvate 5a and oxazinones 6



Method A. A 0.3 M solution of diazoester **3** (2–2.5 equiv) in DCE was added dropwise (0.5 mL/h) via a syringe pump to a 0.1 M solution of pyrrole **2a–r** (0.15–0.45 mmol) and $Rh_2(OAc)_4$ (0.0015–0.0045 mmol) in DCE at 84 °C. After the reaction was completed (control by TLC, hexane/EtOAc 5:1), a 0.1 M solution of DBU (0.015–0.045 mmol, 10 mol%) in DCE was added, and the mixture was stirred under reflux for 1 min. The solvent was removed under reduced pressure, and the product was purified by column chromatography on silica gel.

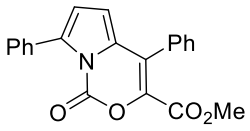
Method B. A 0.3 M solution of diazoester **3** (2–2.5 equiv) in DCE was added dropwise (0.5 mL/h) via a syringe pump to a 0.1 M solution of pyrrole **2a–u** (0.15–0.45 mmol) and $Rh_2(OAc)_4$ (0.0015–0.0045 mmol) in DCE at 84 °C. After the reaction was completed (control by TLC, hexane/EtOAc 5:1), the solvent was removed under reduced pressure, and the product was isolated by column chromatography on silica gel.

Synthesis of methyl 2-(3-methoxy-2,3-dioxo-1-phenylpropyl)-5-phenyl-1*H*-pyrrole-1-carboxylate (5a)



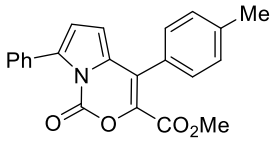
Compound **5a** (76 mg, 33%) was prepared according to method *B* from pyrrole **2a** (150 mg, 0.61 mmol) and dimethyl diazomalonate (**3a**) (288 mg, 1.82 mmol). Colorless solid, mp 123–125 °C (hexane/Et_2O). ^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.43–7.26 (10H, m), 6.29–6.26 (1H, m), 6.11 (1H, d, *J* = 3.5 Hz), 5.70 (1H, dd, *J* = 3.5, 1.2 Hz), 3.84 (3H, s), 3.60 (3H, s). ^{13}C{^{1}H} NMR ($CDCl_3$, 100 MHz) δ 189.3, 160.8, 152.4, 136.7, 134.4, 133.7, 133.3, 130.2, 129.0, 128.31, 128.28, 127.6, 127.1, 115.0, 113.5, 53.7, 53.6, 53.1. HRMS (ESI–TOF): *m/z* calcd for $C_{22}H_{20}NO_5$ $[M+H]^+$ 378.1336; found 378.1345.

Methyl 1-oxo-4,7-diphenyl-1*H*-pyrrolo[1,2-*c*][1,3]oxazine-3-carboxylate (6a)



Compound **6a** (71 mg, 51%) was prepared according to method *A* from pyrrole **2a** (100 mg, 0.41 mmol) and dimethyl diazomalonate (**3a**) (128 mg, 0.81 mmol) using petroleum ether/EtOAc (6:1) as eluent for column chromatography. Colorless solid, mp 167.5–168 °C (from Et_2O). ^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.53–7.45 (5H, m), 7.45–7.33 (5H, m), 6.63 (1H, d, *J* = 3.8 Hz), 6.26 (1H, d, *J* = 3.8 Hz), 3.73 (3H, s). ^{13}C{^{1}H} NMR ($CDCl_3$, 100 MHz) δ 160.4, 142.6, 136.6, 133.0, 132.3, 131.7, 131.1, 129.8, 129.0, 128.9, 128.4, 128.3, 127.7, 122.5, 118.6, 113.4, 52.4. HRMS (ESI–TOF): *m/z* calcd for $C_{21}H_{16}NO_4$ $[M+H]^+$ 346.1074; found 346.1078.

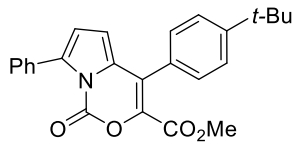
Methyl 4-(4-methylphenyl)-1-oxo-7-phenyl-1*H*-pyrrolo[1,2-*c*][1,3]oxazine-3-carboxylate (6b)



Compound **6b** (90 mg, 65%) was prepared according to method *A* from pyrrole **2b** (100 mg, 0.38 mmol) and dimethyl diazomalonate (**3a**) (151 mg, 0.96 mmol) using petroleum ether/EtOAc (6:1) as eluent for column chromatography. Light pink solid, mp 129–130 °C (from Et_2O). ^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.53–7.46 (2H, m), 7.45–7.39 (3H, m), 7.33–7.27 (4H, m), 6.62 (1H, d, *J* = 3.8 Hz), 6.28 (1H, d, *J* = 3.8 Hz), 3.75 (3H, s), 2.45 (3H, s). ^{13}C{^{1}H} NMR ($CDCl_3$, 100

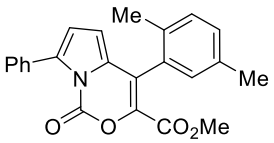
MHz) δ 160.4, 142.6, 138.8, 136.5, 132.9, 132.5, 131.1, 129.7, 129.1, 128.9, 128.6, 128.3, 127.7, 122.7, 118.6, 113.3, 52.3, 21.4. HRMS (ESI–TOF): *m/z* calcd for $C_{22}H_{17}NNaO_4$ $[M+Na]^+$ 382.1050; found 382.1067.

Methyl 4-[4-(*tert*-butyl)phenyl]-1-oxo-7-phenyl-1*H*-pyrrolo[1,2-*c*][1,3]oxazine-3-carboxylate (6c)



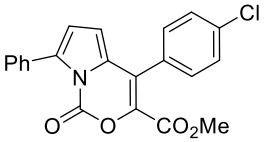
Compound **6c** (86 mg, 64%) was prepared according to method *A* from pyrrole **2c** (100 mg, 0.33 mmol) and dimethyl diazomalonate (**3a**) (104 mg, 0.66 mmol) using petroleum ether/EtOAc (6:1) as eluent for column chromatography. Light pink solid, mp 167–169 °C (from Et_2O). ^1H NMR ($CDCl_3$, 400 MHz) δ 7.53–7.47 (4H, m), 7.44–7.38 (3H, m), 7.35–7.30 (2H, m), 6.62 (1H, d, *J* = 3.8 Hz), 6.31 (1H, d, *J* = 3.8 Hz), 3.74 (3H, s), 1.39 (9H, s). $^{13}C\{^1H\}$ NMR ($CDCl_3$, 100 MHz) δ 160.5, 151.9, 142.6, 136.5, 132.9, 132.5, 131.2, 129.7, 128.8, 128.5, 128.3, 127.7, 125.2, 122.7, 118.6, 113.5, 52.3, 34.8, 31.3. HRMS (ESI–TOF): *m/z* calcd for $C_{25}H_{23}NNaO_4$ $[M+Na]^+$ 424.1519; found 424.1527.

Methyl 4-(2,5-dimethylphenyl)-1-oxo-7-phenyl-1*H*-pyrrolo[1,2-*c*][1,3]oxazine-3-carboxylate (6d)



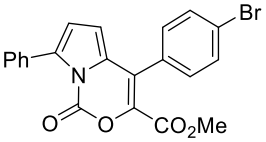
Compound **6d** (69 mg, 51%) was prepared according to method *A* from pyrrole **2d** (100 mg, 0.36 mmol) and dimethyl diazomalonate (**3a**) (115 mg, 0.73 mmol) using petroleum ether/EtOAc (6:1) as eluent for column chromatography. Colorless solid, mp 174.5–175.5 °C (from Et_2O). ^1H NMR ($CDCl_3$, 400 MHz) δ 7.54–7.47 (2H, m), 7.46–7.37 (3H, m), 7.23–7.14 (2H, m), 7.00 (1H, d, *J* = 1.7 Hz), 6.61 (1H, d, *J* = 3.8 Hz), 6.16 (1H, d, *J* = 3.7 Hz), 3.73 (3H, s), 2.36 (3H, s), 2.17 (3H, s). $^{13}C\{^1H\}$ NMR ($CDCl_3$, 100 MHz) δ 160.1, 142.7, 136.5, 135.2, 133.2, 133.1, 131.9, 131.1, 131.0, 129.9, 129.7, 129.6, 129.3, 128.4, 127.7, 121.9, 118.6, 113.1, 52.4, 20.9, 19.0. HRMS (ESI–TOF): *m/z* calcd for $C_{23}H_{19}NNaO_4$ $[M+Na]^+$ 396.1206; found 396.1221.

Methyl 4-(4-chlorophenyl)-1-oxo-7-phenyl-1*H*-pyrrolo[1,2-*c*][1,3]oxazine-3-carboxylate (6e)



Compound **6e** (65 mg, 48%) was prepared according to method *A* from pyrrole **2e** (100 mg, 0.36 mmol) and dimethyl diazomalonate (**3a**) **(**178 mg, 0.89 mmol) using petroleum ether/EtOAc (6:1) as eluent for column chromatography. Light pink solid, mp 143–146 °C (from Et_2O). ^1H NMR ($CDCl_3$, 400 MHz) δ 7.57–7.37 (7H, m), 7.33 (2H, d, *J* = 8.1 Hz), 6.64 (1H, d, *J* = 3.8 Hz), 6.26 (1H, d, *J* = 3.8 Hz), 3.75 (3H, s). $^{13}C\{^1H\}$ NMR ($CDCl_3$, 100 MHz) δ 160.2, 142.4, 136.8, 135.0, 133.0, 131.9, 130.9, 130.5, 130.1, 129.7, 128.7, 128.5, 127.7, 121.4, 118.6, 113.3, 52.5. HRMS (ESI–TOF): *m/z* calcd for $C_{21}H_{14}{}^{35}ClNNaO_4$ $[M+Na]^+$ 402.0504; found 402.0516.

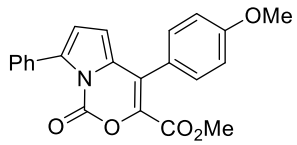
Methyl 4-(4-bromophenyl)-1-oxo-7-phenyl-1*H*-pyrrolo[1,2-*c*][1,3]oxazine-3-carboxylate (6f)



Compound **6f** (86 mg, 74%) was prepared according to method *A* from pyrrole **2f** (100 mg, 0.27 mmol) and dimethyl diazomalonate (**3a**) (108 mg, 0.68 mmol) using petroleum ether/EtOAc (6:1) as eluent for column chromatography. Colorless solid, mp 155–156 °C (from Et_2O). ^1H NMR ($CDCl_3$, 400 MHz) δ 7.66–7.59 (2H, m), 7.51–7.46 (2H, m), 7.45–7.39 (3H, m), 7.29–7.24 (2H, m), 6.63 (1H, d, *J* = 3.8 Hz), 6.25 (1H, d, *J* = 3.8 Hz), 3.75 (3H, s). $^{13}C\{^1H\}$ NMR ($CDCl_3$, 100 MHz) δ 160.3, 142.4, 136.8, 132.9, 131.8, 131.7, 130.9, 130.8, 130.6, 129.8, 128.5, 127.7, 123.2, 121.5, 118.7, 113.3, 52.5. HRMS (ESI–TOF): *m/z* calcd for $C_{21}H_{14}{}^{79}BrNNaO_4$ $[M+Na]^+$ 445.9998; found 446.0006.

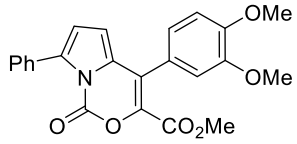
Large-scale (1.6 mmol) synthesis of 6f. Compound **6f** (0.315 g, 46%) was prepared according to method *A* from pyrrole **2f** (0.523 g, 1.6 mmol) and dimethyl diazomalonate **3a** (1.941 g, 12.3 mmol).

Methyl 4-(4-methoxyphenyl)-1-oxo-7-phenyl-1*H*-pyrrolo[1,2-*c*][1,3]oxazine-3-carboxylate (6g)



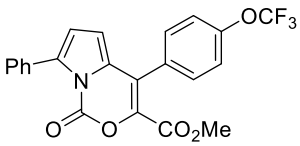
Compound **6g** (44 mg, 65%) was prepared according to method *A* from pyrrole **2g** (100 mg, 0.18 mmol) and dimethyl diazomalonate (**3a**) (75 mg, 0.475 mmol) using petroleum ether/EtOAc (6:1) as eluent for column chromatography. Colorless solid, mp 144–145 °C (from Et_2O/hexane). ^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.53–7.46 (2H, m), 7.46–7.38 (3H, m), 7.35–7.28 (2H, m), 7.05–6.97 (2H, m), 6.63 (1H, d, *J* = 3.7 Hz), 6.31 (1H, d, *J* = 3.8 Hz), 3.88 (3H, s), 3.75 (3H, s). ^{13}C{^{1}H} NMR ($CDCl_3$, 100 MHz) δ 160.5, 160.0, 142.6, 136.5, 132.9, 132.6, 131.1, 130.4, 129.7, 128.3, 127.6, 123.5, 122.4, 118.6, 113.8, 113.4, 55.2, 52.4. HRMS (ESI–TOF): *m/z* calcd for $C_{22}H_{18}NO_5$ $[M+H]^+$ 376.1179; found 376.1187.

Methyl 4-(3,4-dimethoxyphenyl)-1-oxo-7-phenyl-1*H*-pyrrolo[1,2-*c*][1,3]oxazine-3-carboxylate (6h)



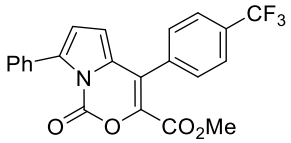
Compound **6h** (30 mg, 45%) was prepared according to method *A* from pyrrole **2h** (50 mg, 0.16 mmol) and dimethyl diazomalonate (**3a**) (64 mg, 0.41 mmol) using petroleum ether/EtOAc (5:1) as eluent for column chromatography. Light pink solid, mp 165–166 °C (from $CHCl_3$). ^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.51–7.47 (2H, m), 7.44–7.38 (3H, m), 7.00–6.92 (2H, m), 6.90 (1H, d, *J* = 1.6 Hz), 6.63 (1H, d, *J* = 3.7 Hz), 6.32 (1H, d, *J* = 3.7 Hz), 3.95 (3H, s), 3.89 (3H, s), 3.75 (3H, s). ^{13}C{^{1}H} NMR ($CDCl_3$, 100 MHz) δ 160.4, 149.5, 148.8, 142.6, 136.5, 133.0, 132.6, 131.1, 129.7, 128.4, 127.7, 123.9, 122.3, 121.8, 118.6, 113.3, 112.4, 110.9, 56.0, 55.9, 52.4. HRMS (ESI-TOF): *m/z* calcd for $C_{23}H_{20}NO_6$ $[M+H]^+$ 406.1285; found 406.1291.

Methyl 1-oxo-7-phenyl-4-[4-(trifluoromethoxy)phenyl]-1*H*-pyrrolo[1,2-*c*][1,3]oxazine-3-carboxylate (6i)



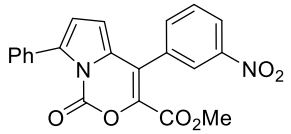
Compound **6i** (60 mg, 58%) was prepared according to method *A* from pyrrole **2i** (80 mg, 0.212 mmol) and of dimethyl diazomalonate (**3a**) (95 mg, 0.60 mmol) using petroleum ether/EtOAc (6:1) as eluent for column chromatography. Colorless solid, mp 114–117 °C (from $CHCl_3$). ^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.52–7.47 (2H, m), 7.46–7.40 (5H, m), 7.37–7.32 (2H, m), 6.65 (1H, d, *J* = 3.8 Hz), 6.26 (1H, d, *J* = 3.8 Hz), 3.74 (3H, s). ^{13}C{^{1}H} NMR ($CDCl_3$, 100 MHz) δ 160.2, 149.6, 142.4, 136.9, 133.1, 131.9, 130.9, 130.8, 130.3, 129.7, 128.5, 127.7, 121.3, 120.7, 120.5 (q, *J* = 258.2 Hz), 118.7, 113.4, 52.5. ^{19}F NMR ($CDCl_3$, 376 MHz) δ -57.7. HRMS (ESI–TOF): *m/z* calcd for $C_{22}H_{14}F_3NNaO_5$ $[M+Na]^+$ 452.0716; found 452.0717.

Methyl 1-oxo-7-phenyl-4-[4-(trifluoromethyl)phenyl]-1*H*-pyrrolo[1,2-*c*][1,3]oxazine-3-carboxylate (6j)



Compound **6j** (66 mg, 50%) was prepared according to method *A* from pyrrole **2j** (100 mg, 0.32 mmol) and dimethyl diazomalonate (**3a**) (125 mg, 0.79 mmol) using petroleum ether/EtOAc (6:1) as eluent for column chromatography. Light pink solid, mp 166–167 °C (from Et_2O) ^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.76 (2H, d, *J* = 8.0 Hz), 7.56–7.47 (4H, m), 7.45–7.41 (3H, m), 6.65 (1H, d, *J* = 3.8 Hz), 6.22 (1H, d, *J* = 3.8 Hz), 3.75 (3H, s). ^{13}C{^{1}H} NMR ($CDCl_3$, 100 MHz) δ 160.2, 142.3, 137.0, 135.6, 133.0, 131.6, 131.2, 130.9, 129.8, 129.6, 128.6, 127.7, 125.4 (q, *J* = 3.9 Hz), 121.3, 118.7, 113.4, 52.5. ^{19}F NMR ($CDCl_3$, 376 MHz) δ -62.7. HRMS (ESI–TOF): *m/z* calcd for $C_{22}H_{15}F_3NO_4$ $[M+H]^+$ 414.0948; found 414.0961.

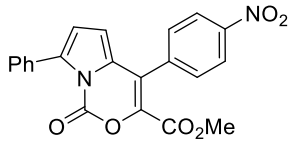
Methyl 4-(3-nitrophenyl)-1-oxo-7-phenyl-1*H*-pyrrolo[1,2-*c*][1,3]oxazine-3-carboxylate (6k)



Compound **6k** (68 mg, 51%) was prepared according to method *A* from pyrrole **2k** (100 mg, 0.34 mmol) and dimethyl diazomalonate (**3a**) (108 mg, 0.68 mmol) using petroleum ether/EtOAc (5:1) as eluent for column chromatography. Gray solid, mp 59–60 °C (from Et_2O). ^{1}H NMR ($CDCl_3$, 400 MHz) δ 8.37 (1H, ddd, *J* = 8.0, 2.2, 1.4 Hz), 8.29 (1H, t, *J* =1.9 Hz), 7.74 (1H, dt, *J* = 7.7, 1.4 Hz), 7.69 (1H, t, *J* = 7.7 Hz), 7.53–7.46 (2H, m), 7.46–7.39 (3H, m), 6.66 (1H, d, *J* = 3.8 Hz), 6.22 (1H, d, *J* = 3.8 Hz), 3.76 (3H, s). ^{13}C{^{1}H} NMR ($CDCl_3$, 100 MHz) δ 160.0, 148.2, 142.1, 137.3, 135.4, 133.5, 133.3, 131.3, 130.7, 129.8, 129.4, 128.6, 127.7, 124.4, 123.9, 120.3,

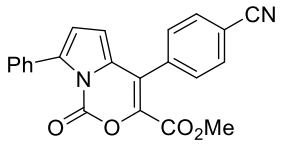
118.8, 113.3, 52.7. HRMS (ESI–TOF): *m/z* calcd for $C_{21}H_{14}N_2NaO_6$ $[M+Na]^+$ 413.0744; found 413.0740.

Methyl 4-(4-nitrophenyl)-1-oxo-7-phenyl-1*H*-pyrrolo[1,2-*c*][1,3]oxazine-3-carboxylate (6l)



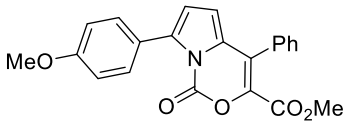
Compound **6l** (62 mg, 46%) was prepared according to method *A* from pyrrole **2l** (100 mg, 0.34 mmol) and dimethyl diazomalonate (**3a**) (108 mg, 0.68 mmol) using petroleum ether/EtOAc (5:1) as eluent for column chromatography. Pink solid, mp 164–167 °C (from Et_2O). ^{1}H NMR ($CDCl_3$, 400 MHz) δ 8.39–8.31 (2H, m), 7.63–7.55 (2H, m), 7.53–7.47 (2H, m), 7.43 (3H, dt, *J* = 4.7, 2.9 Hz), 6.66 (1H, d, *J* = 3.8 Hz), 6.21 (1H, d, *J* = 3.8 Hz), 3.75 (3H, s). ^{13}C{^{1}H} NMR ($CDCl_3$, 100 MHz) δ 160.0, 148.1, 142.1, 138.6, 137.2, 132.9, 131.0, 130.7, 130.3, 129.7, 128.6, 127.7, 123.6, 120.6, 118.8, 113.3, 52.6. HRMS (ESI–TOF): *m/z* calcd for $C_{21}H_{15}N_2O_6$ $[M+H]^+$ 391.0925; found 391.0940.

Methyl 4-(4-cyanophenyl)-1-oxo-7-phenyl-1*H*-pyrrolo[1,2-*c*][1,3]oxazine-3-carboxylate (6m)



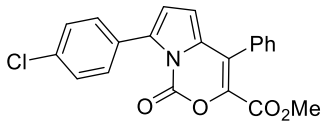
Compound **6m** (63 mg, 46%) was prepared according to method *A* from of pyrrole **2m** (100 mg, 0.37 mmol) and dimethyl diazomalonate (**3a**) (128 mg, 0.91 mmol) using petroleum ether/EtOAc (5:1) as eluent for column chromatography. Light pink solid, mp 193–196 °C (from Et_2O). ^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.82–7.76 (2H, m), 7.54–7.46 (4H, m), 7.45–7.40 (3H, m), 6.65 (1H, d, *J* = 3.8 Hz), 6.20 (1H, d, *J* = 3.8 Hz), 3.75 (3H, s). ^{13}C{^{1}H} NMR ($CDCl_3$, 100 MHz) δ 160.0, 142.1, 137.1, 136.7, 132.9, 132.2, 131.2, 130.7, 130.0, 129.7, 128.6, 127.7, 120.9, 118.7, 118.3, 113.3, 112.9, 52.6. HRMS (ESI–TOF): *m/z* calcd for $C_{22}H_{14}N_2NaO_4$ $[M+Na]^+$ 393.0846; found 393.0855.

Methyl 7-(4-methoxyphenyl)-1-oxo-4-phenyl-1*H*-pyrrolo[1,2-*c*][1,3]oxazine-3-carboxylate (6n)



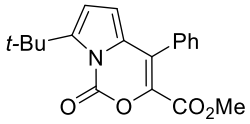
Compound **6n** (72 mg, 53%) was prepared according to method *A* from pyrrole **2n** (100 mg, 0.36 mmol) and dimethyl diazomalonate (**3a**) (143 mg, 0.91 mmol) using petroleum ether/EtOAc (6:1) as eluent for column chromatography. Light pink solid, mp 168–169 °C (from Et_2O). ^1H NMR ($CDCl_3$, 400 MHz) δ 7.51–7.46 (3H, m), 7.43 (2H, d *J* = 8.7 Hz), 7.39–7.36 (2H, m), 6.95 (2H, d *J* = 8.7 Hz),, 6.57 (1H, d, *J* = 3.8 Hz), 6.24 (1H, d, *J* = 3.8 Hz), 3.86 (3H, s), 3.72 (3H, s). $^{13}C\{^1H\}$ NMR ($CDCl_3$, 100 MHz) δ 160.4, 159.8, 142.7, 136.6, 132.7, 131.9, 131.8, 131.1, 129.0, 128.8, 128.3, 123.5, 122.6, 118.0, 113.4, 113.2, 55.3, 52.3. HRMS (ESI–TOF): *m/z* calcd for $C_{22}H_{17}NNaO_5$ $[M+Na]^+$ 398.0999; found 398.0994.

Methyl 7-(4-chlorophenyl)-1-oxo-4-phenyl-1*H*-pyrrolo[1,2-*c*][1,3]oxazine-3-carboxylate (6o)



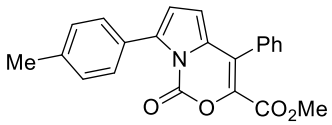
Compound **6o** (83 mg, 62%) was prepared according to method *A* from pyrrole **2o** (100 mg, 0.36 mmol) and dimethyl diazomalonate (**3a**) (140 mg, 0.89 mmol) using petroleum ether/EtOAc (6:1) as eluent for column chromatography. Light pink solid, mp 166–167 °C (from Et_2O). ^1H NMR ($CDCl_3$, 400 MHz): δ 7.54–7.46 (3H, m), 7.45–7.33 (6H, m), 6.62 (1H, d, *J* = 3.7 Hz), 6.26 (1H, d, *J* = 3.7 Hz), 3.73 (3H, s). $^{13}C\{^1H\}$ NMR ($CDCl_3$, 100 MHz): δ 160.3, 142.6, 135.2, 134.6, 133.1, 132.5, 131.5, 131.0, 129.5, 129.0, 128.9, 128.4, 127.9, 122.5, 118.8, 113.4, 52.4. HRMS (ESI–TOF): *m/z* calcd for $C_{21}H_{14}{}^{35}ClNNaO_4$ $[M+Na]^+$ 402.0504; found 402.0496.

Methyl 7-(*tert*-butyl)-1-oxo-4-phenyl-1*H*-pyrrolo[1,2-*c*][1,3]oxazine-3-carboxylate (6p)



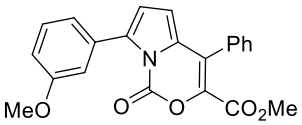
Compound **6p** (52 mg, 34%) was prepared according to method *A* from pyrrole **2p** (108 mg, 0.48 mmol) and dimethyl diazomalonate (**3a**) (150 mg, 0.95 mmol) using petroleum ether/EtOAc (6:1) as eluent for column chromatography. Light pink solid, mp 130–131 °C (from Et_2O). ^1H NMR ($CDCl_3$, 400 MHz) δ 7.49–7.42 (3H, m), 7.35–7.29 (2H, m), 6.45 (1H, d, *J* = 3.9 Hz), 6.05 (1H, d, *J* = 3.9 Hz), 3.71 (3H, s), 1.53 (9H, s). $^{13}C\{^1H\}$ NMR ($CDCl_3$, 100 MHz) δ 160.3, 147.2, 143.0, 132.8, 132.5, 131.9, 129.0, 128.7, 128.2, 122.5, 114.7, 112.7, 52.3, 33.9, 30.4. HRMS (ESI–TOF): *m/z* calcd for $C_{19}H_{19}NNaO_4$ $[M+Na]^+$ 348.1206; found 348.1221.

Methyl 7-(4-methylphenyl)-1-oxo-4-phenyl-1*H*-pyrrolo[1,2-*c*][1,3]oxazine-3-carboxylate (6q)



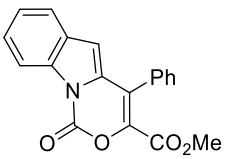
Compound **6q** (80 mg, 58%) was prepared according to method *A* from pyrrole **2q** (100 mg, 0.38 mmol) and dimethyl diazomalonate (**3a**) (119 mg, 0.75 mmol) using petroleum ether/EtOAc (6:1) as eluent for column chromatography. Light pink solid, mp 157–160 °C (from Et_2O). ^1H NMR ($CDCl_3$, 400 MHz) δ 7.52–7.46 (3H, m), 7.43–7.36 (4H, m), 7.26–7.21 (2H, m), 6.61–6.60 (1H, m), 6.27–6.25 (1H, m), 3.73 (3H, s), 2.42 (3H, s). $^{13}C\{^1H\}$ NMR ($CDCl_3$, 100 MHz) δ 160.4, 142.6, 138.4, 136.7, 132.8, 132.1, 131.8, 129.6, 129.0, 128.8, 128.4, 128.3, 128.2, 122.6, 118.3, 113.4, 52.3, 21.3. HRMS (ESI–TOF): *m/z* calcd for $C_{22}H_{17}NNaO_4$ $[M+Na]^+$ 382.1050; found 382.1058.

Methyl 7-(3-methoxyphenyl)-1-oxo-4-phenyl-1*H*-pyrrolo[1,2-*c*][1,3]oxazine-3-carboxylate (6r)



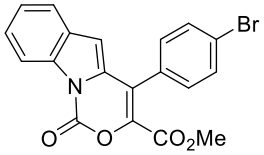
Compound **6r** (73 mg, 54%) was prepared according to method *A* from pyrrole **1r** (100 mg, 0.36 mmol) and dimethyl diazomalonate (**3a**) (143 mg, 0.91 mmol) using petroleum ether/EtOAc (6:1) as eluent for column chromatography. Light pink solid, mp 119–121 °C (from Et_2O). ^1H NMR ($CDCl_3$, 400 MHz) δ 7.52–7.46 (3H, m), 7.41–7.36 (2H, m), 7.35–730 (1H, m), 7.11–7.06 (1H, m), 7.05–7.02 (1H, m), 6.96 (1H, dd, *J* = 8.2, 2.4 Hz), 6.63 (1H, d, *J* = 3.8 Hz), 6.26 (1H, d, *J* = 3.8 Hz), 3.85 (3H, s), 3.73 (3H, s). $^{13}C\{^1H\}$ NMR ($CDCl_3$, 100 MHz) δ 160.4, 158.8, 142.5, 136.3, 133.0, 132.4, 132.3, 131.7, 129.0, 128.9, 128.7, 128.3, 122.5, 122.3, 118.7, 115.4, 114.3, 113.3, 55.3, 52.4. HRMS (ESI–TOF): *m/z* calcd for $C_{22}H_{17}NNaO_5$ $[M+Na]^+$ 398.0999; found 398.1016.

Methyl 1-oxo-4-phenyl-1*H*-[1,3]oxazino[3,4-*a*]indole-3-carboxylate (6s)



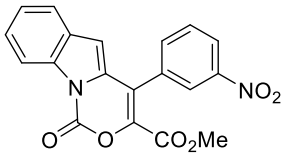
Compound **6s** (53 mg, 37%) was prepared according to method *B* from indole **2s** (100 mg, 0.452 mmol) and dimethyl diazomalonate (**3a**) (220 mg, 2.72 mmol) using petroleum ether/EtOAc (6:1) as eluent for column chromatography. Colorless solid, mp 138–139 °C (from Et_2O). ^1H NMR ($CDCl_3$, 400 MHz) δ 8.51 (1H, d, *J* = 8.2 Hz), 7.60 (1H, d, *J* = 7.8 Hz), 7.55–7.46 (4H, m), 7.44–7.35 (3H, m), 6.49 (1H, s), 3.76 (3H, s). $^{13}C\{^1H\}$ NMR ($CDCl_3$, 100 MHz) δ 160.2, 143.1, 135.3, 134.2, 134.0, 131.5, 130.1, 130.0, 129.0, 128.9, 128.5, 126.1, 125.1, 121.9, 121.2, 115.8, 108.3, 52.6. HRMS (ESI–TOF): *m/z* calcd for $C_{19}H_{13}NNaO_4$ $[M+Na]^+$ 342.0737; found 342.0748.

Methyl 4-(4-bromophenyl)-1-oxo-1*H*-[1,3]oxazino[3,4-*a*]indole-3-carboxylate (6t)



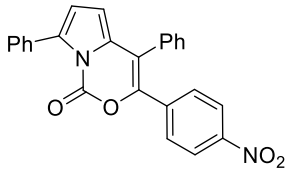
Compound **6t** (71 mg, 53%) was prepared according to method *A* from indole **2t** (100 mg, 0.33 mmol) and dimethyl diazomalonate (**3a**) (988 mg, 6.25 mmol) using petroleum ether/EtOAc (6:1) as eluent for column chromatography. Colorless solid, mp 179–182 °C (from Et_2O). ^1H NMR ($CDCl_3$, 400 MHz) δ 8.53–8.48 (1H, m), 7.68–7.58 (3H, m), 7.54–7.49 (1H, m), 7.44–7.39 (1H, m), 7.31–7.27 (2H, m), 6.48 (1H, s), 3.78 (3H, s). $^{13}C\{^1H\}$ NMR ($CDCl_3$, 100 MHz) δ 160.1, 142.9, 135.4, 134.2, 133.6, 131.8, 130.7, 130.5, 130.0, 126.4, 125.3, 123.4, 121.3, 120.9, 115.9, 108.3, 52.7. HRMS (ESI–TOF): *m/z* calcd for $C_{19}H_{12}{}^{79}BrNNaO_4$ $[M+Na]^+$ 419.9842; found 419.9843.

Methyl 4-(3-nitrophenyl)-1-oxo-1*H*-[1,3]oxazino[3,4-a]indole-3-carboxylate (6u)



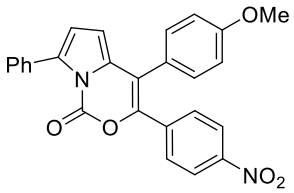
Compound **6u** (34 mg, 25%) was prepared according to method *B* from indol **2u** (100 mg, 0.38 mmol) and dimethyl diazomalonate (**3a**) (283 mg, 1.79 mmol) using petroleum ether/EtOAc (6:1) as eluent for column chromatography. Colorless solid, mp 190–193 °C (from Et_2O/hexane). ^1H NMR ($CDCl_3$, 400 MHz) δ 8.52 (1H, d, *J* = 8.3 Hz), 8.38 (1H, dt, *J* = 8.0, 1.8 Hz), 8.31 (1H, t, *J* = 2.0 Hz), 7.77–7.69 (2H, m), 7.62 (1H, d, *J* = 7.9 Hz), 7.54–7.49 (1H, m), 7.47–7.41 (1H, m), 6.45 (1H, s), 3.79 (3H, s). $^{13}C\{^1H\}$ NMR ($CDCl_3$, 100 MHz) δ 159.9, 148.3, 142.6, 135.8, 135.3, 134.3, 133.3, 130.1, 129.9, 129.6, 126.7, 125.5, 124.3, 124.0, 121.4, 119.8, 115.9, 108.4, 52.9. HRMS (ESI–TOF): *m/z* calcd for $C_{19}H_{12}N_2NaO_6$ $[M+Na]^+$ 387.0588; found 387.0600.

3-(4-Nitrophenyl)-4,7-diphenyl-1*H*-pyrrolo[1,2-*c*][1,3]oxazin-1-one (6v)



Compound **6v** (32 mg, 32%) was prepared according to method *B* from pyrrole **2a** (60 mg, 0.24 mmol) and diazo compound **3b** (126 mg, 0.57 mmol) using petroleum ether/EtOAc (5:1) as eluent for column chromatography. Orange glassy solid. ^{1}H NMR ($CDCl_3$, 400 MHz) δ 8.09–8.01 (2H, m), 7.56–7.35 (12H, m), 6.63 (1H, d, *J* = 3.7 Hz), 6.23 (1H, d, *J* = 3.7 Hz). ^{13}C{^{1}H} NMR ($CDCl_3$, 100 MHz) δ 147.1, 143.4, 141.1, 137.5, 134.9, 133.1, 132.3, 131.4, 129.9, 129.7, 129.5, 129.3, 128.8, 128.1, 127.6, 123.3, 118.4, 115.3, 110.3. HRMS (ESI–TOF): *m/z* calcd for $C_{25}H_{16}N_2NaO_4$ $[M+Na]^+$ 431.1008; found 431.1002.

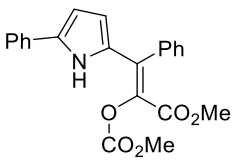
4-(4-Methoxyphenyl)-3-(4-nitrophenyl)-7-phenyl-1*H*-pyrrolo[1,2-*c*][1,3]oxazin-1-one (6w)



Compound **6w** (62 mg, 65%) was prepared according to method *B* from pyrrole **2g** (60 mg, 0.22 mmol) and diazo compound **3b** (113 mg, 0.51 mmol) using petroleum ether/EtOAc (6:1) as eluent for column chromatography. Red solid, mp 181–183 °C (from Et_2O). ^{1}H NMR ($CDCl_3$, 400 MHz) δ 8.09–8.04 (2H, m), 7.54–7.48 (4H, m), 7.46–7.38 (3H, m), 7.31–7.27 (2H, m), 7.03–6.98 (2H, m), 6.63 (1H, d, *J* = 3.8 Hz), 6.26 (1H, d, *J* = 3.8 Hz), 3.89 (3H, s). ^{13}C{^{1}H} NMR ($CDCl_3$, 100 MHz) δ 160.3, 147.0, 143.5, 141.1, 137.7, 134.9, 133.4, 131.5, 131.1, 129.6, 128.8, 128.1, 127.6, 124.1, 123.3, 118.3, 115.01, 114.97, 110.3, 55.3. HRMS (ESI–TOF): *m/z* calcd for $C_{26}H_{18}N_2NaO_5$ $[M+Na]^+$ 461.1108; found 461.1124.

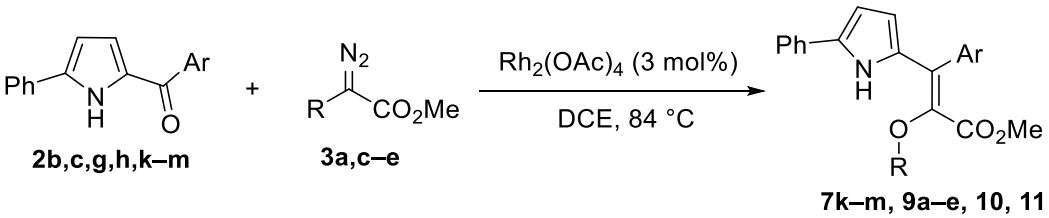
7. Synthesis of cinnamates 7–11

Synthesis of methyl (*Z*)-2-[(methoxycarbonyl)oxy]-3-phenyl-3-(5-phenyl-1*H*-pyrrol-2-yl)acrylate (7a)



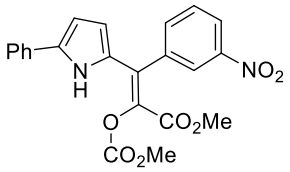
Compound **7a** (45 mg) was obtained as a mixture (4 : 1 molar ratio) with compound **6a** after heating under reflux of compound **6a** (60 mg, 0.17 mmol) in MeOH (5 mL) for 1 h. Colorless solid. ^{1}H NMR ($CDCl_3$, 400 MHz) δ 9.29 (1H, br.s), 7.51–7.28 (10H, m), 6.55 (1H, br.s), 6.20 (1H, br.s), 4.01 (3H, s), 3.57 (3H, s). $^{13}C\{^{1}H\}$ NMR ($CDCl_3$, 100 MHz) δ 162.7, 153.2, 136.6, 135.6, 133.1, 131.4, 129.7, 129.3, 129.2, 129.1, 128.2, 127.9, 127.5, 124.2, 119.9, 108.2, 56.1, 51.9. HRMS (ESI–TOF): *m/z* calcd for $C_{22}H_{20}NO_5^+$ $[M+H]^+$ 378.1336; found 378.1334.

Synthesis of cinnamates 7k−l, 9, 10, 11



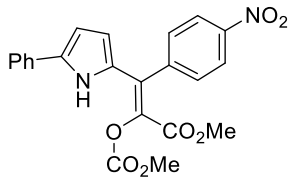
General procedure. A 0.3 M solution of diazoester **3** (2–2.5 equiv) in DCE was added dropwise (0.5 mL/h) via a syringe pump to a 0.1 M solution of pyrrole **2** (0.15–0.45 mmol) and $Rh_2(OAc)_4$ (0.0015–0.0045 mmol) in DCE at 84 °C. After the reaction was complieted (control by TLC, hexane/EtOAc 5:1), the solvent was removed under reduced pressure, and the product was isolated by column chromatography on silica gel.

Methyl (*Z*)-2-[(methoxycarbonyl)oxy]-3-(3-nitrophenyl)-3-(5-phenyl-1*H*-pyrrol-2-yl)acrylate (7k)



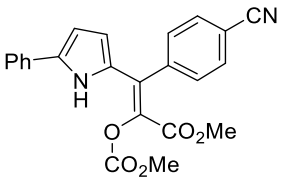
Compound **7k** (94 mg, 65%) was obtained according to the general procedure from pyrrole **1k** (100 mg, 0.34 mmol) and dimethyl diazomalonate (**3a**) (131 mg, 0.83 mmol) using petroleum ether/EtOAc (6:1) as eluent for chromatography. Yellow solid, mp 137–138 °C (from Et_2O). ^{1}H NMR ($CDCl_3$, 400 MHz) δ 9.58 (1H, br.s), 8.31 (1H, ddd, *J* 8.2, 2.3, 1.2 Hz), 8.22 (1H, t, *J* = 1.9 Hz), 7.69 (1H, dt, *J* = 7.6, 1.4 Hz), 7.61 (1H, t, *J* = 7.9 Hz), 7.55–7.48 (2H, m), 7.43 (2H, dd, *J* = 8.5, 6.9 Hz), 7.35–7.31 (1H, m), 6.53 (1H, dd, *J* = 4.0, 2.6 Hz), 5.92 (1H, dd, *J* = 4.0, 2.6 Hz), 4.01 (3H, s), 3.60 (3H, s). $^{13}C\{^{1}H\}$ NMR ($CDCl_3$, 100 MHz) δ 162.2, 152.9, 147.9, 137.8, 137.5, 135.6, 131.1, 130.9, 129.6, 129.2, 128.8, 128.7, 127.9, 124.5, 124.3, 123.2, 120.6, 108.3, 56.3, 52.2. HRMS (ESI–TOF): *m/z* calcd for $C_{22}H_{19}N_2O_7$ $[M+H]^+$ 423.1187; found 423.1186.

Methyl (*Z*)-2-[(methoxycarbonyl)oxy]-3-(4-nitrophenyl)-3-(5-phenyl-1*H*-pyrrol-2-yl)acrylate (7l)



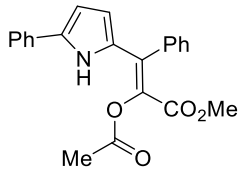
Compound **7l** (70 mg, 48%) was prepared according to the general procedure from pyrrole **2l** (100 mg, 0.34 mmol) and dimethyl diazomalonate (**3a**) (108 mg, 0.68 mmol) using petroleum ether/EtOAc (6:1) as eluent for column chromatography. Yellow solid, mp 158–160 °C (from Et_2O). ^{1}H NMR ($CDCl_3$, 400 MHz) δ 9.54 (1H, br.s), 8.34–8.26 (2H, m), 7.55–7.49 (4H, m), 7.43 (2H, t, *J* = 7.7 Hz), 7.36–7.28 (1H, m), 6.53 (1H, dd, *J* = 4.0, 2.5 Hz), 5.93 (1H, dd, *J* = 4.0, 2.5 Hz), 4.01 (3H, s), 3.58 (3H, s). ^{13}C{^{1}H} NMR ($CDCl_3$, 100 MHz) δ 162.2, 152.9, 147.7, 142.8, 137.7, 131.3, 131.0, 130.4, 129.2, 128.3, 127.9, 124.3, 123.2, 120.5, 108.3, 56.3, 52.2. HRMS (ESI–TOF): *m/z* calcd for $C_{22}H_{19}N_2O_7$ $[M+H]^+$ 423.1187; found 423.1166.

Methyl (*Z*)-3-(4-cyanophenyl)-2-((methoxycarbonyl)oxy)-3-(5-phenyl-1*H*-pyrrol-2-yl)acrylate (7m)



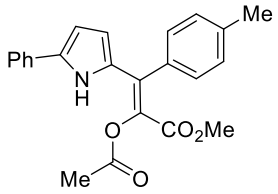
Compound **7m** (24 mg, 20%) was prepared according to the general procedure from pyrrole **2q** (80 mg, 0.29 mmol) and dimethyl diazomalonate (**3a**) (116 mg, 0.74 mmol) using petroleum ether/EtOAc (6:1) as eluent for column chromatography. Colorless solid, mp 137–140 °C (from Et_2O). ^{1}H NMR ($CDCl_3$, 400 MHz) δ 9.51 (br.s), 7.76–7.69 (2H, m), 7.53–7.40 (6H, m), 7.36–7.28 (1H, m), 6.52 (1H, dd, *J* = 4.0, 2.5 Hz), 5.93 (1H, dd, *J* = 4.0, 2.5 Hz), 4.00 (3H, s), 3.58 (3H, s). ^{13}C{^{1}H} NMR ($CDCl_3$, 100 MHz) δ 162.2, 152.9, 140.8, 137.6, 131.7, 131.5, 131.0, 130.1, 129.25, 129.18, 128.4, 127.9, 124.3, 120.4, 118.6, 112.1, 108.2, 56.3, 52.1. HRMS (ESI–TOF): *m/z* calcd for $C_{23}H_{17}N_2O_5$ $[M–H]^–$ 401.1143; found 401.1133.

Methyl (*Z*)-2-acetoxy-3-phenyl-3-(5-phenyl-1*H*-pyrrol-2-yl)acrylate (9a)



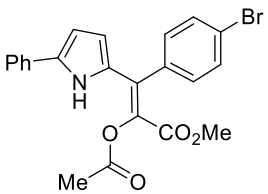
Compound **9a** (85 mg, 58%) was obtained according to the general procedure from pyrrole **2a** (100 mg, 0.41 mmol) and methyl 2-diazo-3-oxobutanoate (**3c**) (379 mg, 2.67 mmol) using petroleum ether/EtOAc (6:1) as eluent for column chromatography. Colorless solid, mp 137–138 °C (Et_2O). ^{1}H NMR ($CDCl_3$, 400 MHz) δ 8.85 (1H, br.s), 7.47–7.42 (3H, m), 7.42–7.32 (7H, m), 6.54 (1H, dd, *J* 3.9, 2.6 Hz), 6.31 (1H, dd, *J* 3.9, 2.5 Hz), 3.50 (3H, s), 2.44 (3H, s). ^{13}C{^{1}H} NMR ($CDCl_3$, 100 MHz) δ 168.5, 163.0, 135.9, 135.7, 132.5, 131.5, 130.2, 129.3, 129.2, 129.1, 128.2, 128.0, 127.3, 124.0, 118.3, 108.3, 51.8, 21.1. HRMS (ESI–TOF): *m/z* calcd for $C_{22}H_{20}NO_4$ $[M+H]^+$ 362.1387; found 362.1392.

Methyl (*Z*)-2-acetoxy-3-(4-methylphenyl)-3-(5-phenyl-1*H*-pyrrol-2-yl)acrylate (9b)



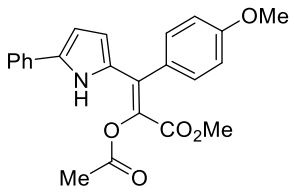
Compound **9b** (6 mg, 12%) was obtained according to the general procedure from pyrrole **2b** (35 mg, 0.13 mmol) and methyl 2-diazo-3-oxobutanoate (**3c**) (114 mg, 0.81 mmol) using petroleum ether/EtOAc (6:1) as eluent for column chromatography. Colorless solid, mp 149–151 °C (from Et_2O). ^{1}H NMR ($CDCl_3$, 400 MHz) δ 8.77 (1H, br.s), 7.41–7.34 (4H, m), 7.24 (5H, d, *J* = 9.1 Hz), 6.54 (1H, dd, *J* = 3.9, 2.6 Hz), 6.35 (1H, dd, *J* = 3.9, 2.5 Hz), 3.53 (3H, s), 2.43 (6H, s). ^{13}C{^{1}H} NMR ($CDCl_3$, 100 MHz) δ 168.7, 163.1, 138.1, 135.6, 132.78, 132.77, 131.6, 130.2, 129.5, 129.2, 129.1, 128.9, 127.4, 124.1, 118.2, 108.4, 51.9, 21.4, 21.1. HRMS (ESI–TOF): calcd for $C_{23}H_{21}NNaO_4$ $[M+Na]^+$ 398.1363; found 398.1368.

Methyl (*Z*)-2-acetoxy-3-(4-bromophenyl)-3-(5-phenyl-1*H*-pyrrol-2-yl)acrylate (9c)



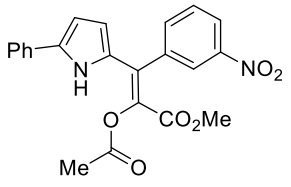
Compound **9c** (63 mg, 31%) was obtained according to the general procedure from pyrrole **2f** (150 mg, 0.46 mmol) and methyl 2-diazo-3-oxobutanoate (**3c**) (393 mg, 2.77 mmol) using petroleum ether/EtOAc (6:1) as eluent for column chromatography. Colorless solid, mp 122–124 °C (from Et_2O). ^{1}H NMR ($CDCl_3$, 400 MHz) δ 8.99 (1H, br.s), 7.59–7.55 (2H, m), 7.44–7.37 (4H, m), 7.31–7.27 (1H, m), 7.25–7.21 (2H, m), 6.53 (1H, dd, *J* = 3.7, 2.8 Hz), 6.20 (1H, dd, *J* = 3.7, 2.7 Hz), 3.54 (3H, s), 2.44 (3H, s). ^{13}C{^{1}H} NMR ($CDCl_3$, 100 MHz) δ 168.4, 162.8, 136.2, 134.9, 131.6, 131.4, 131.2, 131.1, 130.0, 129.2, 129.1, 127.6, 124.1, 122.5, 118.9, 108.3, 52.0, 21.0. HRMS (ESI–TOF): *m/z* calcd for $C_{22}H_{17}BrNO_4$ $[M–H]^-$ 438.0346; found 438.0324.

Methyl (*Z*)-2-acetoxy-3-(4-methoxyphenyl)-3-(5-phenyl-1*H*-pyrrol-2-yl)acrylate (9d)



Compound **9d** (95 mg, 67%) was obtained according to the general procedure from pyrrole **2g** (100 mg, 0.36 mmol) and methyl 2-diazo-3-oxobutanoate (**3c**) (241 mg, 2.10 mmol) using petroleum ether/EtOAc (6:1) as eluent for column chromatography. Colorless solid, mp 149–150 °C (from Et_2O). ^{1}H NMR ($CDCl_3$, 400 MHz) δ 8.79 (1H, br.s), 7.42–7.34 (4H, m), 7.31–7.27 (2H, m), 6.99–6.94 (2H, m), 6.55 (1H, dd, *J* = 3.9, 2.6 Hz), 6.35 (1H, dd, *J* = 3.9, 2.5 Hz), 3.88 (3H, s), 3.54 (3H, s), 2.42 (3H, s). ^{13}C{^{1}H} NMR ($CDCl_3$, 100 MHz) δ 168.7, 163.2, 159.7, 135.5, 132.5, 131.6, 130.7, 130.2, 129.7, 129.1, 127.9, 127.4, 124.1, 118.2, 113.5, 108.4, 55.2, 51.9, 21.1. HRMS (ESI–TOF): *m/z* calcd for $C_{23}H_{21}NNaO_5$ $[M+Na]^+$ 414.1312; found 414.1304.

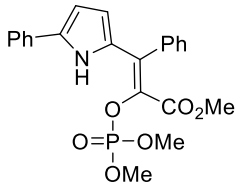
Methyl (*Z*)-2-acetoxy-3-(3-nitrophenyl)-3-(5-phenyl-1*H*-pyrrol-2-yl)acrylate (9e)



Compound **9e** (33 mg, 24%) was obtained according to the general procedure from pyrrole **2k** (50 mg, 0.34 mmol) and methyl 2-diazo-3-oxobutanoate (**3c**) (146 mg, 2.06 mmol) using petroleum ether/EtOAc (6:1) as eluent for column chromatography. Yellow solid, mp 136–138 °C (from Et_2O). ^{1}H NMR ($CDCl_3$, 400 MHz) δ 9.26 (1H, br.s), 8.31 (1H, ddd, *J* = 8.1, 2.3, 1.2 Hz), 8.22 (1H, t, *J* = 1.9 Hz), 7.70 (1H, dt, *J* = 7.6, 1.4 Hz), 7.61 (1H, t, *J* = 7.9 Hz), 7.47–7.37 (4H, m), 7.35-7.28 (1H, m), 6.52 (1H, dd, *J* = 4.0, 2.6 Hz), 5.99 (1H, dd, *J* = 4.0, 2.5 Hz), 3.54

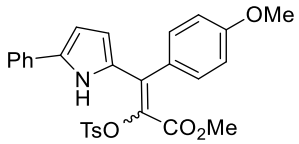
(3H, s), 2.47 (3H, s). $^{13}C\{^{1}H\}$ NMR ($CDCl_3$, 100 MHz) δ 168.2, 162.4, 148.0, 137.8, 137.0, 135.7, 131.3, 130.3, 129.3, 128.9, 128.8, 127.9, 127.6, 124.5, 124.2, 123.2, 119.7, 108.4, 52.2, 21.1. HRMS (ESI–TOF): *m/z* calcd for $C_{22}H_{17}N_2O_6$ $[M–H]^-$ 405.1092; found 405.1085.

Methyl (*Z*)-2-[(dimethoxyphosphoryl)oxy]-3-phenyl-3-(5-phenyl-1*H*-pyrrol-2-yl)acrylate (10)



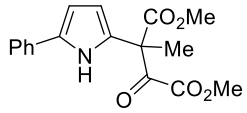
Compound **10** (74 mg, 43%) was prepared according to the general procedure from pyrrole **2a** (100 mg, 0.40 mmol) and methyl 2-diazo-2-(dimethoxyphosphoryl)acetate (**3d**) (253 mg, 1.22 mmol) using petroleum ether/EtOAc (6:1) as eluent for column chromatography. Yellow oil. ^{1}H NMR ($CDCl_3$, 400 MHz) δ 10.68 (1H, br.s), 7.72–7.68 (2H, m), 7.45–7.39 (5H, m), 7.33–7.27 (2H, m), 6.52 (1H, dd, *J* = 4.0, 2.5 Hz), 5.89 (1H, dd, *J* = 4.0, 2.5 Hz), 3.96 (6H, d, *J* = 11.6 Hz), 3.49 (3H, s). $^{13}C\{^{1}H\}$ NMR ($CDCl_3$, 100 MHz) δ 163.9, 137.1, 136.8, 131.9 (d, *J* 6.6 Hz), 131.7, 129.38, 129.37, 129.1 (d, *J* = 1.5 Hz), 128.9, 128.3 (d, *J* = 8.8 Hz), 127.9, 127.6, 127.1, 124.2, 120.1, 107.3, 55.5 (d, *J* = 6.6 Hz), 51.8. HRMS (ESI–TOF): *m/z* calcd for $C_{22}H_{23}NO_6P$ $[M+H]^+$ 428.1258; found 428.1268.

Methyl 3-(4-methoxyphenyl)-3-(5-phenyl-1*H*-pyrrol-2-yl)-2-(tosyloxy)acrylate (11)



Compound **11** (17 mg, 19%) was prepared according to the general procedure from pyrrole **2g** (45 mg, 0.18 mmol) and methyl 2-diazo-2-tosylacetate (**3e**) (112 mg, 0.44 mmol) using petroleum ether/EtOAc (6:1) as eluent for column chromatography. Yellow oil. ^{1}H NMR ($CDCl_3$, 400 MHz) δ 10.11 (1H, br.s), 7.93–7.88 (2H, m), 7.64–7.59 (2H, m), 7.42 (2H, t, *J* = 7.7 Hz), 7.32–7.27 (3H, m), 7.23–7.19 (2H, m), 6.96–6.89 (2H, m), 6.50 (1H, dd, *J* = 4.0, 2.5 Hz), 5.97 (1H, dd, *J* = 3.9, 2.6 Hz), 3.86 (3H, s), 3.40 (3H, s), 2.40 (3H, s). $^{13}C\{^{1}H\}$ NMR ($CDCl_3$, 100 MHz) δ 163.3, 159.7, 145.5, 137.7, 136.0, 133.3, 131.5, 130.8, 129.6, 129.1, 129.0, 128.5, 128.3, 127.5, 127.4, 124.5, 121.4, 113.2, 107.6, 55.2, 51.7, 21.7. HRMS (ESI–TOF): *m/z* calcd for $C_{28}H_{25}NNaO_6S$ $[M+Na]^+$ 526.1295; found 526.1275.

8. Synthesis of compound 8



Dimethyl 2-methyl-3-oxo-2-(5-phenyl-1*H*-pyrrol-2-yl)succinate **8** (71 mg, 41%) was prepared from pyrrole **2v** (100 mg, 0.541 mmol) and dimethyl diazomalonate (**3a**) (171 mg, 1.082 mmol) according to the general procedure for the synthesis of compounds **7** using petroleum ether/EtOAc (6:1) as eluent for column chromatography. Yellow oil. ^{1}H NMR ($CDCl_3$, 400 MHz) δ 9.76 (1H, br.s), 7.52–7.46 (2H, m), 7.41–7.34 (2H, m), 7.24–7.18 (1H, m), 6.43 (1H, dd, *J* = 3.7, 2.8 Hz), 6.05 (1H, dd, *J* = 3.7, 2.6 Hz), 3.83 (3H, s), 3.81 (3H, s), 1.85 (3H, s). ^{13}C{^{1}H} NMR ($CDCl_3$, 100 MHz) δ 184.0, 171.9, 161.1, 133.5, 132.4, 128.9, 126.5, 125.3, 123.9, 110.1, 106.2, 55.7, 53.4, 53.0, 21.9. HRMS (ESI–TOF): calcd for $C_{17}H_{17}NNaO_5$ $[M+Na]^+$ 338.0999; found 338.1010.

9. X-Ray Data

Compound 6l (CCDC 2198285)

Single crystal of compound **6l** was grown by slow evaporation of hexane/$CHCl_3$ solution. A suitable crystal was selected and studied on a diffractometer. The crystal was kept at 99.94(18) K during data collection. Using Olex2,[13] the structure was solved with the SHELXT[14] structure solution program using Intrinsic Phasing and refined with the SHELXL[15] refinement package using Least Squares minimisation.

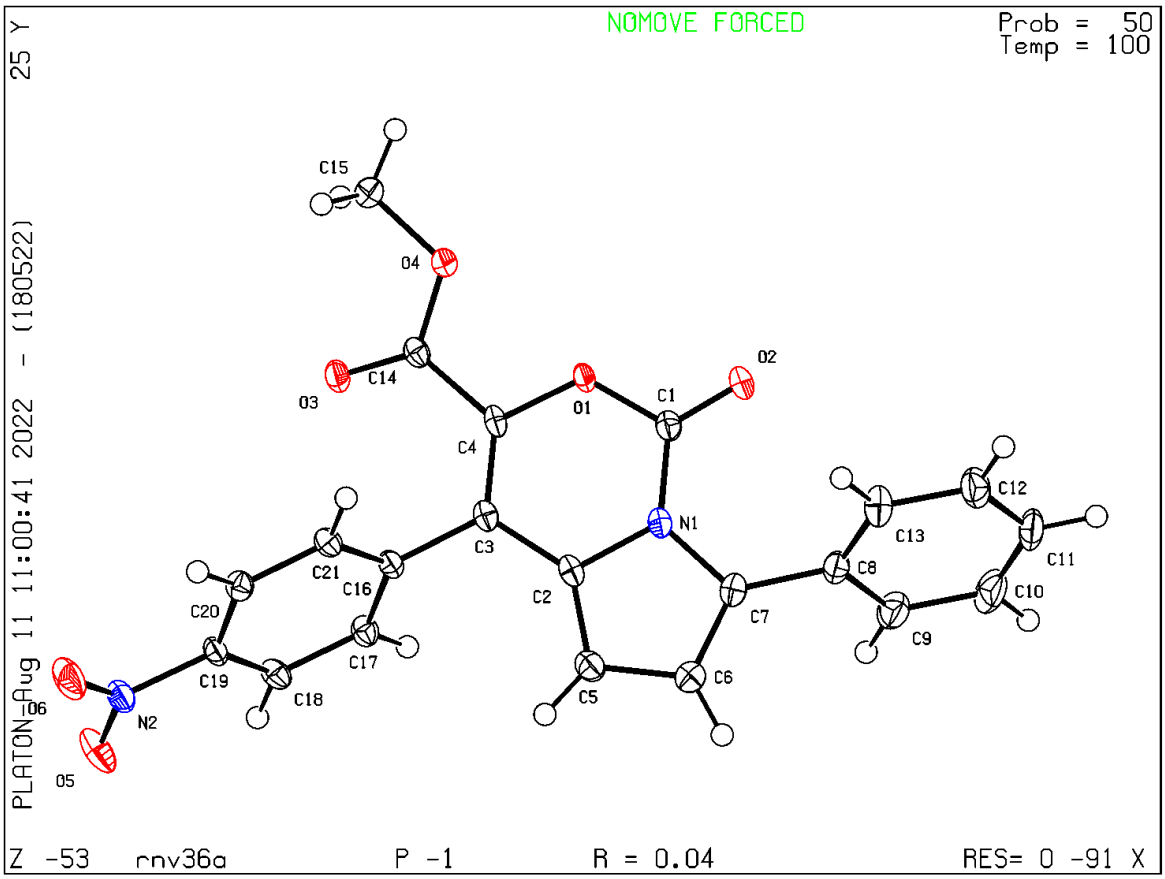


Table S-2. Crystal Data and Structure Refinement for Compound **6l**

Identification code	rnv-36a
Empirical formula	$C_{21}H_{14}N_2O_6$
Formula weight	442.17
Temperature/K	100(2)
Crystal system	triclinic
Space group	P-1 (no. 2)
a/Å	8.1668(3)
b/Å	9.5156(5)
c/Å	12.1149(7)

α/°	101.349(5)
β/°	103.088(4)
γ/°	91.725(4)
Volume/Å^3	896.33(8)
Z	2
ρ_{calc}g/cm^3	1.446
μ(MoKα)/ mm^{-1}	0.108
F(000)	404.0
Crystal size/mm^3	0.34 × 0.22 × 0.14
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	5.5 to 54.998
Index ranges	$-10 \leq h \leq 10$, $-12 \leq k \leq 12$, $-15 \leq l \leq 15$
Reflections collected	14733
Independent reflections	4101 [R_{int} = 0.0280, R_{sigma} = 0.0286]
Data/restraints/parameters	4101/0/263
Goodness-of-fit on F^2	1.022
Final R indexes [I>=2σ (I)]	R_1 = 0.0369, wR_2 = 0.0840
Final R indexes [all data]	R_1 = 0.0453, wR_2 = 0.0901

Compound 7l (CCDC 2172286)

Single crystal of compound **7l** was grown by slow evaporation of hexane/$CHCl_3$ solution. A suitable crystal was selected and studied on a diffractometer. The crystal was kept at 99.94(18) K during data collection. Using Olex2,[13] the structure was solved with the SHELXT[14] structure solution program using Intrinsic Phasing and refined with the SHELXL[15] refinement package using Least Squares minimisation.

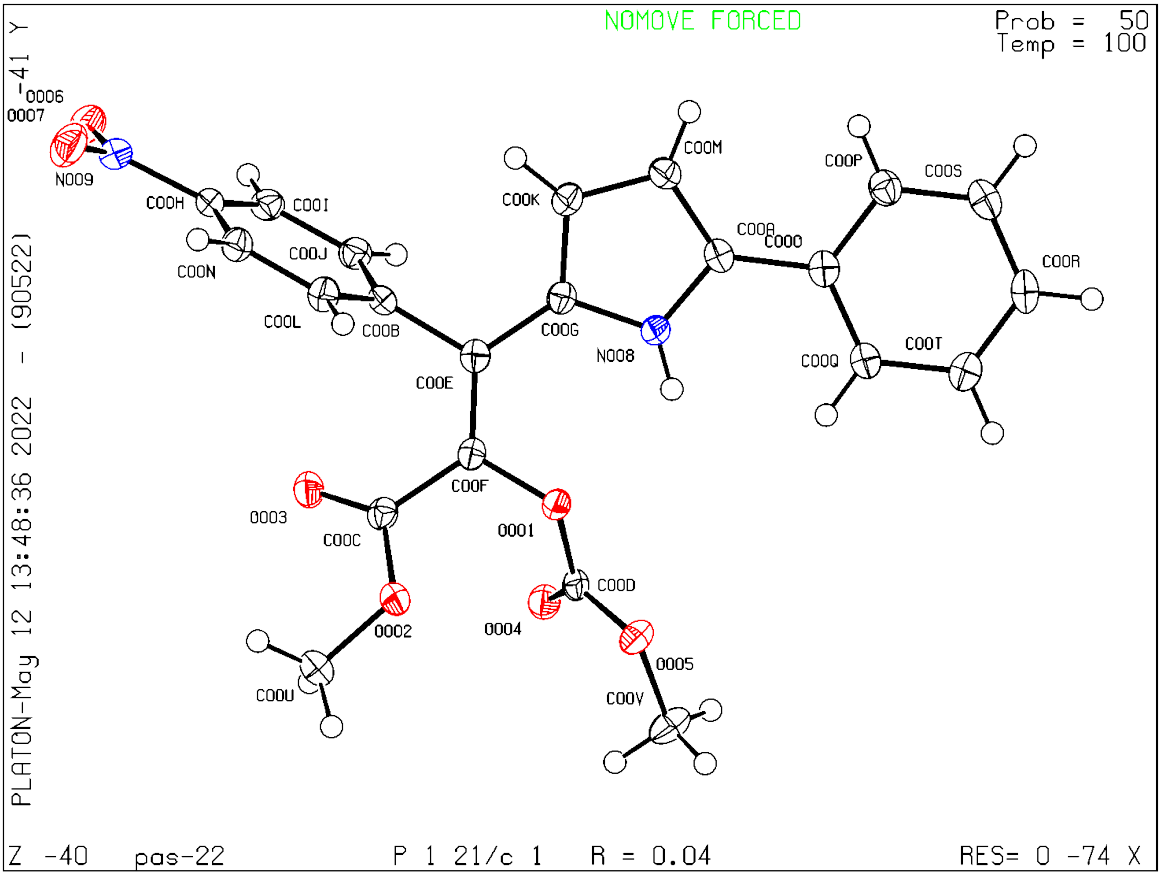


Table S-3. Crystal data and structure refinement for compound **7l**.

Identification code	PAS-22
Empirical formula	$C_{22}H_{18}N_2O_7$
Formula weight	422.38
Temperature/K	99.94(18)
Crystal system	monoclinic
Space group	$P2_1/c$
a/Å	10.4249(3)
b/Å	13.8287(3)
c/Å	13.7118(3)

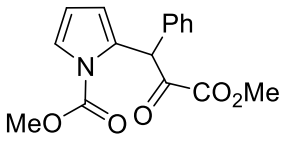
α/°	90
β/°	97.515(2)
γ/°	90
Volume/Å^3	1959.75(8)
Z	4
ρ_{calc}g/cm^3	1.432
μ/mm^{-1}	0.911
F(000)	880.0
Crystal size/mm^3	0.25 × 0.21 × 0.18
Radiation	Cu Kα (λ = 1.54184)
2Θ range for data collection/°	8.556 to 140.982
Index ranges	$-12 \leq h \leq 12$, $-15 \leq k \leq 16$, $-16 \leq l \leq 16$
Reflections collected	12997
Independent reflections	3732 [R_{int} = 0.0387, R_{sigma} = 0.0348]
Data/restraints/parameters	3732/0/282
Goodness-of-fit on F^2	1.046
Final R indexes [I>=2σ (I)]	R_1 = 0.0388, wR_2 = 0.0995
Final R indexes [all data]	R_1 = 0.0449, wR_2 = 0.1035
Largest diff. peak/hole / e Å^{-3}	0.28/-0.23

10. Calculation details

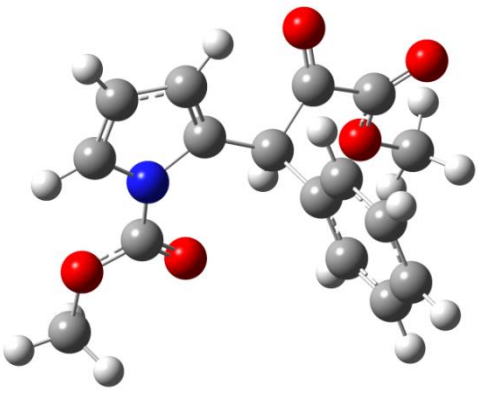
All calculations were performed by using the Gaussian 09 suite of quantum chemical programs.[16] Geometry optimizations of compounds **5x**, **7x**, **12x**, **14−21**, complexes **6x**×**2w**×MeOH, *Z*-**18**×**2w**, **12x**×**2w**, **12x**×**12x**, **7x**×**12x** and transition states TS1−TS14 were performed at the DFT B3LYP/6-31+G(d,p) level using PCM model for 1,2-dichloroethane. 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. The intrinsic reaction coordinate (IRC) calculations were performed to establish the unique connection given between the TSs and the corresponding minima.

Table S-4. Energies (au) and cartesian coordinates of stationary points for compounds **5x**, **7x**, **12x**, **14−21**, complexes **6x**×**2w**×Methanol, *Z*-**18**×**2w**, **12x**×**2w**, **12x**×**12x**, **7x**×**12x** and transition states TS1−TS14 (DFT B3LYP/6-31+G(d,p), PCM for DCE, 357 K).

Compound **5x**

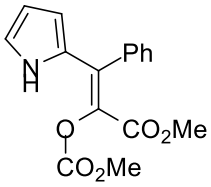


Zero-point correction = 0.286255
Thermal correction to Energy = 0.314789
Thermal correction to Enthalpy = 0.315920
Thermal correction to Gibbs Free Energy = 0.217698
E_0 = -1049.382726, E = -1049.354192,
H = -1049.353061, G = -1049.451282.
Imaginary frequency = 0.

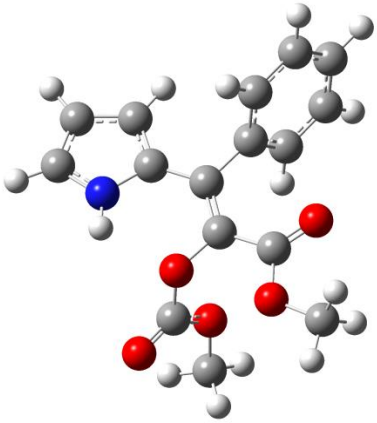


C	-2.35345379	-1.31061864	-2.35262516
C	-2.97104479	-0.79515164	-1.25066616
N	-1.98446779	-0.45499364	-0.31594316

Compound **7x**



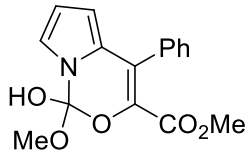
Zero-point correction = 0.286471
Thermal correction to Energy = 0.314764
Thermal correction to Enthalpy = 0.315895
Thermal correction to Gibbs Free Energy = 0.219529
E_0 = -1049,387191, E = -1049,358898,
H = -1049,357767, G = -1049,454133.
Imaginary frequency = 0.



C	1.85272601	3.62104560	0.01788738
C	0.57127701	3.71270460	0.54930938
N	0.06215101	2.45559560	0.65730638

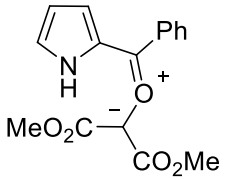
C	-0.71517879	-0.77134364	-0.85906616	C	0.99078701	1.52119760	0.21761338
C	-0.94119579	-1.29311964	-2.10926116	C	2.11947201	2.25097860	-0.18640162
C	0.57423921	-0.44838564	-0.15014716	C	0.80750501	0.08458660	0.20663338
C	1.08550521	0.98327536	-0.42644916	C	2.04706901	-0.69981540	-0.10627062
C	1.33809121	1.40863336	-1.73924916	C	2.22728801	-1.25002840	-1.38254462
C	1.80624321	2.70055736	-1.98773916	C	3.40443801	-1.93282540	-1.69589662
C	2.03017321	3.58309136	-0.92550716	C	4.41043501	-2.07686440	-0.73468462
C	1.78396021	3.16465936	0.38499484	C	4.23678801	-1.52553940	0.53845838
C	1.31797621	1.86982536	0.63375184	C	3.06484501	-0.83009040	0.84837538
O	1.78710121	-2.15911764	-1.41717916	O	-1.51786099	0.24575960	0.71017238
C	1.72701221	-1.39276064	-0.47885216	C	-0.38156499	-0.54638940	0.43885238
C	2.96892921	-1.32049164	0.45411084	C	-0.58818499	-2.00095440	0.60324338
C	-2.26035279	0.05551936	0.95846684	C	-2.54254899	0.31939660	-0.17895662
O	4.10058021	-1.48410464	0.04913684	O	0.26936401	-2.86379040	0.49037238
O	2.62371121	-1.10846564	1.72542684	O	-1.87278399	-2.27889440	0.92161538
C	3.70230621	-1.06601464	2.69573084	C	-2.19116399	-3.67316440	1.11346538
O	-1.42505979	0.25934736	1.82112184	O	-3.56307099	0.90621460	0.10795938
O	-3.57097179	0.28764736	1.10365784	O	-2.26503899	-0.27551140	-1.33526862
C	-3.98473479	0.80082436	2.39214984	C	-3.31536399	-0.24485540	-2.33414762
H	-2.84909779	-1.67137764	-3.24312516	H	2.51135901	4.45110360	-0.19500962
H	-4.01204879	-0.64629164	-1.01944616	H	-0.00582399	4.57322060	0.85551938
H	0.41782921	-0.51874464	0.92647484	H	-0.84070399	2.22005260	1.04188038
H	-0.17136079	-1.63464964	-2.78291416	H	3.02515701	1.82203360	-0.58844962
H	1.15974521	0.73353836	-2.57136516	H	1.44394301	-1.14418940	-2.12724562
H	1.99639121	3.01639436	-3.00929116	H	3.53454301	-2.35321440	-2.68891462
H	2.39277721	4.58835436	-1.11887116	H	5.32375301	-2.61222240	-0.97726362
H	1.95202321	3.84398036	1.21565784	H	5.01419001	-1.63086840	1.28961138
H	1.12322421	1.55045336	1.65243184	H	2.93551801	-0.39589340	1.83547138
H	3.21683521	-0.90122164	3.65533784	H	-3.25247199	-3.69379240	1.35625338
H	4.24302221	-2.01392264	2.69019284	H	-1.99410799	-4.23686440	0.19906038
H	4.38123521	-0.24601864	2.45572784	H	-1.60146299	-4.08711740	1.93403438
H	-5.06440479	0.91449936	2.31505684	H	-2.90628999	-0.77921840	-3.18933462
H	-3.50771079	1.76349936	2.58322384	H	-3.54786299	0.78802860	-2.59760462
H	-3.72612279	0.09135236	3.17996384	H	-4.20552299	-0.74739540	-1.95278262

Compound **12x**

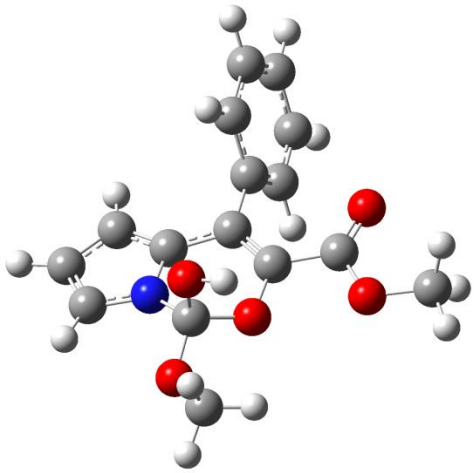


Zero-point correction = 0.286557
Thermal correction to Energy = 0.314082
Thermal correction to Enthalpy = 0.315213
Thermal correction to Gibbs Free Energy = 0.222142
E_0 = -1049.365290, E = -1049.337766,
H = -1049.336635, G = -1049.429706.
Imaginary frequency = 0.

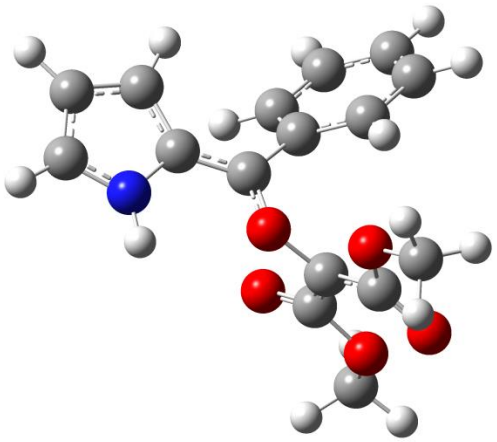
Carbonyl ylide **14**



Zero-point correction = 0.285682
Thermal correction to Energy = 0.314123
Thermal correction to Enthalpy = 0.315254
Thermal correction to Gibbs Free Energy = 0.218456
E_0 = -1049.347524, E = -1049.319083,
H = -1049.317952, G = -1049.414751.
Imaginary frequency = 0.

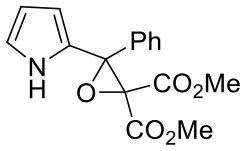


C	1.06362436	-3.51700859	-0.53022766
C	2.15903236	-2.68009559	-0.38944766
N	1.69003736	-1.39363759	-0.30418466
C	0.30186836	-1.38952559	-0.35410066
C	-0.10482164	-2.71297059	-0.50449666
C	-0.40188264	-0.13471059	-0.27426566
C	-1.89024564	-0.18388659	-0.17362066
C	-2.69100764	0.11907441	-1.28443766
C	-4.08119164	0.01743041	-1.20107566
C	-4.68677464	-0.38727359	-0.00665466
C	-3.89336864	-0.69884159	1.10132934
C	-2.50125964	-0.60752459	1.01543234
O	1.72774236	0.92768341	-0.50083566
C	0.34864836	1.00439241	-0.31127366
C	-0.16147164	2.38725841	-0.20014566
C	2.41455136	-0.19359159	0.02804734
O	-1.33051364	2.68649141	-0.00384266
O	0.82133936	3.30191341	-0.33283366
C	0.41321536	4.68352041	-0.23967666
O	2.47969836	-0.09708359	1.42638534
O	3.64499936	-0.27585259	-0.58307266
C	4.61065236	0.73308841	-0.23214366
H	1.10683836	-4.59090859	-0.64585966
H	3.21630436	-2.88977859	-0.34683966
H	2.59464236	0.83317441	1.67563734
H	-1.12770864	-3.04549559	-0.60617866
H	-2.22347164	0.43744841	-2.21142266
H	-4.69065164	0.25537941	-2.06807666
H	-5.76834764	-0.46207759	0.05840434
H	-4.35505664	-1.01684159	2.03162034
H	-1.88679164	-0.85560859	1.87601434
H	1.32706436	5.26105641	-0.37076666
H	-0.30702564	4.92077641	-1.02550266
H	-0.03126364	4.88357041	0.73761334
H	4.89975036	0.64497441	0.81883834
H	4.22303136	1.73358141	-0.44283066
H	5.47489936	0.53530741	-0.86507766

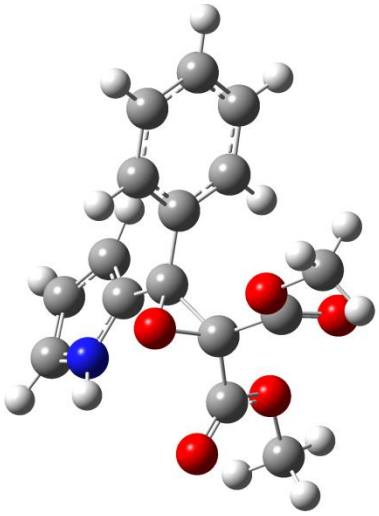


C	-4.08922735	0.84226849	-0.54552957
C	-3.31885235	1.90708349	-0.05220657
N	-2.01769435	1.57158849	-0.12833557
C	-1.89205335	0.29013149	-0.65350857
C	-3.20355935	-0.16877551	-0.92162157
C	-0.63456535	-0.29999751	-0.87470557
C	-0.48619535	-1.70092951	-1.29102157
C	-1.21192135	-2.72251851	-0.65534657
C	-1.10224535	-4.03912351	-1.10461657
C	-0.28034735	-4.34105051	-2.19394357
C	0.44104165	-3.32463751	-2.83328057
C	0.35159765	-2.01114451	-2.38043057
O	0.38427065	0.52723749	-0.77824957
C	1.69594865	0.04486649	-0.47379557
C	2.73281065	0.51251849	-1.32963957
C	1.76646565	-0.66565751	0.76057243
O	3.95062065	0.35863749	-1.18607657
O	2.22643265	1.18119649	-2.42686757
C	3.20174165	1.70806249	-3.33957557
O	0.77540965	-0.93896751	1.45976443
O	3.02308065	-1.04242551	1.12635043
C	3.12676765	-1.75796251	2.36883243
H	-5.16686535	0.82689149	-0.61716457
H	-3.62787935	2.86346749	0.34480243
H	-1.23728835	2.14227249	0.16916443
H	-3.45303335	-1.12134251	-1.36473257
H	-1.82742835	-2.49044451	0.20661043
H	-1.65354135	-4.82679551	-0.60089957
H	-0.19838535	-5.36552251	-2.54422257
H	1.07441065	-3.55745051	-3.68343257
H	0.90394665	-1.22204751	-2.87876157
H	2.62729665	2.20158249	-4.12419857
H	3.85468365	2.42904649	-2.84084457
H	3.81167365	0.90747749	-3.76630157
H	4.18747365	-1.98379151	2.48033043
H	2.54490365	-2.68266751	2.33751043
H	2.78352565	-1.14308351	3.20498043

Oxirane **15**

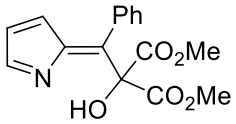


Zero-point correction = 0.285688
Thermal correction to Energy = 0.314081
Thermal correction to Enthalpy = 0.315212
Thermal correction to Gibbs Free Energy = 0.218684
E_0 = -1049.353725, E = -1049.325332,
H = -1049.324201, G = -1049.420729.
Imaginary frequency = 0.

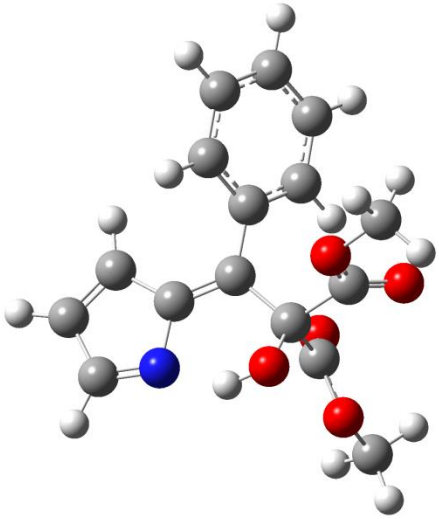


C	2.62925298	2.90714714	0.43309377
C	3.33090998	2.21564414	-0.53923423
N	2.59045998	1.11846214	-0.89395323
C	1.41477698	1.09293314	-0.17345223
C	1.41536498	2.20153014	0.66219077
C	0.41201498	0.01361114	-0.34772423
C	-1.00011302	0.37473114	0.03188877
C	-1.41547302	0.30415014	1.36764277
C	-2.71441402	0.68482314	1.71864577
C	-3.60227102	1.13474614	0.73728377
C	-3.18844802	1.20302214	-0.59765523
C	-1.89054402	0.82690614	-0.94995123
O	0.58203498	-0.76375286	-1.55559323
C	0.82394698	-1.44607486	-0.33427123
C	-0.16931902	-2.52675786	0.06744177
C	2.28132998	-1.81425986	-0.08841623
O	-0.09570902	-3.13745586	1.11743277
O	-1.10234502	-2.71791386	-0.86382423
C	-2.11247702	-3.71297386	-0.56371323
O	3.07644498	-2.00045686	-0.99055923
O	2.55953898	-1.88772286	1.20892377
C	3.91331798	-2.27033886	1.56437777
H	2.94848398	3.81929814	0.91781777
H	4.28088398	2.41981214	-1.01074623
H	2.83624598	0.44897014	-1.61060823
H	0.63132298	2.46648214	1.35666477
H	-0.72915002	-0.04935686	2.13190877

Compound **16**



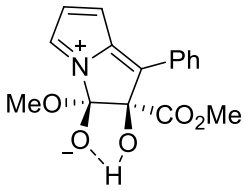
Zero-point correction = 0.285562
Thermal correction to Energy = 0.313799
Thermal correction to Enthalpy = 0.314931
Thermal correction to Gibbs Free Energy = 0.220691
E_0 = -1049.354795, E = -1049.326558,
H = -1049.325427, G = -1049.419666.
Imaginary frequency = 0.



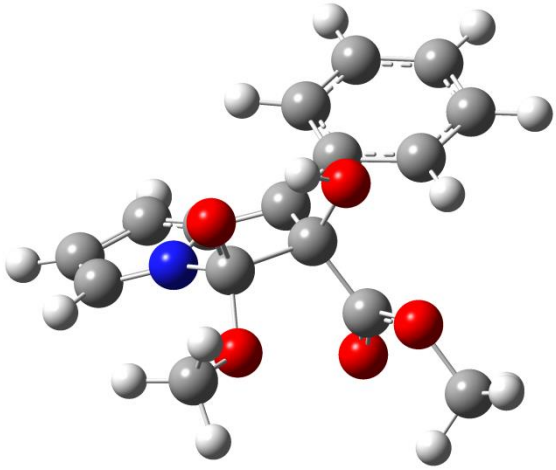
C	-0.98373685	3.42395688	0.04269028
C	-2.13625085	2.71973988	0.58798128
N	-1.96078985	1.42283488	0.63147628
C	-0.65818085	1.18686088	0.12197828
C	-0.05675585	2.46926488	-0.24523372
C	-0.16061785	-0.07650612	-0.02710072
C	1.23270115	-0.30283512	-0.47165772
C	1.53990915	-1.16656612	-1.54142172
C	2.86435415	-1.35412212	-1.93859972
C	3.90469015	-0.70359112	-1.26742672
C	3.61255915	0.14427388	-0.19494072
C	2.28931215	0.34673588	0.19858328
O	-1.84660585	-1.06672412	1.46986728
C	-1.09215685	-1.28029512	0.30070528
C	-0.29014385	-2.58383312	0.56187928
C	-1.99201885	-1.55714612	-0.94363672
O	-0.35640585	-3.56966112	-0.14695172
O	0.44215815	-2.48612512	1.66672528
C	1.21559215	-3.65482612	2.03673728
O	-1.64825685	-1.30784012	-2.08407572
O	-3.15859185	-2.09574912	-0.60361172
C	-4.05880485	-2.42127512	-1.69151372
H	-0.90801685	4.49242588	-0.10943872
H	-3.05977085	3.17431088	0.93217528
H	-2.23006685	-0.15782512	1.38060328
H	0.91575915	2.60475288	-0.69571772
H	0.73793515	-1.65598612	-2.08131272

H	-3.03049502	0.62534614	2.75581777	H	3.08216115	-2.00883212	-2.77708372
H	-4.61183102	1.42803914	1.00957177	H	4.93428415	-0.85920612	-1.57542772
H	-3.87564202	1.54852414	-1.36430323	H	4.41361915	0.64496488	0.34051628
H	-1.56935802	0.87470314	-1.98594123	H	2.07020615	0.98468288	1.04840128
H	-2.77115602	-3.71854486	-1.42992723	H	1.73185315	-3.37557812	2.95307328
H	-1.64487902	-4.68940786	-0.42532723	H	0.54966015	-4.50200112	2.20954828
H	-2.65904902	-3.42985986	0.33759377	H	1.92882215	-3.89454612	1.24619428
H	3.92631898	-2.28749886	2.65218877	H	-4.93993685	-2.84572812	-1.21410172
H	4.62108198	-1.53469986	1.17882077	H	-3.59037685	-3.14763312	-2.35809172
H	4.13904698	-3.25753286	1.15758477	H	-4.31609385	-1.51719412	-2.24626272

Compound *cis*-**17**

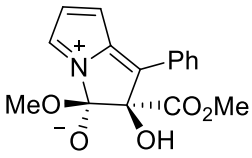


Zero-point correction = 0.285524
Thermal correction to Energy = 0.313015
Thermal correction to Enthalpy = 0.314146
Thermal correction to Gibbs Free Energy = 0.222057
E_0 = -1049.336770, E = -1049.309280,
H = -1049.308149, G = -1049.400238.
Imaginary frequency = 0.

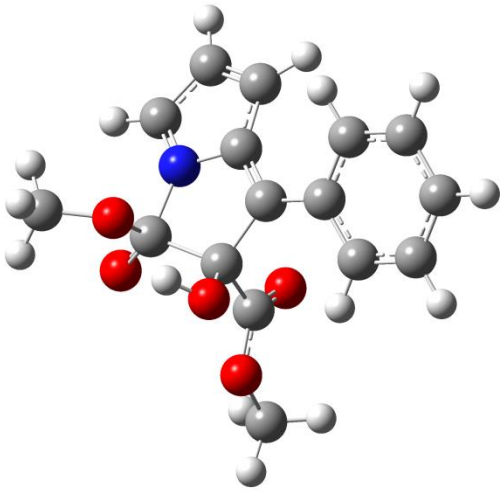


C	0.92057731	-3.23737440	-0.84628147
C	1.93698931	-2.38037740	-0.30616447
N	1.38239931	-1.23685540	0.04779353
C	0.00428131	-1.27681840	-0.19972247
C	-0.27797969	-2.56135540	-0.77769547
C	-0.61279169	-0.09802340	0.15509653
C	-2.03555569	0.17901560	0.19789353
C	-2.50708869	1.51105760	0.26022253
C	-3.87149569	1.78276660	0.27008353
C	-4.79722569	0.73417560	0.23957553
C	-4.34992169	-0.59241040	0.20949153
C	-2.98733569	-0.86850140	0.19297753
O	0.16462831	1.46216160	1.84119053
C	0.44920231	0.92666960	0.58359753
C	0.62664931	1.98720560	-0.50567547
C	1.84578531	0.07203460	0.76715953
O	0.41919831	1.76465060	-1.68761747
O	1.03800531	3.15914360	-0.02017247
C	1.30262631	4.19830960	-0.99083547

Compound *trans*-**17**



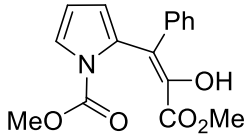
Zero-point correction = 0.285225
Thermal correction to Energy = 0.313023
Thermal correction to Enthalpy 0.314154
Thermal correction to Gibbs Free Energy = 0.221805
E_0 = -1049.332348, E = -1049.304551,
H = -1049.303420, G = -1049.395769.
Imaginary frequency = 0.



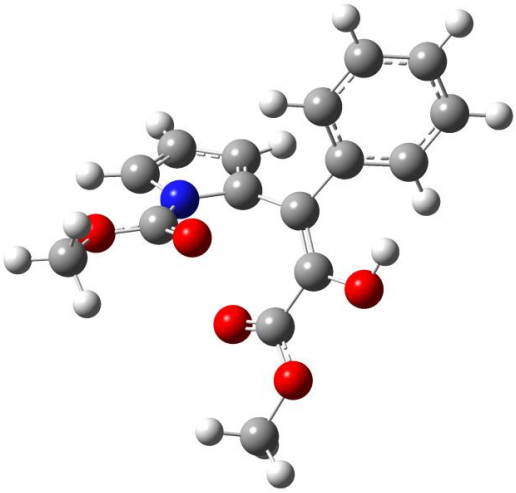
C	1.08006316	-3.58655371	-1.78759157
C	2.05034016	-2.70792671	-1.19302757
N	1.41213616	-1.75775371	-0.54141457
C	0.03077516	-1.93325071	-0.66690957
C	-0.17257984	-3.11582771	-1.45659457
C	-0.66408884	-0.87901571	-0.11927657
C	-2.09871384	-0.77681171	0.05964743
C	-2.72207284	0.48579429	0.18691143
C	-4.10445484	0.58174429	0.31378243
C	-4.89034784	-0.57606671	0.34197843
C	-4.28627784	-1.83575671	0.24682643
C	-2.90598984	-1.93735971	0.10884743
O	0.01809216	0.80965829	1.52218143
C	0.32543216	0.22128729	0.28774743
C	0.41942016	1.27121529	-0.83087657
C	1.80269116	-0.50177171	0.33933043
O	0.30969116	0.99000229	-2.01172257
O	0.66009916	2.49431429	-0.36475357
C	0.84021316	3.53309429	-1.35711557

O	2.12659131	-0.09798940	2.00654253	O	2.82816316	0.11846129	-0.04762257
O	2.83181231	0.65393260	-0.07422147	O	1.79411516	-1.03366071	1.69771343
C	4.19004631	0.49799360	0.35138653	C	3.07787516	-1.39417171	2.21524243
H	1.09085931	-4.23049540	-1.23803647	H	1.31513616	-4.45072271	-2.39341657
H	2.99192631	-2.57881940	-0.17667147	H	3.13045516	-2.75705471	-1.22788957
H	0.84070331	1.00109960	2.41191553	H	0.53332216	0.29750629	2.17561243
H	-1.23584869	-2.90971940	-1.13332747	H	-1.12281484	-3.51282471	-1.78235057
H	-1.80687869	2.33607260	0.29747053	H	-2.12547984	1.38986329	0.17807143
H	-4.21404169	2.81181160	0.30727053	H	-4.57020684	1.55842829	0.39718243
H	-5.86151069	0.94820260	0.25407853	H	-5.96779784	-0.49795271	0.45059543
H	-5.06458769	-1.40914940	0.21281953	H	-4.89134284	-2.73559271	0.29224143
H	-2.65764169	-1.89979540	0.21538953	H	-2.44301784	-2.91697171	0.07673643
H	1.61887331	5.06092360	-0.40682747	H	1.02739816	4.44145929	-0.78728657
H	2.09495931	3.88172260	-1.67204647	H	1.69197716	3.29467429	-1.99651657
H	0.39721931	4.42653560	-1.55663647	H	-0.06233384	3.63533029	-1.96274557
H	4.52777231	-0.54118540	0.25525253	H	3.78680416	-0.56907271	2.11545343
H	4.31788431	0.82240760	1.38648253	H	3.47413116	-2.27823071	1.70041943
H	4.78111831	1.12800260	-0.31551247	H	2.92177016	-1.63253871	3.26899143

Enol *E*-**18**

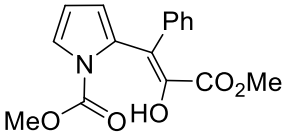


Zero-point correction = 0.286116
Thermal correction to Energy = 0.314597
Thermal correction to Enthalpy = 0.315728
Thermal correction to Gibbs Free Energy = 0.219280
E_0 = -1049.378568, E = -1049.350087,
H = -1049.348956, G = -1049.445405.
Imaginary frequency = 0.

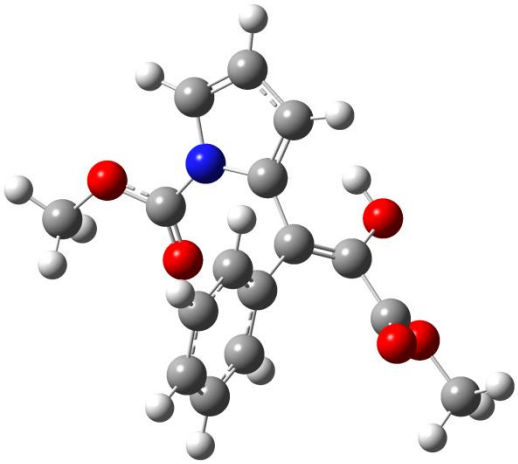


C	-0.17142311	2.86998976	-2.35182937
C	-1.09048211	2.86716676	-1.33931137
N	-0.73792811	1.86607976	-0.42915837
C	0.41893489	1.21229476	-0.89931737
C	0.78041689	1.84091576	-2.06965237
C	1.11787489	0.07501076	-0.26876037
C	2.54866089	0.32083376	0.08684363
C	3.57306089	-0.53895324	-0.35458737
C	4.90850489	-0.28596124	-0.02671737

Enol *Z*-**18**



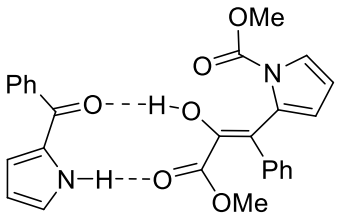
Zero-point correction = 0.286093
Thermal correction to Energy = 0.314629
Thermal correction to Enthalpy = 0.315760
Thermal correction to Gibbs Free Energy = 0.219072
E_0 = -1049.379384, E = -1049.350848,
H = -1049.349717, G = -1049.446404.
Imaginary frequency = 0.



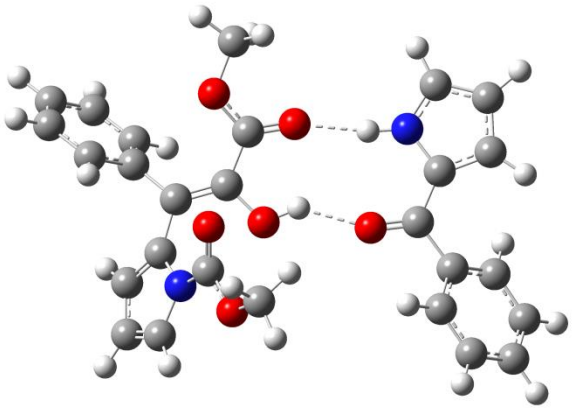
C	-2.09430577	-1.65890316	-1.56567788
C	-2.68798177	-0.97291416	-0.54140988
N	-1.69312777	-0.30271516	0.17169212
C	-0.44340777	-0.56793116	-0.42435888
C	-0.68854477	-1.40462916	-1.49477488
C	0.83052623	0.08528684	-0.05217388
C	0.90659023	1.57023384	-0.14982288
C	0.40002723	2.22027784	-1.28884188
C	0.46155323	3.61094584	-1.40540488

C	5.24322689	0.82695876	0.74881063	C	1.01952623	4.37810284	-0.37817888
C	4.23461289	1.69252176	1.18785763	C	1.50691223	3.74307684	0.76944912
C	2.90255789	1.44583776	0.85546663	C	1.44258023	2.35412584	0.88578512
O	1.18457889	-2.13657424	0.67170263	O	1.77568523	-2.05774616	0.50377912
C	0.55349889	-1.13676624	-0.01454037	C	1.87352723	-0.70801316	0.30404312
C	-0.82428711	-1.52146324	-0.44301637	C	3.28578523	-0.23417816	0.48389612
C	-1.39613911	1.63992576	0.78660963	C	-1.89437777	0.35979584	1.39437412
O	-1.51769611	-0.87540924	-1.21345537	O	3.83331323	0.59329884	-0.22346688
O	-1.21359511	-2.68718724	0.09865563	O	3.89138023	-0.86686616	1.50071912
C	-2.52723711	-3.15444224	-0.27813437	C	5.27901023	-0.53031016	1.72965512
O	-0.97683111	0.92817176	1.67862963	O	-1.00087977	0.66249484	2.15798312
O	-2.54644311	2.32666976	0.83485663	O	-3.19666577	0.59676784	1.59122012
C	-3.29721211	2.21424776	2.06622863	C	-3.54121477	1.22857784	2.84783412
H	-0.17159911	3.53730476	-3.20236137	H	-2.60423477	-2.27476316	-2.29304988
H	-1.94704611	3.49300676	-1.15322537	H	-3.71618677	-0.91550316	-0.22439288
H	2.03972889	-1.81364524	0.99871563	H	0.85063123	-2.32614816	0.36639612
H	1.63149589	1.56295176	-2.67611537	H	0.06681723	-1.75131016	-2.18715188
H	3.32763689	-1.39050024	-0.98317837	H	-0.03050777	1.63088184	-2.09332588
H	5.68473689	-0.95454424	-0.38709437	H	0.07529623	4.09314284	-2.29887588
H	6.28036889	1.02318476	1.00374463	H	1.06531423	5.45969784	-0.46602088
H	4.48644889	2.56164176	1.78848263	H	1.92523023	4.33114484	1.58140912
H	2.12650689	2.12480976	1.19518163	H	1.79107823	1.87297684	1.79417712
H	-2.65562411	-4.09967224	0.24674363	H	5.58854323	-1.15019816	2.56930312
H	-3.28795911	-2.43517124	0.03246463	H	5.87276723	-0.75749816	0.84201912
H	-2.58092411	-3.30297724	-1.35858237	H	5.37469923	0.52897384	1.97664212
H	-2.70017311	2.57461176	2.90589163	H	-4.62551577	1.31985884	2.82862912
H	-3.58985311	1.17641976	2.23405063	H	-3.07175877	2.21141284	2.91303912
H	-4.17405911	2.84226476	1.91954263	H	-3.22024077	0.60319484	3.68265712

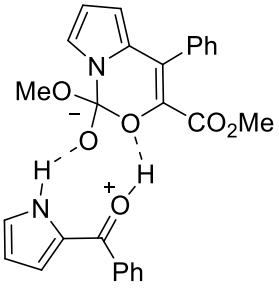
Complex *Z*-**18**×**2w**



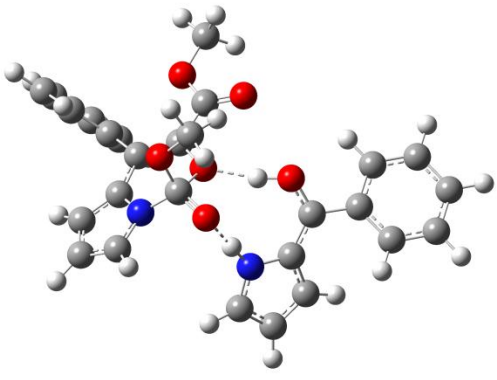
Zero-point correction = 0.460644
Thermal correction to Energy = 0.505933
Thermal correction to Enthalpy = 0.507064
Thermal correction to Gibbs Free Energy = 0.367092
E_0 = -1603.827643, E = -1603.782354,
H = -1603.781223, G = -1603.921195.
Imaginary frequency = 0.



Complex **19**



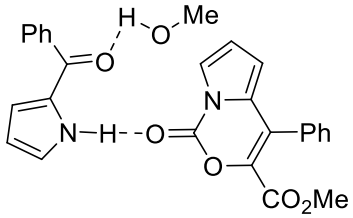
Zero-point correction = 0.459857
Thermal correction to Energy = 0.503339
Thermal correction to Enthalpy = 0.504470
Thermal correction to Gibbs Free Energy = 0.372240
E_0 = -1603.794011, E = -1603.750529,
H = -1603.749398, G = -1603.881628.
Imaginary frequency = 0.



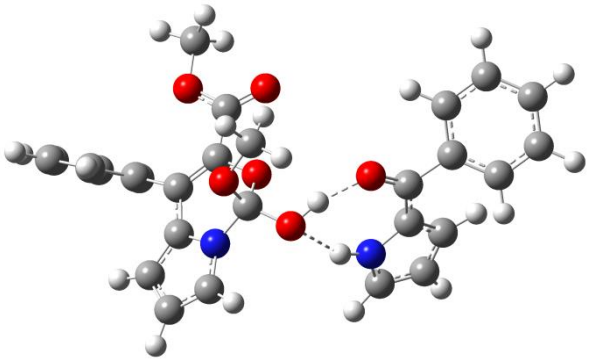
C	2.86813388	1.66694379	-0.60029331
C	3.58264388	2.29066379	-1.60747731
C	3.29702788	3.68743779	-1.57498931
C	2.41979388	3.90290179	-0.54411431
N	2.15089888	2.67813779	0.06631669
C	1.49000088	2.55692179	1.30294769
C	2.76755188	0.22315979	-0.35304731
O	0.42174888	0.37103179	-0.30546531
C	1.55316488	-0.36930321	-0.15287831
O	1.68634088	1.66694279	2.10374969
O	0.64212388	3.57851079	1.47670469
C	4.04511788	-0.53000321	-0.50484431
C	-0.03251512	3.62697179	2.75586969
C	4.19050488	-1.51627421	-1.49484831
C	5.40420388	-2.18740921	-1.66064631
C	6.49499988	-1.87970221	-0.84136531
C	6.36594188	-0.88843021	0.13784669
C	5.15498888	-0.21182321	0.29629469
C	1.29918388	-1.77160621	0.26583769
O	0.16759088	-2.25401321	0.22428969
O	2.35154288	-2.43287221	0.74608669
C	2.12544488	-3.79832821	1.16486769
H	4.21184588	1.77609479	-2.32006831
H	3.69555788	4.44644879	-2.23351431
H	1.98836588	4.81006079	-0.15346731
H	-0.39110112	-0.13450121	-0.09759431
H	-0.65047412	4.52208479	2.71548569
H	-0.65002112	2.73691179	2.88639869
H	0.69779088	3.69781279	3.56412869
H	3.35000088	-1.74901821	-2.14239031
H	5.49949788	-2.94370021	-2.43465031
H	7.43944888	-2.40037921	-0.97037131
H	7.20914288	-0.63936921	0.77578669
H	5.06175788	0.56113079	1.05353269
H	1.39587588	-3.82692021	1.97647369
H	1.76981388	-4.39692521	0.32384769
H	3.09575588	-4.15345121	1.50712869
N	-2.71117612	-2.71626721	0.32070569
H	-1.72741412	-2.46314721	0.24758269
C	-3.19351212	-3.94720821	0.61716069
H	-2.52829412	-4.78213521	0.78507869
C	-4.58689312	-3.88248521	0.64738369
H	-5.25502812	-4.70381921	0.86514669
C	-4.94440212	-2.55260921	0.34918269
H	-5.94485612	-2.14748121	0.31466669
C	-3.75832012	-1.83132121	0.14096969
C	-3.48384312	-0.43109621	-0.12174031
O	-2.32419512	0.01795179	-0.03211931
C	-4.60263112	0.49495279	-0.48212331
C	-5.65950212	0.10817679	-1.32320631
H	-5.68798512	-0.89561021	-1.73277931
C	-4.55407412	1.81638979	-0.00525631
H	-3.72770512	2.11692379	0.63055169
C	-5.55887612	2.72421279	-0.33720431
H	-5.52037912	3.73830579	0.04935569
C	-6.61174812	2.33066879	-1.17186531
H	-7.38997012	3.04019579	-1.43729431
C	-6.65448212	1.02551679	-1.67054331
H	-7.45858012	0.72149179	-2.33401831

C	-3.39707340	-1.65584406	-0.10887233
C	-4.24660540	-2.54160806	-0.77677133
C	-3.80611440	-3.85501906	-0.47979733
C	-2.70682440	-3.74660206	0.36282667
N	-2.45849340	-2.41850506	0.56662167
C	-1.48613240	-1.86061106	1.52315067
C	-3.33569640	-0.21549106	-0.04874333
O	-1.17668740	-0.46910006	0.91284167
C	-2.21960340	0.34410294	0.51189667
O	-0.37771540	-2.49468806	1.63077767
O	-2.22065040	-1.62129706	2.69795767
C	-4.49450940	0.52756994	-0.62818733
C	-1.43533640	-1.20649806	3.82310467
C	-4.37823240	1.17873594	-1.86539033
C	-5.47980240	1.82158494	-2.43507333
C	-6.71291840	1.82114394	-1.77457733
C	-6.83898940	1.16678794	-0.54527033
C	-5.73872740	0.51572494	0.01962667
C	-1.93735940	1.77234594	0.77973867
O	-0.86939240	2.16720194	1.23194667
O	-2.96092240	2.60003094	0.49788667
C	-2.73146740	4.00280894	0.74304767
H	-5.07143940	-2.25835806	-1.41512833
H	-4.23371440	-4.78010206	-0.84139333
H	-2.09363040	-4.49975606	0.83405067
H	0.44936260	-0.16143306	0.83053967
H	-2.14400340	-1.05243506	4.63838467
H	-0.71059740	-1.97728306	4.09824667
H	-0.91106340	-0.26875706	3.61046667
H	-3.42128740	1.18142494	-2.37917133
H	-5.37516340	2.32080494	-3.39421533
H	-7.56914140	2.32255394	-2.21651933
H	-7.79362740	1.15824594	-0.02703033
H	-5.84086440	0.00271394	0.97146167
H	-1.89887240	4.36538894	0.13605067
H	-3.65784940	4.49850894	0.45636267
H	-2.51592840	4.17473394	1.79992267
H	0.44916360	-4.14071006	-1.47496833
C	1.10697160	-3.28287306	-1.50896133
C	2.08665360	-2.94380106	-2.46594933
H	2.31051060	-3.49739606	-3.36638433
C	2.68420060	-1.76927306	-2.02757333
H	3.44938160	-1.20024806	-2.53430833
N	1.07400860	-2.35706406	-0.54260733
H	0.46736060	-2.42340006	0.34310567
C	2.04743860	-1.39694706	-0.80879333
C	2.25747060	-0.25770106	-0.01341033
O	1.39752360	0.17568094	0.87407367
C	3.47683360	0.55704694	-0.10534033
C	4.73403160	-0.01957006	-0.37143433
H	4.82497660	-1.09347406	-0.48754833
C	3.38461760	1.94561894	0.12028567
H	2.41756660	2.38610094	0.33558767
C	4.52330860	2.74299894	0.04352667
H	4.44295460	3.81383394	0.20134267
C	5.76782660	2.16465294	-0.23412433
C	5.87156160	0.78414694	-0.43306633
H	6.83946060	0.33174294	-0.62395233
H	6.65568060	2.78758494	-0.28538433

Complex **6x**×**2w**×Methanol

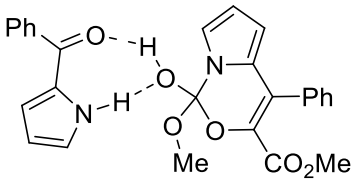


Zero-point correction = 0.459818
Thermal correction to Energy = 0.505825
Thermal correction to Enthalpy = 0.506956
Thermal correction to Gibbs Free Energy = 0.362791
E_0 = -1603.833329, E = -1603.787322,
H = -1603.786191, G = -1603.930356.
Imaginary frequency = 0.

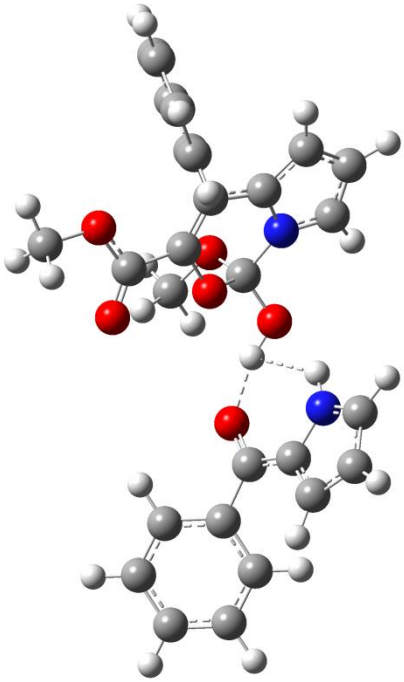


C	3.27450980	-1.62130467	-0.52866488
C	4.10524880	-2.73541367	-0.42608488
C	3.39109880	-3.84673567	-0.94322588
C	2.14657880	-3.39641267	-1.35639888
N	2.07879480	-2.05529167	-1.08231788
C	1.06370080	-1.10598467	-1.47970988
C	3.42156180	-0.23103667	-0.17032788
O	1.07593480	-0.02390067	-0.55933588
C	2.30288280	0.54896933	-0.24228288
O	-0.16685020	-1.70391967	-1.40823288
O	1.41226480	-0.67407867	-2.76457988
C	4.77458880	0.21558333	0.27504012
C	0.49325380	0.23635933	-3.39443188
C	5.02969480	0.47471733	1.62992912
C	6.31078180	0.83843533	2.05103012
C	7.35175580	0.94675733	1.12294812
C	7.10618380	0.68078133	-0.22755988
C	5.82664280	0.30758433	-0.64798488
C	2.14082680	1.99523533	0.03279412
O	1.05108680	2.54856733	0.08595912
O	3.30620080	2.64334433	0.20131612

Complex **12x**×**2w**



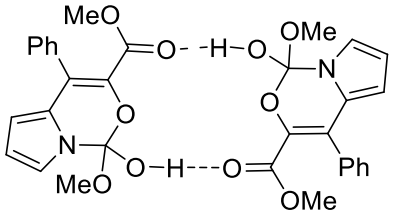
Zero-point correction = 0.461415
Thermal correction to Energy = 0.505298
Thermal correction to Enthalpy = 0.506429
Thermal correction to Gibbs Free Energy = 0.370095
E_0 = -1603.812802, E = -1603.768918,
H = -1603.767787, G = -1603.904121.
Imaginary frequency = 0.



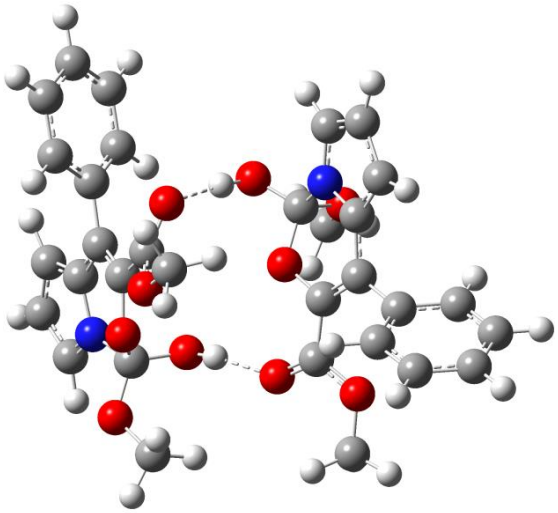
C	3.08126138	-1.48267508	-0.50011021
C	3.91200038	-2.59678408	-0.39753021
C	3.19785038	-3.70810608	-0.91467121
C	1.95333038	-3.25778308	-1.32784421
N	1.88554638	-1.91666208	-1.05376321
C	0.87045238	-0.96735508	-1.45115521
C	3.22831338	-0.09240708	-0.14177321
O	0.88268638	0.11472892	-0.53078121
C	2.10963438	0.68759892	-0.21372821
O	-0.36009862	-1.56529008	-1.37967821
O	1.21901638	-0.53544908	-2.73602521
C	4.58134038	0.35421292	0.30359479
C	0.30000538	0.37498892	-3.36587721
C	4.83644638	0.61334692	1.65848379
C	6.11753338	0.97706492	2.07958479
C	7.15850738	1.08538692	1.15150279
C	6.91293538	0.81941092	-0.19900521
C	5.63339438	0.44621392	-0.61943021
C	1.94757838	2.13386492	0.06134879
O	0.85783838	2.68719692	0.11451379
O	3.11295238	2.78197392	0.22987079

C	3.21542980	4.05379133	0.49526012	C	3.02218138	4.19242092	0.52381479
H	5.10083480	-2.73840867	-0.00656188	H	4.90758638	-2.59977908	0.02199279
H	3.73964680	-4.86830567	-1.00334688	H	3.54639838	-4.72967608	-0.97479221
H	1.31814080	-3.91244667	-1.81649088	H	1.12489238	-3.77381708	-1.78793621
H	-0.91901120	-1.04277467	-1.34590288	H	-1.11225962	-0.90414508	-1.31734821
H	0.97348280	0.53894833	-4.32495588	H	0.78023438	0.67757792	-4.29640121
H	-0.45531320	-0.26081267	-3.61898588	H	-0.64856162	-0.12218308	-3.59043121
H	0.31781680	1.11504233	-2.76725288	H	0.12456838	1.25367192	-2.73869821
H	4.22256380	0.39215833	2.35191312	H	4.02931538	0.53078792	2.38046779
H	6.49535580	1.03605633	3.10304012	H	6.30210738	1.17468592	3.13159479
H	8.34718180	1.23207733	1.45065012	H	8.15393338	1.37070692	1.47920479
H	7.90962280	0.75922433	-0.95425688	H	7.71637438	0.89785392	-0.92570221
H	5.63958280	0.09631333	-1.69675988	H	5.44633438	0.23494292	-1.66820521
H	2.65503380	4.21447033	1.41875712	H	2.46178538	4.35309992	1.44731179
H	4.24561280	4.38785133	0.60851912	H	4.05236438	4.52648092	0.63707379
H	2.72827880	4.58265733	-0.32676088	H	2.53503038	4.72128692	-0.29820621
H	-0.95287620	-3.29124667	2.57710712	H	-1.14612462	-3.15261708	2.60566179
C	-1.73715520	-2.59045567	2.32908912	C	-1.93040362	-2.45182608	2.35764379
C	-2.80138520	-2.11653267	3.09642512	C	-2.99463362	-1.97790308	3.12497979
H	-3.01462420	-2.38912567	4.12015612	H	-3.20787262	-2.25049608	4.14871079
C	-3.52453020	-1.22061667	2.28864212	C	-3.71777862	-1.08198708	2.31719679
H	-4.39439020	-0.65115567	2.57981512	H	-4.58763862	-0.51252608	2.60836979
N	-1.79626620	-2.01343767	1.10551112	N	-1.98951462	-1.87480808	1.13406579
H	-1.12140220	-2.15209167	0.35838312	H	-1.31465062	-2.01346208	0.38693779
C	-2.89068720	-1.16367267	1.03557512	C	-3.08393562	-1.02504308	1.06412979
C	-3.16194720	-0.37116067	-0.14319988	C	-3.35519562	-0.23253108	-0.11464521
O	-2.34804820	-0.29641067	-1.09459188	O	-2.54129662	-0.15778108	-1.06603721
C	-4.43409120	0.40492133	-0.23945888	C	-4.62733962	0.54355092	-0.21090421
C	-5.66783620	-0.11663167	0.18517112	C	-5.86108462	0.02199792	0.21372579
H	-5.72004020	-1.11438067	0.60704712	H	-5.91328862	-0.97575108	0.63560179
C	-4.39375420	1.67770033	-0.83567888	C	-4.58700262	1.81632992	-0.80712421
H	-3.44169820	2.07249233	-1.17475788	H	-3.63494662	2.21112192	-1.14620321
C	-5.56081320	2.42739733	-0.97498788	C	-5.75406162	2.56602692	-0.94643321
H	-5.51692820	3.41693933	-1.41989688	H	-5.71017662	3.55556892	-1.39134221
C	-6.78625220	1.90396033	-0.54588188	C	-6.97950062	2.04258992	-0.51732721
C	-6.83821320	0.62892433	0.02472112	C	-7.03146162	0.76755392	0.05327579
H	-7.78928320	0.21115133	0.34082512	H	-7.98253162	0.34978092	0.36937979
H	-7.69633320	2.48498333	-0.66226988	H	-7.88958162	2.62361292	-0.63371521

Complex **12x**×**12x**

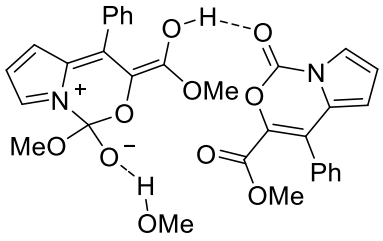


Zero-point correction = 0.575119
Thermal correction to Energy = 0.631787
Thermal correction to Enthalpy = 0.632918
Thermal correction to Gibbs Free Energy = 0.471352
E_0 = -2098.747853, E = -2098.691186,
H = -2098.690055, G = -2098.851621.
Imaginary frequency = 0.

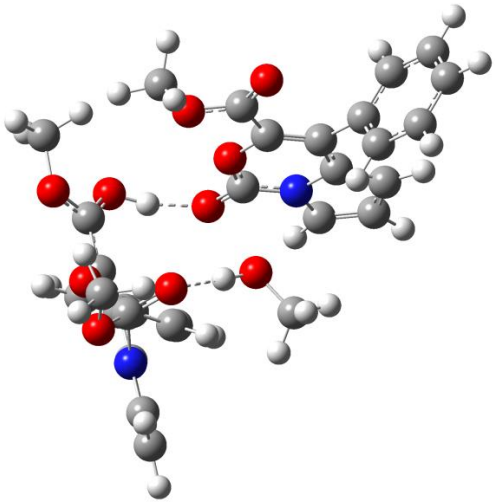


C	2.23780802	1.41786971	0.44913934
C	3.00684902	2.50415571	0.86557234
C	2.23119402	3.67324871	0.66505534
C	1.01218502	3.28617471	0.12763834
N	1.01764502	1.92105971	0.02055334
C	0.04059302	1.07756971	-0.64880866
C	2.45677102	-0.00426329	0.42151734
O	0.12123202	-0.22361229	-0.05953766
C	1.37720402	-0.78965029	0.12331034
O	-1.23795598	1.52839071	-0.49120966
O	0.38542102	1.05607771	-1.99167966
C	3.82830602	-0.48802329	0.75736834
C	-0.49547098	0.30977171	-2.85590566
C	4.08685202	-1.10211729	1.99185934
C	5.38294002	-1.50177529	2.32478034
C	6.43553002	-1.29260829	1.42755334
C	6.18586702	-0.67324029	0.19923434
C	4.89077502	-0.26417929	-0.13052066
C	1.30639302	-2.25779329	0.01227034
O	0.25044102	-2.88578929	-0.06072266
O	2.49876202	-2.86156029	-0.01819266
C	2.49526802	-4.30507829	-0.09604566
H	4.00125702	2.44467371	1.28388634
H	2.52135802	4.68927971	0.89327334
H	0.15467802	3.86351871	-0.18218266

Complex **20**



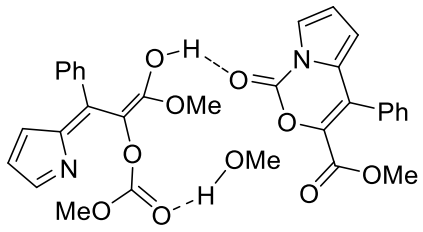
Zero-point correction = 0.571594
Thermal correction to Energy = 0.629953
Thermal correction to Enthalpy = 0.631084
Thermal correction to Gibbs Free Energy = 0.463178
E_0 = -2098.727899, E = -2098.669540,
H = -2098.668409, G = -2098.836315.
Imaginary frequency = 0.



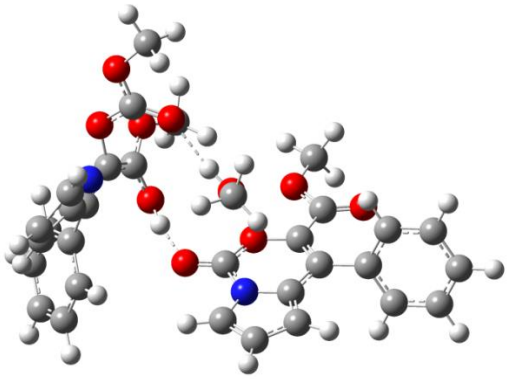
C	2.60625823	1.54797793	0.40115439
C	3.15800223	2.58009993	-0.33410161
C	2.19351523	3.62808493	-0.39726661
C	1.06889723	3.23104293	0.28938939
N	1.31574423	1.96238393	0.78482639
C	0.45530423	1.17027493	1.49933539
C	3.05307223	0.24919093	0.80555539
O	0.92627623	-0.01888907	1.88192239
C	2.19036823	-0.50245307	1.54444939
O	-0.67258477	1.53356693	1.82416939
O	-0.16905177	-0.25382007	-0.96357161
C	4.41365623	-0.18534207	0.37053639
C	-0.02181677	-0.04111507	-2.36050061
C	5.55078423	0.32680393	1.01050539
C	6.82696423	-0.04040207	0.57465239
C	6.97518923	-0.90741707	-0.51176061
C	5.84175123	-1.40680407	-1.16178461
C	4.56533523	-1.04723807	-0.72468661
C	2.44900023	-1.85264807	2.09920139
O	3.51830323	-2.43162007	1.99940539
O	1.37775323	-2.35993807	2.72826539
C	1.54366723	-3.68564107	3.28149539
H	4.14388523	2.57768893	-0.77476261
H	2.31386123	4.57764593	-0.89938461
H	0.12458623	3.71753093	0.47353239

H	-1.53070298	1.41173571	0.44496234	H	-1.67976977	0.62918093	2.58848939
H	-0.00399498	0.30051571	-3.82883066	H	0.47019923	-0.89017507	-2.85662561
H	-1.46821798	0.80068971	-2.93218866	H	0.60216923	0.84664593	-2.50200761
H	-0.62043598	-0.71360829	-2.49272966	H	-0.98817977	0.13439193	-2.85462961
H	3.27131502	-1.26610829	2.69004334	H	5.43769223	1.00148893	1.85405639
H	5.57011202	-1.97467429	3.28451334	H	7.70223623	0.35308893	1.08300839
H	7.44289202	-1.60564829	1.68596334	H	7.96705123	-1.19055207	-0.85150761
H	6.99803602	-0.50366229	-0.50164166	H	5.94979823	-2.07766307	-2.00890161
H	4.70063602	0.22121371	-1.08323966	H	3.68592923	-1.43866807	-1.22680761
H	1.98552802	-4.72938929	0.77115334	H	0.58140723	-3.93164907	3.72627739
H	3.54585802	-4.58992629	-0.10200566	H	2.33093623	-3.68292707	4.03805439
H	2.00148802	-4.63255829	-1.01294866	H	1.79306223	-4.39437007	2.48972939
C	-5.10612298	-1.47120429	0.37888734	C	-4.06160477	-0.53769507	-0.72925261
C	-6.36704198	-1.43911029	-0.21503766	C	-4.76495877	0.14404393	-1.74548561
C	-6.65621998	-2.75078229	-0.66783566	C	-4.86732377	-0.72789207	-2.83851661
C	-5.57418698	-3.55806829	-0.34872866	C	-4.22890177	-1.92415007	-2.48089261
N	-4.65254298	-2.78067829	0.30067034	N	-3.76991477	-1.80695707	-1.21548061
C	-3.29678998	-3.11522729	0.68336234	C	-2.84608877	-2.73584907	-0.47245161
C	-4.28422798	-0.48310329	1.03025434	C	-3.67323177	-0.17202407	0.58990239
O	-2.93752998	-2.30428129	1.80319834	O	-3.31363177	-2.50227707	0.97693939
C	-3.18276098	-0.93993429	1.69743834	C	-3.21197877	-1.20867007	1.40318339
O	-2.46849098	-2.86328629	-0.39385366	O	-1.60516977	-2.52171507	-0.64063861
O	-3.31628698	-4.42818429	1.10992234	O	-3.35319177	-4.01676407	-0.75342661
C	-4.72635598	0.93898371	0.98597434	C	-3.91062577	1.22708693	1.03175539
C	-2.04006298	-5.04355429	1.36102034	C	-2.45265077	-5.09075807	-0.46432961
C	-4.84597398	1.60605071	-0.24314166	C	-3.40875877	2.30951093	0.28955239
C	-5.29659698	2.92769271	-0.29050166	C	-3.68718577	3.62242193	0.67322139
C	-5.64961598	3.59251271	0.88764634	C	-4.47778177	3.87406593	1.79852939
C	-5.54966598	2.92825671	2.11463534	C	-4.99160877	2.80354593	2.53792339
C	-5.09186298	1.61030071	2.16362434	C	-4.71253477	1.49052893	2.15680139
C	-2.18911198	-0.10555829	2.39526834	C	-2.69426177	-1.05550707	2.72647439
O	-1.95266298	1.07361071	2.12479134	O	-2.17332777	0.02134693	3.24014539
O	-1.54726298	-0.76614529	3.36481034	O	-2.75490377	-2.10812507	3.50573039
C	-0.52429298	-0.03377629	4.07938534	C	-2.14380177	-2.05140907	4.82372039
H	-7.00362598	-0.56925629	-0.28724966	H	-5.16453777	1.14468593	-1.66858061
H	-7.55736498	-3.07894829	-1.16667466	H	-5.35674177	-0.53507407	-3.78300261
H	-5.39028998	-4.60604229	-0.52624866	H	-4.08428177	-2.83608007	-3.04046961
H	-1.52426498	-2.76745329	-0.12809066	H	-0.73817977	-1.05202407	-0.82511461
H	-2.27092898	-6.04963029	1.71017834	H	-2.97190477	-6.00106707	-0.76930961
H	-1.44572698	-5.09659629	0.44564634	H	-1.52036077	-4.98489207	-1.02525861
H	-1.49193498	-4.50117529	2.13627634	H	-2.22820277	-5.13985807	0.60687839
H	-4.57119998	1.09373471	-1.15990866	H	-2.78274077	2.11821493	-0.57537161
H	-5.37225298	3.43554371	-1.24755666	H	-3.28488077	4.44818893	0.09377239
H	-6.00418598	4.61838171	0.84998034	H	-4.69680377	4.89582093	2.09425939
H	-5.83119398	3.43423371	3.03352734	H	-5.61841777	2.98965093	3.40494739
H	-5.02263298	1.09528171	3.11726534	H	-5.13514277	0.66381193	2.71995339
H	-0.11737998	-0.74357729	4.79747534	H	-2.24793677	-3.06045107	5.21610639
H	0.24914502	0.30456571	3.38772234	H	-1.09417777	-1.76996107	4.73524139
H	-0.96363198	0.82391571	4.59216334	H	-2.67936877	-1.33601807	5.44901639

Complex **21**

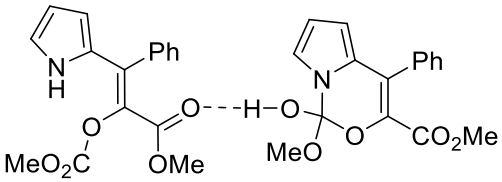


Zero-point correction = 0,571540
Thermal correction to Energy = 0,631168
Thermal correction to Enthalpy = 0,632299
Thermal correction to Gibbs Free Energy = 0,460334
E_0 = -2098.734249, E = -2098.674621,
H = -2098.673490, G = -2098.845456.
Imaginary frequency = 0.

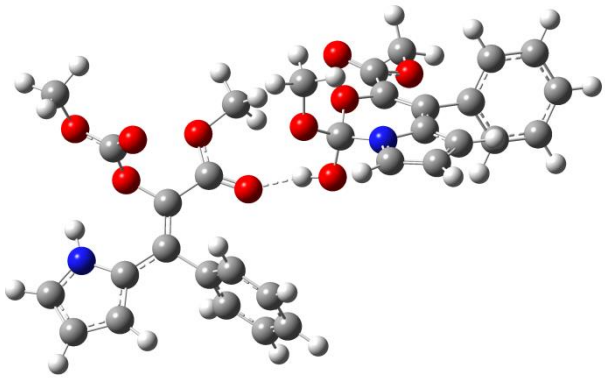


C	-1.97164023	0.68642945	0.82993358
C	-2.32888423	1.63885145	1.76669658
C	-1.18447723	2.45174045	2.01257458
C	-0.14520423	1.99052245	1.23677258
N	-0.62062023	0.91602145	0.50663358
C	0.09368877	0.12437145	-0.35976142
C	-2.65324523	-0.39481155	0.18389058
O	-0.59366823	-0.85661955	-0.95784442
C	-1.93781823	-1.13385655	-0.71015942
O	1.27500877	0.31327645	-0.62119742
O	0.41652477	-1.79007555	1.82978358
C	-4.07708323	-0.64115355	0.55641558
C	0.36891377	-1.50719655	3.22756858
C	-5.07734523	0.24453745	0.13145358
C	-6.40497323	0.04317845	0.51907158
C	-6.73909823	-1.03196955	1.34746958
C	-5.74010623	-1.90713955	1.78675958
C	-4.41434323	-1.71348055	1.39455258
C	-2.45127423	-2.24391955	-1.54790542
O	-3.62313323	-2.58173555	-1.58377542
O	-1.48311123	-2.82535455	-2.27523042
C	-1.90981623	-3.90152655	-3.14183242
H	-3.30422123	1.73687545	2.21972658
H	-1.12926923	3.28862245	2.69435158
H	0.87844677	2.31293345	1.13553758
H	2.22196577	-0.74901755	-1.45248442
H	0.25797377	-2.42288855	3.82379158
H	-0.50309923	-0.87185755	3.40194158
H	1.26631777	-0.97298155	3.56447158
H	-4.82017823	1.08120845	-0.51140142

Complex **7x**×**12x**



Zero-point correction = 0.574421
Thermal correction to Energy = 0.632601
Thermal correction to Enthalpy = 0.633732
Thermal correction to Gibbs Free Energy = 0.463762
E_0 = -2098.763122, E = -2098.704942,
H = -2098.703811, G = -2098.873781.
Imaginary frequency = 0.



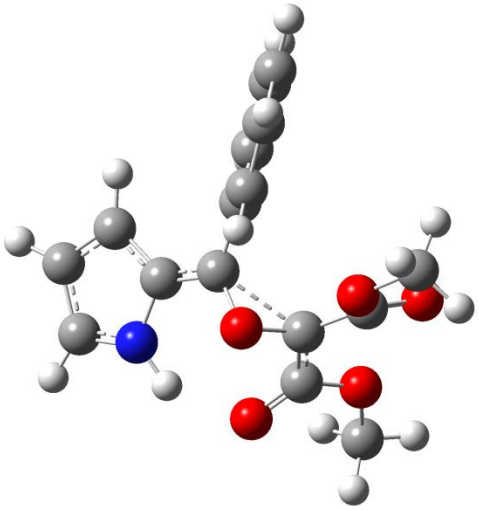
C	3.42103650	0.46548021	2.17505105
C	4.14125068	-0.00265008	3.27145984
C	3.20308140	-0.48731558	4.21951837
C	1.93561888	-0.31540297	3.68719748
N	2.07488430	0.28537995	2.46120362
C	1.04631630	0.49225358	1.45511590
C	3.79918450	1.05110828	0.91224959
O	1.48261648	1.53718109	0.58988609
C	2.79185217	1.53911476	0.13205690
O	0.85791951	-0.69185659	0.78597421
O	-0.15763093	0.88857099	2.00670492
C	5.25658187	1.09795122	0.59216442
C	-0.19978596	2.18423058	2.63852958
C	5.94720235	-0.07970592	0.27080103
C	7.32074412	-0.04715560	0.01491297
C	8.02204804	1.15982752	0.09539912
C	7.34200532	2.33470172	0.43256166
C	5.96755842	2.30392154	0.68035556
C	2.86834027	2.18762057	-1.19840738
O	1.93294777	2.79251931	-1.70377176
O	4.05934251	2.03258121	-1.80093521
C	4.21262295	2.67109783	-3.08652479
H	5.21680813	0.02037518	3.37074702
H	3.42374548	-0.91225146	5.18882259
H	0.96034847	-0.56835303	4.07429853
H	0.08914227	-0.61490539	0.17626934
H	-0.10922176	2.97905740	1.89550614
H	0.59203666	2.27922793	3.38735772
H	-1.17390292	2.23468530	3.12478753
H	5.40578630	-1.01931469	0.21094814

H	-7.17463523	0.72792345	0.17548658
H	-7.77031323	-1.18594555	1.65117358
H	-5.99202823	-2.74152255	2.43457658
H	-3.64004123	-2.39496355	1.73342858
H	-2.32839423	-4.71813955	-2.55032142
H	-1.00912923	-4.22471155	-3.66059942
H	-2.65498223	-3.54015955	-3.85306442
C	4.96527577	-0.33398655	1.53070058
C	5.70759677	0.83605045	1.96541558
C	5.84494177	0.72137545	3.32640758
C	5.17982177	-0.51056855	3.68256758
N	4.67456677	-1.14449155	2.63975458
C	3.83183277	-3.72908855	1.39531258
C	4.58005077	-0.65317855	0.22797958
O	4.66175977	-3.04957855	0.58633858
C	4.14254877	-1.96461555	-0.14605442
O	2.62634777	-3.58478655	1.48922358
O	4.55513677	-4.63653055	2.04751958
C	4.74941177	0.36979045	-0.84432542
C	3.82799077	-5.48954155	2.96121158
C	4.24020277	1.67125845	-0.69779342
C	4.44293077	2.63119345	-1.69141342
C	5.16621577	2.30890245	-2.84350142
C	5.68214477	1.01738445	-2.99875342
C	5.46985577	0.05487945	-2.01183342
C	3.38013977	-2.30899755	-1.25276142
O	2.64635777	-1.48541955	-1.98017242
O	3.36956277	-3.58277655	-1.63560842
C	2.37768077	-4.01392855	-2.59897142
H	6.09644677	1.61780745	1.32819258
H	6.35181277	1.39858245	4.00245358
H	5.07649877	-0.91541655	4.68545758
H	1.20830377	-2.32878655	1.65483258
H	4.57763677	-6.15836255	3.38030658
H	3.36583977	-4.88995155	3.74736458
H	3.06521377	-6.05551055	2.42334458
H	3.66443677	1.91906145	0.18674658
H	4.03223777	3.62888045	-1.56656542
H	5.32643477	3.05669445	-3.61467142
H	6.25263277	0.76086145	-3.88657542
H	5.88113877	-0.94277655	-2.13262142
H	2.48889877	-5.09594255	-2.64338442
H	1.37700477	-3.74158855	-2.25979942
H	2.57935477	-3.56953455	-3.57490342

H	7.84144834	-0.96482095	-0.24305790
H	9.09040862	1.18426025	-0.09871035
H	7.88054900	3.27528547	0.50441329
H	5.44194296	3.21758381	0.94255793
H	3.50068408	2.25658170	-3.80347412
H	5.23460164	2.45355380	-3.39280276
H	4.05884076	3.74860446	-2.99674271
C	-5.15662135	-3.00568506	-1.24175576
C	-5.53204408	-4.28723041	-0.80780258
C	-6.85901345	-4.52000326	-1.22302921
C	-7.27677693	-3.38536722	-1.91042494
N	-6.25781389	-2.48498067	-1.90973829
C	-5.19488045	0.72549426	-1.08317493
C	-3.88351777	-2.34302381	-1.06078344
O	-4.70312548	-0.26065617	-1.88204690
C	-3.64343952	-1.03156008	-1.36500512
O	-4.85921172	0.94562119	0.05878750
O	-6.11686029	1.37687845	-1.78852053
C	-2.80214454	-3.21550289	-0.49582504
C	-6.78662656	2.46192570	-1.09981340
C	-2.45324052	-3.11889541	0.85795577
C	-1.48356197	-3.96712692	1.39652032
C	-0.85041537	-4.91546097	0.58659413
C	-1.19938284	-5.01839161	-0.76329692
C	-2.17927340	-4.17919184	-1.30050575
C	-2.33431192	-0.35441102	-1.36185960
O	-1.28086195	-0.84953404	-0.96843525
O	-2.41385534	0.88156883	-1.87896057
C	-1.17950046	1.63383307	-1.95734598
H	-4.90230855	-4.96210491	-0.24755539
H	-7.45030693	-5.40719449	-1.04620473
H	-8.21595198	-3.16054335	-2.39490936
H	-6.27080275	-1.58367267	-2.36351982
H	-7.49934109	2.85613487	-1.82152935
H	-7.30133524	2.08309123	-0.21532761
H	-6.06218685	3.22696494	-0.81589022
H	-2.93717872	-2.37624651	1.48524373
H	-1.21958993	-3.88322150	2.44662726
H	-0.09119147	-5.56970908	1.00501265
H	-0.71377655	-5.75353028	-1.39842597
H	-2.45403710	-4.26544711	-2.34774090
H	-1.45514383	2.58299896	-2.41339818
H	-0.76065898	1.79109616	-0.96374277
H	-0.45623392	1.10472970	-2.57981344

TS1

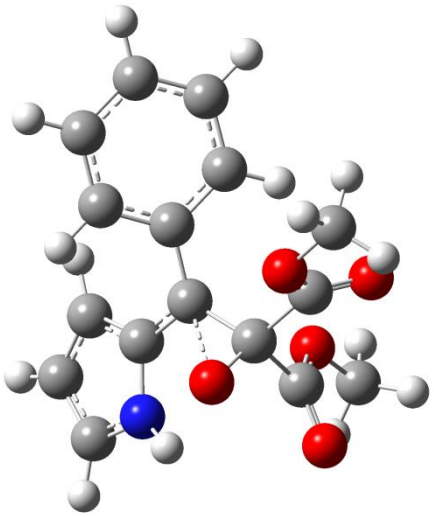
Zero-point correction = 0.284649
Thermal correction to Energy = 0.311958
Thermal correction to Enthalpy = 0.313089
Thermal correction to Gibbs Free Energy = 0.221025
E_0 = -1049.335604, E = -1049.308296,
H = -1049.307165, G = -1049.399229.
Imaginary frequency = 1.



C	1.96558089	3.16716142	0.18716169
C	2.88782289	2.29477342	-0.41840331
N	2.29071689	1.11165542	-0.63845531
C	0.98635689	1.14935142	-0.15766431
C	0.77957489	2.45509342	0.36126769
C	0.08239789	0.08111542	-0.33067031
C	-1.31072811	0.19318642	0.14531069
C	-1.60059911	0.59350042	1.46259469
C	-2.92375011	0.75798942	1.87029869
C	-3.96909411	0.53733642	0.96637069
C	-3.68692811	0.13742642	-0.34408231
C	-2.36630211	-0.04650158	-0.75308531
O	0.40999789	-0.91145858	-1.22172231
C	0.62862089	-1.87874058	-0.18795931
C	-0.41000411	-2.88179958	0.02601169
C	2.01780089	-2.08128258	0.15791369
O	-0.46141511	-3.67765558	0.95967269
O	-1.35077011	-2.85864458	-0.95477131
C	-2.43325211	-3.79663858	-0.80993531
O	2.96634789	-1.47355958	-0.36790431
O	2.23085089	-3.02001558	1.10264969
C	3.60725189	-3.30260658	1.42342969
H	2.15130189	4.19948942	0.44687669
H	3.91985389	2.46011042	-0.69396731
H	2.73485789	0.21795042	-0.88394431
H	-0.14979111	2.82992442	0.76274469
H	-0.79132611	0.74524842	2.16953569
H	-3.13914911	1.05128542	2.89310569
H	-4.99890211	0.67007442	1.28423069
H	-4.49593711	-0.03507258	-1.04736731
H	-2.14353511	-0.36400158	-1.76477831
H	-3.09079811	-3.61188458	-1.65895531
H	-2.05835111	-4.82255658	-0.83605131
H	-2.96576611	-3.62839458	0.12907069

TS2

Zero-point correction = 0.284647
Thermal correction to Energy = 0.312398
Thermal correction to Enthalpy = 0.313529
Thermal correction to Gibbs Free Energy = 0.220325
E_0 = -1049.330647, E = -1049.302896,
H = -1049.301765, G = -1049.394969.
Imaginary frequency = 1.

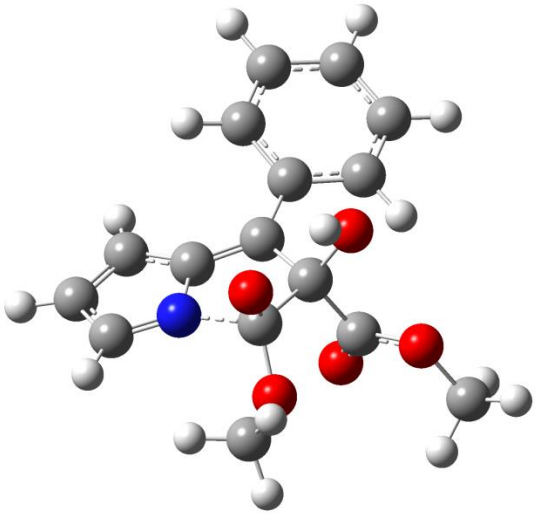


C	-2.75177824	-3.23702136	-0.16466257
C	-3.43297524	-2.28016136	-0.92686557
N	-2.63646724	-1.19890736	-1.07773057
C	-1.40749924	-1.42844236	-0.47292757
C	-1.47846024	-2.71896436	0.10463943
C	-0.38588324	-0.45575636	-0.38405757
C	0.96901576	-0.90460336	-0.04371457
C	1.70327276	-0.26297236	0.97627243
C	2.96330476	-0.73407936	1.33734243
C	3.52517276	-1.82646836	0.66581543
C	2.81442176	-2.45993636	-0.35847357
C	1.53959576	-2.01283136	-0.70303257
O	-0.89068324	0.69685264	-2.08118057
C	-0.71800324	0.97768964	-0.76184057
C	0.40566376	2.03336964	-0.49726157
C	-1.97570324	1.55160364	-0.03913157
O	0.36392076	2.85906764	0.40018343
O	1.38176176	1.96023764	-1.39865057
C	2.45264376	2.92447464	-1.26934057
O	-2.81541524	2.22638464	-0.60126257
O	-2.01688424	1.20978564	1.25363343
C	-3.11706824	1.73708364	2.03379443
H	-3.14829424	-4.19139536	0.15031043
H	-4.41481424	-2.31761436	-1.37683557
H	-2.76240024	-0.42853536	-1.72846657
H	-0.70274824	-3.17589536	0.70115743
H	1.27175276	0.57566964	1.51199043
H	3.50864076	-0.24827036	2.14036543
H	4.51489176	-2.17989836	0.93888343
H	3.25233876	-3.29998436	-0.88837257
H	0.99176976	-2.49344836	-1.50640557
H	3.13030876	2.71127864	-2.09410657
H	2.05547676	3.93826664	-1.34718357
H	2.95938676	2.79755264	-0.31041857

H	3.56647989	-4.08775258	2.17760569	H	-2.96946924	1.34820864	3.03974943
H	4.09986289	-2.41410658	1.82489369	H	-4.06770124	1.39249064	1.62229343
H	4.14637089	-3.65109358	0.53951569	H	-3.08522124	2.82832864	2.03324943

TS3

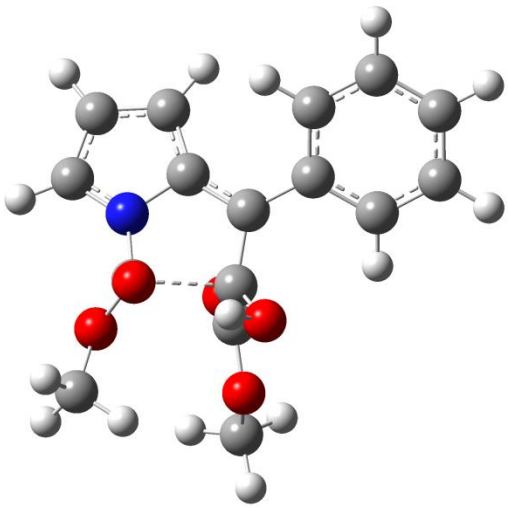
Zero-point correction = 0.284687
Thermal correction to Energy = 0.311892
Thermal correction to Enthalpy = 0.313023
Thermal correction to Gibbs Free Energy = 0.220995
E_0 = -1049.335439, E = -1049.308234,
H = -1049.307103, G -1049.399130.
Imaginary frequency = 1.



C	-1.31879126	3.52591979	-1.05496333
C	-2.42196026	2.76359179	-0.51003333
N	-1.99803226	1.58794679	-0.10767733
C	-0.61959226	1.50941479	-0.32699833
C	-0.19439926	2.74953079	-0.93773233
C	-0.06859626	0.31243279	0.04713767
C	1.35506674	-0.00120321	0.09632367
C	1.81785874	-1.33098321	-0.01350333
C	3.18057774	-1.61482421	0.00904867
C	4.11292274	-0.58355321	0.16586067
C	3.67149474	0.73610979	0.30994767
C	2.30984674	1.02501279	0.27906267
O	-0.77210726	-1.29680021	1.70731567
C	-1.13482626	-0.70086421	0.48758967
C	-1.35519026	-1.74362321	-0.62290733
C	-2.52558726	0.07740579	0.76675667
O	-1.19853726	-1.49451321	-1.80559433
O	-1.74496626	-2.92465021	-0.14376833
C	-2.04624226	-3.94644121	-1.12339333
O	-2.74996726	0.32927979	1.97122267
O	-3.51873026	-0.41391721	-0.05687633
C	-4.86341626	-0.08178221	0.32222867
H	-1.39338226	4.51815979	-1.47932333
H	-3.45645026	3.07053979	-0.41986933
H	-1.33711026	-0.83600221	2.36799567
H	0.80210274	2.98780079	-1.27908733
H	1.11643174	-2.14788921	-0.12820733
H	3.51568974	-2.64245721	-0.08987033
H	5.17470574	-0.80884621	0.19188067
H	4.38736874	1.53777979	0.46207267
H	1.97941474	2.04384679	0.44300367

TS4

Zero-point correction = 0.284408
Thermal correction to Energy = 0.311637
Thermal correction to Enthalpy = 0.312768
Thermal correction to Gibbs Free Energy = 0.222001
E_0 = -1049.329746, E = -1049.302517,
H = -1049.301386, G = -1049.392153.
Imaginary frequency = 1.



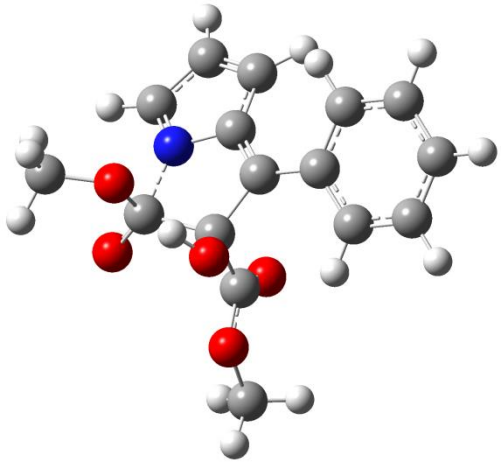
C	-0.70981167	3.89326561	-1.23998798
C	-1.76355467	3.32158161	-0.48703798
N	-1.33422967	2.15421261	0.00981502
C	-0.01863367	1.91612161	-0.39722298
C	0.38418133	3.03442561	-1.16929998
C	0.45638133	0.65835961	-0.01738198
C	1.86566833	0.32571861	0.12258402
C	2.29281633	-1.01604639	0.00232702
C	3.64472833	-1.33480039	0.07477602
C	4.59461533	-0.32615239	0.28283702
C	4.18591133	1.00504261	0.42121902
C	2.83380833	1.33018661	0.34544702
O	-0.45389267	-1.03405939	1.45306702
C	-0.64700967	-0.24311839	0.33382202
C	-1.40660767	-0.84776039	-0.79103598
C	-1.94001367	1.18834861	0.95088502
O	-1.43346967	-0.40666739	-1.93402598
O	-2.09878867	-1.93689139	-0.40448498
C	-2.89227067	-2.57641839	-1.42603398
O	-1.68706267	1.23921861	2.17537502
O	-3.20749367	0.93317561	0.48152202
C	-4.11756767	0.34346461	1.42891402
H	-0.76336867	4.83804661	-1.76276298
H	-2.74913367	3.70643561	-0.26891698
H	-0.71990467	-0.45510339	2.20293302
H	1.33527033	3.14576861	-1.66932498
H	1.55980533	-1.79748339	-0.16369198
H	3.96203233	-2.36743739	-0.03089298
H	5.64878333	-0.57901139	0.34481102
H	4.91947833	1.78473661	0.60055902
H	2.51681833	2.35724061	0.49110402

H	-2.33246426	-4.82201421	-0.54340633
H	-2.86890426	-3.62027121	-1.76278633
H	-1.16482726	-4.15732721	-1.73195833
H	-5.02878226	0.99926279	0.26957767
H	-5.08080026	-0.43344421	1.33312767
H	-5.50415826	-0.58606121	-0.40139833

H	-3.35943467	-3.42873239	-0.93439098
H	-3.65088567	-1.88824639	-1.80511998
H	-2.25728467	-2.91060539	-2.24943798
H	-4.21958067	0.97772161	2.31182502
H	-3.77388867	-0.65077339	1.72524102
H	-5.06896967	0.26734161	0.90264402

TS5

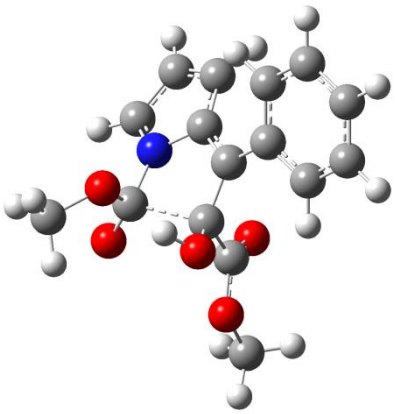
Zero-point correction = 0.284636
Thermal correction to Energy = 0.311895
Thermal correction to Enthalpy = 0.313026
Thermal correction to Gibbs Free Energy = 0.221597
E_0 = -1049.332038, E = -1049.304779,
H = -1049.303648, G = -1049.395076.
Imaginary frequency = 1.



C	0.90917628	-3.97667917	-1.64807086
C	1.94544628	-3.13463317	-1.09020886
N	1.39600828	-2.13514917	-0.44182086
C	0.00610028	-2.24290417	-0.52516986
C	-0.29843772	-3.43008017	-1.28933386
C	-0.64857072	-1.17053617	0.02436014
C	-2.08603772	-1.04016217	0.21103214
C	-2.70320572	0.22990683	0.25469914
C	-4.08396472	0.34261583	0.39218614
C	-4.87563472	-0.80460417	0.51644114
C	-4.27687172	-2.06953017	0.50705014
C	-2.89796072	-2.18799417	0.35774314
O	0.00043228	0.54430583	1.64618714
C	0.34247928	-0.06923217	0.42637414
C	0.43456528	0.97682283	-0.70404086
C	1.82086328	-0.71777417	0.53725314
O	0.33776528	0.68329383	-1.88169286
O	0.65361228	2.20691983	-0.24616086
C	0.82622928	3.23943683	-1.24691486
O	2.82219428	-0.12181517	0.10770814
O	1.83041428	-1.28895617	1.83415514
C	3.12158728	-1.66003317	2.33426814
H	1.07845728	-4.86352317	-2.24386286
H	3.01904328	-3.26066717	-1.15749886
H	0.45569028	0.03008083	2.33659314
H	-1.28170572	-3.77436417	-1.57467986
H	-2.10598972	1.12980483	0.17125914
H	-4.54305072	1.32598783	0.40914014
H	-5.95112972	-0.71286017	0.63363214
H	-4.88354172	-2.96137117	0.62858914

TS6

Zero-point correction = 0.284150
Thermal correction to Energy = 0.311595
Thermal correction to Enthalpy = 0.312726
Thermal correction to Gibbs Free Energy = 0.221221
E_0 = -1049.325894, E = -1049.298449,
H = -1049.297318, G = -1049.388823.
Imaginary frequency = 1.

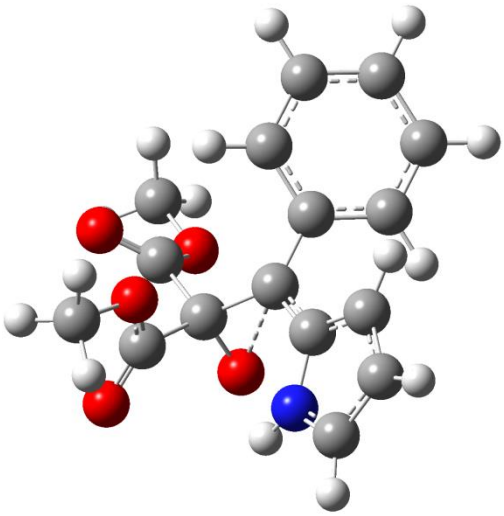


C	0.25905394	-3.45841198	-2.07302309
C	1.28669794	-2.90464298	-1.26924909
N	0.77159194	-1.87481398	-0.59061009
C	-0.56863806	-1.69611298	-0.93342609
C	-0.90336706	-2.72413998	-1.85159909
C	-1.11092706	-0.52432198	-0.40208309
C	-2.53541806	-0.29423798	-0.20950709
C	-3.05123306	1.02122002	-0.18389809
C	-4.42012106	1.23879302	-0.06656509
C	-5.29833806	0.15275202	0.04425491
C	-4.80093506	-1.15511698	0.03773591
C	-3.43169206	-1.37897598	-0.08510509
O	-0.28769106	1.14629602	1.15956491
C	-0.04437906	0.39633202	0.01584091
C	0.64673394	1.14535202	-1.07902609
C	1.37131994	-0.94077198	0.39955991
O	0.72525994	0.76220502	-2.23801409
O	1.21194394	2.27618002	-0.63021309
C	1.95317194	3.04404702	-1.60365609
O	2.55002394	-0.59425798	0.23925891
O	0.89337194	-1.29581798	1.68205191
C	1.87729894	-1.24639398	2.73412391
H	0.37630994	-4.30882398	-2.73028009
H	2.31181594	-3.21903898	-1.13541609
H	-0.24436406	0.51626702	1.89999791
H	-1.85675306	-2.84488898	-2.34535609
H	-2.37425506	1.86325402	-0.27029109
H	-4.80614106	2.25324702	-0.06073609
H	-6.36556706	0.32671902	0.14308291
H	-5.47863206	-1.99687198	0.13974391

H	-2.43973572	-3.16979917	0.39477414	H	-3.04510006	-2.39211498	-0.05530809
H	0.98935928	4.15667683	-0.68404686	H	2.32034294	3.91403802	-1.06124109
H	1.69015928	3.01032883	-1.87331786	H	2.78517394	2.45526002	-1.99493309
H	-0.07054072	3.31815183	-1.86440786	H	1.29997794	3.35000302	-2.42360809
H	3.80744828	-0.81035917	2.31331514	H	2.29449394	-0.24228998	2.84164991
H	3.54125228	-2.48279717	1.74488914	H	2.68587194	-1.95646098	2.54252091
H	2.95851228	-1.99153117	3.36047814	H	1.33792194	-1.52802198	3.63937491

TS7

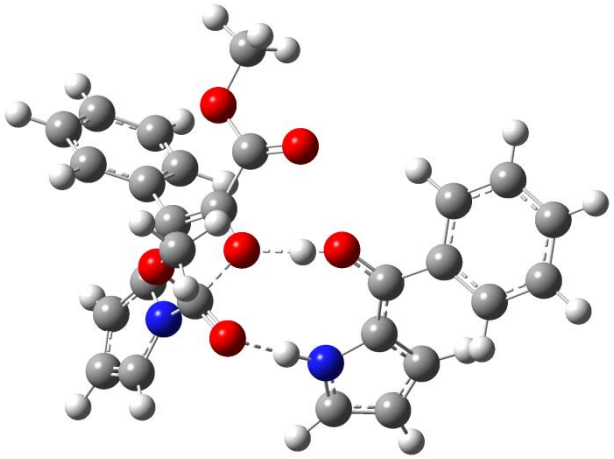
Zero-point correction = 0.284647
Thermal correction to Energy = 0.312398
Thermal correction to Enthalpy = 0.313529
Thermal correction to Gibbs Free Energy = 0.220325
E_0 = -1049.330647, E = -1049.302896,
H = -1049.301765, G = -1049.394969.
Imaginary frequency = 1.



C	-2.52912424	-3.17558633	0.02812555
C	-3.21032124	-2.21872633	-0.73407745
N	-2.41381324	-1.13747233	-0.88494245
C	-1.18484524	-1.36700733	-0.28013945
C	-1.25580624	-2.65752933	0.29742755
C	-0.16322924	-0.39432133	-0.19126945
C	1.19166976	-0.84316833	0.14907355
C	1.92592676	-0.20153733	1.16906055
C	3.18595876	-0.67264433	1.53013055
C	3.74782676	-1.76503333	0.85860355
C	3.03707576	-2.39850133	-0.16568545
C	1.76224976	-1.95139633	-0.51024445
O	-0.66802924	0.75828767	-1.88839245
C	-0.49534924	1.03912467	-0.56905245
C	0.62831776	2.09480467	-0.30447345
C	-1.75304924	1.61303867	0.15365655
O	0.58657476	2.92050267	0.59297155
O	1.60441576	2.02167267	-1.20586245
C	2.67529776	2.98590967	-1.07655245
O	-2.59276124	2.28781967	-0.40847445
O	-1.79423024	1.27122067	1.44642155
C	-2.89441424	1.79851867	2.22658255
H	-2.92564024	-4.12996033	0.34309855
H	-4.19216024	-2.25617933	-1.18404745
H	-2.53974624	-0.36710033	-1.53567845
H	-0.48009424	-3.11446033	0.89394555
H	1.49440676	0.63710467	1.70477855

TS8

Zero-point correction = 0.459159
Thermal correction to Energy = 0.502149
Thermal correction to Enthalpy = 0.503280
Thermal correction to Gibbs Free Energy = 0.372448
E_0 = -1603.794208, E = -1603.751218,
H = -1603.750087, G = -1603.880919.
Imaginary frequency = 1.



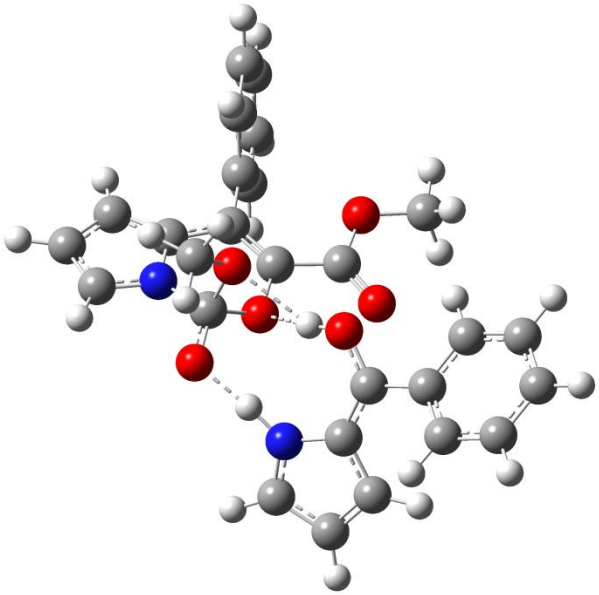
C	-3.21681050	-1.85213219	0.28555219
C	-4.15385850	-2.70345119	-0.30139681
C	-3.75328750	-4.03755419	-0.02974281
C	-2.58667950	-3.97885219	0.71489719
N	-2.26010550	-2.65667519	0.88864119
C	-1.20831050	-2.18196119	1.77886419
C	-3.08656950	-0.41057519	0.28398719
O	-0.85199850	-0.69577219	1.01478019
C	-1.88882650	0.12413881	0.67619219
O	-0.12248750	-2.82006219	1.80557319
O	-1.81767750	-1.79435019	2.95831819
C	-4.25641450	0.36513381	-0.22331781
C	-0.92275850	-1.42509119	4.01860119
C	-4.18773450	1.05006881	-1.44662281
C	-5.29864950	1.73786781	-1.94156781
C	-6.49777050	1.74686681	-1.22160981
C	-6.57945350	1.05778981	-0.00723081
C	-5.46930450	0.36536981	0.48331519
C	-1.53899650	1.56689581	0.75693019
O	-0.38401650	1.97325481	0.73317919
O	-2.59939850	2.38394781	0.89129619
C	-2.31749650	3.79886081	0.92031019
H	-5.01083650	-2.38614119	-0.87821481
H	-4.25274450	-4.94231619	-0.34809981
H	-1.97131150	-4.75664519	1.14092719
H	0.64821450	-0.38706719	1.04909119
H	-1.56145650	-1.14976819	4.85844019

H	3.73129476	-0.18683533	2.33315355
H	4.73754576	-2.11846333	1.13167155
H	3.47499276	-3.23854933	-0.69558445
H	1.21442376	-2.43201333	-1.31361745
H	3.35296276	2.77271367	-1.90131845
H	2.27813076	3.99970167	-1.15439545
H	3.18204076	2.85898767	-0.11763045
H	-2.74681524	1.40964367	3.23253755
H	-3.84504724	1.45392567	1.81508155
H	-2.86256724	2.88976367	2.22603755

H	-0.27893050	-2.26406519	4.29303419
H	-0.30823550	-0.56871519	3.72435719
H	-3.25980650	1.04000781	-2.01145481
H	-5.22839550	2.26239381	-2.89036681
H	-7.36180050	2.28147081	-1.60573281
H	-7.50732650	1.05668881	0.55776719
H	-5.53757350	-0.17044919	1.42559419
H	-1.81572350	4.10668181	0.00013719
H	-3.28920350	4.28280181	1.00671419
H	-1.68933950	4.04369781	1.77963519
H	0.68077550	-4.21224919	-1.54000581
C	1.34147750	-3.35732819	-1.49772281
C	2.32140550	-2.93465119	-2.41601681
H	2.54427850	-3.40317919	-3.36367381
C	2.92610750	-1.80692519	-1.86893281
H	3.69563150	-1.19807219	-2.31991881
N	1.31484750	-2.51986219	-0.45061381
H	0.72813350	-2.65816919	0.41195319
C	2.29230050	-1.54419519	-0.62450881
C	2.50630750	-0.48392319	0.28040219
O	1.63593950	-0.12452019	1.17989619
C	3.74570350	0.30611981	0.28202119
C	4.99501150	-0.26926619	-0.02010881
H	5.06637850	-1.32897019	-0.23701781
C	3.67469450	1.66979381	0.63187219
H	2.70995150	2.10554681	0.86688219
C	4.82946850	2.44747881	0.64610419
H	4.76717750	3.50106281	0.89951019
C	6.06729150	1.87129281	0.33525519
C	6.14855050	0.51334981	0.00999919
H	7.11083350	0.06163581	-0.20902981
H	6.96753050	2.47811781	0.35474619

TS9

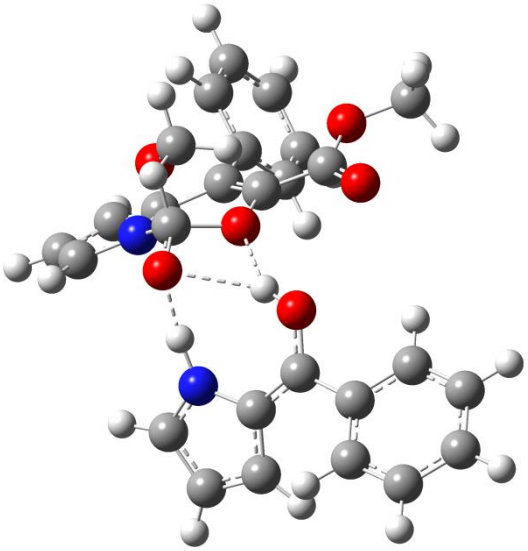
Zero-point correction = 0.459562
Thermal correction to Energy = 0.502324
Thermal correction to Enthalpy = 0.503455
Thermal correction to Gibbs Free Energy = 0.373251
E_0 = -1603.787349, E = -1603.744587,
H = -1603.743456, G = -1603.873660.
Imaginary frequency = 1.



C	3.02650000	-1.43138900	-0.22665000
C	4.21545600	-2.14804400	-0.38594900
C	3.86278000	-3.49790600	-0.63285200
C	2.47467200	-3.57733400	-0.62424900
N	1.98185000	-2.32846800	-0.37025700
C	0.57099400	-1.89667000	-0.40866500
C	2.73889000	-0.05751300	0.10529500
O	0.48200400	-0.74256600	0.48965300
C	1.44488100	0.24906300	0.42472500
O	-0.27522500	-2.80986200	-0.07883000
O	0.31361600	-1.25529000	-1.68692200
C	3.89258800	0.89141600	0.10379900
C	0.16371100	-2.14847100	-2.79220400
C	4.49111300	1.29005200	1.30813400
C	5.60553200	2.13241100	1.30156700
C	6.13726300	2.58548200	0.08959500
C	5.55250000	2.18370300	-1.11530800
C	4.44259000	1.33401600	-1.10812400
C	0.86175800	1.56002300	0.78813900
O	-0.30480700	1.70010900	1.13534200
O	1.72361800	2.58969500	0.69098400
C	1.20650500	3.88929500	1.04267200
H	5.21192300	-1.73774800	-0.30240700
H	4.53939400	-4.32627100	-0.79246100
H	1.80808600	-4.41272800	-0.77370600
H	-1.36932100	-0.43542600	-0.68628600
H	1.10542900	-2.66814600	-3.00801900
H	-0.62340400	-2.88447900	-2.60053100
H	-0.10903900	-1.53123200	-3.65046100
H	4.07812500	0.94154400	2.25029000
H	6.05824200	2.43332900	2.24211200

TS10

Zero-point correction = 0.459573
Thermal correction to Energy = 0.502323
Thermal correction to Enthalpy = 0.503454
Thermal correction to Gibbs Free Energy = 0.373208
E_0 = -1603.792620, E = -1603.49870,
H = -1603.748739, G = -1603.878985.
Imaginary frequency = 1.

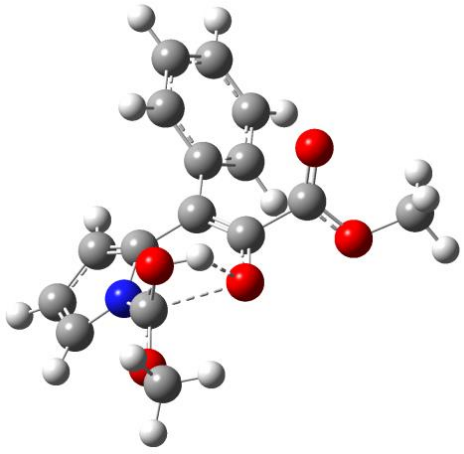


C	-2.59760283	-1.46941815	0.04135486
C	-3.37576983	-2.46186115	-0.55954214
C	-2.80282183	-3.71223615	-0.21716214
C	-1.69636883	-3.46040915	0.58453186
N	-1.57235383	-2.10632415	0.71996386
C	-0.63776083	-1.39583415	1.61108886
C	-2.66228183	-0.02718915	0.03360886
O	-0.47660683	-0.04597615	0.97669086
C	-1.58865883	0.64805585	0.54651686
O	0.54288917	-1.91753615	1.71438286
O	-1.35839583	-1.21883915	2.81535186
C	-3.87957983	0.58908185	-0.57264914
C	-0.59325483	-0.68027515	3.89958586
C	-3.81877983	1.20397185	-1.83233814
C	-4.97103683	1.72934985	-2.42211014
C	-6.20067883	1.64442085	-1.76049914
C	-6.27139983	1.02355585	-0.50952814
C	-5.11951983	0.49105685	0.07614686
C	-1.39820983	2.11009185	0.69075186
O	-0.32579183	2.62114585	0.98821586
O	-2.51748383	2.82967085	0.48305986
C	-2.38280883	4.26206985	0.58495686
H	-4.23961183	-2.28925115	-1.18564914
H	-3.14986283	-4.68992215	-0.52245014
H	-1.00274583	-4.12941515	1.07092786
H	1.47560817	-0.07876315	1.02080186
H	-1.29136383	-0.57300415	4.73167486
H	0.21868617	-1.35698715	4.18032786
H	-0.17925683	0.30072185	3.64215786
H	-2.86527483	1.27032285	-2.34840914
H	-4.90843983	2.20224985	-3.39812814

H	7.00259300	3.24202000	0.08435700	H	-7.09652083	2.05399585	-2.21827614
H	5.96134900	2.52700600	-2.06139900	H	-7.22260983	0.94966485	0.00989686
H	3.99345700	1.01963100	-2.04585000	H	-5.17807483	0.00507685	1.04567686
H	0.85763400	3.89448600	2.07771500	H	-1.65629683	4.63021285	-0.14295714
H	2.04469800	4.57341300	0.91786000	H	-3.37413683	4.65851585	0.36997286
H	0.38461900	4.16562400	0.37827900	H	-2.06720983	4.54470085	1.59176286
H	-2.11834700	-3.35398900	2.78251100	H	1.31743917	-3.89807415	-1.36305314
C	-2.70384000	-2.53549300	2.38590500	C	2.00350217	-3.06241715	-1.39280714
C	-3.85612600	-1.91733800	2.92231700	C	3.00800317	-2.76284815	-2.33985514
H	-4.33021500	-2.16769500	3.86023800	H	3.23177617	-3.33715515	-3.22719114
C	-4.23174600	-0.93177200	2.02470500	C	3.62440617	-1.59505915	-1.91460614
H	-5.04587900	-0.23089100	2.13159300	H	4.41028417	-1.05384615	-2.41977214
N	-2.37078700	-1.96020500	1.22733900	N	1.98225417	-2.12482615	-0.44020914
H	-1.52366400	-2.27672700	0.64071400	H	1.33784917	-2.11136815	0.42489086
C	-3.29718800	-0.95571400	0.94409500	C	2.98127317	-1.18981215	-0.70790014
C	-3.24283200	-0.10707600	-0.16659400	C	3.20056317	-0.04859915	0.07628986
O	-2.20540500	-0.00466900	-0.97309400	O	2.35616817	0.37153785	0.99336686
C	-4.35779200	0.76909200	-0.55396400	C	4.39446317	0.79609685	-0.05300214
C	-5.69706500	0.34513700	-0.45862000	C	5.66078417	0.24475085	-0.32897114
H	-5.92598700	-0.65787700	-0.11682100	H	5.77728417	-0.82883815	-0.42290914
C	-4.06971000	2.04731400	-1.07274400	C	4.27103217	2.18604885	0.14652486
H	-3.03796100	2.37086400	-1.15207400	H	3.29775117	2.60914285	0.36830786
C	-5.10598700	2.89667400	-1.45168100	C	5.38831717	3.00915685	0.03326986
H	-4.87822200	3.88729900	-1.83224400	H	5.28356517	4.08068885	0.17028786
C	-6.43606900	2.47387700	-1.34267100	C	6.64185417	2.45616585	-0.25437014
C	-6.72805500	1.19645300	-0.85435900	C	6.77656517	1.07477885	-0.42658014
H	-7.75745300	0.85832300	-0.79182300	H	7.75196017	0.64207085	-0.62464614
H	-7.24183900	3.13531500	-1.64611600	H	7.51281017	3.09953285	-0.33414514

TS11

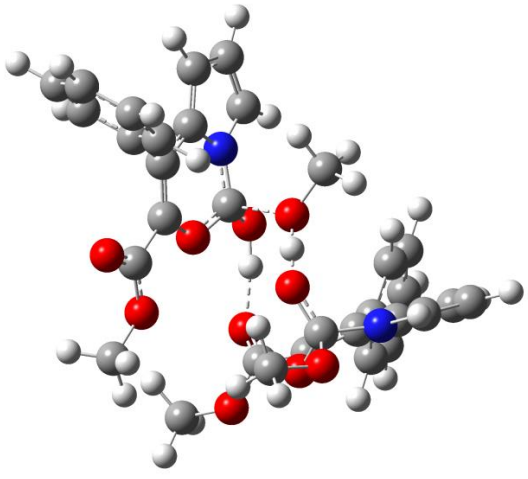
Zero-point correction = 0.283396
Thermal correction to Energy = 0.311013
Thermal correction to Enthalpy = 0.312144
Thermal correction to Gibbs Free Energy = 0.218343
E_0 = -1049.322407, E = -1049.294790,
H = -1049.293659, G = -1049.387460.
Imaginary frequency = 1.



C	1.89130441	-3.63385489	-0.96446368	C	-2.05347493	1.92295690	0.02797885
C	2.84092141	-2.68803789	-0.70032568	C	-2.67394093	3.02955690	0.58118285
N	2.18077441	-1.59553189	-0.10121068	C	-1.72366493	4.08981190	0.60509785
C	0.78021341	-1.84176889	-0.07007068	C	-0.53534193	3.62525890	0.08451585
C	0.61381341	-3.11698089	-0.58282668	N	-0.73877193	2.30793190	-0.28423415
C	-0.21192559	-0.81080889	0.17403232	C	0.17654007	1.38761190	-0.74258715
C	-1.62830059	-1.28168189	0.25043132	C	-2.46890393	0.58718890	-0.29614515

TS12

Zero-point correction = 0,569179
Thermal correction to Energy = 0,625513
Thermal correction to Enthalpy = 0,626644
Thermal correction to Gibbs Free Energy = 0,466556
E_0 = -2098.712643, E = -2098.656308,
H = -2098.655177, G = -2098.815266.
Imaginary frequency = 1.



C	-2.56098259	-0.96015789	-0.74960168
C	-3.88434159	-1.40568289	-0.66759268
C	-4.29351159	-2.19573589	0.40981332
C	-3.36972759	-2.53793189	1.40439632
C	-2.05097159	-2.08708489	1.32286732
O	1.31387541	1.03697311	0.02349732
C	0.10666441	0.53087011	0.12062932
C	-0.97427659	1.58813811	0.24885232
C	2.81822941	-0.53175889	0.45482732
O	-1.69658959	1.72622911	1.22197632
O	-0.98379459	2.41674311	-0.80853968
C	-1.89876059	3.53439011	-0.74301668
O	2.55939141	-0.13416489	1.69020632
O	3.94136441	-0.21362189	-0.11569068
C	4.82567441	0.75524311	0.52720132
H	2.08681841	-4.60880989	-1.38963668
H	3.91481541	-2.69005789	-0.79142268
H	2.02545841	0.70011211	1.55924832
H	-0.34183259	-3.59621989	-0.73389668
H	-2.24481859	-0.36491489	-1.60187768
H	-4.59045059	-1.14213689	-1.45011768
H	-5.31992459	-2.54541689	0.47348032
H	-3.67823659	-3.15154489	2.24624232
H	-1.34072259	-2.34938189	2.10211232
H	-1.75623359	4.07771711	-1.67577168
H	-2.92749159	3.17800711	-0.65859368
H	-1.65765159	4.16886311	0.11257032
H	5.04107841	0.43762911	1.54647832
H	4.34852841	1.73502111	0.51168932
H	5.72143041	0.75097411	-0.08839568

O	-0.31994293	0.28866290	-1.31535315
C	-1.58483693	-0.19943410	-0.97158815
O	1.28398507	1.85506490	-1.21796415
O	0.78021407	0.57420490	0.91882985
C	-3.83717193	0.16444490	0.12591485
C	0.52640407	1.18898290	2.17878485
C	-4.96194993	0.63602890	-0.56478615
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C	-6.41382693	-0.53289610	0.98294985
C	-5.29272593	-0.99262310	1.68193885
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H	3.35798407	-1.18573310	-4.67758215

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Zero-point correction = 0.570821
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Thermal correction to Enthalpy = 0.630074
Thermal correction to Gibbs Free Energy = 0.462629
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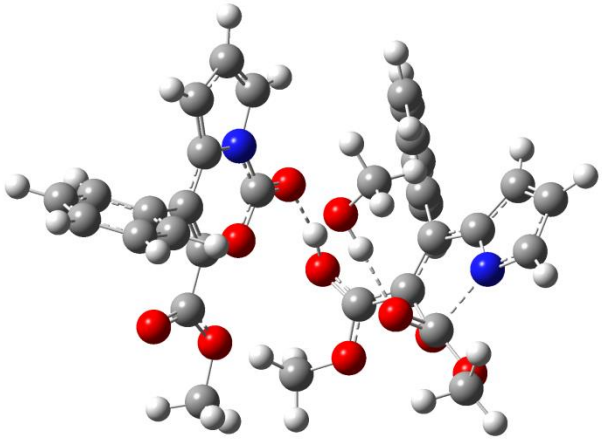
H = -2098.659376, G = -2098.826821.
Imaginary frequency = 1.



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C	2.00514874	2.82398168	-2.00762928
C	0.90410674	2.44242868	-1.27514928
N	1.19109674	1.21201868	-0.71051928
C	0.35742074	0.44241368	0.06214072
C	2.96972474	-0.45507132	-0.62172428
O	0.86604674	-0.71283032	0.50401972
C	2.13914974	-1.18045732	0.17817272
O	-0.77280726	0.79578468	0.37990672
O	-0.26922026	-1.15994432	-2.28541728
C	4.32983474	-0.88496832	-1.06109728
C	-0.42980626	-0.91383432	-3.67791228
C	5.46842774	-0.27276532	-0.51887628
C	6.74188374	-0.63811332	-0.96418628
C	6.88532874	-1.60391032	-1.96445328
C	5.74980774	-2.20432632	-2.51839428
C	4.47660574	-1.84641632	-2.07104328
C	2.44888474	-2.48035332	0.82030072
O	3.54423974	-3.01576632	0.77139572
O	1.39212174	-2.99572232	1.46785772
C	1.61211974	-4.27163532	2.11208872
H	3.97221674	1.79783368	-2.36304928
H	2.09281874	3.74464068	-2.56709028
H	-0.04776426	2.91734568	-1.10008728
H	-1.83242626	-0.10691332	1.18403472
H	-0.11275126	-1.77346532	-4.28487728
H	0.19970974	-0.05817832	-3.93832828
H	-1.47038526	-0.67141332	-3.93329028
H	5.35927374	0.47837568	0.25790972
H	7.61858574	-0.16611132	-0.53063028

TS14

Zero-point correction = 0,566234
Thermal correction to Energy = 0,623784
Thermal correction to Enthalpy = 0,624915
Thermal correction to Gibbs Free Energy = 0,460626
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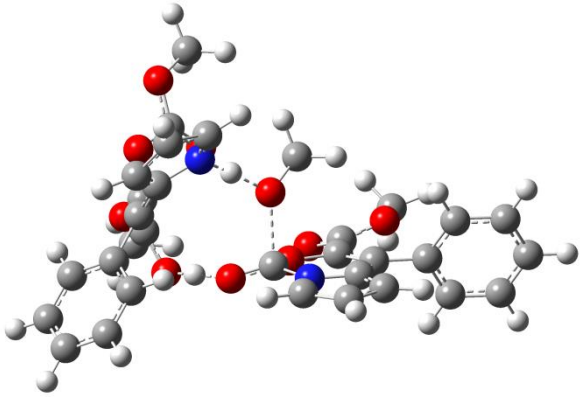
H = -2098.650385, G = -2098.814674.
Imaginary frequency = 1.



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C	-0.41485451	-1.51462354	-1.16808425
C	2.40966649	-1.32751154	-0.86599625
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C	1.66362749	-0.30817854	-1.37821625
O	-1.57600051	-1.68317954	-1.59531425
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C	-0.00198251	0.16437146	1.37254575
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C	6.14709149	-1.34951054	-1.53334325
C	6.66263949	-1.34073554	-0.23315225
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O	1.41312749	1.75610946	-2.54308525
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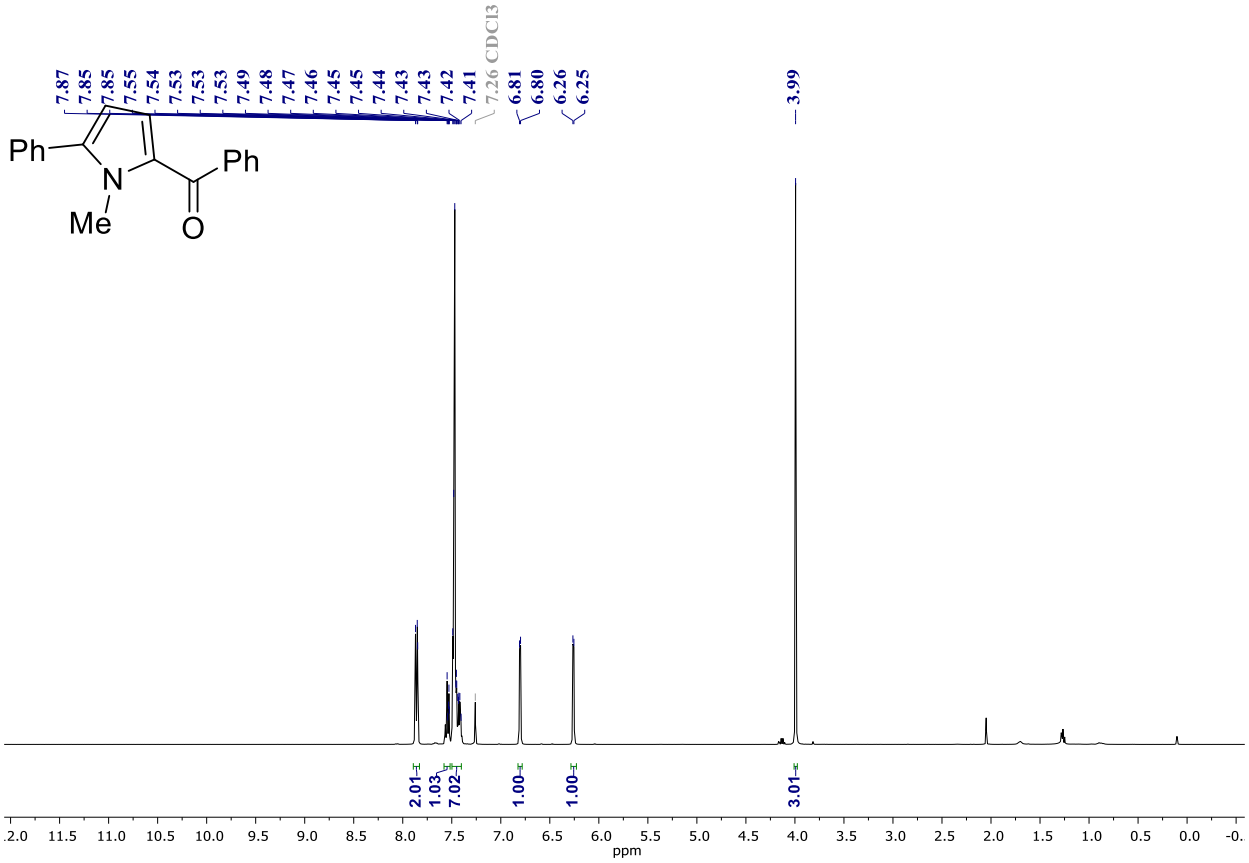
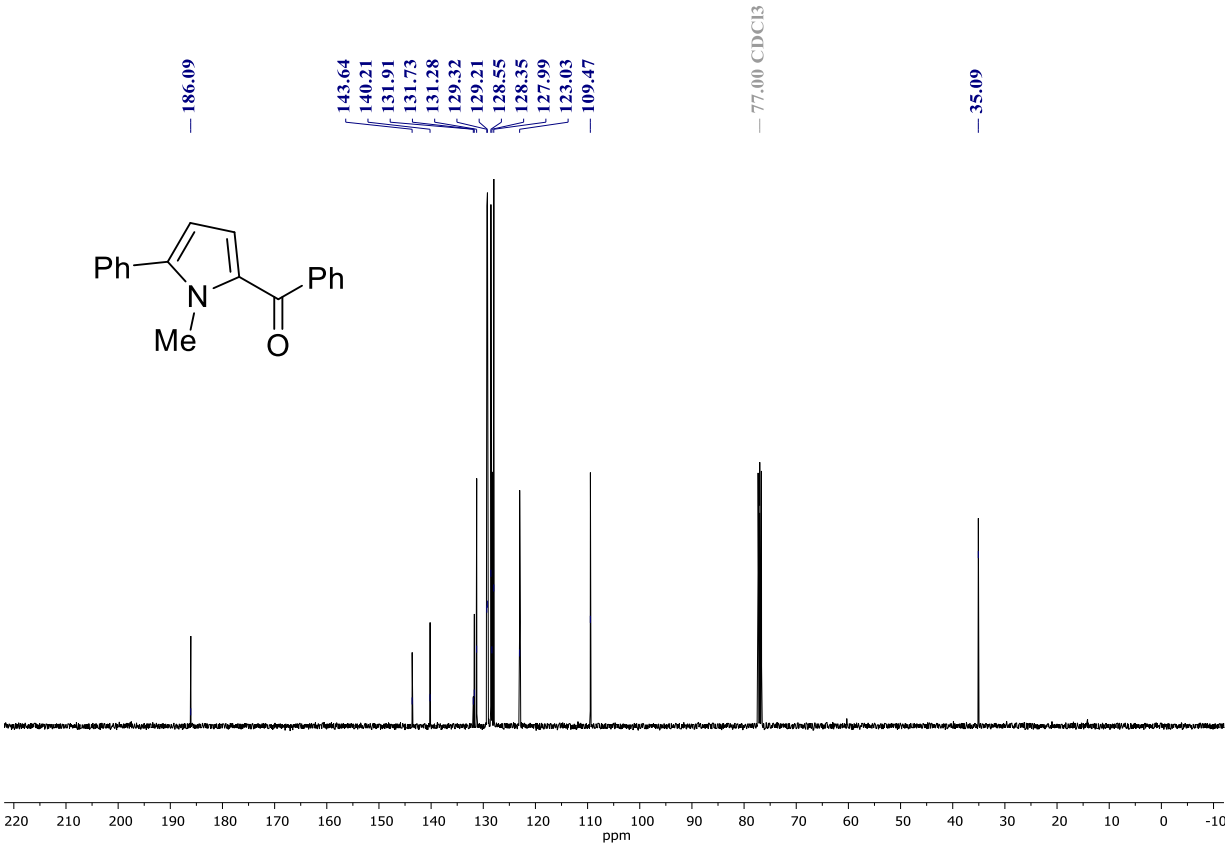
12. NMR spectra of new compounds

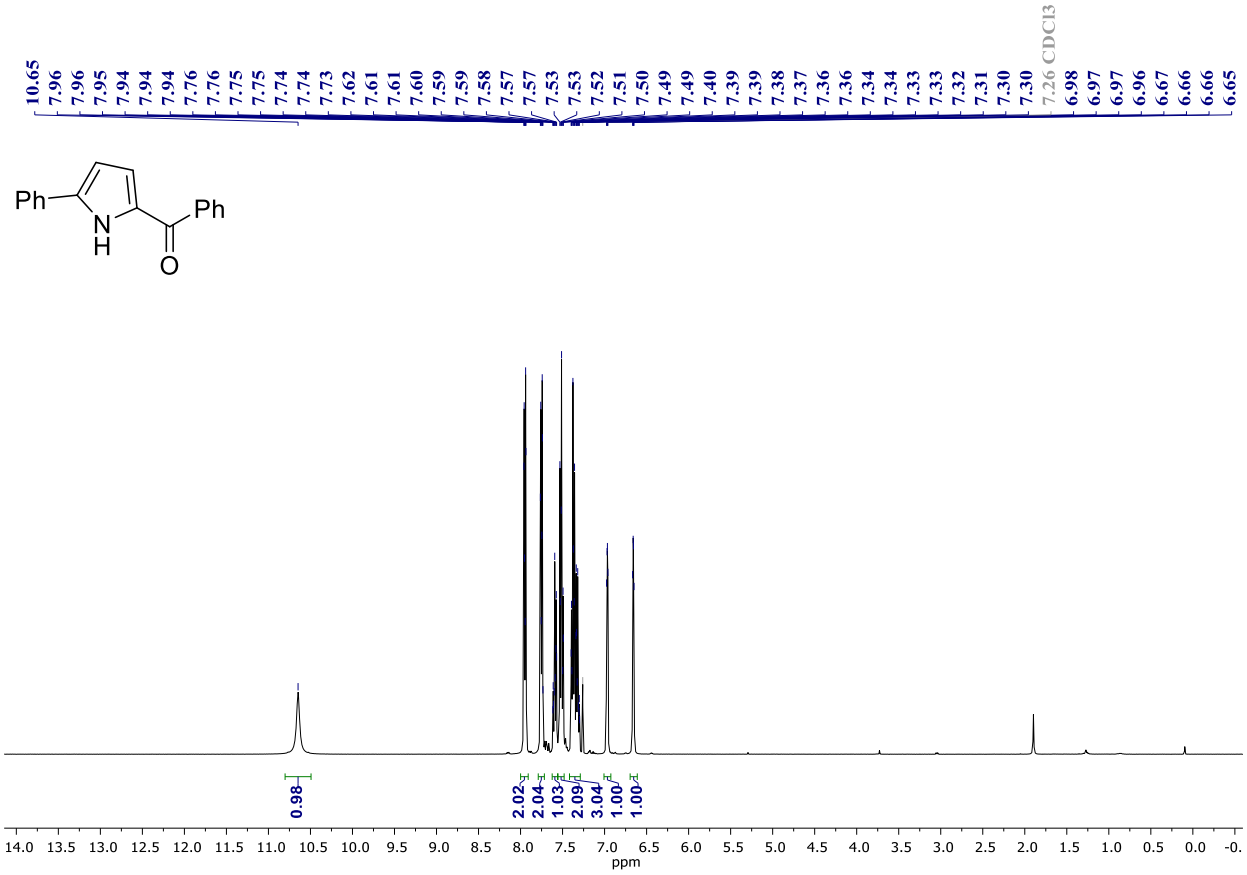
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound **1**



^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) spectrum of compound **1**



^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound **2a**



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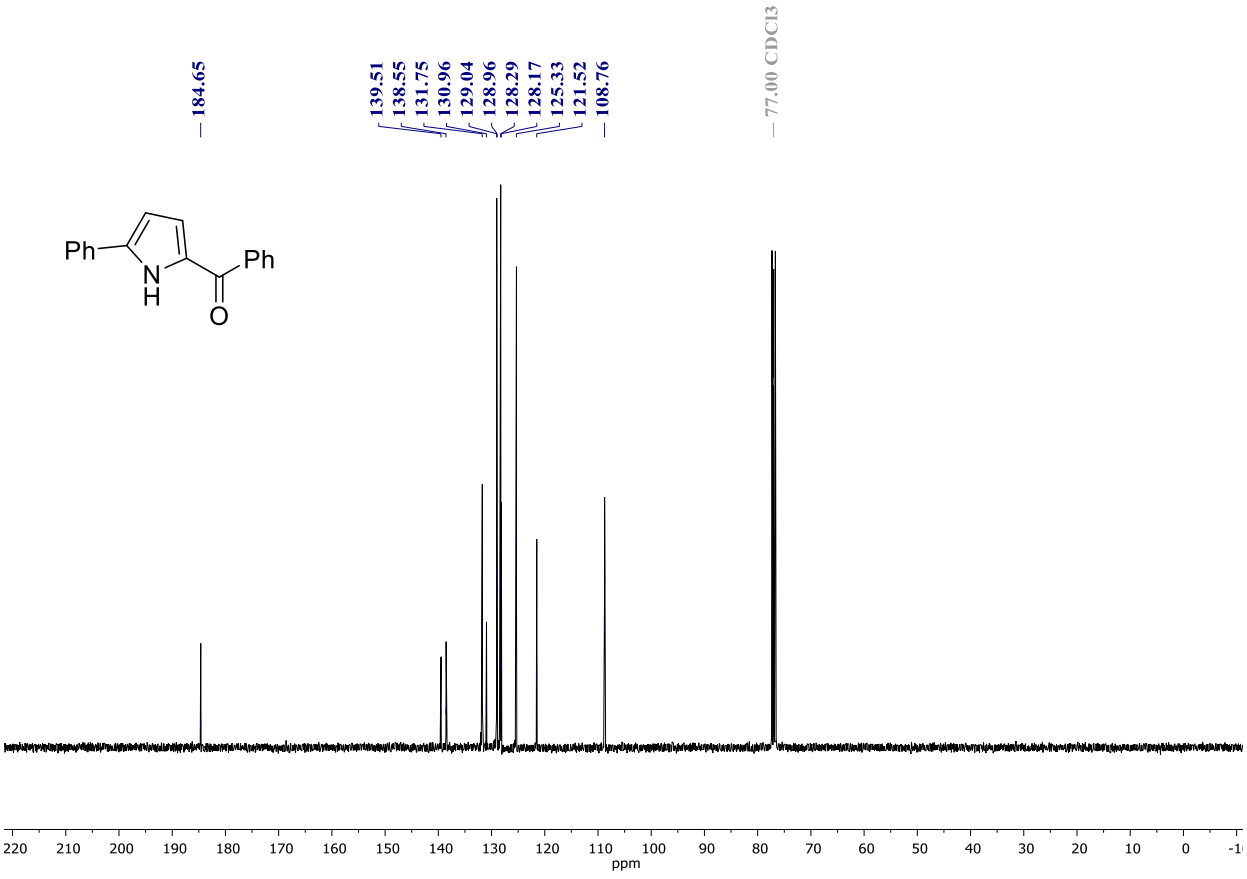
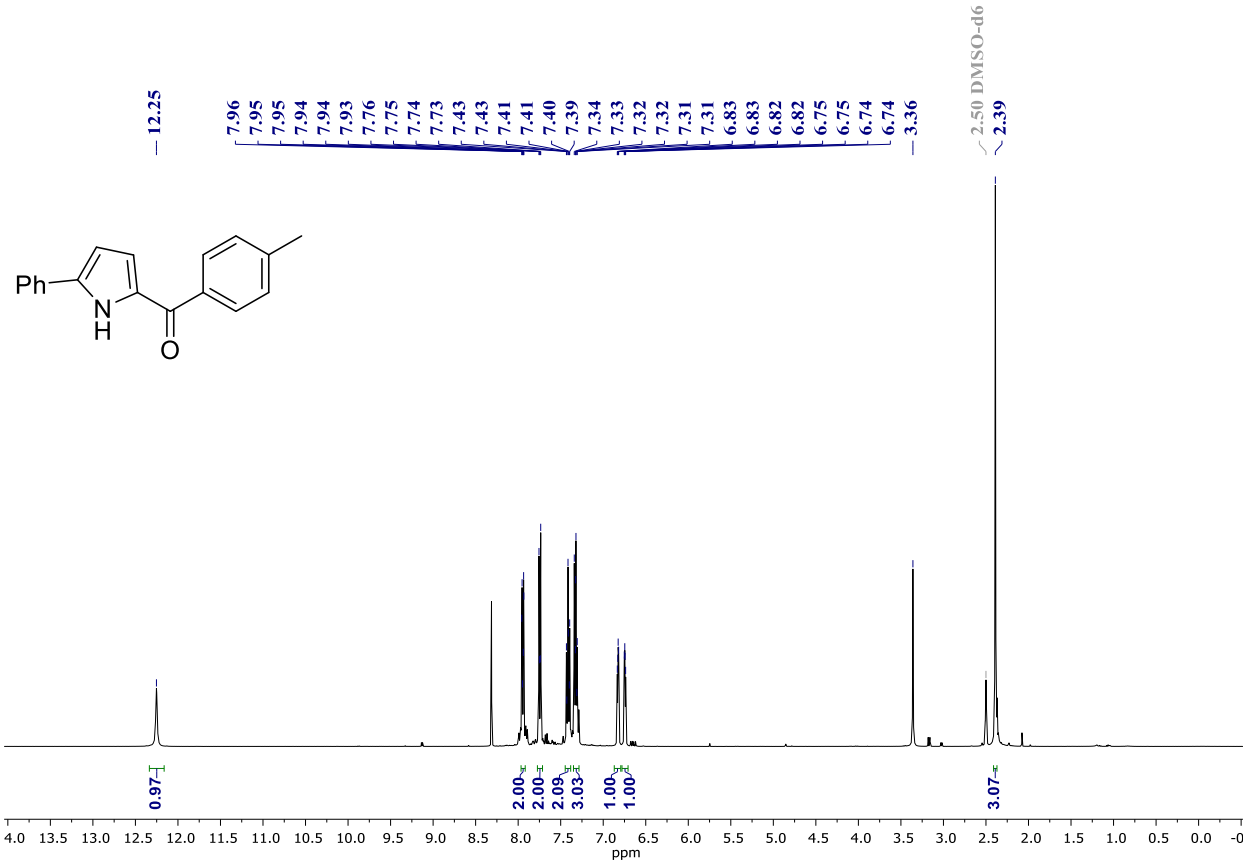
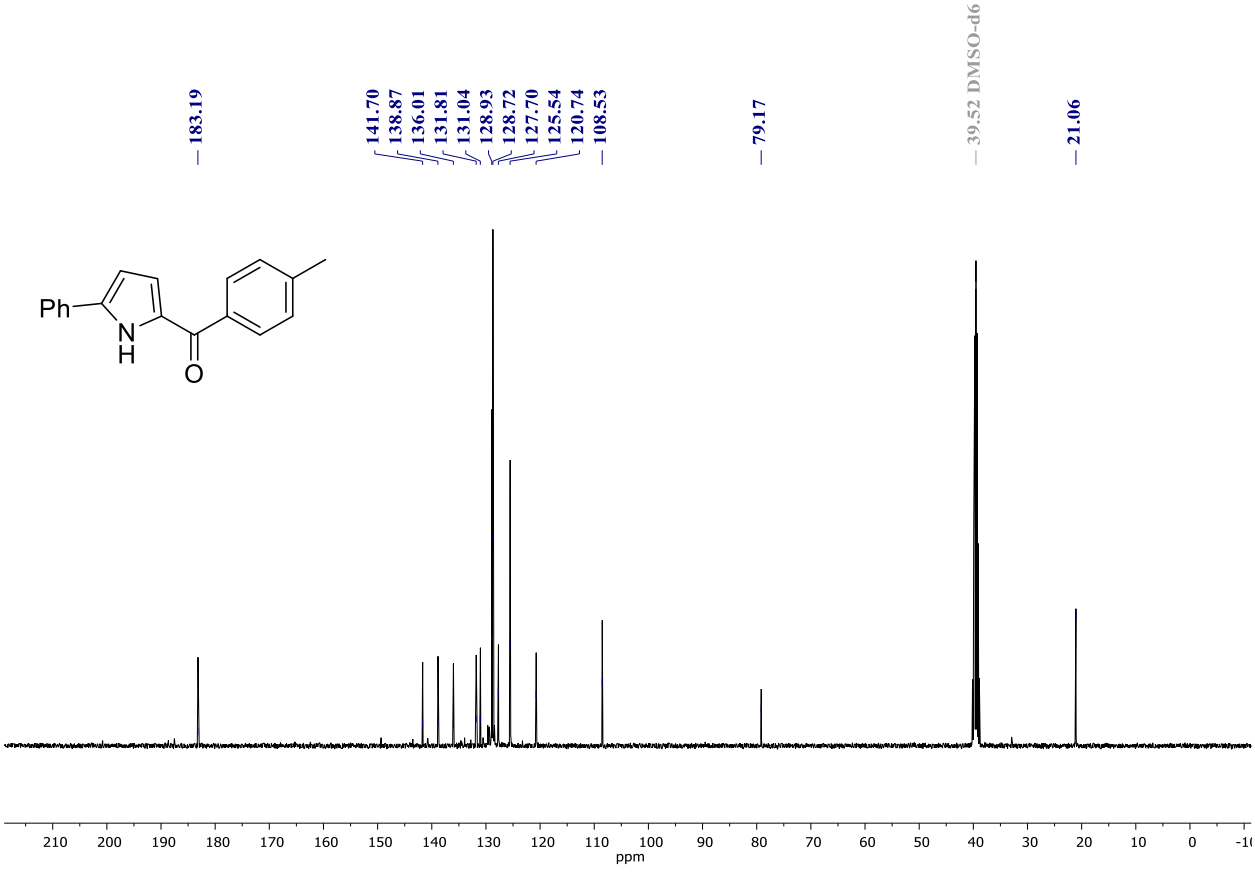


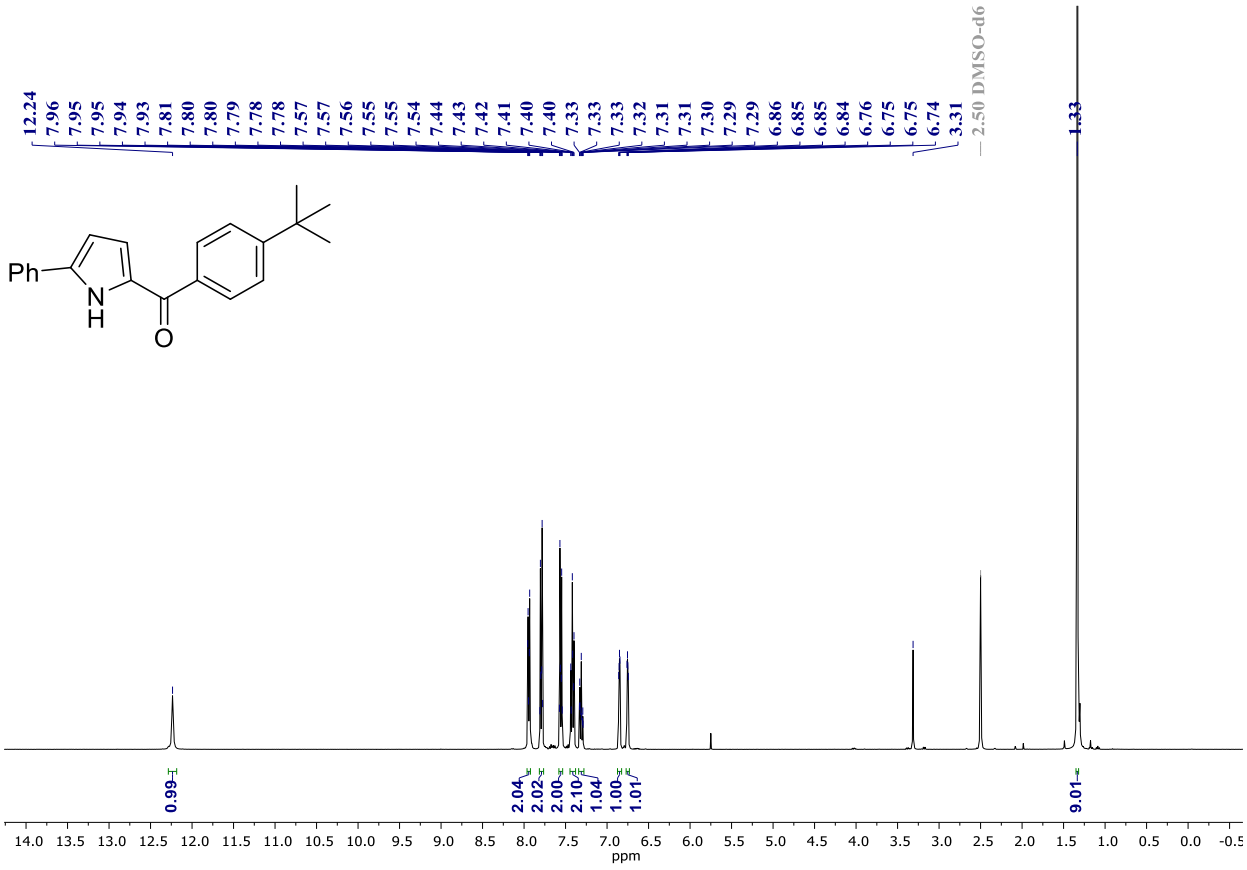
^{1}H NMR (400 MHz, $CDCl_3$/DMSO-d_6) spectrum of compound **2b**



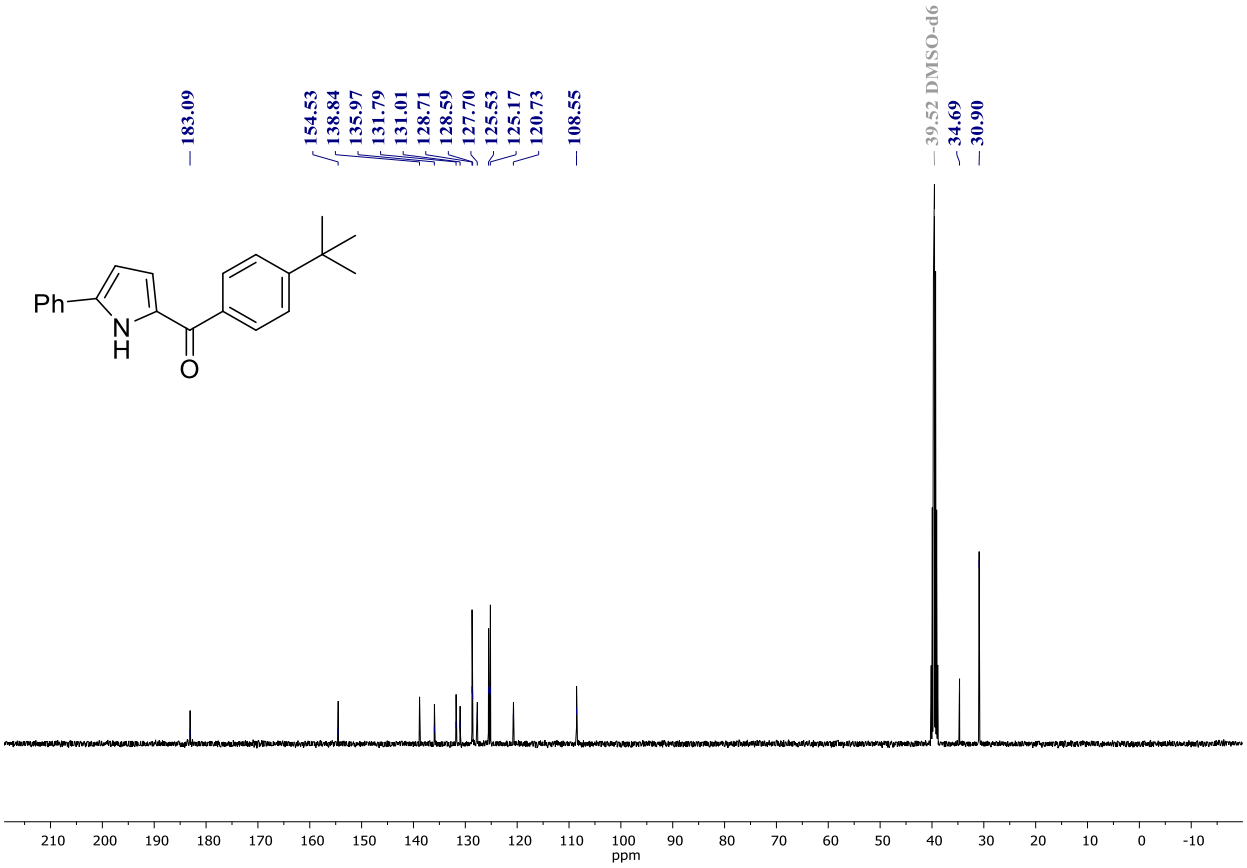
^{13}C{^{1}H} NMR (100 MHz, DMSO-d_6) spectrum of compound **2b**



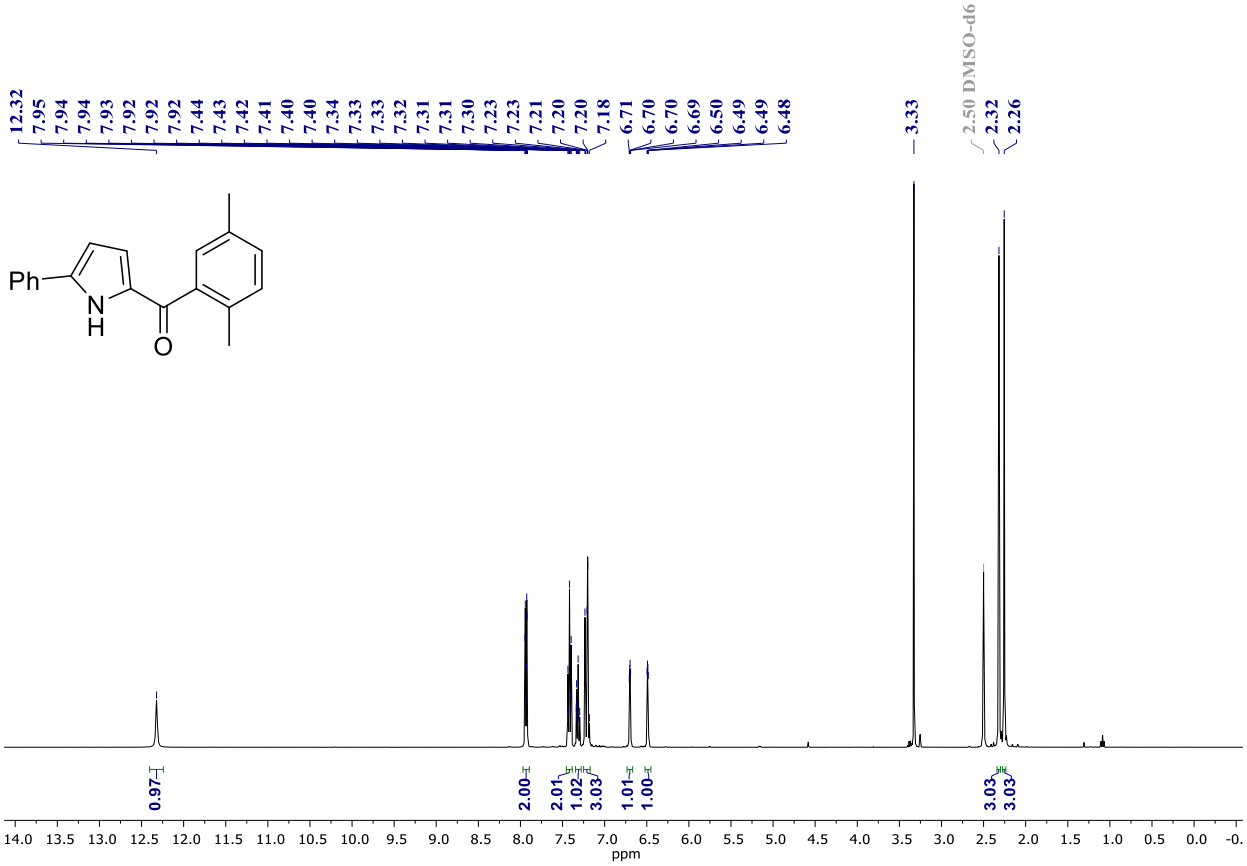
^{1}H NMR (400 MHz, DMSO-d_6) spectrum of compound **2c**



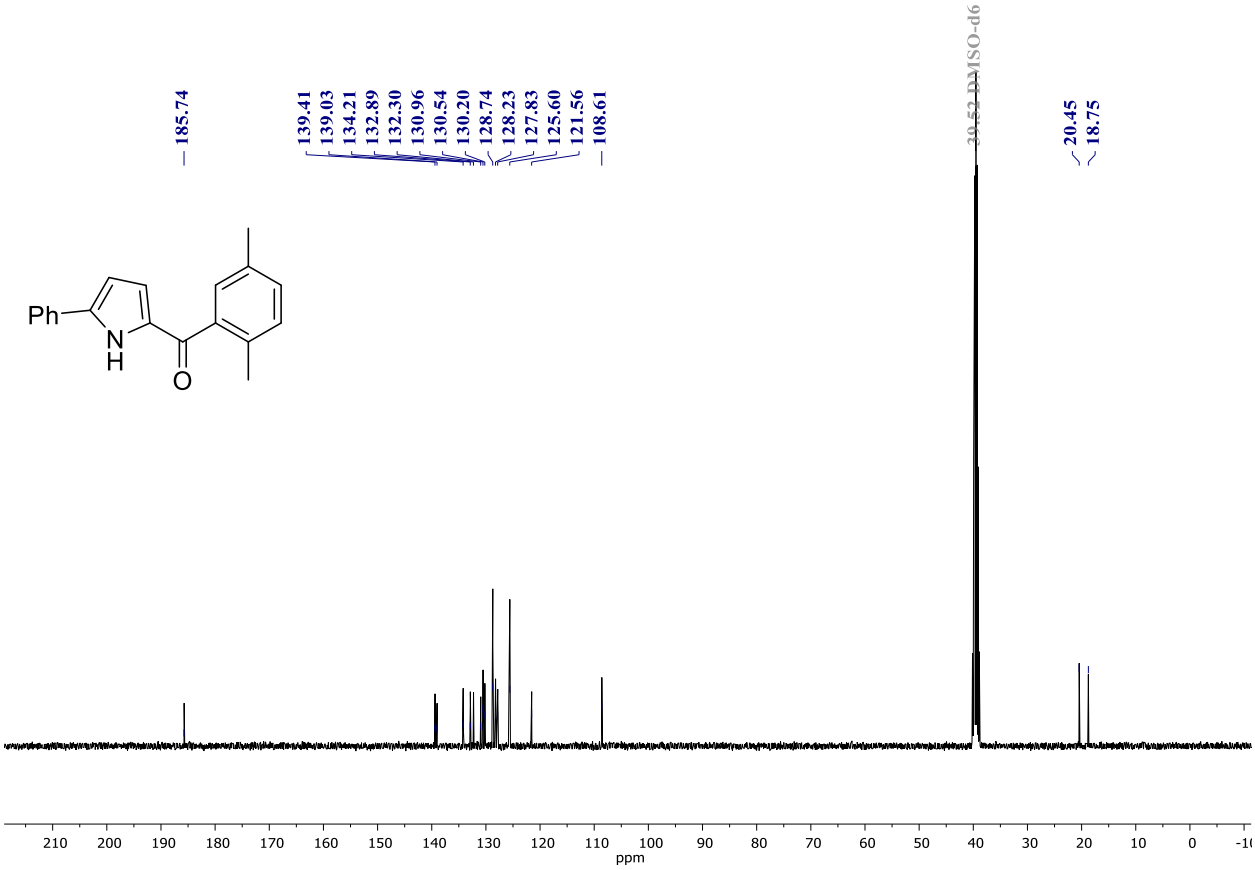
^{13}C{^{1}H} NMR (100 MHz, DMSO-d_6) spectrum of compound **2c**



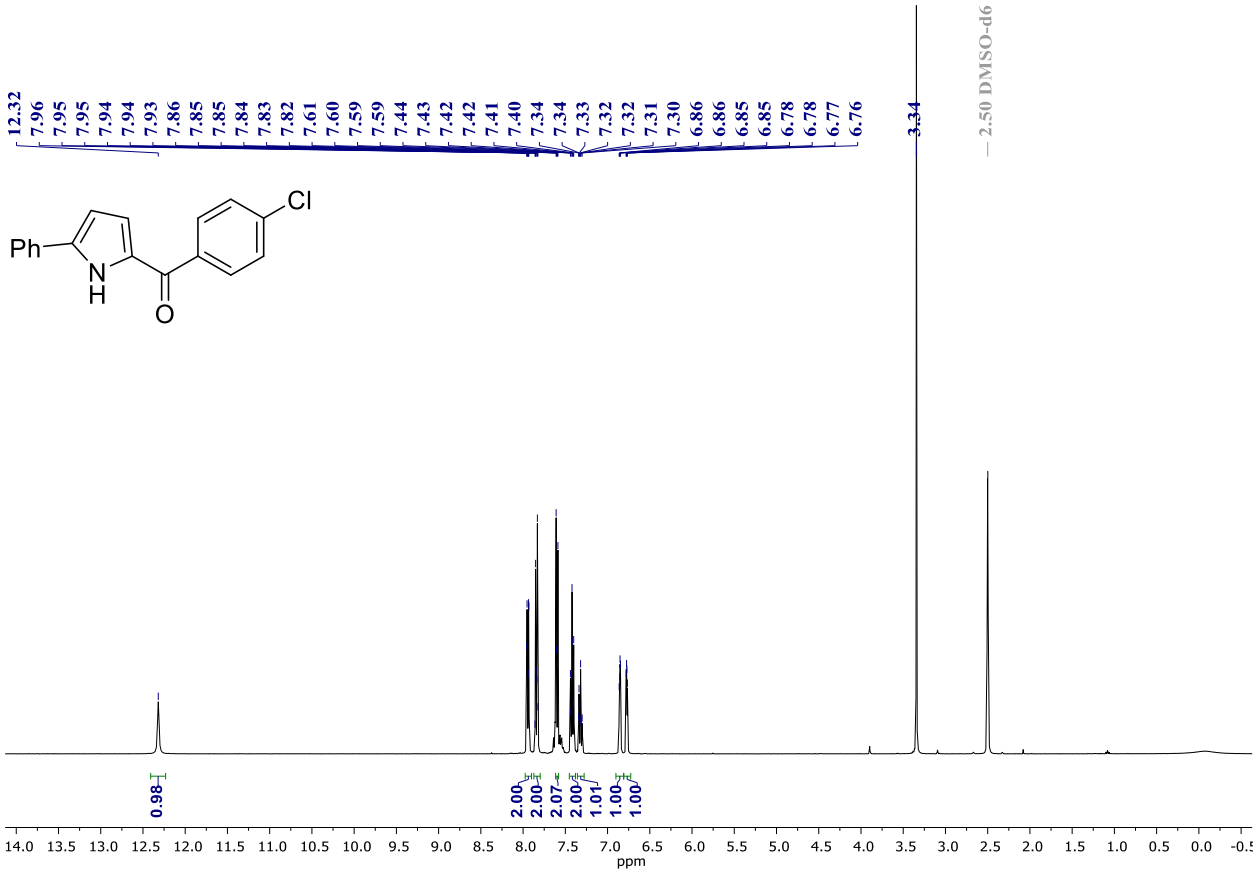
^{1}H NMR (400 MHz, DMSO-d_6) spectrum of compound **2d**



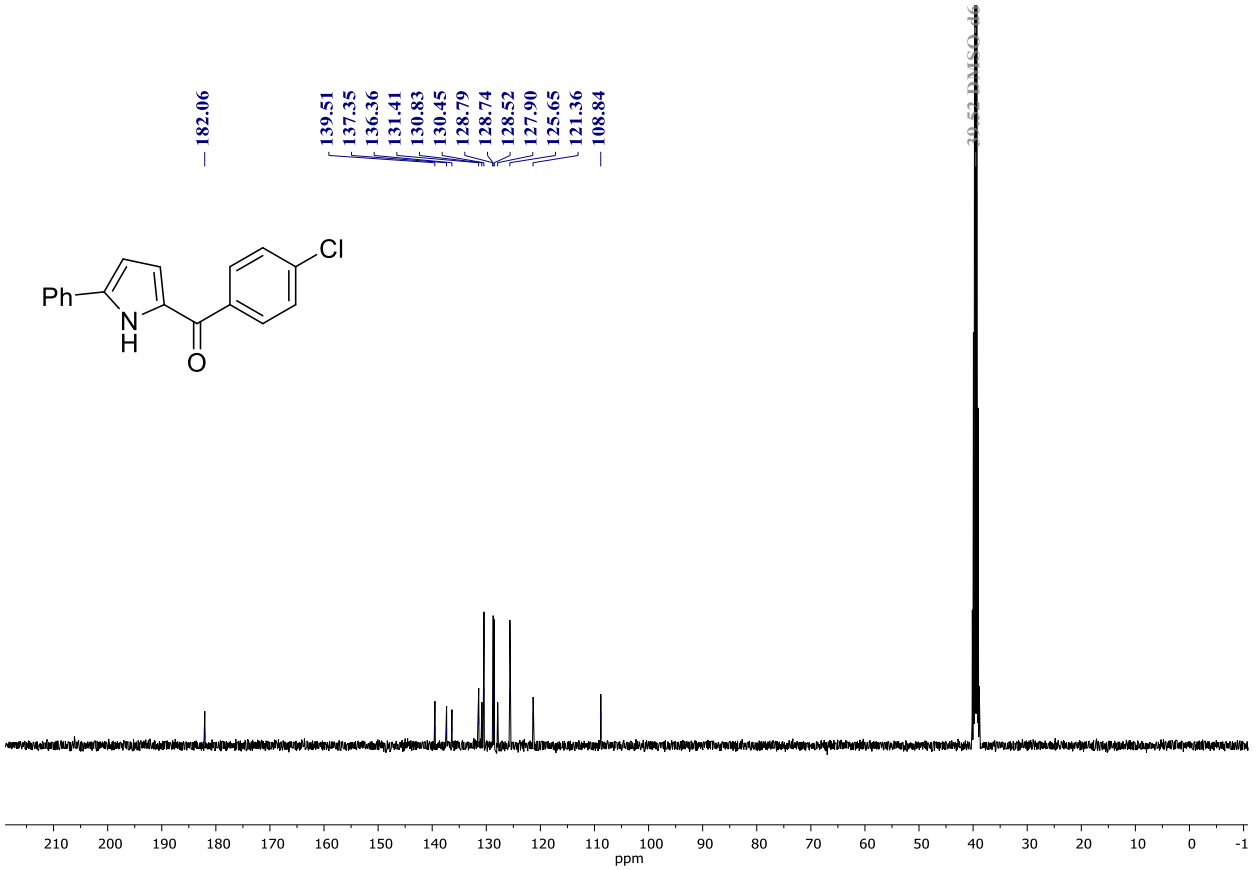
^{13}C{^{1}H} NMR (100 MHz, DMSO-d_6) spectrum of compound **2d**



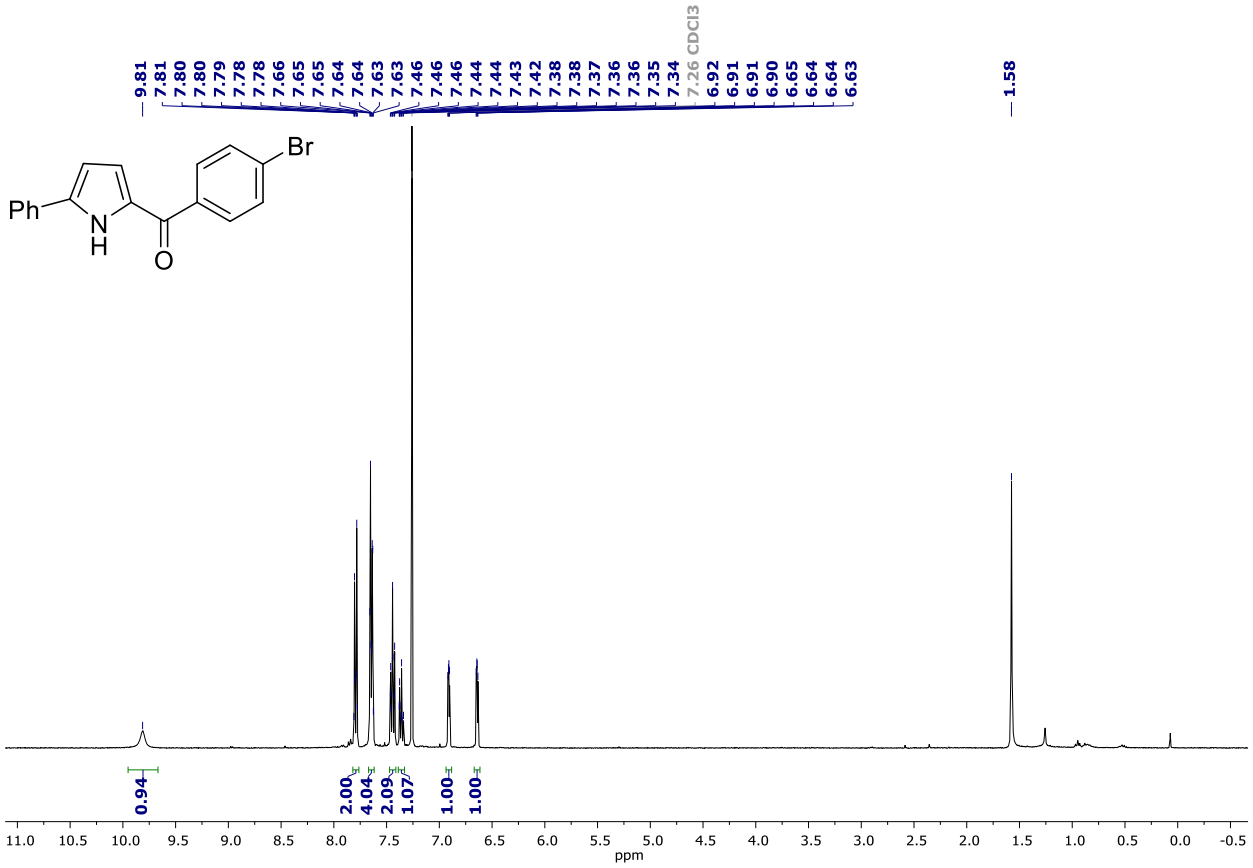
^{1}H NMR (400 MHz, DMSO-d_6) spectrum of compound **2e**



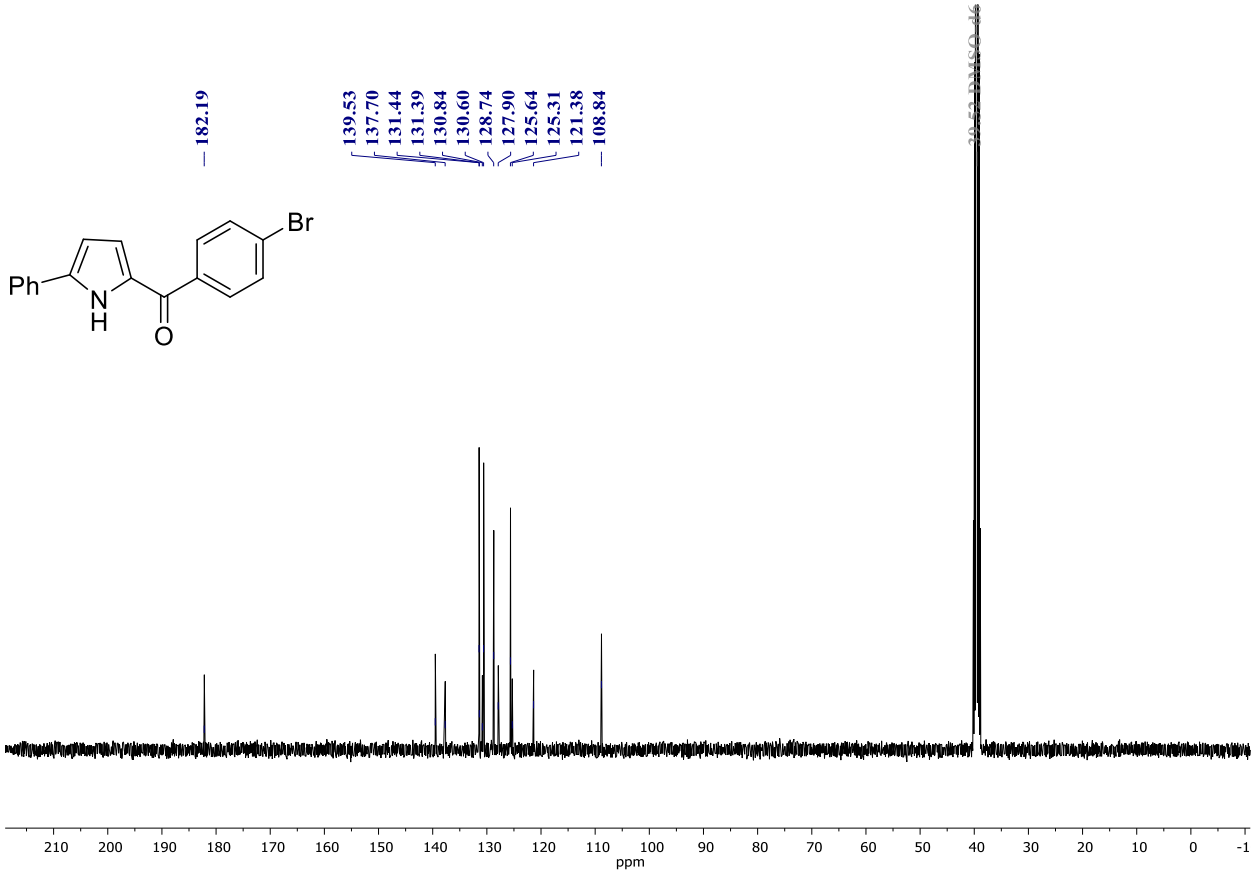
^{13}C{^{1}H} NMR (100 MHz, DMSO-d_6) spectrum of compound **2e**



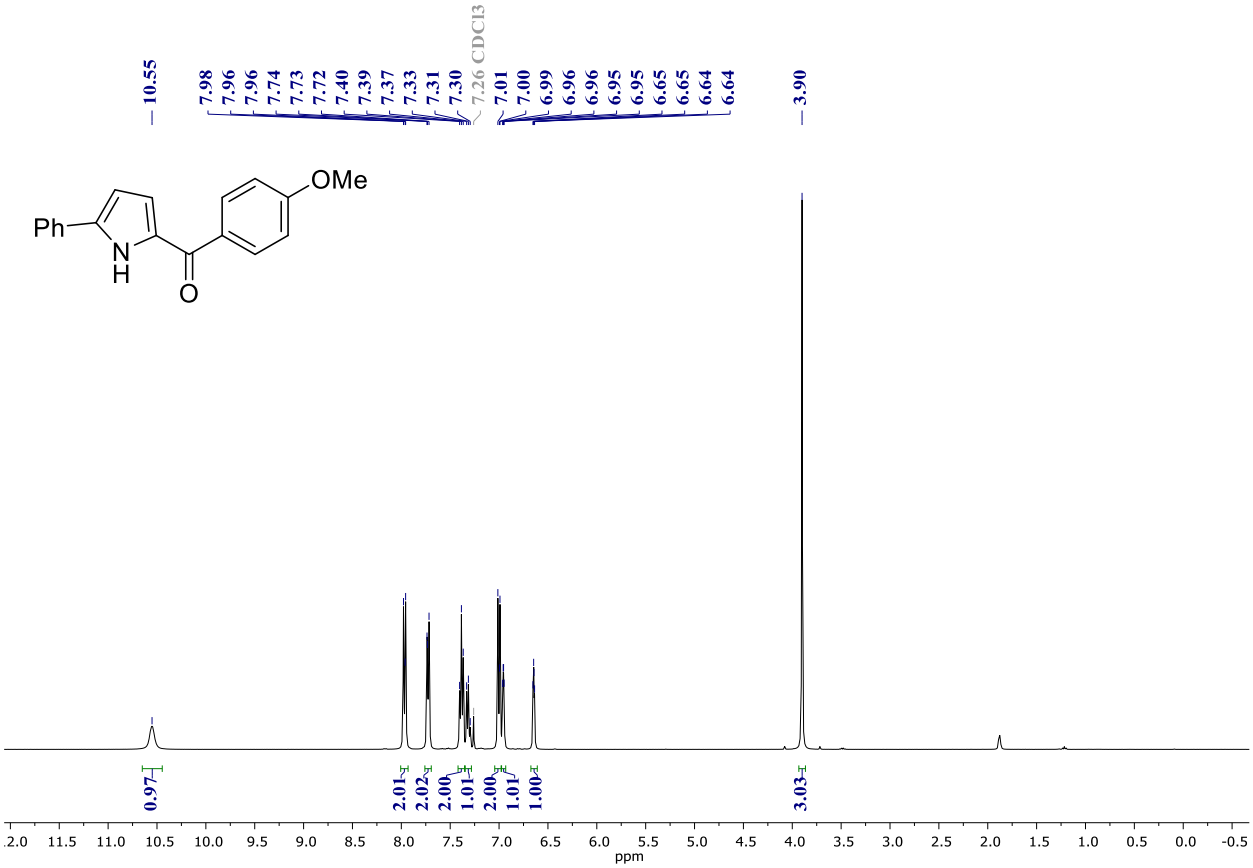
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound **2f**



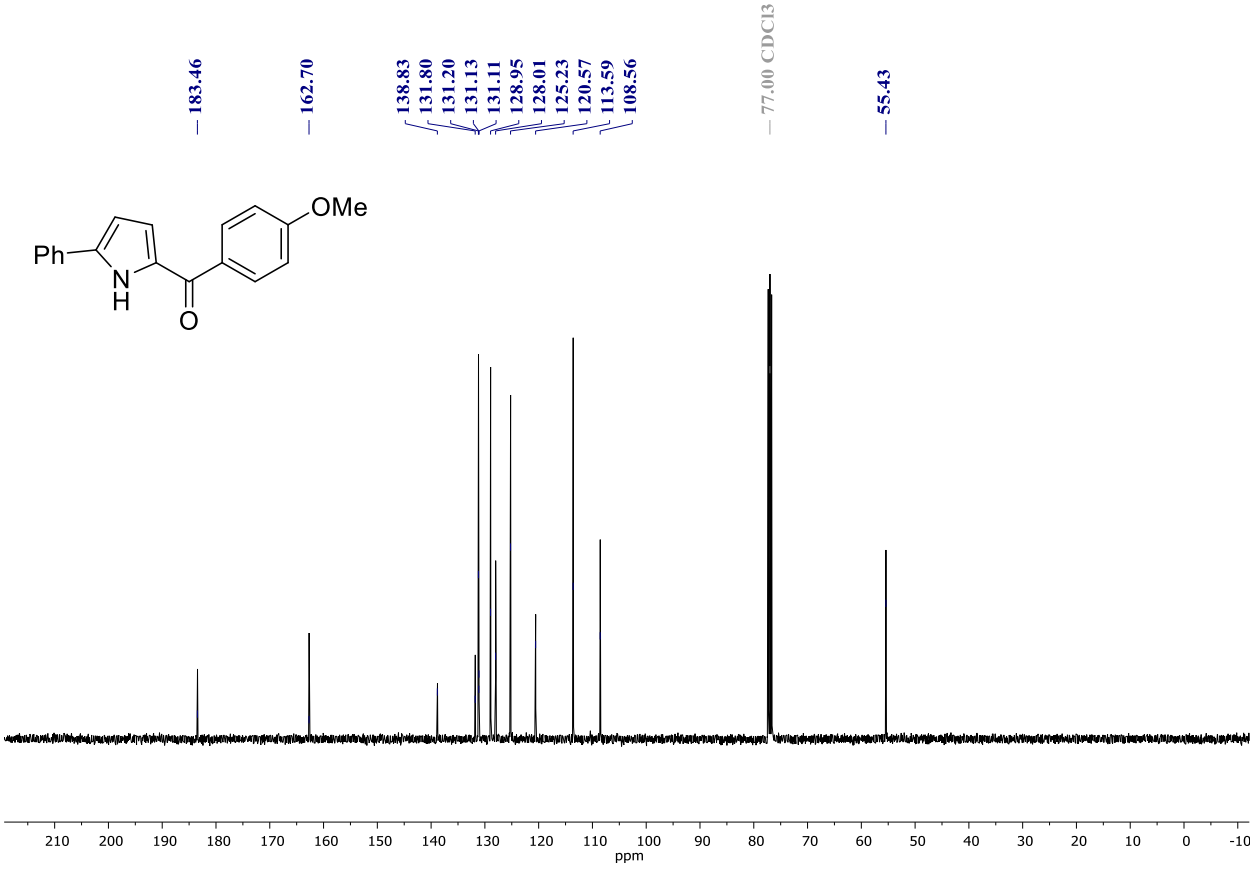
^{13}C{^{1}H} NMR (100 MHz, DMSO-d_6) spectrum of compound **2f**



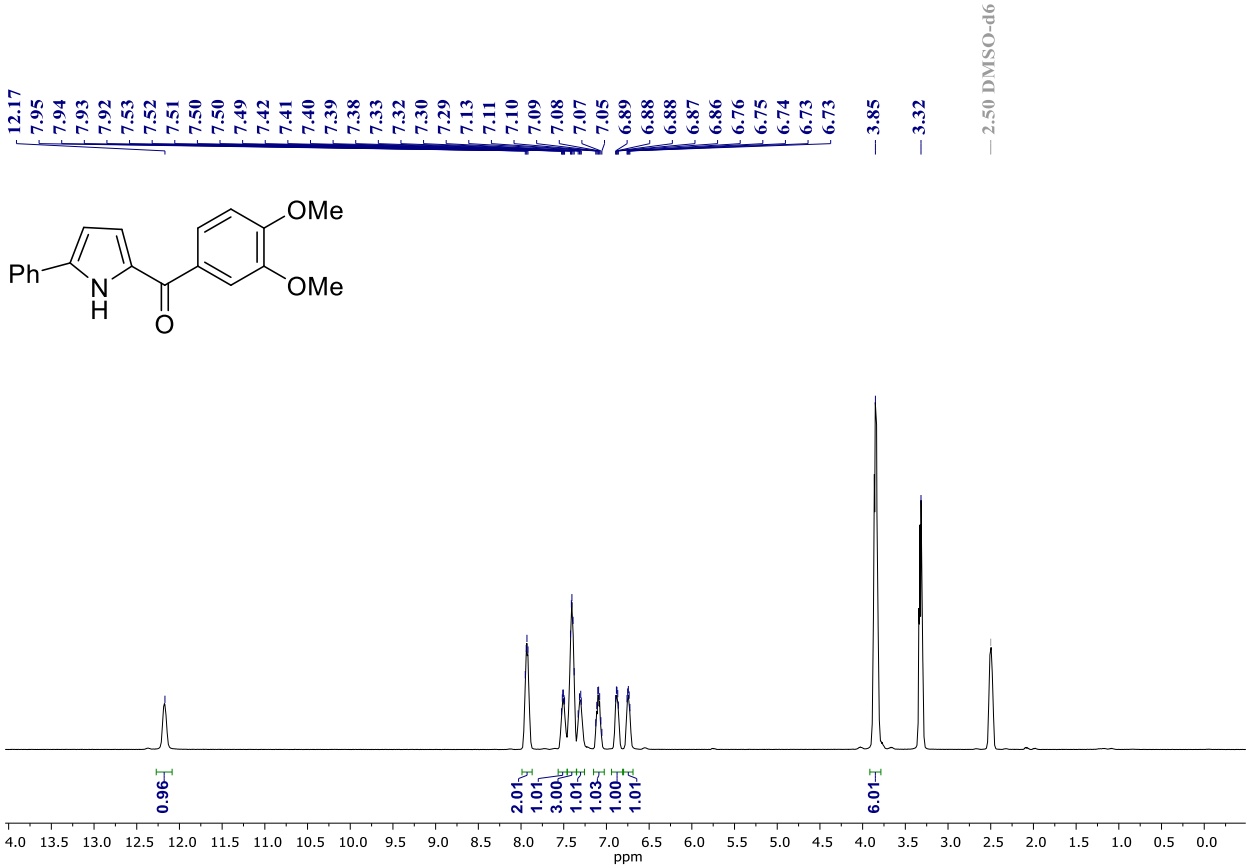
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound **2g**



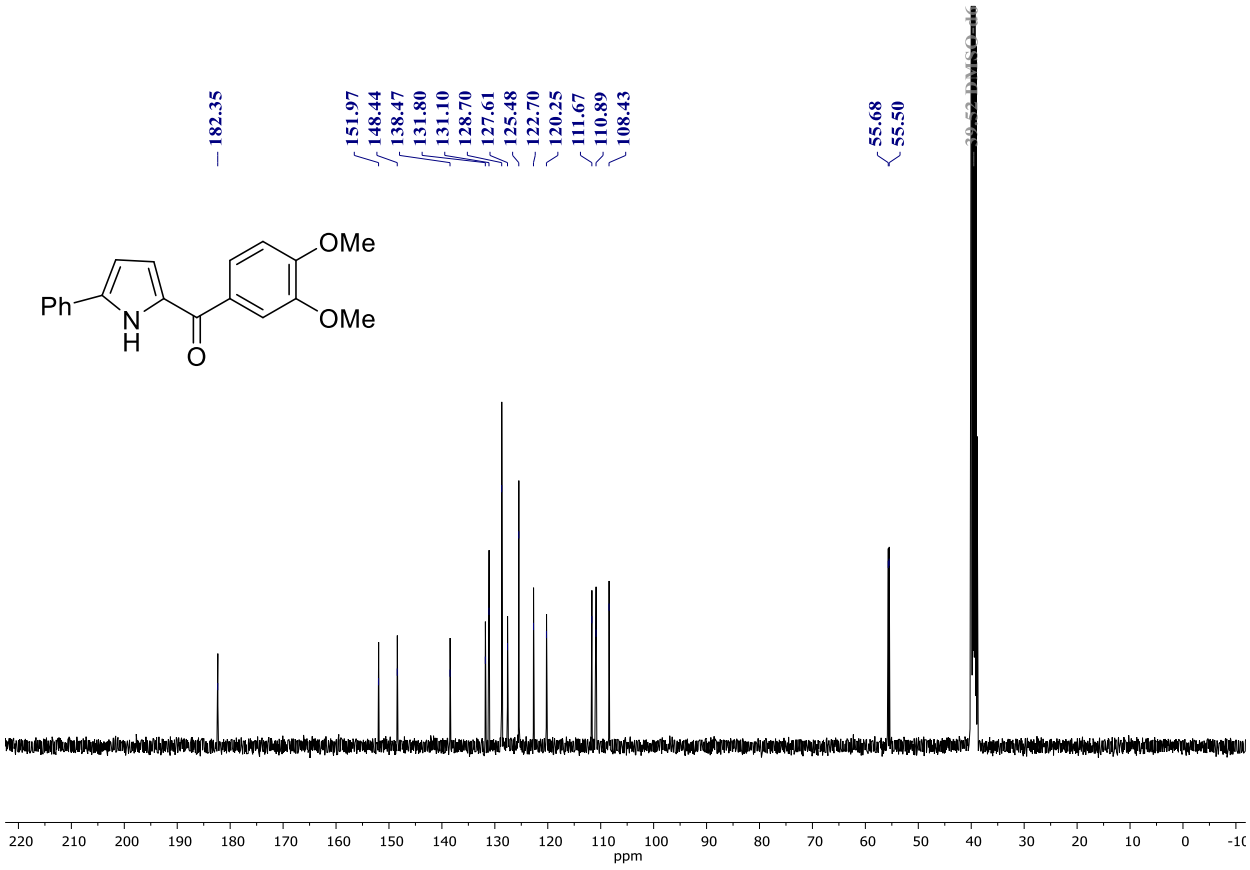
^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) spectrum of compound **2g**



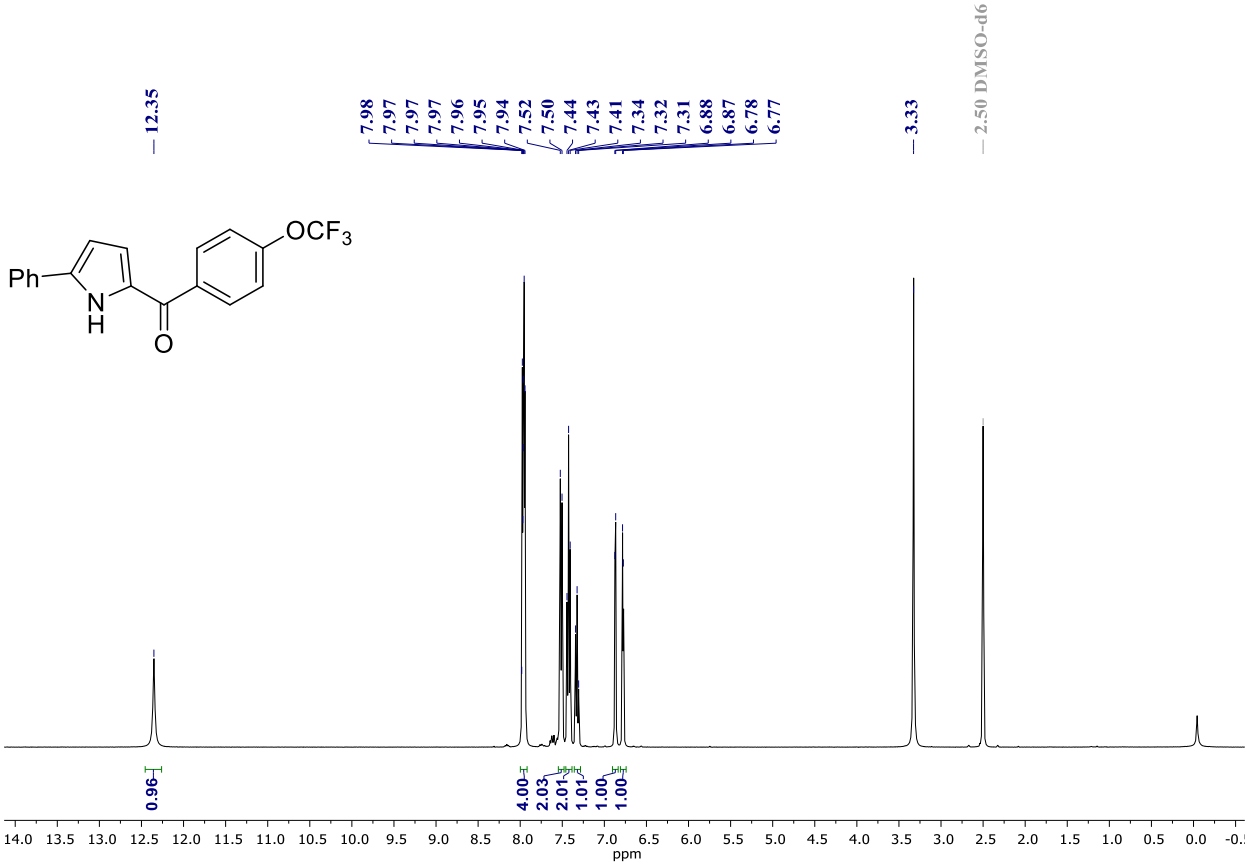
^{1}H NMR (400 MHz, DMSO-d_6) spectrum of compound **2h**



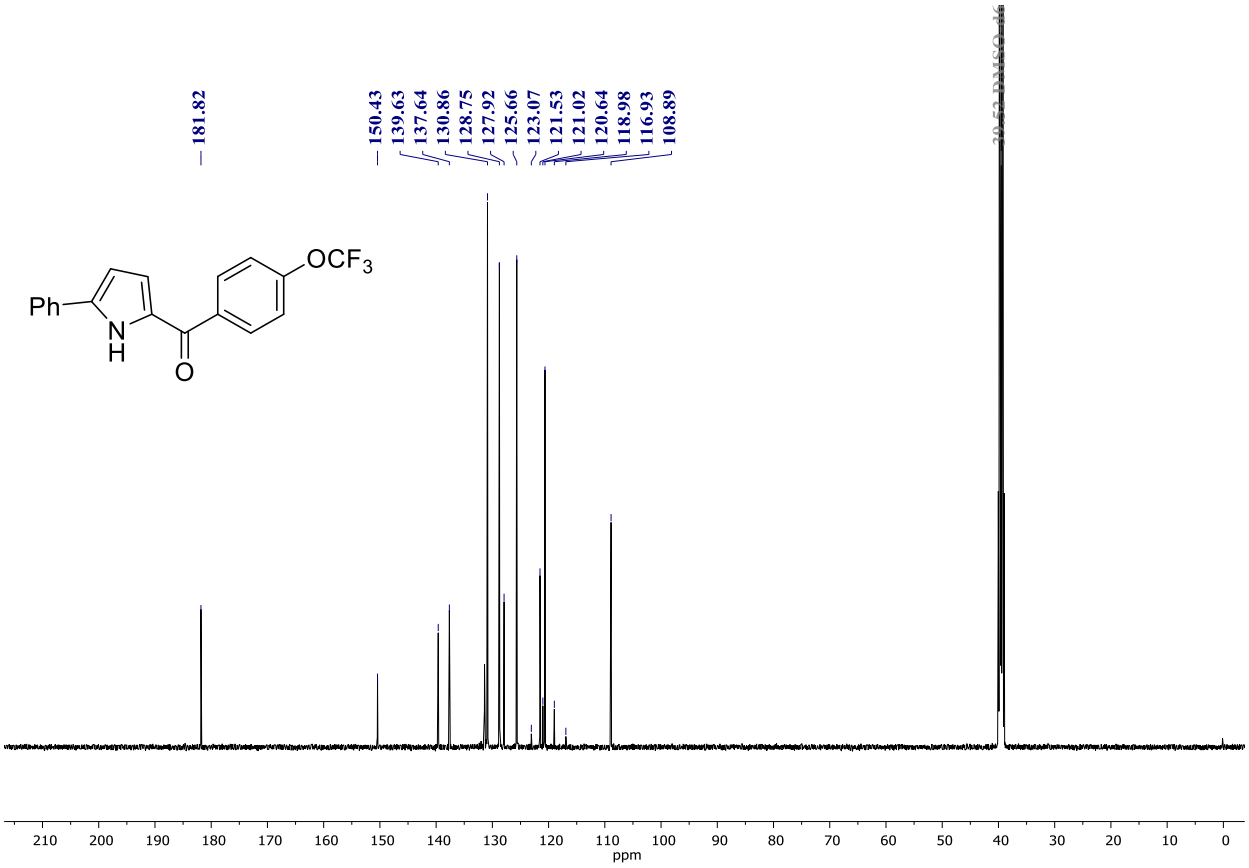
^{13}C{^{1}H} NMR (100 MHz, DMSO-d_6) spectrum of compound **2h**



^{1}H NMR (400 MHz, DMSO-d_6) spectrum of compound **2i**

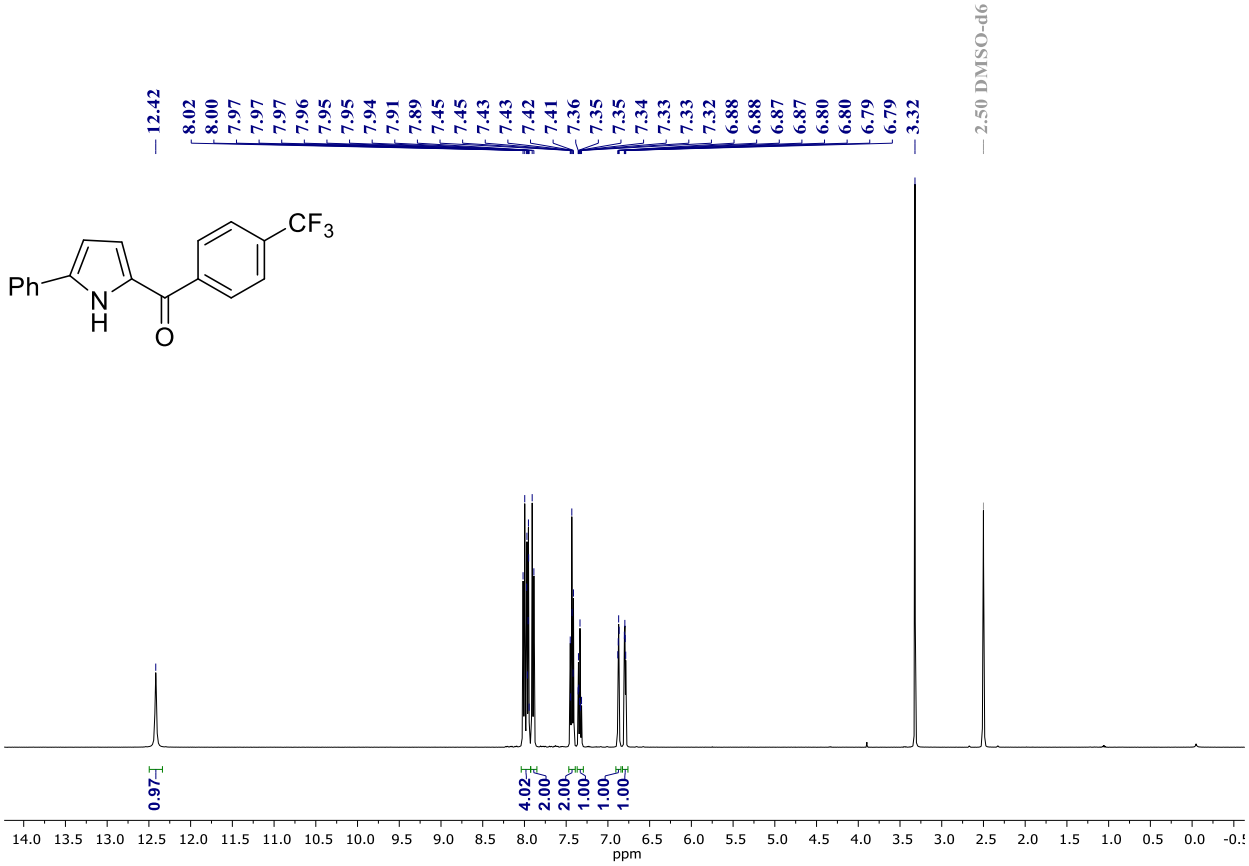


^{13}C{^{1}H} NMR (100 MHz, DMSO-d_6) spectrum of compound **2i**

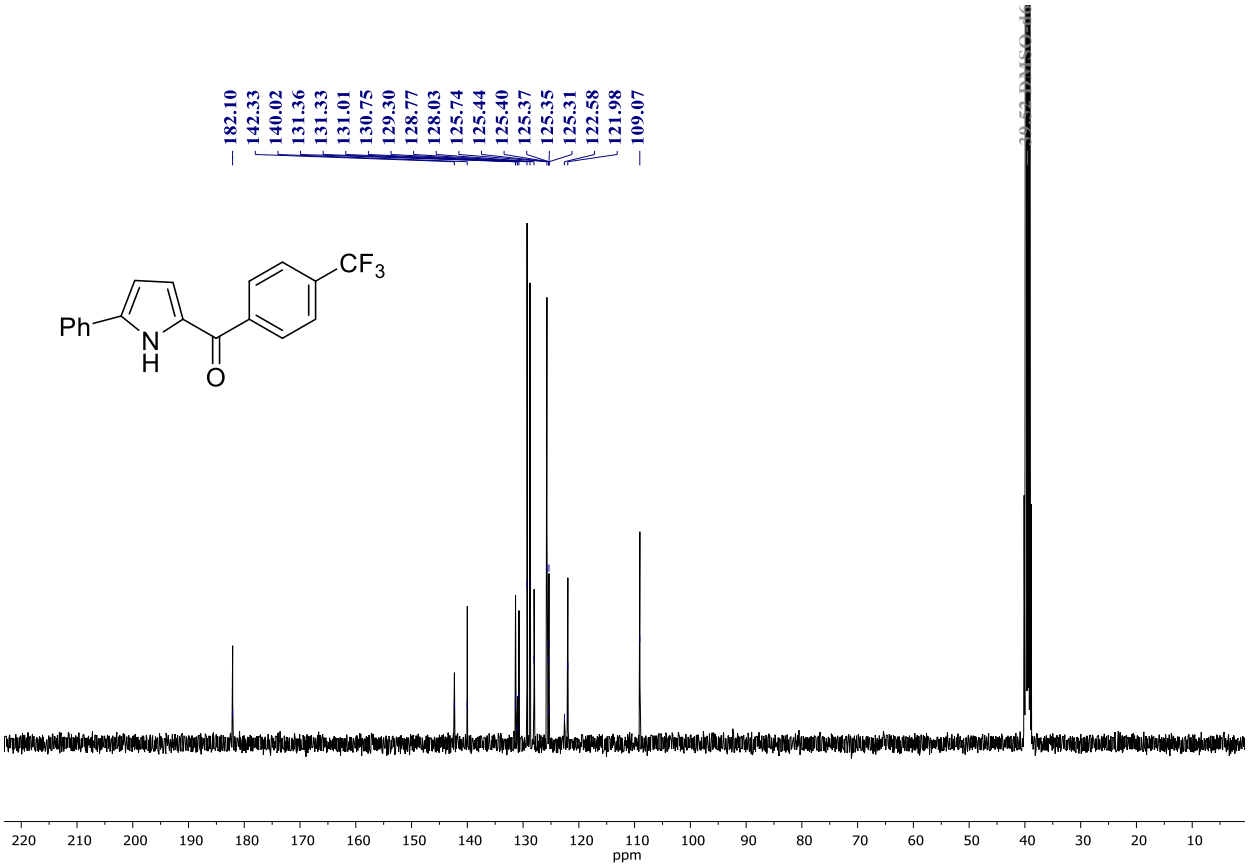


^{19}F NMR (376 MHz, DMSO-d_6) spectrum of compound **2i**

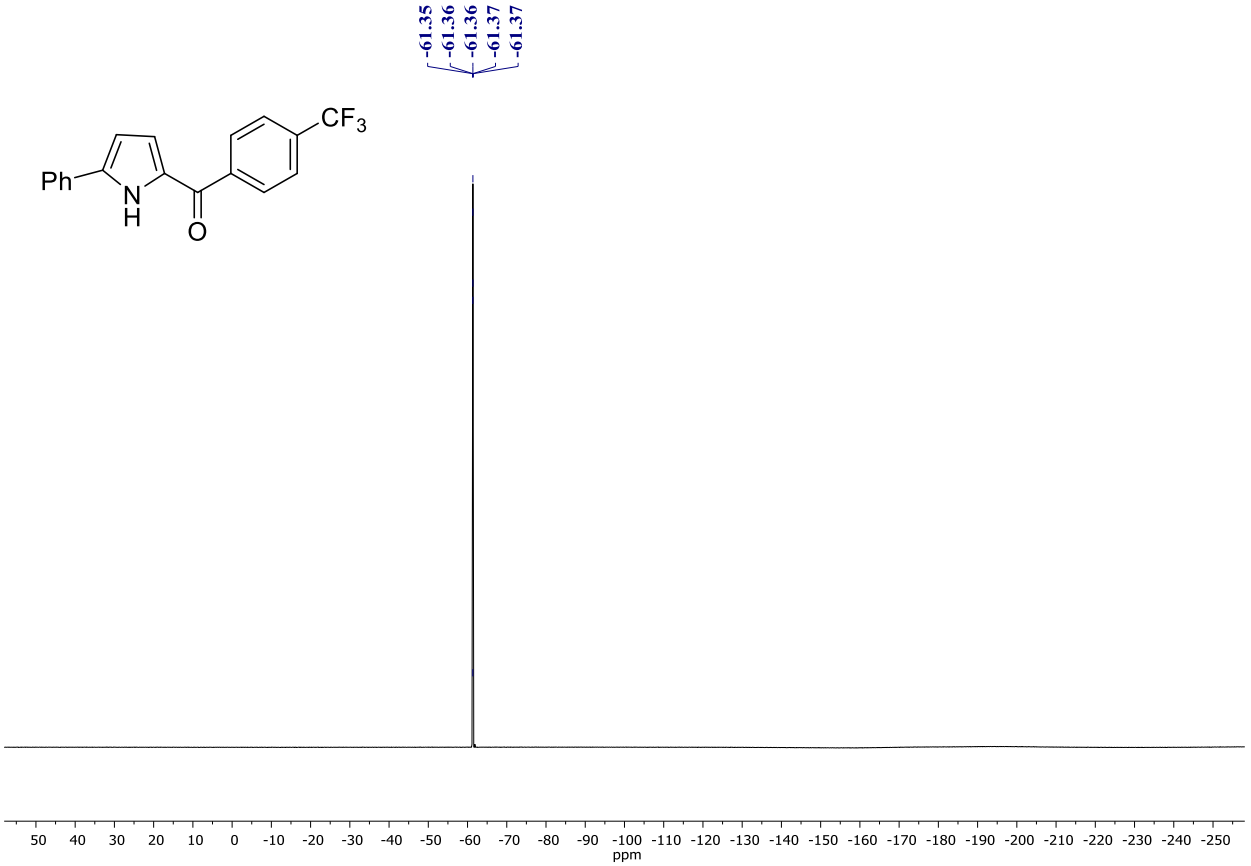
^{1}H NMR (400 MHz, DMSO-d_6) spectrum of compound **2j**



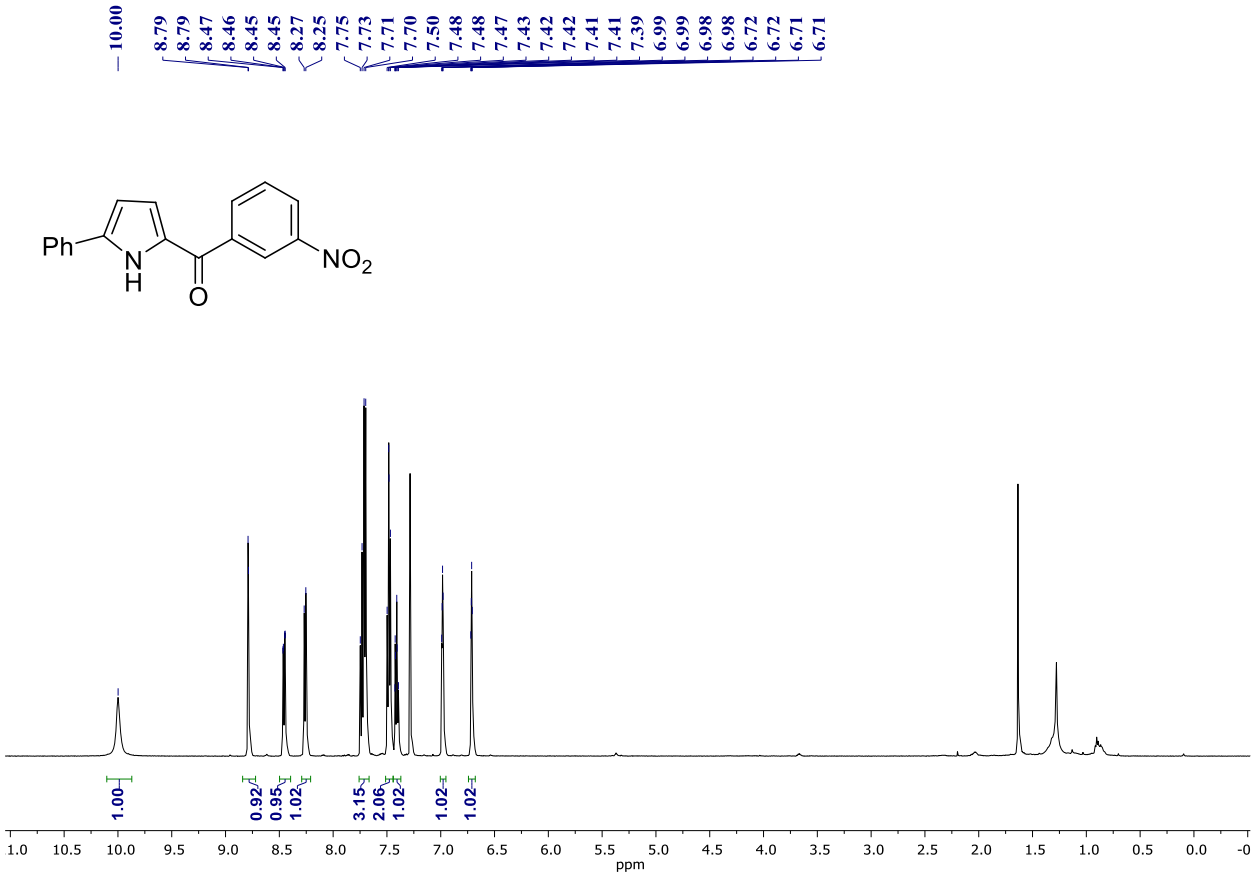
^{13}C{^{1}H} NMR (100 MHz, DMSO-d_6) spectrum of compound **2j**



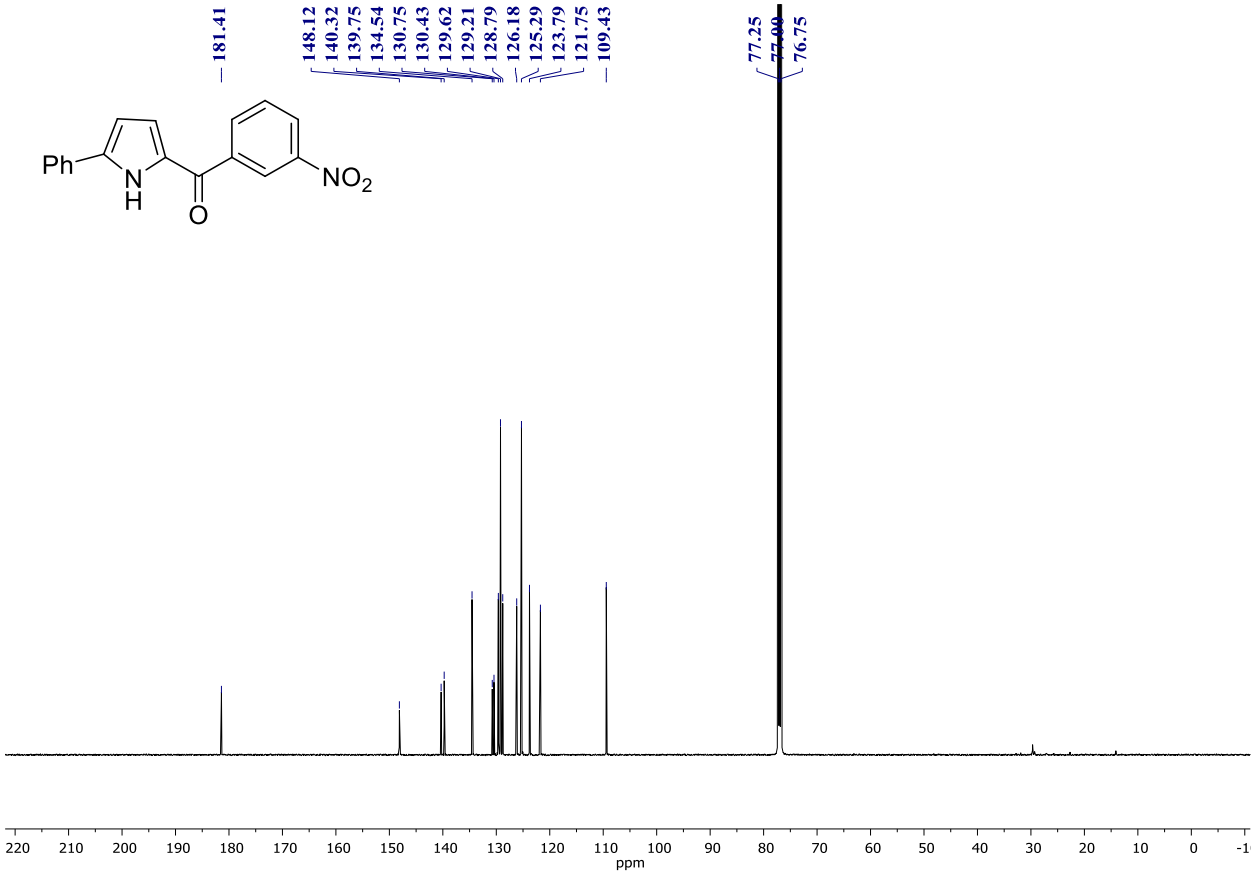
^{19}F NMR (376 MHz, DMSO-d_6) spectrum of compound **2j**



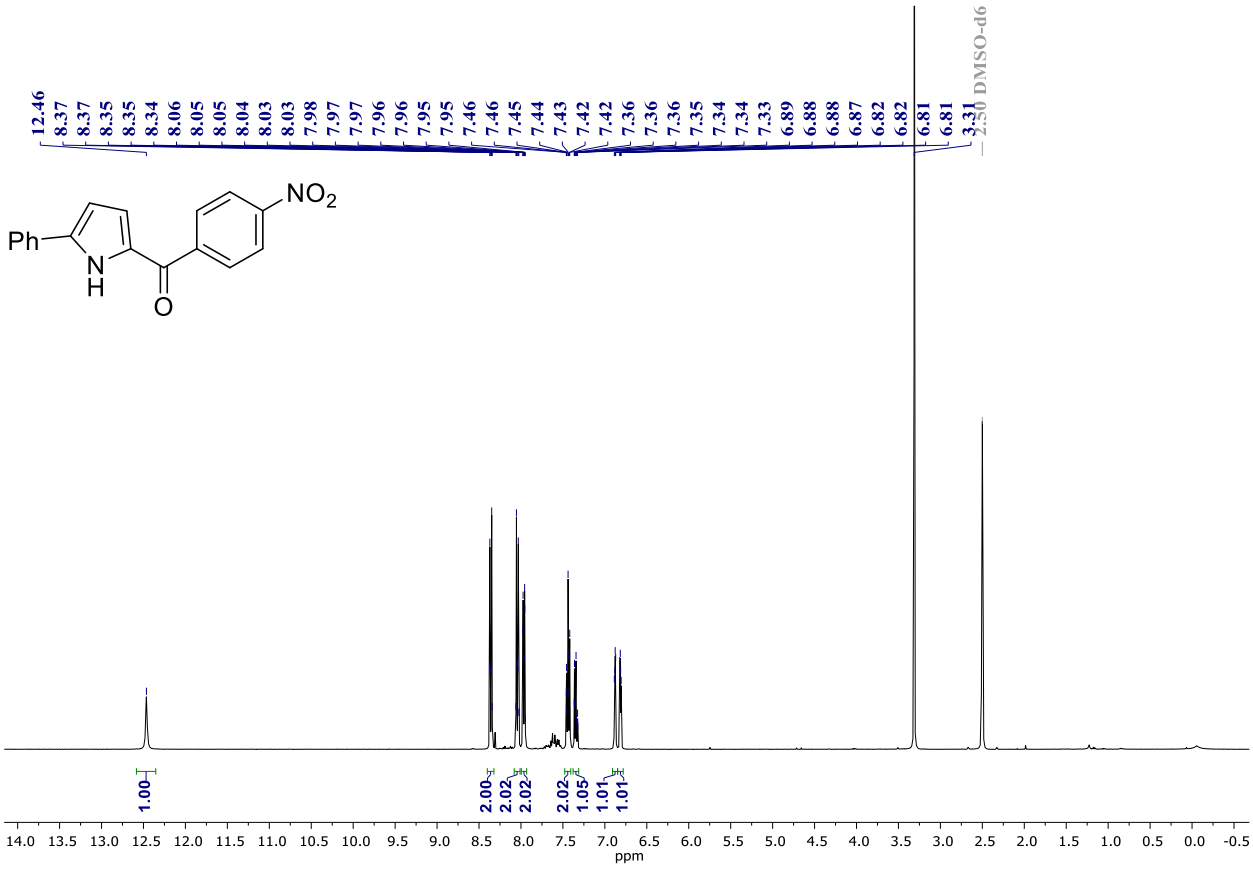
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound **2k**



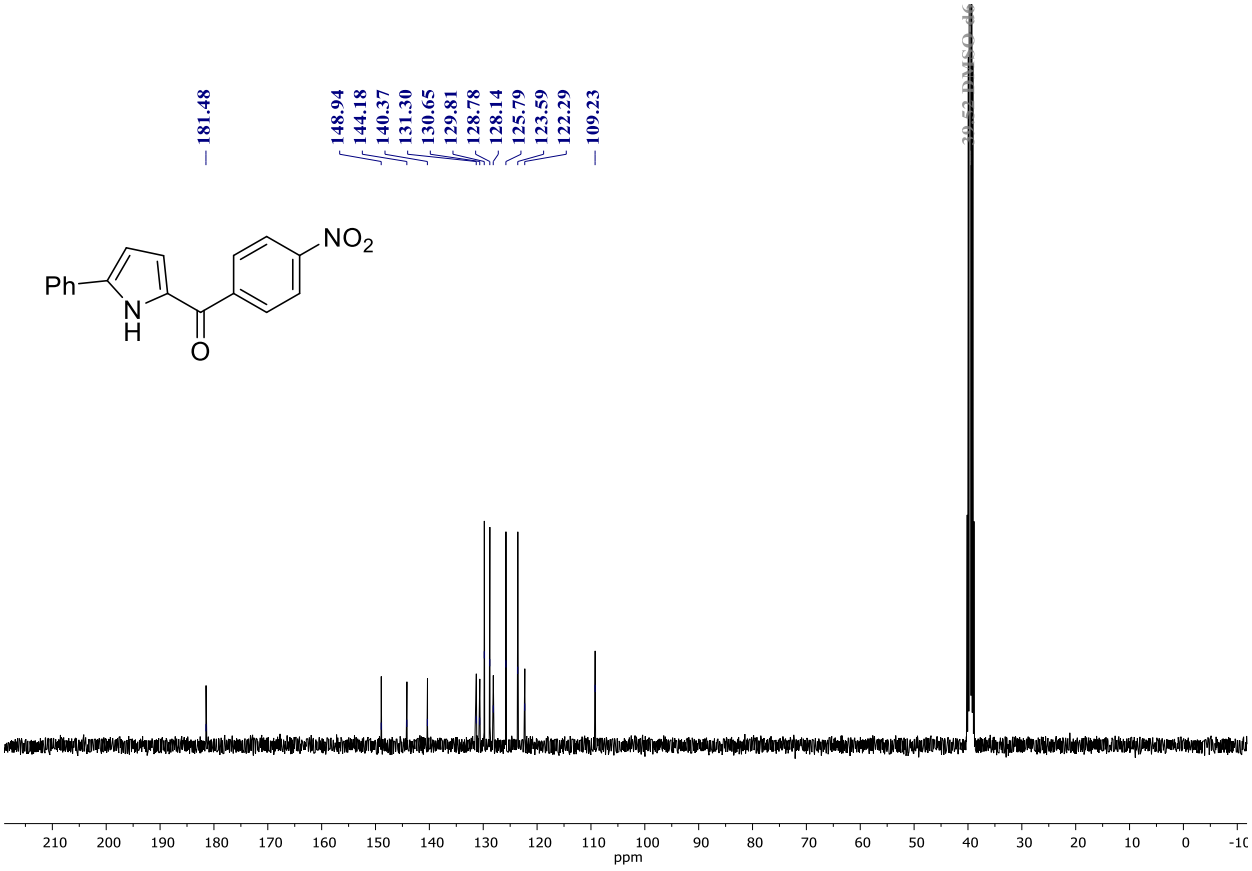
^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) spectrum of compound **2k**



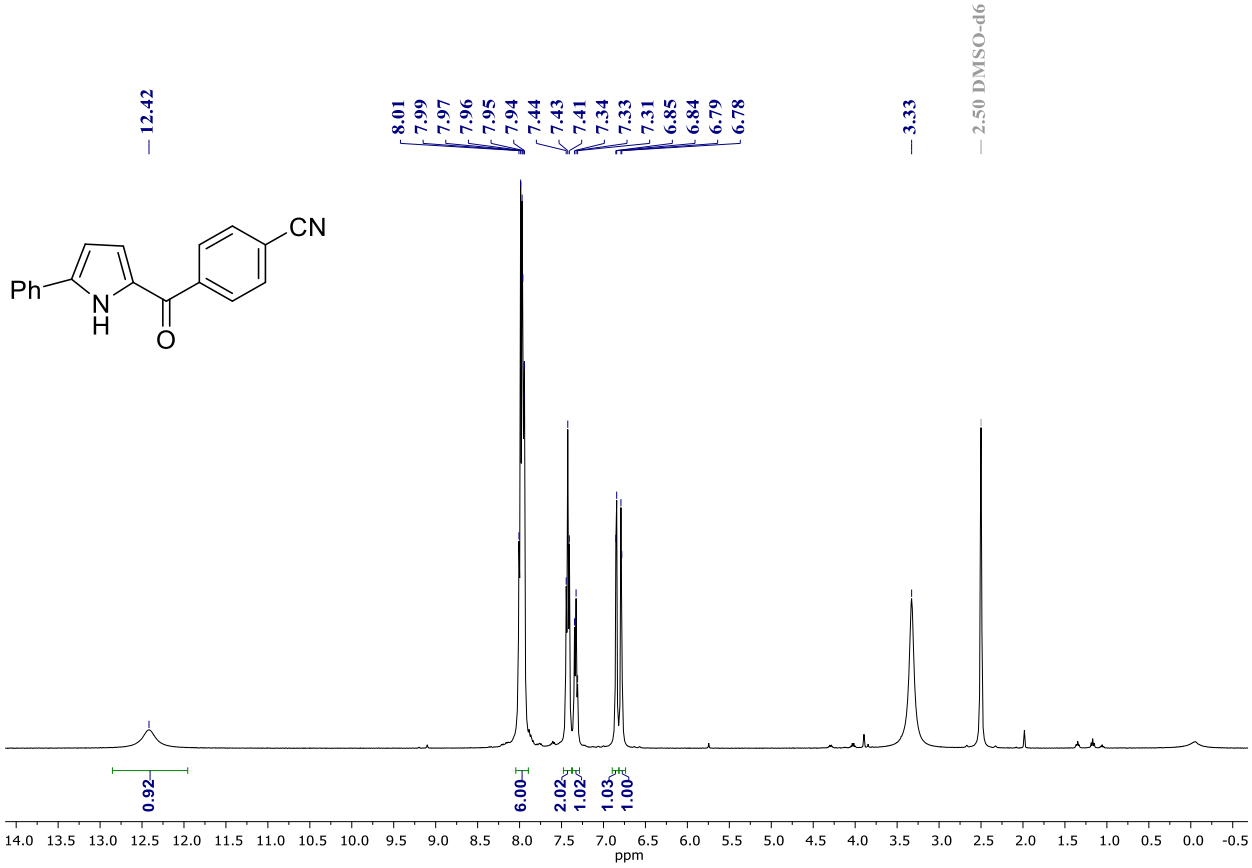
^{1}H NMR (400 MHz, DMSO-d_6) spectrum of compound **2l**



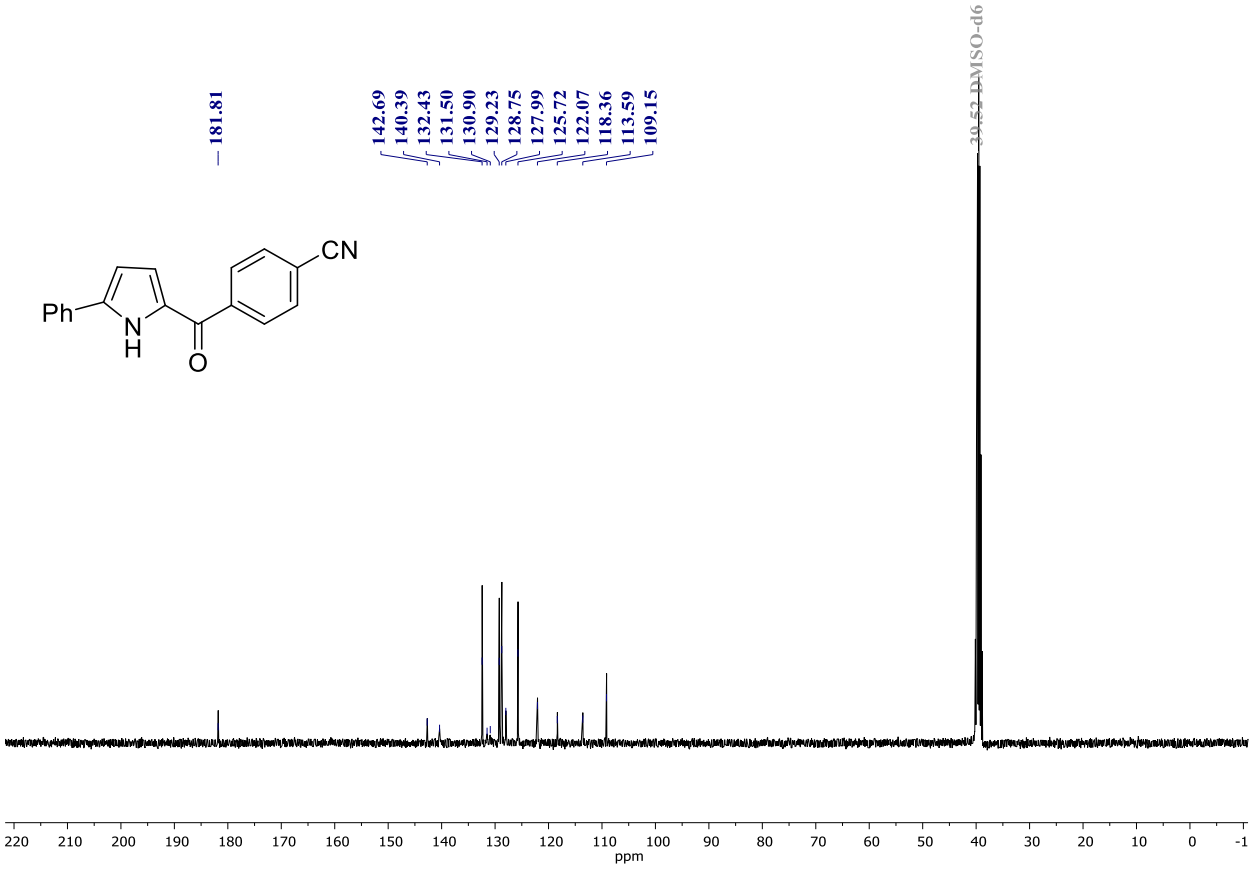
^{13}C{^{1}H} NMR (100 MHz, DMSO-d_6) spectrum of compound **2l**



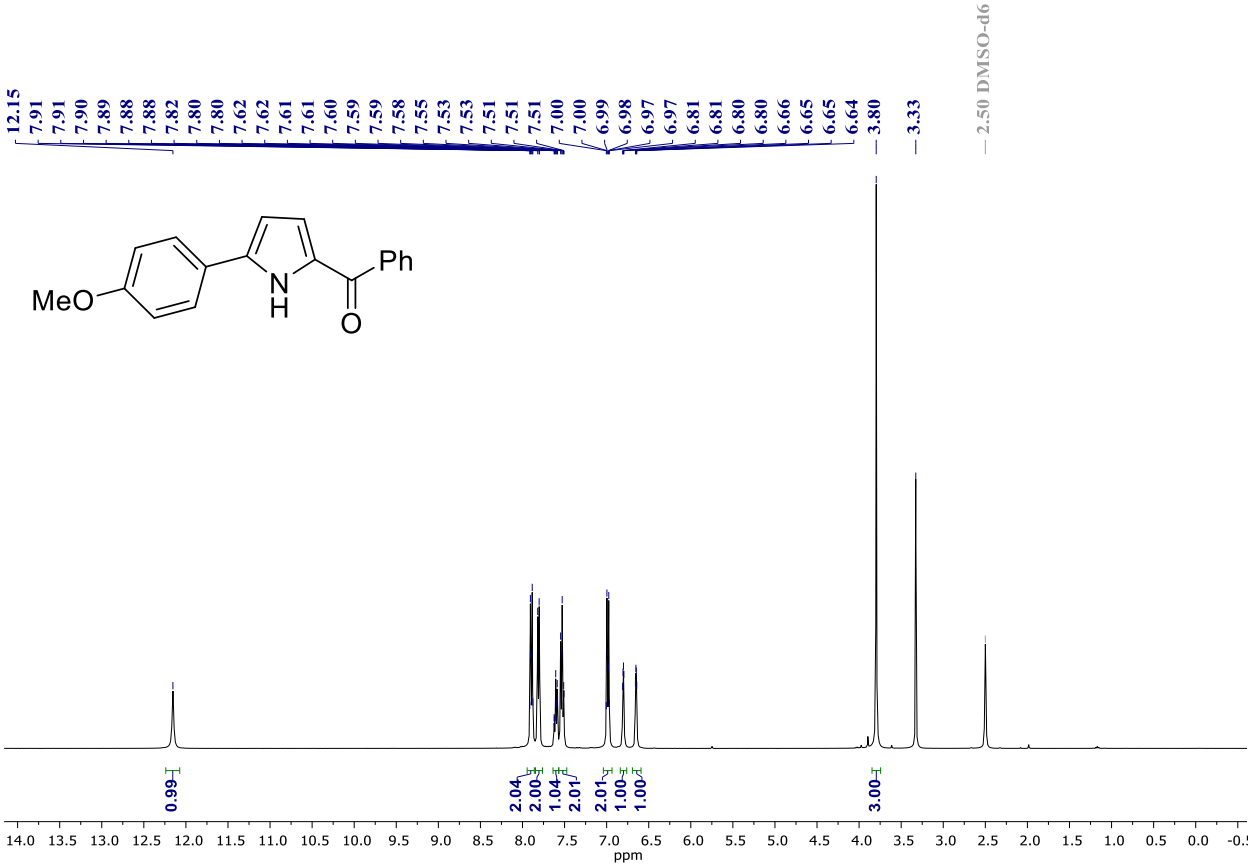
^{1}H NMR (400 MHz, DMSO-d_6) spectrum of compound **2m**



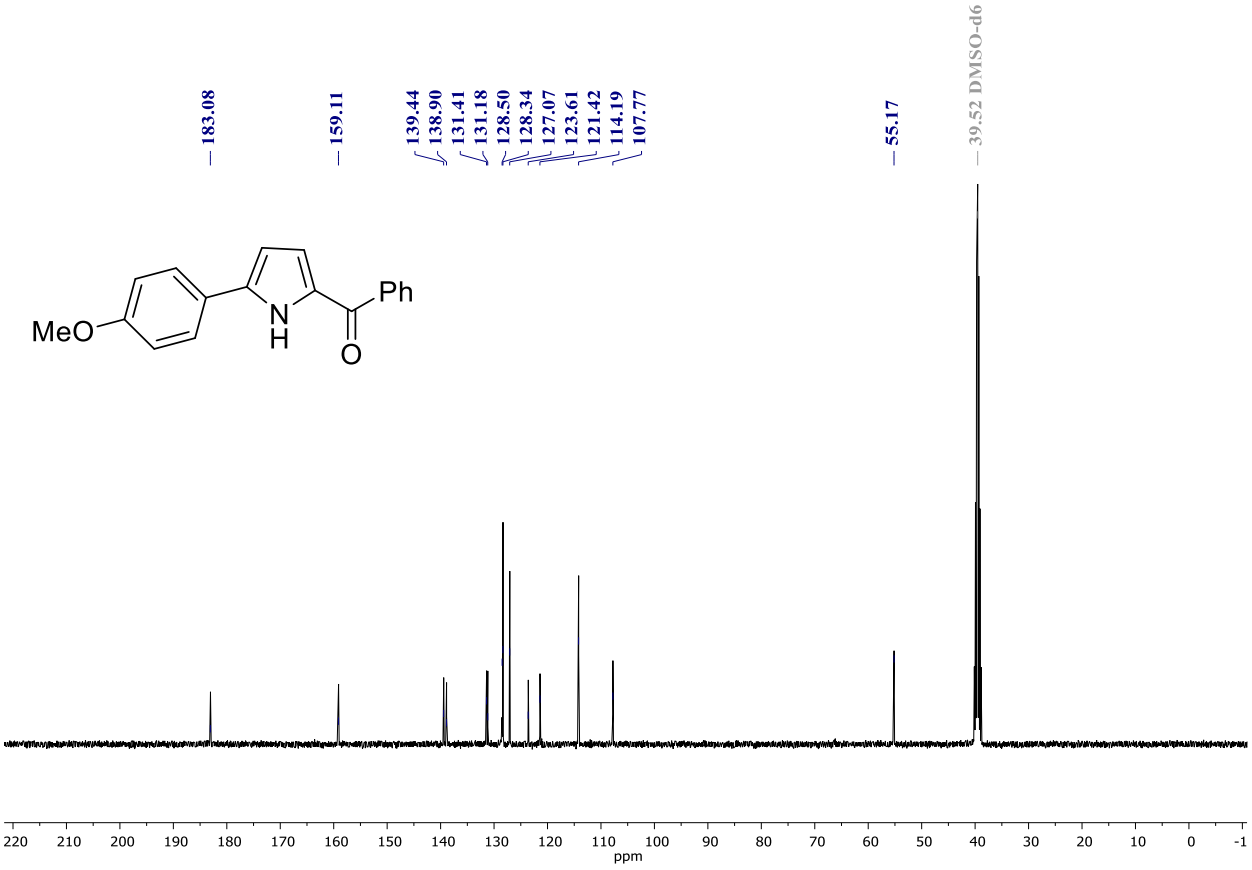
^{13}C{^{1}H} NMR (100 MHz, DMSO-d_6) spectrum of compound **2m**



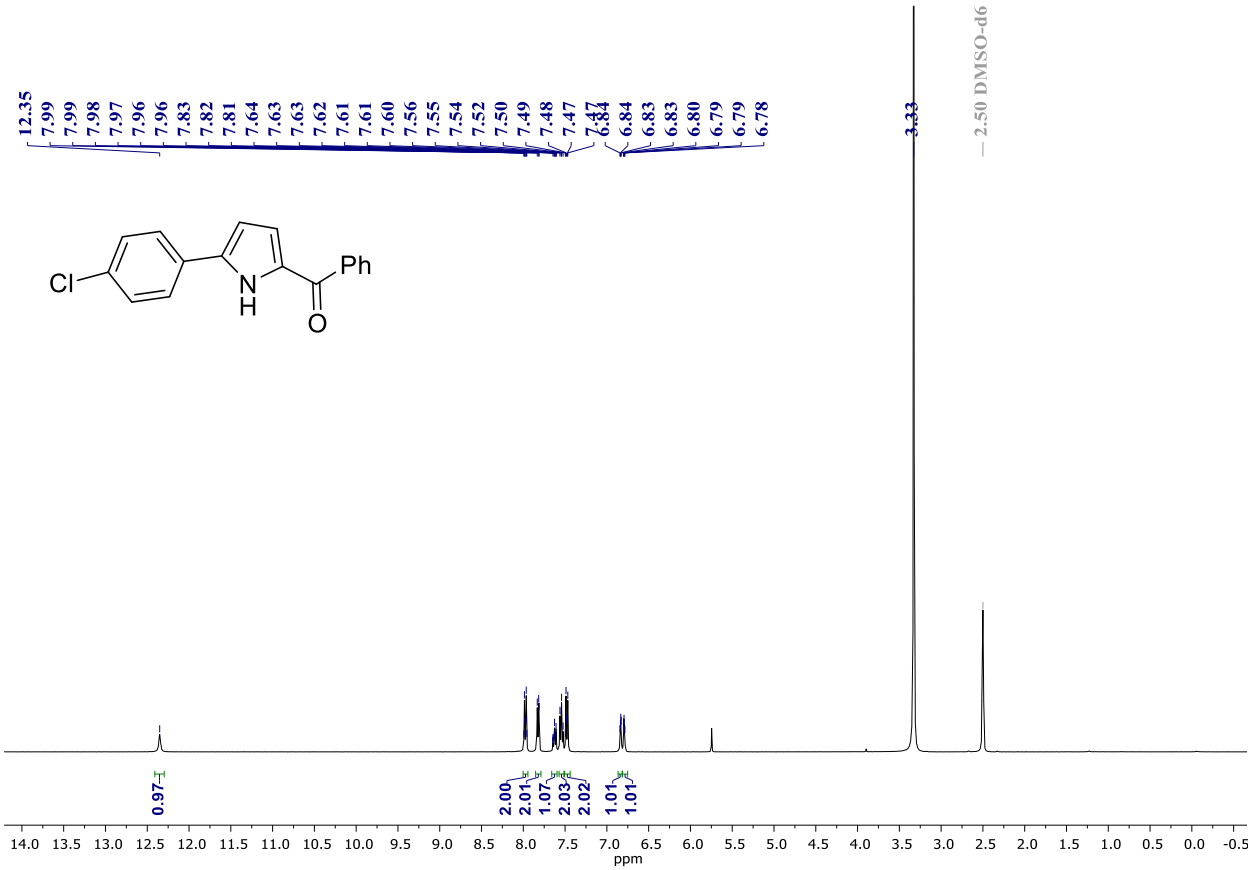
^{1}H NMR (400 MHz, DMSO-d_6) spectrum of compound **2n**



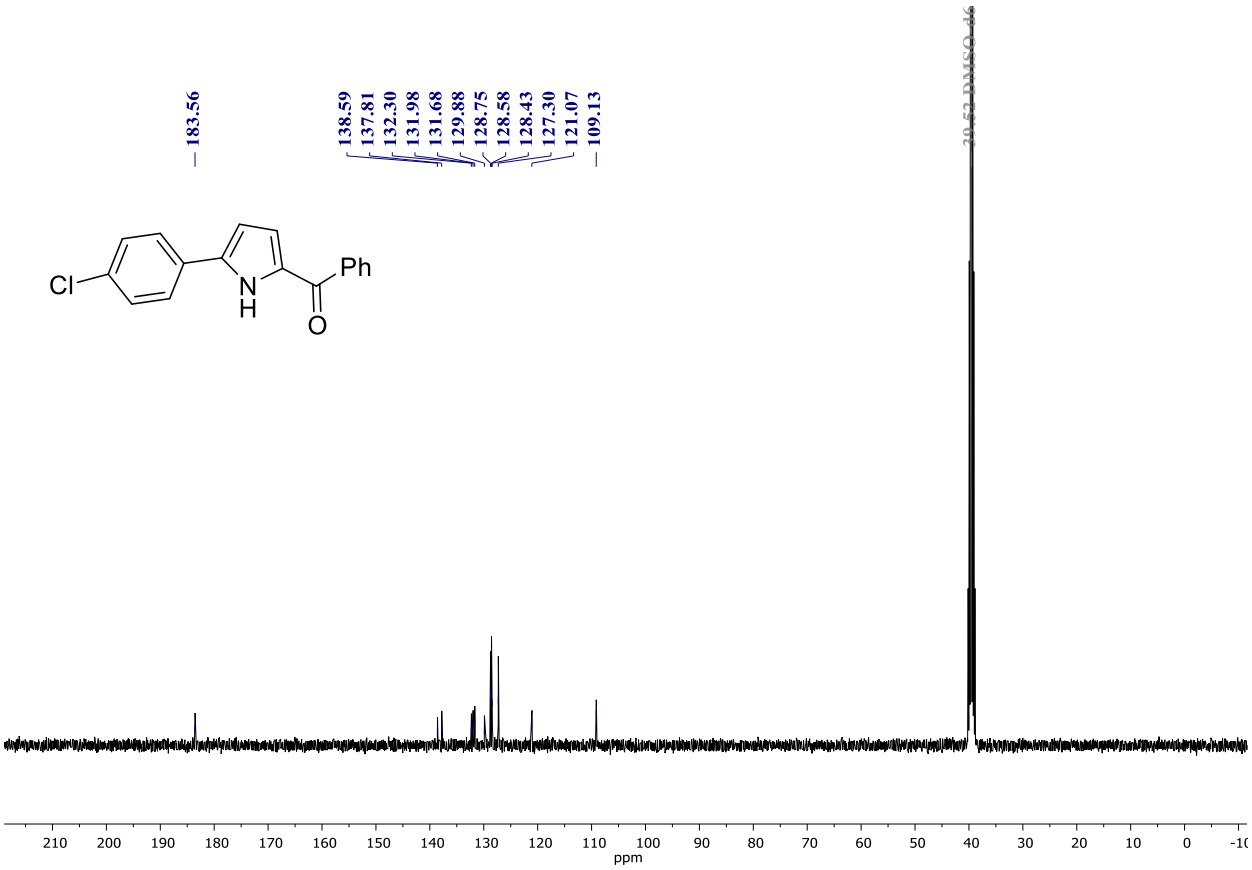
^{13}C{^{1}H} NMR (100 MHz, DMSO-d_6) spectrum of compound **2n**



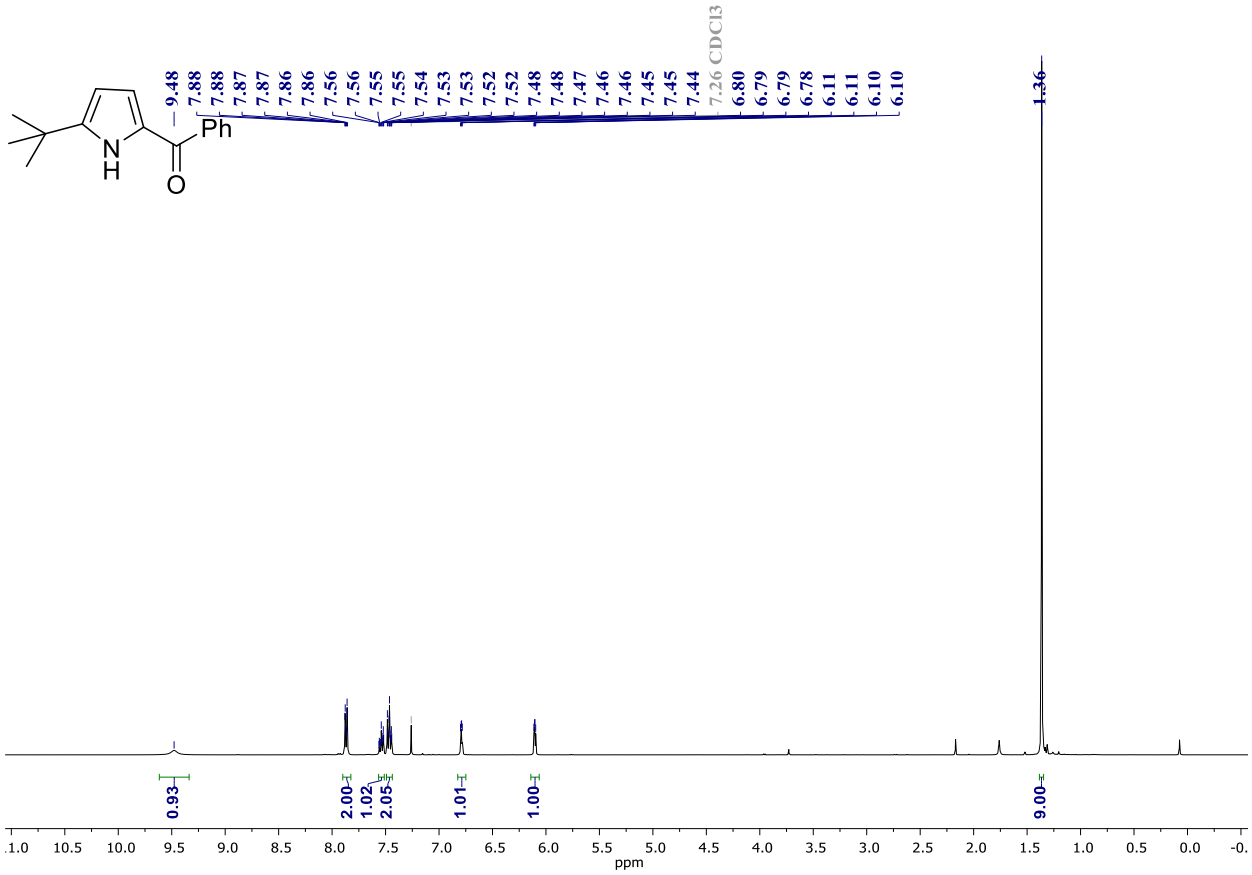
^{1}H NMR (400 MHz, DMSO-d_6) spectrum of compound **2o**



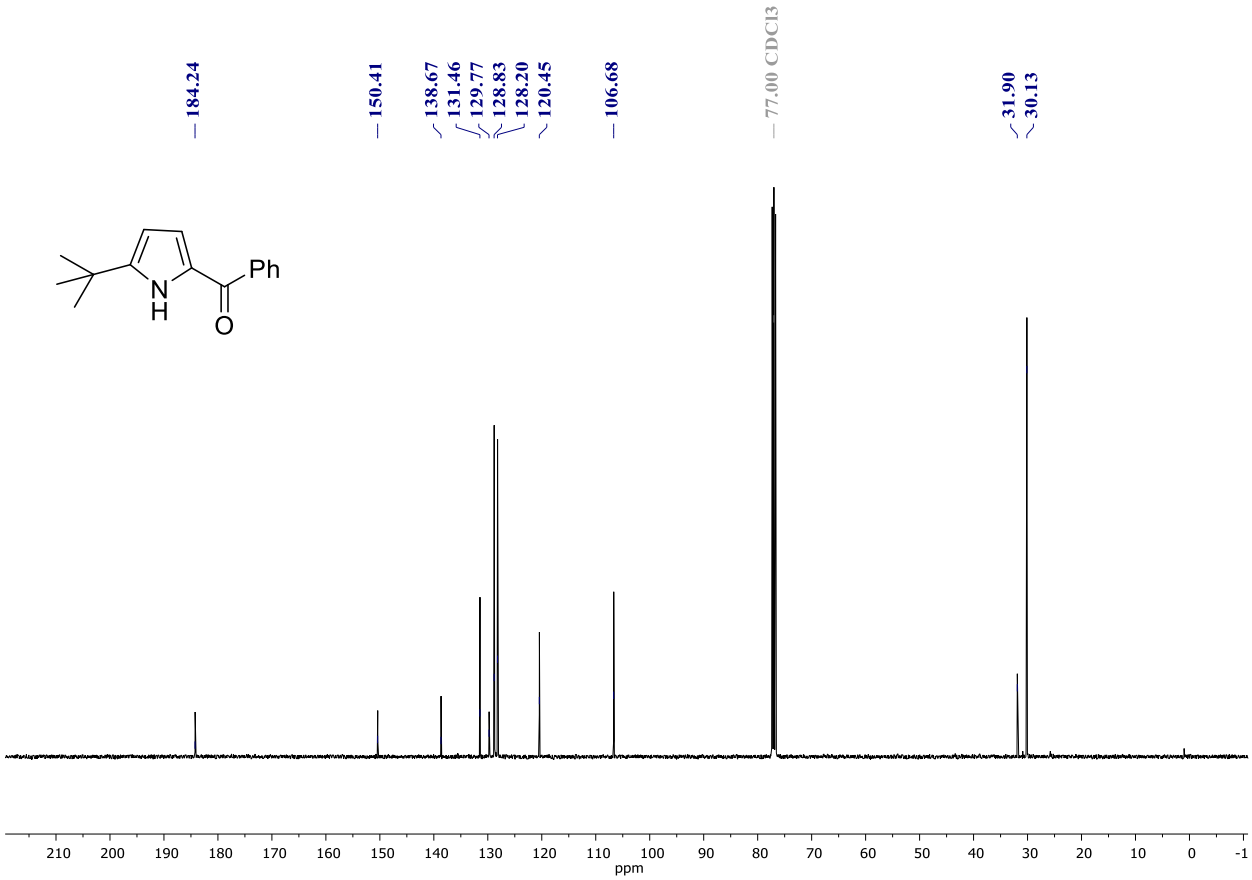
^{13}C{^{1}H} NMR (100 MHz, DMSO-d_6) spectrum of compound **2o**



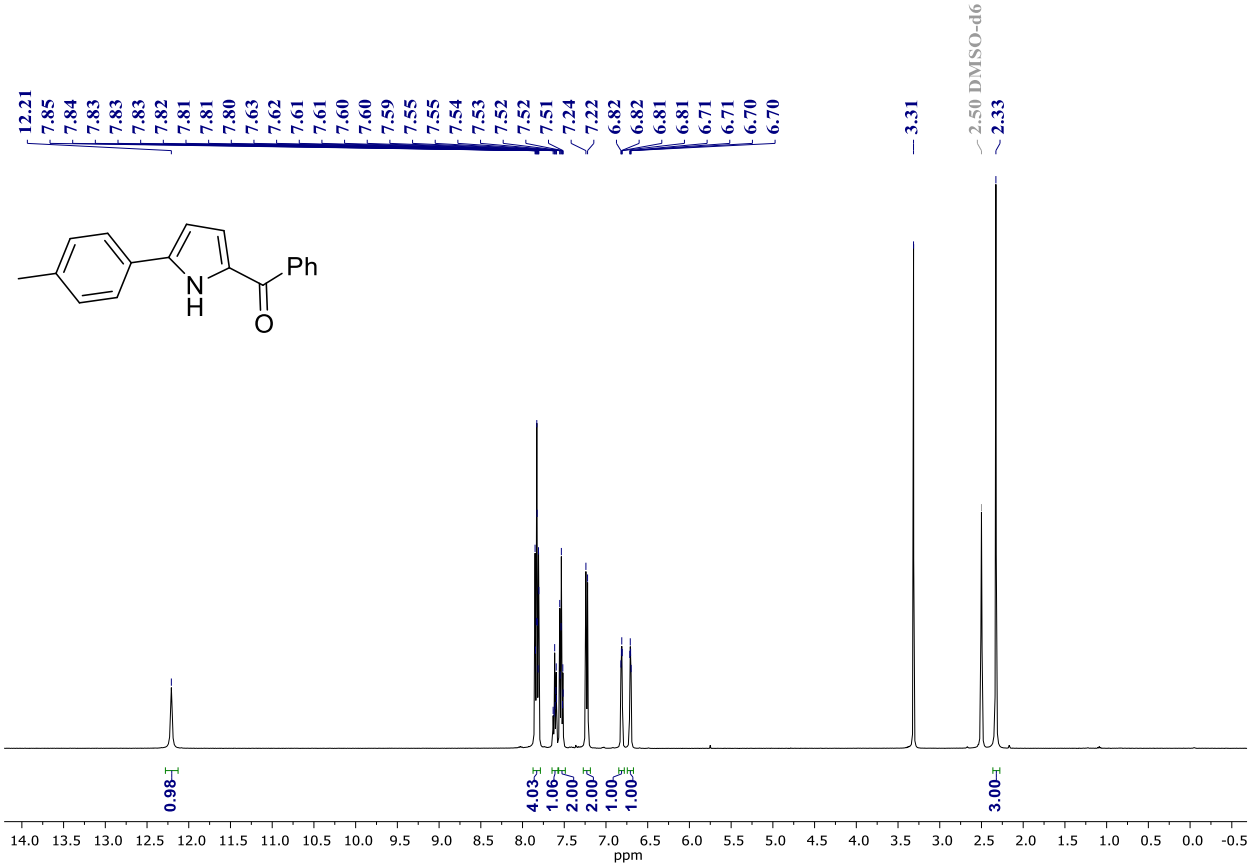
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound **2p**



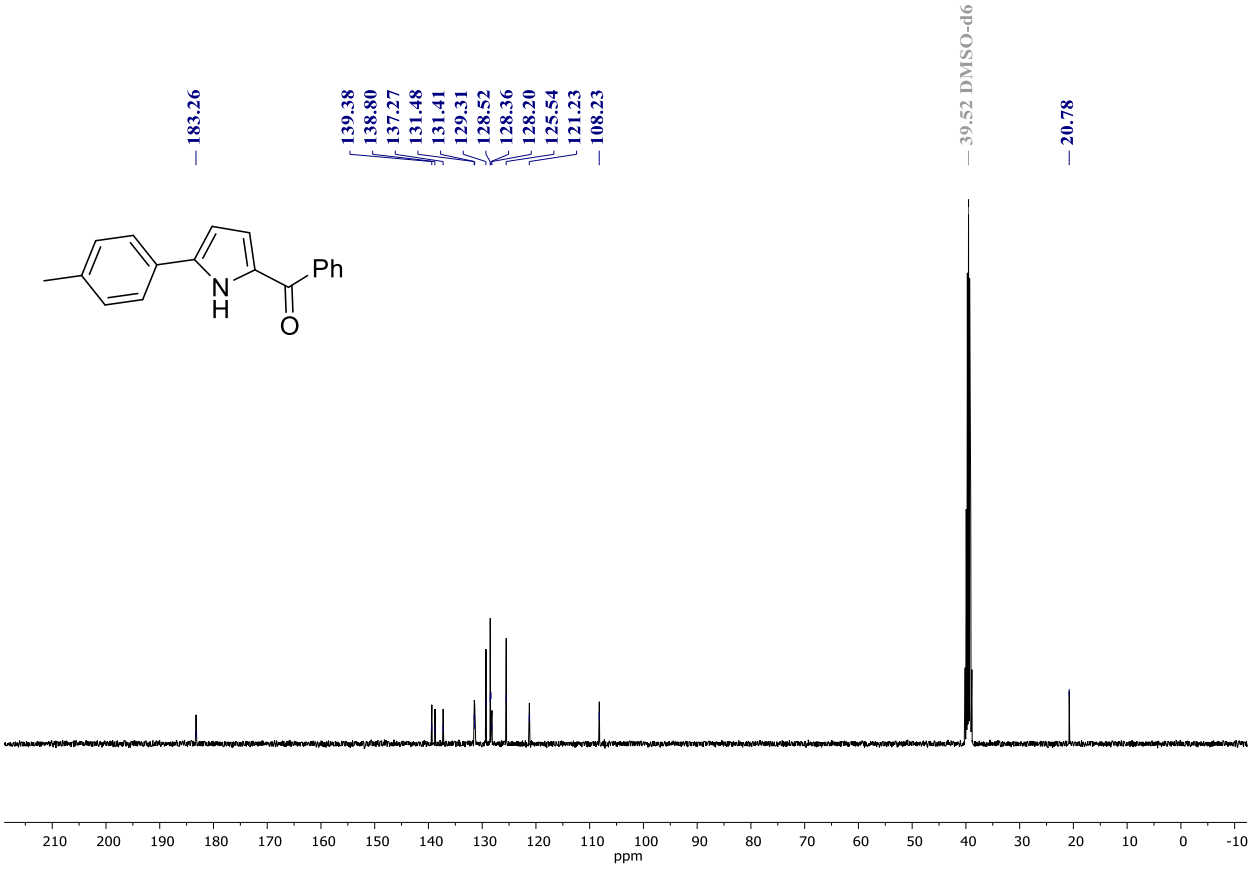
^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) spectrum of compound **2p**



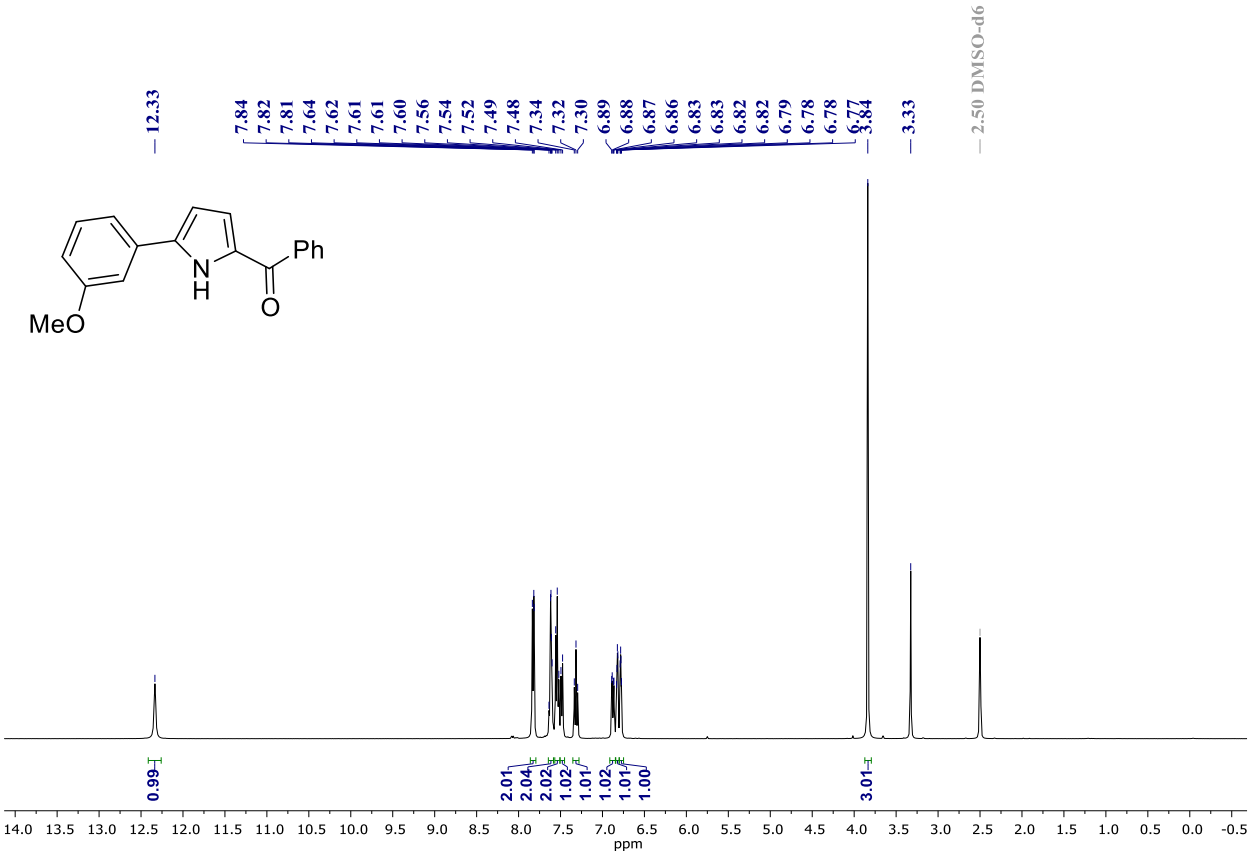
^{1}H NMR (400 MHz, DMSO-d_6) spectrum of compound **2q**



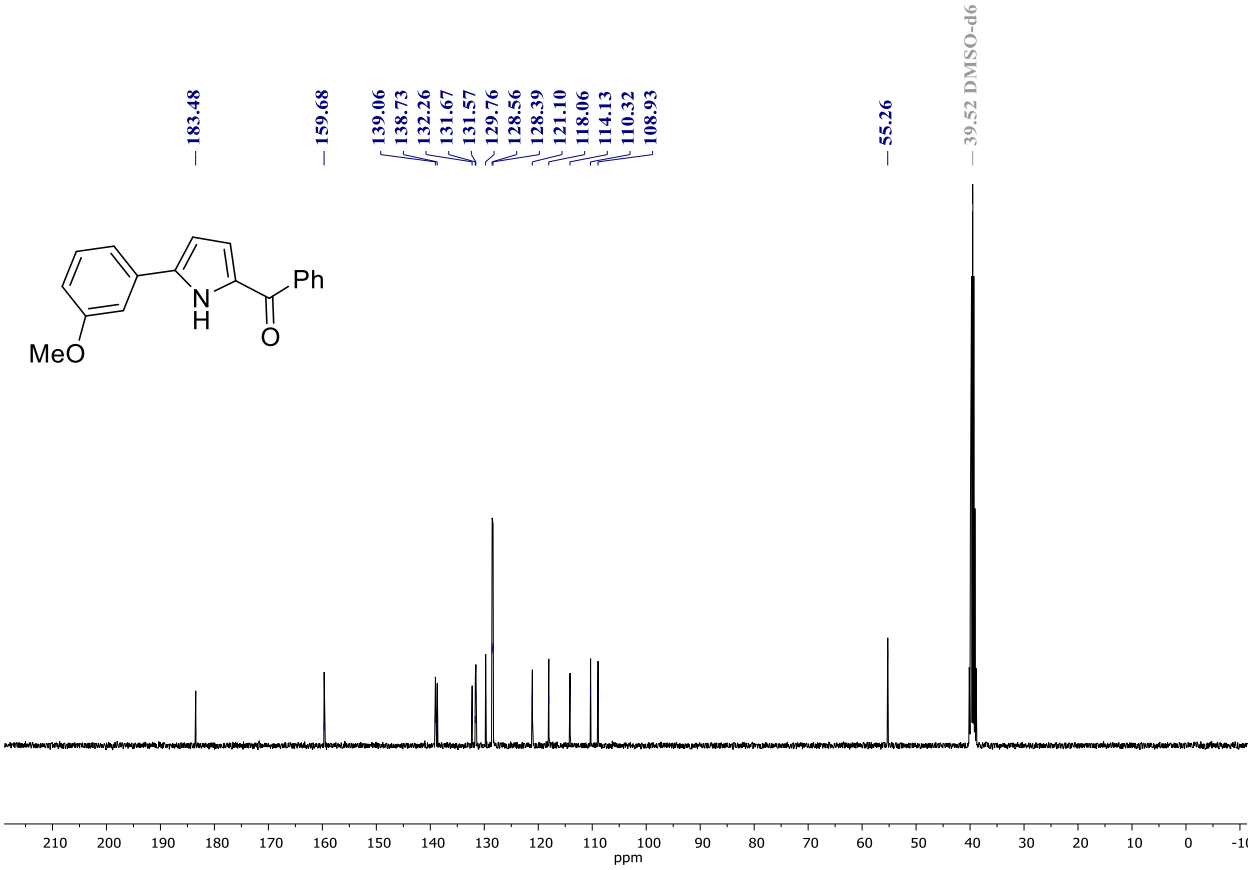
^{13}C{^{1}H} NMR (100 MHz, DMSO-d_6) spectrum of compound **2q**



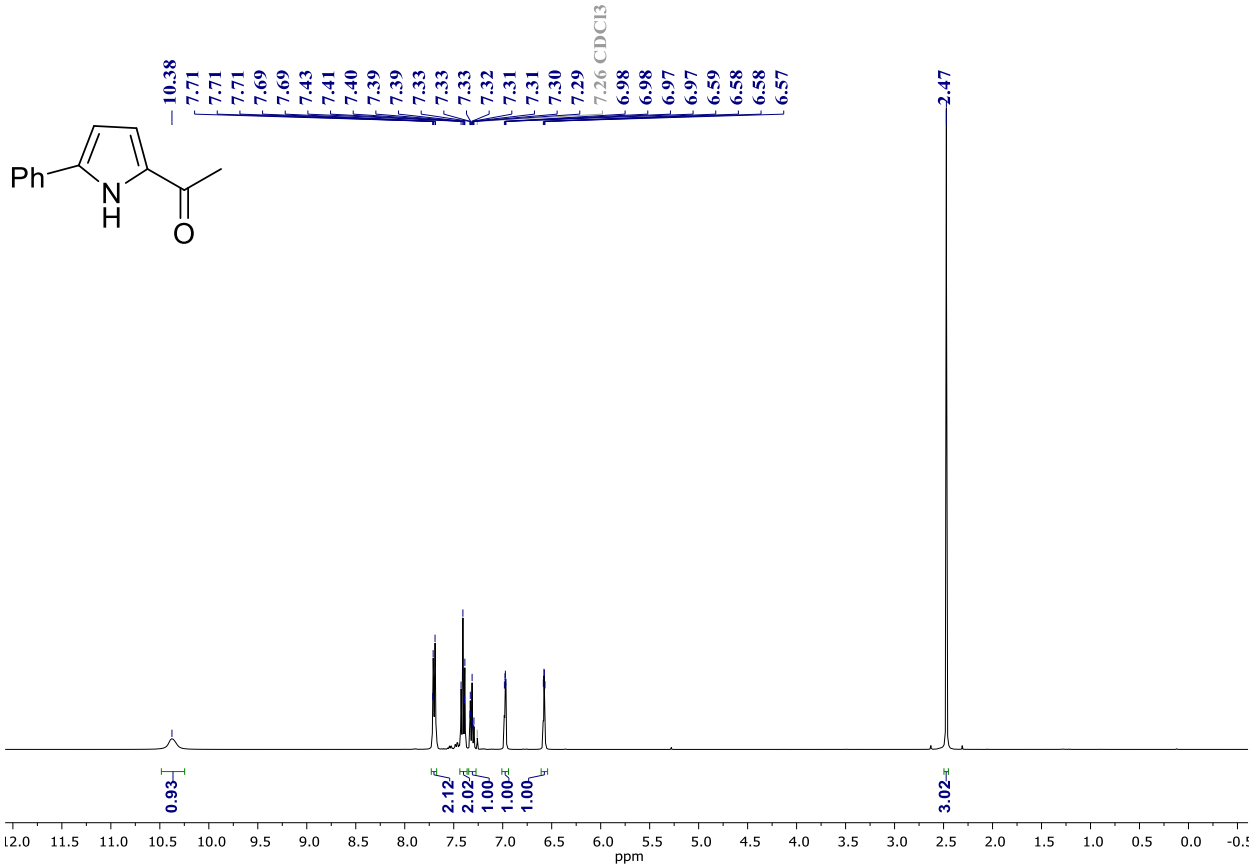
^{1}H NMR (400 MHz, DMSO-d_6) spectrum of compound **2r**



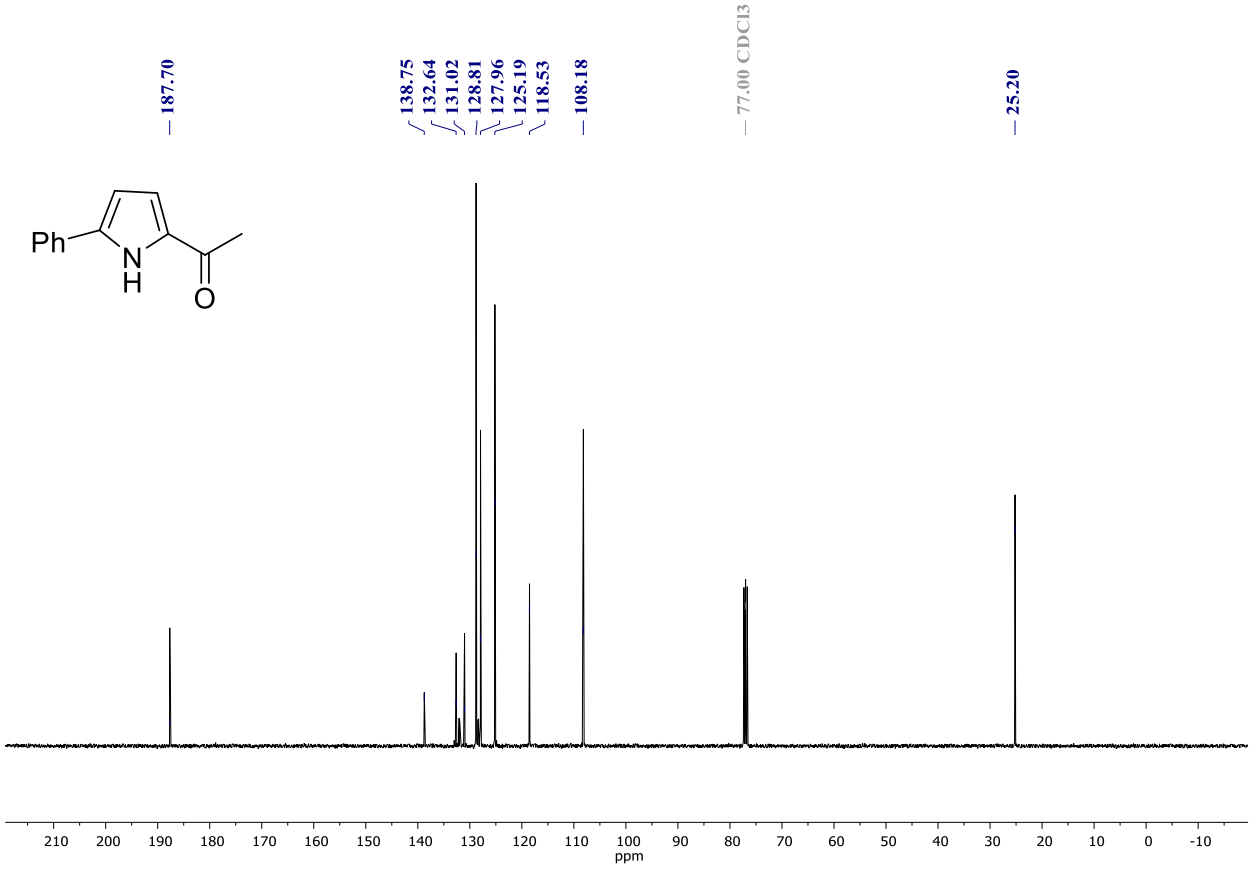
^{13}C{^{1}H} NMR (100 MHz, DMSO-d_6) spectrum of compound **2r**



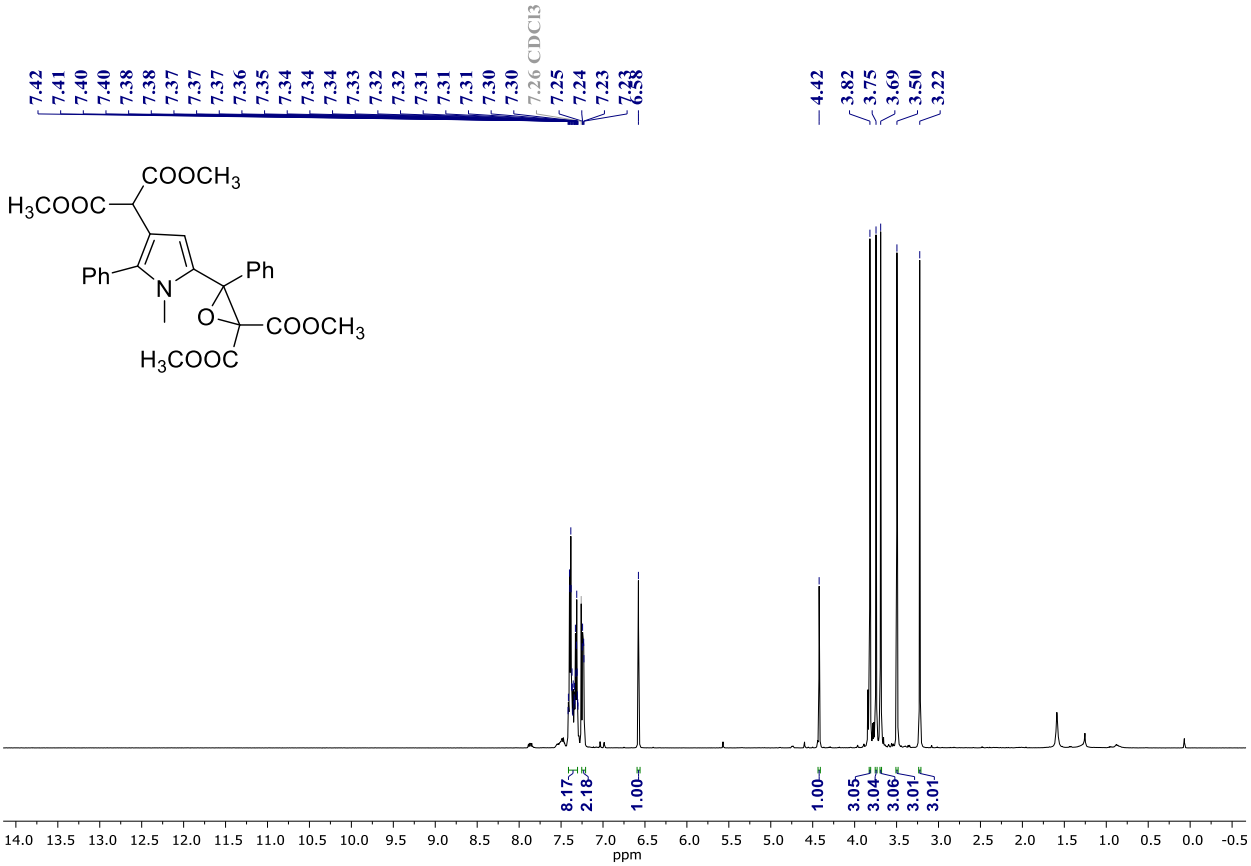
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound **2v**



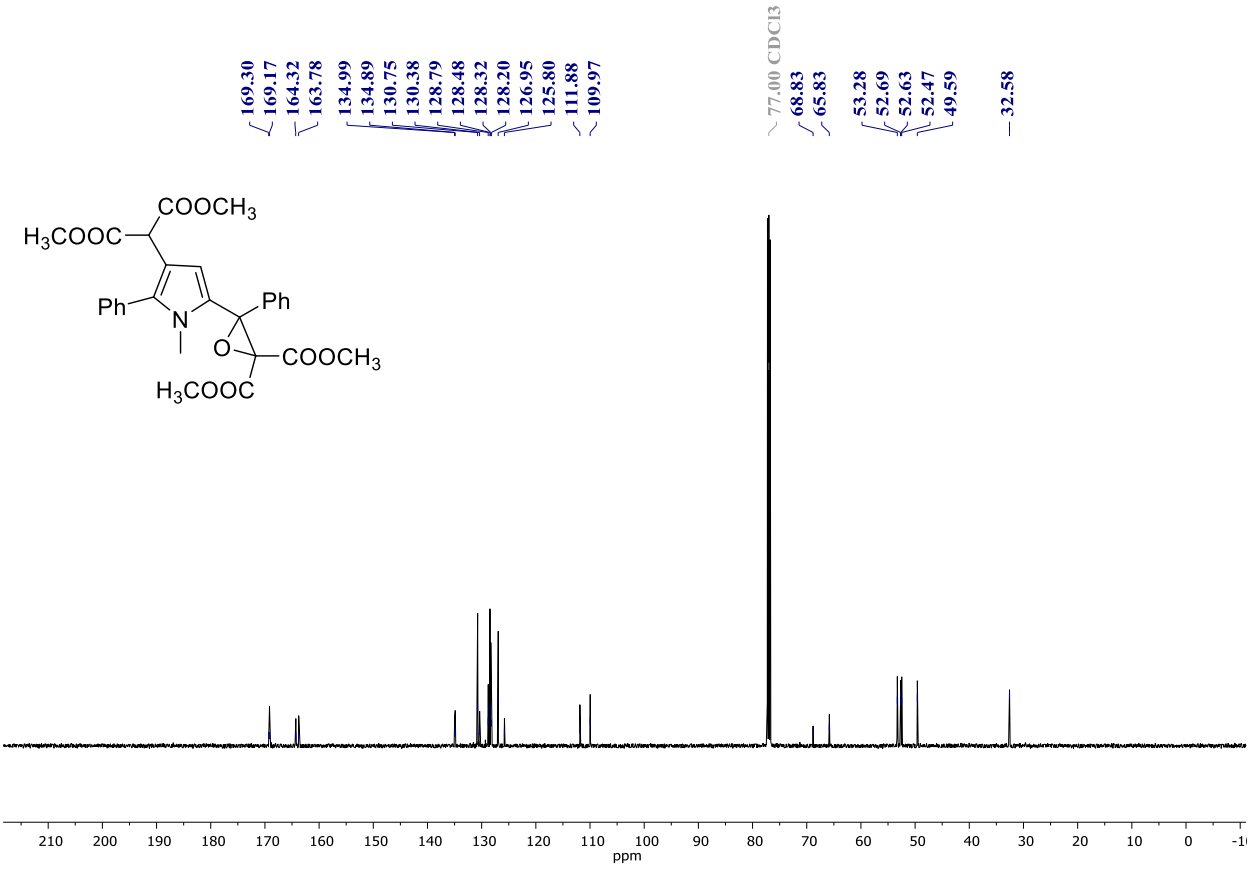
^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) spectrum of compound **2v**



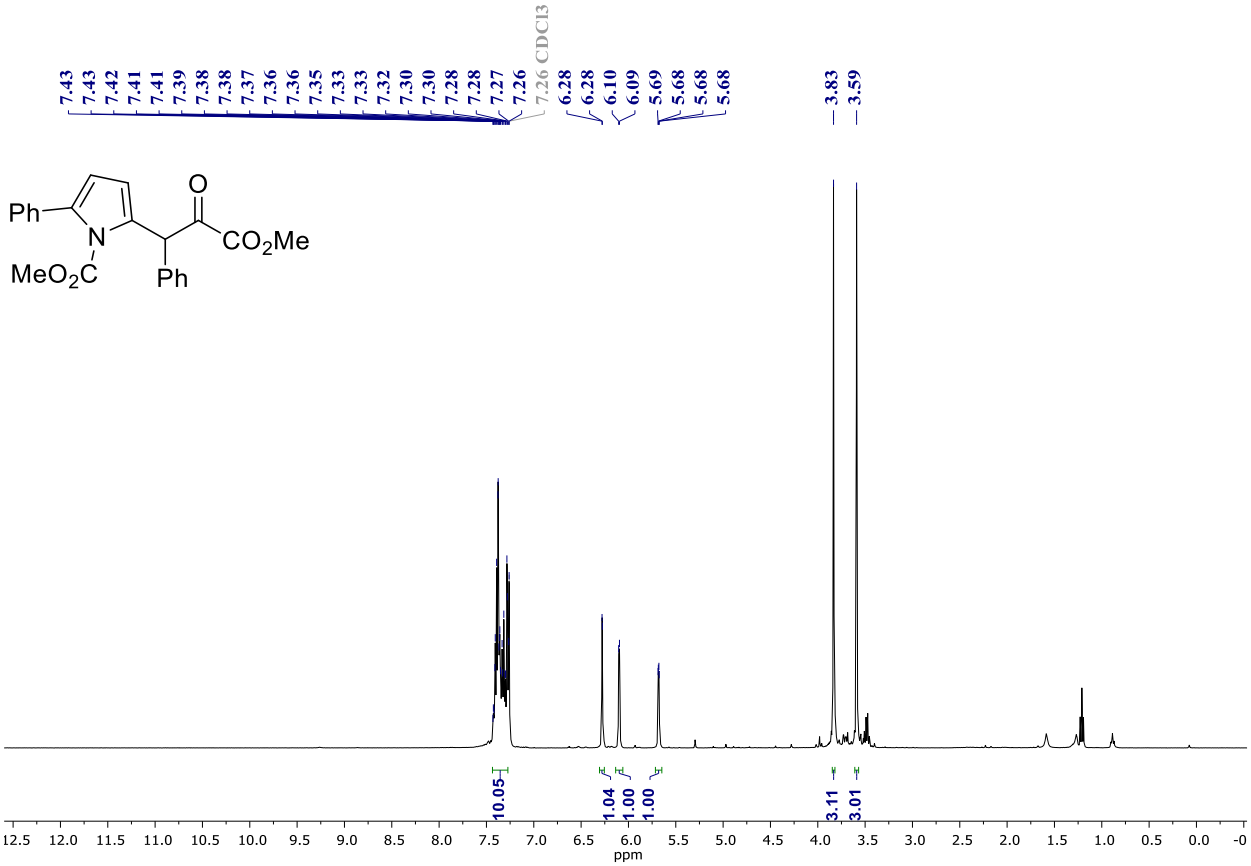
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound **4**



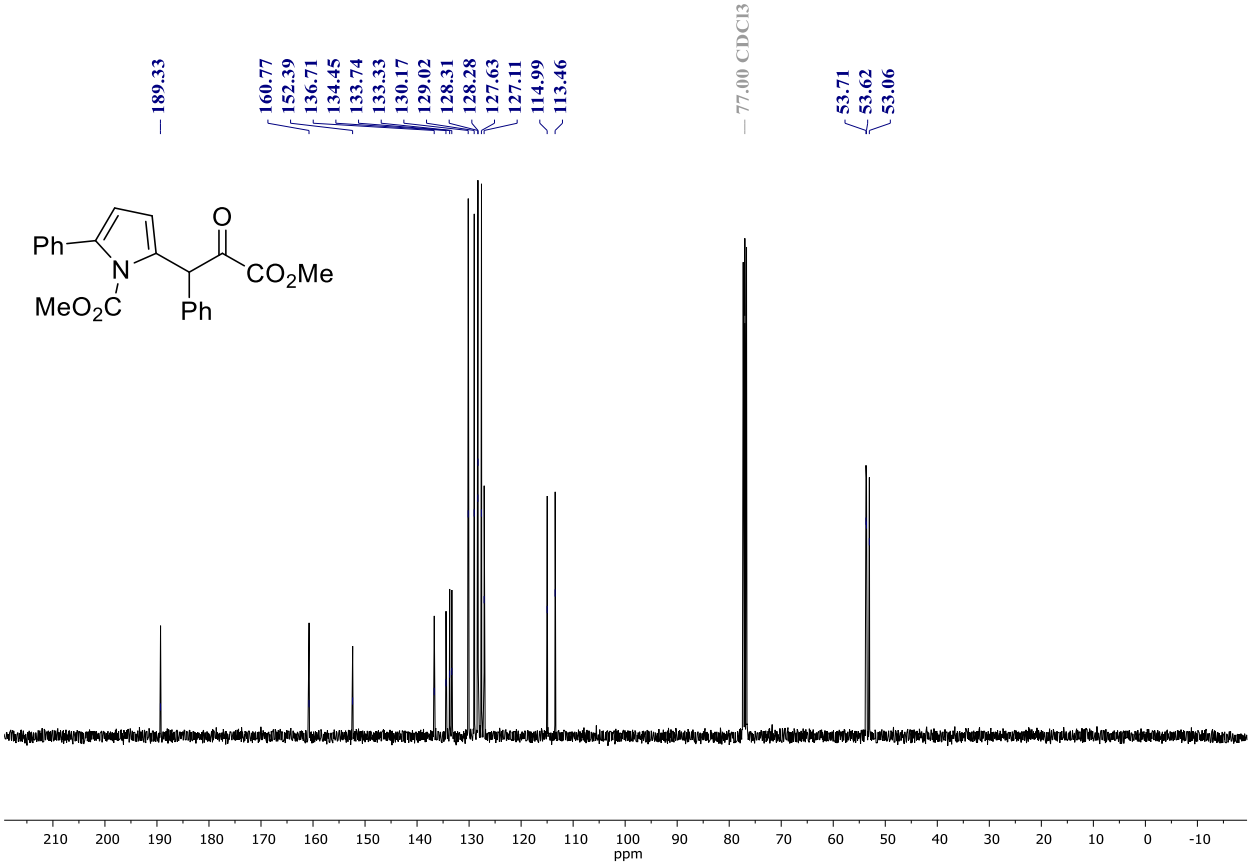
^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) spectrum of compound **4**



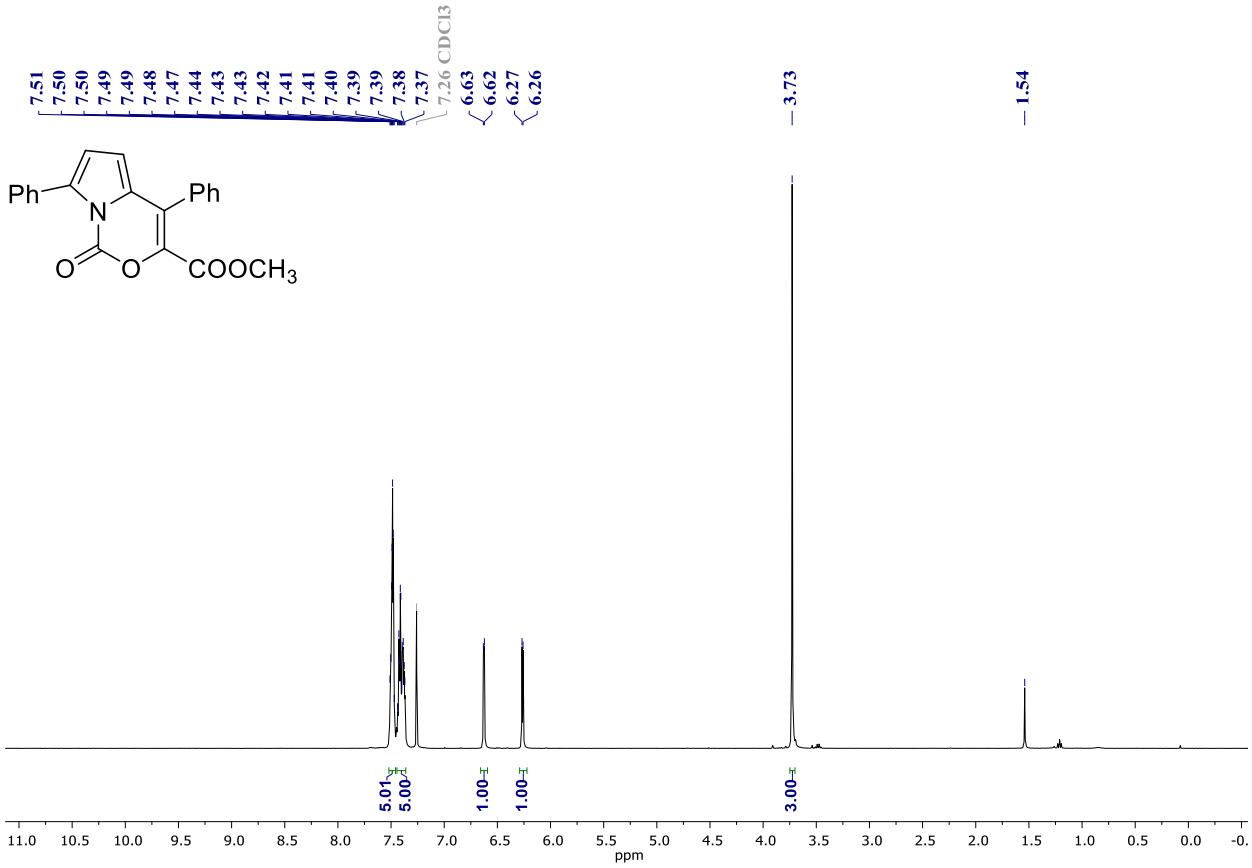
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound **5a**



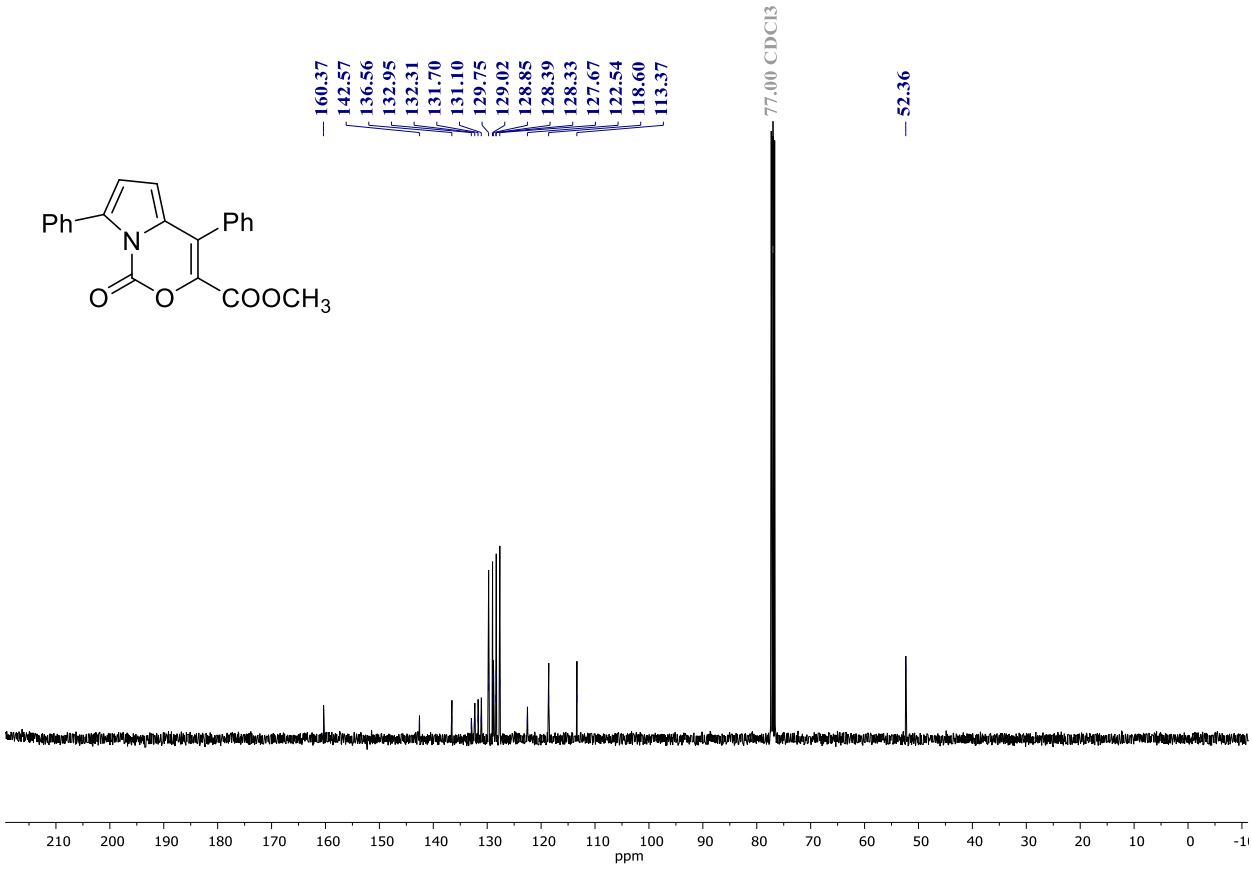
^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) spectrum of compound **5a**



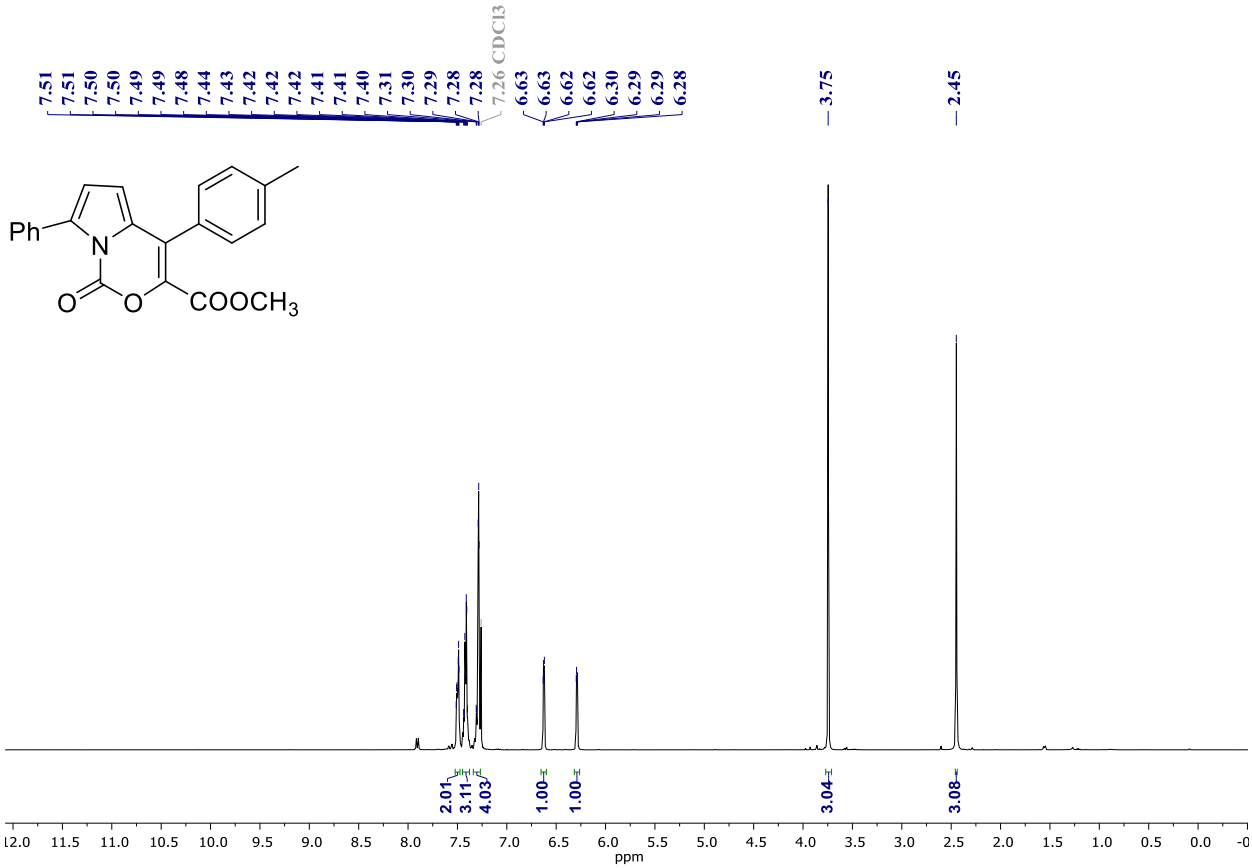
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound **6a**



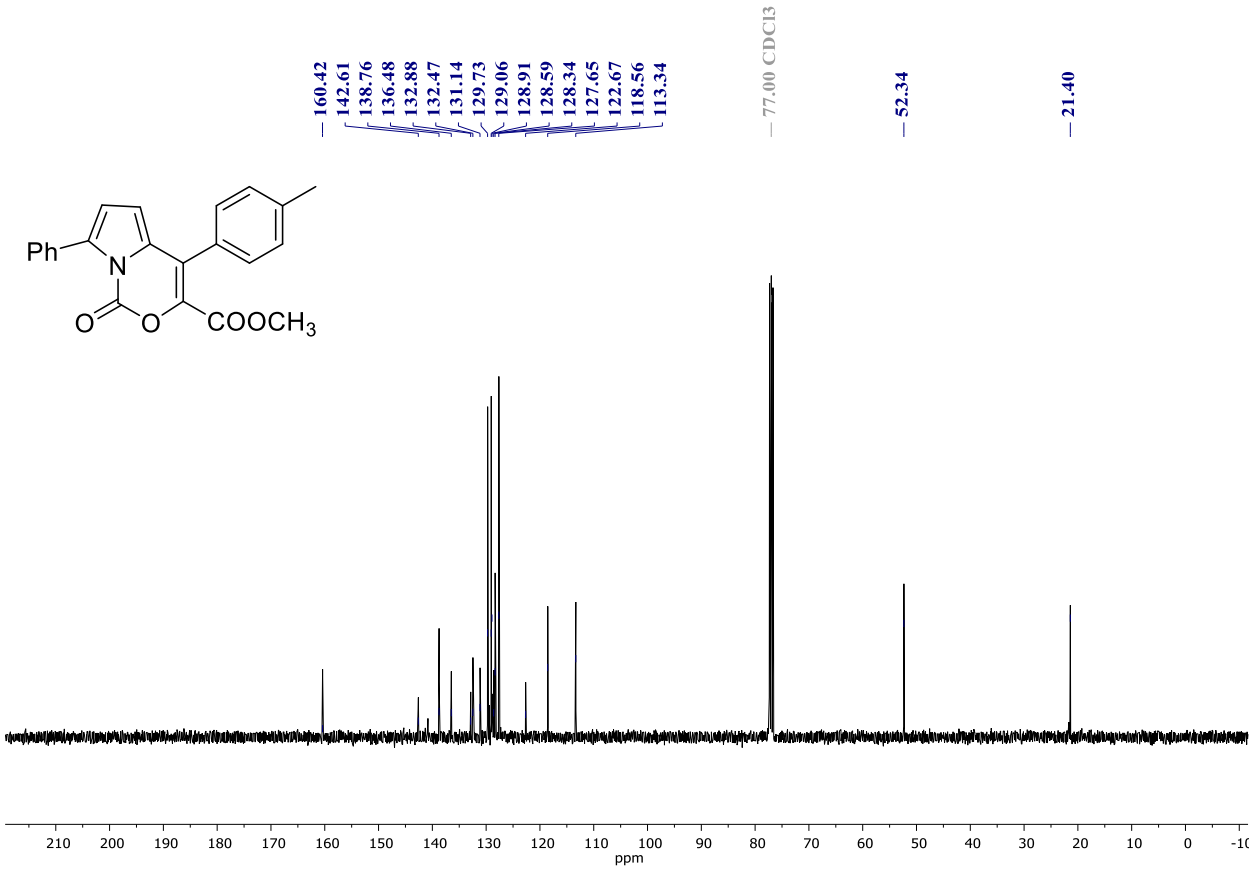
^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) spectrum of compound **6a**



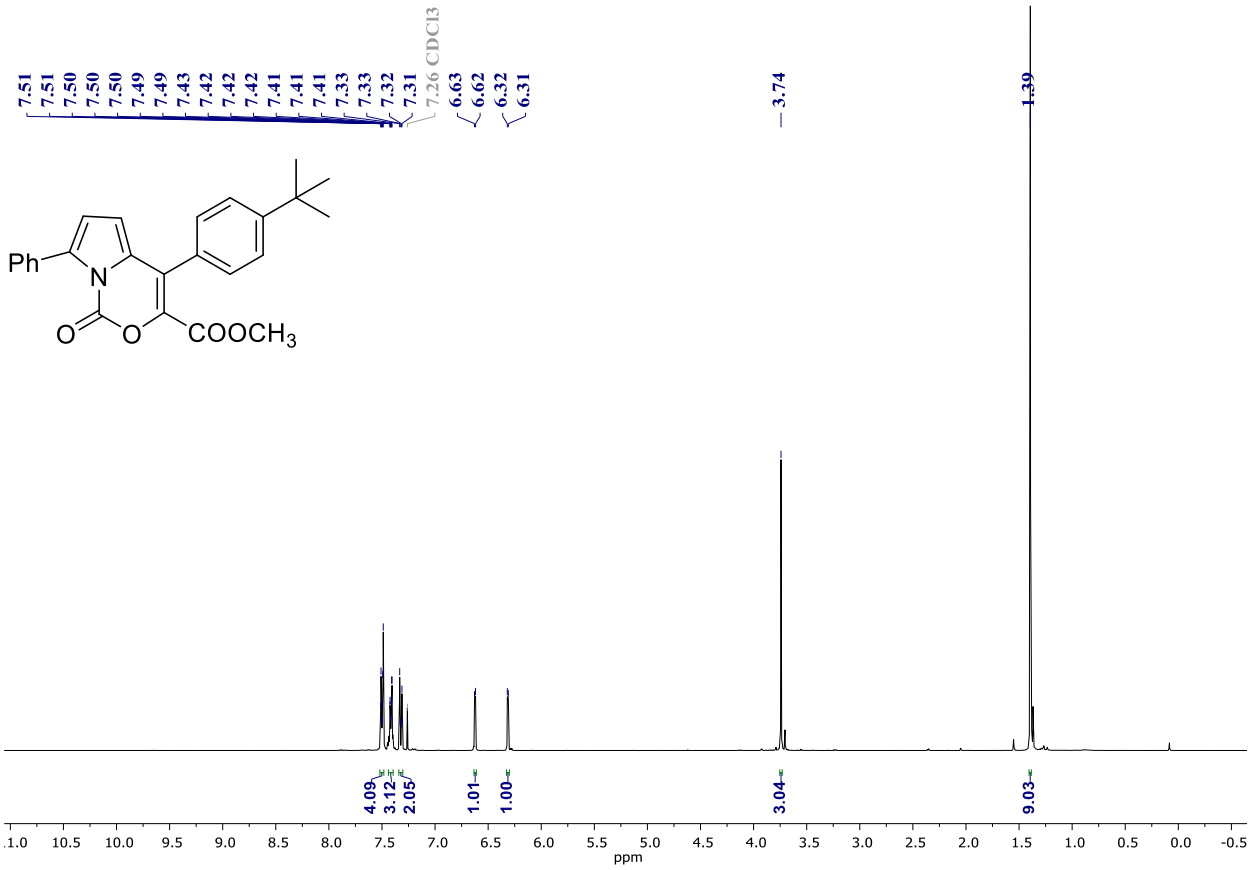
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound **6b**



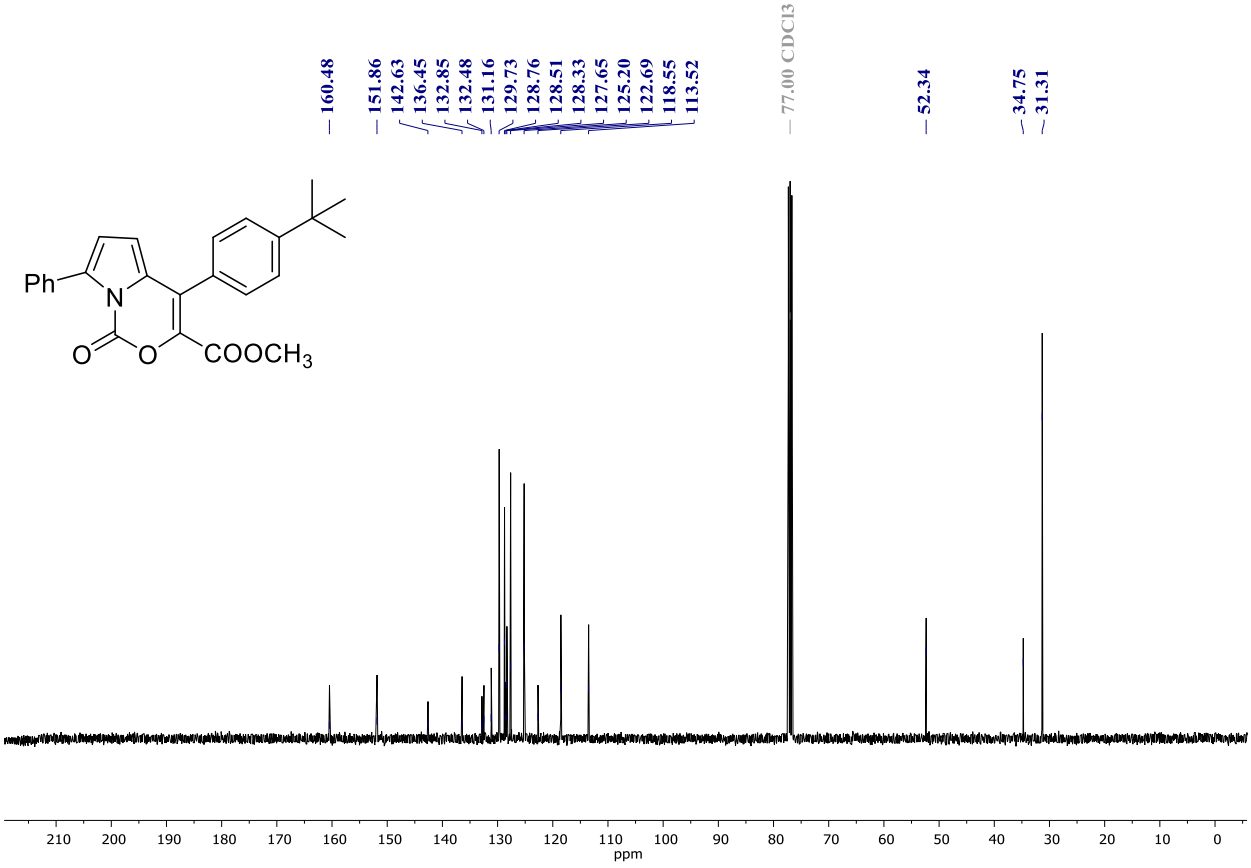
^{13}C{^{1}H} NMR (100MHz, $CDCl_3$) spectrum of compound **6b**



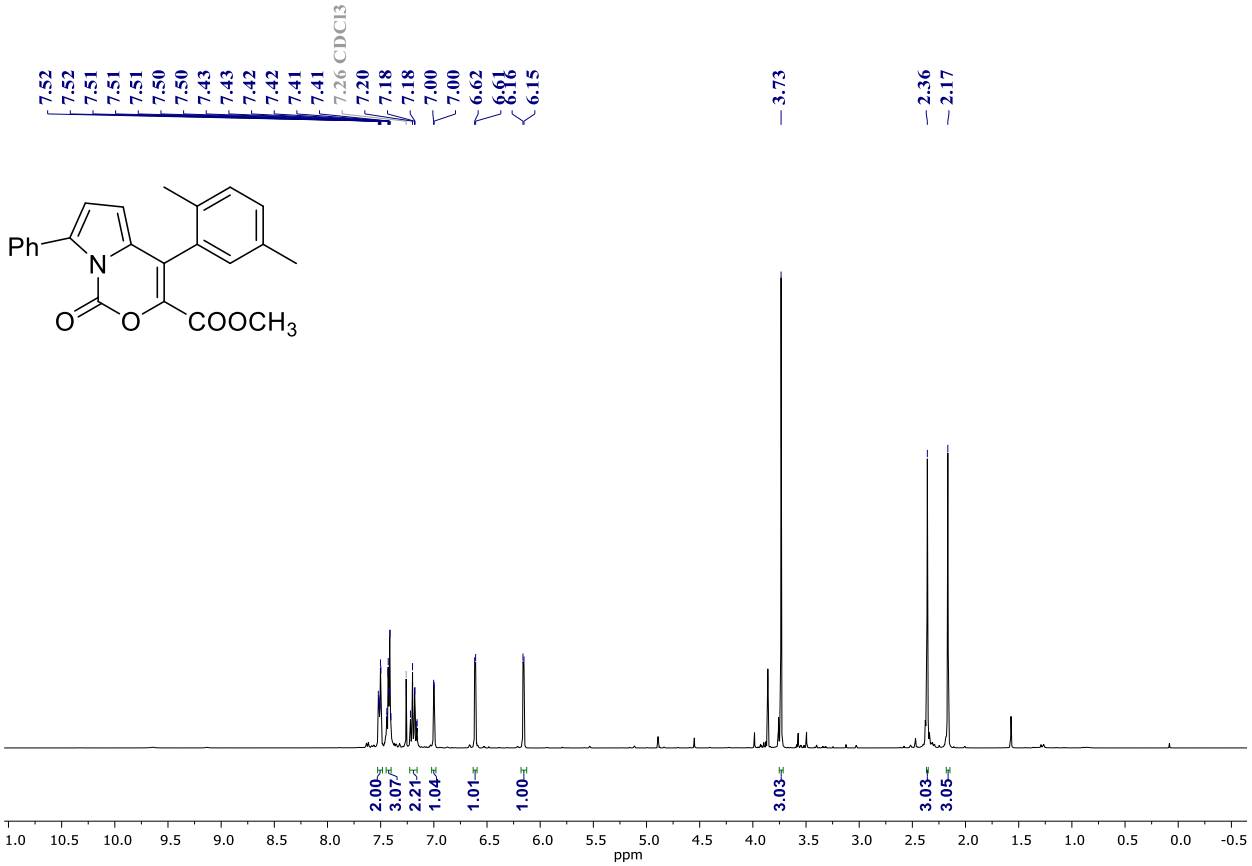
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound **6c**



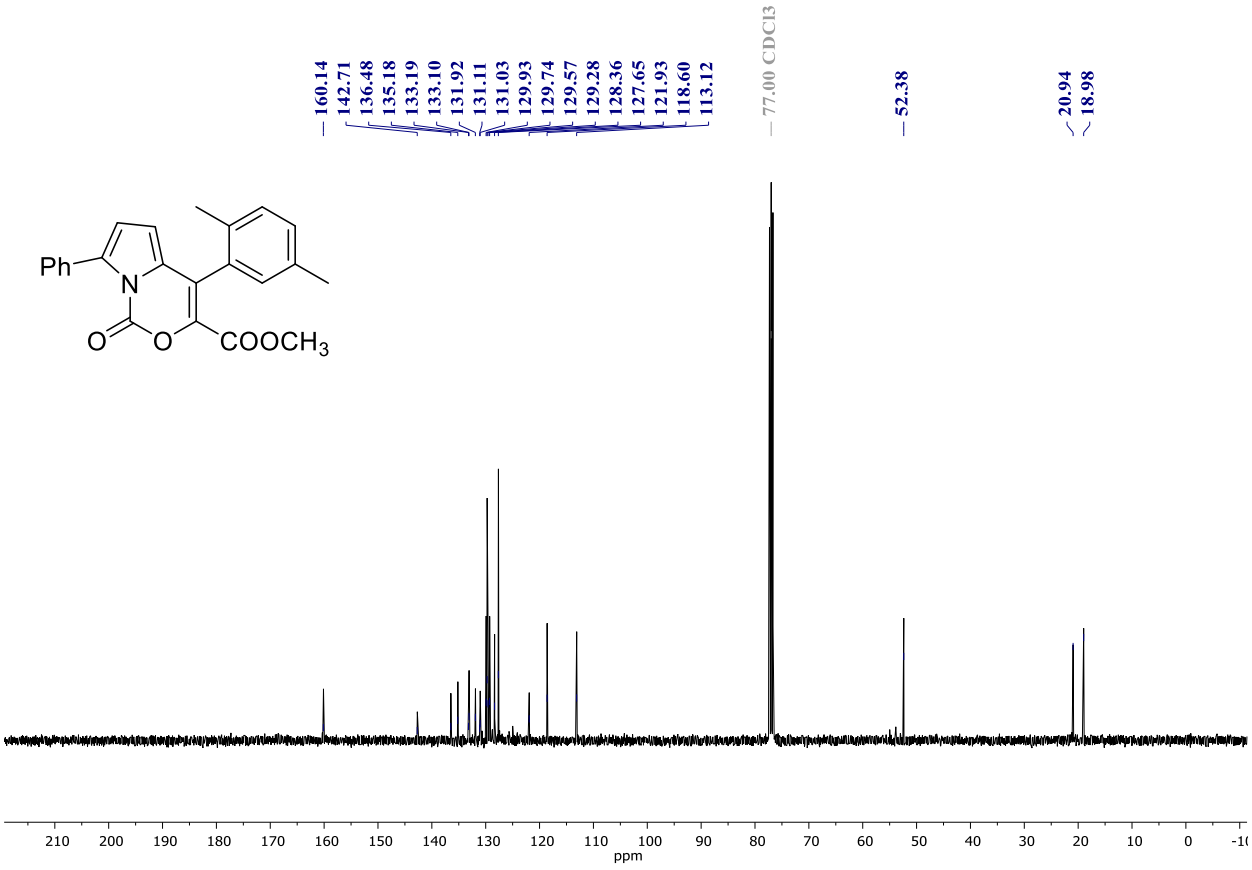
^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) spectrum of compound **6c**



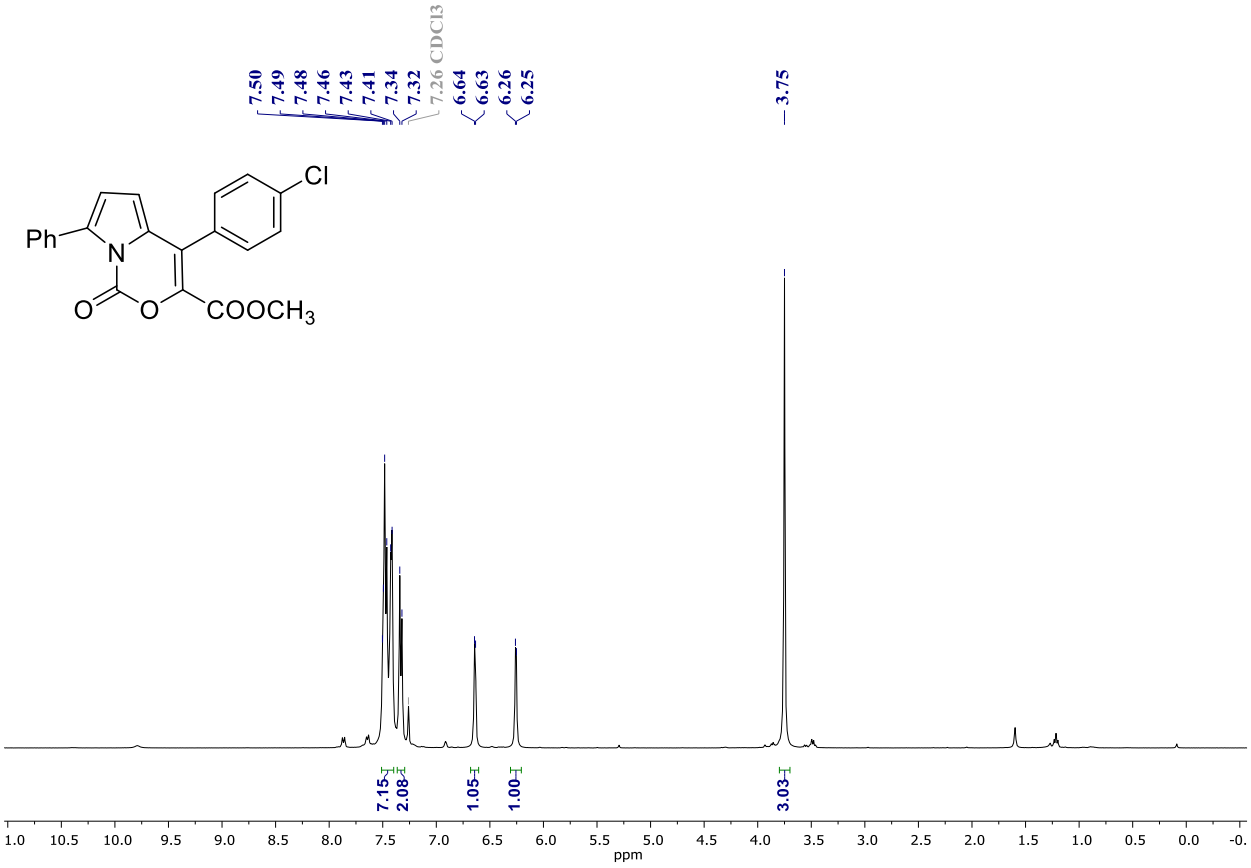
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound **6d**



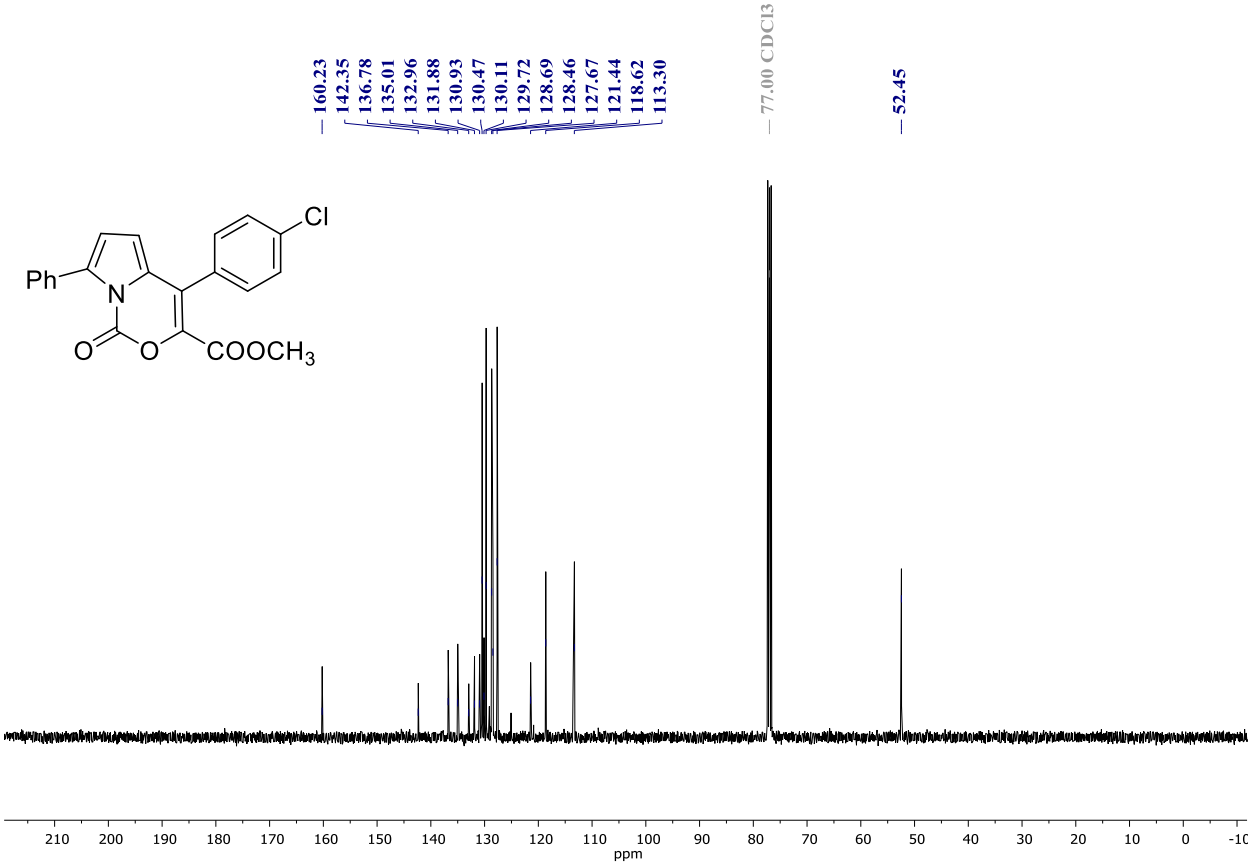
^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) spectrum of compound **6d**



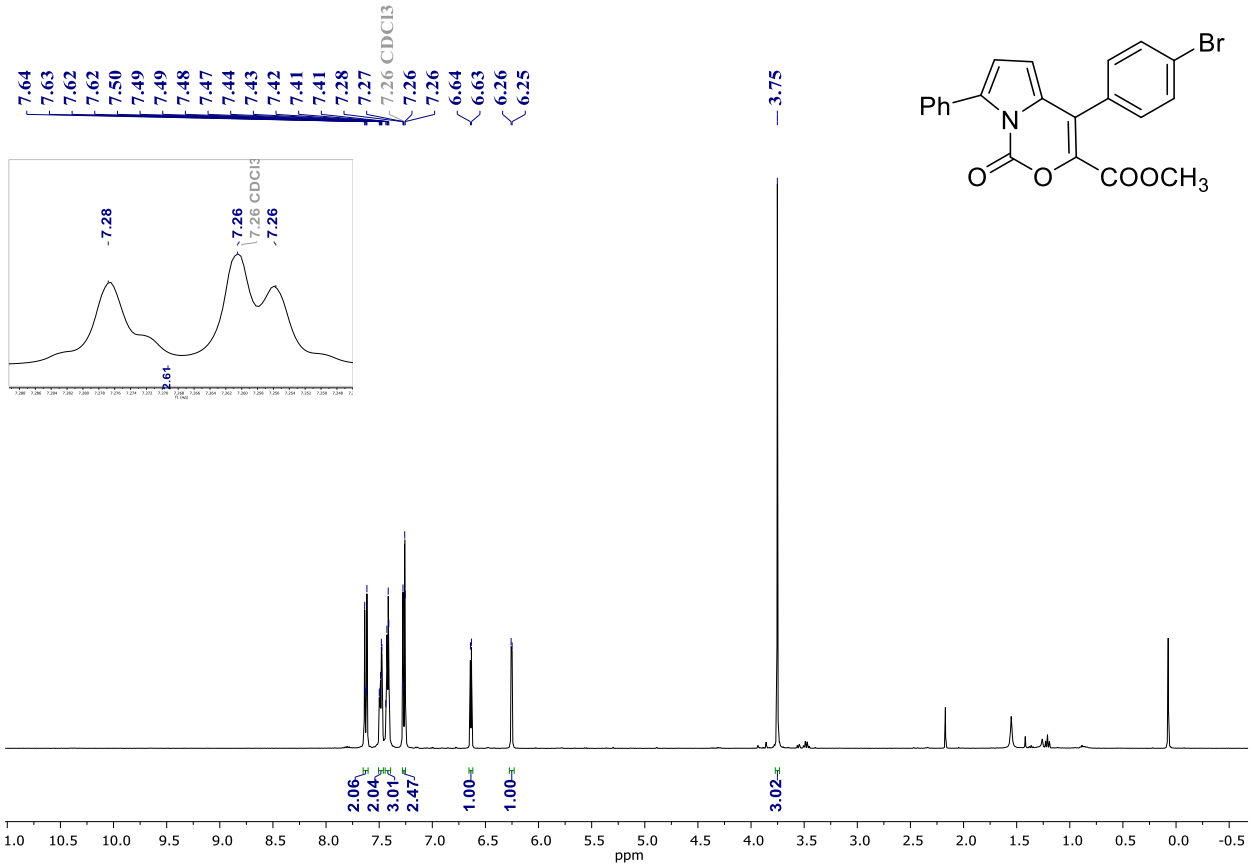
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound **6e**



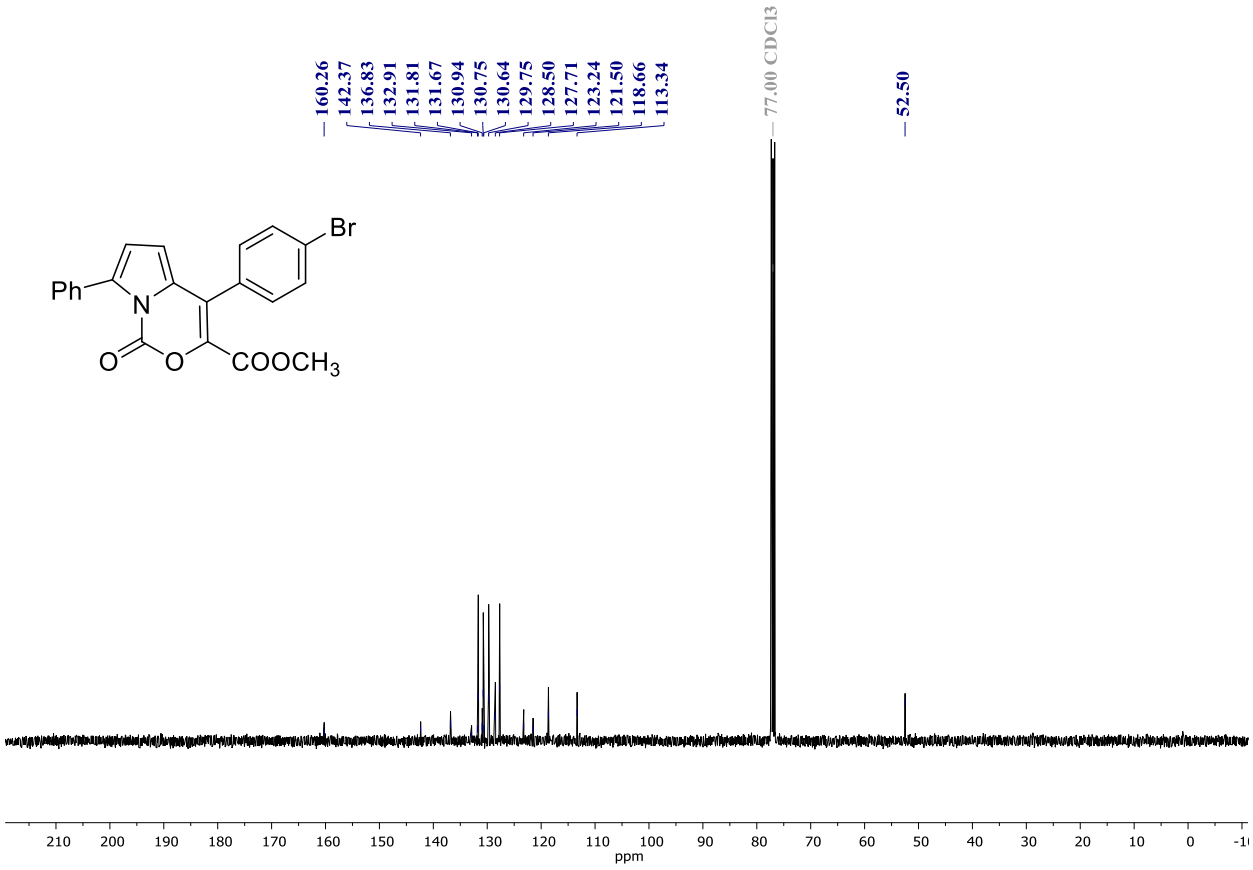
^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) spectrum of compound **6e**



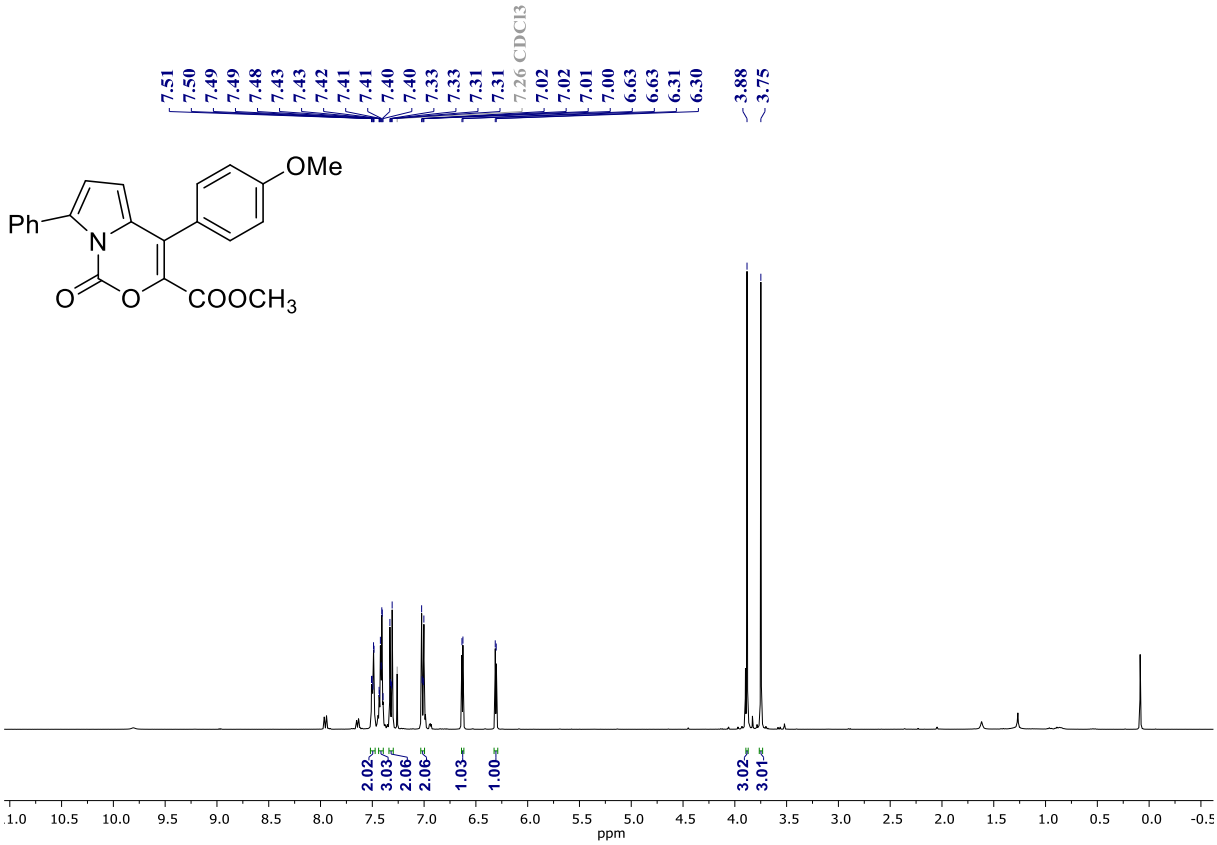
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound **6f**



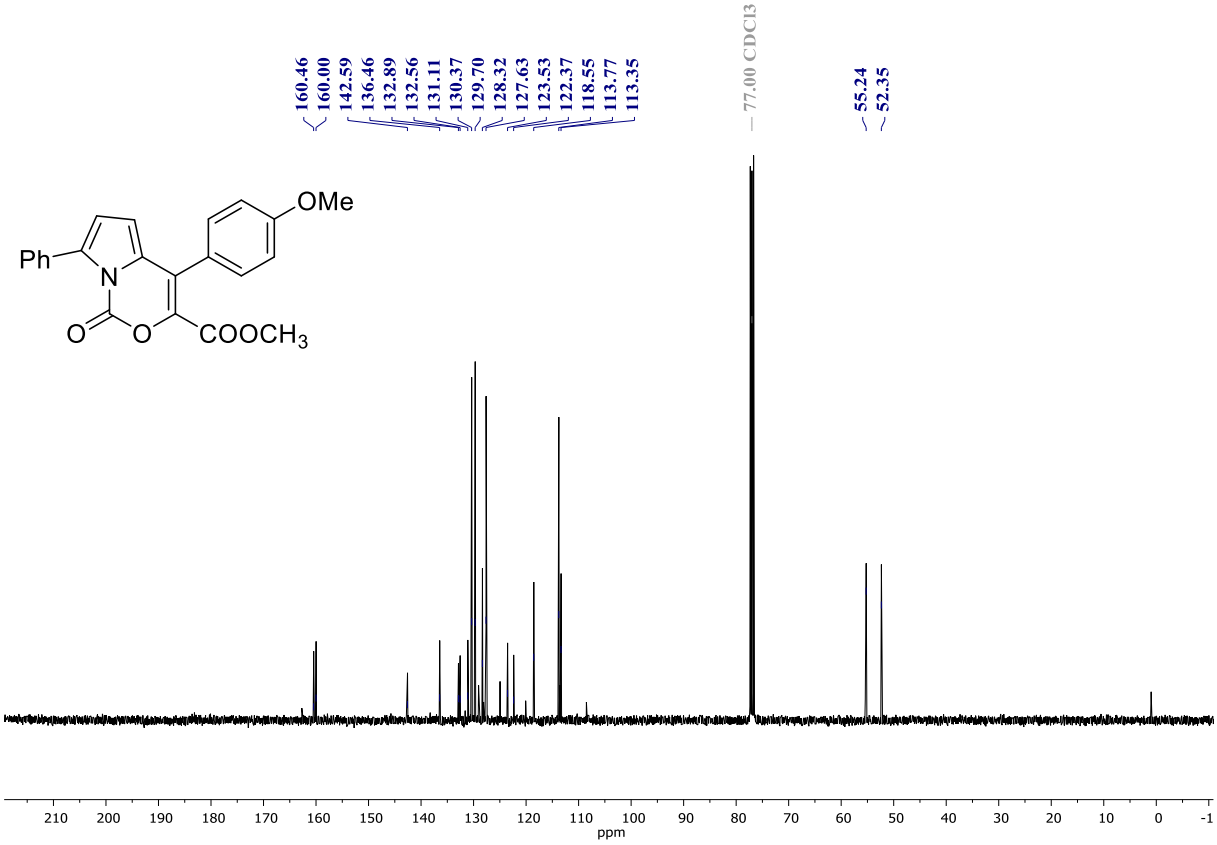
^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) spectrum of compound **6f**



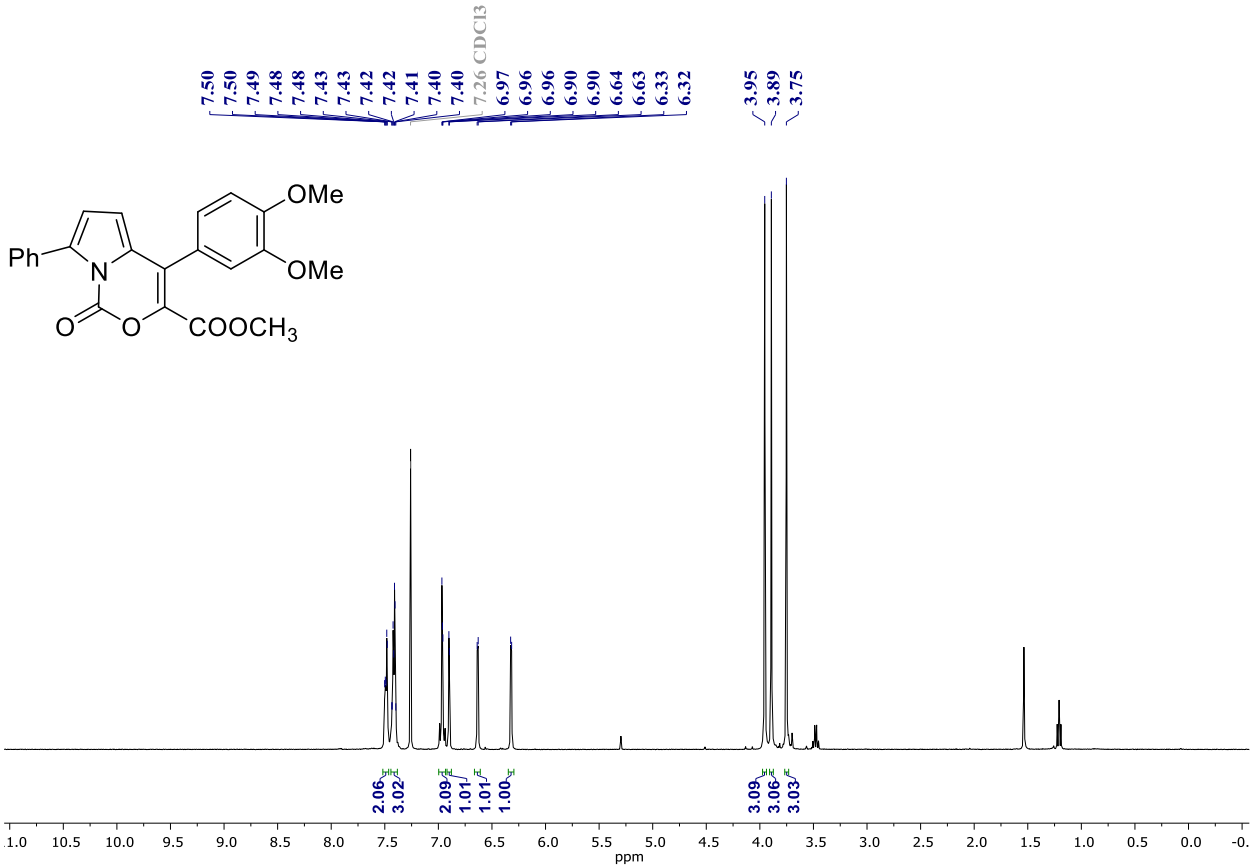
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound **6g**



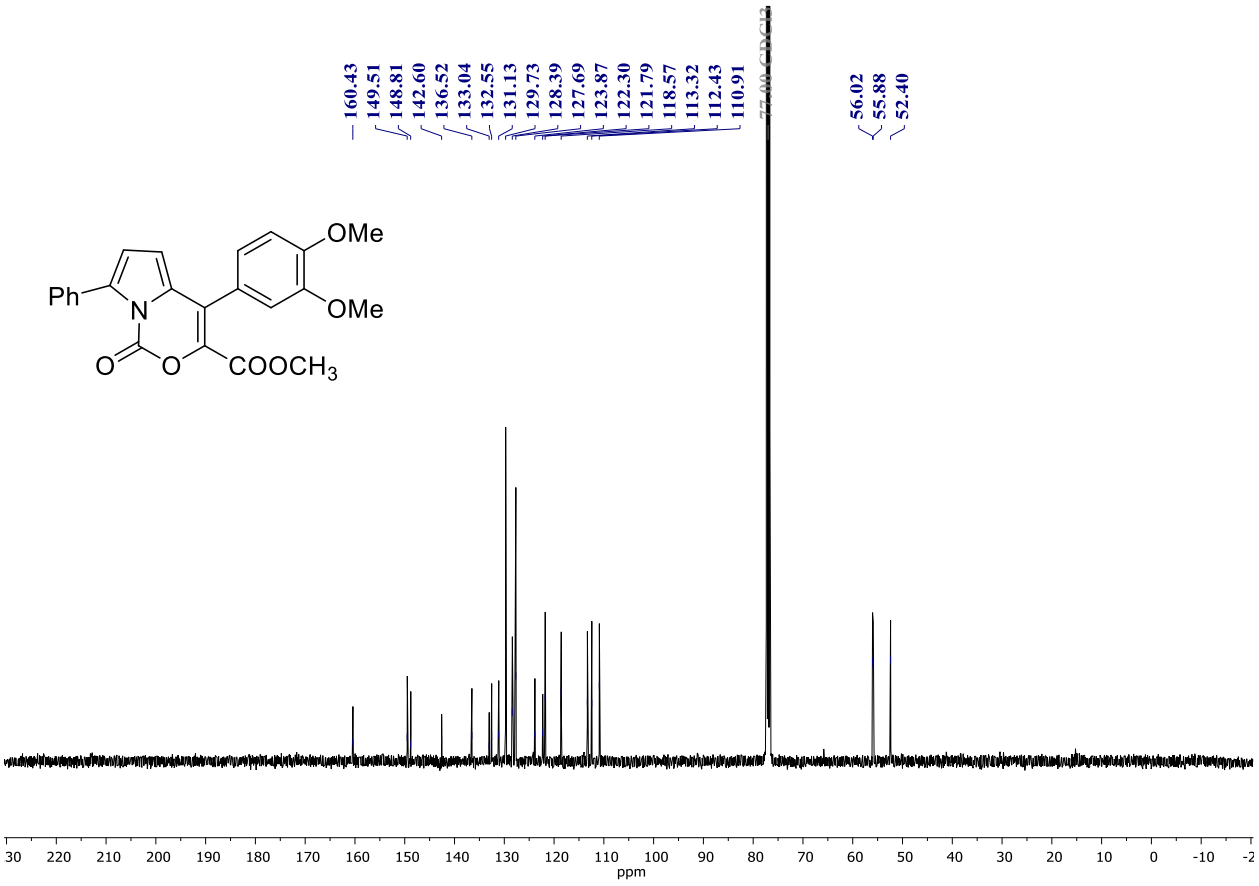
^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) spectrum of compound **6g**



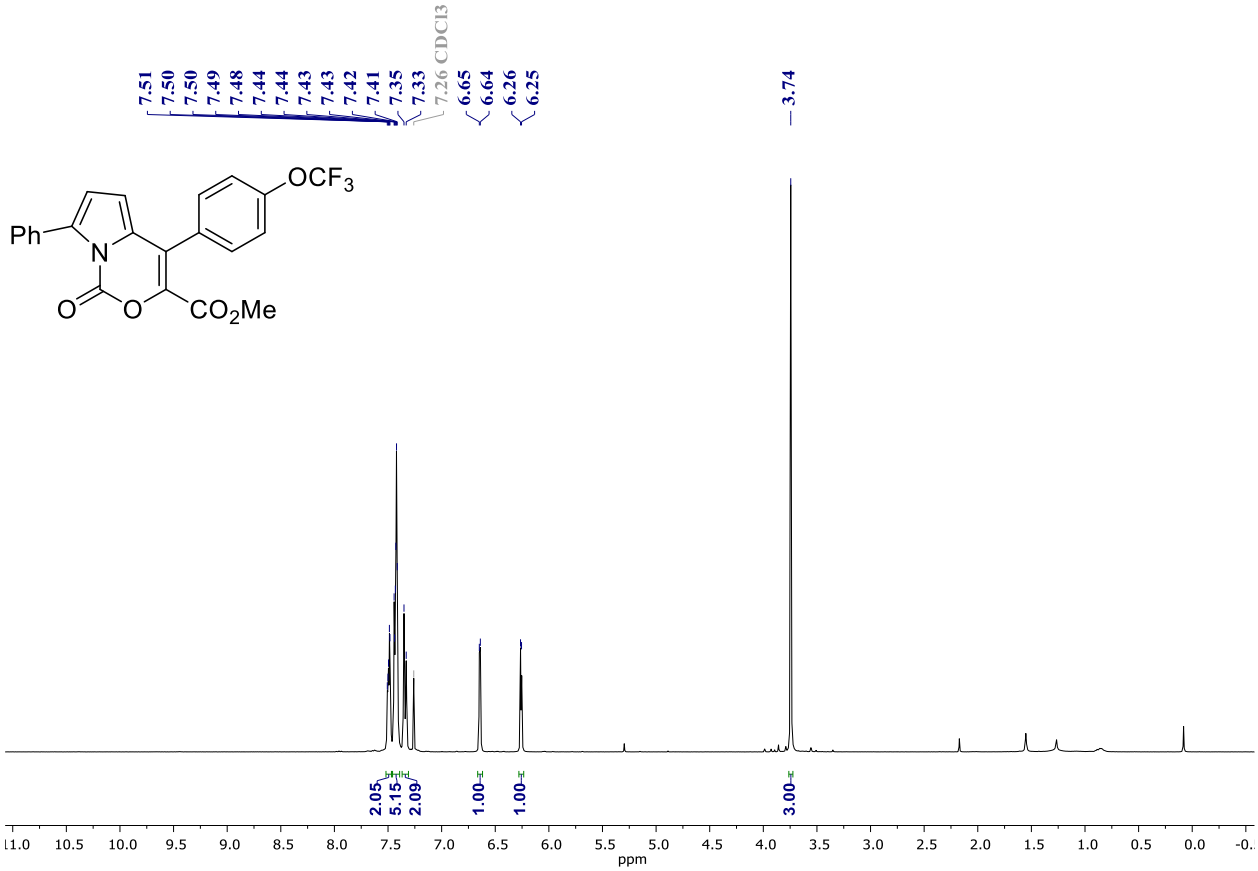
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound **6h**



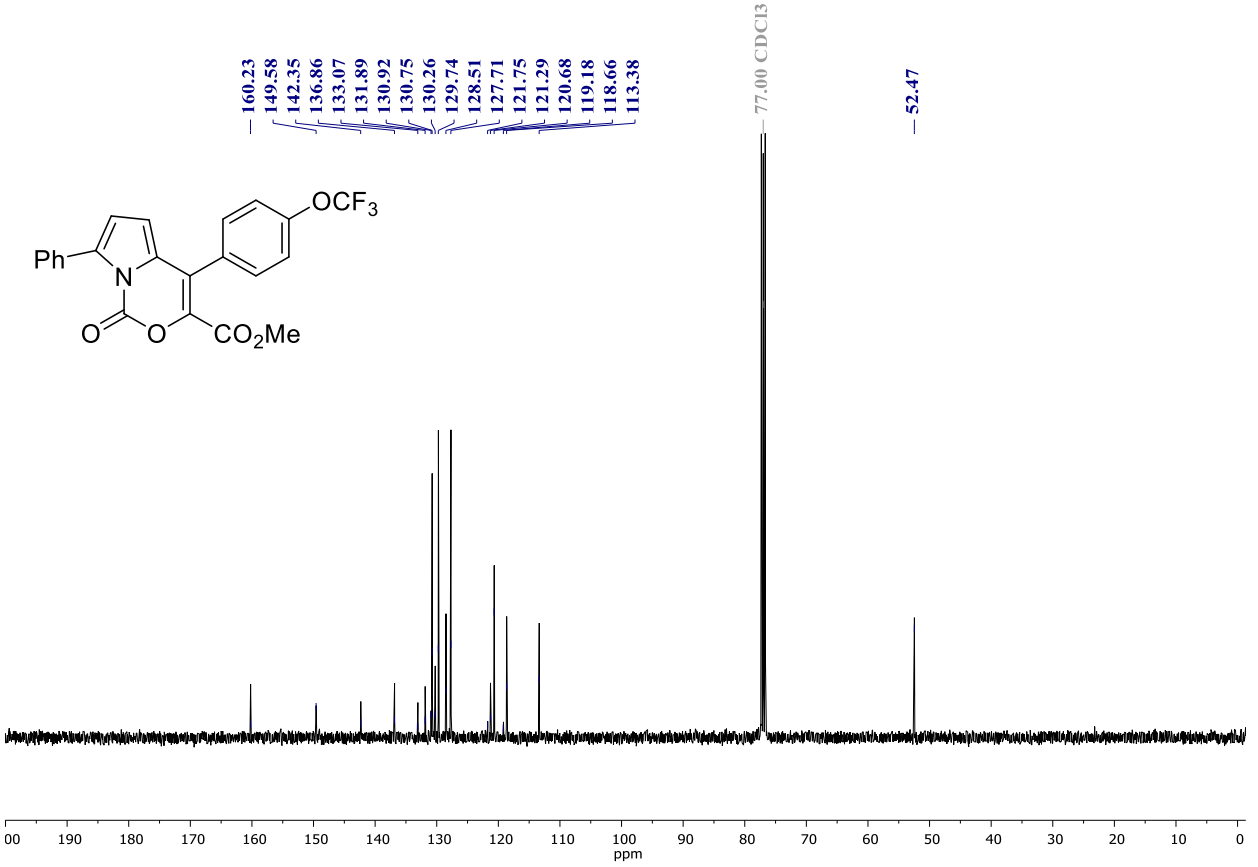
^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) spectrum of compound **6h**



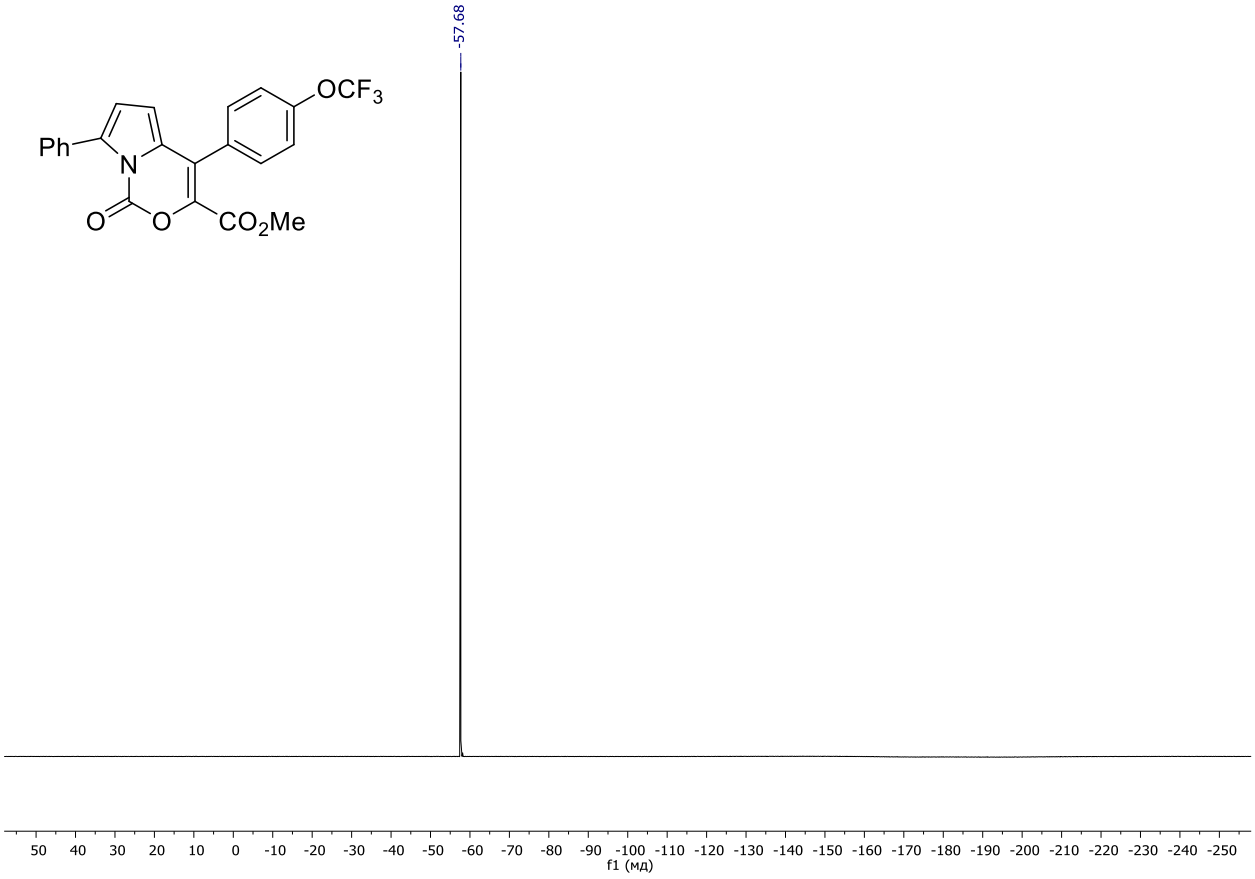
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound **6i**



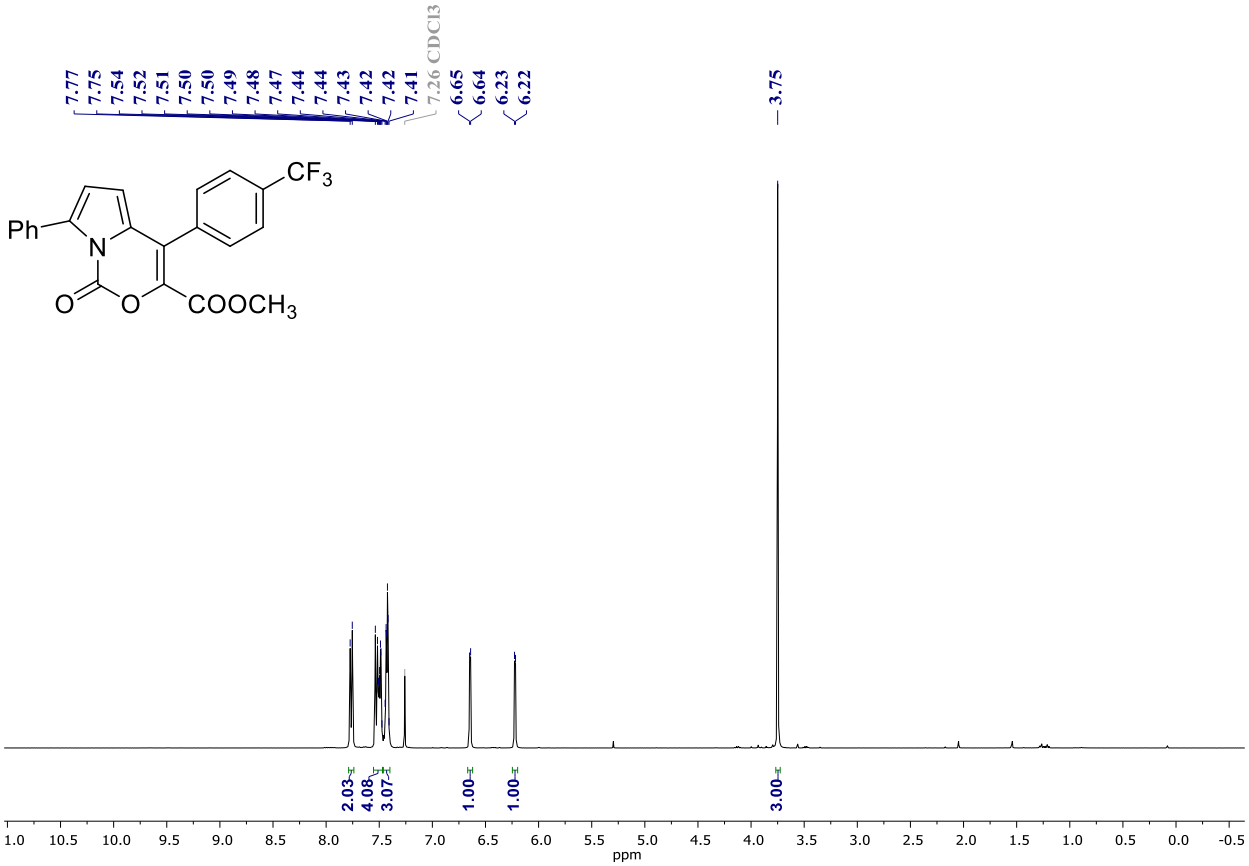
^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) spectrum of compound **6i**



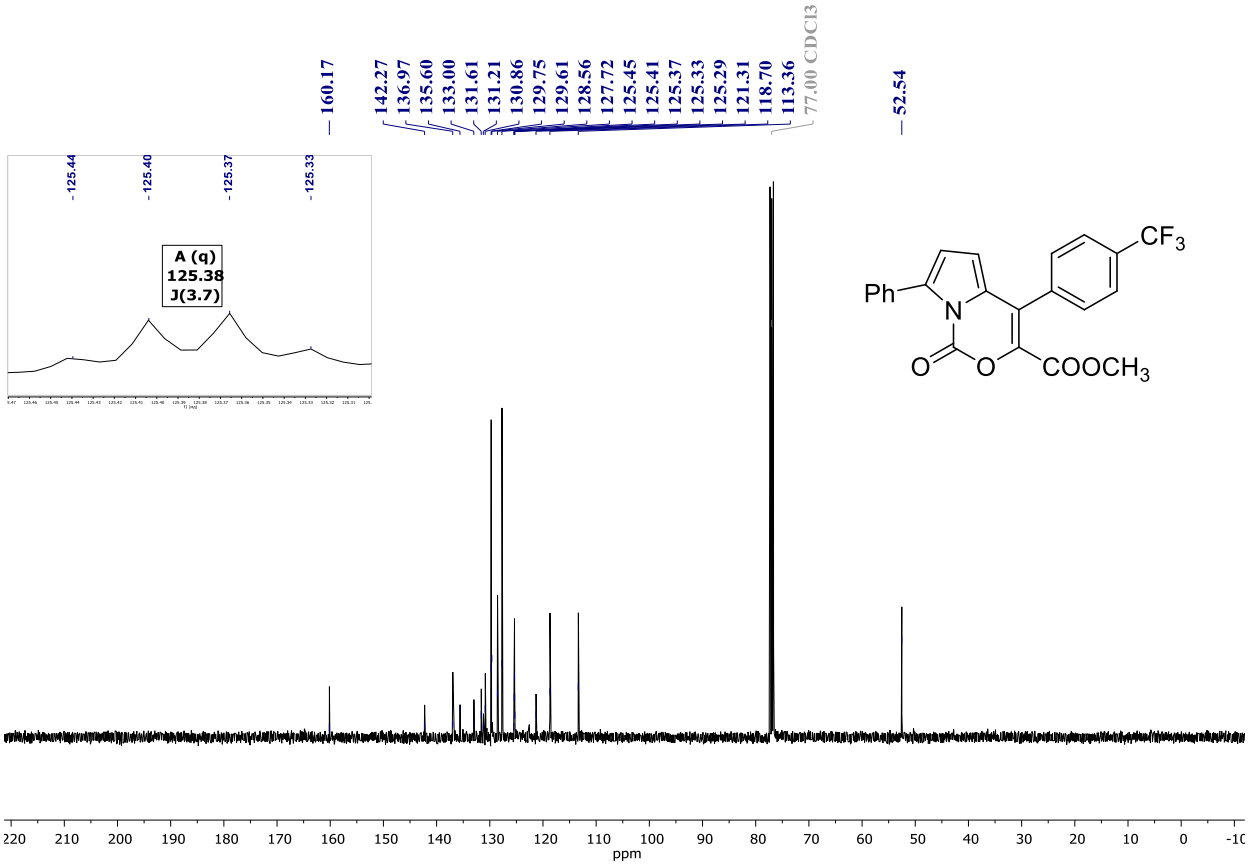
^{19}F NMR (376 MHz, DMSO-d_6) spectrum of compound **6i**



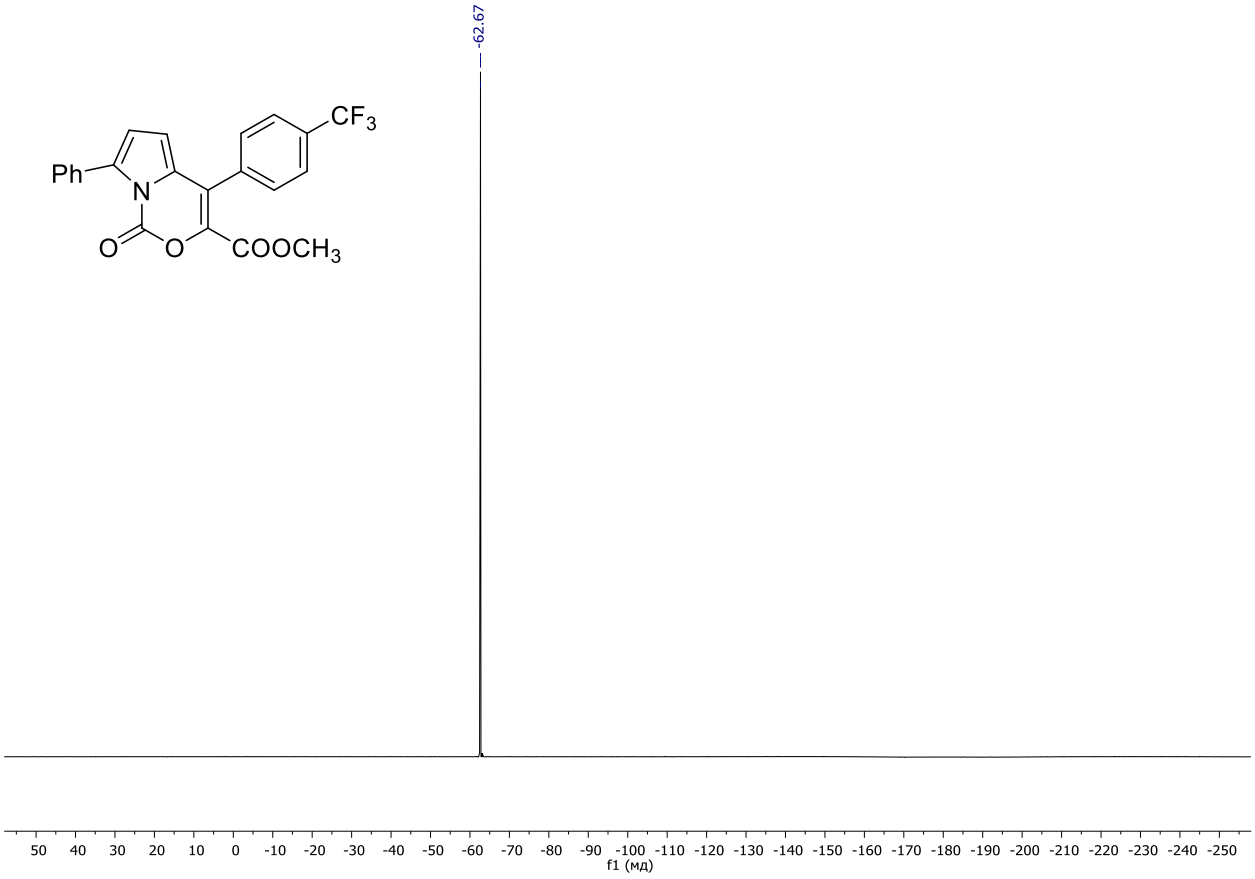
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound **6j**



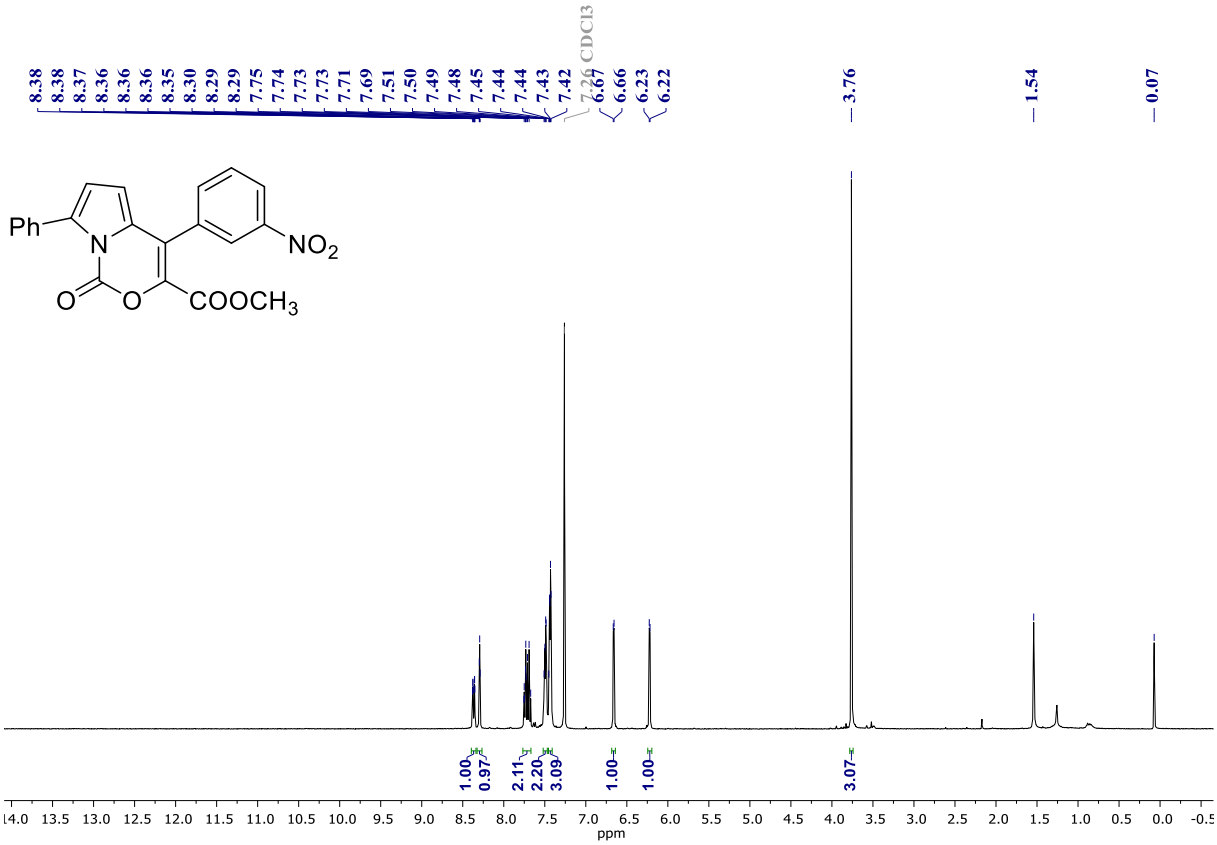
^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) spectrum of compound **6j**



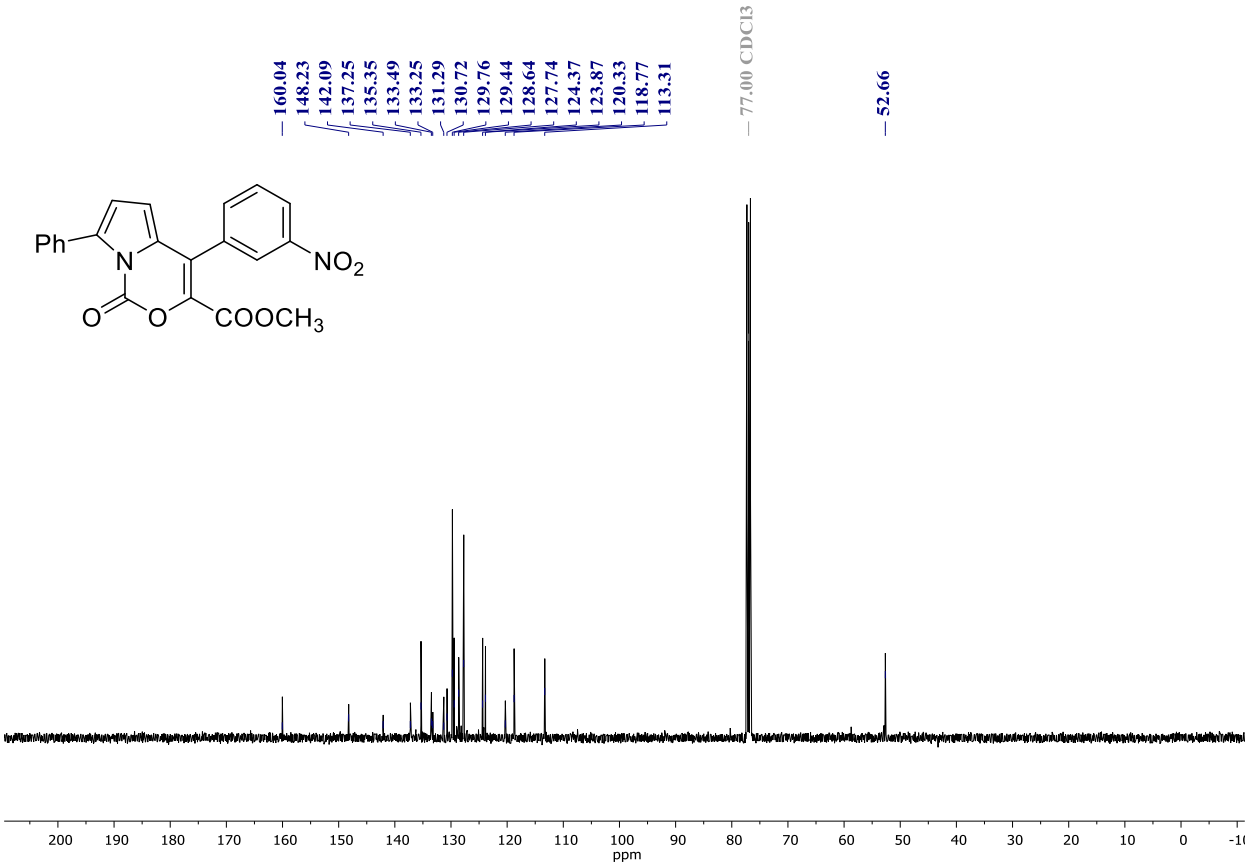
^{19}F NMR (376 MHz, DMSO-d_6) spectrum of compound **6j**



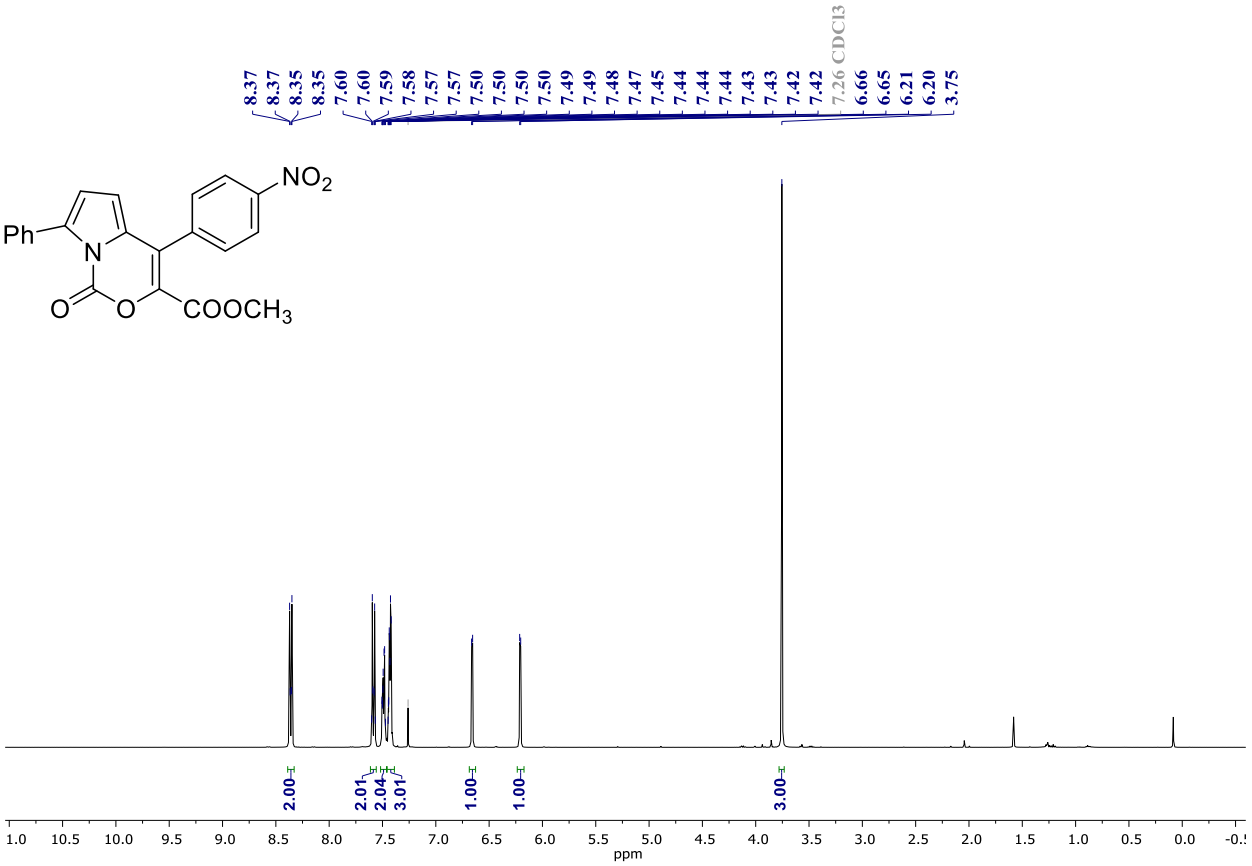
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound **6k**



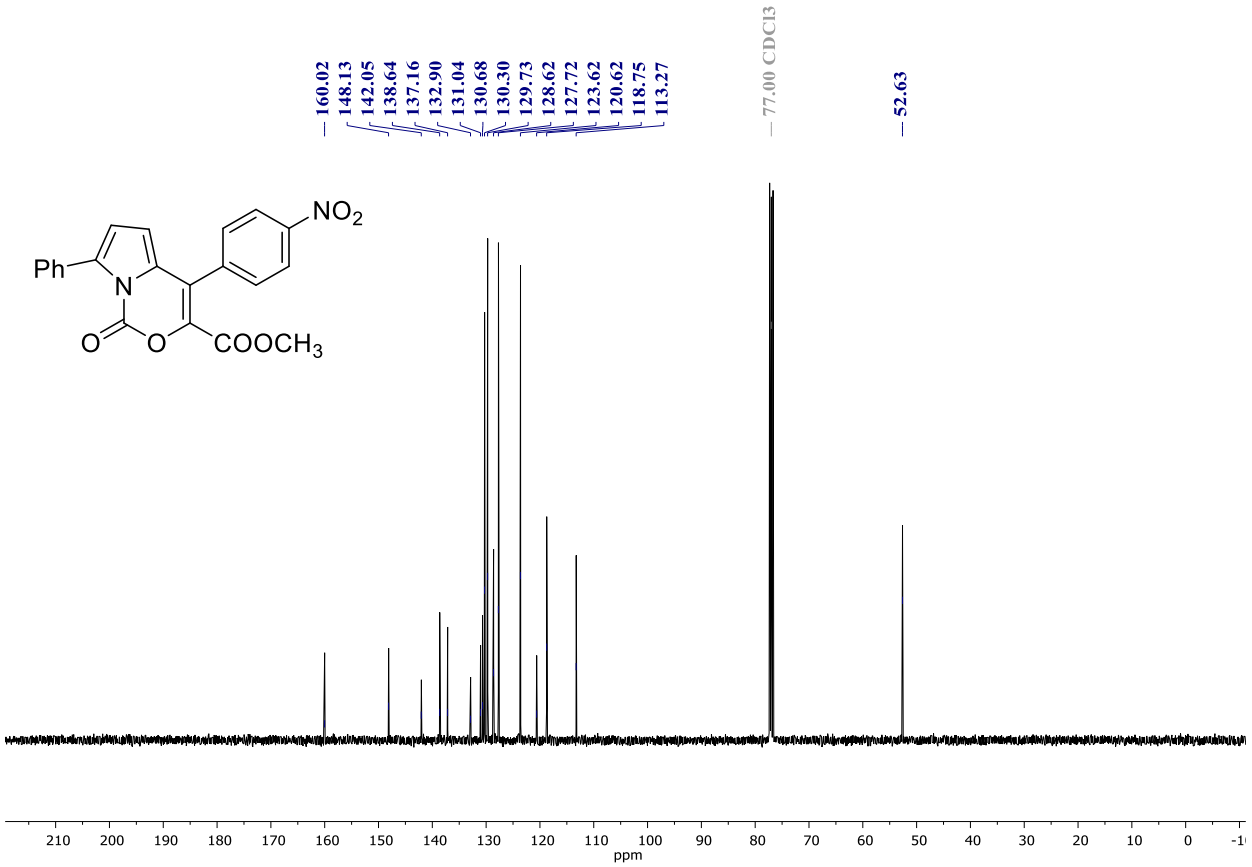
^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) spectrum of compound **6k**



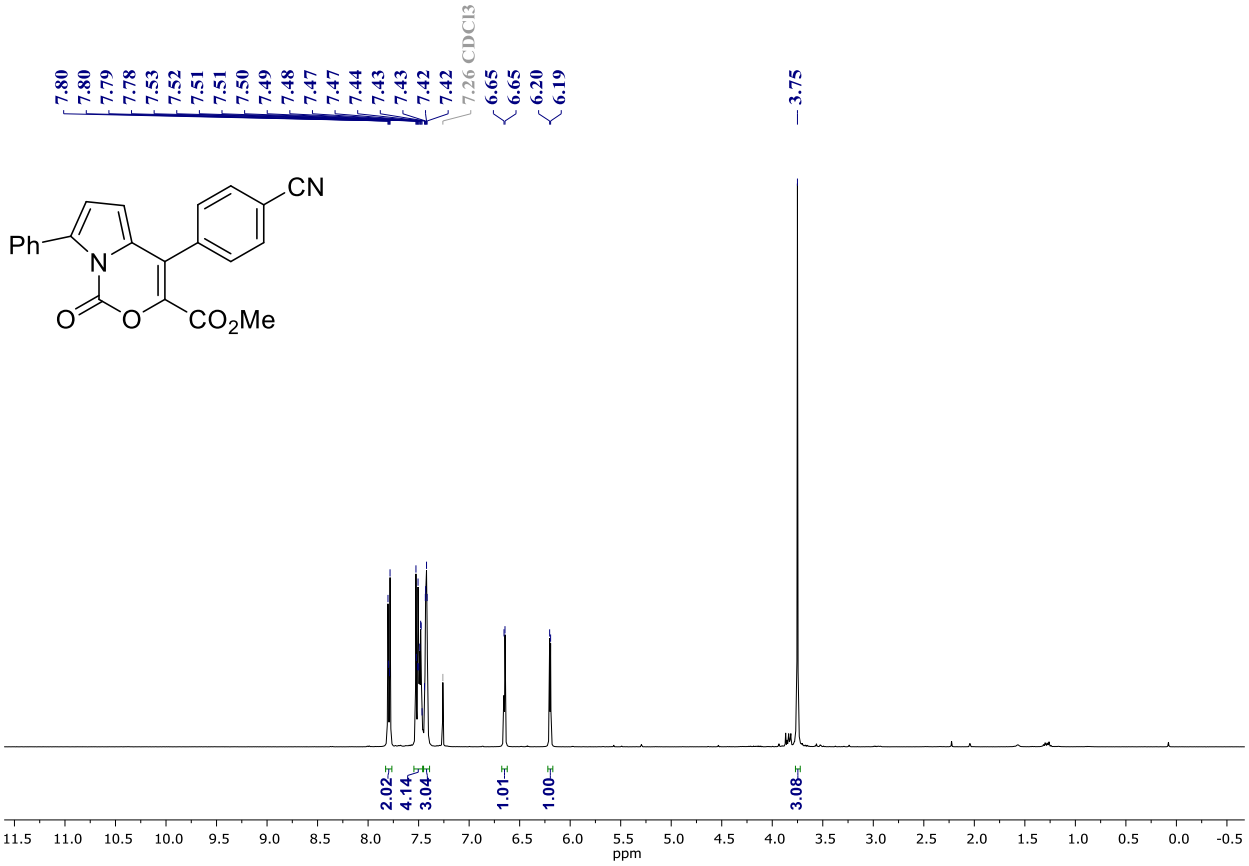
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound **6l**



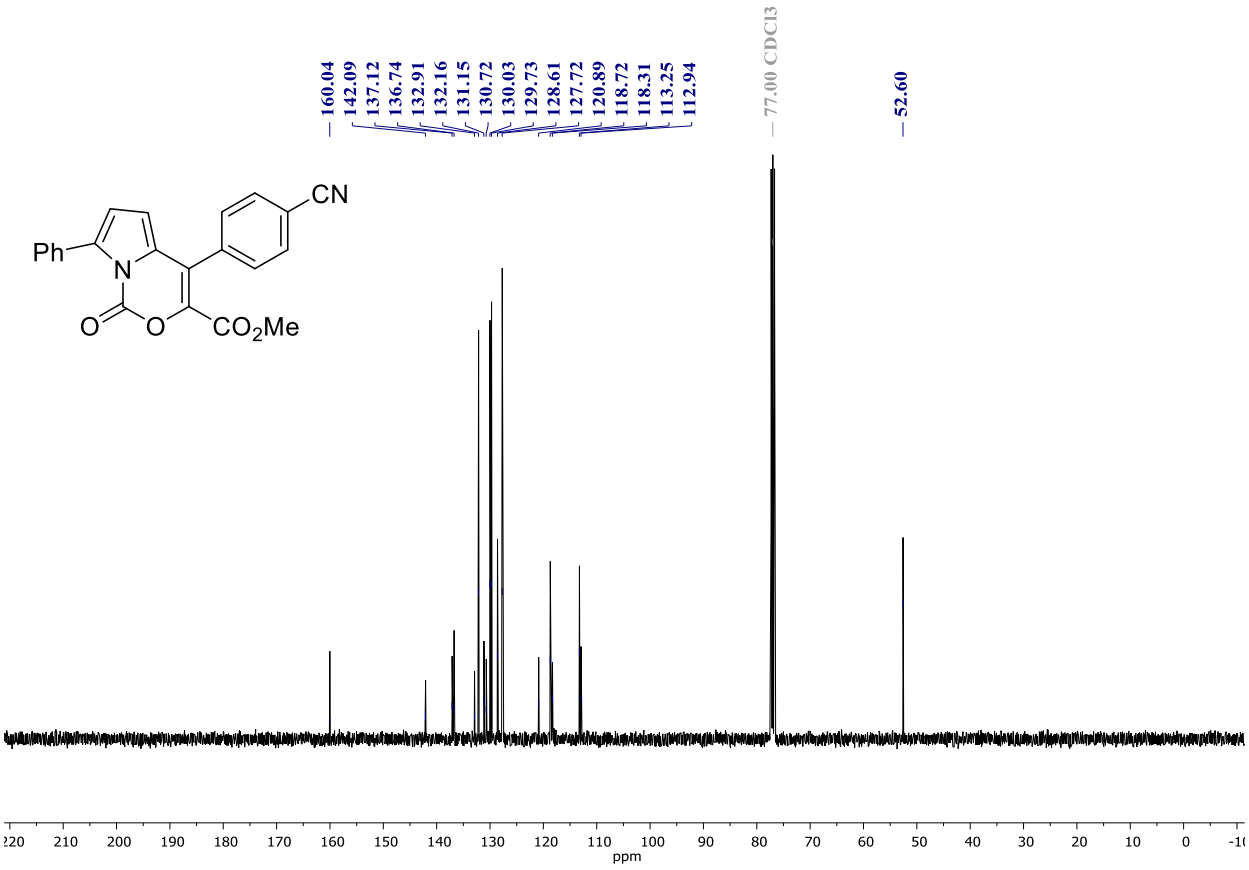
^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) spectrum of compound **6l**



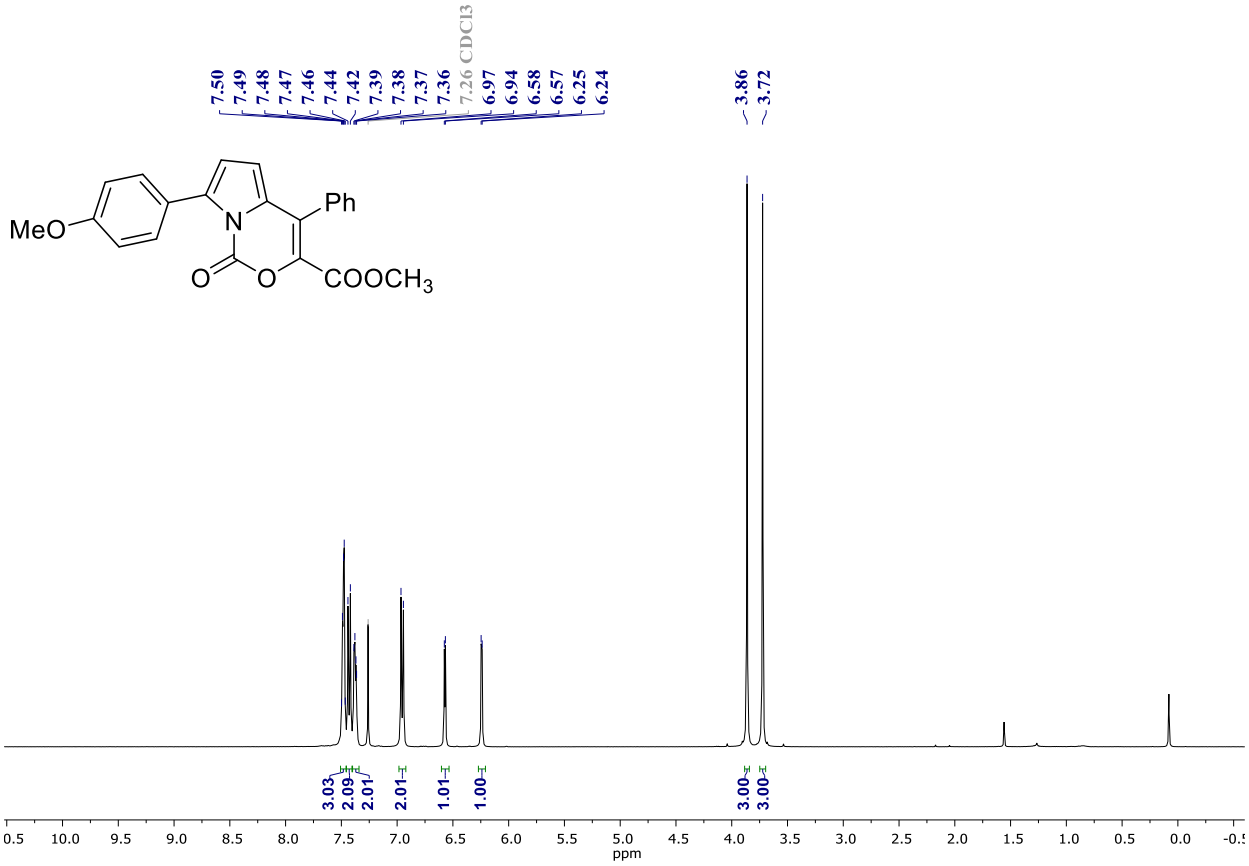
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound **6m**



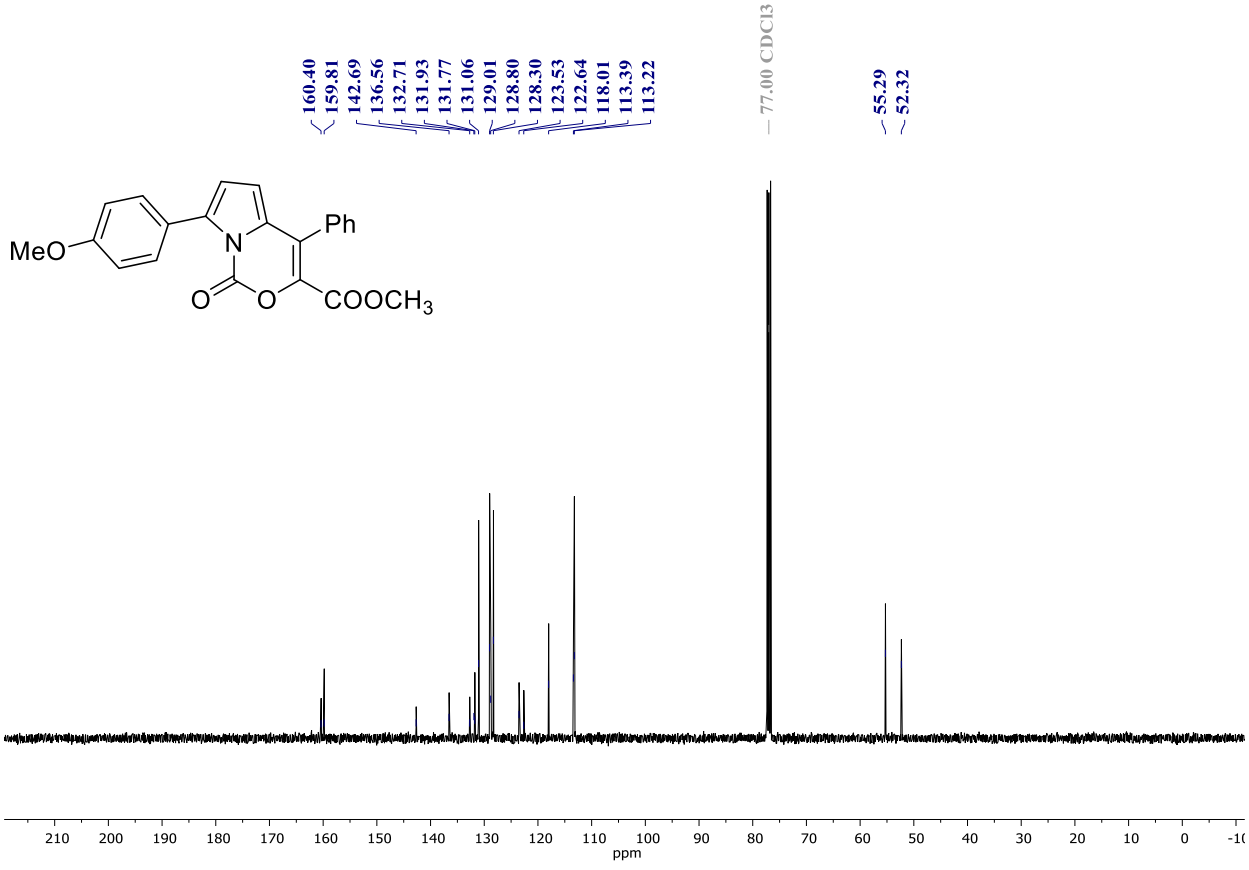
^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) spectrum of compound **6m**



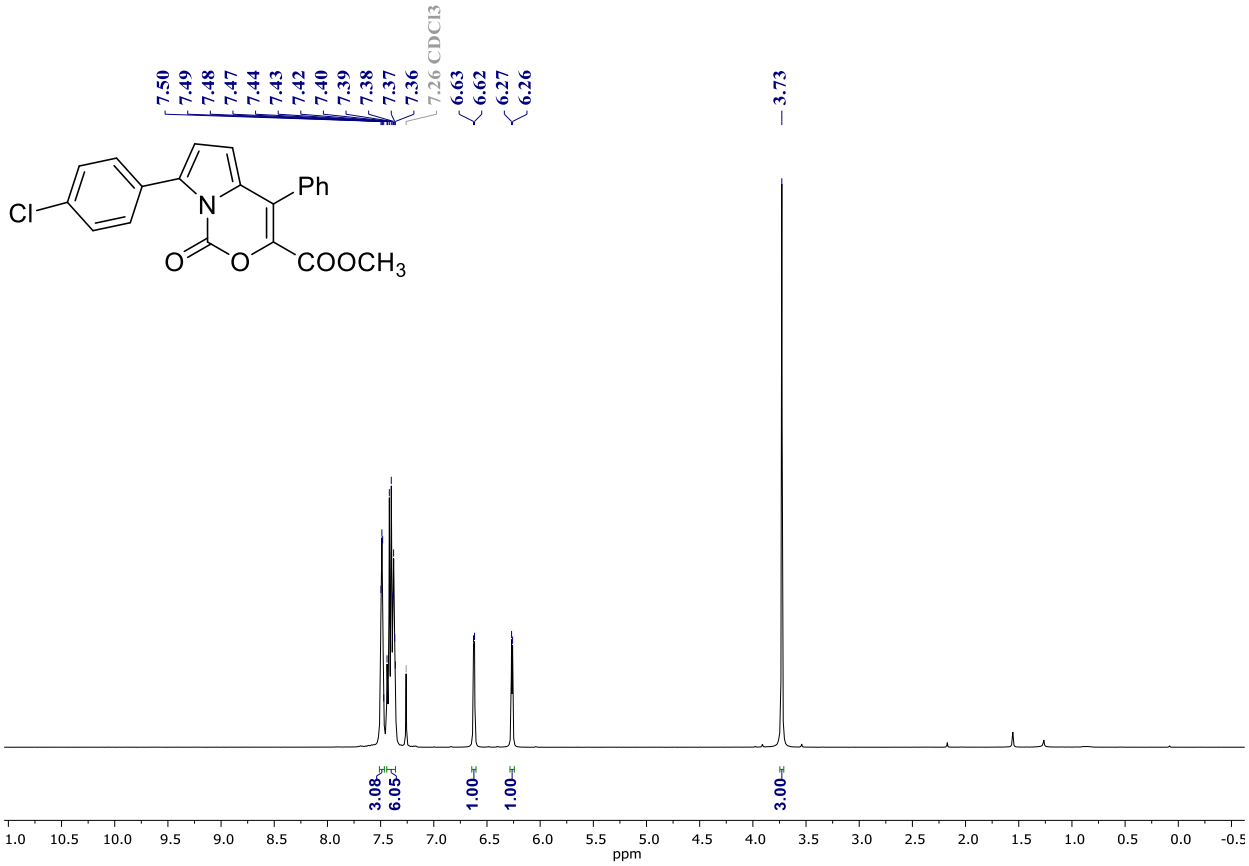
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound **6n**



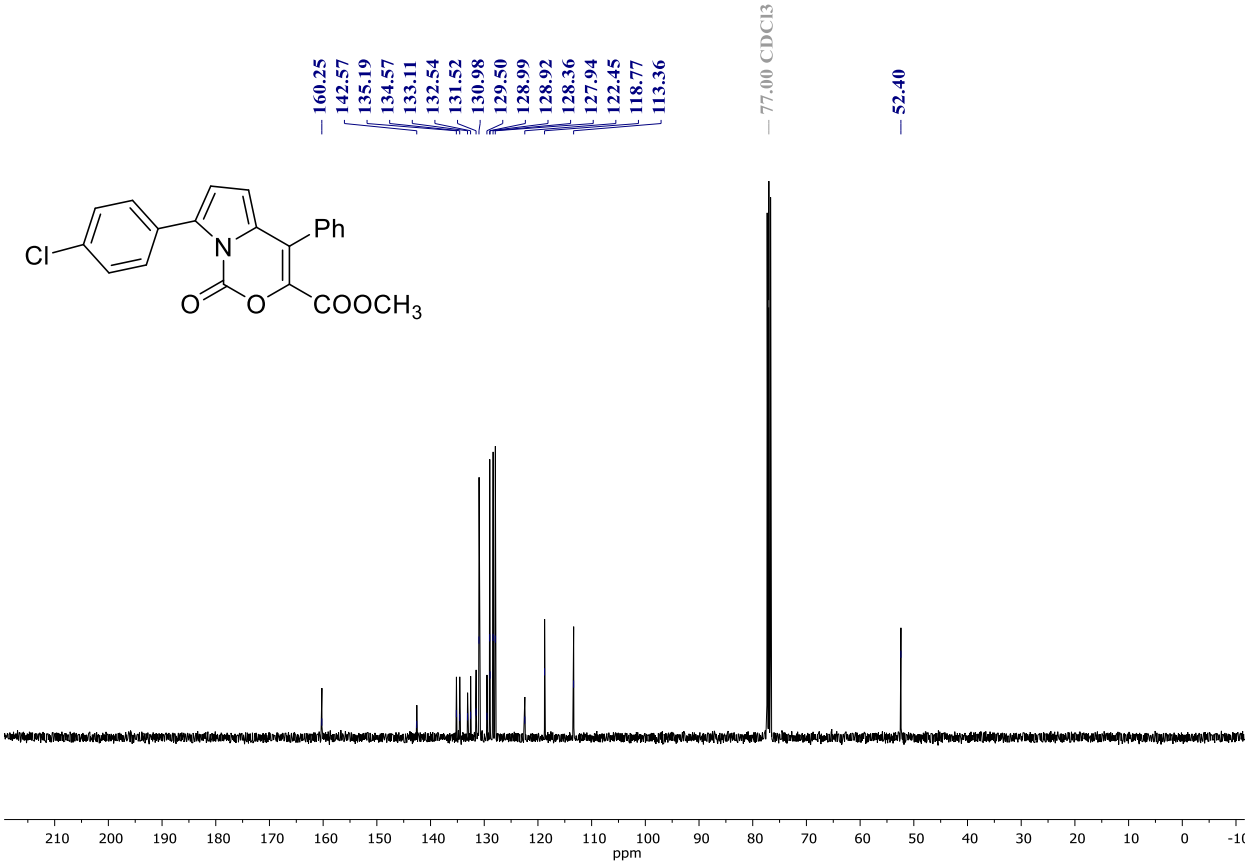
^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) spectrum of compound **6n**



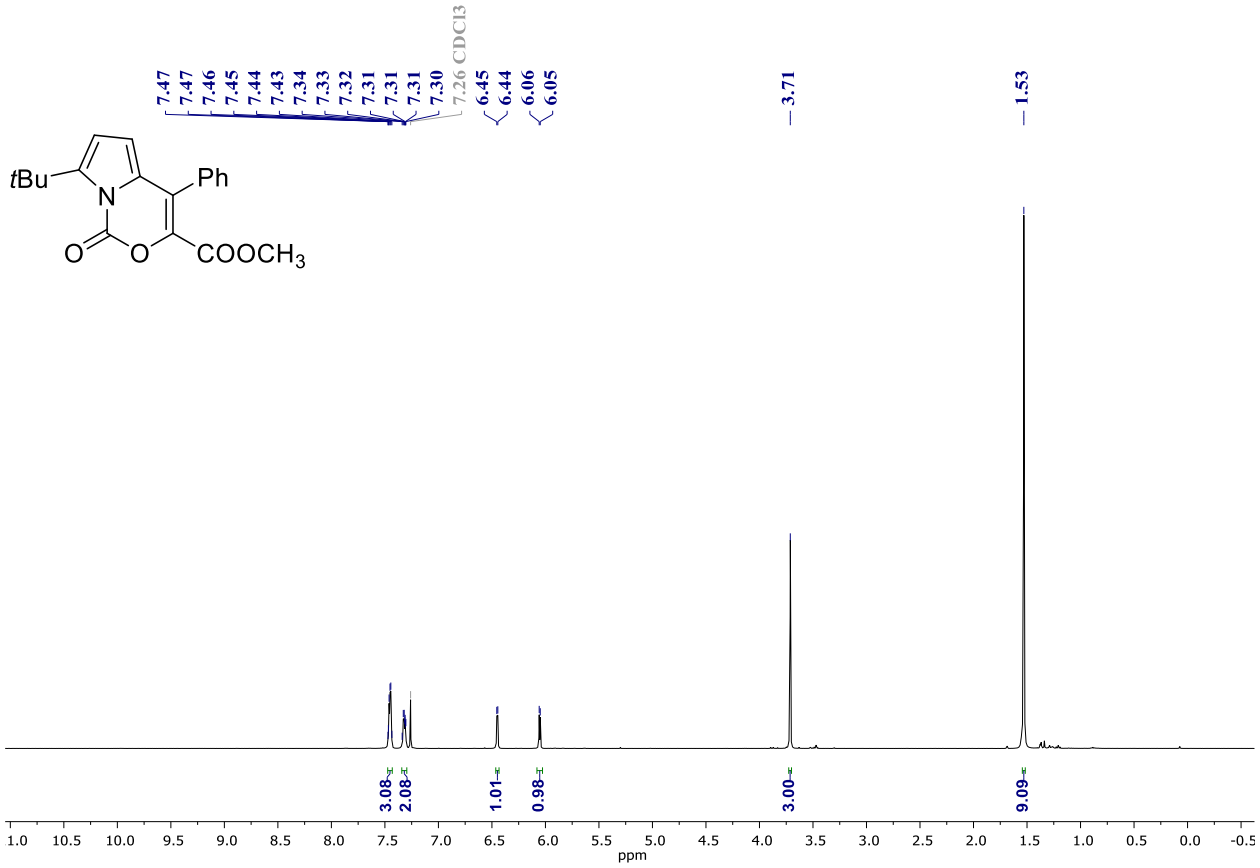
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound **6o**



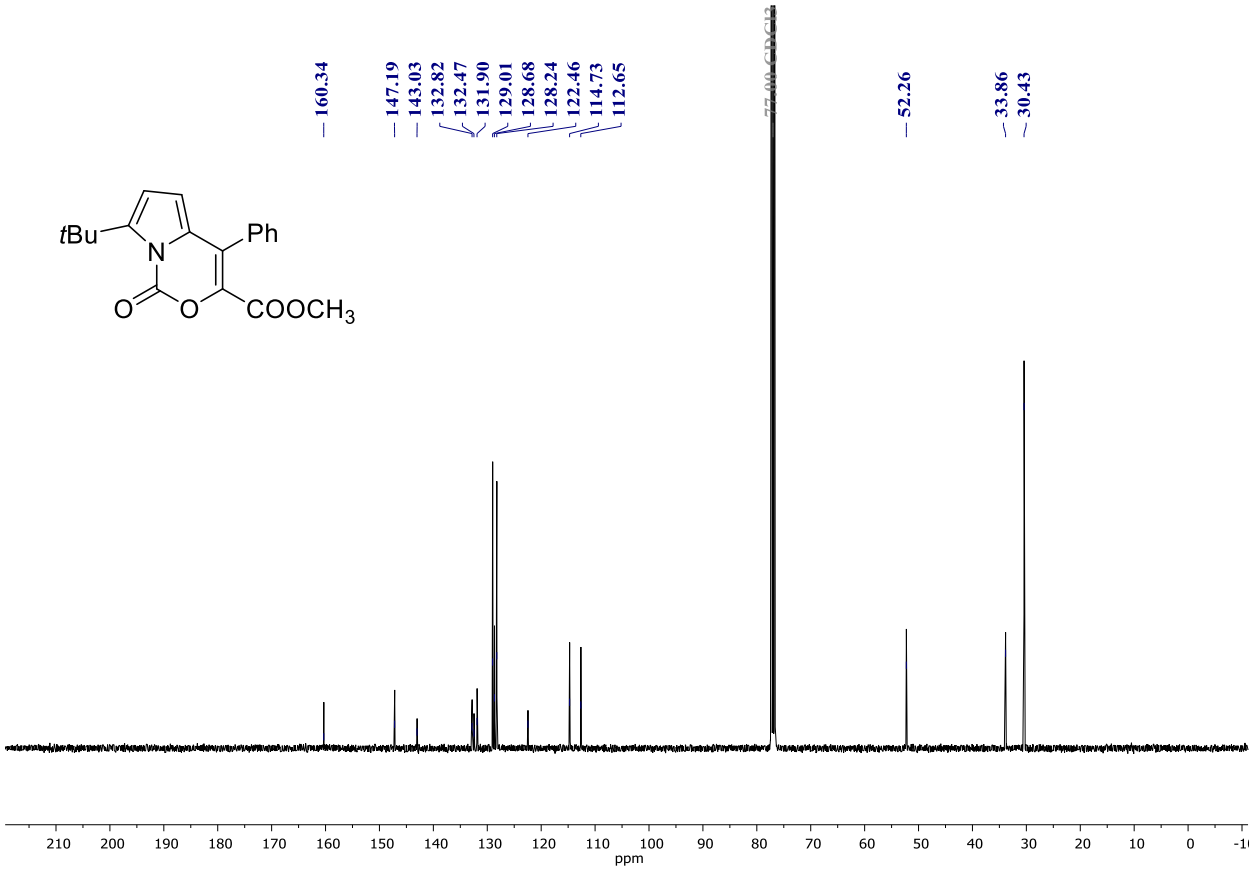
^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) spectrum of compound **6o**



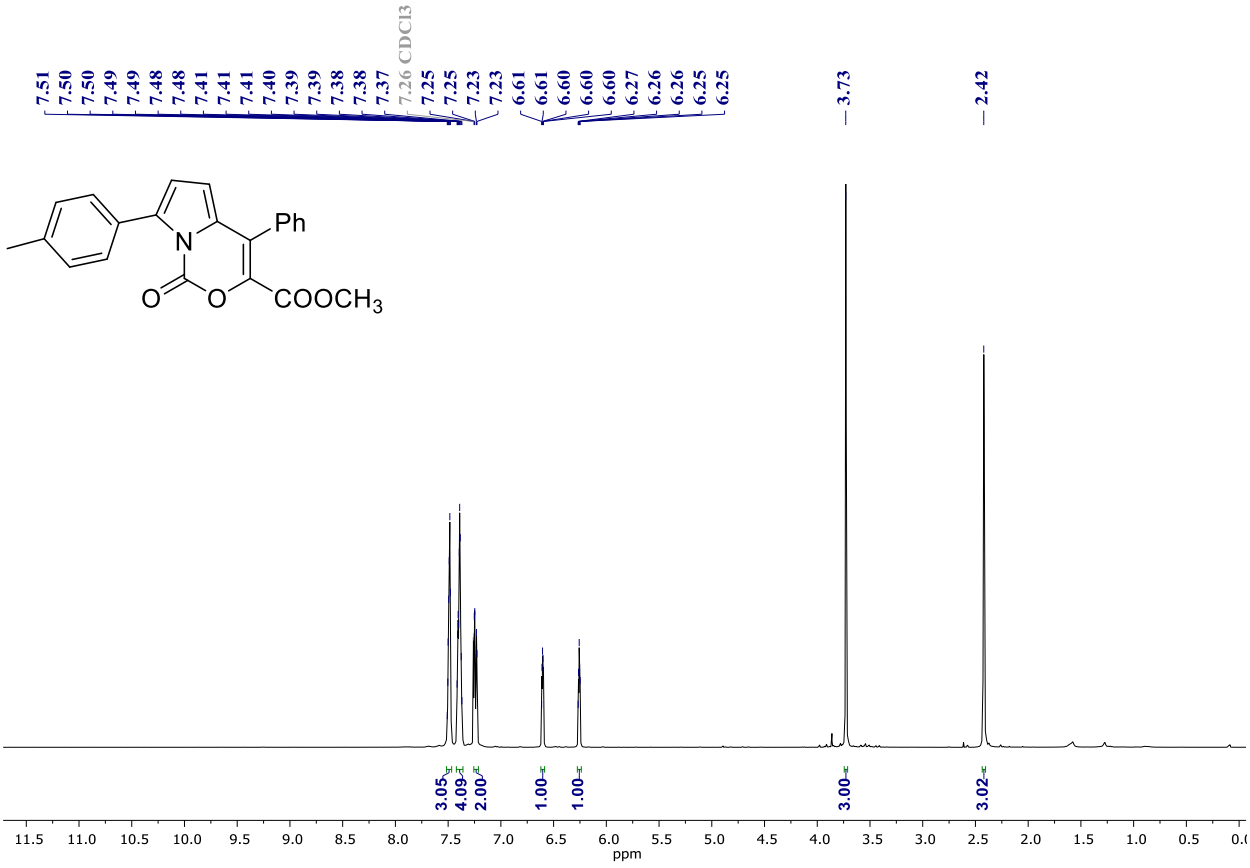
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound **6p**



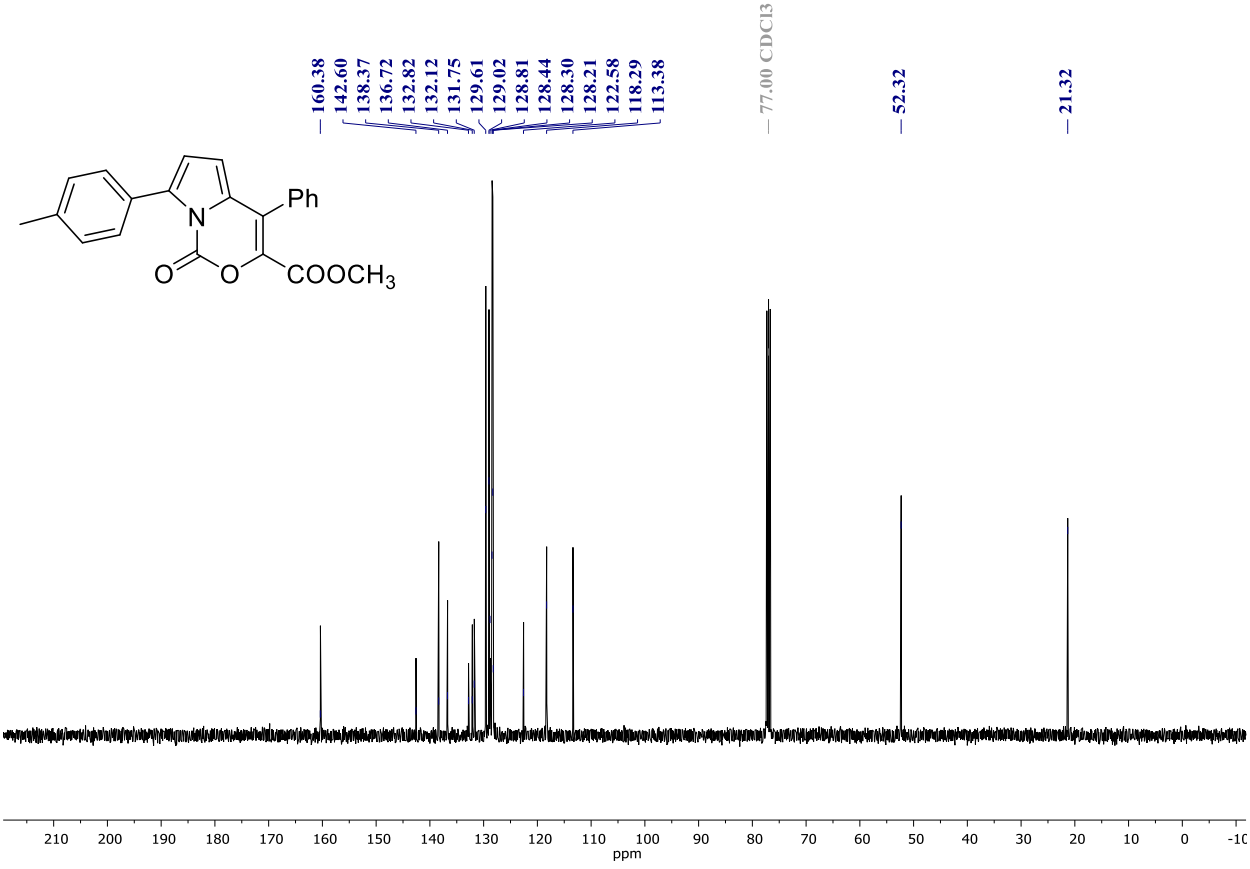
^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) spectrum of compound **6p**



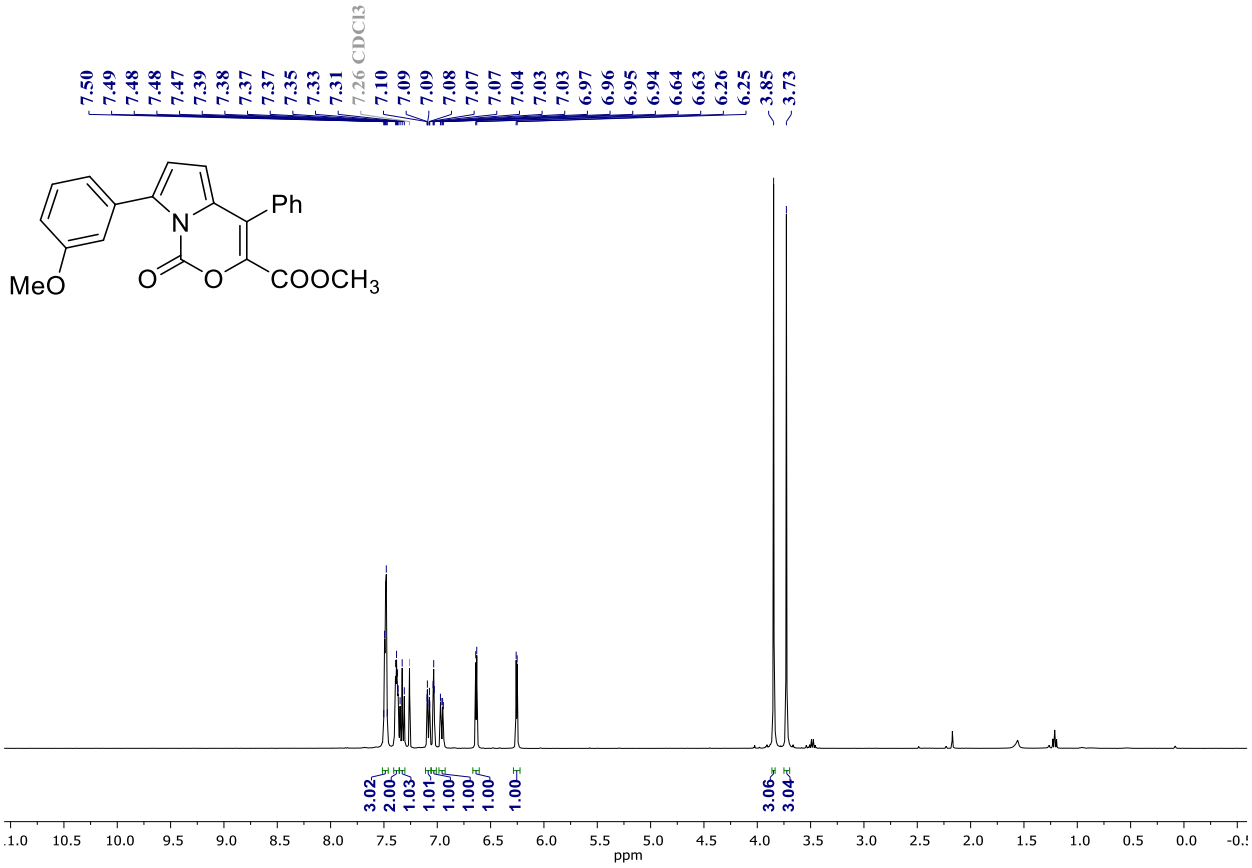
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound **6q**



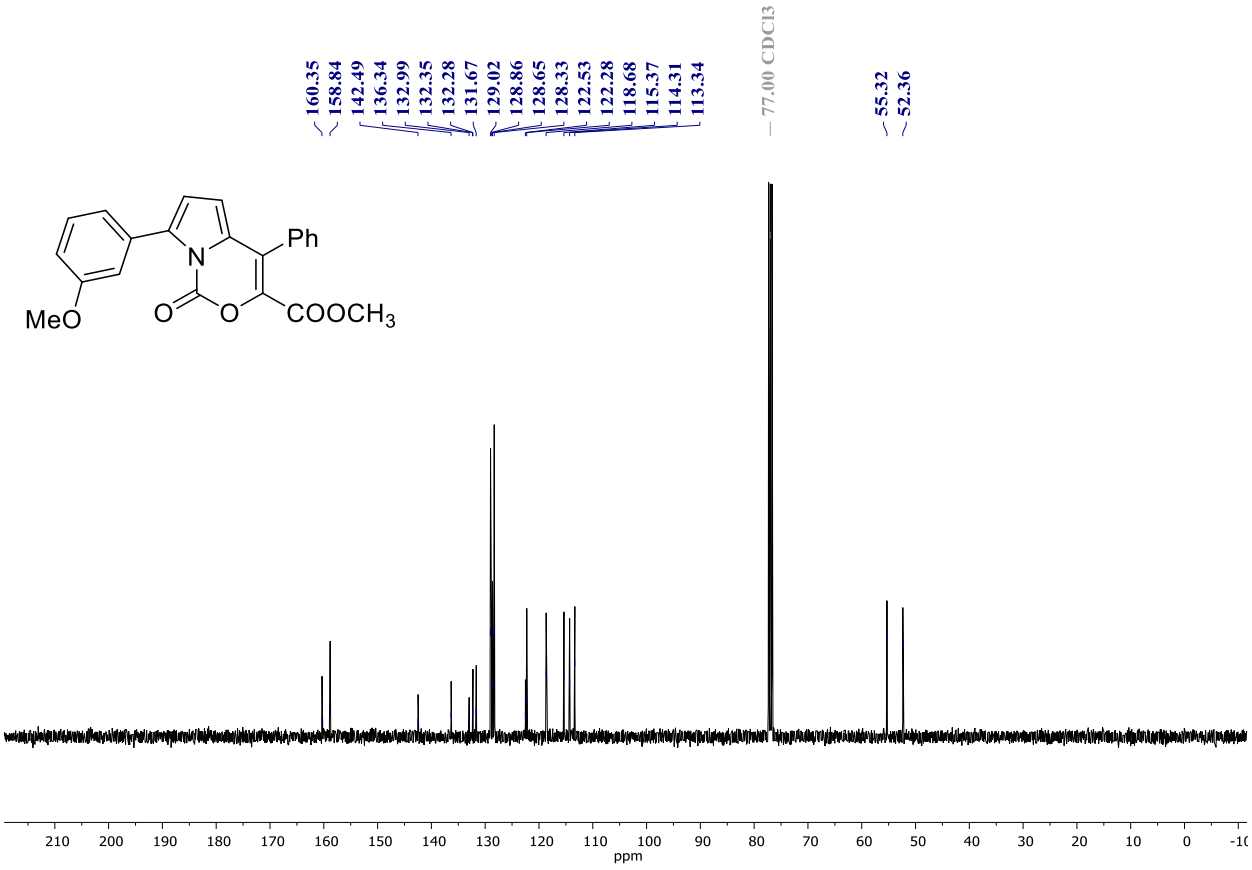
^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) spectrum of compound **6q**



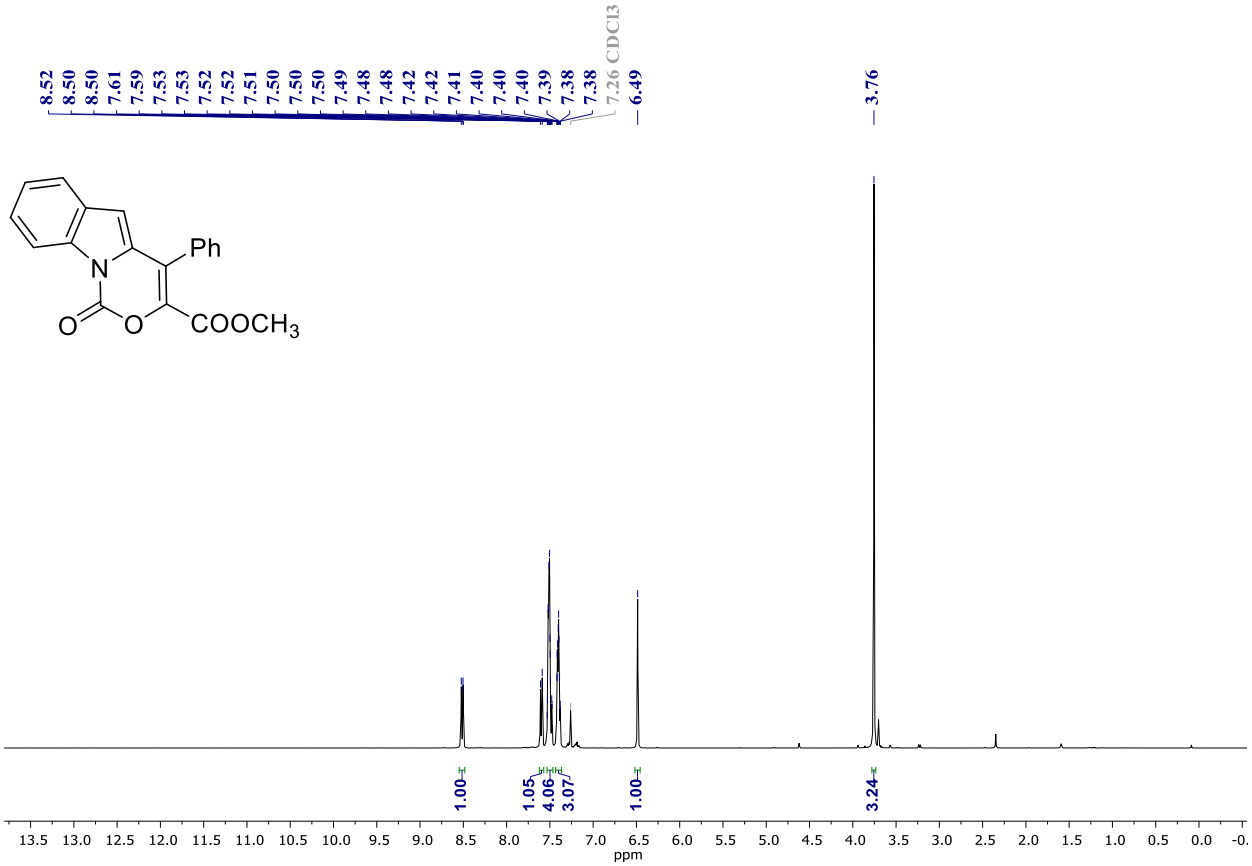
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound **6r**



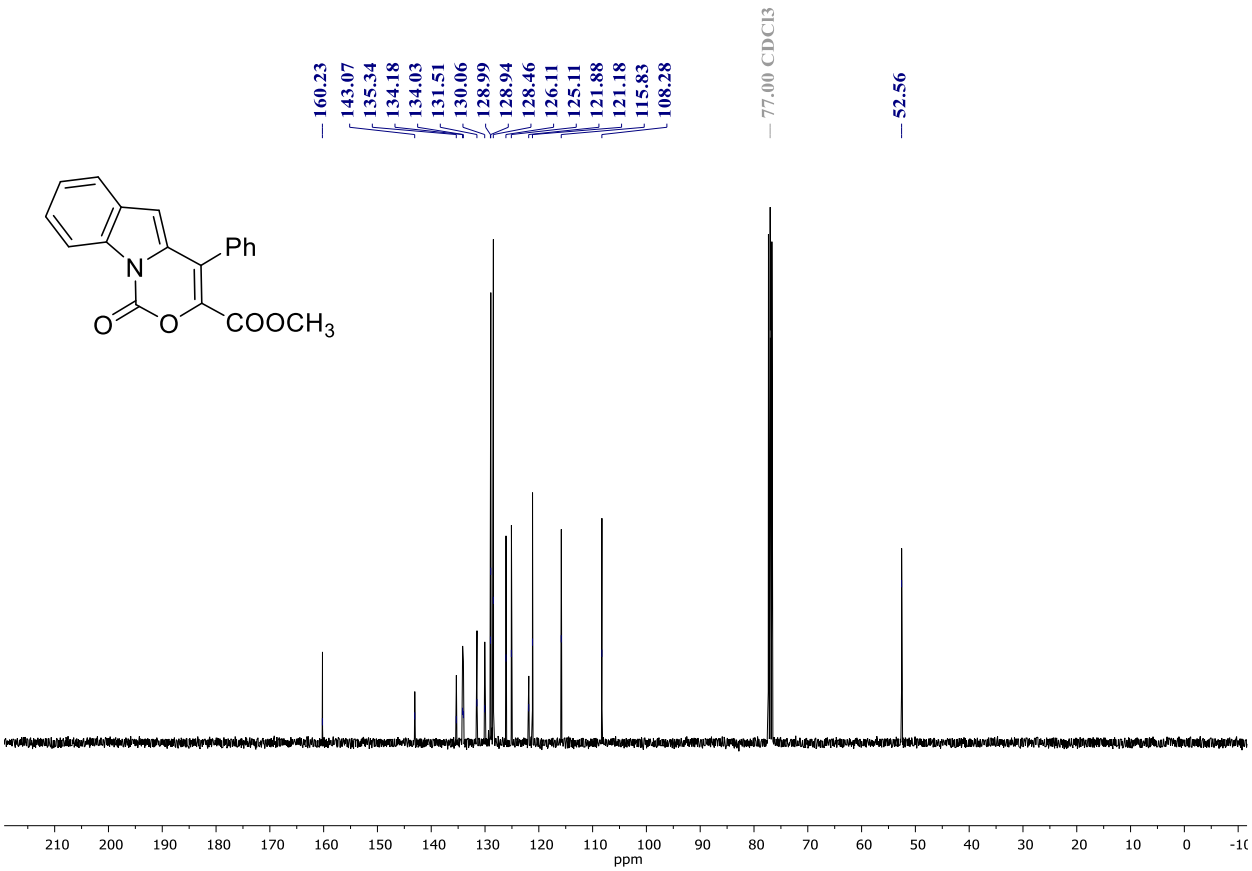
^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) spectrum of compound **6r**



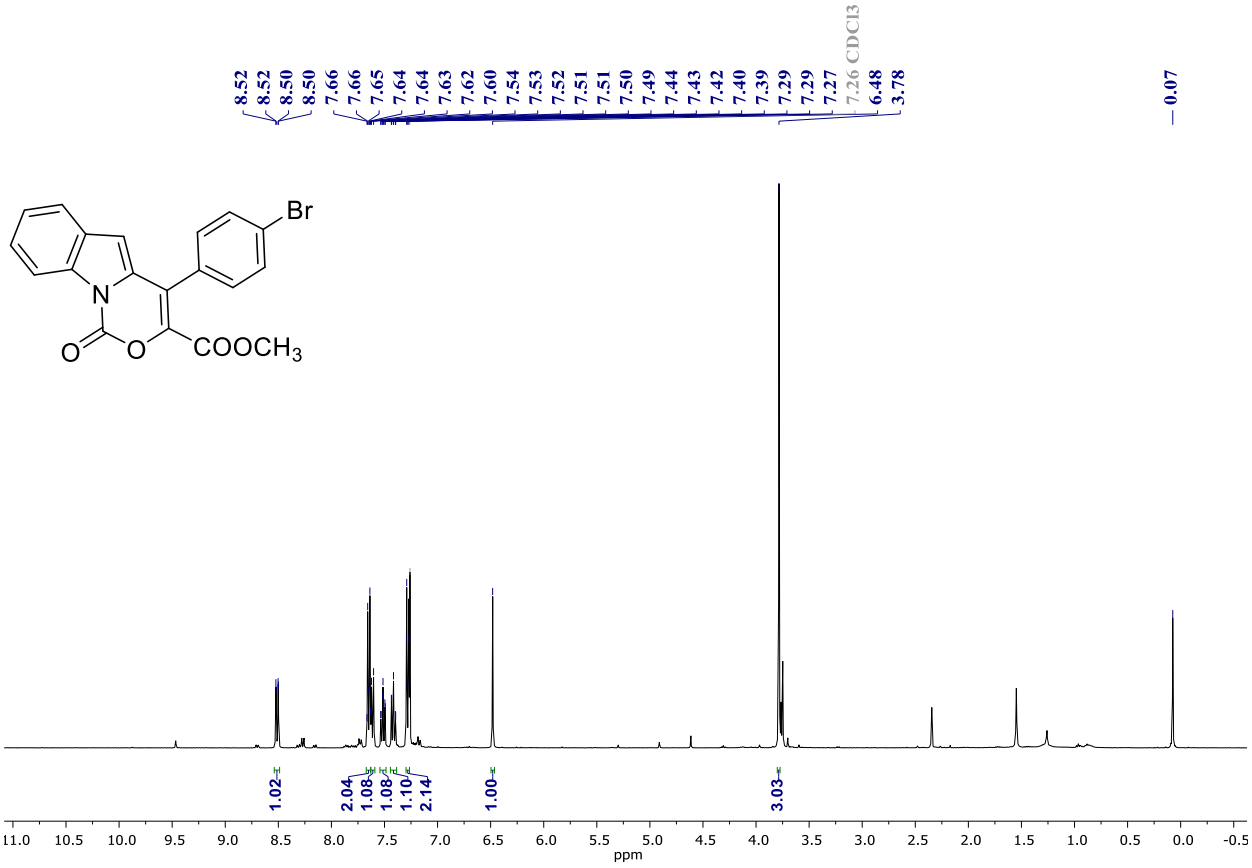
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound **6s**



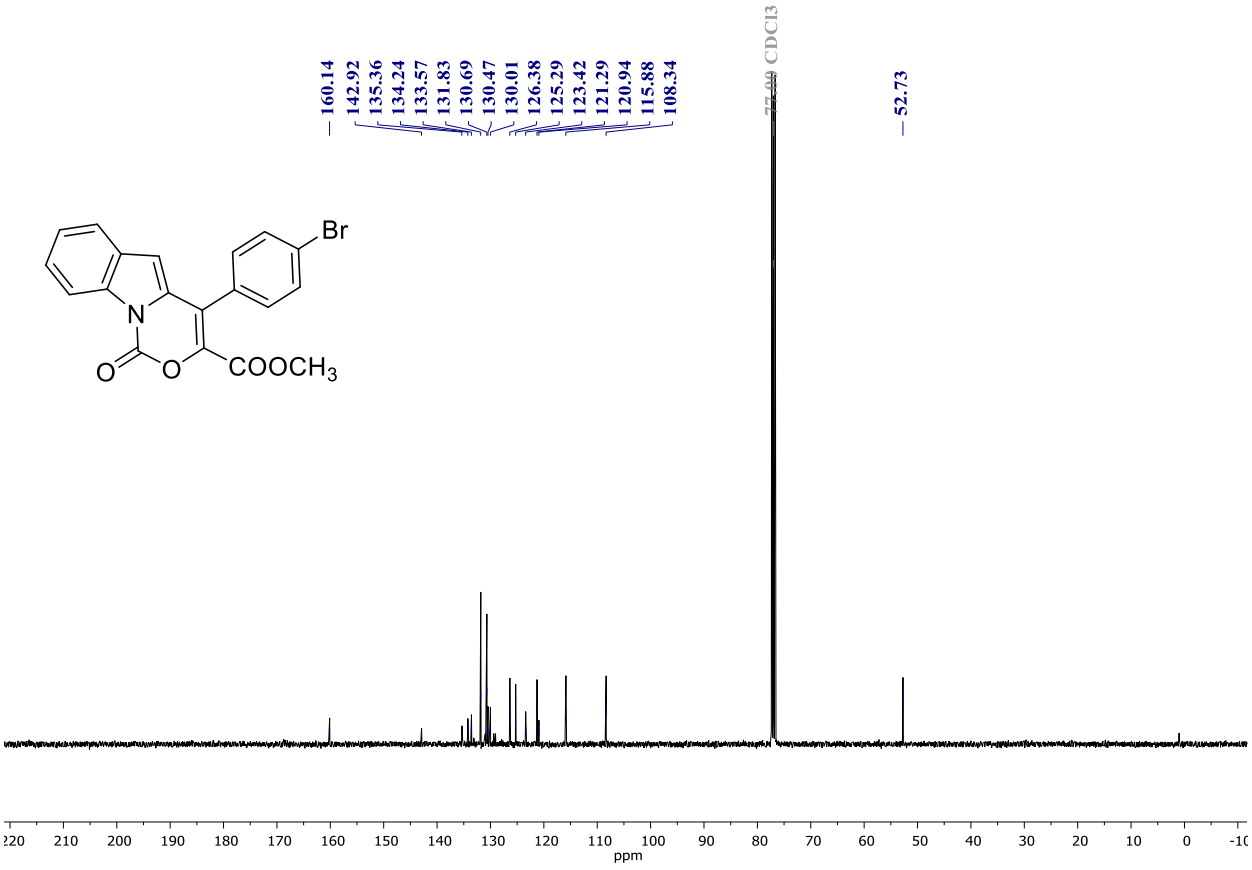
^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) spectrum of compound **6s**



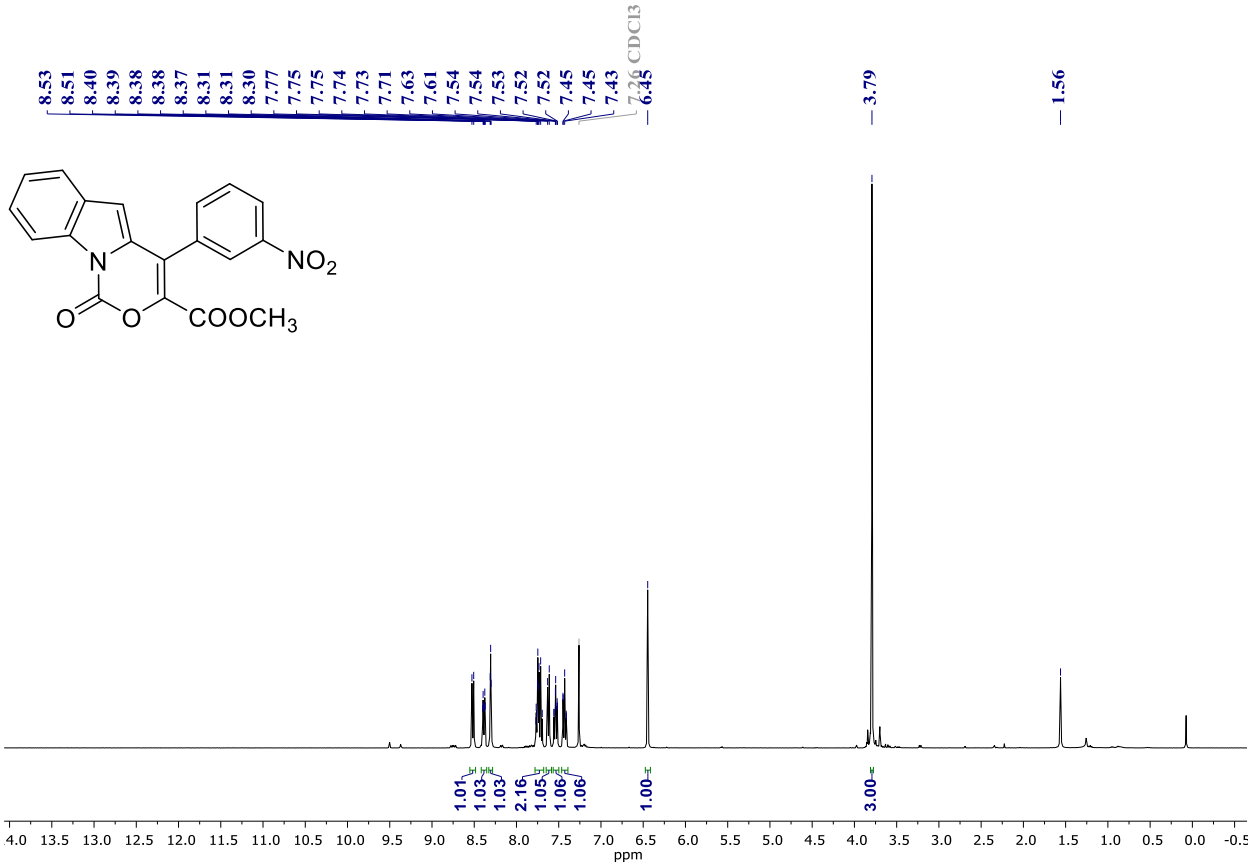
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound **6t**



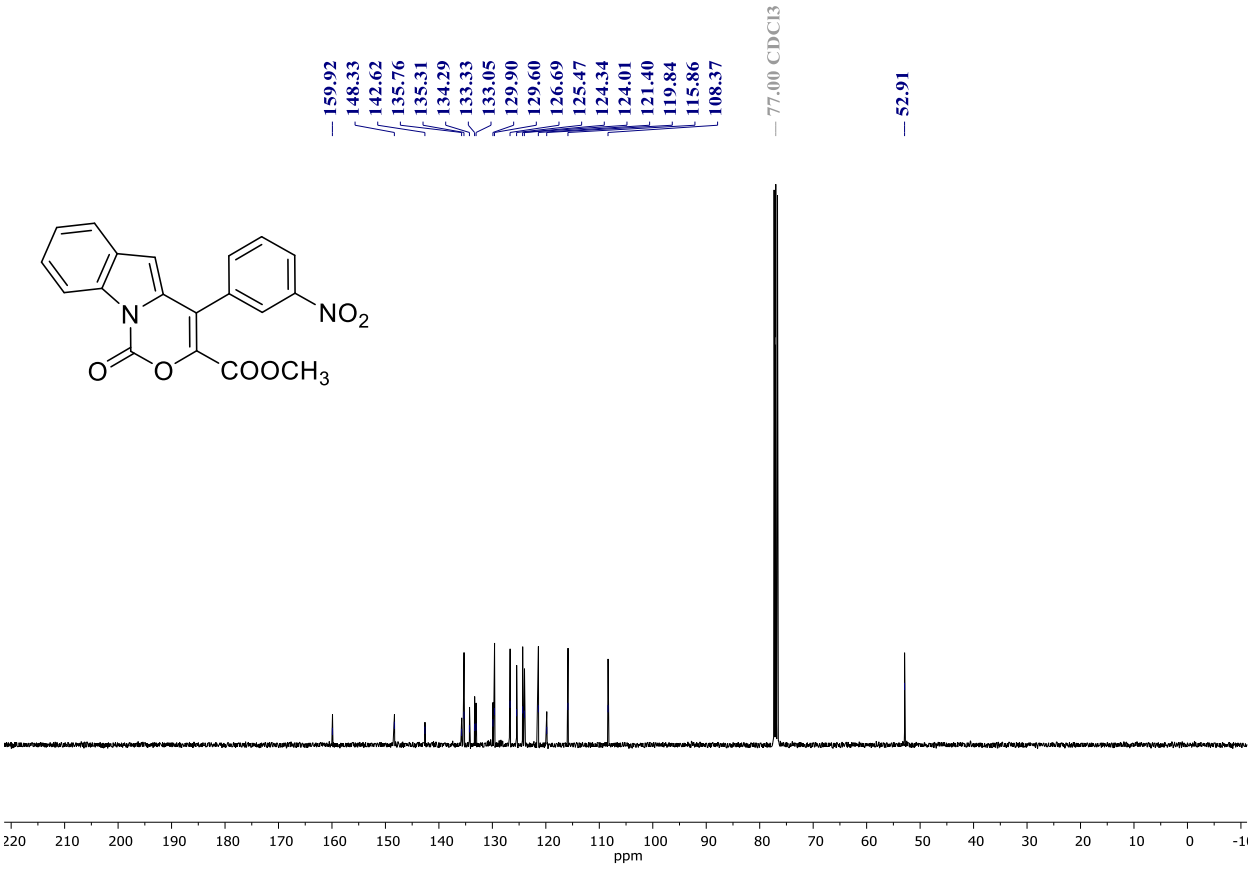
^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) spectrum of compound **6t**



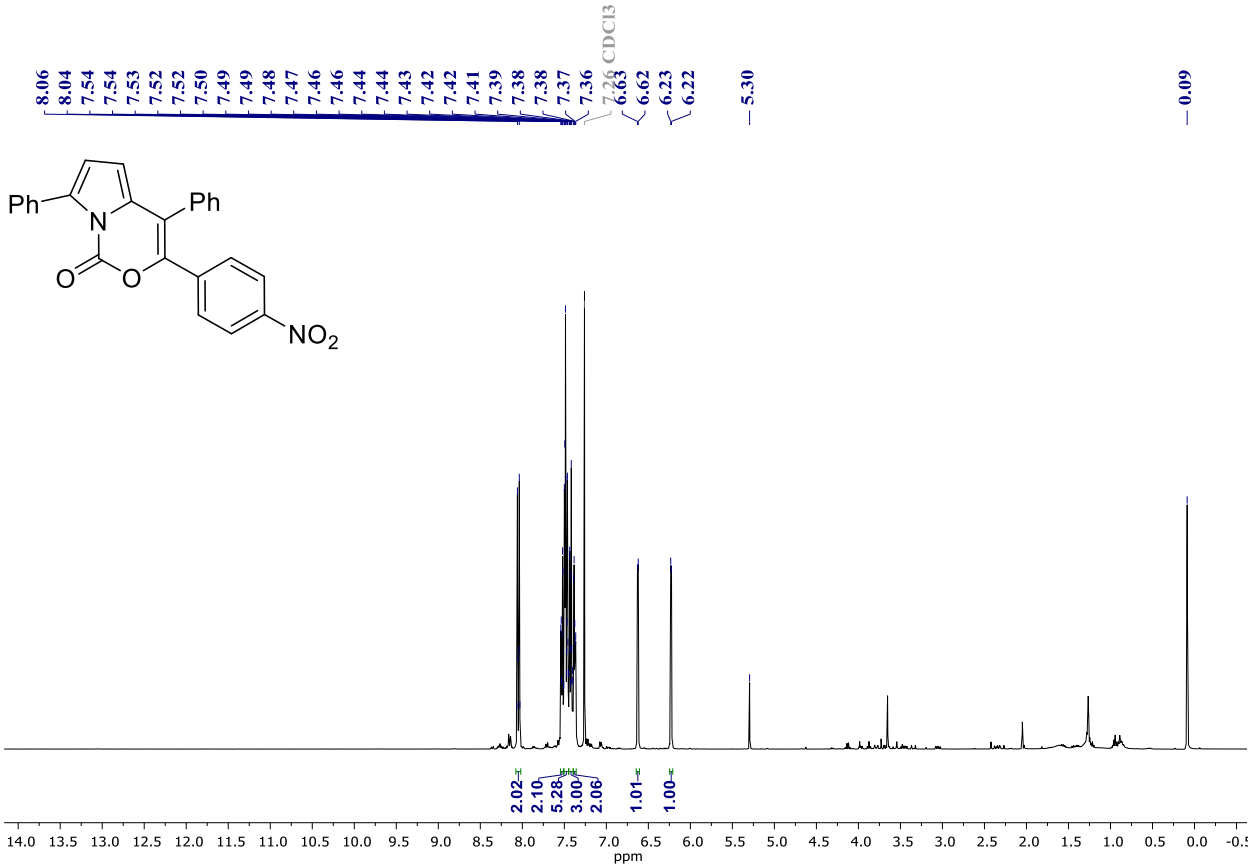
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound **6u**



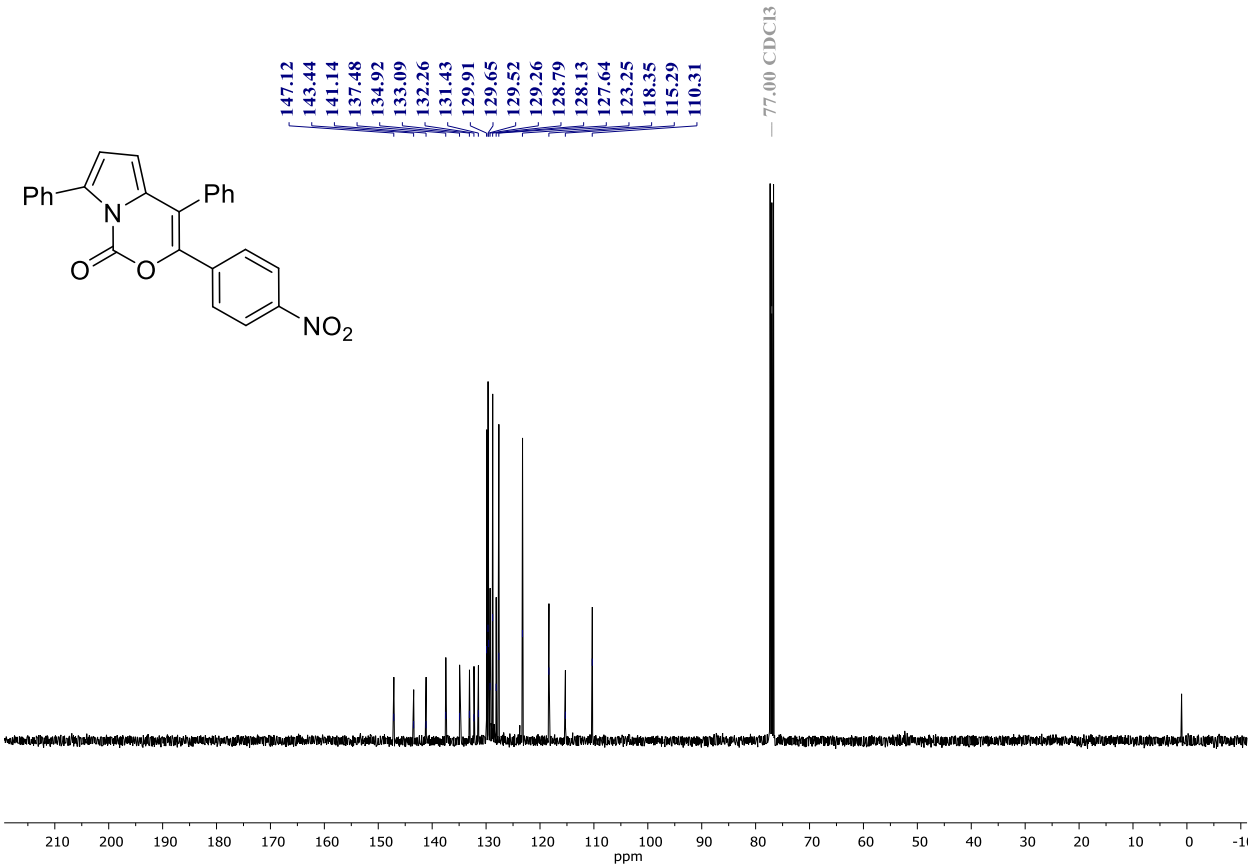
^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) spectrum of compound **6u**



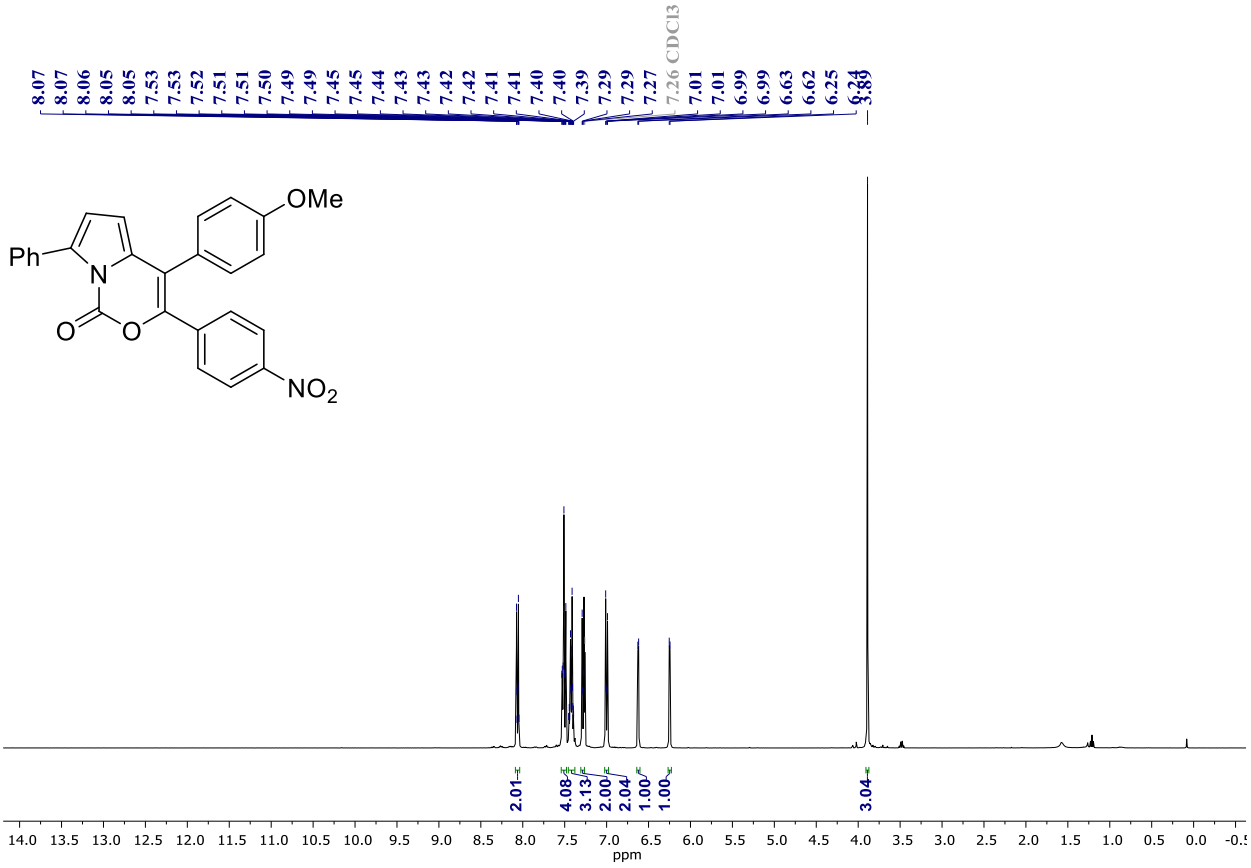
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound **6v**



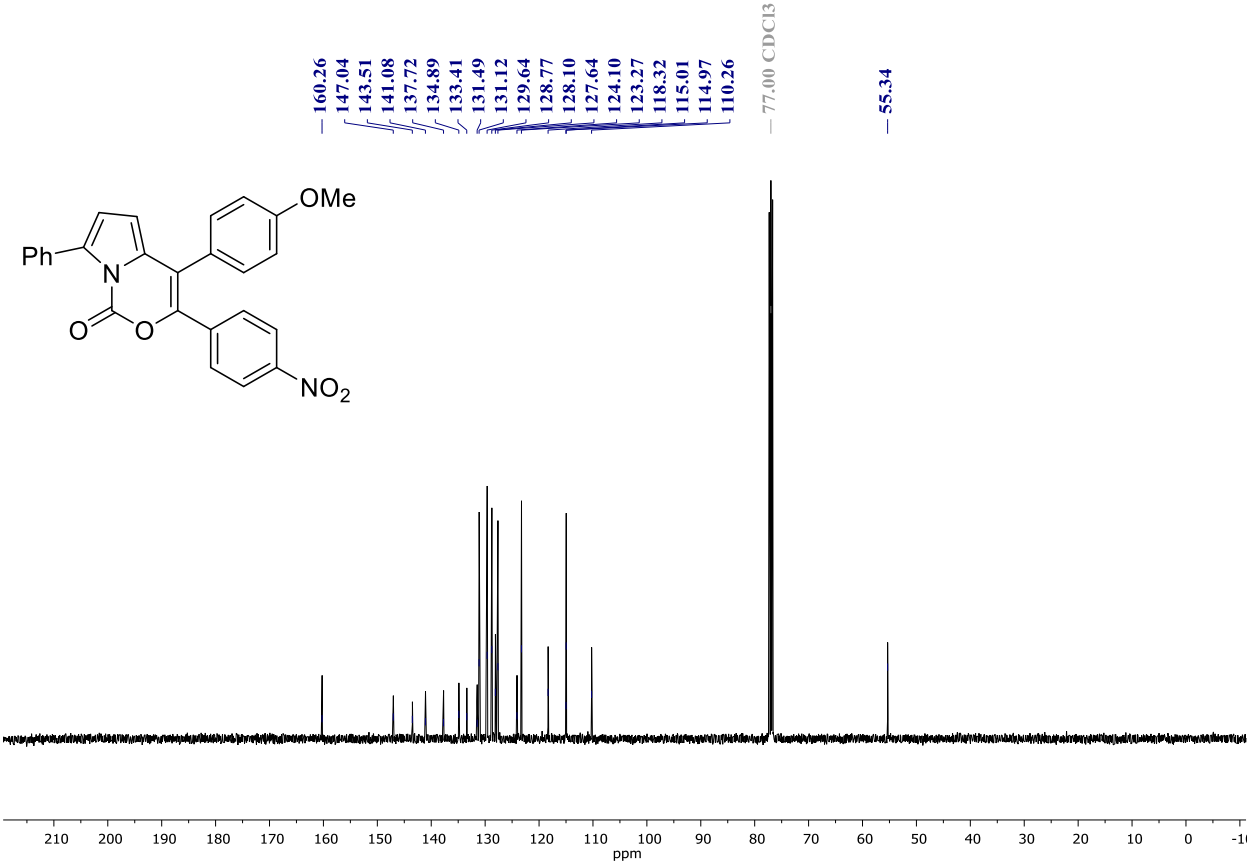
^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) spectrum of compound **6v**



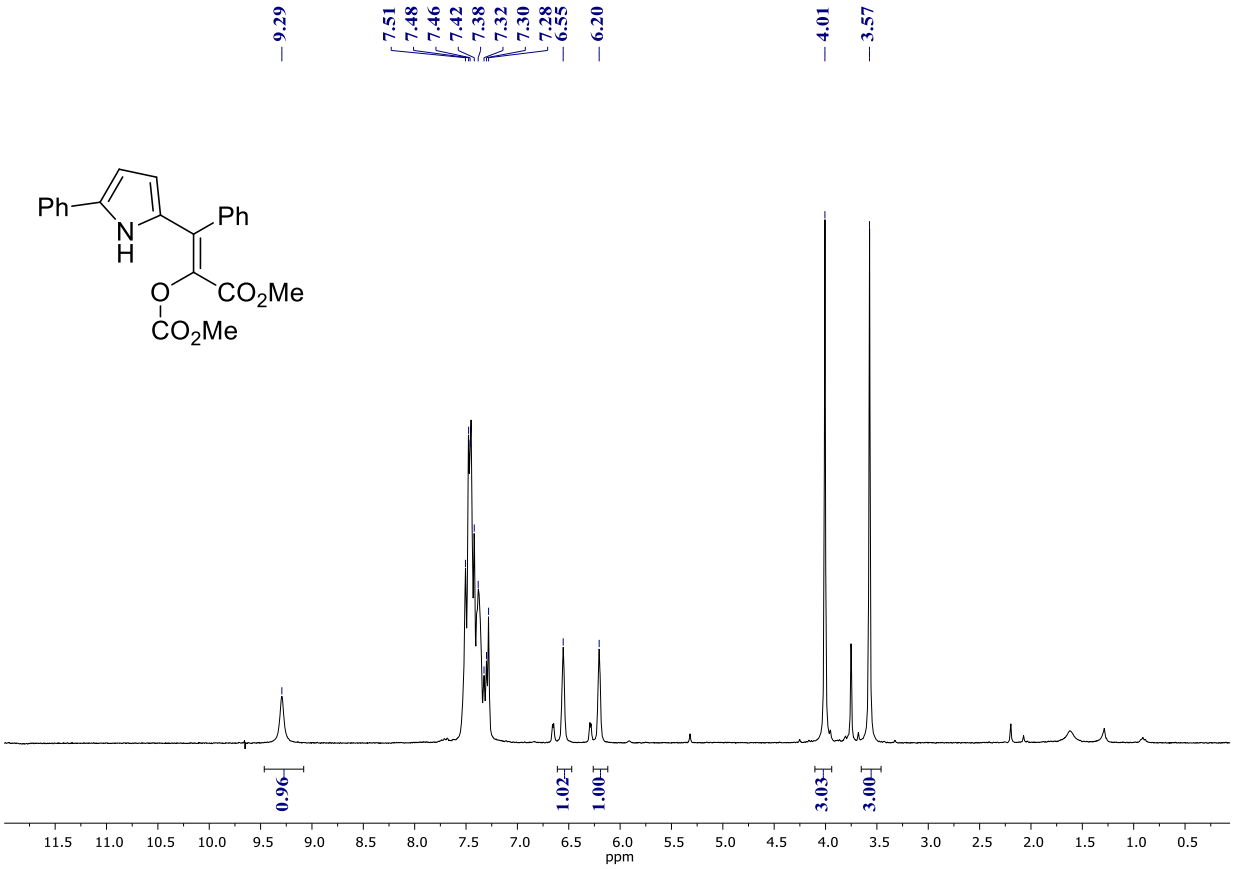
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound **6w**



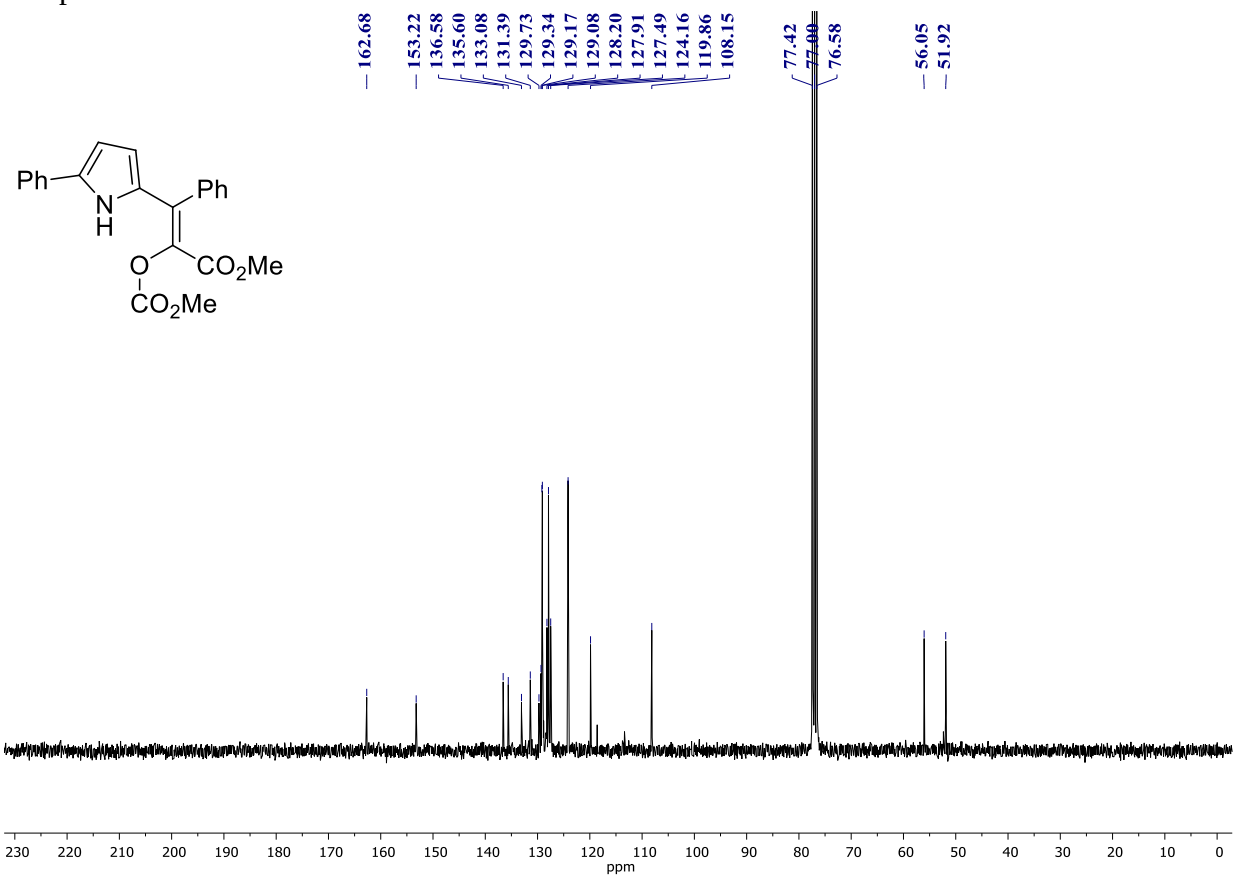
^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) spectrum of compound **6w**



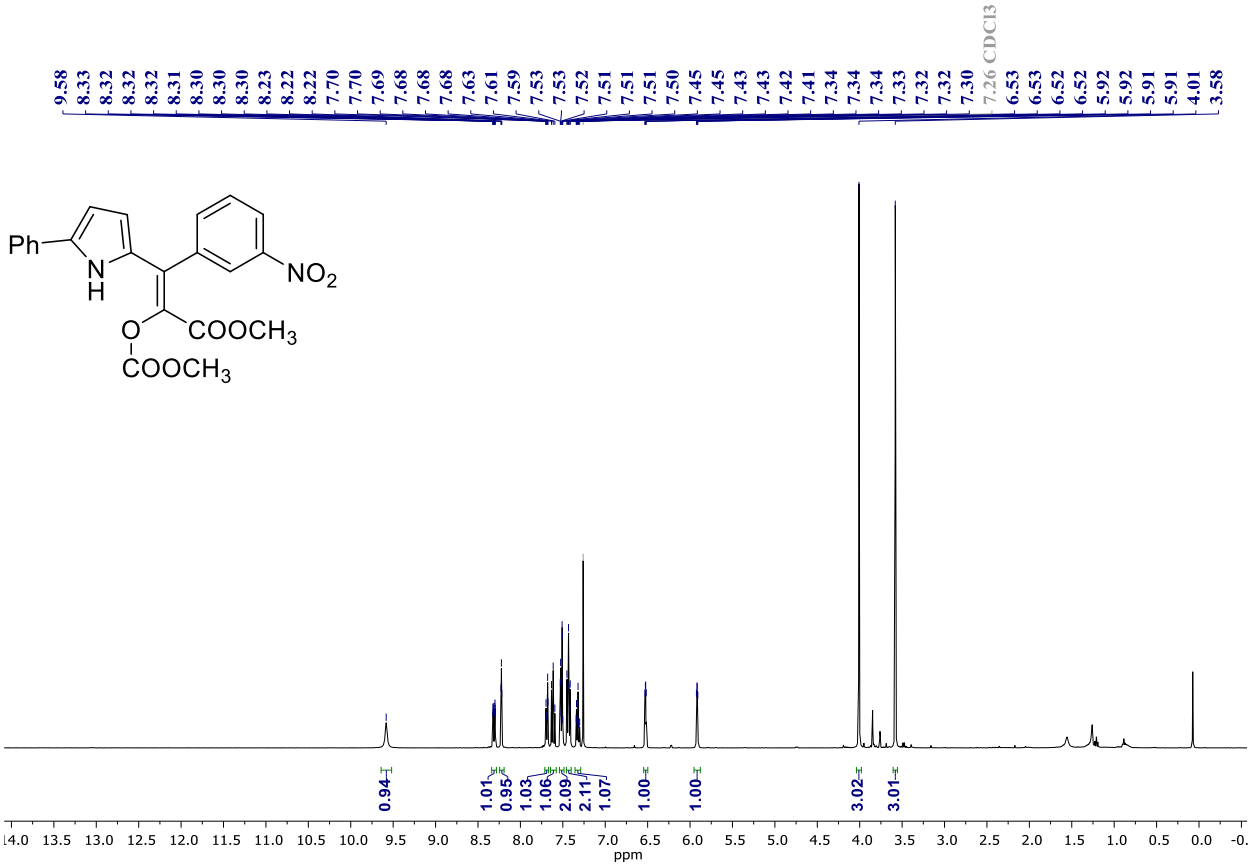
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound **7a** with 20% impurity of compound **6a**



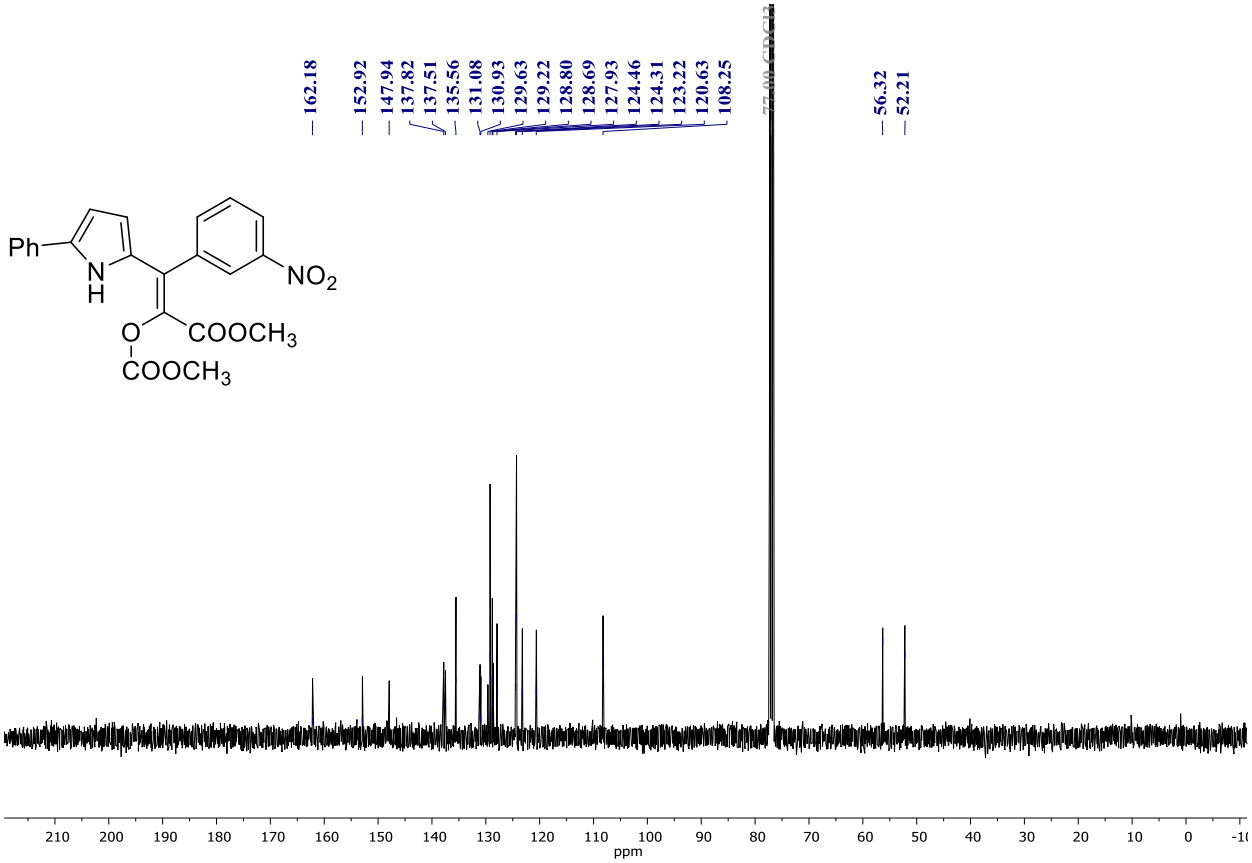
^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) spectrum of compound **7a** with 20% impurity of compound **6a**



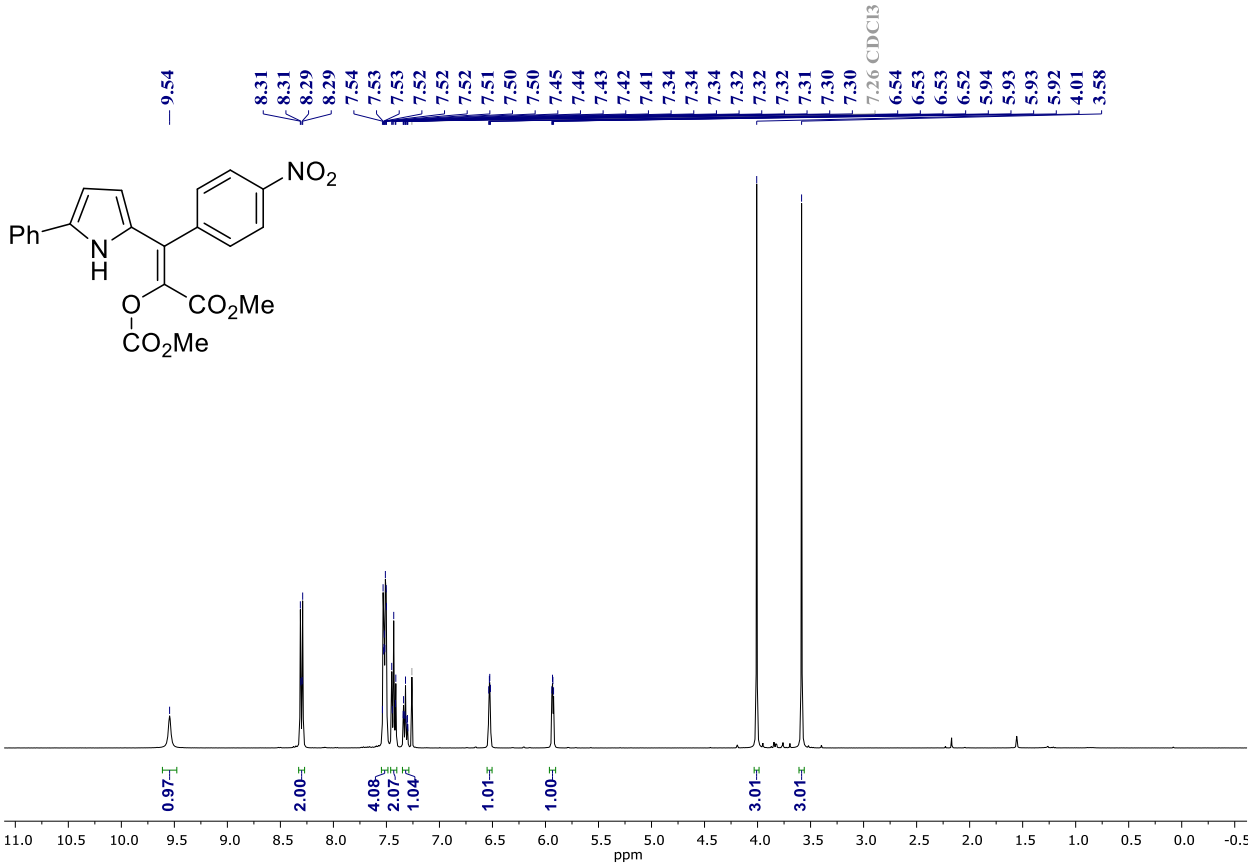
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound **7k**



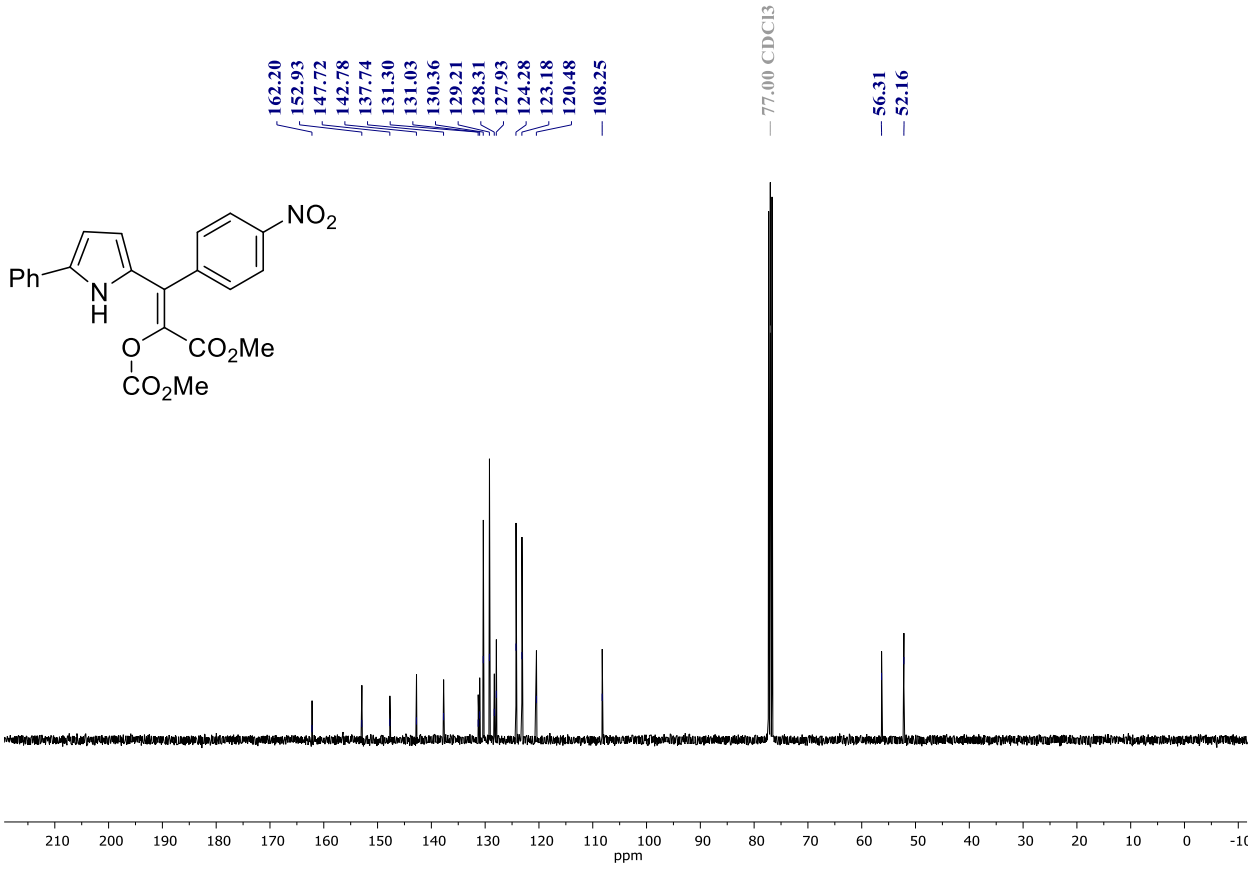
^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) spectrum of compound **7k**



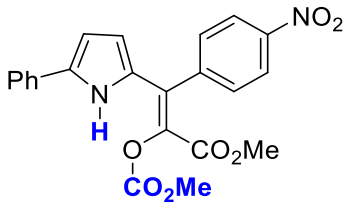
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound **7l**

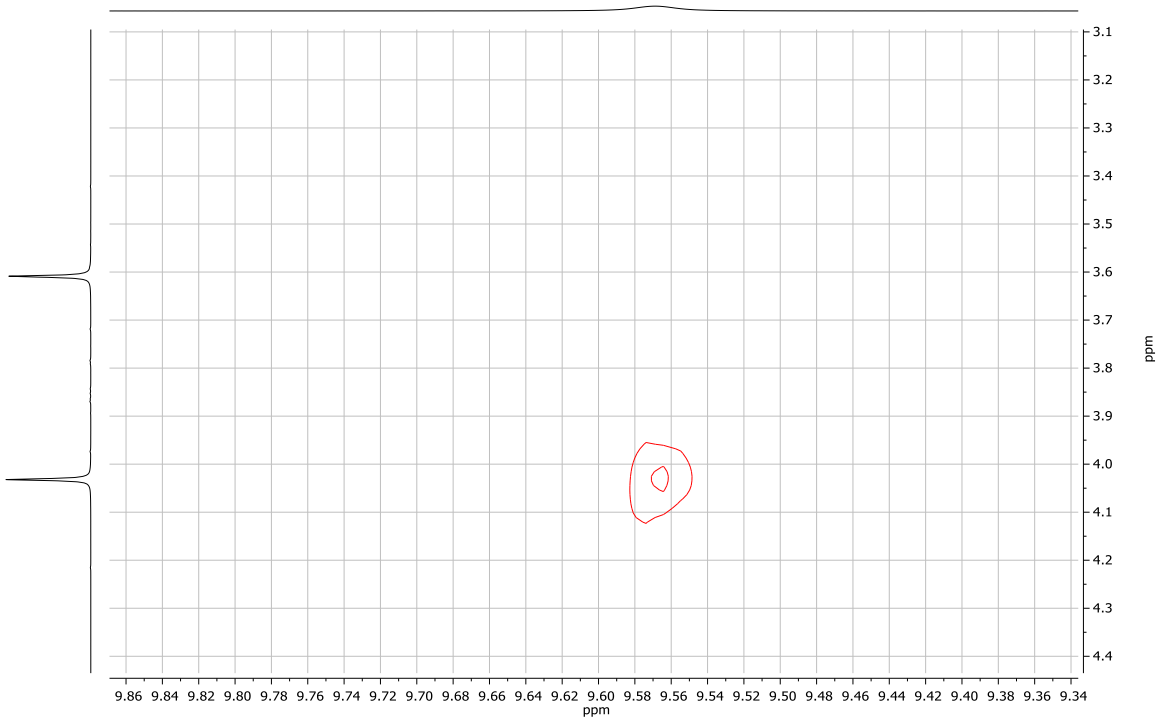


^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) spectrum of compound **7l**

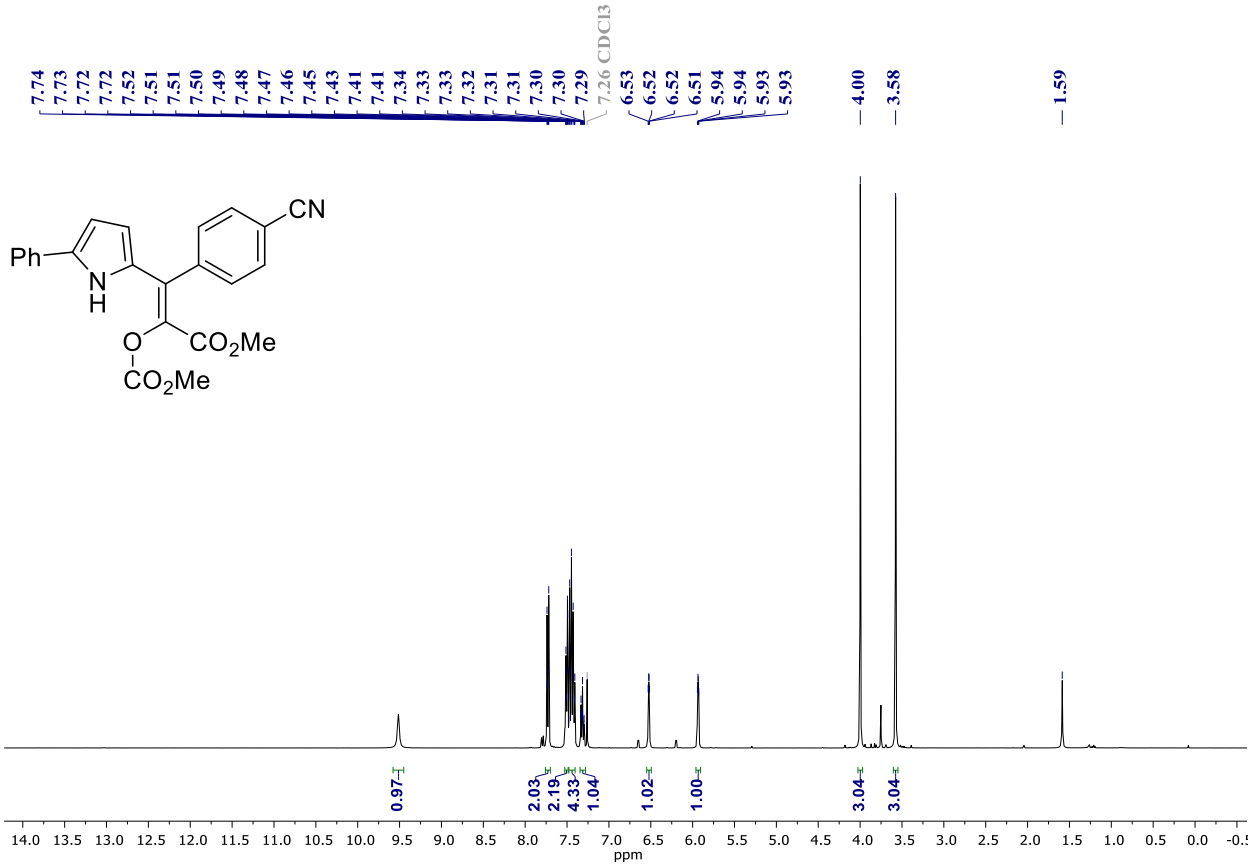


^{1}H-^{1}H NOESY (400 MHz, $CDCl_3$) spectrum of compound **7l** with correlation of highlighted atoms

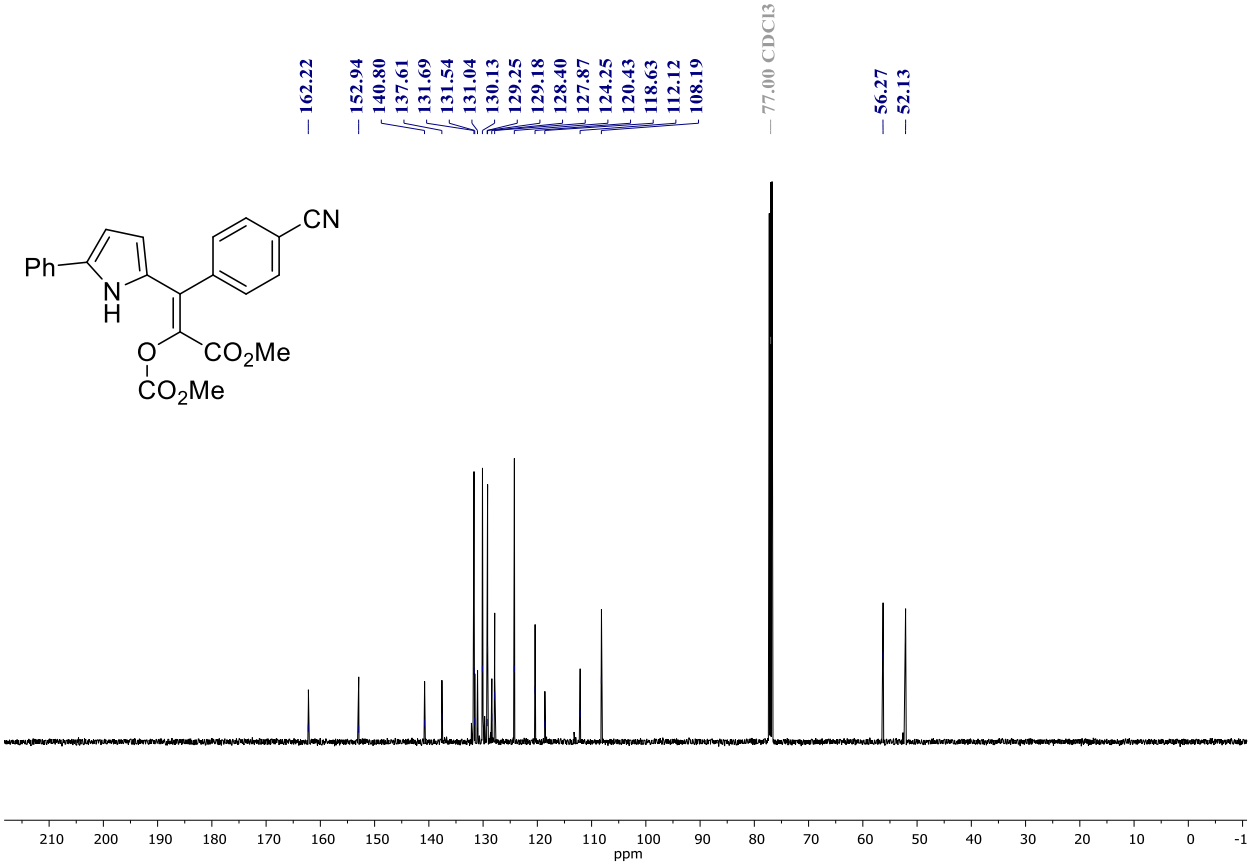




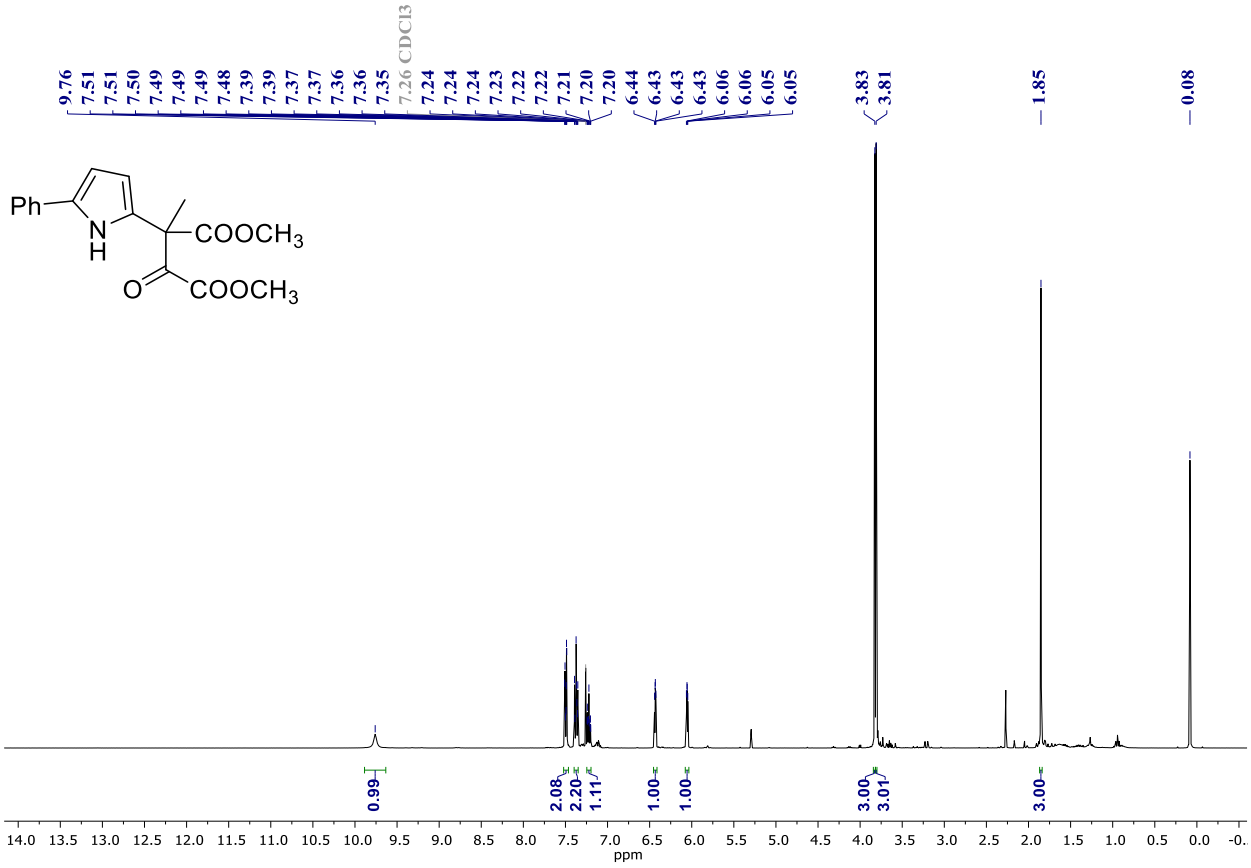
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound **7m**



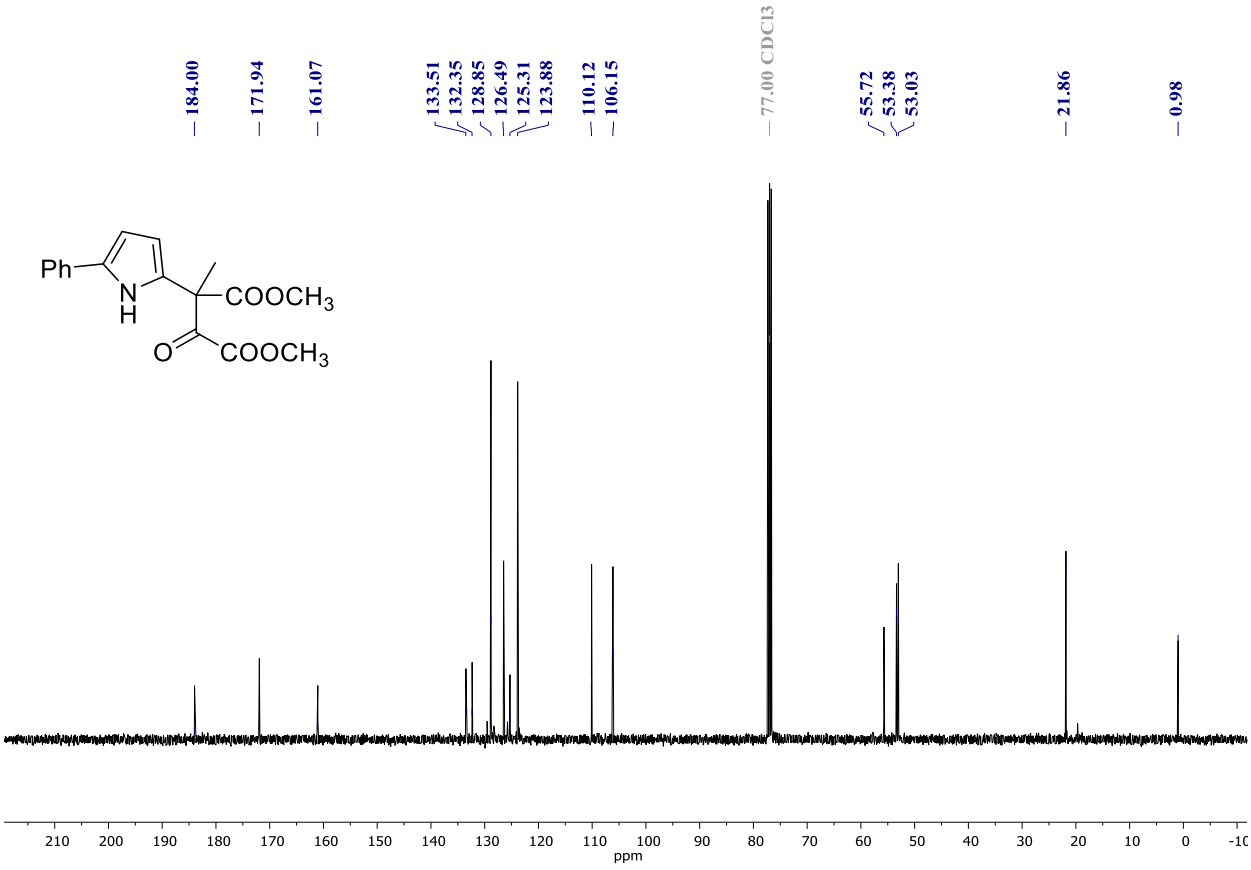
^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) spectrum of compound **7m**



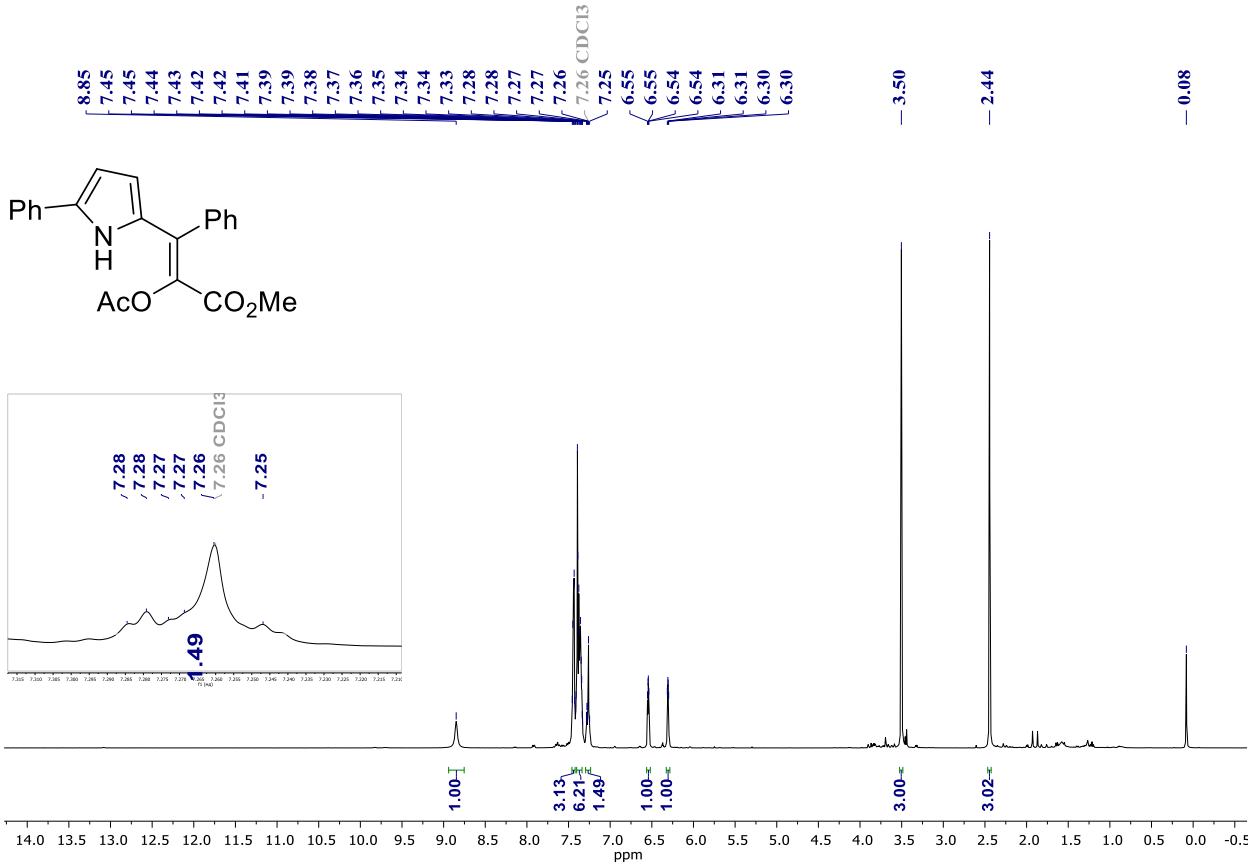
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound **8**



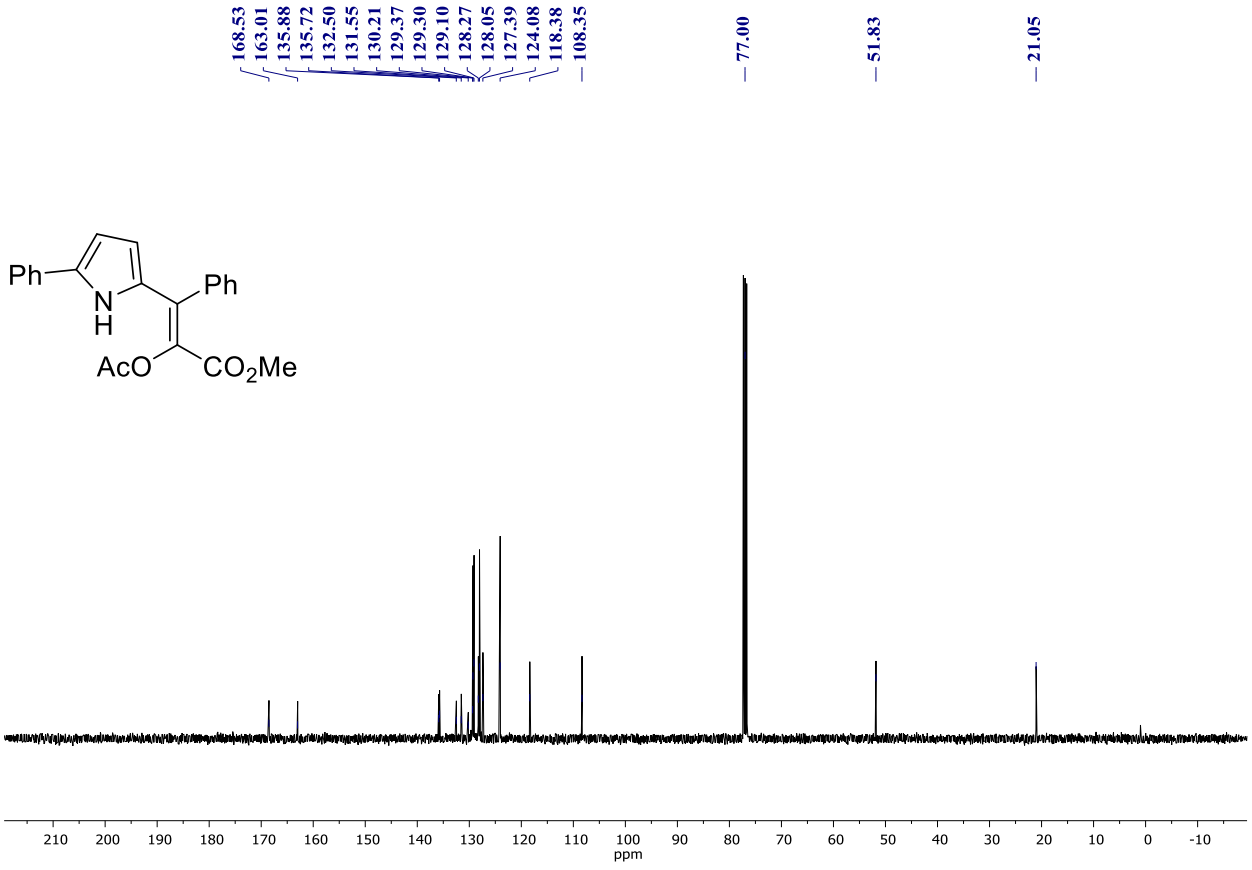
^{13}C{^{1}H} NMR (100MHz, $CDCl_3$) spectrum of compound **8**



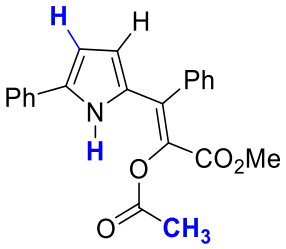
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound **9a**

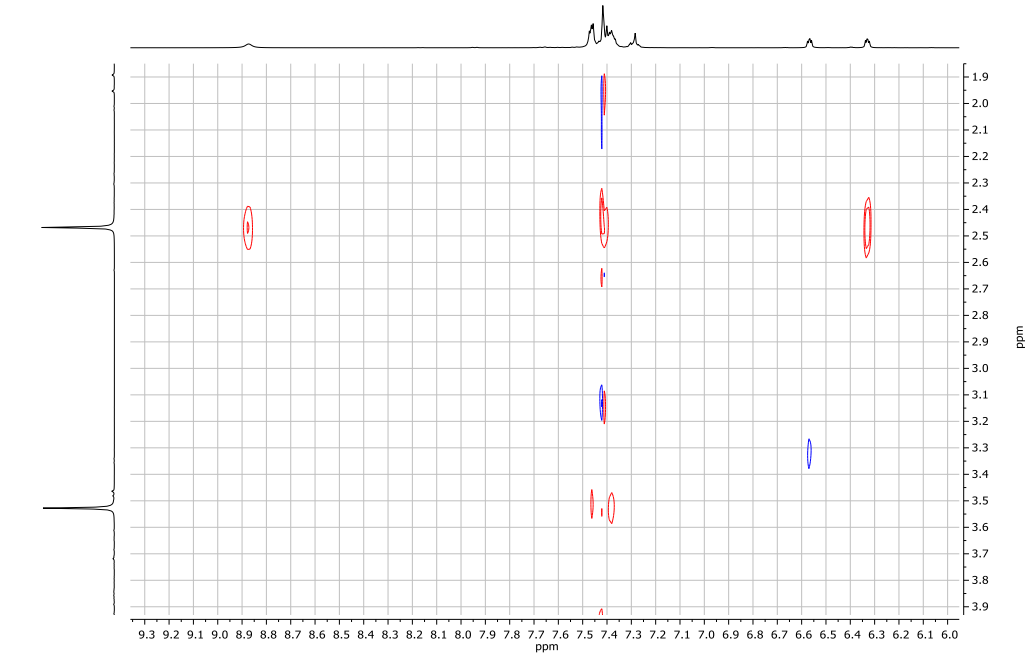


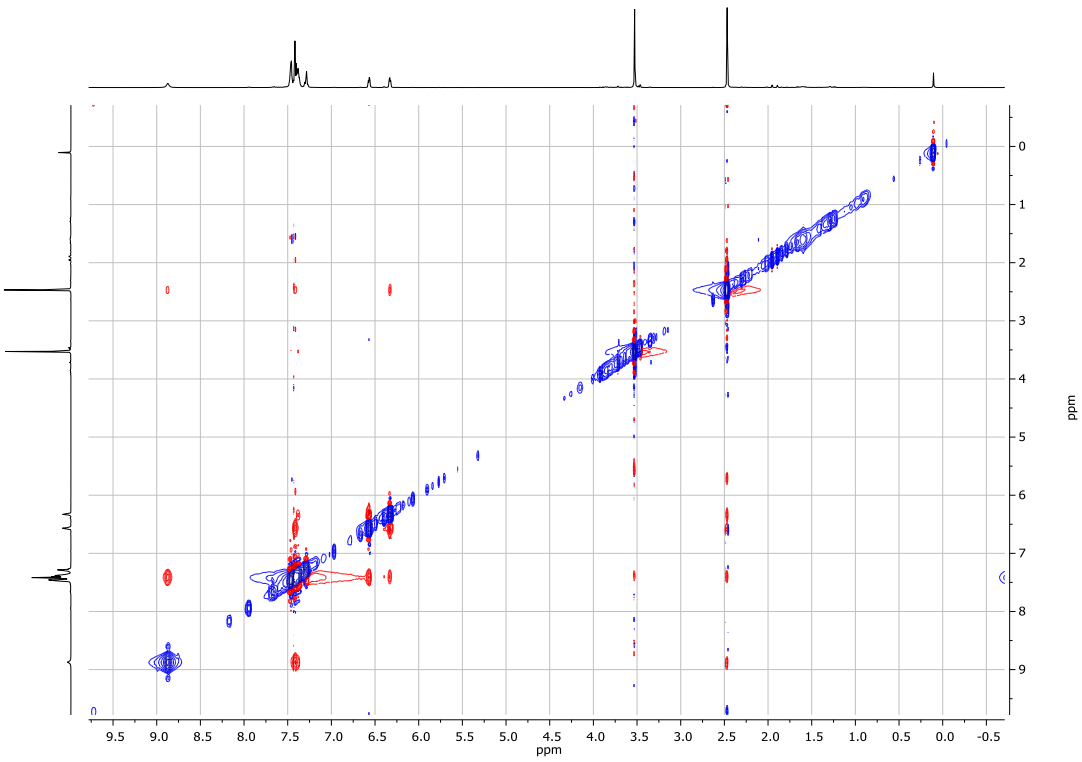
^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) spectrum of compound **9a**



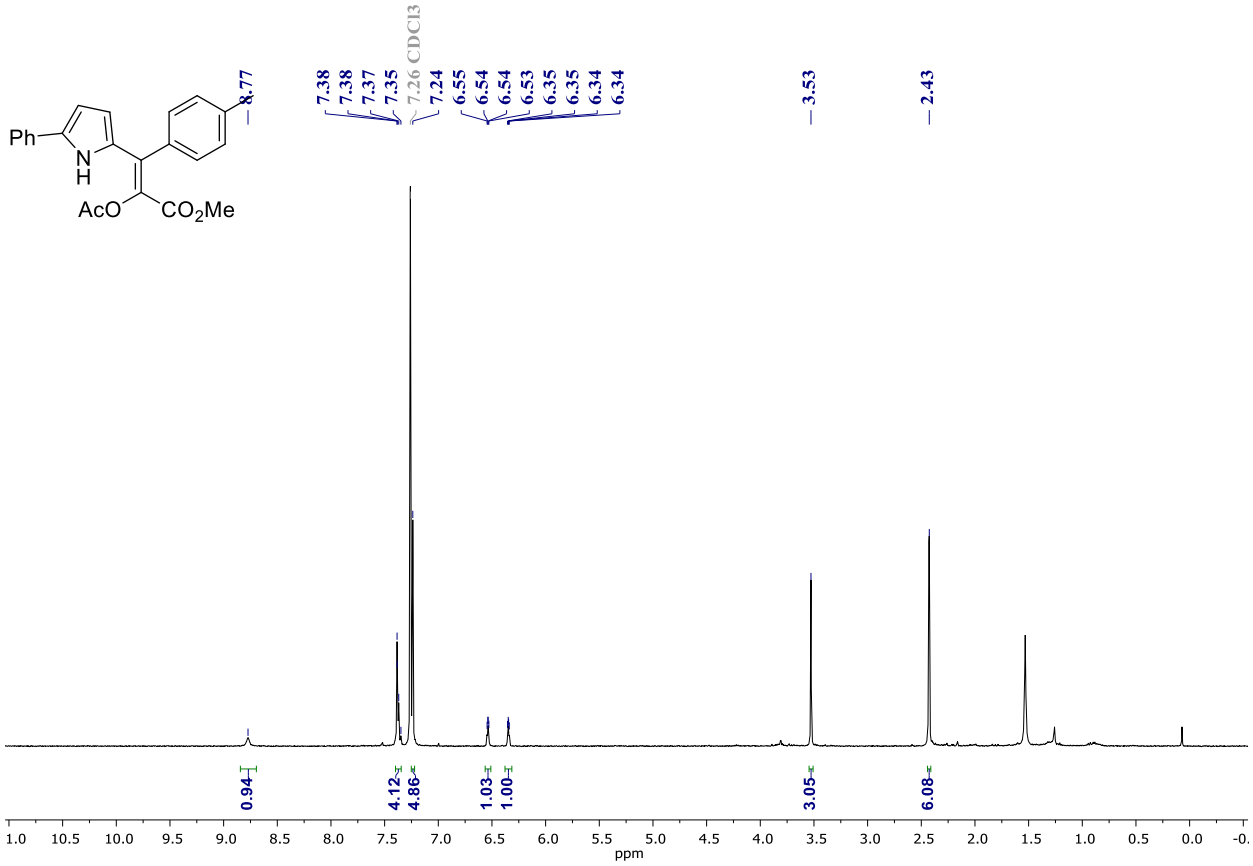
^{1}H-^{1}H NOESY (400 MHz, $CDCl_3$) spectrum of compound **9a** with correlation of highlighted atoms



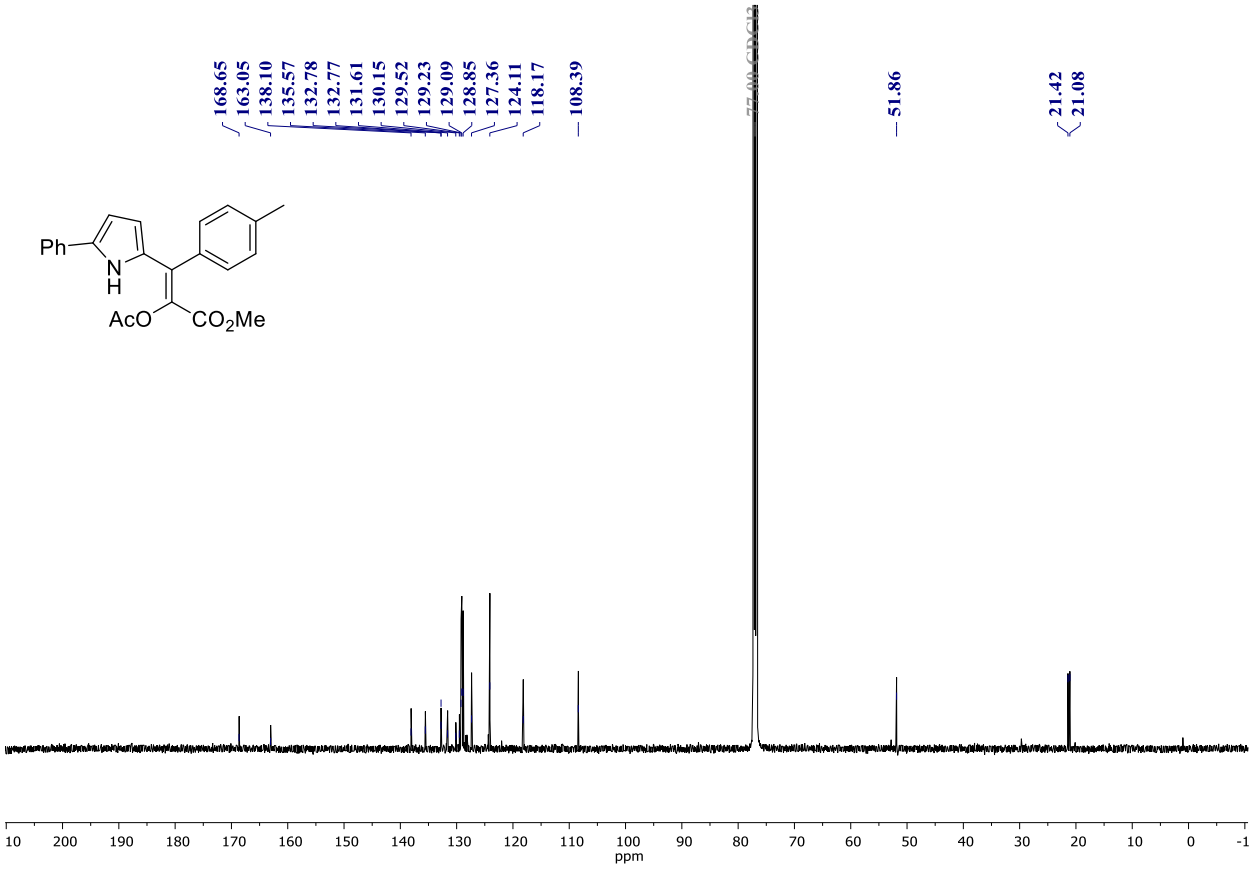




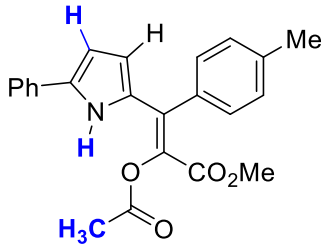
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound **9b**

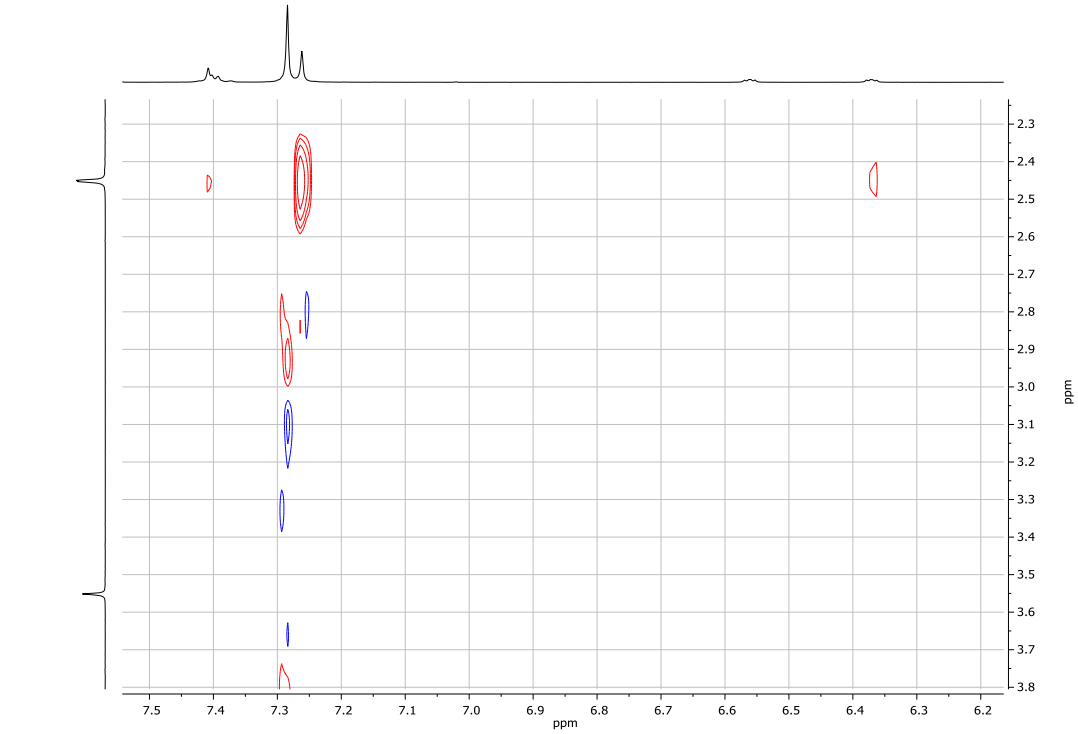


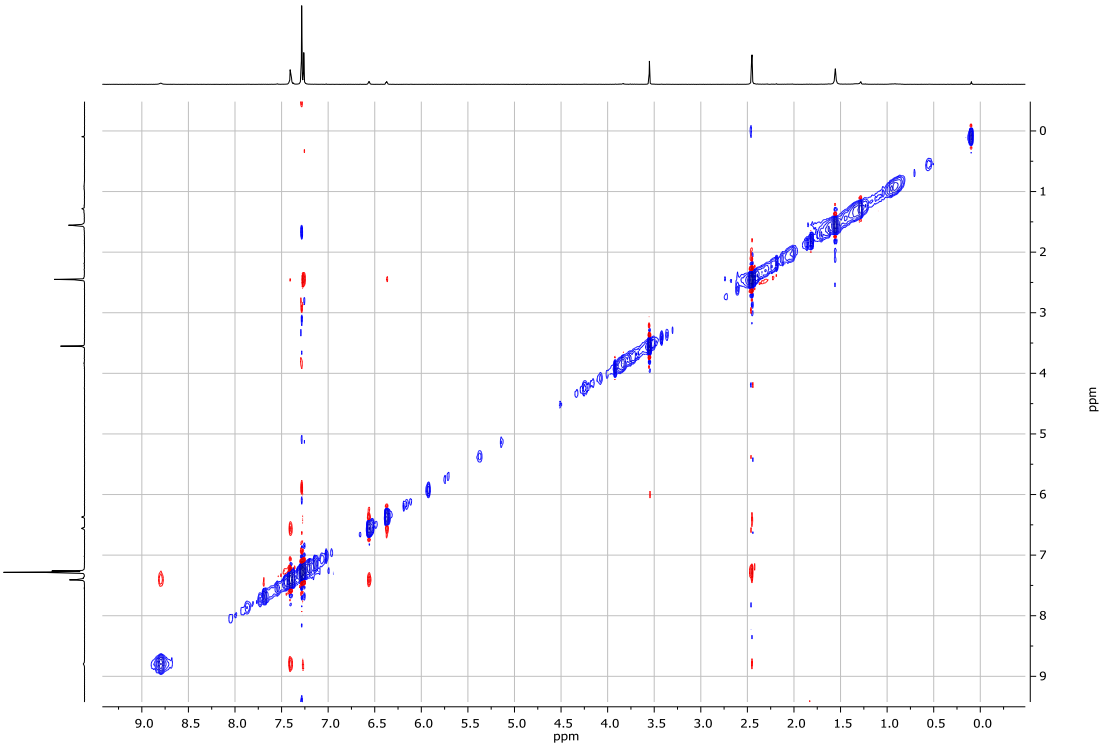
^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) spectrum of compound **9b**



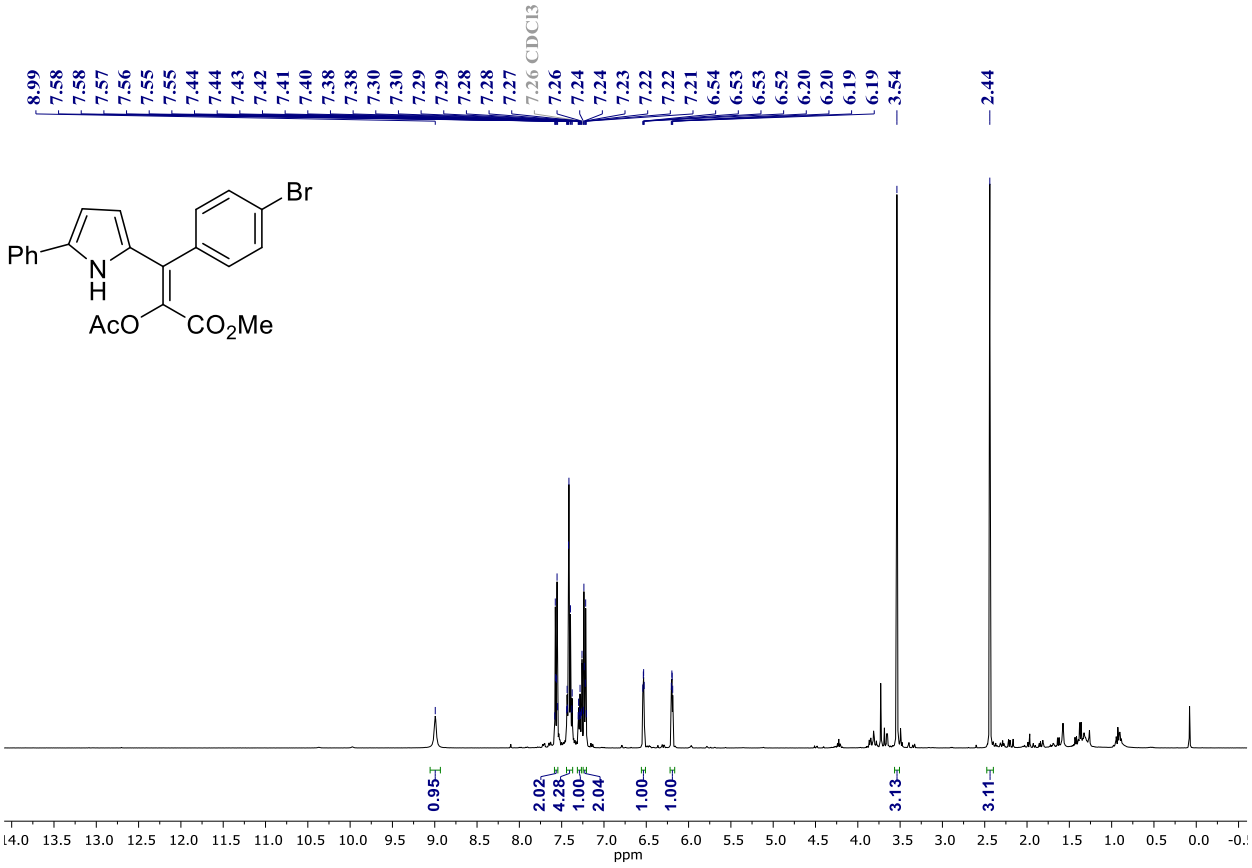
^{1}H-^{1}H NOESY (400 MHz, $CDCl_3$) spectrum of compound **9b** with correlation of highlighted atoms



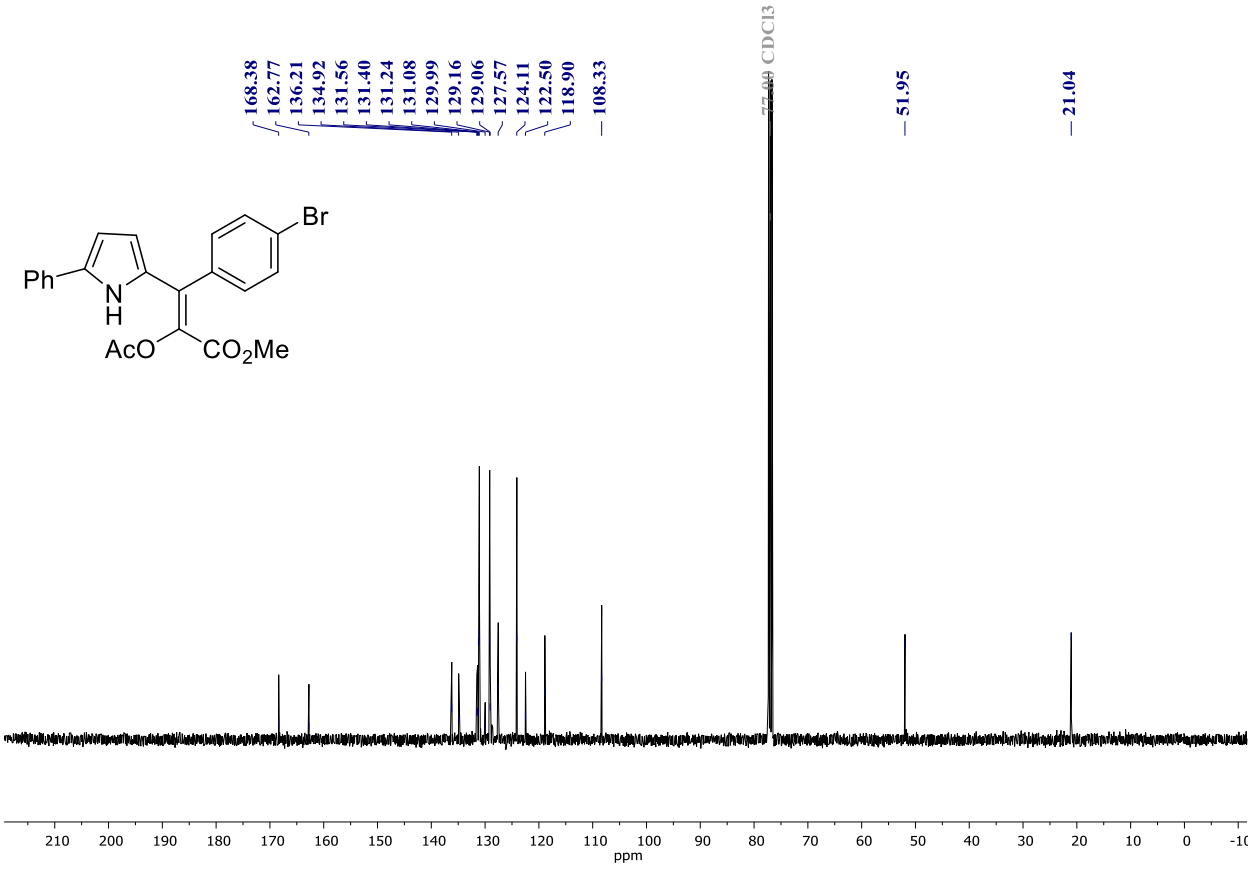




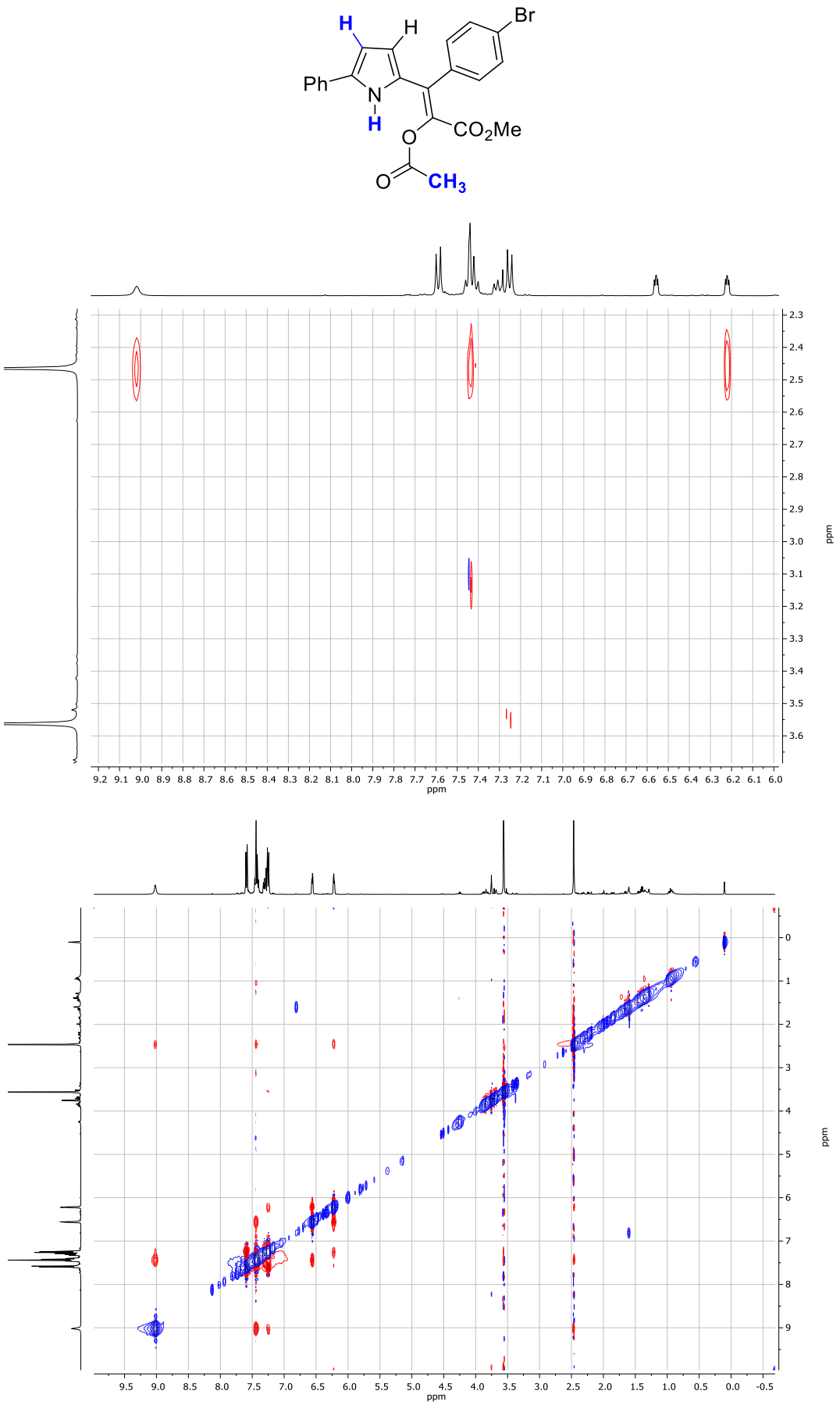
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound **9c**



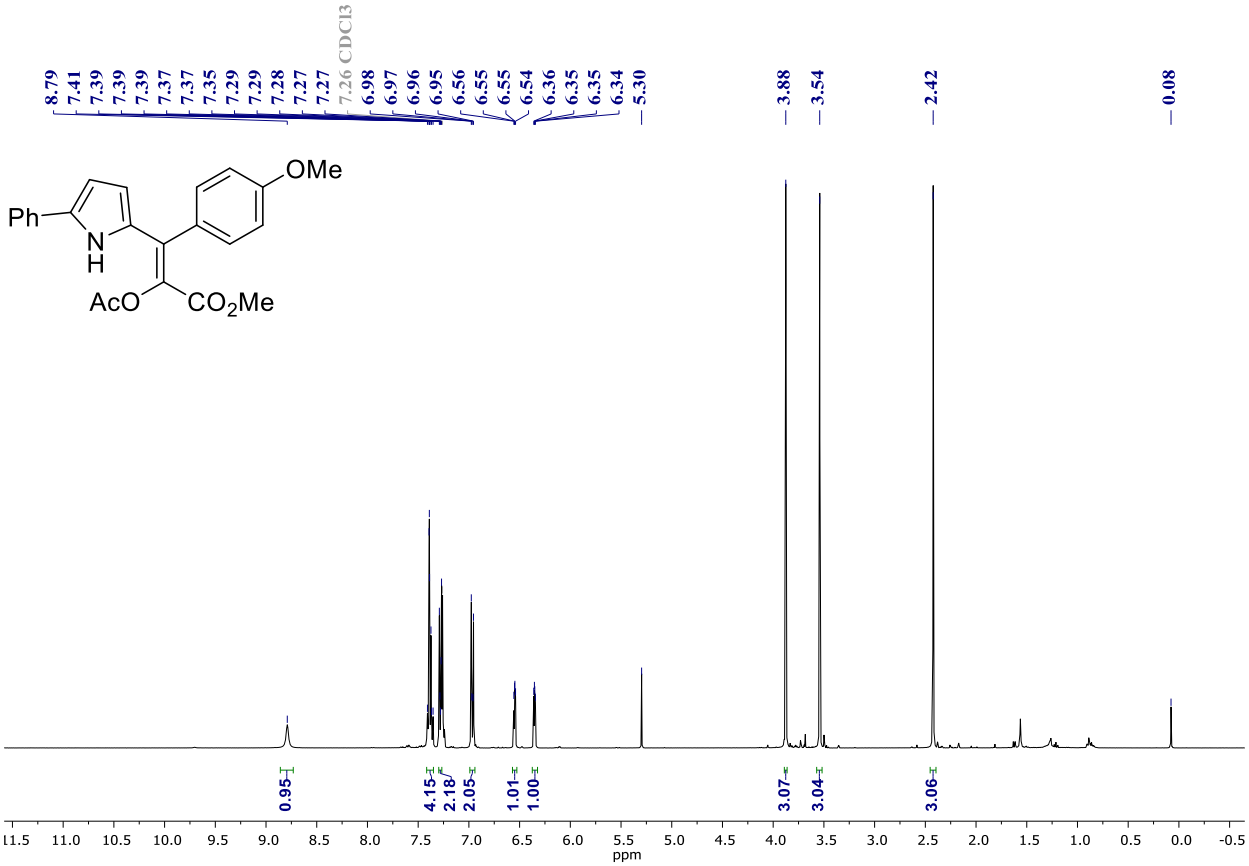
^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) spectrum of compound **9c**



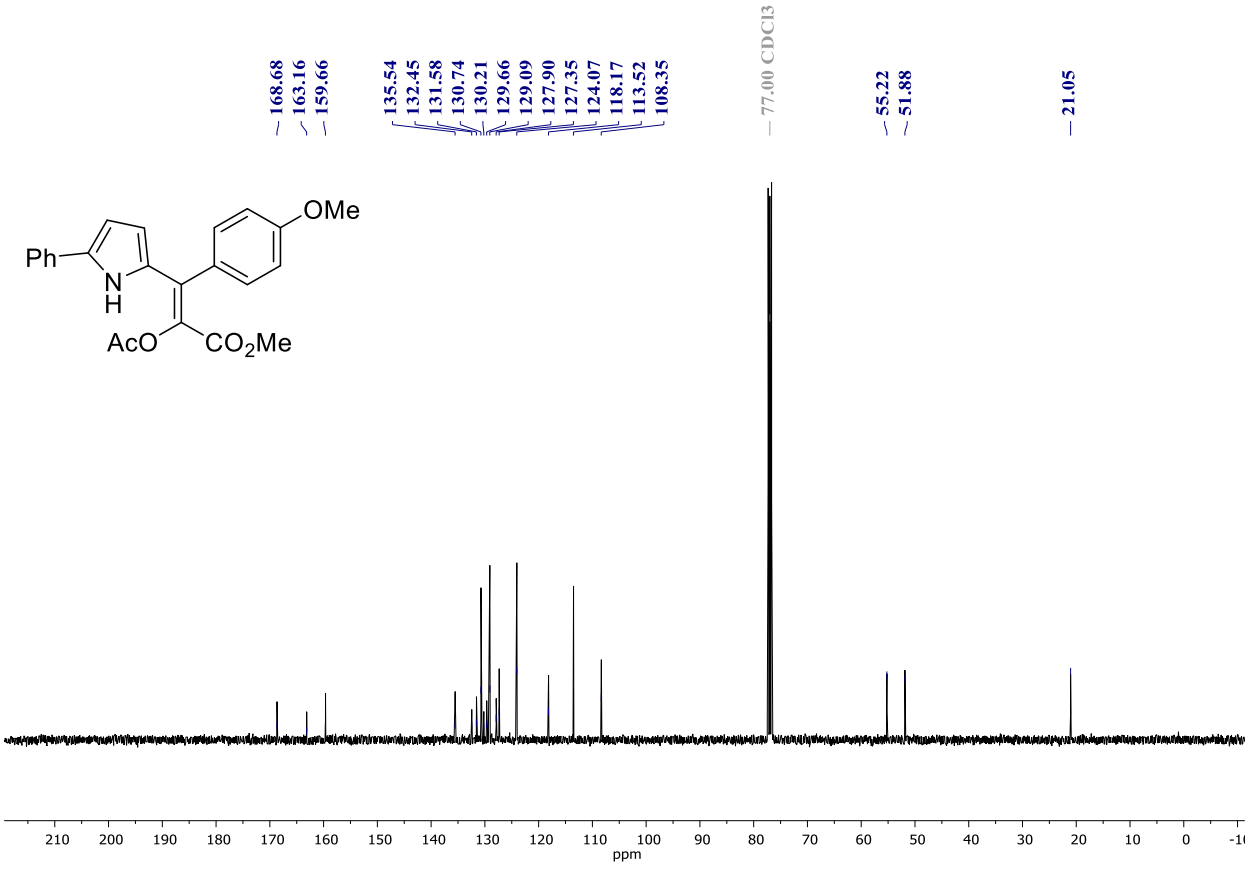
^{1}H-^{1}H NOESY (400 MHz, $CDCl_3$) spectrum of compound **9c** with correlation of highlighted atoms



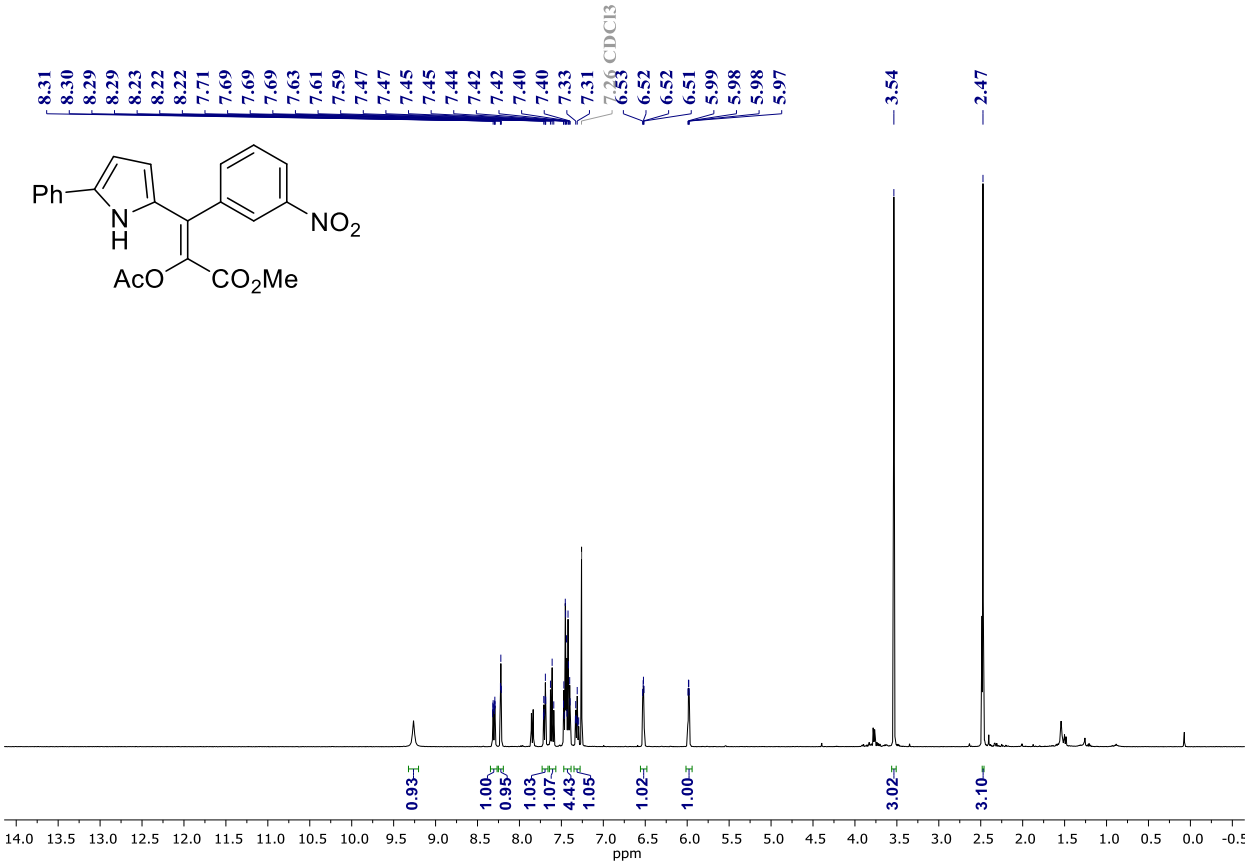
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound **9d**



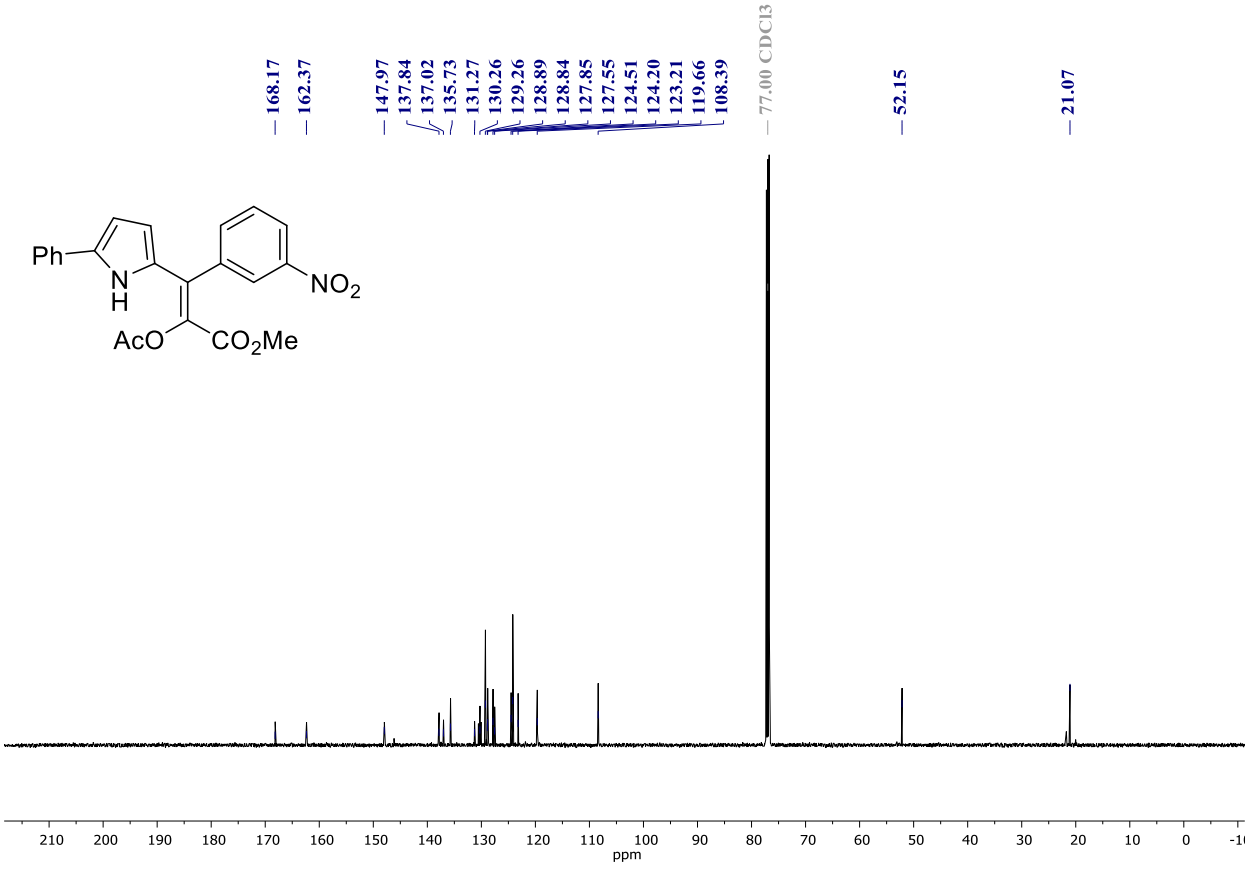
^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) spectrum of compound **9d**



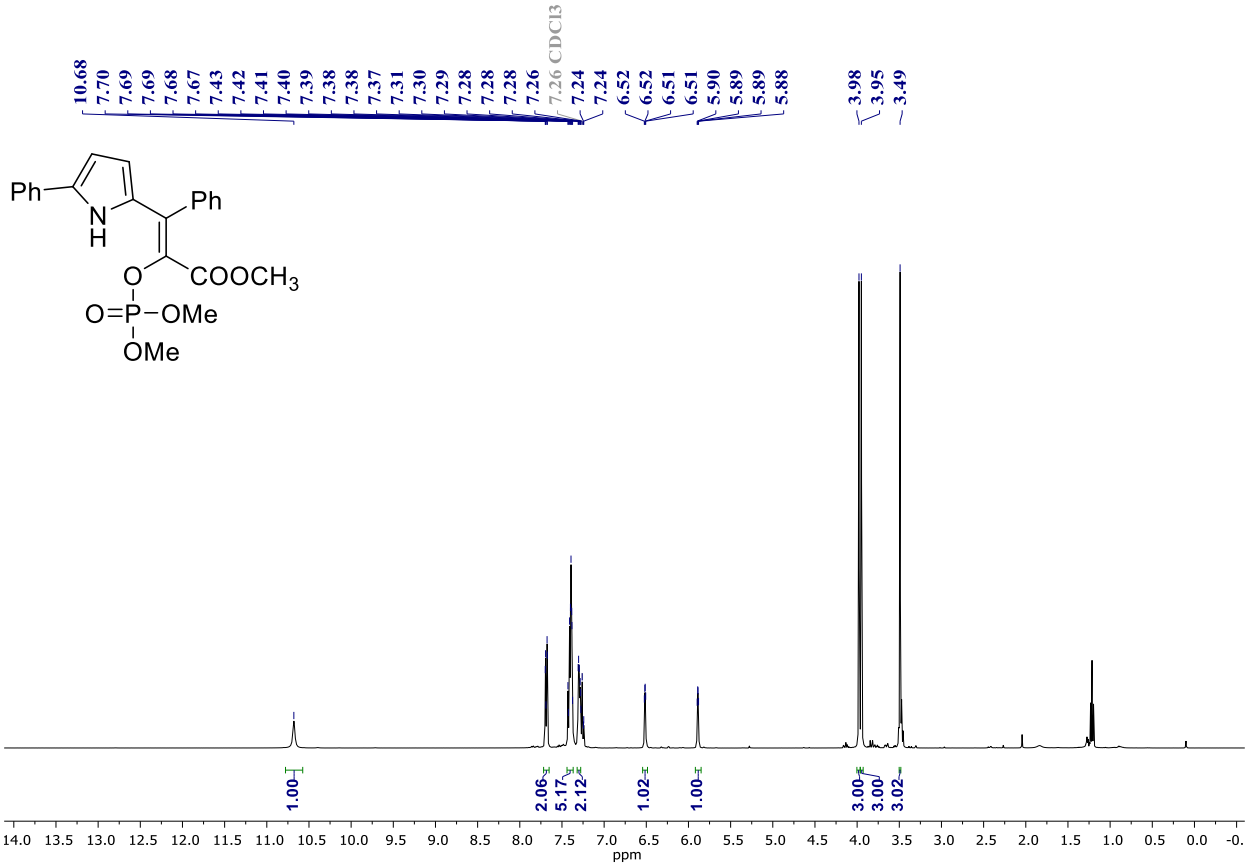
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound **9e**



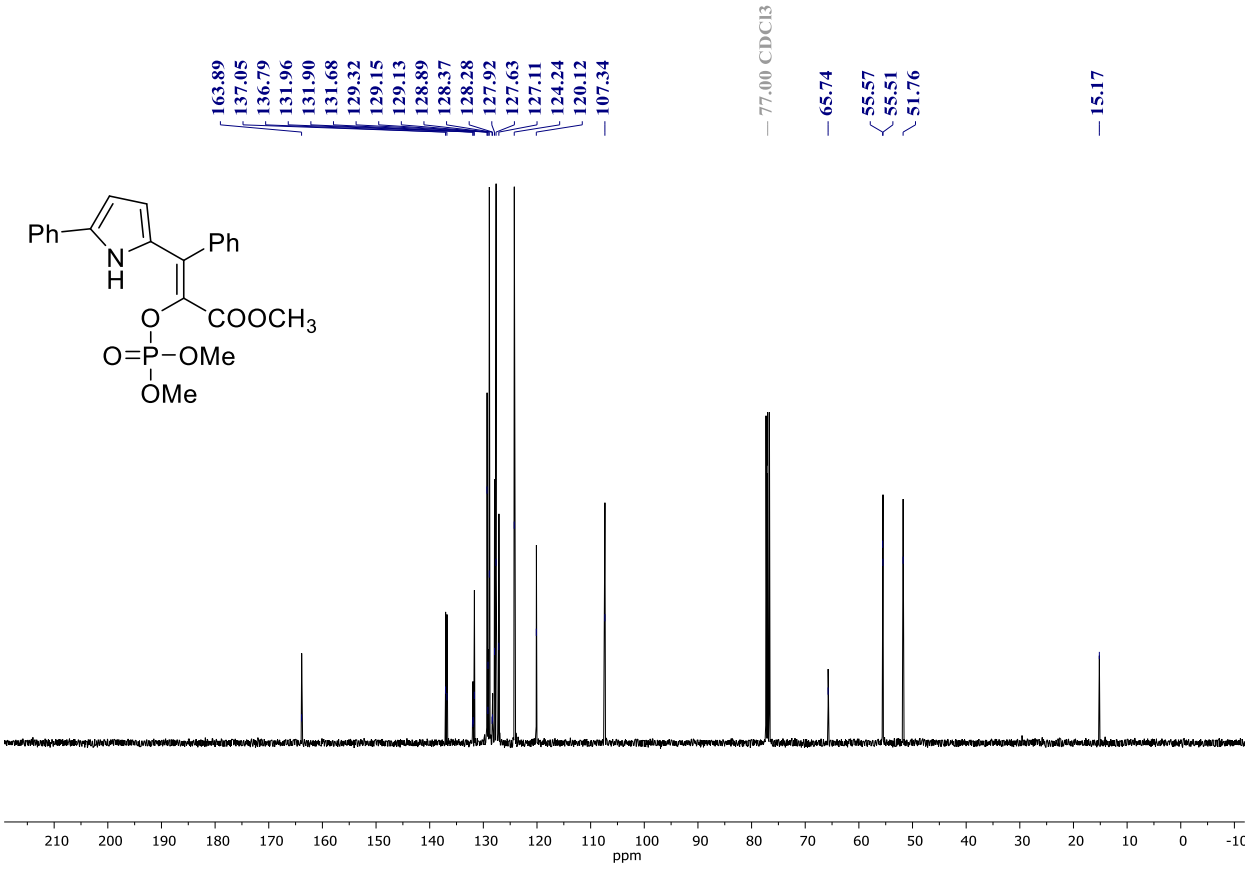
^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) spectrum of compound **9e**



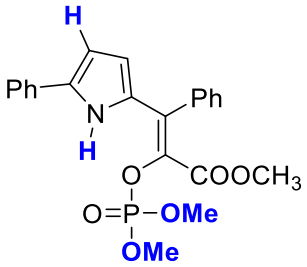
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound **10**

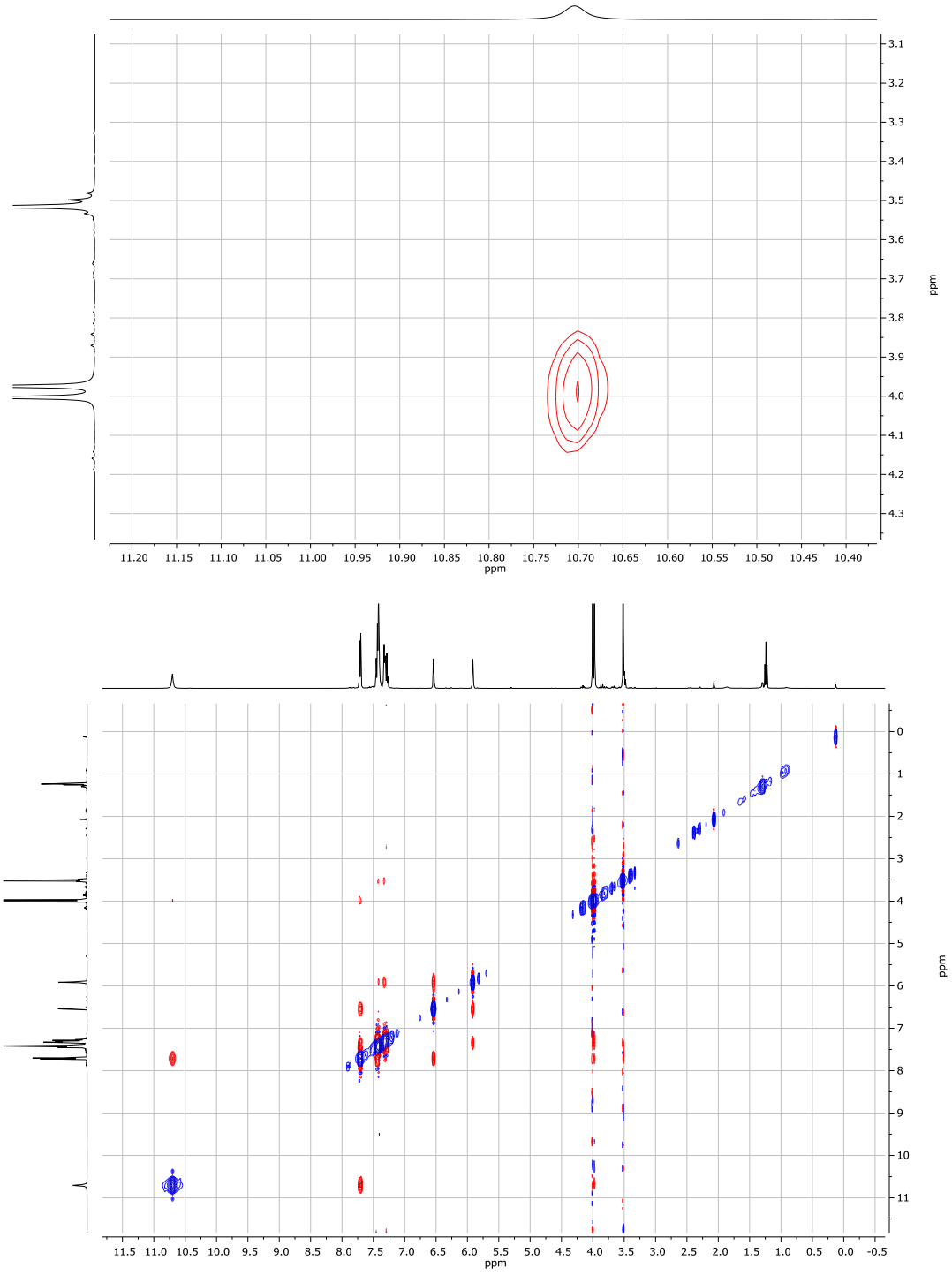


^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) spectrum of compound **10**

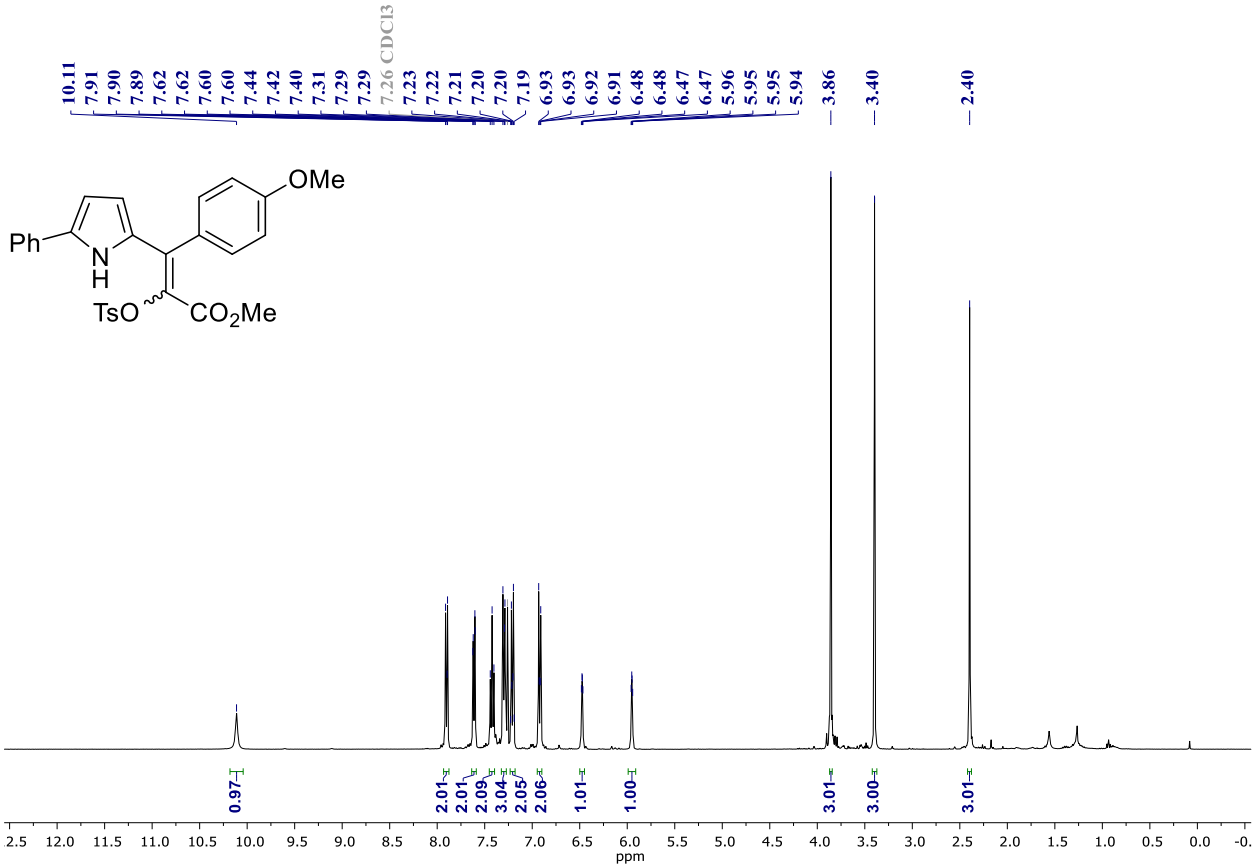


^{1}H-^{1}H NOESY (400 MHz, $CDCl_3$) spectrum of compound **10** with correlation of highlighted atoms

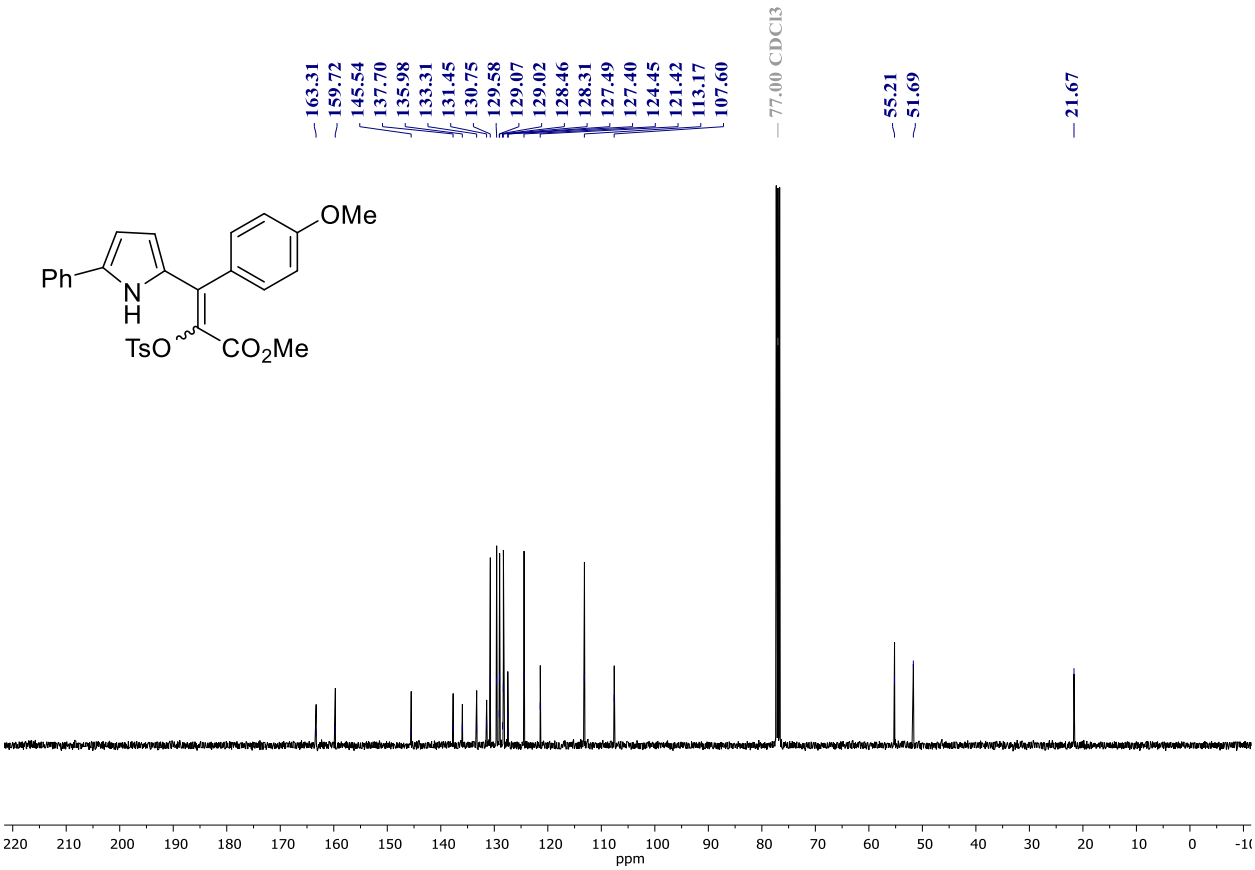




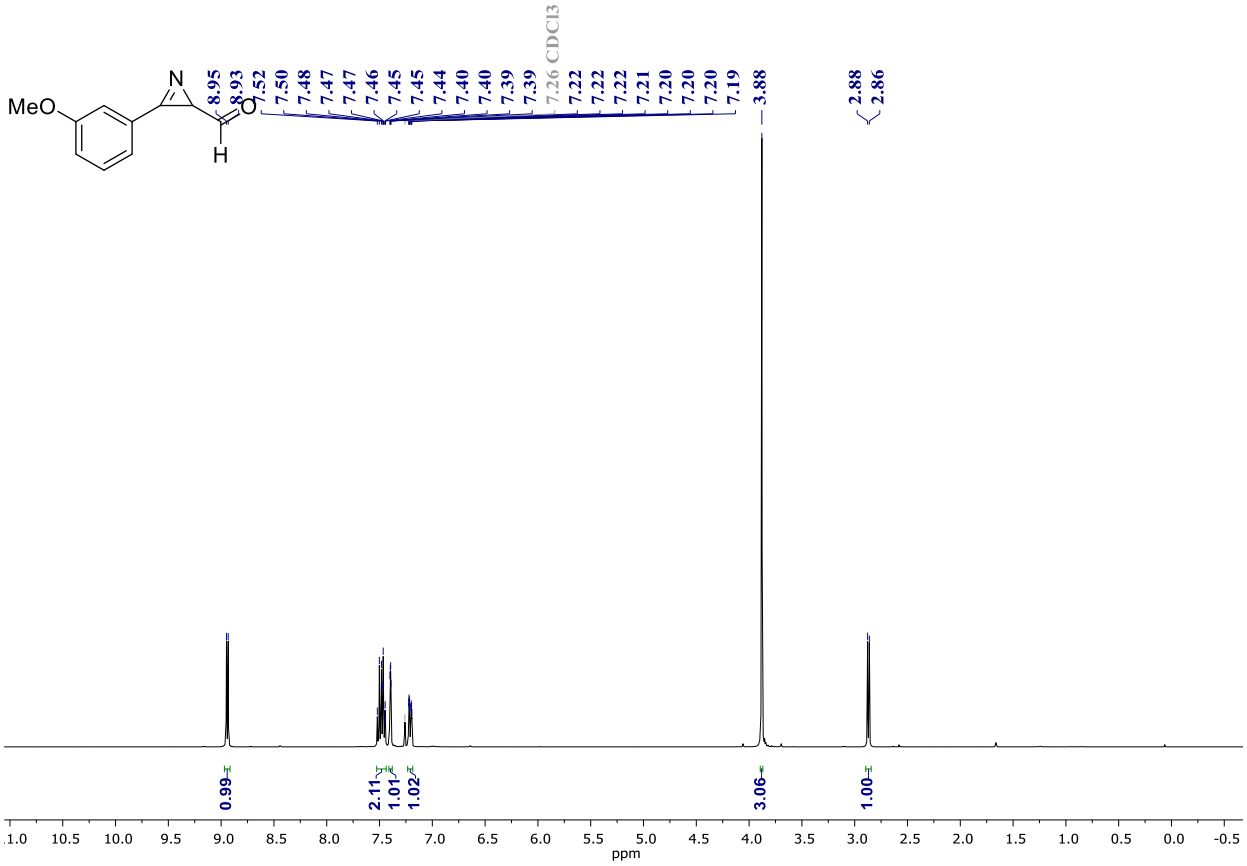
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound **11**



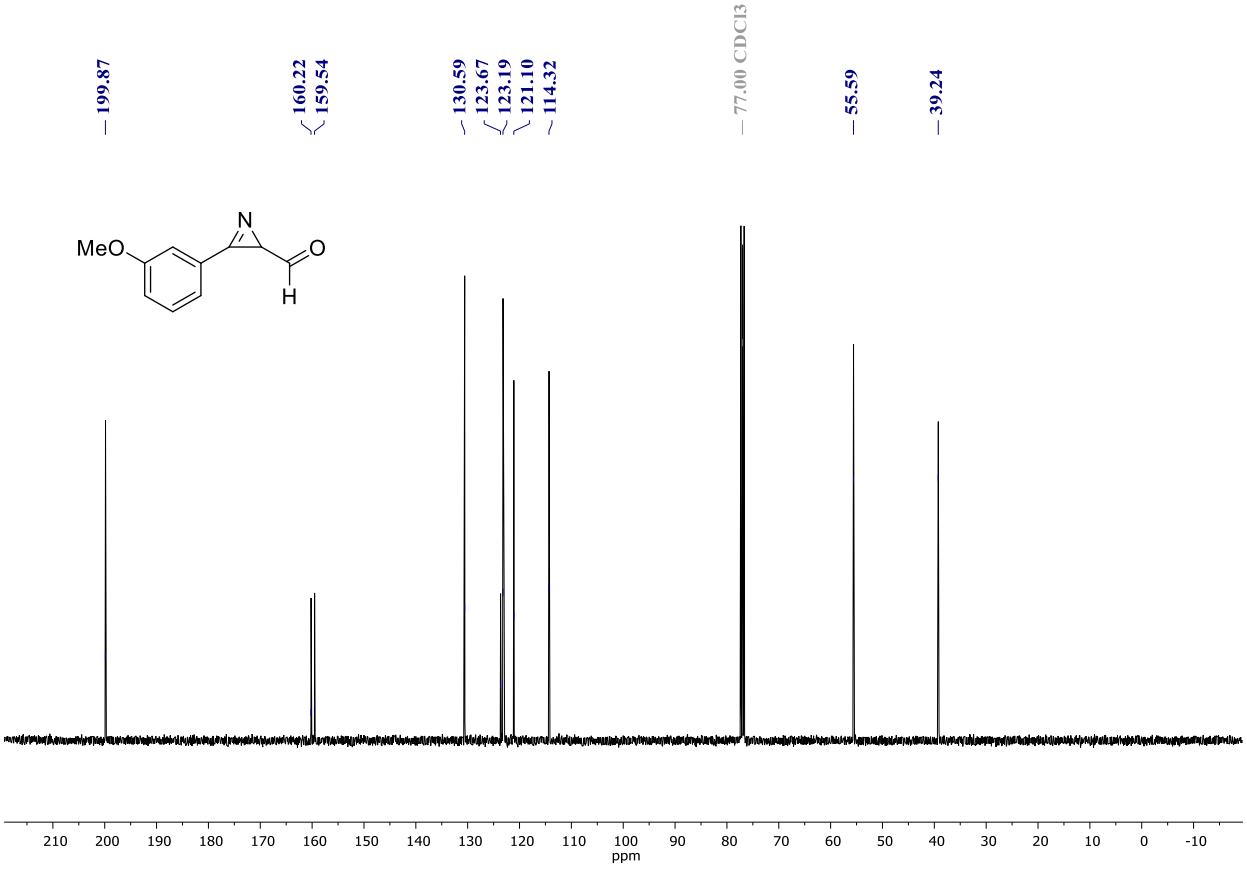
^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) spectrum of compound **11**



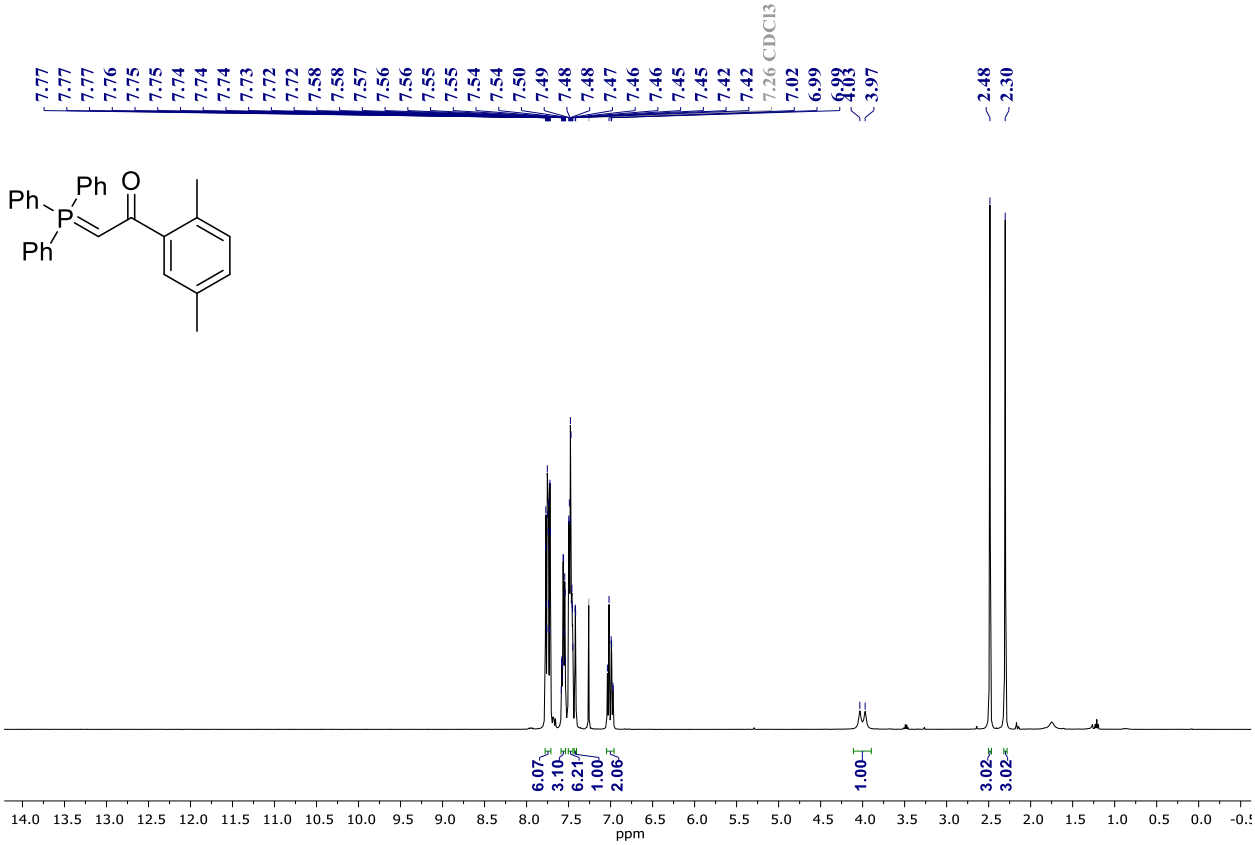
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of 3-(3-methoxyphenyl)-2*H*-azirine-2-carbaldehyde



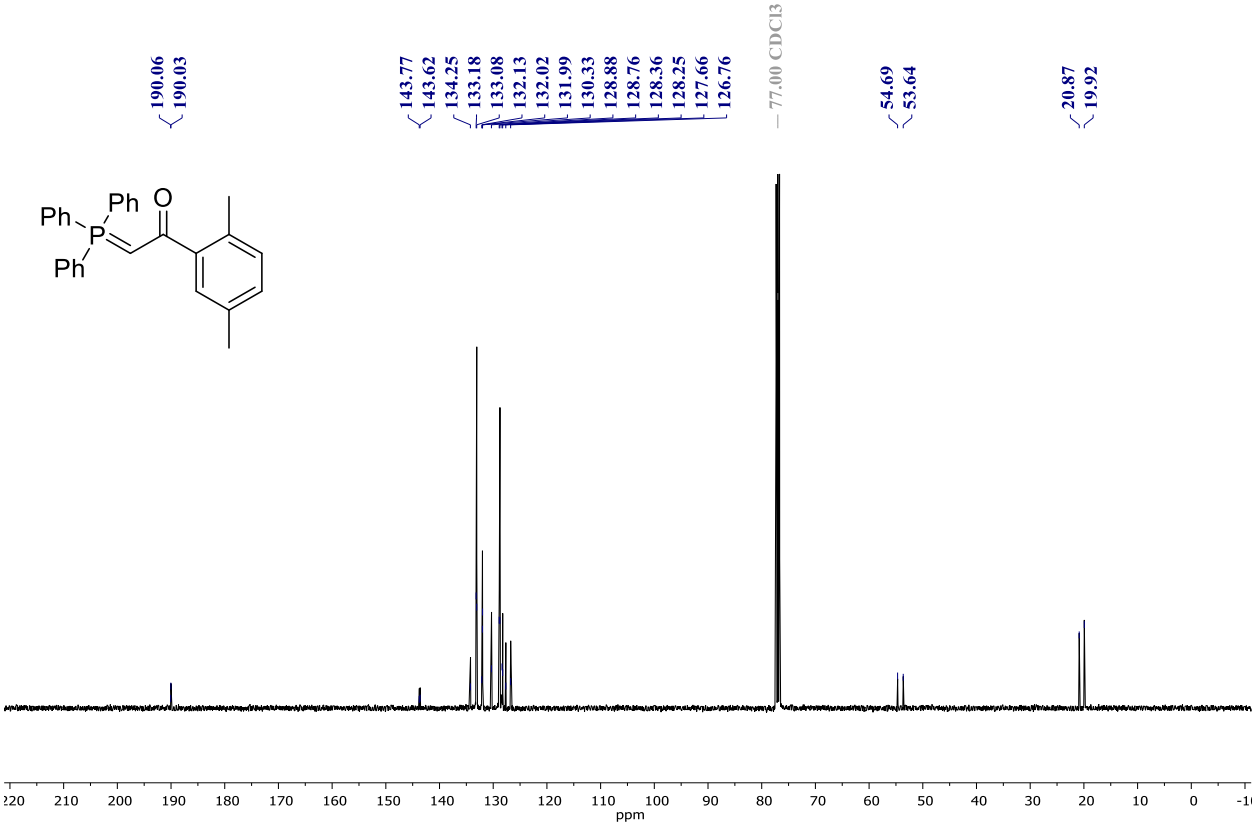
^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) spectrum of 3-(3-methoxyphenyl)-2*H*-azirine-2-carbaldehyde



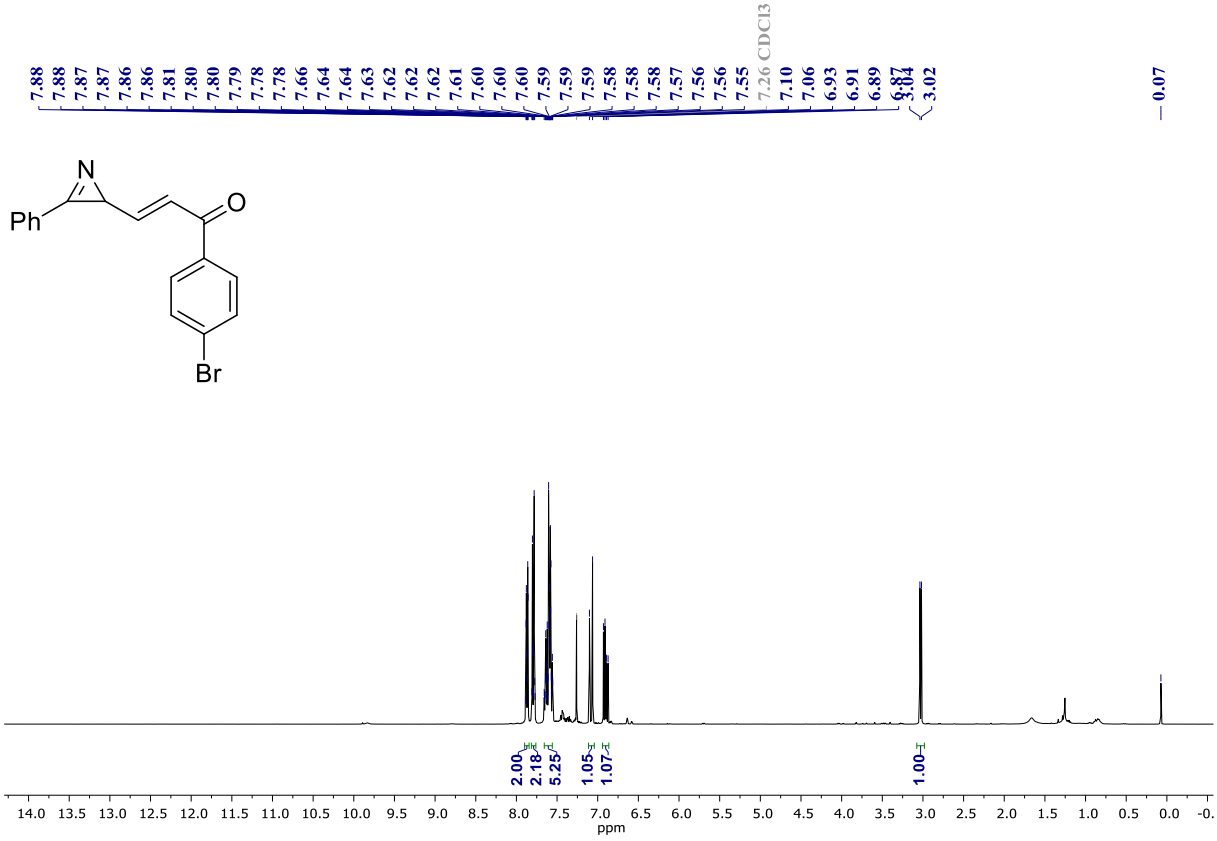
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of 1-(2,5-dimethylphenyl)-2-(triphenyl-λ^5-phosphanylidene)ethan-1-one



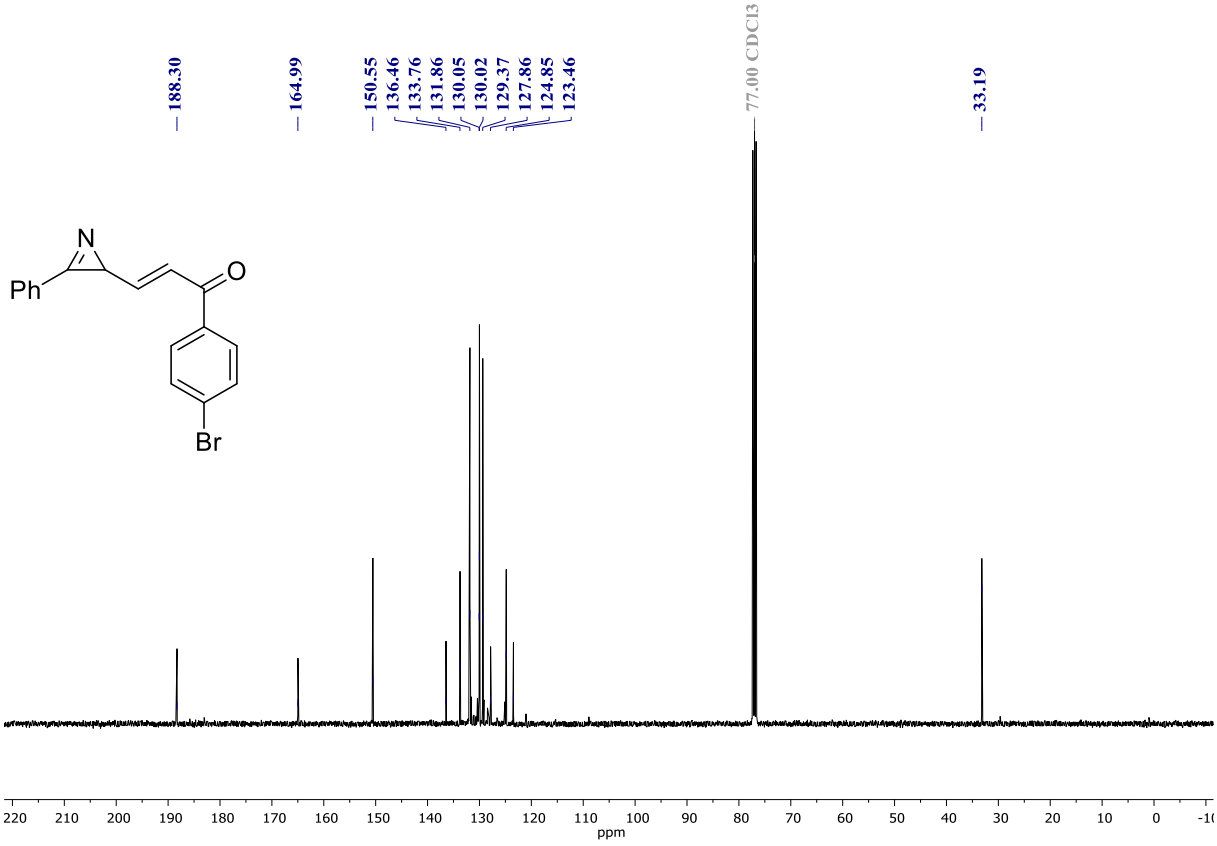
^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) spectrum of 1-(2,5-dimethylphenyl)-2-(triphenyl-λ^5-phosphanylidene)ethan-1-one



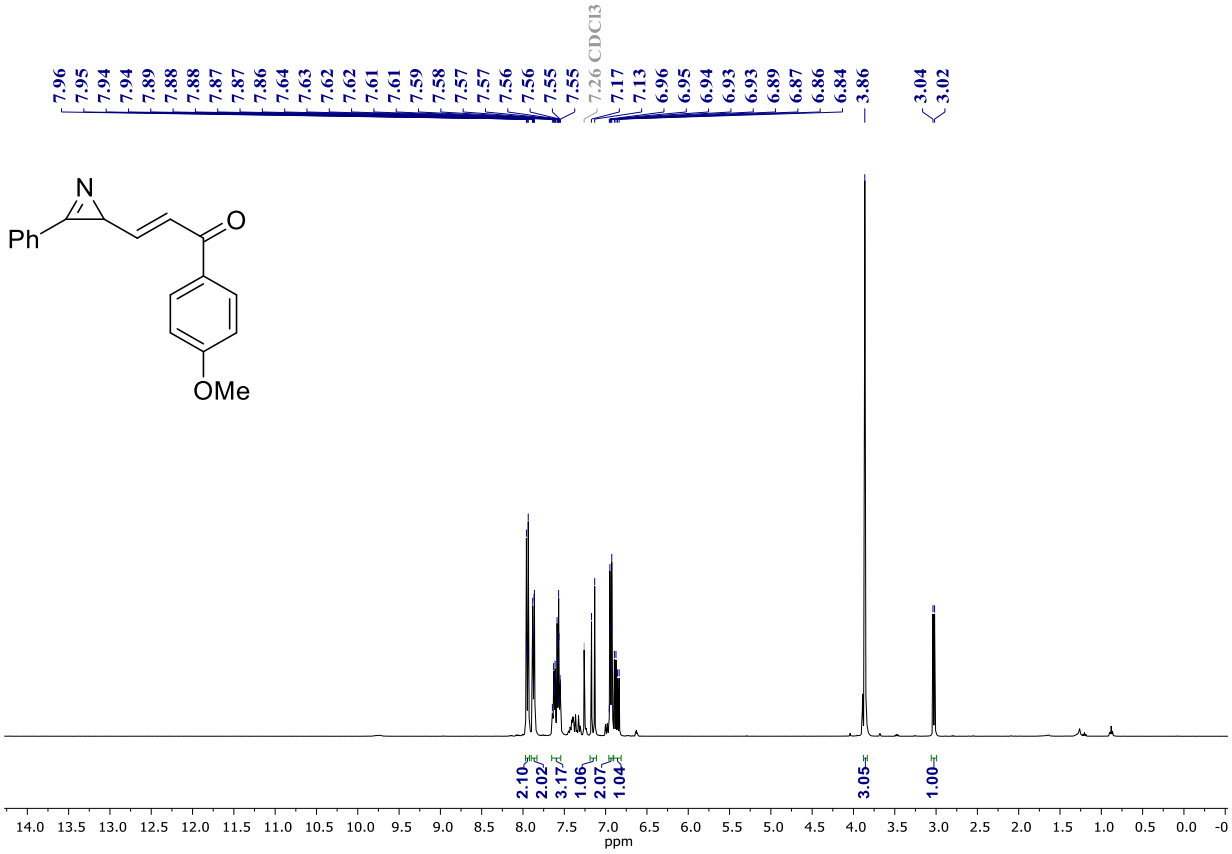
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of (*E*)-1-(4-bromophenyl)-3-(3-phenyl-2*H*-azirin-2-yl)prop-2-en-1-one



^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) spectrum of (*E*)-1-(4-bromophenyl)-3-(3-phenyl-2*H*-azirin-2-yl)prop-2-en-1-one



^{1}H NMR (400 MHz, $CDCl_3$) spectrum of (*E*)-1-(4-methoxyphenyl)-3-(3-phenyl-2*H*-azirin-2-yl)prop-2-en-1-one



^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) spectrum of (*E*)-1-(4-methoxyphenyl)-3-(3-phenyl-2*H*-azirin-2-yl)prop-2-en-1-one