Supporting Information

Visible Light-induced Aerobic Oxidation of Diarylalkynes to α-Diketones Catalyzed by Copper-superoxo at Room Temperature

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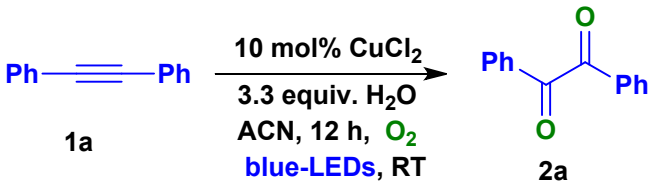
Experimental section

General: All reactions were conducted in oven-dried glasswares. All reactions were conducted using a blue light-emitting diode (LED) array (30 lamps, power density: 40 mW/cm^2 at 460 nm) as the visible-light source under oxygen (O_2) atmosphere in all reactions. All solvents were dried according to known methods and distilled prior to use. Starting materials were commercially available (Sigma-Aldrich or Alfa-Aesar or TCI-chemicals) and used as received. ^{1}H NMR and ^{13}C NMR spectra were recorded at 600 MHz using deuterated $CDCl_3$ or $CDCl_3$-DMSO-d_6 mixture. Chemical shifts (δ) were reported as parts per million (ppm) and the following abbreviations were used to identify the multiplicities: s= singlet, d= doublet, t= triplet, q= quartet, m= multiplet, b= broad and all combinations thereof can be explained by their integral parts. Unless otherwise specified, the proton/carbon signal of 2 residual solvents (at δ 7.24 or 2.50 and δ 77.00 or 39.51 ppm, respectively) was used as the internal reference.

General procedure for the synthesis of α-diketones:

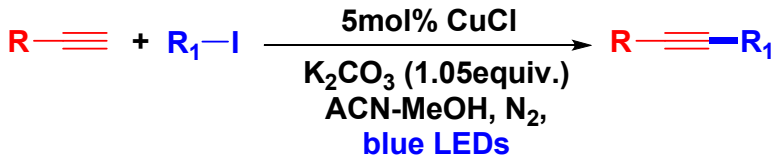
Scheme S1: Current photochemical process for the synthesis of α-diketones



To a dry test tube (20 mL) containing 10 mol% $CuCl_2$ and internal alkyne (diarylacetylenes) (0.5 mmol), was added 5 mL of ACN, followed by the addition of 30 μL of water. The reaction mixture was then irradiated with blue LEDs (40 mW/cm^2 at 460 nm) under an oxygen atmosphere at room temperature (25-28 ^{o}C) until completion of the reaction (monitored by TLC). The reaction mixture was then diluted with 40 % ethyl acetate in hexane and stirred for 10 min. The mixture was filtered through celite and silica gel pads and washed with ethyl acetate. The filtrate was concentrated and the residue was purified by column chromatography on silica gel.

General procedure for the preparation of starting materials (internal alkynes)[s1]:

Scheme S2: Photo induced Sonogashira coupling

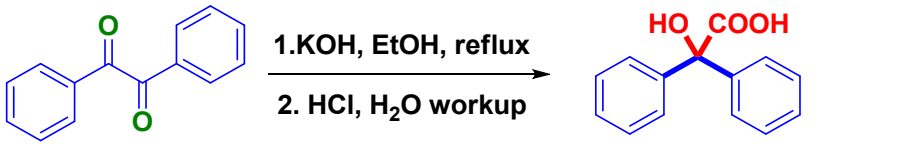


A dry test tube (20 mL) with a rubber septum and a magnetic stirrer bar was charged with aryl or alkyl iodides (0.50 mmol, 1.0 equiv.), K_2CO_3 (0.52 mmol, 1.05 equiv.) and 5 mol% CuCl. The test tube was evacuated and purged with dry N_2 gas for three times and then dry ACN (2 mL) and MeOH (2 mL) were added via syringe, and finally the terminal acetylene (0.60 mmol, 1.2 equiv.) using syringe. The transparent suspension was irradiated with blue light output from a blue LED array (power density 40 mW/cm^2 at 460 nm) at room temperature for 4–12 h until completion of the cross-coupling reaction (as determined by thin layer chromatography). The reaction mixture was diluted with 40% ethyl acetate in hexane and stirred for 10 min. The mixture was filtered through celite and silica gel pads and washed with ethyl acetate. The filtrate was concentrated and the residue was purified by flash column chromatography on silica gel to afford the desired cross-coupling product.

Procedures for the further transformations from the a-diketones:

a) Formation of benzillic acid from a-diketones[s2]

Scheme S3: Formation of benzillic acid from α-diketones



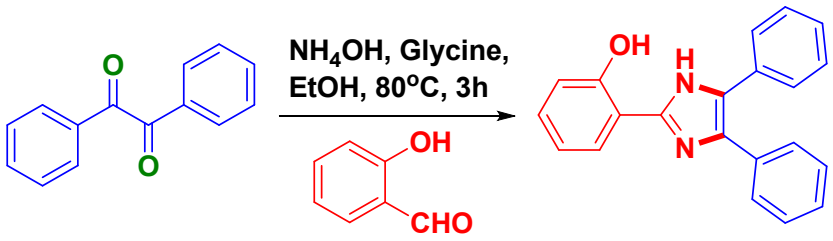
2-hydroxy-2,2-diphenylacetic acid
(Benzillic acid)

After cooled to room temperature, the mixture was washed with ether (50 mL x 3). The aqueous layer was cooled to 0 ^oC, acidified with 12 N HCl (5 mL) and extracted with DCM (50 mL x 2). The combined organic layers were washed with brine, dried over $MgSO_4$ and the filtrate was concentrated in vacuo to get benzillic acid **(3)** (yield 89%).

b) Synthesis of Trifenagrel drug:

Step1: Preparation of 2-(4,5-diphenyl-1H-imidazol-2-yl)phenol[s3]

Scheme S4: Preparation of 2-(4,5-diphenyl-1H-imidazol-2-yl)phenol from α-diketones

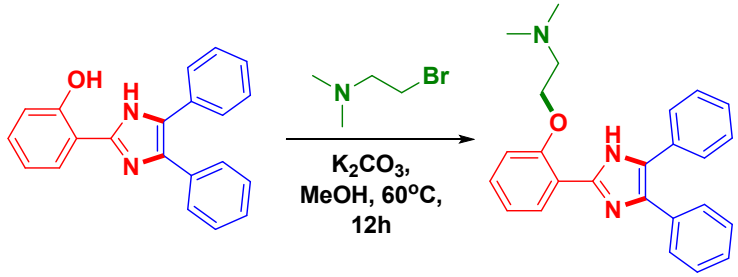


2-(4,5-diphenyl-1*H*-imidazol-2-yl)phenol

A mixture of benzil (0.525 g; 2.5 mmol), salicylaldehyde (0.3053 g; 2.5 mmol), ammonium acetate (0.5g;6mmol) and glycine (0.05 g, 0.6 mmol) was stirred in ethanol (10ml) for 3 h at 80 °C. The completion of the reaction was monitored by TLC. Ensuring the completion of reaction, the reaction mixture was poured into crush ice: cold ethanol mixture (1:1) and filtered to afford 2-(2-Hydroxyphenyl)-4,5-diphenyl-1H-imidazole **(4)** in **93% yield** (pale yellow precipitate).

Step2: Preparation of 2-(2-(4,5-diphenyl-1H-imidazol-2-yl)phenoxy)-N,N-dimethylethanamine (Trifenagrel)[s3]

Scheme S5: Synthesis of Trifenagrel (4')



2-(4,5-diphenyl-1*H*-imidazol-2-yl)phenol

Trifenagrel

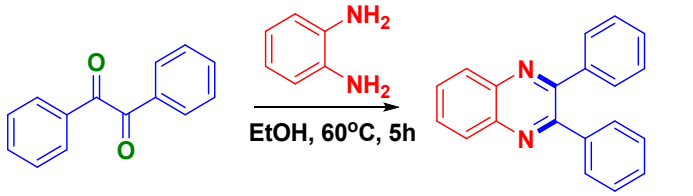
2-(2-(4,5-diphenyl-1*H*-imidazol-2-yl)phenoxy)-*N*,*N*-dimethylethanamine

2-(2-Hydroxyphenyl)-4,5-diphenylimidazole (0.2 g, 0.6 mmol) and K_2CO_3 (1.5 equiv., 0.12 g) was dissolved in MeOH (15 mL) and stirred for 15 mins at room temperature. Then, the solution of 2-bromo-N,N-dimethylethanamine (1.5 equiv., 0.15 g, 1.0 mmol) in 3 mL of MeOH was added dropwise into the reaction mixture over the period of 10mins. The reaction mixture was then stirred for 12 h at 60 °C. After completion of reaction, the reaction mixture was then concentrated (to remove MeOH) and then diluted with ether and layers were separated. The

filtrate was then concentrated and the residue was purified by column chromatography on silica gel (yield 85%).

c) Preparation of 2,3-diphenylquinoxaline from a-diketones[s4]:

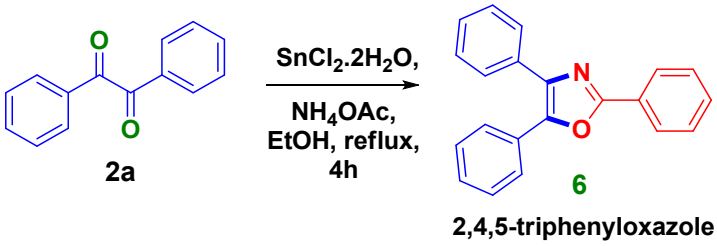
Scheme S6: Preparation of 2,3-diphenylquinoxaline (5) from α-diketones



Benzil (0.21 g, 1 mmol) and o-phenyldiamine (0.11g, 1.05 equiv., 1.05 mmol) was dissolved in ethanol and stirred at 60 °C for 3 h. The reaction mixture was then concentrated and the residue was purified by column chromatography on silica gel **(yield 96%)**.

d) Preparation of 2,4,5-triphenyloxazole (6)

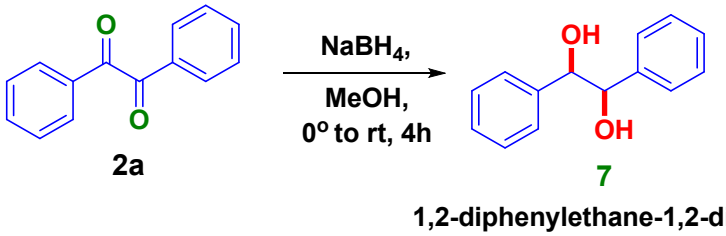
Scheme S7: Preparation of 2,4,5-triphenyloxazole (6)



Benzil (1.0 mmol), NH4OAc (5.0 mmol) and $SnCl_2.2H_2O$ (0.05 mmol) was dissolved in EtOH (4 mL). The reaction mixture was stirred and refluxed for 4 h. After completion of reaction, the reaction mixture was then concentrated (to remove EtOH) and then diluted with ether and layers were separated. The filtrate was then concentrated and the residue was purified by column chromatography on silica gel (yield 73%).

e) Preparation of 1,2-diphenylethane-1,2-diol (7)

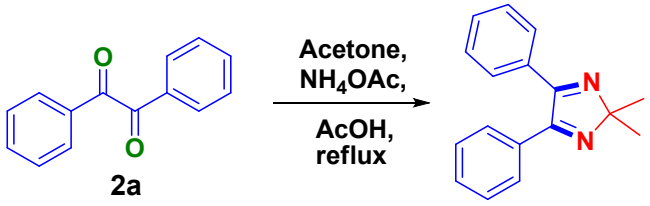
Scheme S8: Preparation of 1,2-diphenylethane-1,2-diol (7)



Benzil (1.0 mmol) was dissolved in EtOH (15 mL) and stirred for 5min at 0 °C. To this solution, $NaBH_4$ (2.0 equiv.) was added slowly and the reaction mixture was further stirred for 4 h at room temperature. After completion of reaction, the reaction mixture was then concentrated (to remove EtOH) and then the layers were separated. The filtrate was then concentrated and the residue was purified by column chromatography on silica gel (yield 88%).

f) Preparation of 2,2-dimethyl-4,5-diphenyl-2H-imidazole (8)

Scheme S9: Preparation of 2,2-dimethyl-4,5-diphenyl-2H-imidazole (8)



8

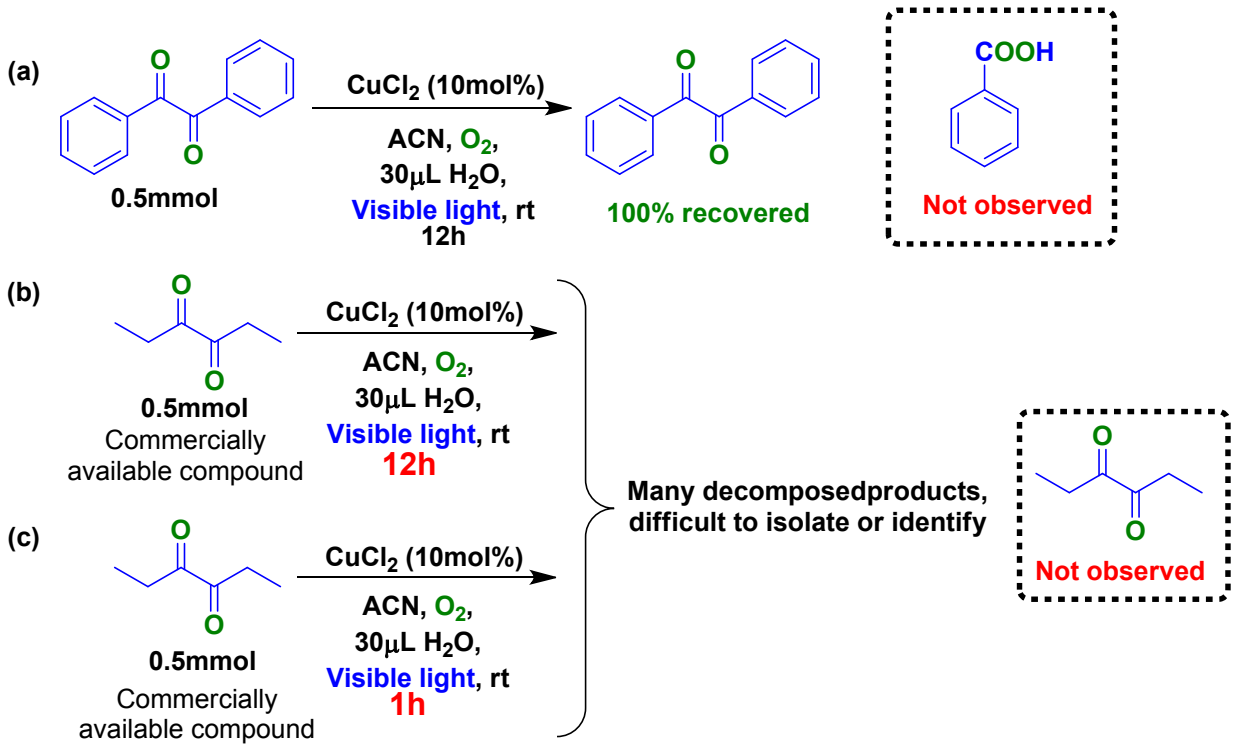
2,2-dimethyl-4,5-diphenyl-2*H*-imidazole

Benzil (1.0 mmol) and NH_4OAc (5.0 mmol) was dissolved in AcOH (5 mL). To this solution, acetone (4.0 equiv.) was added. The reaction mixture was stirred and refluxed (120 °C) for 4 h. After completion of reaction, the reaction mixture was then concentrated and the layers were separated. The filtrate was then concentrated and the residue was purified by column chromatography on silica gel (yield 78%).

Control Reactions:

Control reaction presented in the **Scheme S10** showed that the aryl diketones are stable. In contrast, alkyl diketones are not stable and undergo over oxidation (cleavage) to form various (oxidized products) unidentified products in the presence of copper superoxide. The decomposition of 3,4-hexadione under current reaction conditions forms various products which are difficult to identify and isolate.

Scheme S10: Control reactions to check the stability of aryl and alkyl α-diketones in the presence of copper superoxo species.



EPR measurements: EPR spectra were recorded at room temperature on a Bruker ESP-300E(X band, 9.8 GHz) with parameters setting as shown below: receiver gain=30n; receiver phase=0deg; receiver harmonic=1; field modulation frequency=100000 Hz; microwave frequency[Hz]= $9.660469e^{+09}$; field modulation amplitude [T]= 0.00016; receiver time constant[S] = 0.32768; microwave power= 0.015 W; receiver offset [%FS]=0; DMPO (5-,5-dimethyl-1-pyrroline N-oxide) was employed as a radical trap for superoxide.

The reaction under standard condition (**1a**, $CuCl_2$, O_2) in ACN was irradiated with blue LED light for 30 min in the presence of DMPO. The EPR signals shown in Figure S1 is corresponding to DMPO-OO(Cu). This result indicates that copper superoxide free radical was formed in the reaction solution. No superoxide EPR signals were observed from the reaction solution under standard condition in absence of $CuCl_2$ (Figure S2).

EPR spectra of the reaction mixture after blue LEDs irradiation

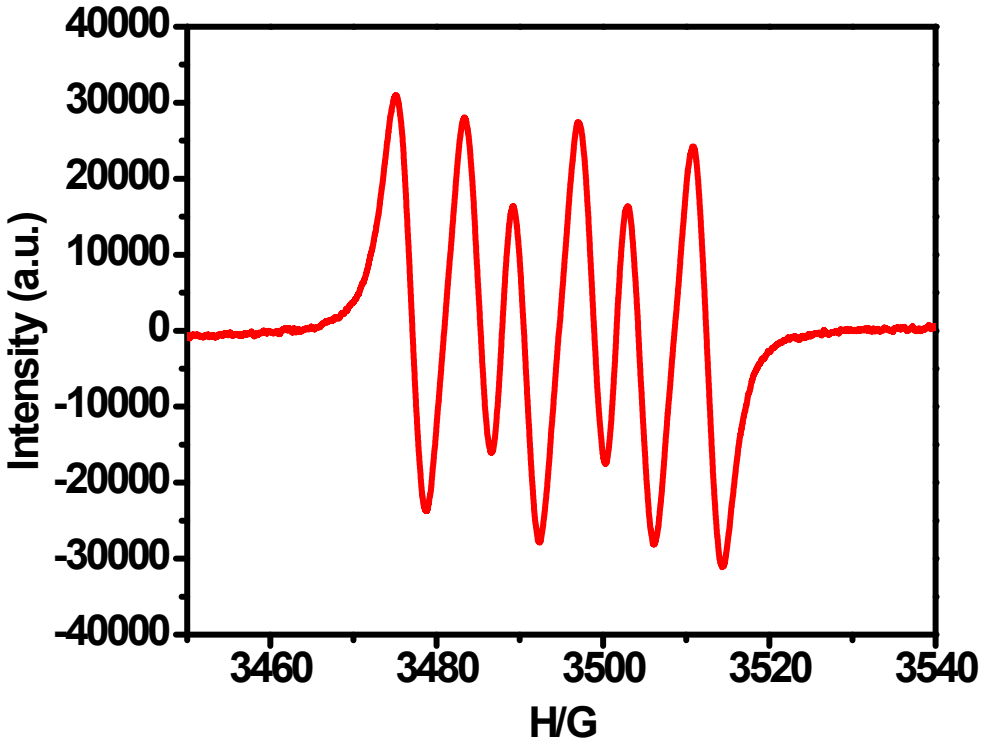


Figure S1: EPR spectra of the reaction mixture: diphenylacetylene (**1a**) (0.5 mmol), and 10 mol% of $CuCl_2$ in ACN (5 mL), 0.5 ml of this reaction solution was taken out into a small vial, followed by the addition of 0.01 mL of DMPO (5 x 10^{-2} M). The mixture was irradiated with blue LEDs at room temperature under an oxygen atmosphere (1 atm) for 30 minutes. The reaction mixture was then analyzed by EPR spectra. There are classical 6 peaks, the signals corresponding to (DMPO-OO(Cu))

EPR spectra of the reaction mixture in the absence of $CuCl_2$

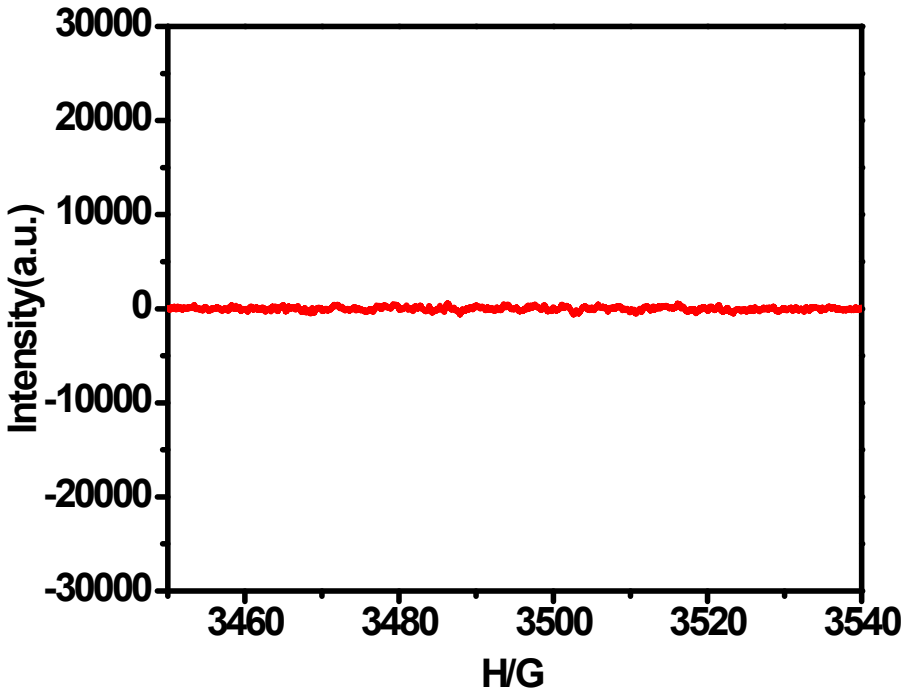


Figure S2: EPR spectra of the reaction mixture: diphenylacetylene (**1a**) (0.5 mmol) in ACN (5 mL), 0.5 ml of this reaction solution was taken out into a small vial, followed by the addition of 0.01 mL of DMPO (5 x 10^{-2} M). The mixture was irradiated with blue LEDs at room temperature under an oxygen atmosphere (1 atm) for 30 minutes. The reaction mixture was then analyzed by EPR spectra. No signals were detected.

Evaluation of Green metrics for the literature reported photochemical process[s5]

Atom economy (%) (AE) = $\frac{\text{Molecular mass of desired product}}{\text{Molecular mass of all reactants}}$ x 100

Reaction mass efficiency (%) (RME) = $\frac{\text{Mass of desired product}}{\text{Mass of all reactants}}$ x 100

Reactant1	**1,2-diphenylethyne**	**1g**	**5.61 mmol**	**FW 178.23**
Reactant2	**4,4'-Dinitrodiphenyl disulfide**	**0.259g**	**0.84 mmol**	**FW 308.33**
Solvent	**ACN**	**15.72g (20mL)**	**----**	**----**
Auxiliary	**----**	**----**	**----**	**----**
Product	**Benzil**	**0.977g**	**4.65 mmol**	**FW 210.22**

Product yield = 83%

E-factor = $\frac{\text{1g + 15.72g + 0.259g - 0.977g}}{\text{0.977g}}$ = **16.0 Kg waste/ 1 Kg product**

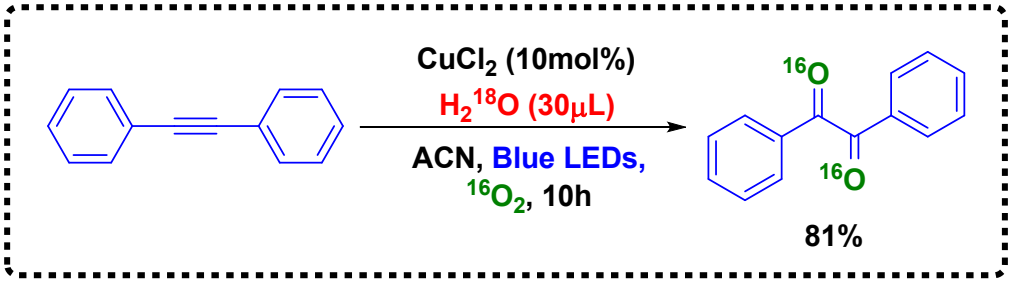
Atom economy = $\frac{210}{210}$ x 100 = **100%**

Atom efficiency = **83% x 100% /100** = **83%**

Carbon efficiency = $\frac{14}{14}$ x 100 = **100%**

Reaction mass efficiency = $\frac{0.977\text{g}}{1\text{g}}$ x 100 = **97.7%**

$H_2{}^{18}O$ experiment



Scheme S11: Reaction in the presence of $H_2{}^{18}O$

Procedure: To a dry test tube (20 mL) containing 10 mol% $CuCl_2$ and diphenylacetylene (0.5 mmol), was added 5 mL of dry ACN, followed by the addition of **30 μL of $H_2{}^{18}O$**. The reaction mixture was then irradiated with blue LEDs (40 mW/cm^2 at 460 nm) under an oxygen atmosphere at room temperature (25-28 ^oC) for 10h. The reaction mixture was then diluted with 40 % ethyl acetate in hexane and stirred for 10 min. The mixture was filtered through celite and silica gel pads and washed with ethyl acetate. The filtrate was concentrated and the residue was purified by column chromatography on silica gel.

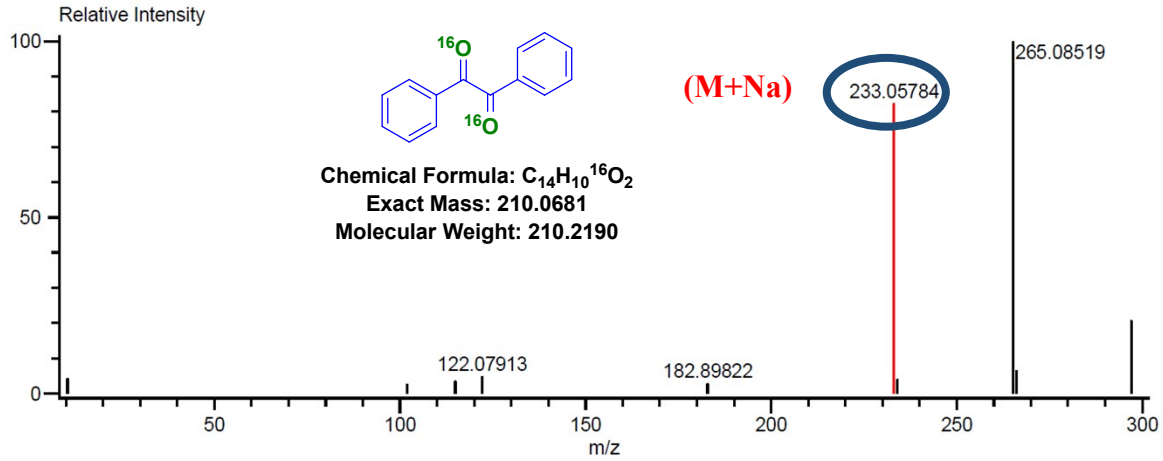
The ESI mass of the crude reaction mixture was detected. In the ESI mass data, we have observed only (M+Na) peak of $^{16}O_2$ product. Thus, this experiment showed that the source of O-atom in the product is only from the molecular O_2.

ESI Mass Data

Data:H2O18-2
Comment:
Description:
Ionization Mode:ESI+
History:Average(MS[1] 1.59..1.62)

Acquired:4/15/2020 3:41:42 PM
Operator:AccuTOF
m/z Calibration File:20200102-1TFANa...
Created:4/16/2020 3:12:00 PM
Created by:AccuTOF

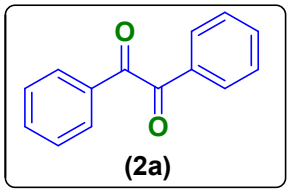
Charge number:1
Tolerance:50.00[ppm], 20.00 .. 20.00[...
Unsaturation Number:-150.0 .. 200.0 (...
Element:^{12}C:14 .. 14, ^{1}H:0 .. 11, ^{23}Na:0 .. 1, ^{16}O:2 .. 2



Mass	Intensity	Calc. Mass	Mass Difference [mDa]	Mass Difference [ppm]	Possible Formula
233.05784	1885.54	233.05785	-0.01	-0.03	$^{12}C_{14}{}^{1}H_{10}{}^{23}Na_{1}{}^{16}O_{2}$

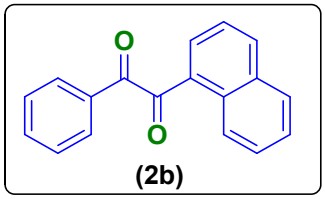
Spectroscopic Data

Benzil (2a)[s6-9]



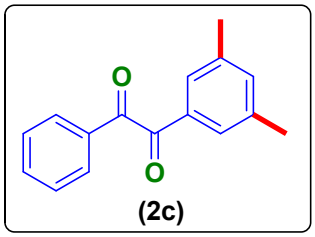
Yellow solid; **^{1}H NMR** (600 MHz, $CDCl_3$): δ 7.94 (t, *J*= 6.0 Hz, 4H), 7.62-7.59 (m, 2H), 7.46 (t, *J*= 12.0 Hz, 4H); **^{13}C NMR** (150 MHz, $CDCl_3$): δ 194.4, 134.7, 132.8, 129.7 and 128.8; ESI-MS calcd for $C_{14}H_{10}O_2$ (M+H): 210.0681, found: 211.0795.

1-(naphthalen-1-yl)-2-phenylethane-1,2-dione (2b)[s6,7]



Yellow solid; **^{1}H NMR** (600 MHz, $CDCl_3$): δ 9.28 (d, *J*= 6.0 Hz, 1H), 8.09 (d, *J*= 6.0 Hz, 1H), 8.01 (t, *J*= 6.0 Hz, 2H), 7.93-7.89 (m, 2H), 7.73 (t, *J*= 6.0 Hz, 1H), 7.65-7.59 (m, 2H), 7.51-7.45 (m, 3H); **^{13}C NMR** (150 MHz, $CDCl_3$): δ 197.1, 194.5, 135.9, 135.0, 134.7, 134.0, 133.3, 130.9, 129.9, 129.4, 129.0, 128.7, 128.6, 127.1, 125.9 and 124.4; **ESI-MS** calcd for $C_{18}H_{12}O_2$ (M+H): 260.0837, found: 261.0913.

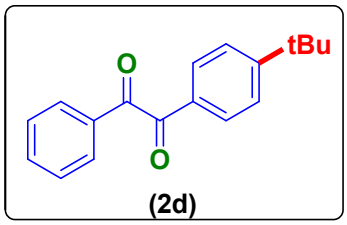
1-(3,5-dimethylphenyl)-2-phenylethane-1,2-dione (2c)[s7]



Pale yellow oil; **^{1}H NMR** (600 MHz, $CDCl_3$): δ 7.95 (d, *J*= 7.2 Hz, 2H), 7.64-7.61 (m, 1H), 7.56 (s, 2H), 7.50-7.46 (m, 2H), 7.26 (s, 1H), 2.34 (s, 6H); **^{13}C NMR** (150 MHz, $CDCl_3$): δ 194.7,

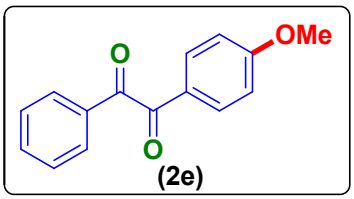
194.4, 138.6, 136.5, 134.5, 132.8, 131.6, 129.7, 128.7, 127.3 and 21.2; **ESI-MS** calcd for $C_{16}H_{14}O_2$ (M+H): 238.0994, found: 239.1075.

1-(4-tert-butylphenyl)-2-phenylethane-1,2-dione (2d)[s7]



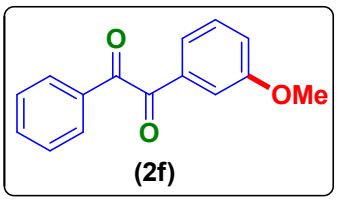
Off white solid; **^{1}H NMR** (600 MHz, $CDCl_3$): δ 7.95 (d, *J*= 7.2 Hz, 2H), 7.89 (d, *J*= 12.0 Hz, 2H), 7.63 (t, *J*= 6.0 Hz, 1H), 7.51-7.47 (m, 4H), 1.32 (s, 9H); **^{13}C NMR** (150 MHz, $CDCl_3$): δ 194.7, 194.2, 159.0, 134.7, 133.0, 130.4, 129.8, 128.9, 126.0, 35.3 and 30.9; **ESI-MS** calcd for $C_{18}H_{18}O_2$ (M+Na): 266.1307, found: 289.1205.

1-(4-methoxyphenyl)-2-phenylethane-1,2-dione (2e)[s6]



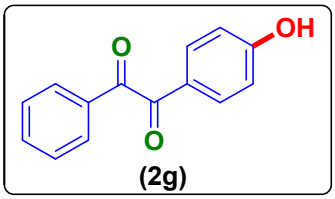
Off white solid; **^{1}H NMR** (600 MHz, $CDCl_3$): δ 7.95-7.92 (m, 4H), 7.62 (t, *J*= 6.0 Hz, 1H), 7.48 (t, *J*= 6.0 Hz, 2H), 7.65 (d, *J*= 6.0 Hz, 2H), 3.86 (s, 3H); **^{13}C NMR** (150 MHz, $CDCl_3$): δ 194.8, 193.1, 164.9, 134.7, 133.1, 132.3, 129.8, 128.9, 126.0, 114.3 and 55.6; **ESI-MS** calcd for $C_{15}H_{12}O_3$ (M+Na): 240.0786, found: 263.0677.

1-(3-methoxyphenyl)-2-phenylethane-1,2-dione (2f)[s6]



Off white solid; **^{1}H NMR** (600 MHz, $CDCl_3$): δ 7.94 (d, *J*= 12.0 Hz, 2H), 7.64-7.62 (m, 1H), 7.52-7.46 (m, 4H), 7.45-7.36 (m, 1H), 7.19-7.17 (m, 1H), 3.84 (s, 3H); **^{13}C NMR** (150 MHz, $CDCl_3$): δ 194.4, 194.4, 160.0, 134.8, 134.1, 132.9, 130.0, 129.8, 128.9, 123.2, 121.8, 112.7, and 55.5; **ESI-MS** calcd for $C_{15}H_{12}O_3$ (M+Na): 240.0786, found: 263.0684.

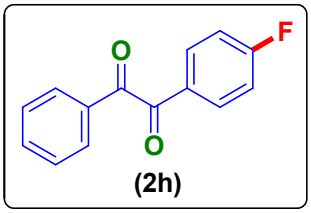
1-(4-hydroxyphenyl)-2-phenylethane-1,2-dione (2g)[s6]



(2g)

Brown solid; **^{1}H NMR** (600 MHz, $CDCl_3$): δ 7.92 (d, *J*= 6.0 Hz, 2H), 7.82 (d, *J*= 6.0 Hz, 2H), 7.62 (t, *J*= 6.0 Hz, 1H), 7.47 (t, *J*= 6.0 Hz, 2H), 6.87 (d, *J*= 12.0 Hz, 2H); **^{13}C NMR** (150 MHz, $CDCl_3$): δ 195.4, 193.6, 162.5, 135.0, 132.9, 132.7, 129.9, 129.0, 125.5 and 116.1; **ESI-MS** calcd for $C_{14}H_{10}O_3$ (M+Na): 226.0630, found: 249.0529

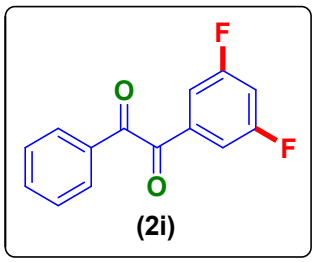
1-(4-fluorophenyl)-2-phenylethane-1,2-dione (2h)[s6]



(2h)

White solid; **^{1}H NMR** (600 MHz, $CDCl_3$): δ 8.01 (d, *J*= 6.0 Hz, 2H), 7.96 (d, *J*= 6.0 Hz, 2H), 7.65 (t, *J*= 6.0 Hz, 1H), 7.50 (t, *J*= 6.0 Hz, 2H), 7.17 (t, *J*= 12.0 Hz, 2H); **^{13}C NMR** (150 MHz, $CDCl_3$): δ 194.0, 192.7, 167.6 (d, $^1J_{C\text{-}F}$=258.0 Hz), 135.0, 132.7 (d, $^3J_{C\text{-}F}$=6.0 Hz), 132.6, 129.9, 129.0, and 116.4 (d, $^2J_{C\text{-}F}$=22.5 Hz); **ESI-MS** calcd for $C_{14}H_9FO_2$ (M+Na): 228.0587, found: 251.0479

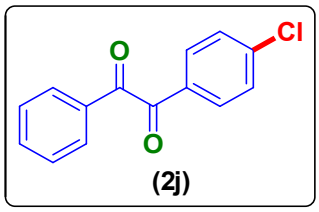
1-(3,5-difluorophenyl)-2-phenylethane-1,2-dione (2i)



(2i)

White solid; **^{1}H NMR** (600 MHz, $CDCl_3$): δ 7.95 (d, *J*= 6.0 Hz, 2H), 7.68 (t, *J*= 6.0 Hz, 1H), 7.54-7.49 (m, 4H), 7.10 (t, *J*= 6.0 Hz, 1H); **^{13}C NMR** (150 MHz, $CDCl_3$): δ 192.7, 191.4, 163.9 (d, $^1J_{C\text{-}F}$=252.0 Hz), 162.2 (d, $^1J_{C\text{-}F}$=252.0 Hz), 135.3, 133.0, 132.4, 130.0, 129.1, 112.7 (q, $^2J_{C\text{-}F}$=15.0, 6.0 Hz), and 110.1 (d, $^2J_{C\text{-}F}$=25.5 Hz); **ESI-MS** calcd for $C_{14}H_8F_2O_2$ (M+Na): 246.0492, found: 269.0400

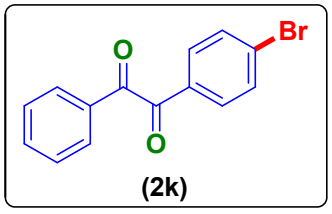
1-(4-chlorophenyl)-2-phenylethane-1,2-dione (2j)[s6]



(2j)

White solid; **^{1}H NMR** (600 MHz, $CDCl_3$): δ 7.94 (d, *J*= 12.0 Hz, 2H), 7.90 (d, *J*= 6.0 Hz, 2H), 7.64 (t, *J*= 6.0 Hz, 1H), 7.51-7.46 (m, 4H); **^{13}C NMR** (150 MHz, $CDCl_3$): δ 193.8, 193.0, 141.5, 135.0, 132.7, 131.3, 131.2, 129.9, 129.4 and 129.0; **ESI-MS** calcd for $C_{14}H_9ClO_2$ (M+Na): 244.0291, found: 267.0189

1-(4-bromophenyl)-2-phenylethane-1,2-dione (2k)[s6]

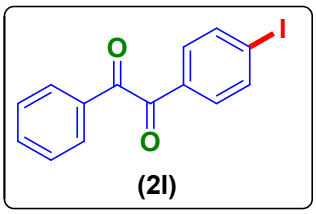


(2k)

Pale yellow solid; **^{1}H NMR** (600 MHz, $CDCl_3$): δ 7.94 (d, J = 7.2 Hz, 2H), 7.83-7.81 (m, 2H), 7.65-7.63 (m, 3H), 7.51-7.49 (m, 2H); **^{13}C NMR** (150 MHz, $CDCl_3$): δ 193.8, 193.2, 135.0, 132.7, 132.4,

131.6, 131.2, 130.4, 129.9, and 129.0; **ESI-MS** calcd for $C_{14}H_9BrO_2$ (M+Na): 287.9786, found: 310.9673.

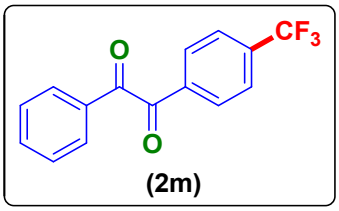
1-(4-iodophenyl)-2-phenylethane-1,2-dione (2l)



(2l)

White solid; **^{1}H NMR** (600 MHz, $CDCl_3$): δ 7.93 (d, *J*= 12.0 Hz, 2H), 7.86 (d, *J*= 6.0 Hz, 2H), 7.65 (d, *J*= 12.0 Hz, 3H), 7.49 (t, *J*= 12.0 Hz, 2H); **^{13}C NMR** (150 MHz, $CDCl_3$): δ 193.8, 193.6, 138.3, 135.0, 132.7, 132.2, 130.9, 129.9, 129.0 and 103.6; **ESI-MS** calcd for $C_{14}H_9IO_2$ (M+Na): 335.9647, found: 358.9521

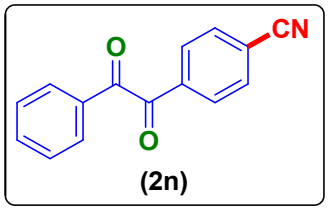
1-phenyl-2-(4-(trifluoromethyl)phenyl)ethane-1,2-dione (2m)[s6,7]



(2m)

Pale yellow solid; **^{1}H NMR** (600 MHz, $CDCl_3$): δ 8.08 (d, *J*= 6.0 Hz, 2H), 7.95 (d, *J*= 6.0 Hz, 2H), 7.76 (d, *J*= 12.0 Hz, 2H), 7.67 (t, *J*= 6.0 Hz, 1H), 7.52 (t, *J*= 6.0 Hz, 2H); **^{13}C NMR** (150 MHz, $CDCl_3$): δ 193.4, 193.0, 135.6, 135.2, 132.6, 130.2, 129.9, 129.1, 128.6 and 126.0; **ESI-MS** calcd for $C_{15}H_9F_3O_2$ (M+Na): 278.0555, found: 301.1433

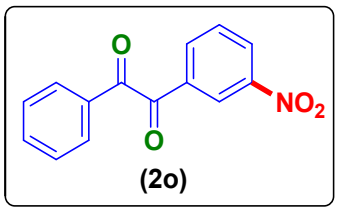
4-(2-oxo-2-phenylacetyl)benzonitrile (2n)[s7]



(2n)

White solid; **^{1}H NMR** (600 MHz, $CDCl_3$): δ 8.06 (d, *J*= 12.0 Hz, 2H), 7.95 (d, *J*= 6.0 Hz, 2H), 7.79 (d, *J*= 12.0 Hz, 2H), 7.67 (t, *J*= 12.0 Hz, 1H), 7.52 (t, *J*= 6.0 Hz, 2H); **^{13}C NMR** (150 MHz, $CDCl_3$): δ 192.9, 192.3, 135.8, 135.3, 132.7, 132.4, 130.1, 129.9, 129.1, 117.8 and 117.5; **ESI-MS** calcd for $C_{15}H_9NO_2$ (M+Na): 235.0633, found: 258.0560.

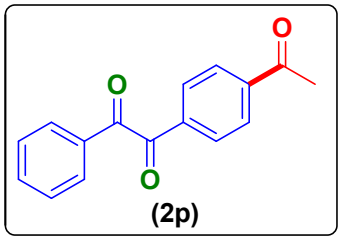
1-(3-nitrophenyl)-2-phenylethane-1,2-dione (2o)[s8]



(2o)

Yellow solid; **^{1}H NMR** (600 MHz, $CDCl_3$): δ 8.79 (d, *J*= 6.0 Hz, 1H), 8.48 (d, *J*= 6.0 Hz, 1H), 8.29 (d, *J*= 6.0 Hz, 1H), 7.98 (d, *J*= 6.0 Hz, 2H), 7.73-7.67 (m, 2H), 7.53 (t, *J*= 6.0 Hz, 2H); **^{13}C NMR** (150 MHz, $CDCl_3$): δ 192.6, 191.4, 148.5, 135.4, 135.2, 134.2, 132.3, 130.3, 130.0, 129.2, 128.8 and 124.5; **ESI-MS** calcd for $C_{14}H_9NO_4$ (M+Na): 255.0532, found: 278.0460.

1-(4-acetylphenyl)-2-phenylethane-1,2-dione (2p)[s7]

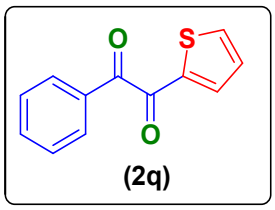


(2p)

White solid; **^{1}H NMR** (600 MHz, $CDCl_3$): δ 8.13 (s, 4H), 8.04 (d, *J*= 6.0 Hz, 2H), 7.74 (t, *J*= 6.0 Hz, 1H), 7.60 (t, *J*= 6.0 Hz, 2H); **^{13}C NMR** (150 MHz, $CDCl_3$): δ 197.2, 193.7, 193.5, 141.2,

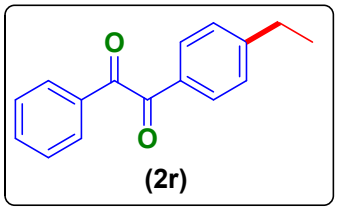
135.9, 135.1, 132.6, 130.0, 129.9, 129.0, 128.6 and 26.8; **ESI-MS** calcd for $C_{16}H_{12}O_3$ (M+Na): 252.0786, found: 275.0677.

1-phenyl-2-(thiophen-2-yl)ethane-1,2-dione (2q)



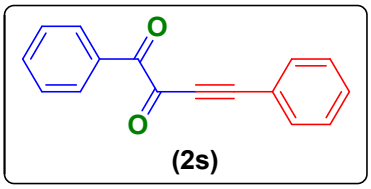
Yellow solid; **^{1}H NMR** (600 MHz, $CDCl_3$): δ 8.03 (d, *J*= 8.4 Hz, 2H), 7.80 (d *J*= 6.0 Hz, 1H), 7.78 (d, *J*= 4.2 Hz, 1H), 7.65-7.62 (m, 1H), 7.51-7.48 (m, 2H), 7.17-7.16 (m, 1H); **^{13}C NMR** (150 MHz, $CDCl_3$): δ 192.0, 185.5, 139.8, 136.8, 136.7, 134.8, 132.5, 130.2, 128.9 and 128.8; **ESI-MS** calcd for $C_{12}H_8O_2S$ (M+Na): 216.0245, found: 239.0142

1-(4-ethylphenyl)-2-phenylethane-1,2-dione (2r)



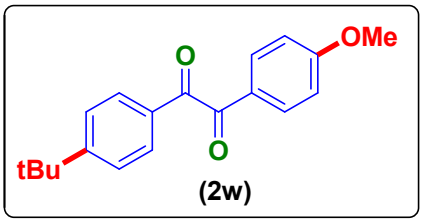
Yellow liquid; **^{1}H NMR** (600 MHz, $CDCl_3$): δ 7.95 (d, *J*= 6.0 Hz, 2H), 7.87 (t, *J*= 6.0 Hz, 2H), 7.63-7.60 (m, 1H), 7.49-7.46 (m, 2H), 7.31 (d, *J*= 6.0 Hz, 2H), 2.70 (q, 2H), 1.23 (t, *J*= 6.0 Hz, 3 H); **^{13}C NMR** (150 MHz, $CDCl_3$): δ 194.7, 194.2, 152.2, 134.7, 133.0, 130.6, 130.0, 129.8, 128.9, 128.5, 29.1 and 14.9; **ESI-MS** calcd for $C_{16}H_{14}O_2$ (M+Na): 238.0994, found: 261.0890.

1,4-diphenylbut-3-yne-1,2-dione (2s)



Yellow oil; **^{1}H NMR** (600 MHz, $CDCl_3$): δ 8.07-8.05 (m, 2H), 7.65-7.62 (m, 3 H), 7.52-7.48 (m, 3H), 7.40-7.37 (m, 2H); **^{13}C NMR** (150 MHz, $CDCl_3$): δ 188.4, 178.5, 134.8, 133.6, 131.6, 130.4, 128.9, 128.7, 119.1, 99.1, and 87.0; **ESI-MS** calcd for $C_{16}H_{10}O_2$ (M+Na): 234.0681, found: 257.0079

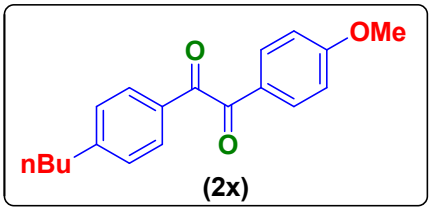
1-(4-tert-butylphenyl)-2-(4-methoxyphenyl)ethane-1,2-dione (2w)



(2w)

Semi solid; **^{1}H NMR** (600 MHz, $CDCl_3$): δ 7.92 (d, *J*= 9.0 Hz, 2H), 7.88 (d, *J*= 8.4 Hz, 2H), 7.49 (d, *J*= 8.4 Hz, 2H), 6.94 (d, *J*= 9.0 Hz, 2H), 3.85 (s, 3H), 1.31 (s, 9H); **^{13}C NMR** (150 MHz, $CDCl_3$): δ 194.5, 193.3, 164.8, 158.7, 132.3, 130.6, 129.8, 126.1, 125.9, 114.2, 55.6, 35.3 and 30.9; **ESI-MS** calcd for $C_{19}H_{20}O_3$ (M+Na): 296.1412, found: 319.1318

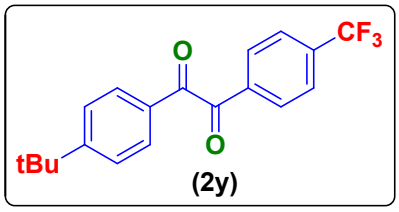
1-(4-butylphenyl)-2-(4-methoxyphenyl)ethane-1,2-dione (2x)



(2x)

White solid; **^{1}H NMR** (600 MHz, $CDCl_3$): δ 7.88 (d, *J*= 12.0 Hz, 2H), 7.81 (d, *J*= 6.0 Hz, 2H), 7.22 (d, *J*= 12.0 Hz, 2H), 6.90 (d, *J*= 12.0 Hz, 2H), 3.82 (s, 3H), 2.61 (t, *J*= 6.0 Hz, 2H), 1.57-1.52 (m, 2H); **^{13}C NMR** (150 MHz, $CDCl_3$): δ 194.6, 193.4, 164.8, 150.8, 132.3, 130.8. 130.0, 129.0, 126.1, 114.2, 55.6, 35.8, 33.1, 22.2 and 13.8; **ESI-MS** calcd for $C_{19}H_{20}O_3$ (M+H): 296.1412, found: 297.1490

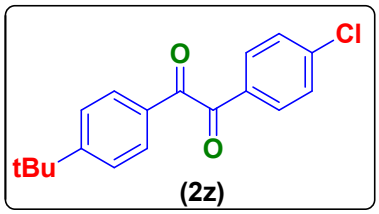
1-(4-tert-butylphenyl)-2-(4-(trifluoromethyl)phenyl)ethane-1,2-dione (2y)



(2y)

White solid; **^{1}H NMR** (600 MHz, $CDCl_3$): δ 8.07 (d, *J*= 6.0 Hz, 2H), 7.89 (d, *J*= 12.0 Hz, 2H), 7.74 (d, *J*= 6.0 Hz, 2H), 7.52 (d, *J*= 6.0 Hz, 2H); **^{13}C NMR** (150 MHz, $CDCl_3$): δ 193.2, 193.1, 159.4, 135.7 (t, $^2J_{C\text{-}F}$=19.3 Hz), 131.3, 131.2, 130.4, 130.1, 130.0, 129.9, 126.1, 125.9, 124.2 (q, $^1J_{C\text{-}F}$=272.2 Hz), 122.4, 35.4 and 30.9; **ESI-MS** calcd for $C_{19}H_{17}F_3O_2$ (M+Na): 334.1181, found: 357.1068

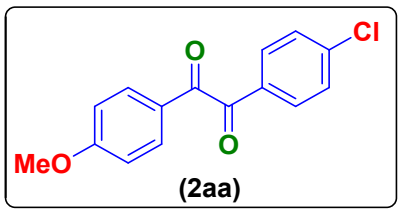
1-(4-tert-butylphenyl)-2-(4-chlorophenyl)ethane-1,2-dione (2z)



(2z)

Yellow solid; **^{1}H NMR** (600 MHz, $CDCl_3$): δ 7.91-7.88 (m, 4H), 7.51 (d, *J*= 6.0 Hz, 2H), 7.46 (d, *J*= 6.0 Hz, 2H), 1.32 (s, 9H); **^{13}C NMR** (150 MHz, $CDCl_3$): δ 193.5, 193.2, 159.2, 141.4, 131.4, 131.1, 130.2, 129.9, 129.3, 126.0, 35.3 and 30.9; **ESI-MS** calcd for $C_{18}H_{17}ClO_2$ (M+Na): 300.0917, found: 323.0805

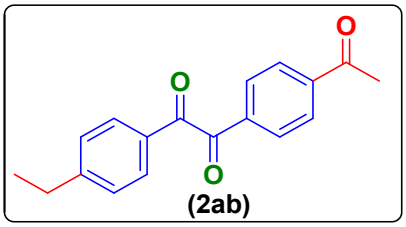
1-(4-chlorophenyl)-2-(4-methoxyphenyl)ethane-1,2-dione (2aa)[s9]



(2aa)

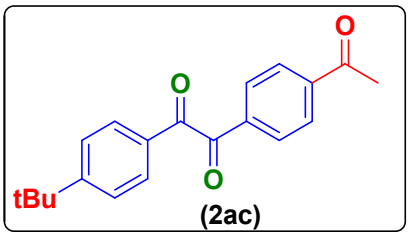
Yellow solid; **^{1}H NMR** (600 MHz, $CDCl_3$): δ 7.90 (t, *J*= 12.0 Hz, 4H), 7.45 (d, *J*= 6.0 Hz, 2H), 6.95 (d, *J*= 6.0 Hz, 2H), 3.87 (s, 3H); **^{13}C NMR** (150 MHz, $CDCl_3$): δ 193.3, 192.4, 165.1, 141.3, 132.4, 131.5, 131.2, 129.3, 125.8, 114.4 and 55.6; **ESI-MS** calcd for $C_{15}H_{11}ClO_3$ (M+Na): 274.0397, found: 297.0294

1-(4-acetylphenyl)-2-(4-ethylphenyl)ethane-1,2-dione (2ab)



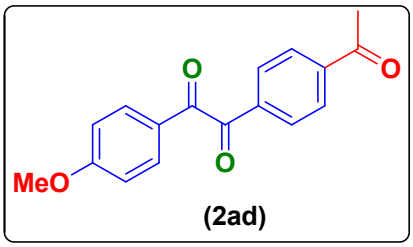
White solid; **^{1}H NMR** (600 MHz, $CDCl_3$): δ 8.03 (s, 4H), 7.86 (d, *J*= 6.0 Hz, 2H), 7.32 (d, *J*= 12.0 Hz, 2H), 2.71 (q, 2H), 2.62 (s, 3H), 1.24 (t, *J*= 6.0 Hz, 3H); **^{13}C NMR** (150 MHz, $CDCl_3$): δ 197.2, 193.7, 193.4, 152.6, 141.2, 136.1, 130.4, 130.1, 130.0, 128.6, 128.6, 29.1, 26.9 and 15.0; **ESI-MS** calcd for $C_{18}H_{16}O_3$ (M+Na): 280.1099, found: 303.0982

1-(4-acetylphenyl)-2-(4-tert-butylphenyl)ethane-1,2-dione (2ac)



White solid; **^{1}H NMR** (600 MHz, $CDCl_3$): δ 8.04 (s, 4H), 7.93 (d, *J*= 8.4 Hz, 2H), 7.52 (d, *J*= 9.0 Hz, 2H), 2.63 (s, 3H), 1.32 (s, 9H); **^{13}C NMR** (150 MHz, $CDCl_3$): δ 197.2, 193.8, 193.4, 159.3, 141.1, 136.0, 130.0, 129.9, 129.8, 128.6, 128.1, 126.1, 35.4, and 30.9; **ESI-MS** calcd for $C_{20}H_{20}O_3$ (M+Na): 308.1412, found: 331.1324

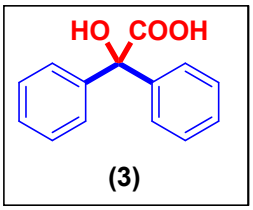
1-(4-acetylphenyl)-2-(4-methoxyphenyl)ethane-1,2-dione (2ad)



White solid; **^{1}H NMR** (600 MHz, $CDCl_3$): δ 8.02 (t, *J*= 6.0 Hz, 4H), 7.92 (d, *J*= 12.0 Hz, 2H), 6.95 (d, *J*= 6.0 Hz, 2H), 3.86 (s, 3H), 2.62 (s, 3H); **^{13}C NMR** (150 MHz, $CDCl_3$): δ 197.2, 193.8,

192.2, 165.2, 141.1, 136.2, 132.4, 130.0, 128.6, 125.7, 114.4, 55.6 and 26.9; **ESI-MS** calcd for $C_{17}H_{14}O_4$ (M+H): 282.0892, found: 283.0969

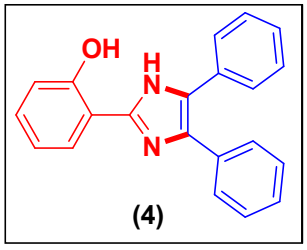
2-hydroxy-2,2-diphenylacetic acid (Benzillic acid) (3)



(3)

White solid; **^{1}H NMR** (600 MHz, $CDCl_3$): δ 7.33 (d, *J*= 12.0 Hz, 4H), 7.16-7.11 (m, 6H), 6.19 (s, 1H); **^{13}C NMR** (150 MHz, $CDCl_3$): δ 175.5, 142.2, 127.4, 127.2, 127.0 and 80.1; **ESI-MS** calcd for $C_{14}H_{12}O_3$ (M-H): 228.0786, found: 227.0707

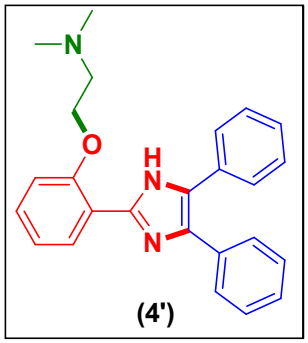
2-(4,5-diphenyl-1H-imidazol-2-yl)phenol (4)



(4)

Pale yellow solid; **^{1}H NMR** (600 MHz, $CDCl_3$): δ 7.83 (d, *J*= 6.0 Hz, 1H), 7.54 (d, *J*= 6.0 Hz, 4H), 7.31 (d, *J*= 12.0 Hz, 4H), 7.28 (d, *J*= 12.0 Hz, 2H), 7.19 (t, *J*= 6.0 Hz, 1H), 7.00 (d, *J*= 6.0 Hz, 1H), 6.84 (t, *J*= 6.0 Hz, 1H); **^{13}C NMR** (150 MHz, $CDCl_3$): δ 157.0, 146.0, 132.5, 132.1, 129.7, 128.3, 127.8, 127.3, 124.2, 118.7, 117.0 and 113.0; **ESI-MS** calcd for $C_{21}H_{16}N_2O$ (M+H): 312.1263, found: 313.1352

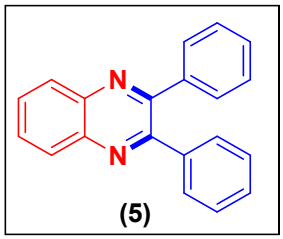
2-(2-(4,5-diphenyl-1H-imidazol-2-yl)phenoxy)-N,N-dimethylethanamine (4')



(4')

Pale yellow liquid; **^{1}H NMR** (600 MHz, $CDCl_3$): δ 12.33 (s, 1H), 8.46 (d, *J*= 6.0 Hz, 1H), 7.60-7.25 (m, 12H), 7.10 (t, *J*= 6.0 Hz, 1H), 6.98 (d, *J*= 6.0 Hz, 1H), 4.18 (t, *J*= 6.0 Hz, 2H), 2.63 (t, *J*= 6.0 Hz, 2H), 1.94 (s, 6H); **^{13}C NMR** (150 MHz, $CDCl_3$): δ 154.9, 143.6, 128.9, 128.7, 128.2, 127.4, 126.4, 122.0, 120.2, 113.5, 65.5, 57.9 and 44.3; **ESI-MS** calcd for $C_{25}H_{25}N_3O$ (M+H): 383.1998, found: 384.2083

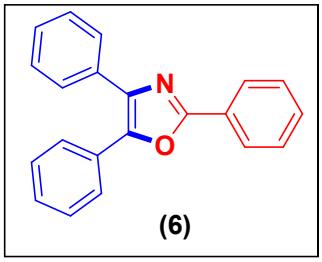
2,3-diphenylquinoxaline (5)



(5)

Yellow solid; **^{1}H NMR** (600 MHz, $CDCl_3$): δ 8.17 (t, *J*= 6.0 Hz, 2H), 7.71 (d, *J*= 6.0 Hz, 2H), 7.53 (d, *J*= 6.0 Hz, 4H), 7.34-7.30 (m, 6H); **^{13}C NMR** (150 MHz, $CDCl_3$): δ 152.9, 140.8, 138.7, 129.5, 128.7, 128.4 and 127.8; **ESI-MS** calcd for $C_{20}H_{14}N_2$ (M+H): 282.1157, found: 283.1238

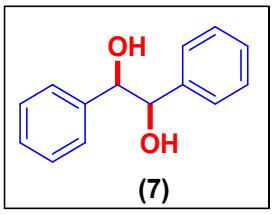
2,4,5-triphenyloxazole (6)



(6)

Pale yellow solid; **^{1}H NMR** (600 MHz, $CDCl_3$): δ 8.18 (d, *J*= 6.0 Hz, 2H), 7.74 (d, *J*= 6.0 Hz, 2H), 7.68 (d, *J*= 6.0 Hz, 2H), 7.48-7.46 (m, 3H), 7.43-7.34 (m, 6H); **^{13}C NMR** (150 MHz, $CDCl_3$): δ 160.0, 145.4, 136.6, 134.8, 132.5, 130.2, 129.8, 128.7, 128.6, 128.5, 128.0, 126.4 and 126.3; **ESI-MS** calcd for $C_{21}H_{15}NO$ (M+H): 297.1154, found: 298.1229

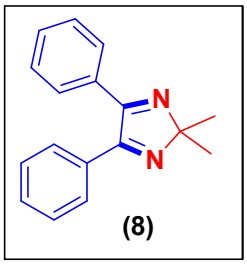
(1R,2R)-1,2-diphenylethane-1,2-diol (7)



(7)

White solid; **^{1}H NMR** (600 MHz, $CDCl_3$): δ 7.03-7.02 (m, 6H), 6.98 (dd, *J*= 6.0 Hz, 4H), 4.64 (s, 2H), 4.07 (s, 2H); **^{13}C NMR** (150 MHz, $CDCl_3$): δ 140.4, 127.1, 126.7 and 77.1; **ESI-MS** calcd for $C_{14}H_{14}O_2$ (M+Na): 214.0994, found: 237.0884

2,2-dimethyl-4,5-diphenyl-2H-imidazole (8)



(8)

White solid; **^{1}H NMR** (600 MHz, $CDCl_3$): δ 7.43 (t, *J*= 6.0 Hz, 4H), 7.33-7.30 (m, 2H), 7.25 (t, *J*= 6.0 Hz, 4H), 1.58 (s, 6H); **^{13}C NMR** (150 MHz, $CDCl_3$): δ 163.8, 132.3, 129.8, 128.5, 127.9, 101.2 and 23.8; **ESI-MS** calcd for $C_{17}H_{16}N_2$ (M+H): 248.1313, found: 249.1389

References:

S1. A. Sagadevan and K. C. Hwang, *Adv. Synth. Catal.,* 2012, 354, 3421.

S2. A. Acharjee, A. Ghoshal and S. K. Ghosh, *World Journal of pharmacy and Pharmaceutical Sciences*, 2015, **6**, 1741.

S3. (a) L. Nagarapu, A. A. Satyender, G. Chandana and R. Bantu, *J. Heterocyclic. Chem*., 2009, **46**, 195; (b) S. Elumalai, D. Somasundaran and S. Guhanathan, *Der. Chemica Sinica*, 2014, **5**, 60.

S4. G. N. Raju, K. B. Sai, R. T. Myneni, N. Navya, R. S. Yasaswini and R. R. Nadendla, *World Journal of Pharmaceutical Research*, 2015, **5**, 2625.

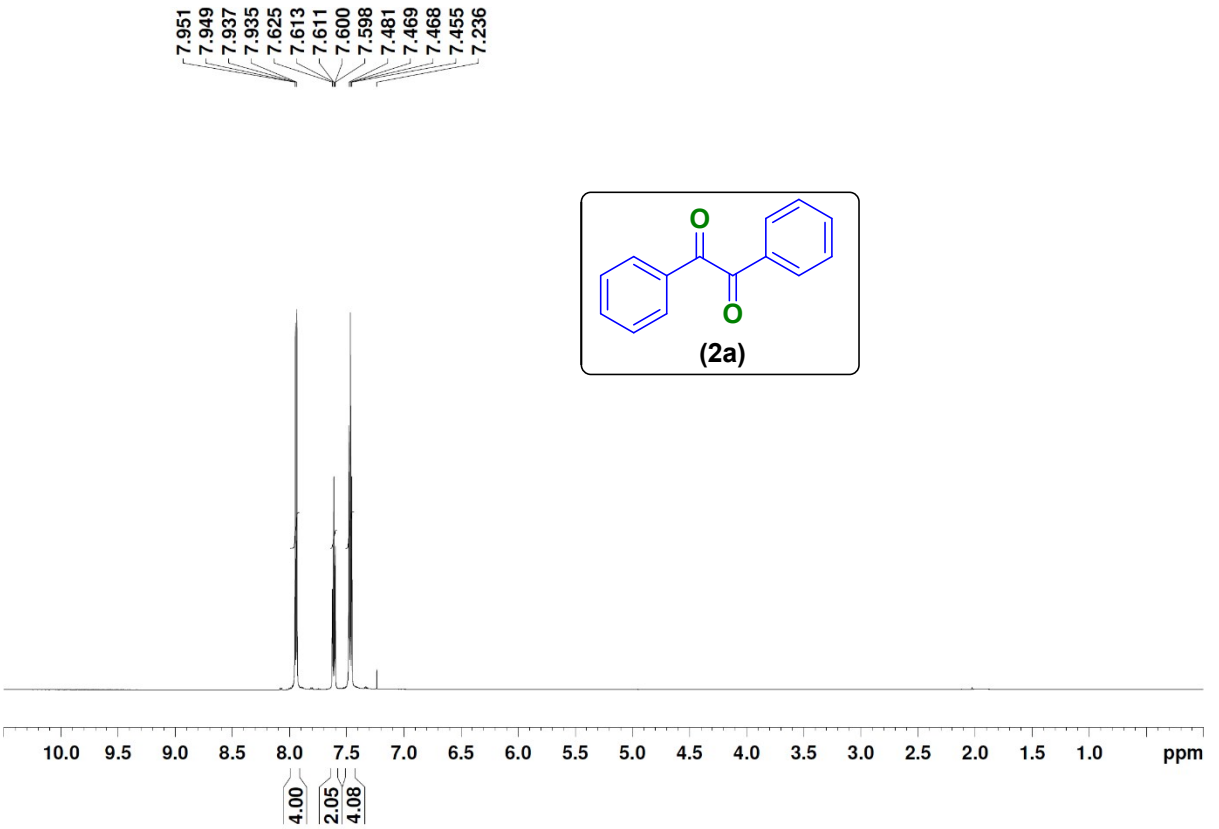
S5. X. Zhu, P. Li, Q. Shi and L. Wang, *Green Chem*, 2016, **18,** 6373**.**

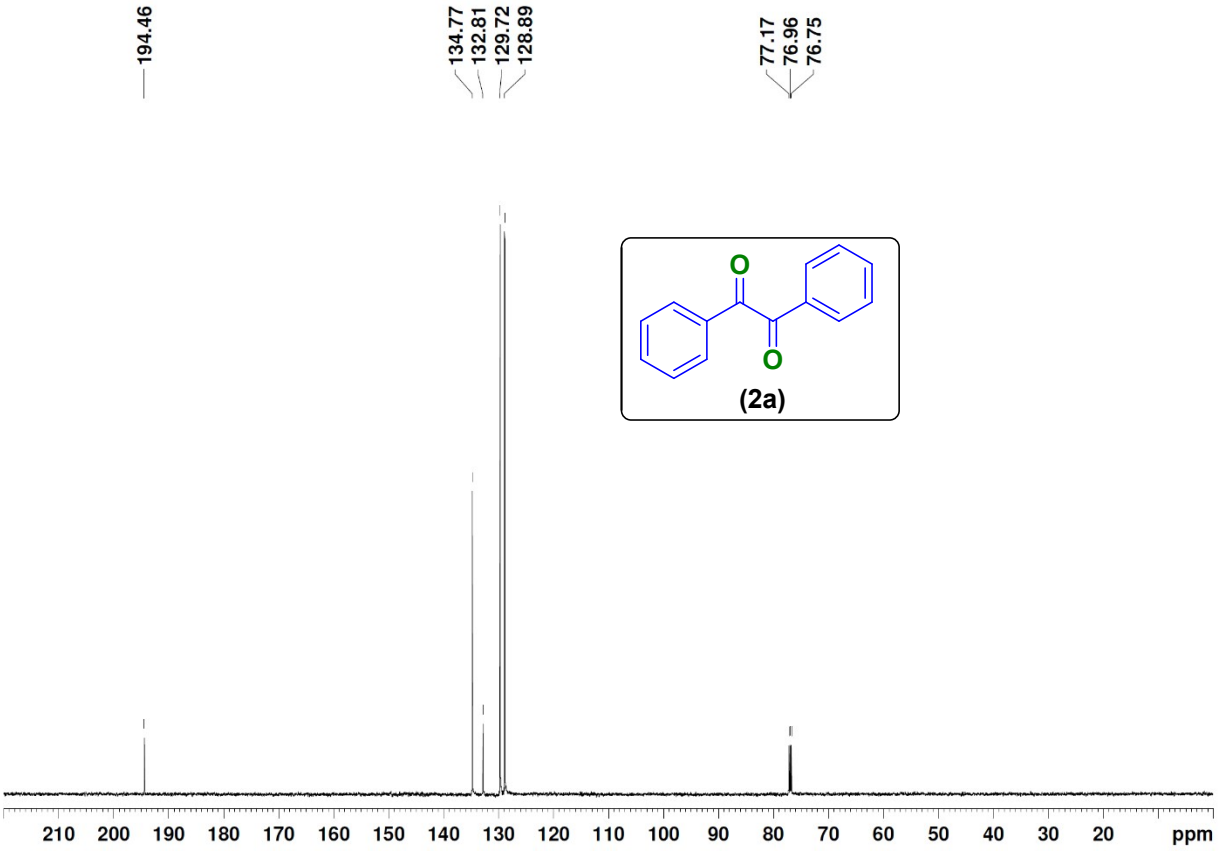
S6. J. W. Xue, M. Zeng, X. Hou, Z. Chen and G. Yin, *Asian J. Org. Chem*., 2018, **7**, 212.

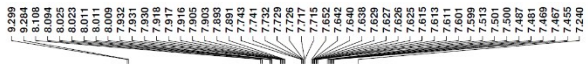
S7. X. Liu, T. Cong, P. Liu and P. Sun, *J. Org. Chem.,* 2016, **81**, 7256.

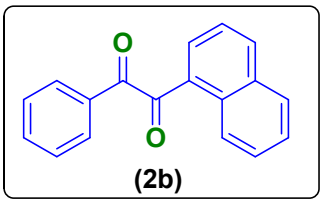
S8. T. Nobuta, N. Tada, K. Hattori, S. I. Hirashima, T. Miura and A. Itoh, *Tetrahedron Lett*., 2011, **52**, 875.

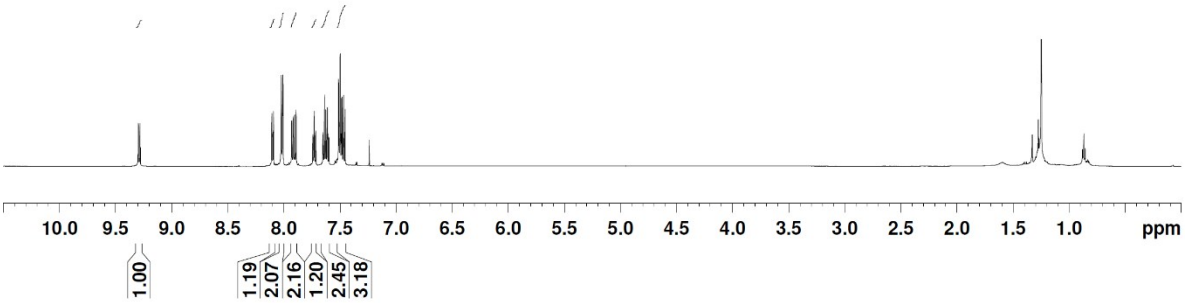
S9. X. F. Xia, Z. Gu, W. Liu, N. Wang, H. Wang, Y. Xia, H. Gao and X. Liu, *Org. Biomol. Chem*., 2014, **12**, 9909.


7.951
7.949
7.937
7.935
7.625
7.613
7.611
7.600
7.598
7.481
7.469
7.468
7.455
7.236
O
O
(2a)
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 ppm
4.00
2.05
4.08


194.46
134.77
132.81
129.72
128.89
77.17
76.96
76.75
O
O
(2a)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm




O
O
(2b)


10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 ppm
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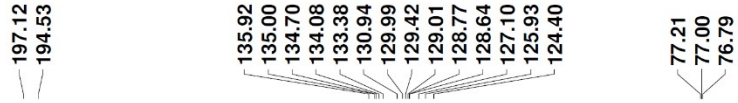
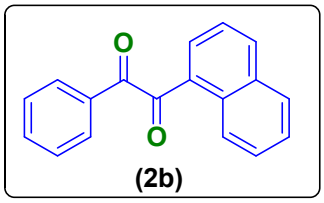
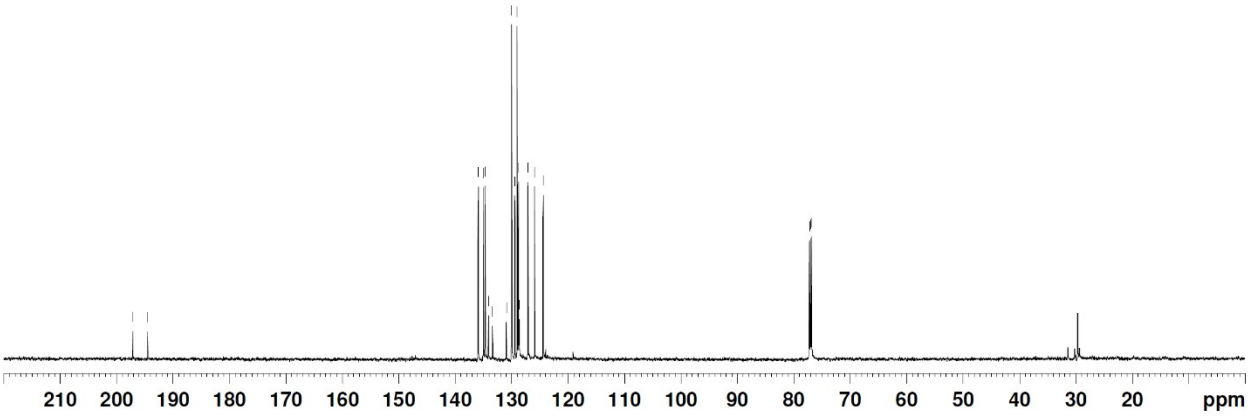
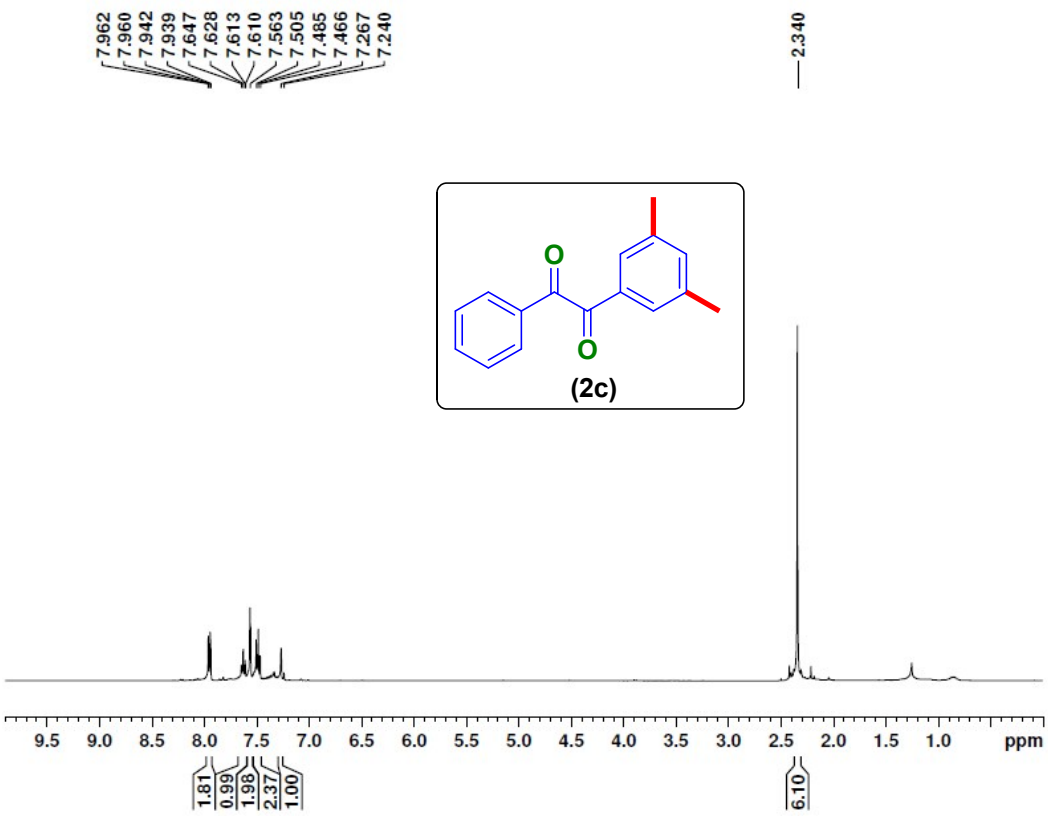
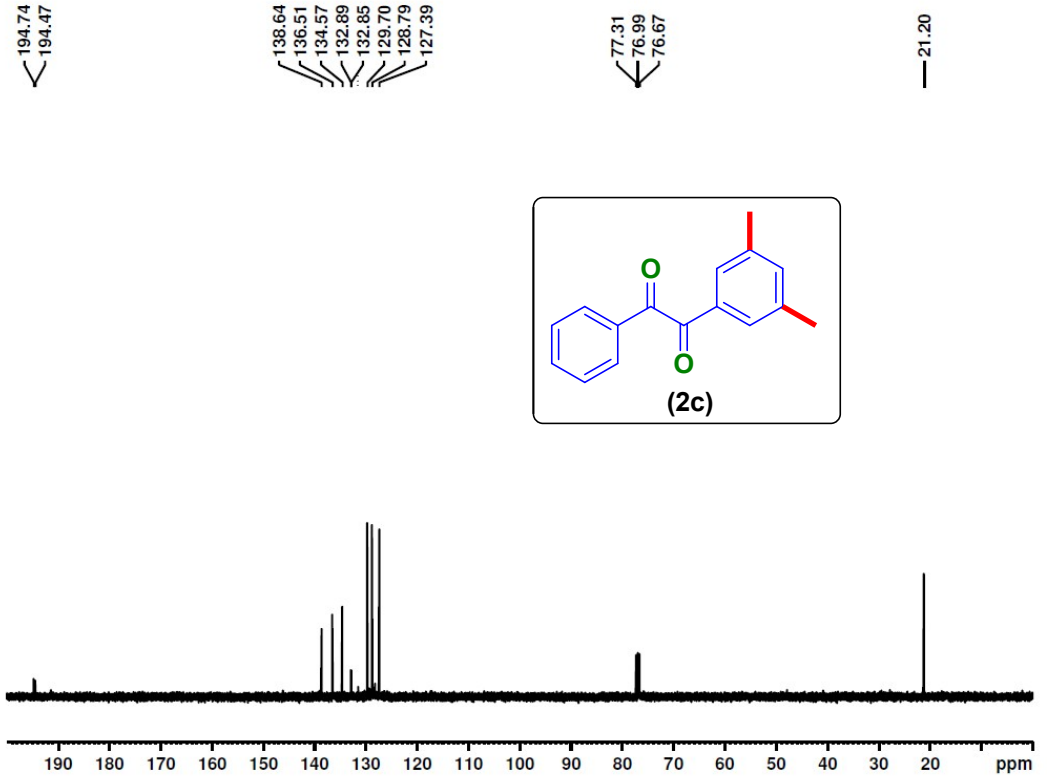
1.19
2.07
2.16
1.20
2.45
3.18

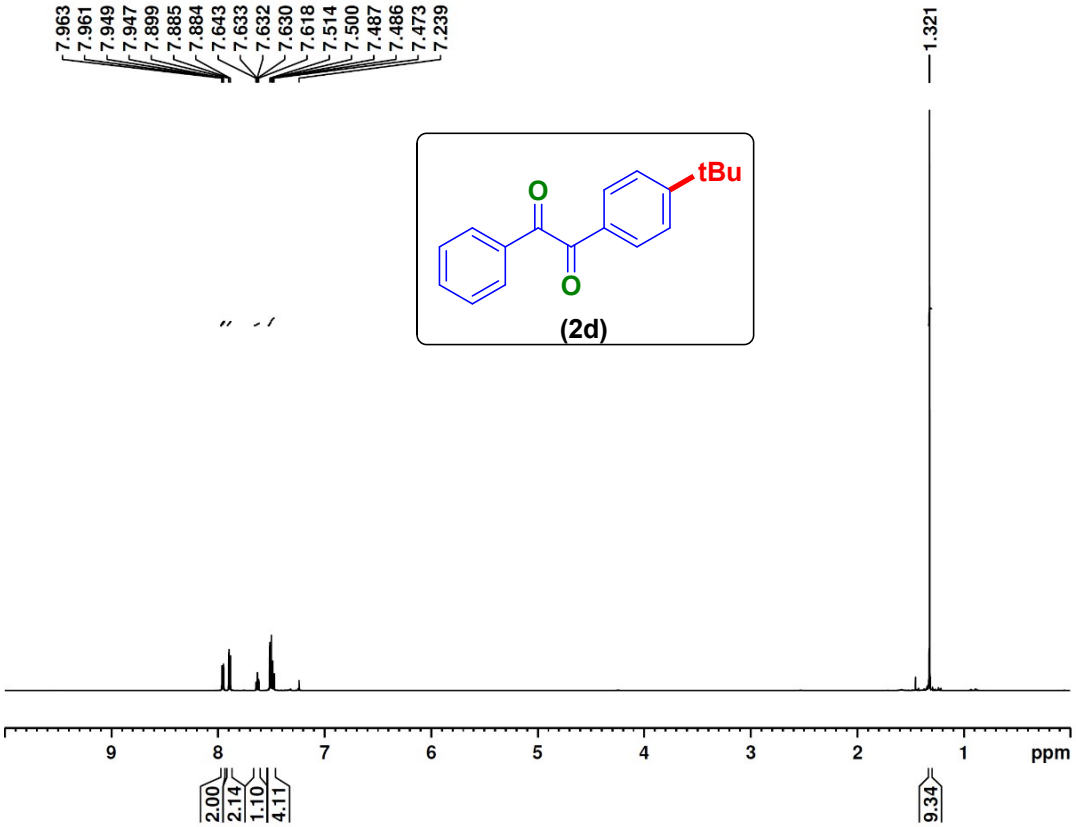

197.12
194.53
135.92
135.00
134.70
134.08
133.38
130.94
129.99
129.42
129.01
128.77
128.64
127.10
125.93
124.40
77.21
77.00
76.79


O
O
(2b)


210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm


7.962
7.960
7.942
7.939
7.647
7.628
7.613
7.610
7.563
7.505
7.485
7.466
7.267
7.240
2.340
O
O
(2c)
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 ppm
1.81
0.99
1.98
2.37
1.00
6.10


194.74
194.47
138.64
136.51
134.57
132.89
132.85
129.70
128.79
127.39
77.31
76.99
76.67
21.20
O
O
(2c)
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm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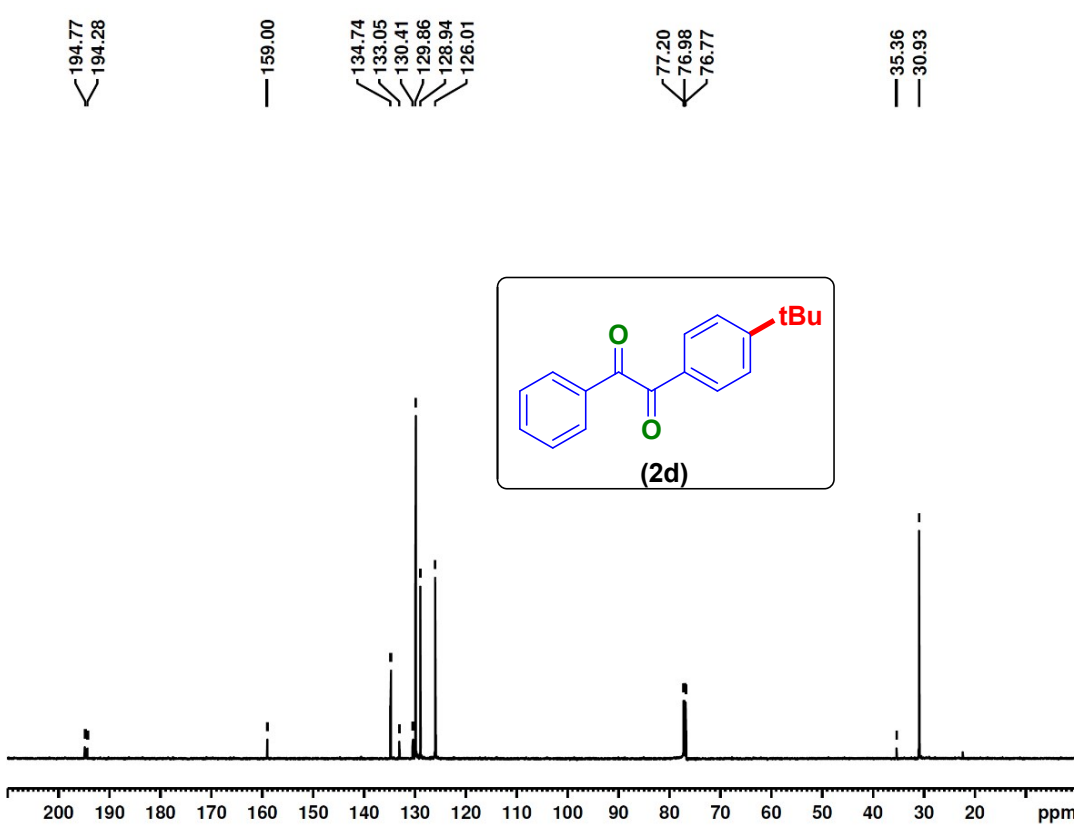
7.961
7.949
7.947
7.899
7.885
7.884
7.643
7.633
7.632
7.630
7.618
7.514
7.500
7.487
7.486
7.473
7.239
1.321
tBu
O
O
(2d)
9
8
7
6
5
4
3
2
1
ppm
2.00
2.14
1.10
4.11
9.34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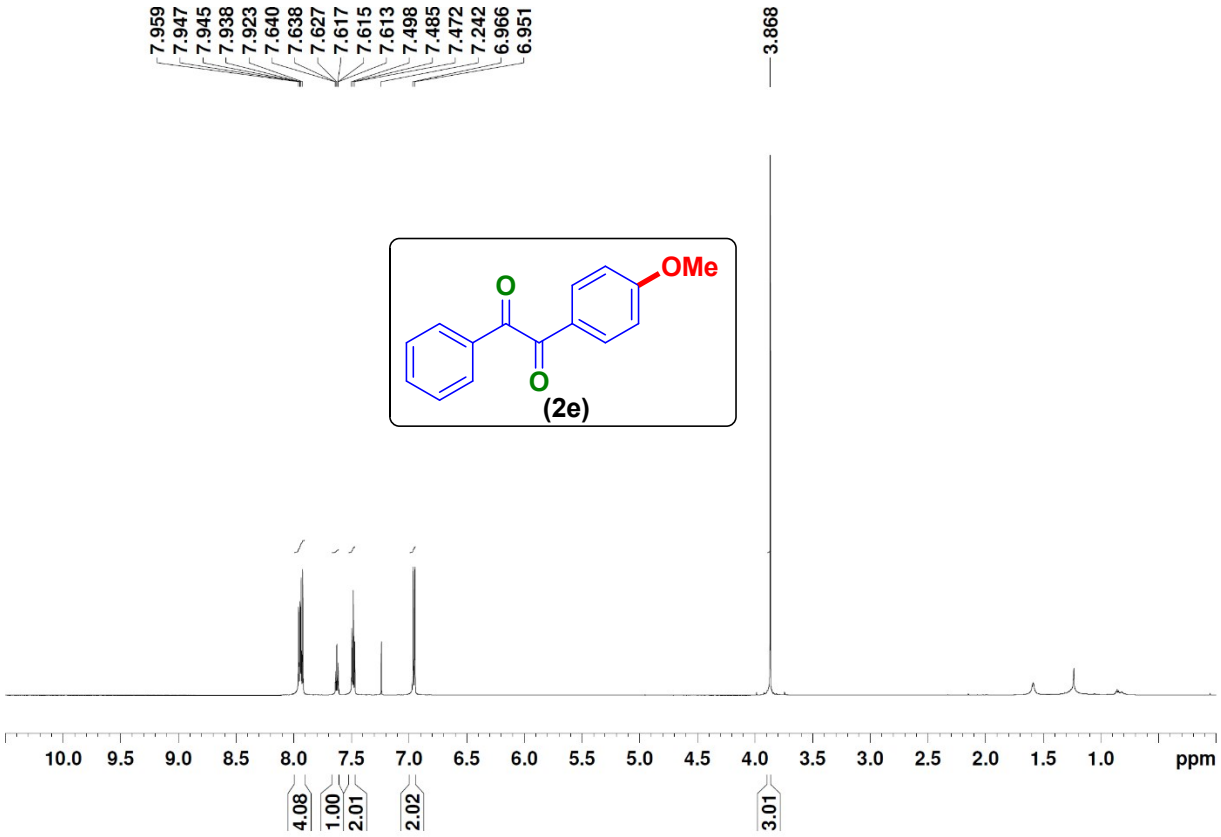
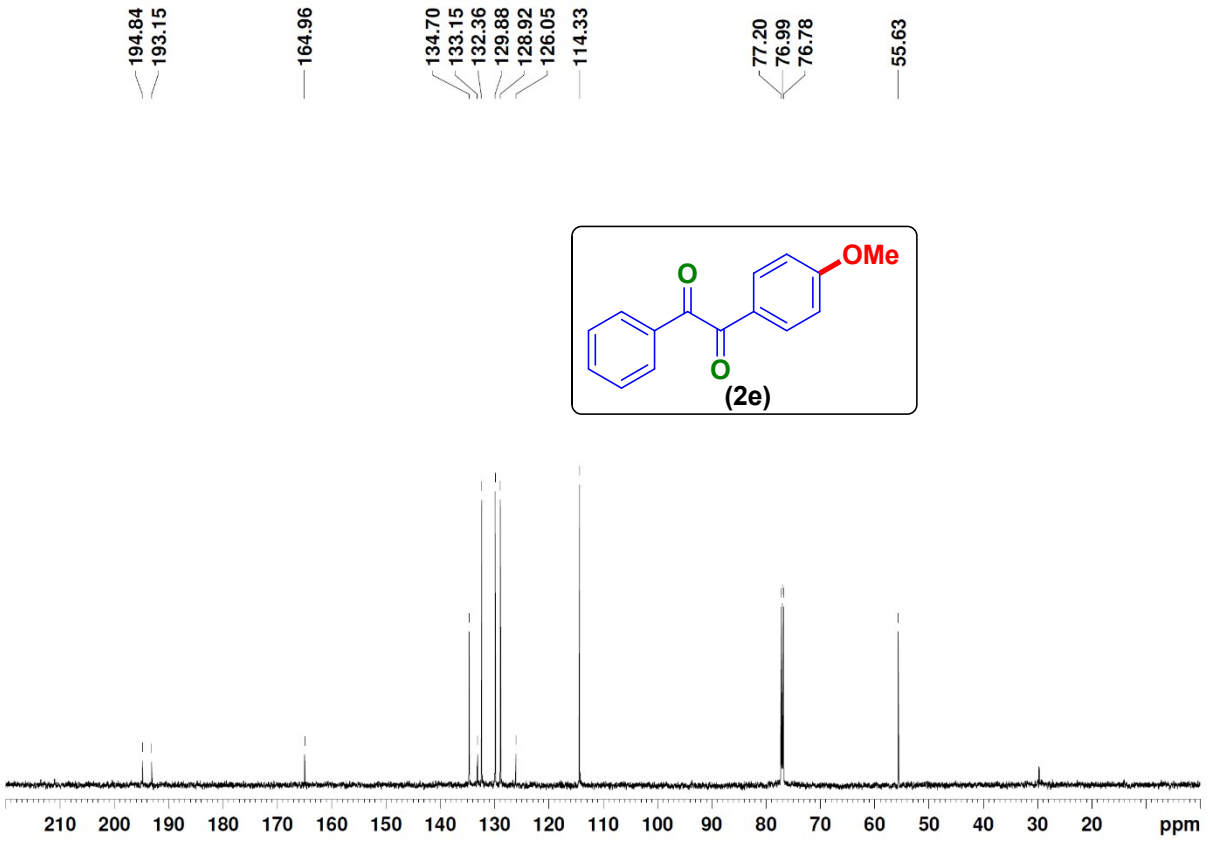
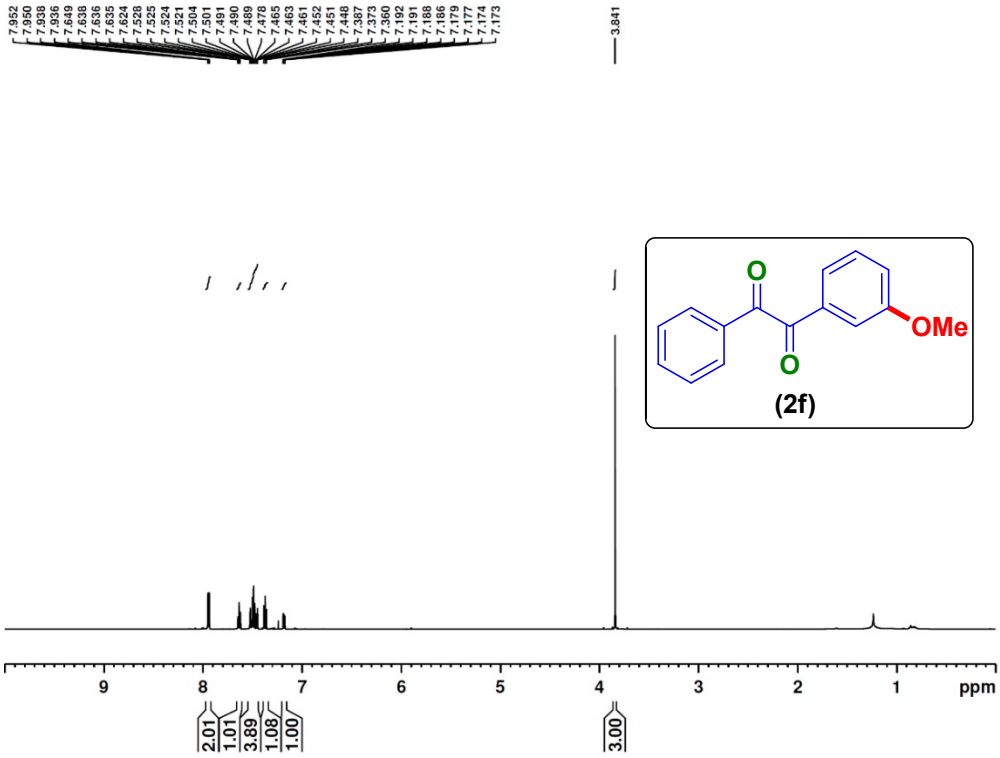
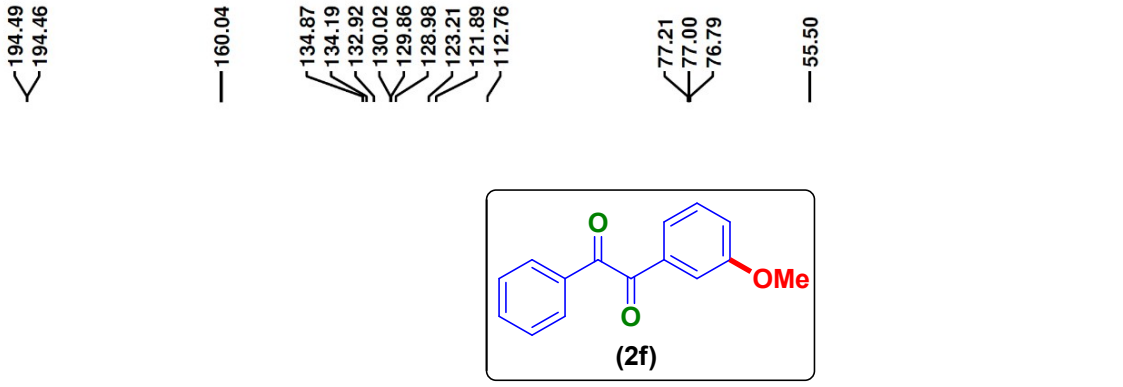
194.28
159.00
134.74
133.05
130.41
129.86
128.94
126.01
77.20
76.98
76.77
35.36
30.93
tBu
O
O
(2d)
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm


7.959
7.947
7.945
7.938
7.923
7.640
7.638
7.627
7.617
7.615
7.613
7.498
7.485
7.472
7.242
6.966
6.951
3.868
OMe
O
O
(2e)
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 ppm
4.08
1.00
2.01
2.02
3.01


194.84
193.15
164.96
134.70
133.15
132.36
129.88
128.92
126.05
114.33
77.20
76.99
76.78
55.63
OMe
O
O
(2e)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm


7.952
7.950
7.938
7.936
7.649
7.638
7.636
7.635
7.624
7.528
7.525
7.524
7.521
7.504
7.501
7.491
7.490
7.489
7.478
7.465
7.463
7.461
7.452
7.451
7.448
7.397
7.373
7.360
7.192
7.191
7.188
7.186
7.179
7.177
7.174
7.173
3.841
OMe
O
O
(2f)
9
8
7
6
5
4
3
2
1
ppm
2.01
1.01
3.89
1.08
1.00
3.00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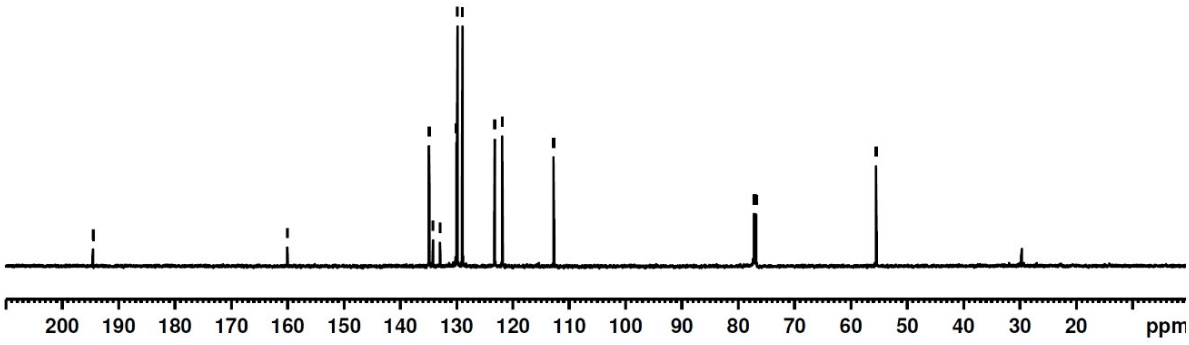
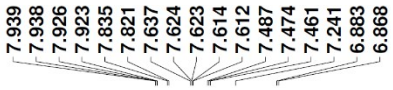
194.46
160.04
134.87
134.19
132.92
130.02
129.86
128.98
123.21
121.89
112.76
77.21
77.00
76.79
55.50
OMe
O
O
(2f)


200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm


7.939
7.938
7.926
7.923
7.835
7.821
7.637
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7.623
7.614
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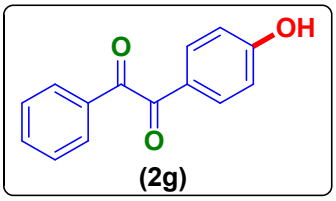
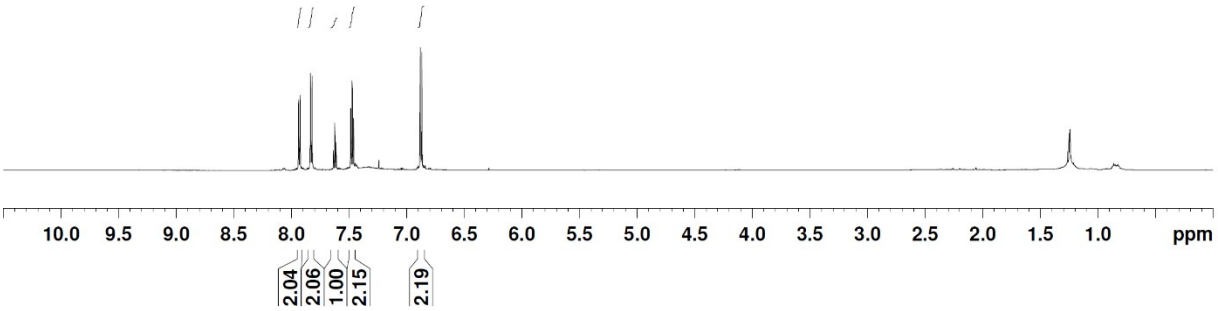
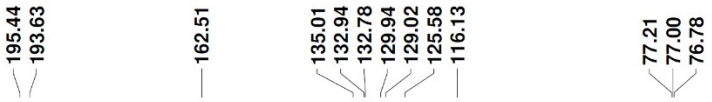
7.474
7.461
7.241
6.883
6.868


OH
O
O
(2g)


10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
ppm
2.04
2.06
1.00
2.15
2.19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132.94
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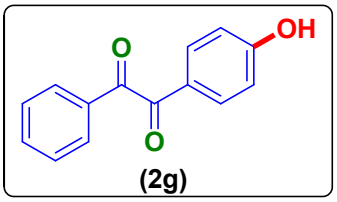
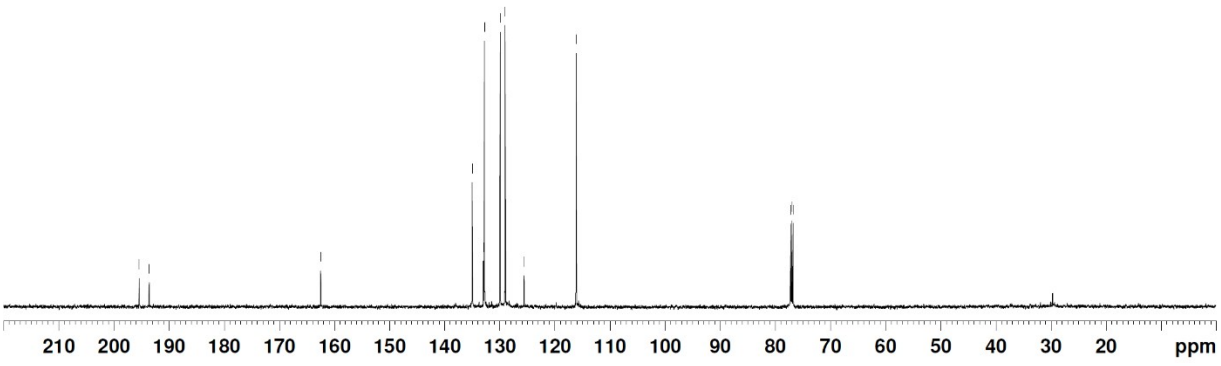
129.94
129.02
125.58
116.13
77.21
77.00
76.78


OH
O
O
(2g)


210
200
190
180
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160
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140
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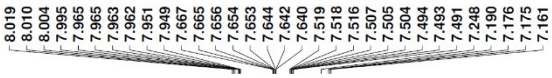
120
110
100
90
80
70
60
50
40
30
20
ppm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8.010
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7.995
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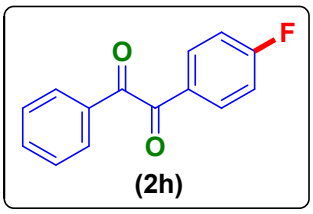
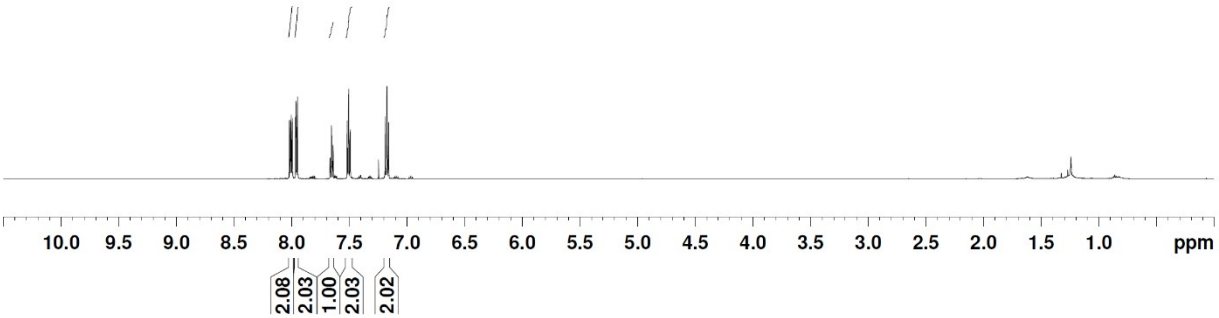
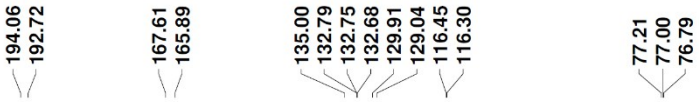
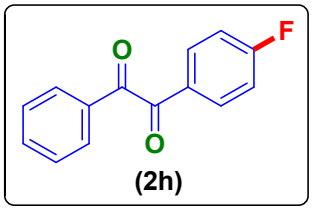
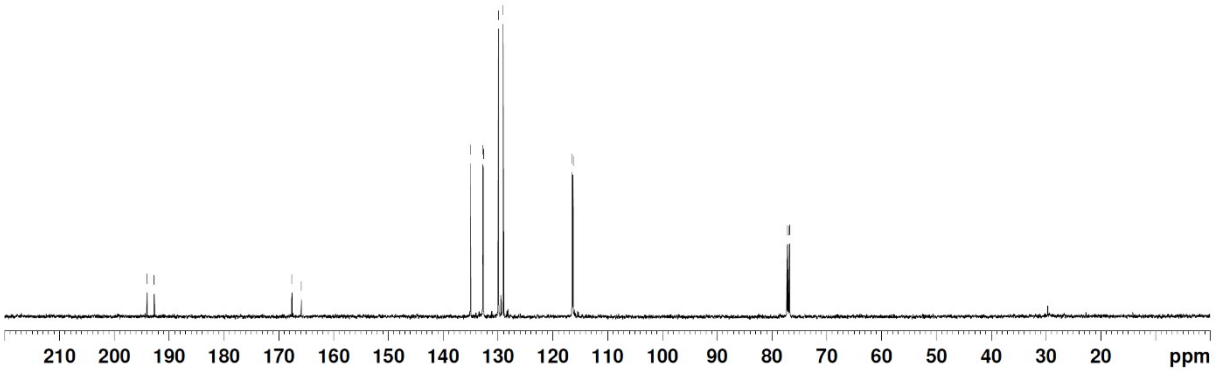
7.965
7.963
7.962
7.951
7.949
7.667
7.665
7.656
7.654
7.653
7.644
7.642
7.640
7.519
7.518
7.516
7.507
7.505
7.504
7.494
7.493
7.491
7.248
7.190
7.176
7.175
7.161

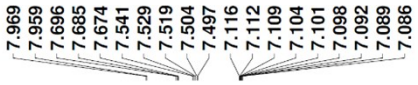

O
F
O
(2h)

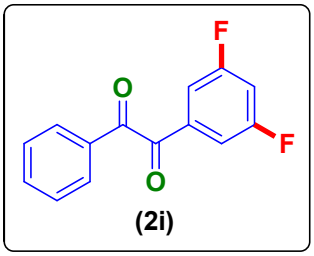

10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 ppm
2.08
2.03
1.00
2.03
2.02

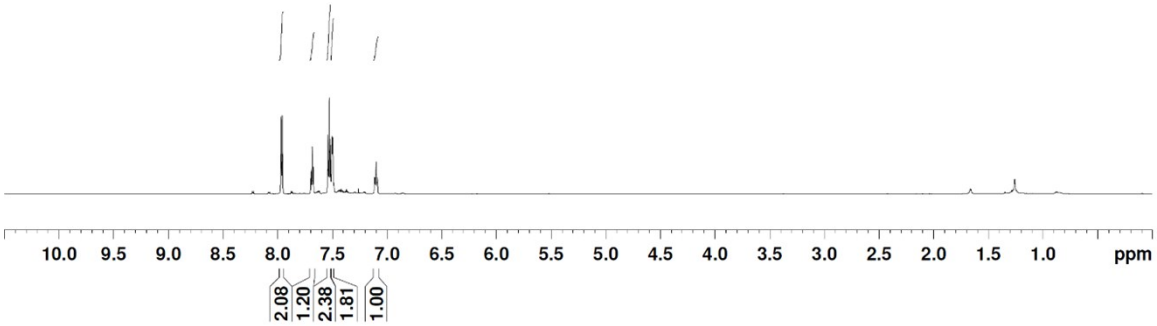

194.06
192.72
167.61
165.89
135.00
132.79
132.75
132.68
129.91
129.04
116.45
116.30
77.21
77.00
76.79

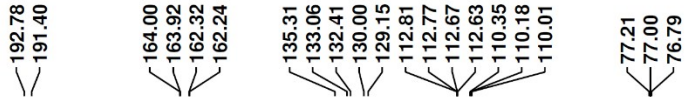

O
F
O
(2h)

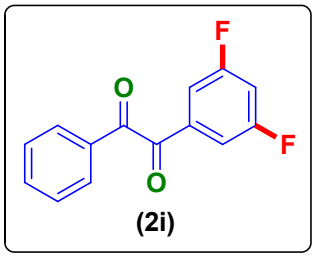

210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

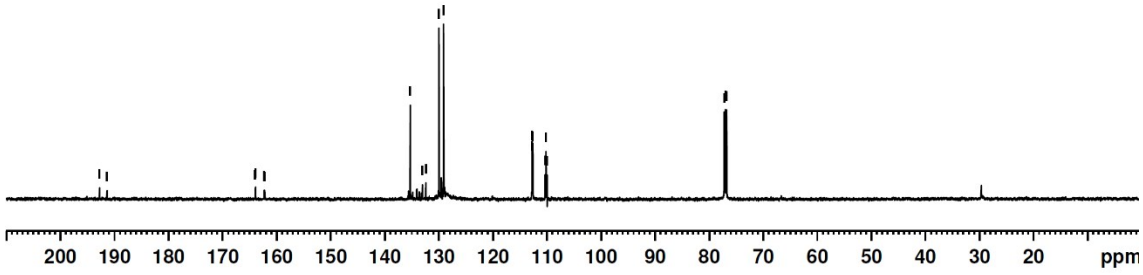

7.969
7.959
7.696
7.685
7.674
7.541
7.529
7.519
7.504
7.497
7.116
7.112
7.109
7.104
7.101
7.098
7.092
7.089
7.086

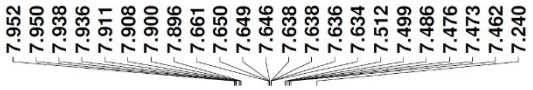

F
O
F
O
(2i)

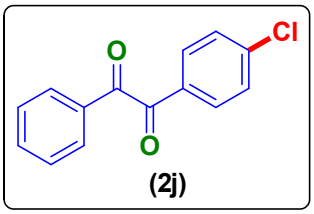

10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 ppm
2.08
1.20
2.38
1.81
1.00

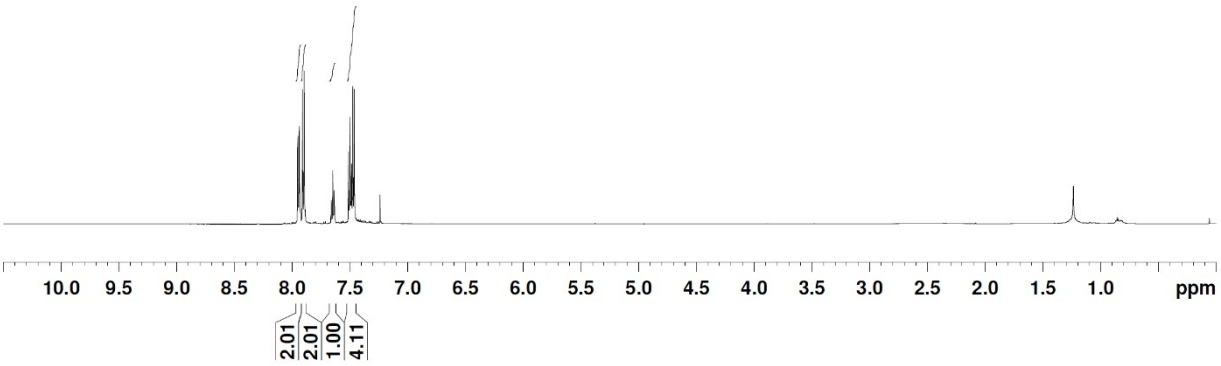

192.78
191.40
164.00
163.92
162.32
162.24
135.31
133.06
132.41
130.00
129.15
112.81
112.77
112.67
112.63
110.35
110.18
110.01
77.21
77.00
76.79

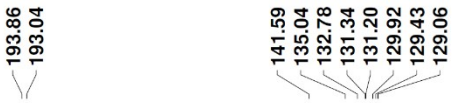

F
O
F
O
(2i)

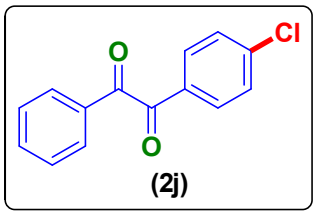

200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

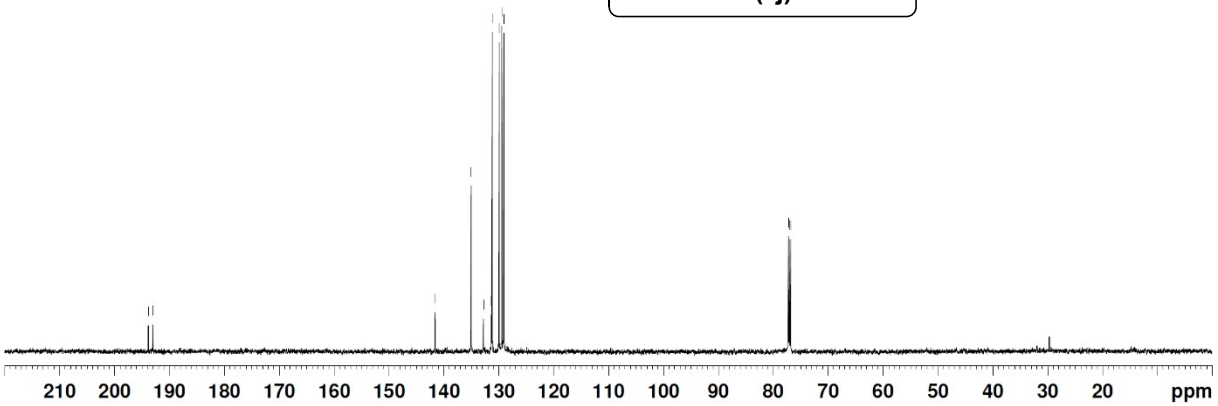

7.952
7.950
7.938
7.936
7.911
7.908
7.900
7.896
7.661
7.650
7.649
7.646
7.638
7.638
7.636
7.634
7.512
7.499
7.486
7.476
7.473
7.462
7.240

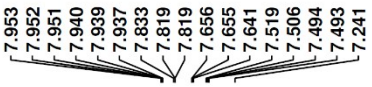

O
Cl
O
(2j)

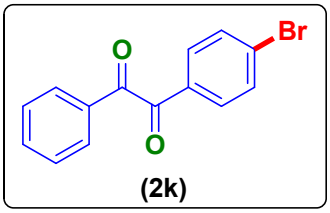

10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 ppm
2.01
2.01
1.00
4.11

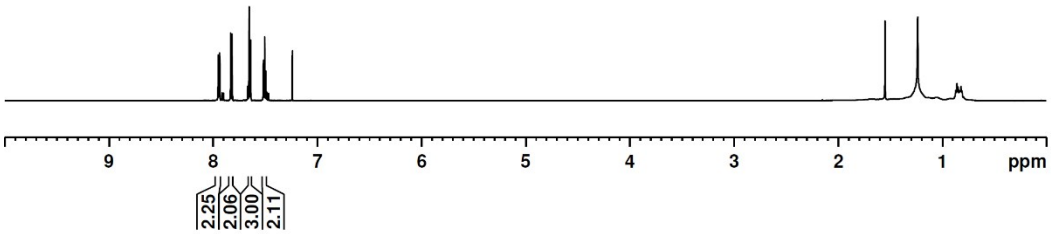

193.86
193.04
141.59
135.04
132.78
131.34
131.20
129.92
129.43
129.06
77.22
77.00
76.79

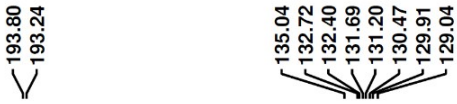

O
Cl
O
(2j)

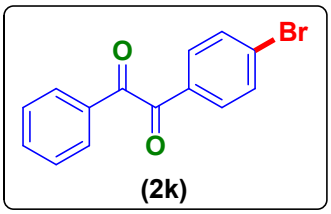

210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

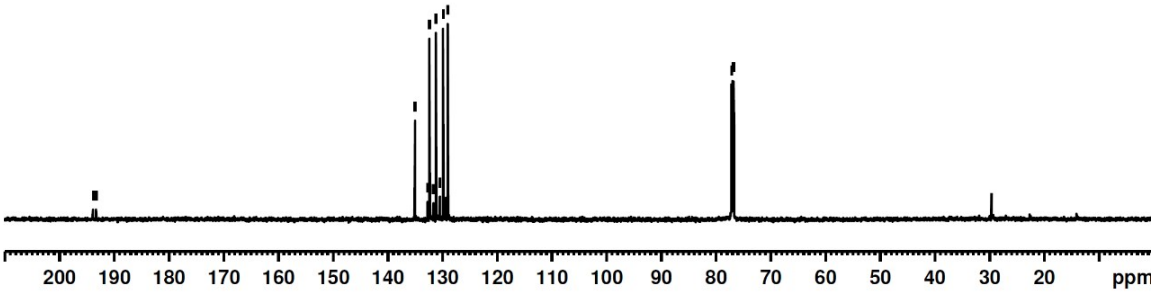

7.953
7.952
7.951
7.940
7.939
7.937
7.833
7.819
7.819
7.656
7.655
7.641
7.519
7.506
7.494
7.493
7.241

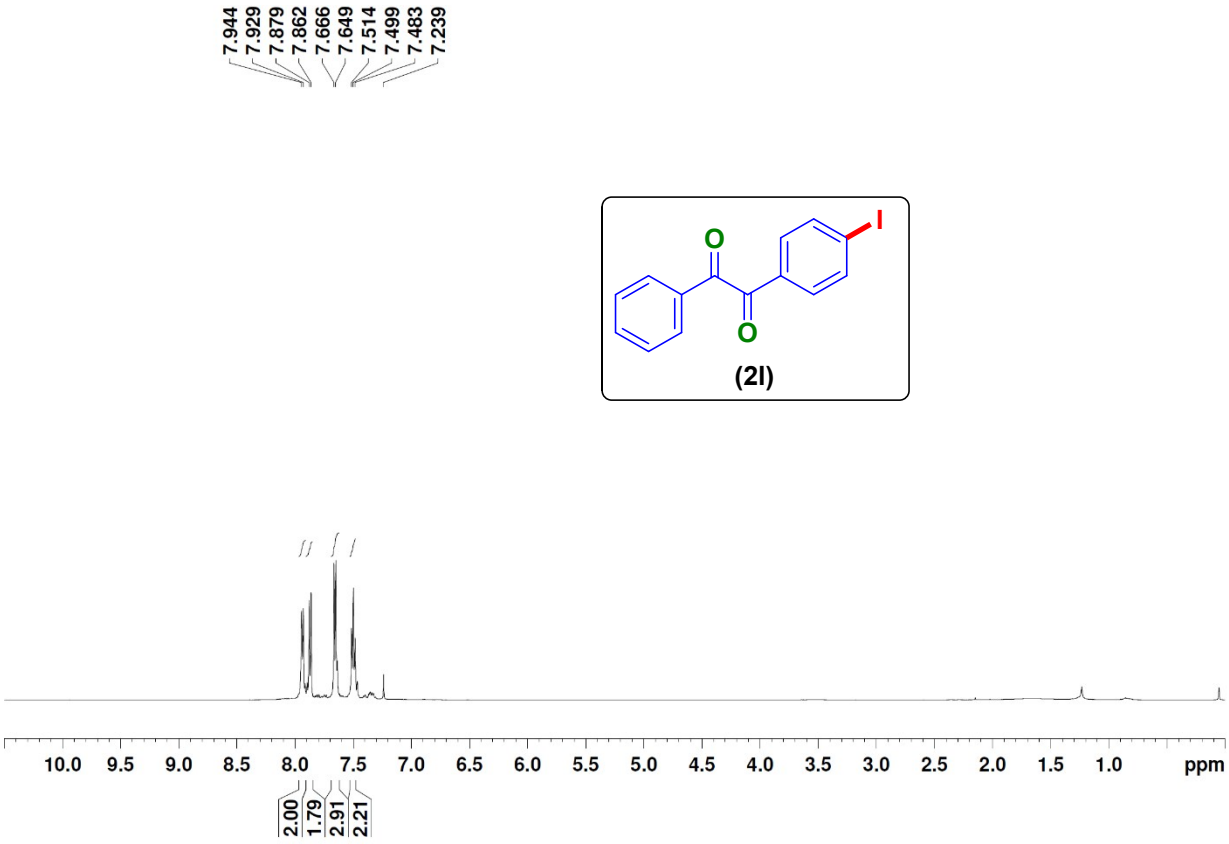

O
Br
O
(2k)

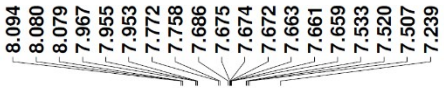

9
8
7
6
5
4
3
2
1
ppm
2.25
2.06
3.00
2.11

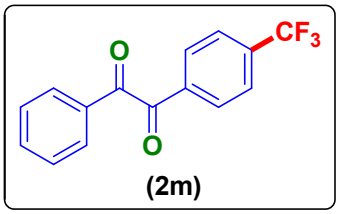

193.80
193.24
135.04
132.72
132.40
131.69
131.20
130.47
129.91
129.04
77.18
76.96
76.75


O
Br
O
(2k)

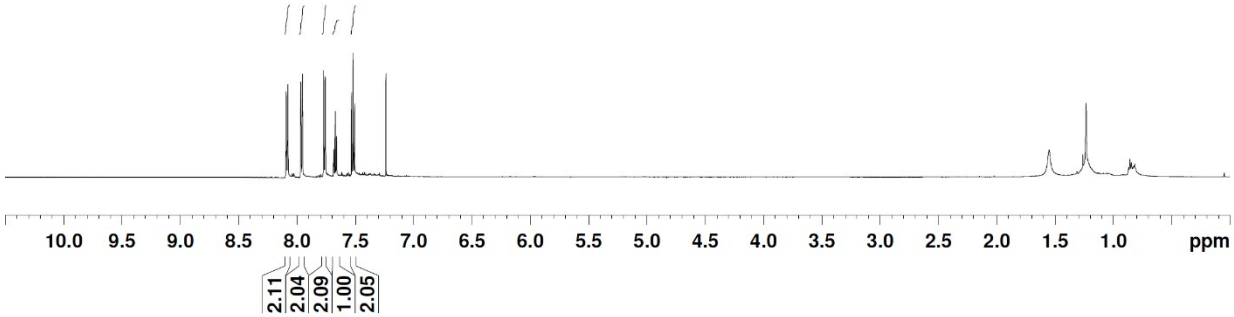

200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

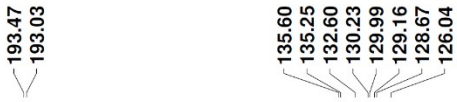

7.944
7.929
7.879
7.862
7.666
7.649
7.514
7.499
7.483
7.239
O
O
I
(2l)
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 ppm
2.00
1.79
2.91
2.21
193.83
193.63
138.39
135.06
132.72
132.20
130.96
129.92
129.06
103.65
O
O
I
(2l)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

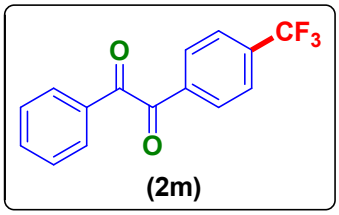

8.094
8.080
8.079
7.967
7.955
7.953
7.772
7.758
7.686
7.675
7.674
7.672
7.663
7.661
7.659
7.533
7.520
7.507
7.239


O
O
CF3

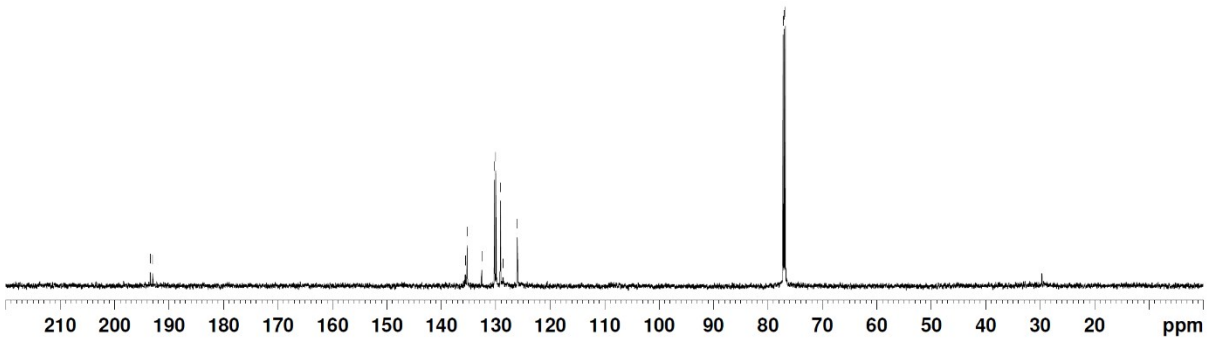
(2m)

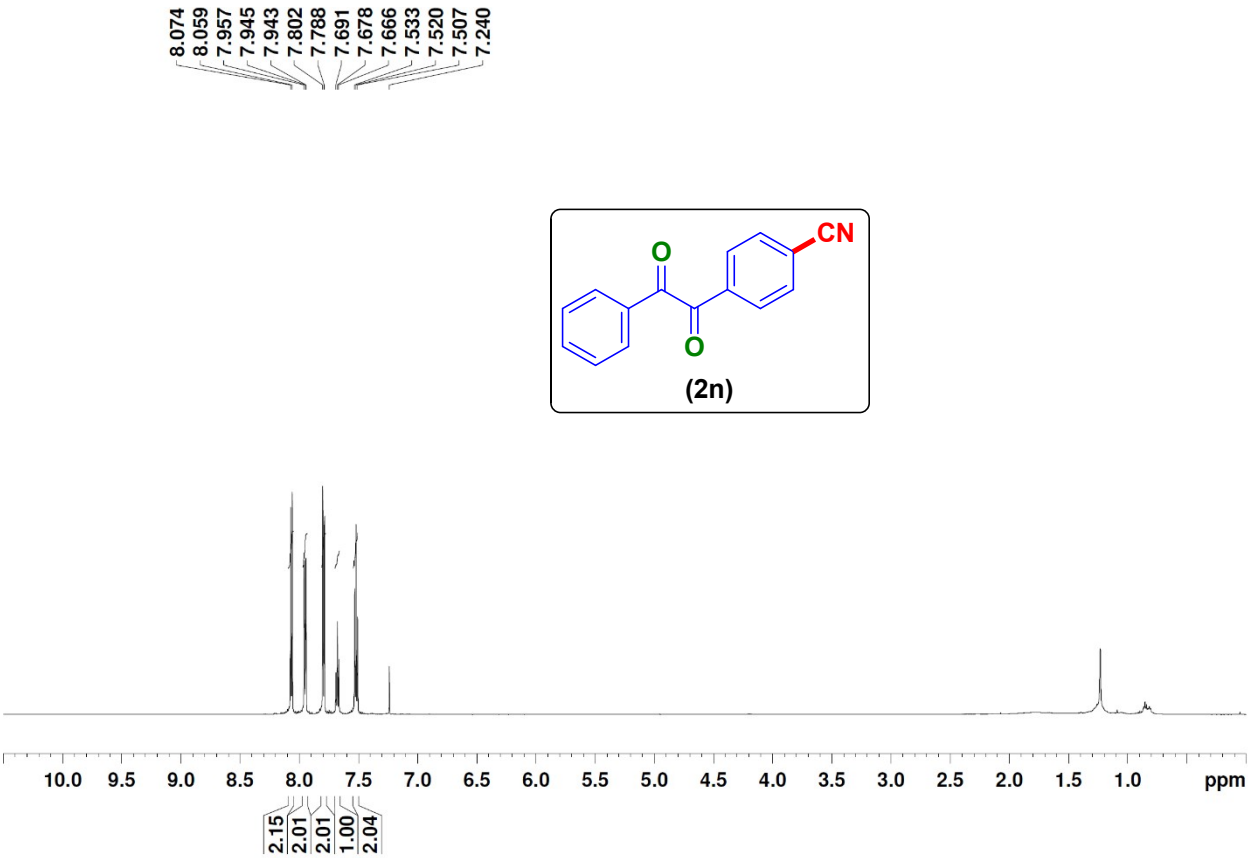

10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 ppm
2.11
2.04
2.09
1.00
2.05

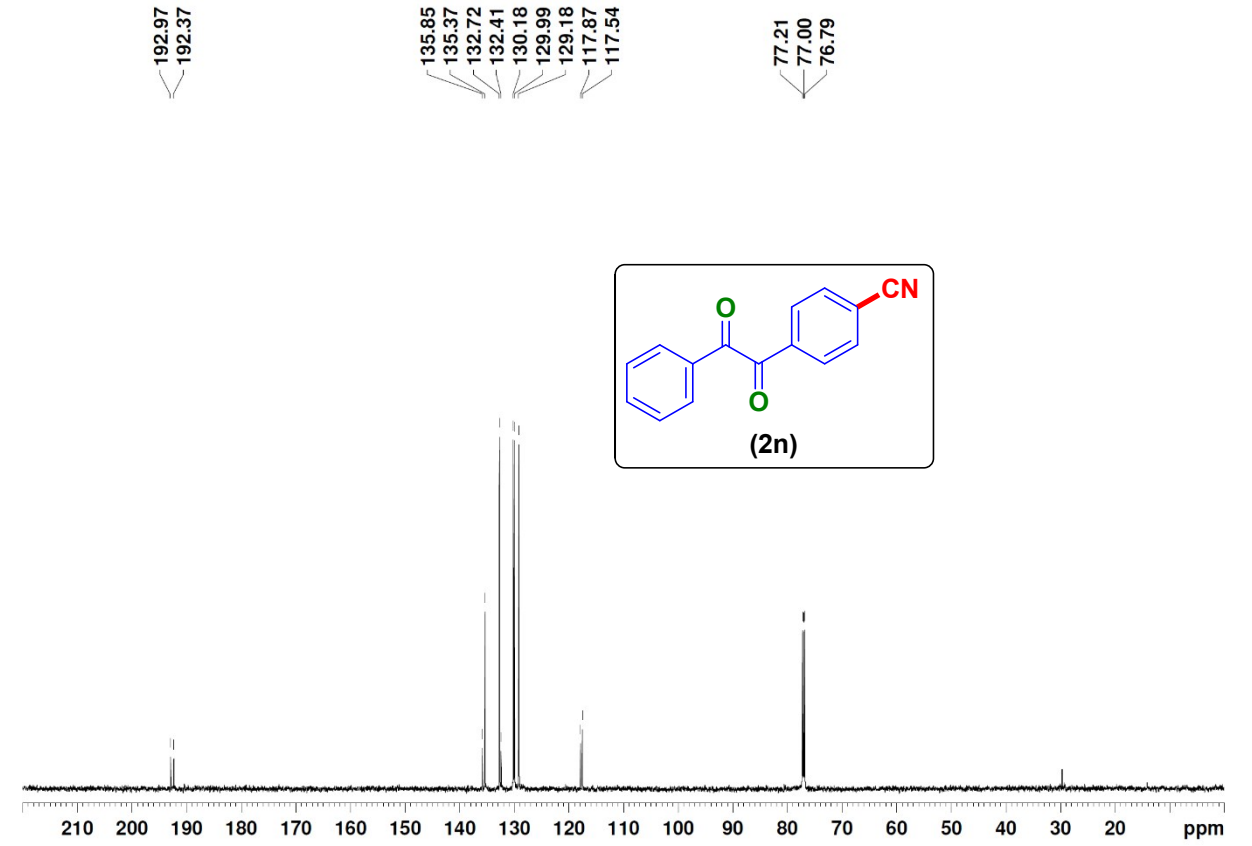

193.47
193.03
135.60
135.25
132.60
130.23
129.99
129.16
128.67
126.04
77.21
77.00
76.79

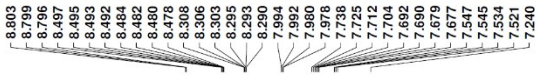

O
O
CF3

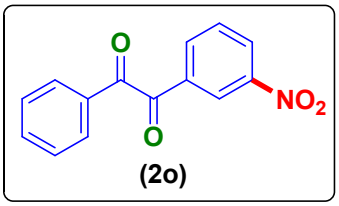
(2m)


210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

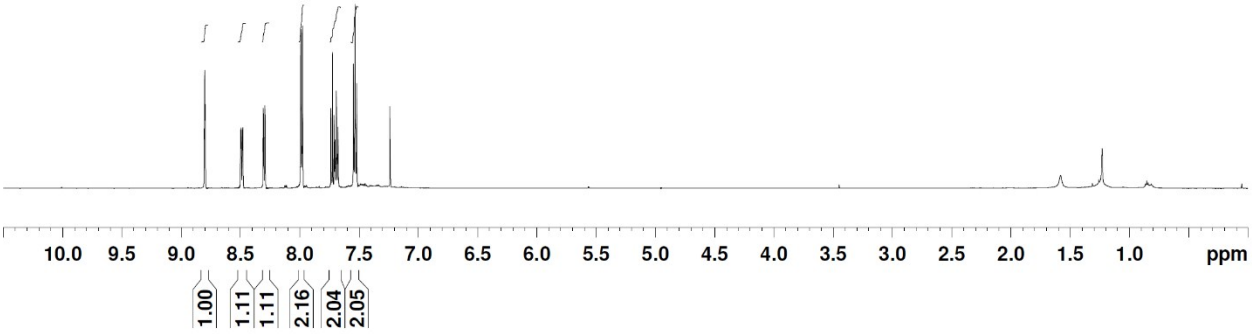

8.074
8.059
7.957
7.945
7.943
7.802
7.788
7.691
7.678
7.666
7.533
7.520
7.507
7.240
CN
O
O
(2n)
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 ppm
2.15
2.01
2.01
1.00
2.04

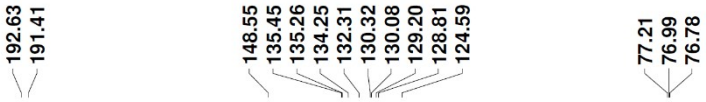

192.97
192.37
135.85
135.37
132.72
132.41
130.18
129.99
129.18
117.87
117.54
77.21
77.00
76.79
CN
O
O
(2n)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

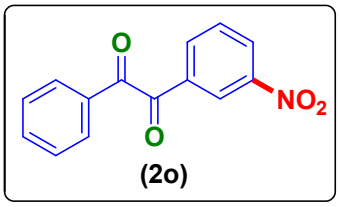

8.803
8.799
8.796
8.497
8.495
8.493
8.492
8.484
8.482
8.480
8.478
8.308
8.306
8.303
8.295
8.293
8.290
7.994
7.992
7.980
7.978
7.738
7.725
7.712
7.704
7.692
7.690
7.679
7.677
7.547
7.545
7.534
7.521
7.240


O
NO2
O

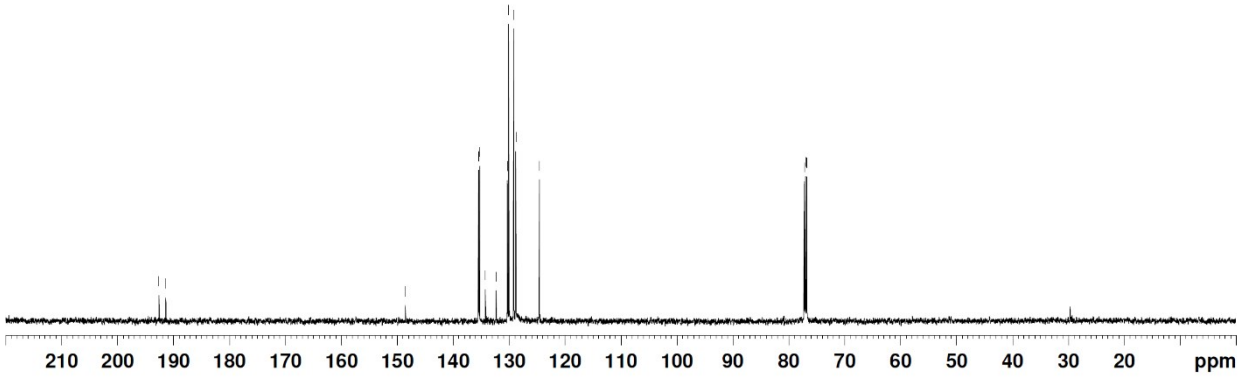
(2o)

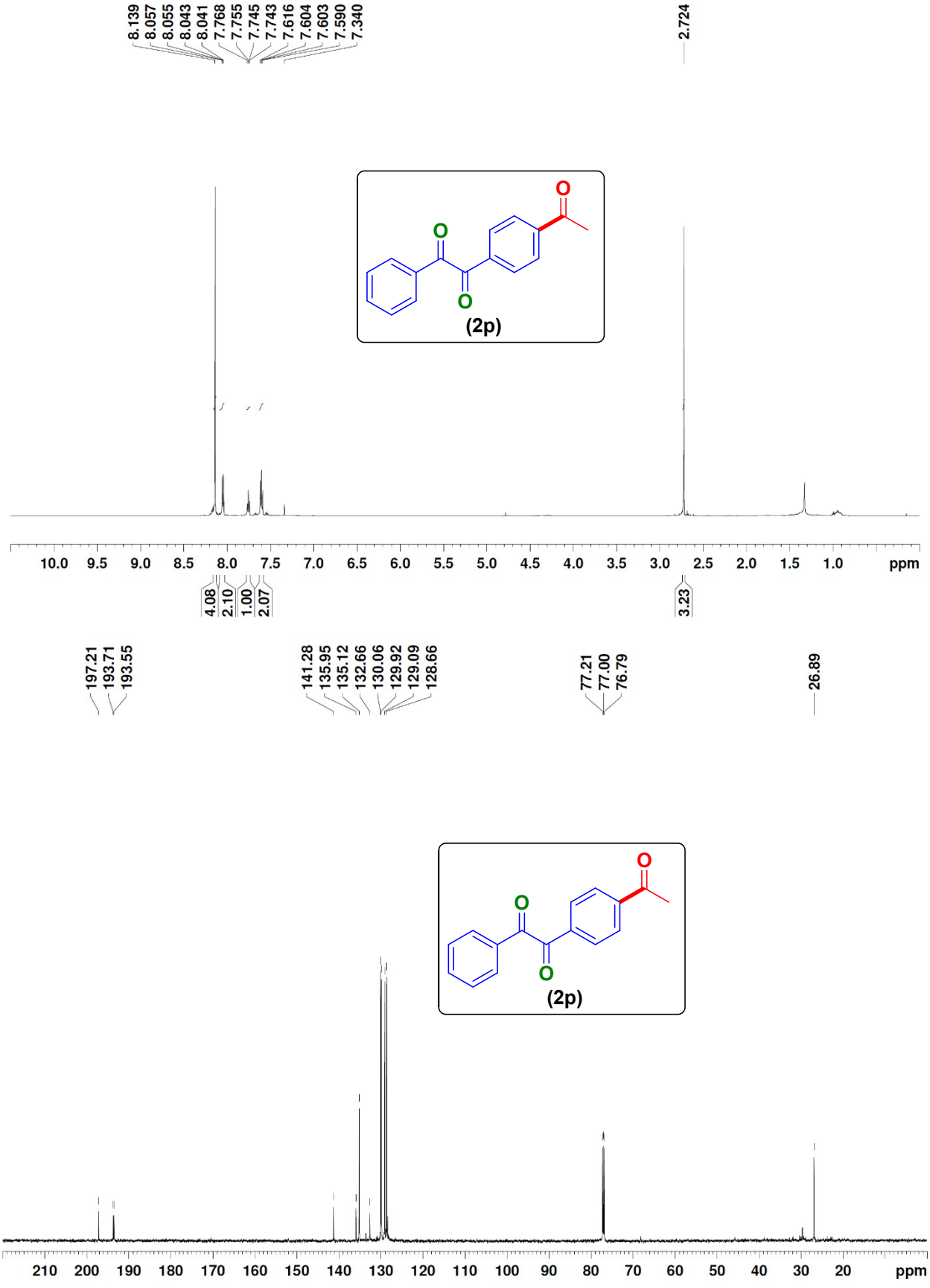

10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 ppm
1.00
1.11
1.11
2.16
2.04
2.05

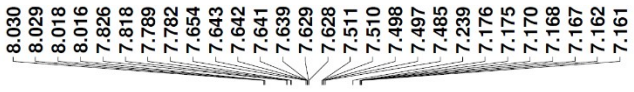

192.63
191.41
148.55
135.45
135.26
134.25
132.31
130.32
130.08
129.20
128.81
124.59
77.21
76.99
76.78

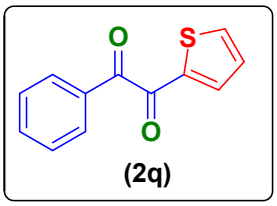

O
NO2
O

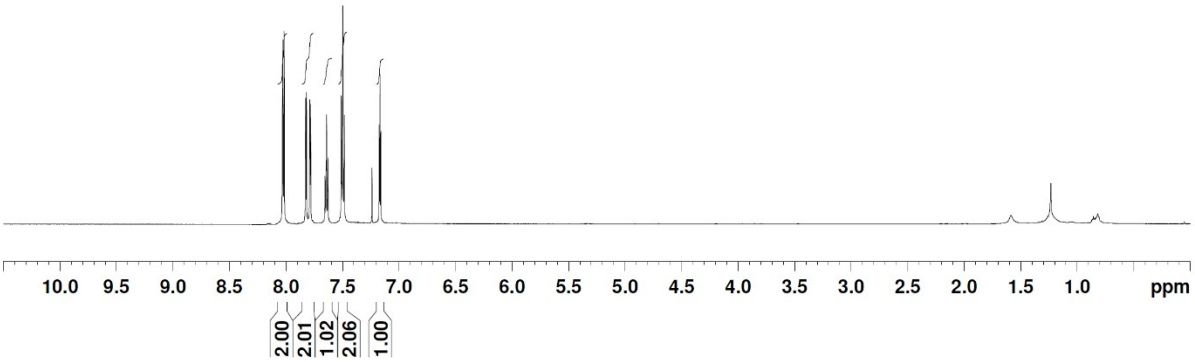
(2o)

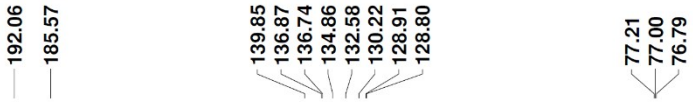

210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

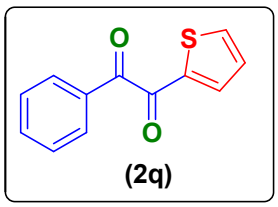

8.139
8.057
8.055
8.043
8.041
7.768
7.755
7.745
7.743
7.616
7.604
7.603
7.590
7.340
2.724
(2p)
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 ppm
4.08
2.10
1.00
2.07
3.23
197.21
193.71
193.55
141.28
135.95
135.12
132.66
130.06
129.92
129.09
128.66
77.21
77.00
76.79
26.89
(2p)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

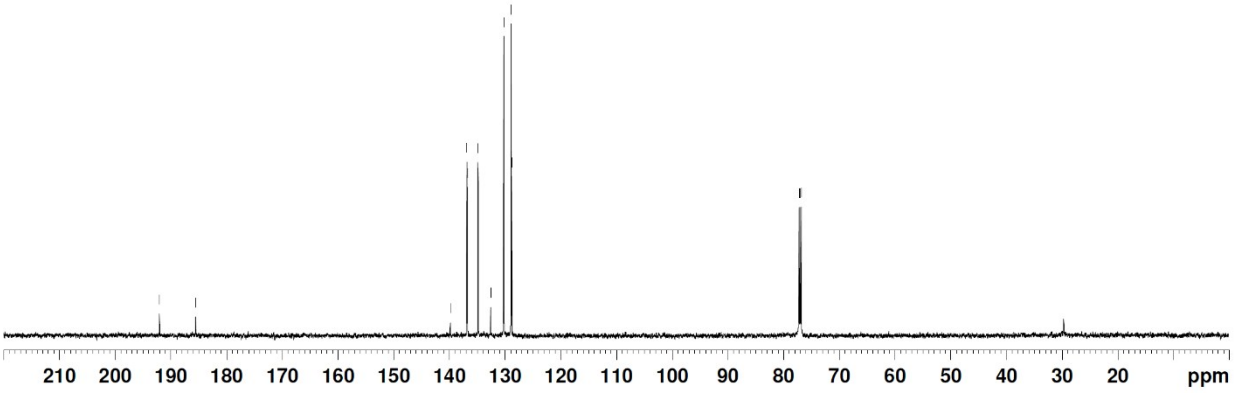

8.030
8.029
8.018
8.016
7.826
7.818
7.789
7.782
7.654
7.643
7.642
7.641
7.639
7.629
7.628
7.511
7.510
7.498
7.497
7.485
7.239
7.176
7.175
7.170
7.168
7.167
7.162
7.161

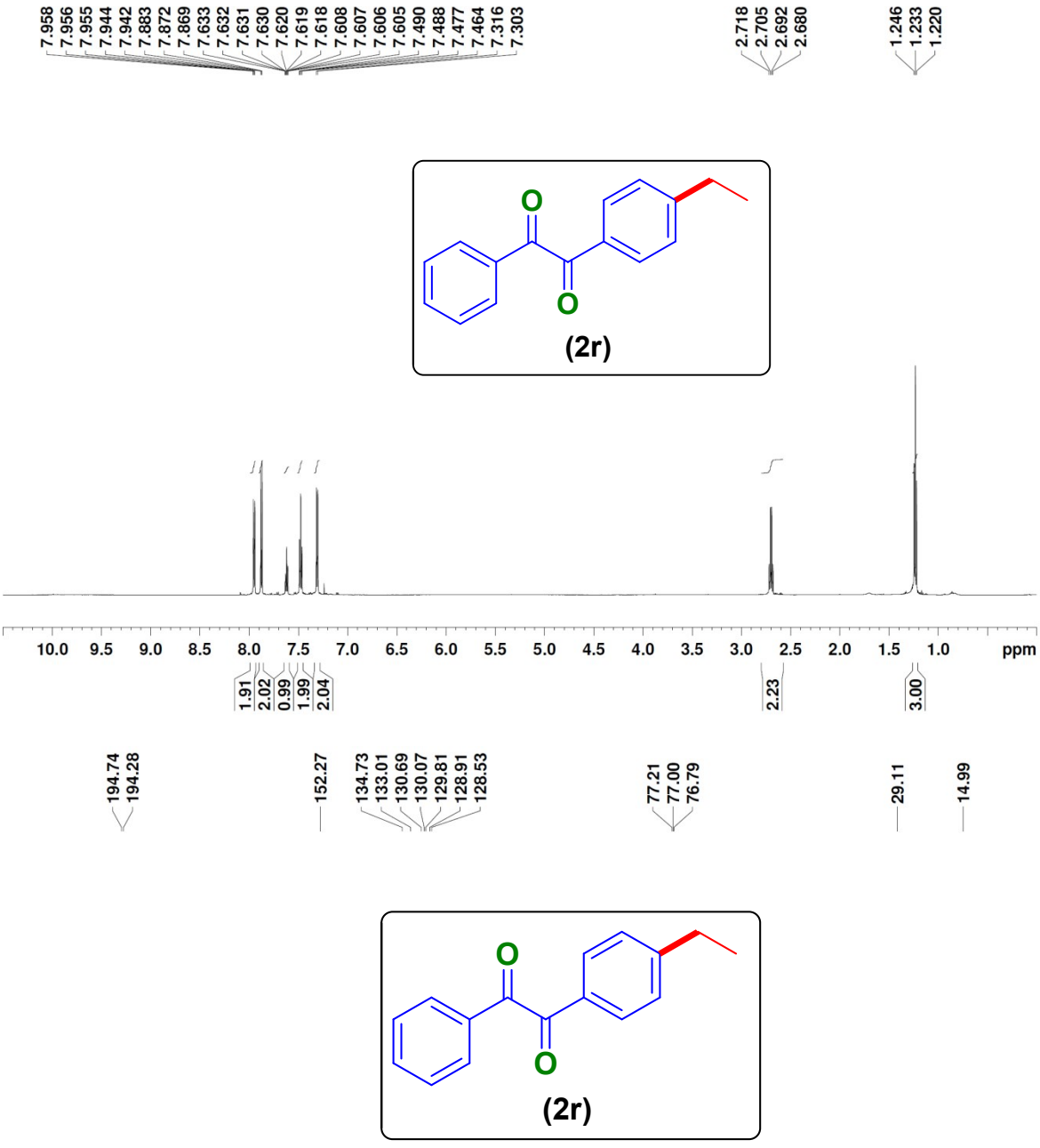

O
S
O
(2q)


10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 ppm
2.00
2.01
1.02
2.06
1.00


192.06
185.57
139.85
136.87
136.74
134.86
132.58
130.22
128.91
128.80
77.21
77.00
76.79

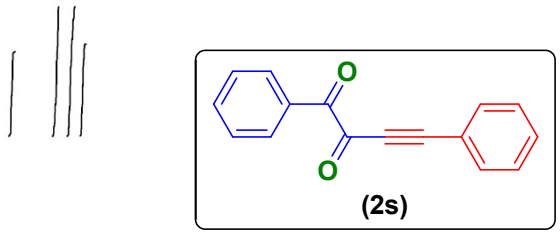

O
S
O
(2q)

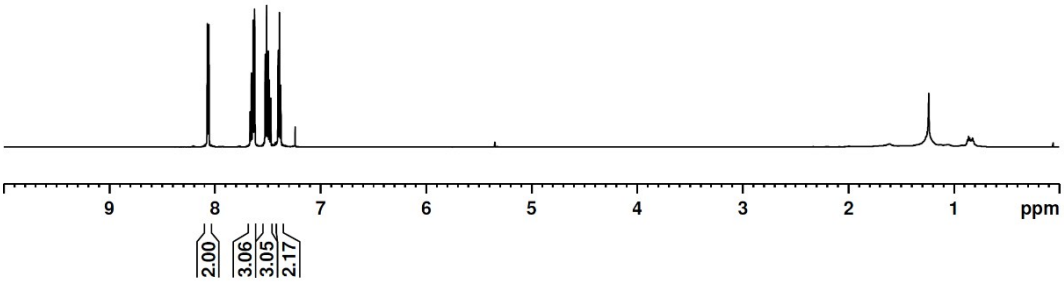

210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

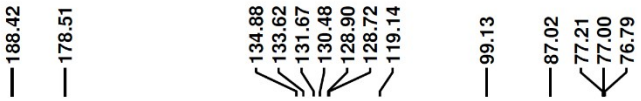

7.958
7.956
7.955
7.944
7.942
7.883
7.872
7.869
7.633
7.632
7.631
7.630
7.620
7.619
7.618
7.608
7.607
7.606
7.605
7.490
7.488
7.477
7.464
7.316
7.303
2.718
2.705
2.692
2.680
1.246
1.233
1.220
(2r)
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 ppm
1.91
2.02
0.99
1.99
2.04
2.23
3.00

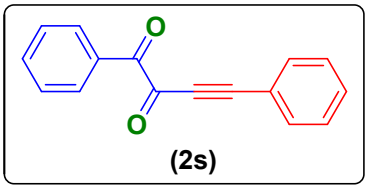
194.74
194.28
152.27
134.73
133.01
130.69
130.07
129.81
128.91
128.53
77.21
77.00
76.79
29.11
14.99
(2r)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

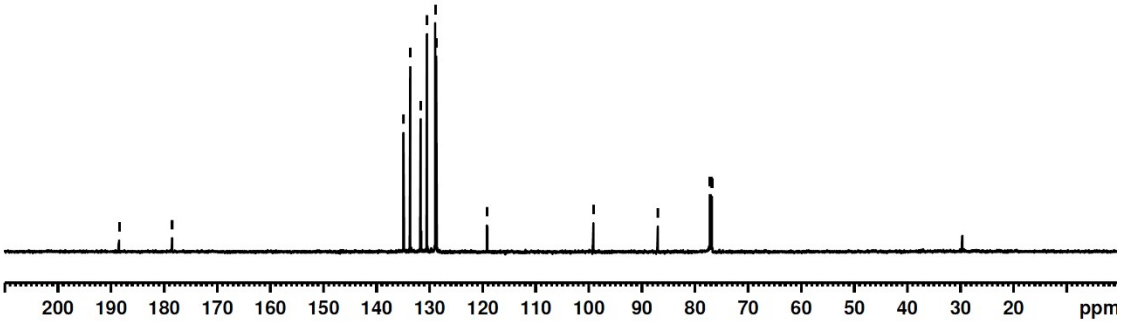

8.072
8.070
8.059
8.056
7.654
7.642
7.639
7.638
7.637
7.625
7.623
7.524
7.512
7.510
7.500
7.499
7.498
7.486
7.485
7.403
7.391
7.390
7.389
7.379
7.377
7.377
7.240

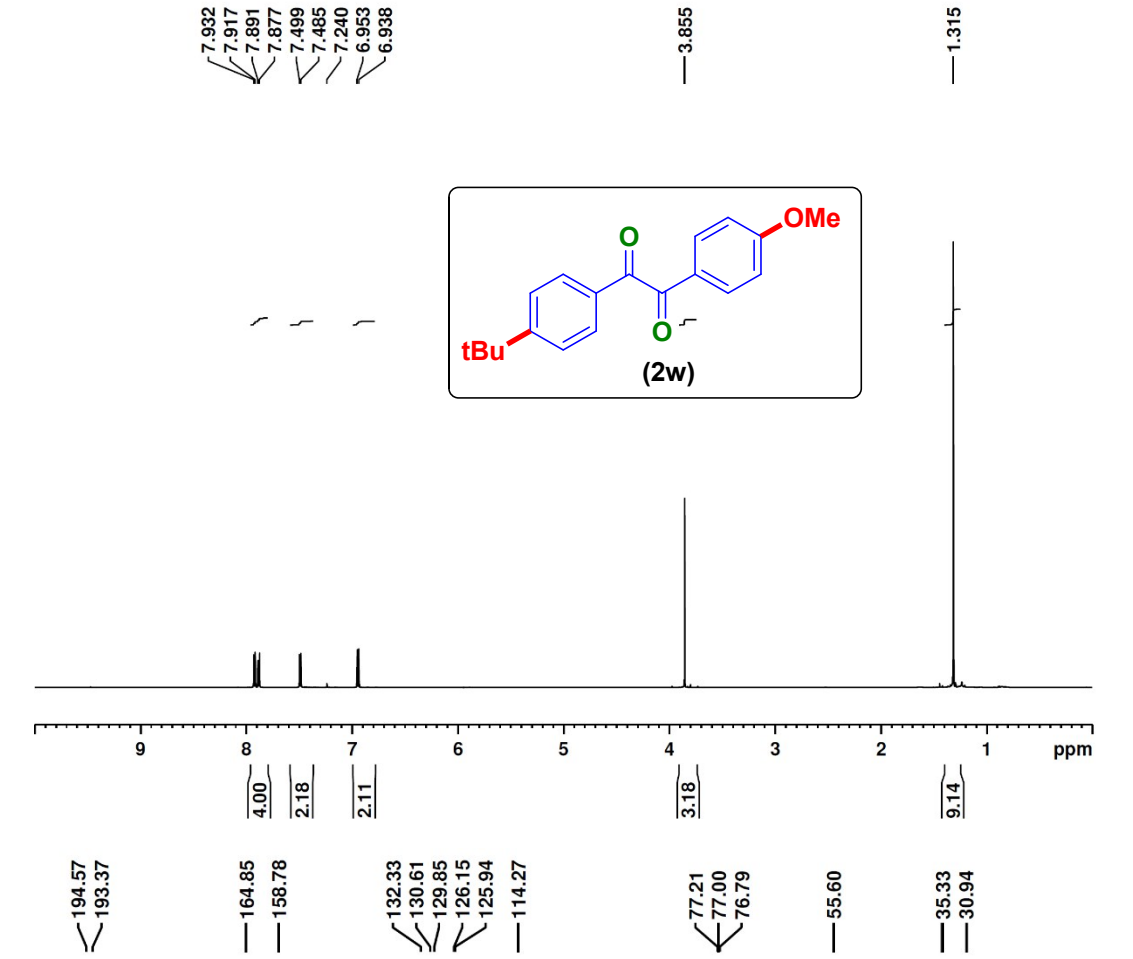

O
O
(2s)

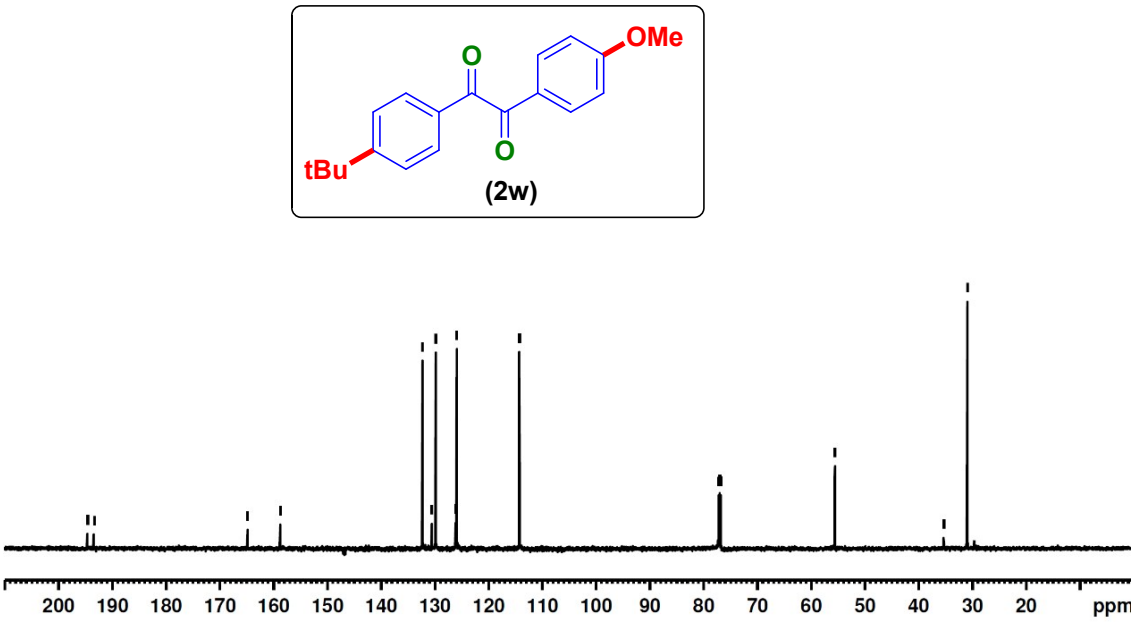

9
8
7
6
5
4
3
2
1
ppm
2.00
3.06
3.05
2.17

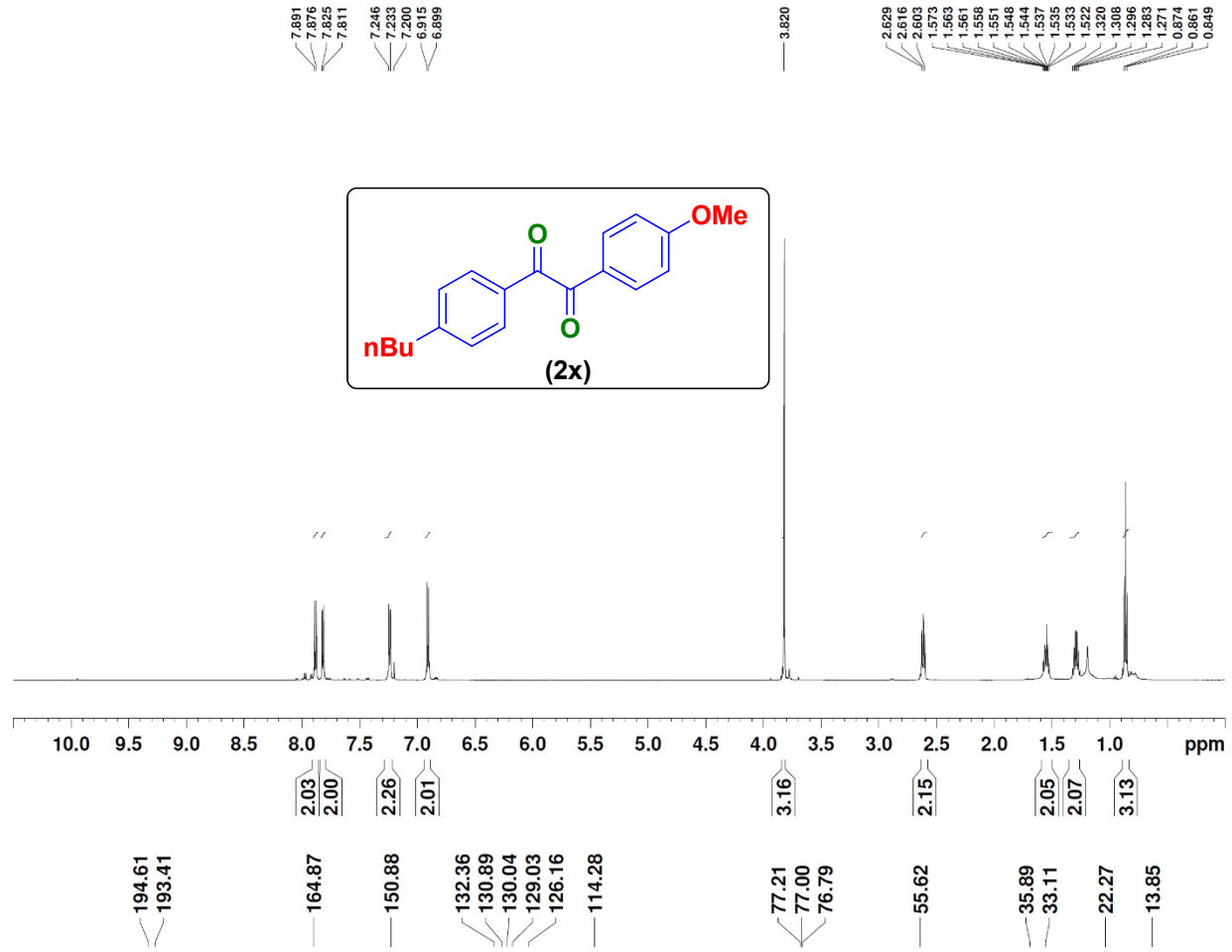

188.42
178.51
134.88
133.62
131.67
130.48
128.90
128.72
119.14
99.13
87.02
77.21
77.00
76.79

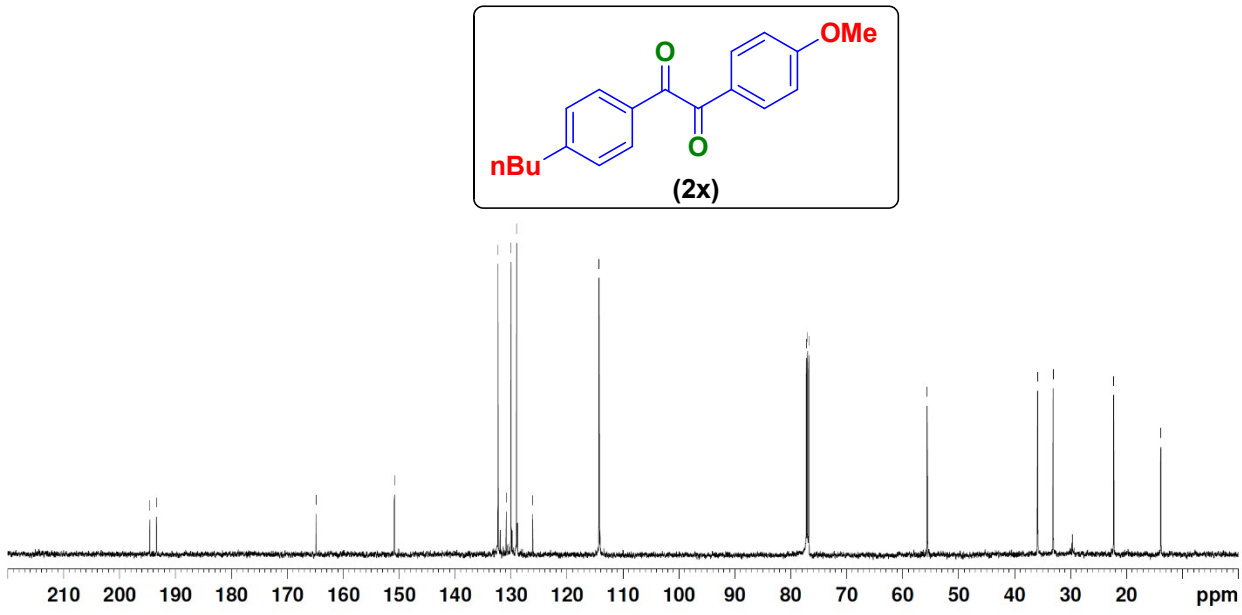

O
O
(2s)

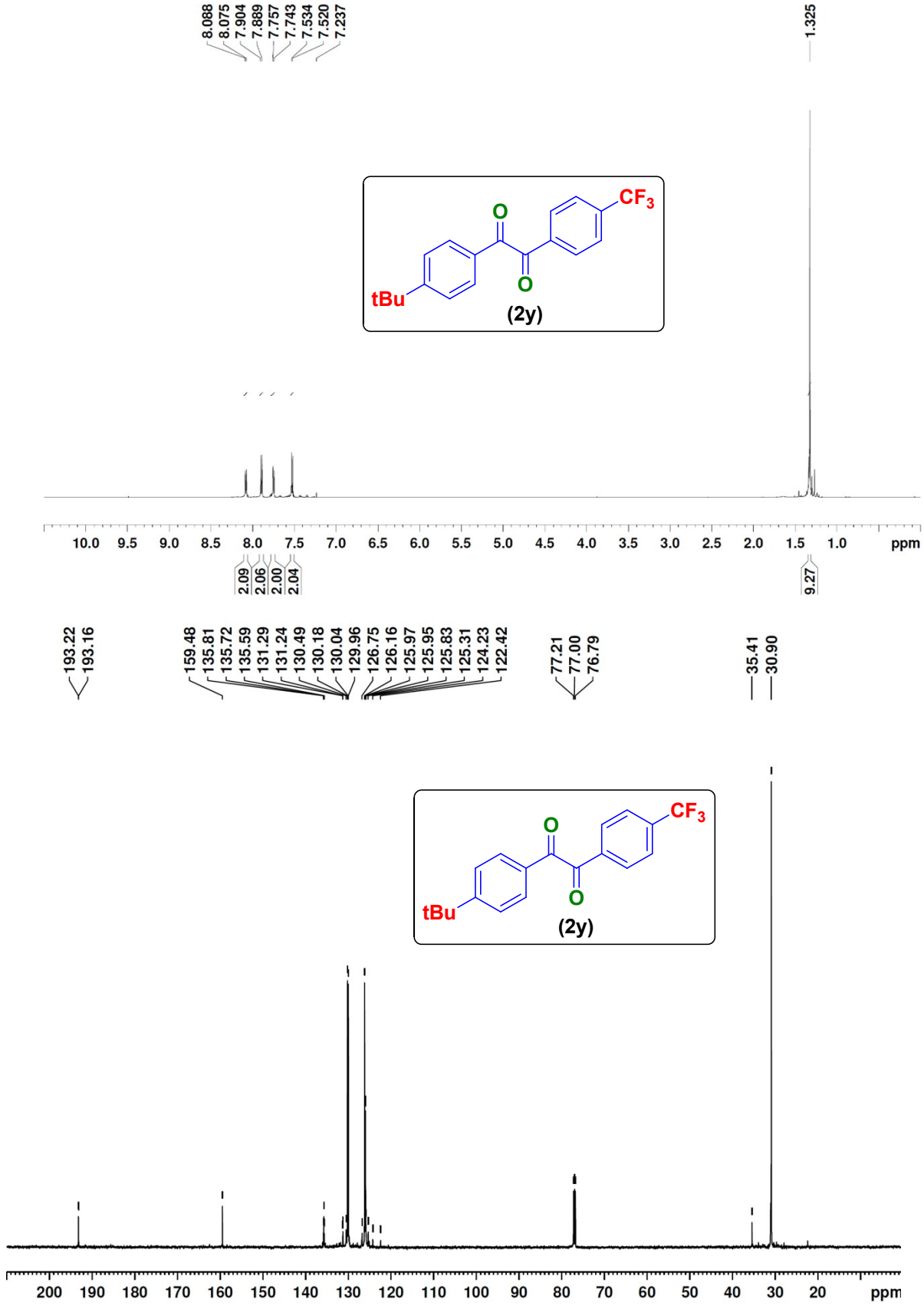

200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

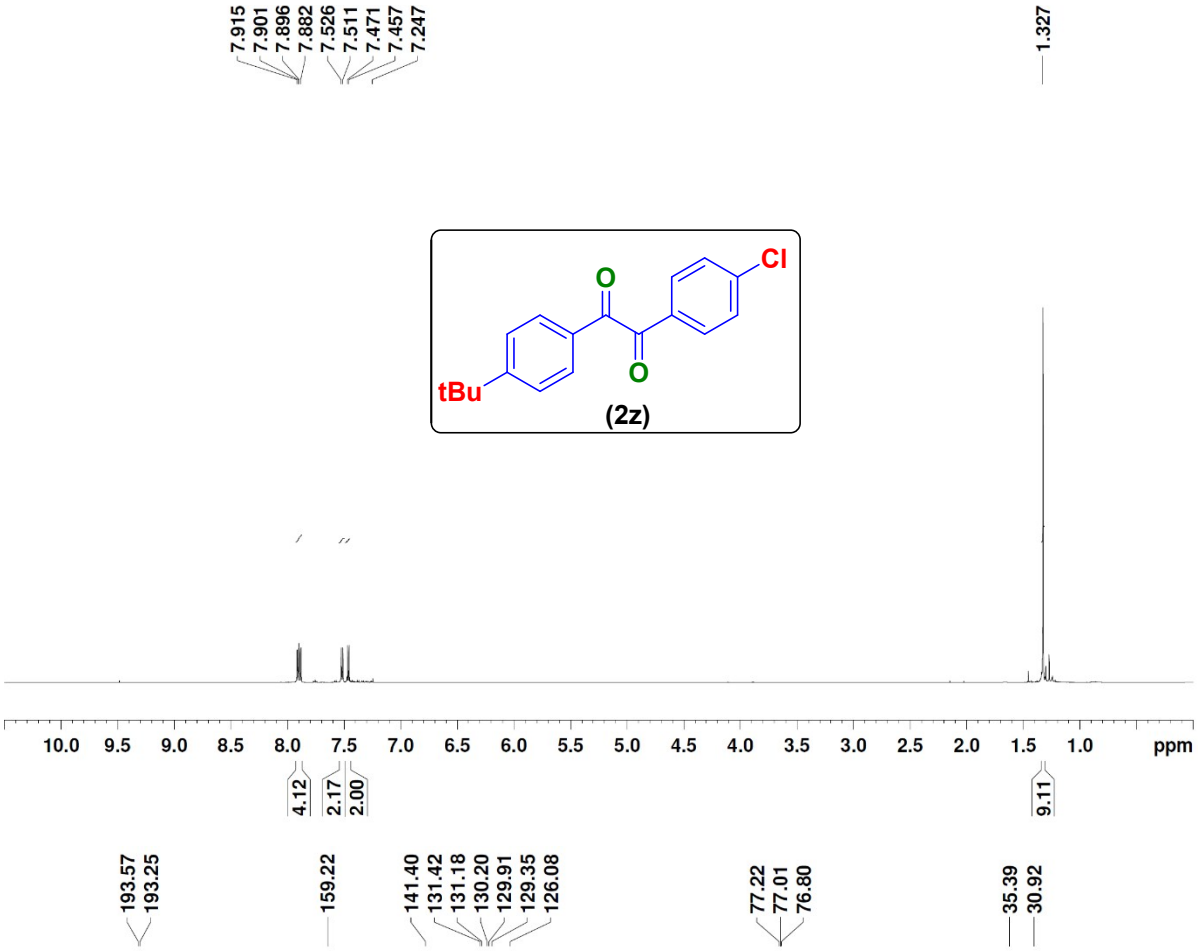

7.932
7.917
7.891
7.877
7.499
7.485
7.240
6.953
6.938
3.855
1.315
OMe
O
O
tBu
(2w)
9
8
7
6
5
4
3
2
1
ppm
4.00
2.18
2.11
3.18
9.14
194.57
193.37
164.85
158.78
132.33
130.61
129.85
126.15
125.94
114.27
77.21
77.00
76.79
55.60
35.33
30.94

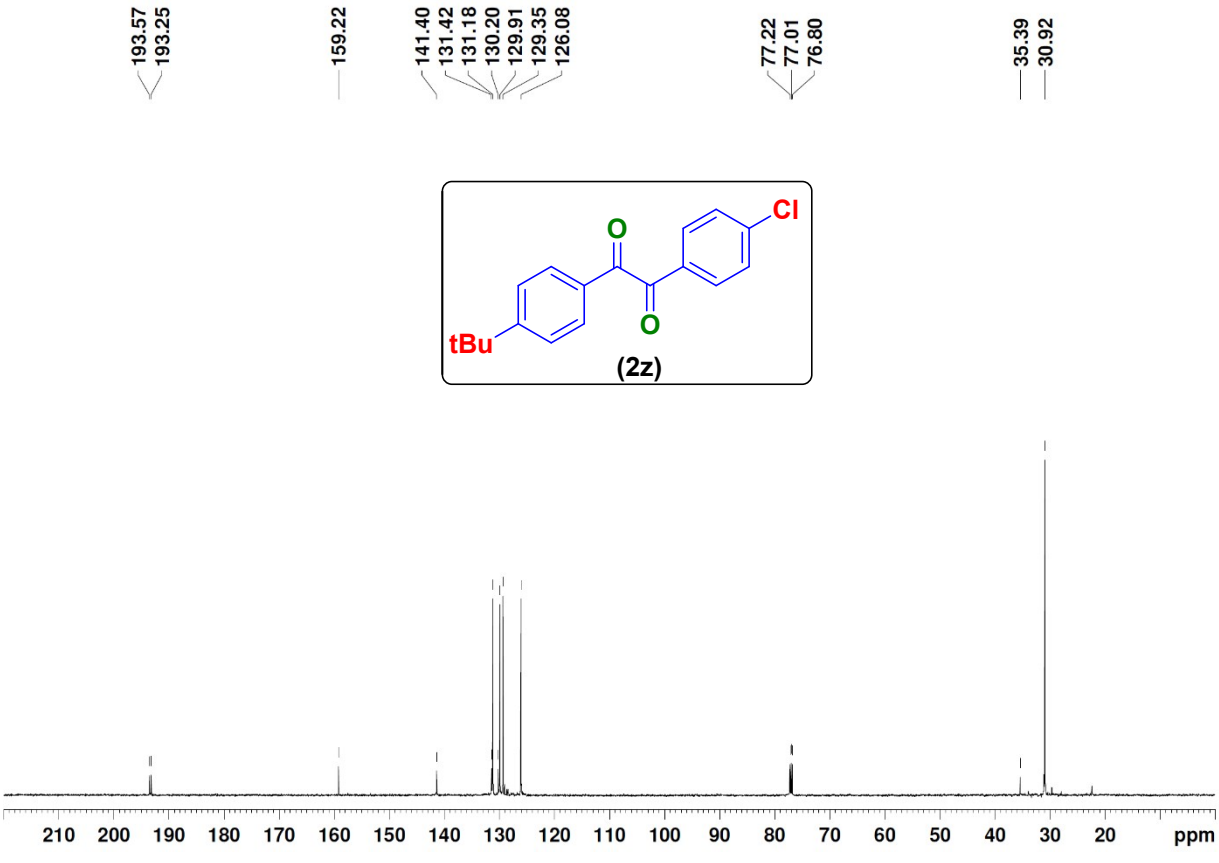

OMe
O
O
tBu
(2w)
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

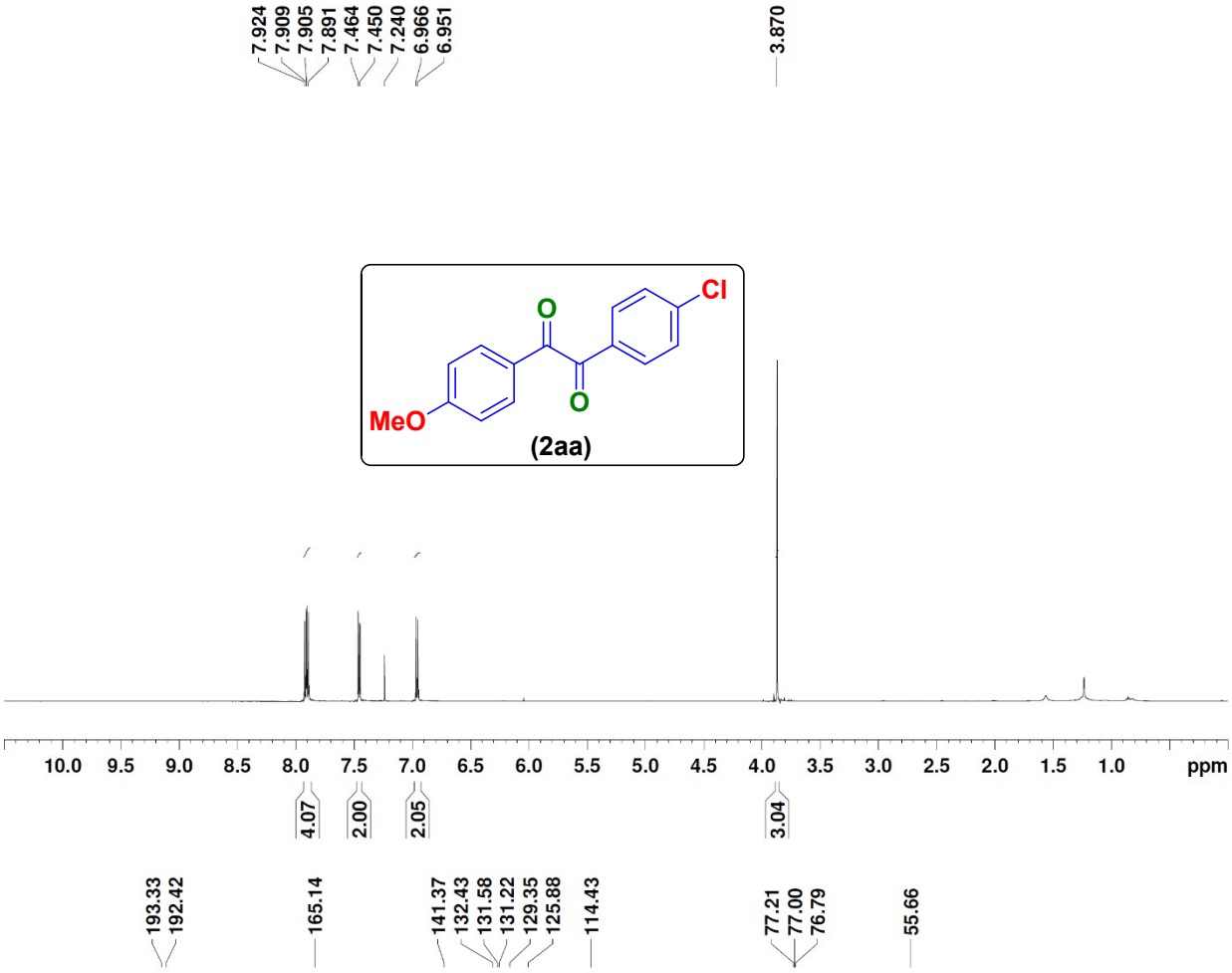

7.891
7.876
7.825
7.811
7.246
7.233
7.200
6.915
6.899
3.820
2.629
2.616
2.603
1.573
1.563
1.561
1.558
1.551
1.548
1.544
1.537
1.535
1.533
1.522
1.320
1.308
1.296
1.283
1.271
0.874
0.861
0.849
OMe
O
O
nBu
(2x)
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 ppm
2.03
2.00
2.26
2.01
3.16
2.15
2.05
2.07
3.13
194.61
193.41
164.87
150.88
132.36
130.89
130.04
129.03
126.16
114.28
77.21
77.00
76.79
55.62
35.89
33.11
22.27
13.85

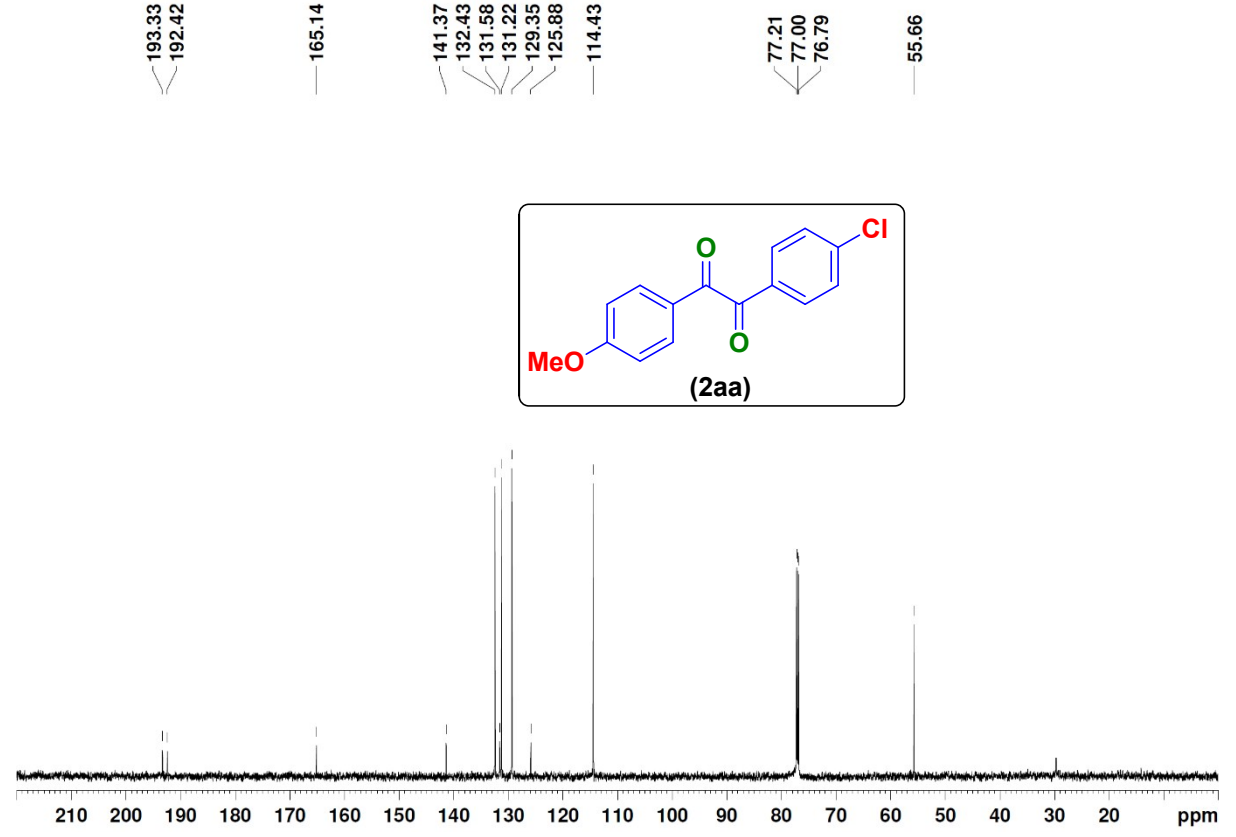

OMe
O
O
nBu
(2x)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

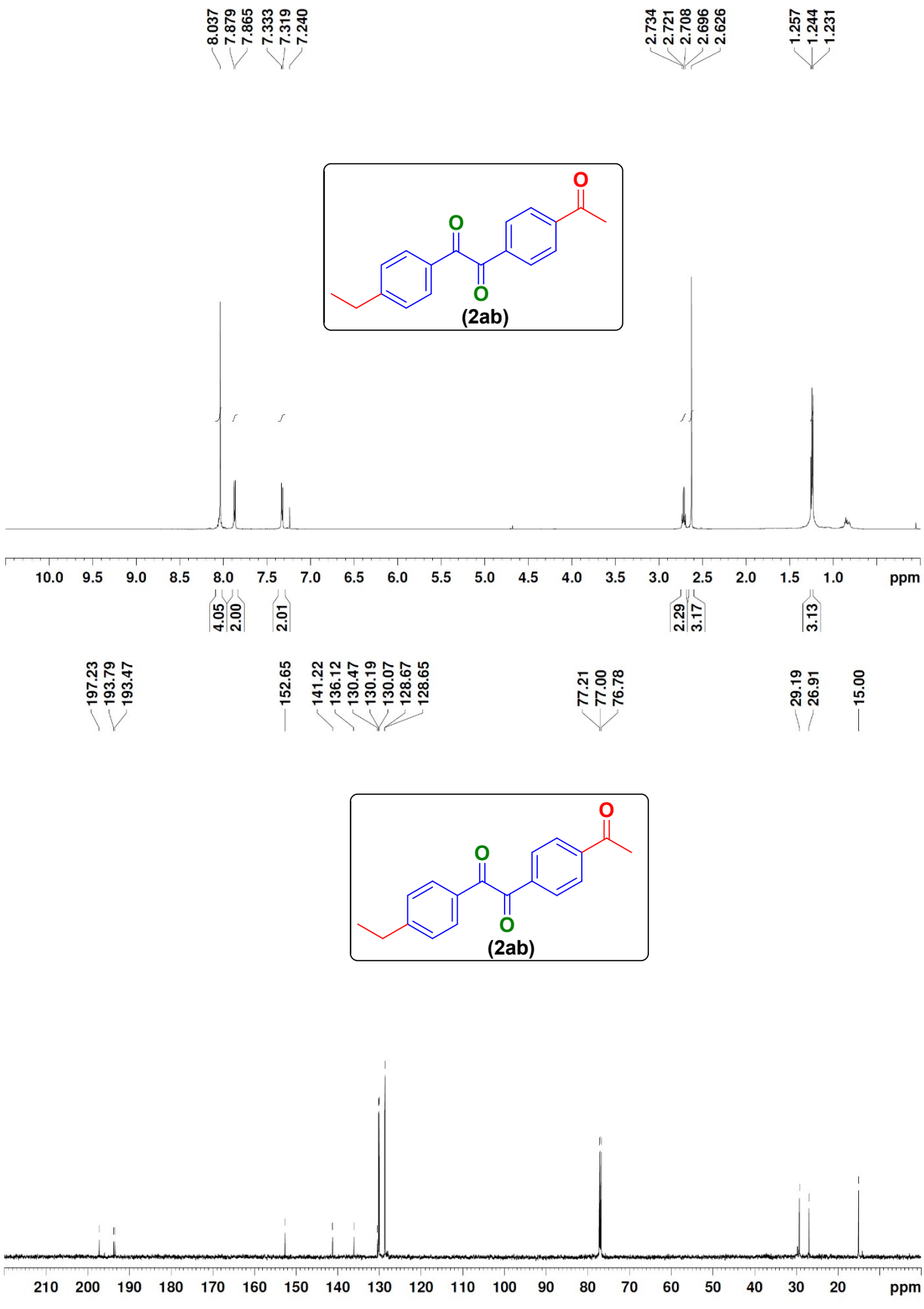

8.088
8.075
7.904
7.889
7.757
7.743
7.534
7.520
7.237
1.325
CF3
O
O
tBu
(2y)
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 ppm
2.09
2.06
2.00
2.04
9.27
193.22
193.16
159.48
135.81
135.72
135.59
131.29
131.24
130.49
130.18
130.04
129.96
126.75
126.16
125.97
125.95
125.83
125.31
124.23
122.42
77.21
77.00
76.79
35.41
30.90
CF3
O
O
tBu
(2y)
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

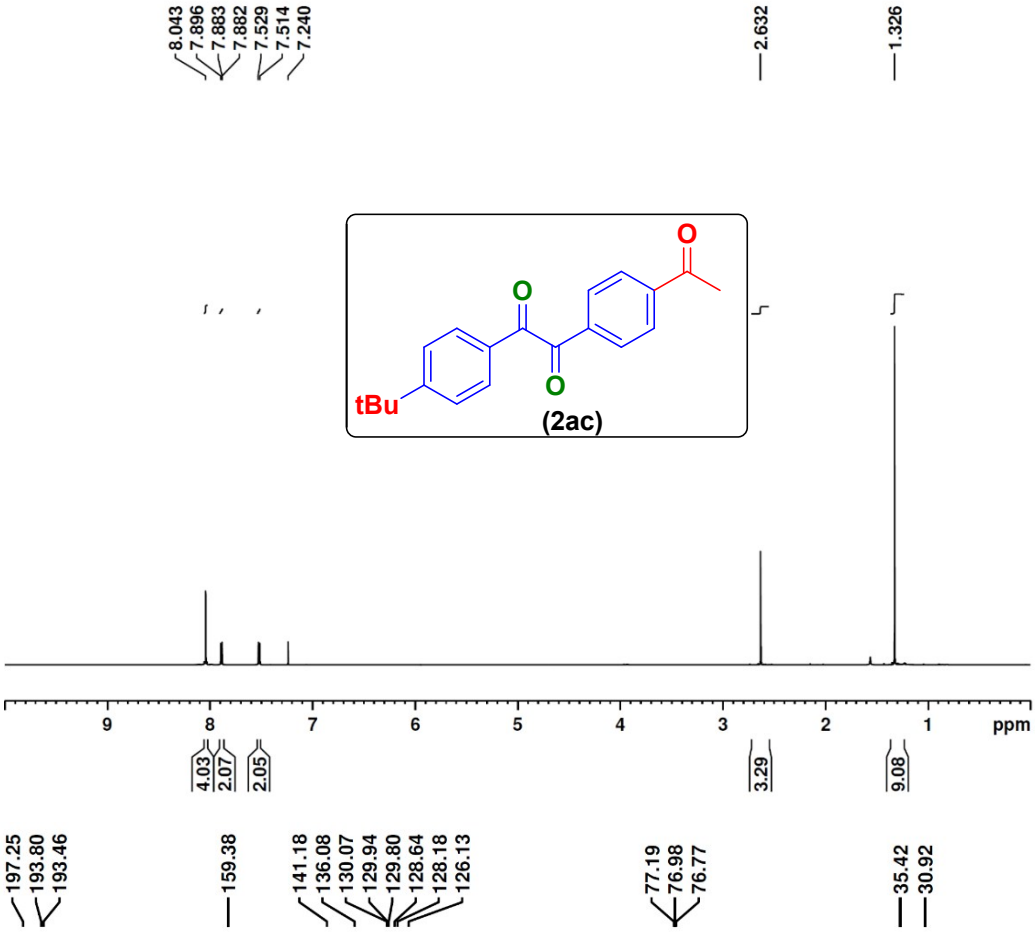

7.915
7.901
7.896
7.882
7.526
7.511
7.471
7.457
7.247
1.327
Cl
O
O
tBu
(2z)
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 ppm
4.12
2.17
2.00
9.11

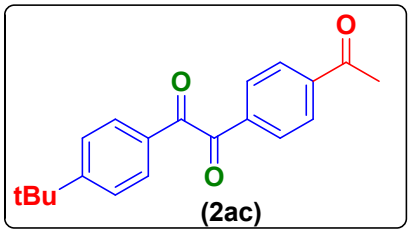

193.57
193.25
159.22
141.40
131.42
131.18
130.20
129.91
129.35
126.08
77.22
77.01
76.80
35.39
30.92
Cl
O
O
tBu
(2z)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

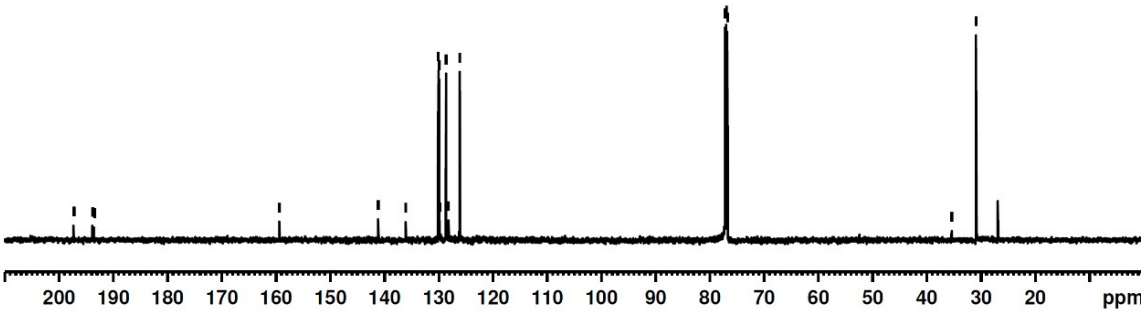

7.924
7.909
7.905
7.891
7.464
7.450
7.240
6.966
6.951
3.870
Cl
O
O
MeO
(2aa)
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 ppm
4.07
2.00
2.05
3.04

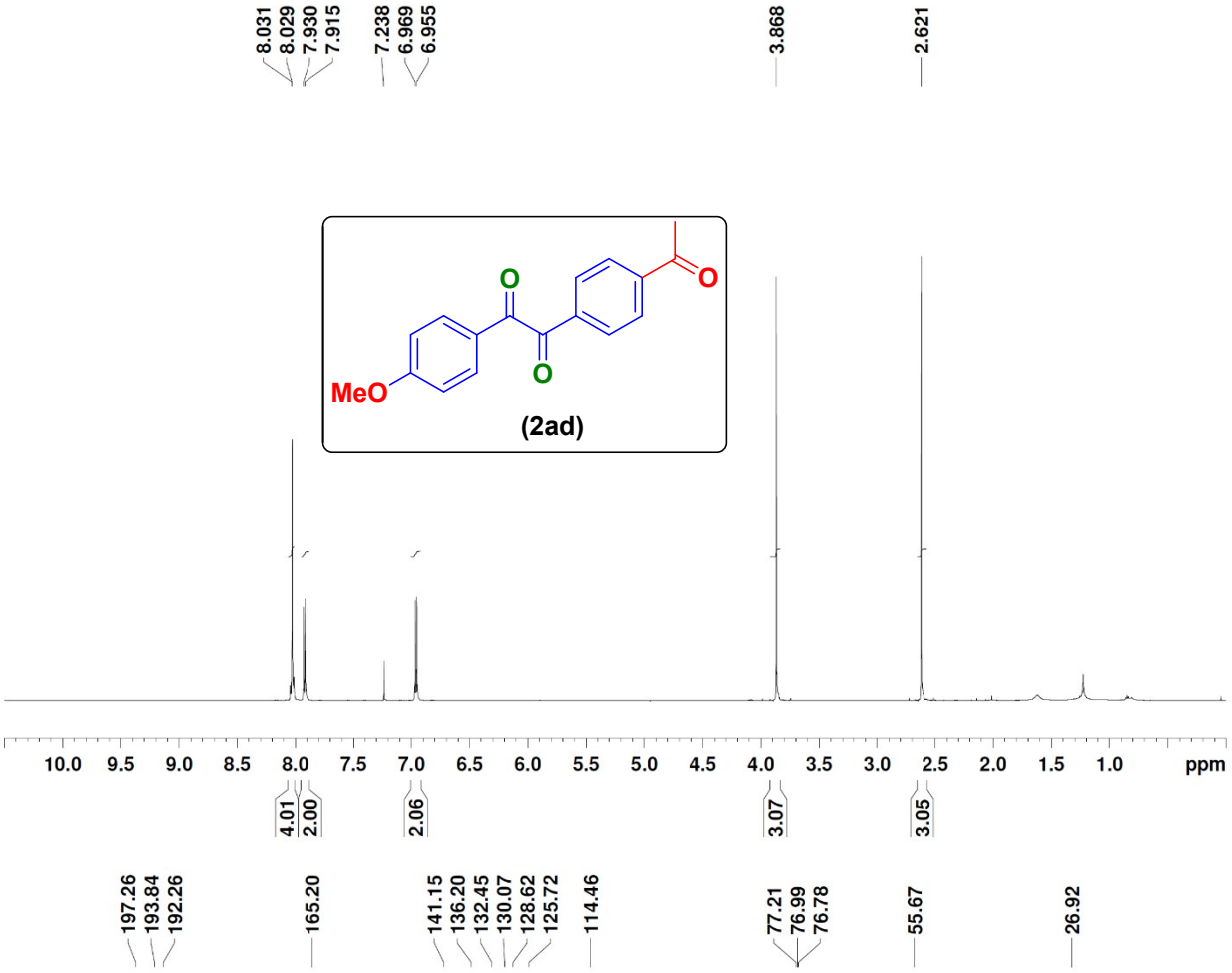

193.33
192.42
165.14
141.37
132.43
131.58
131.22
129.35
125.88
114.43
77.21
77.00
76.79
55.66
Cl
O
O
MeO
(2aa)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

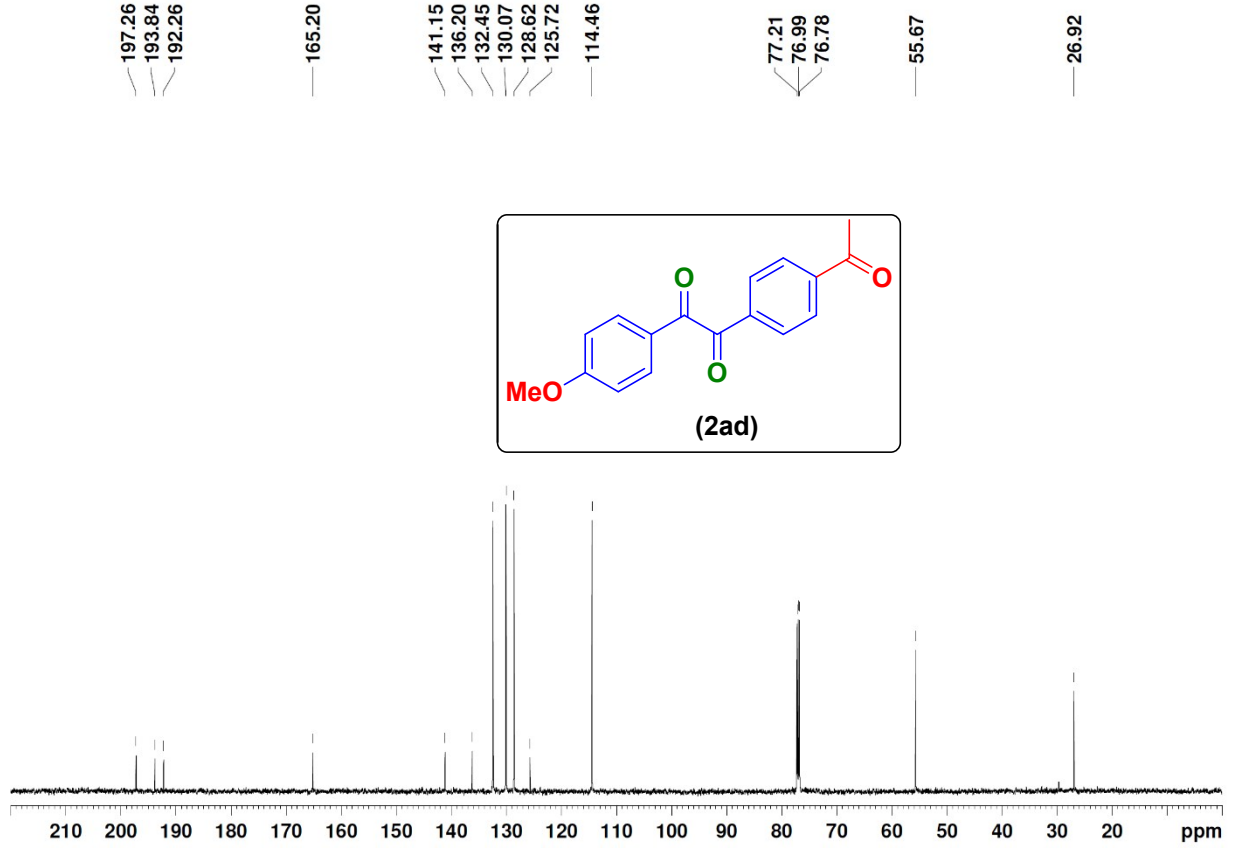

8.037
7.879
7.865
7.333
7.319
7.240
2.734
2.721
2.708
2.696
2.626
1.257
1.244
1.231
O
O
O
(2ab)
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 ppm
4.05
2.00
2.01
2.29
3.17
3.13
197.23
193.79
193.47
152.65
141.22
136.12
130.47
130.19
130.07
128.67
128.65
77.21
77.00
76.78
29.19
26.91
15.00
O
O
O
(2ab)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

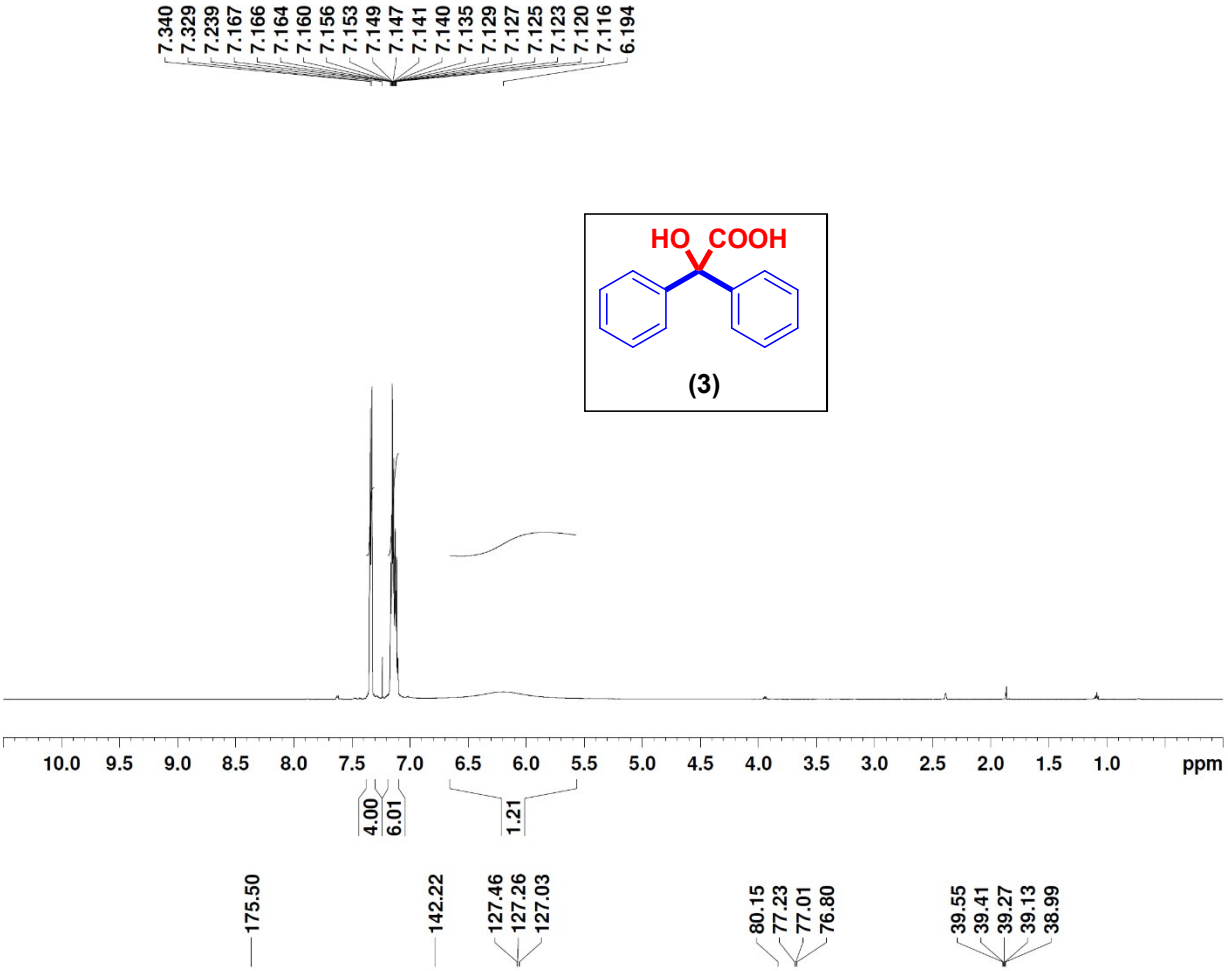

8.043
7.896
7.883
7.882
7.529
7.514
7.240
2.632
1.326
O
O
O
tBu
(2ac)
9
8
7
6
5
4
3
2
1
ppm
4.03
2.07
2.05
3.29
9.08
197.25
193.80
193.46
159.38
141.18
136.08
130.07
129.94
129.80
128.64
128.18
126.13
77.19
76.98
76.77
35.42
30.92


O
O
O
tBu
(2ac)

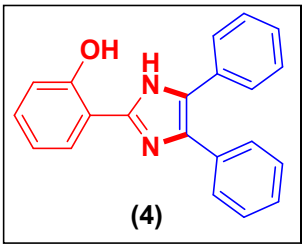

200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm


8.031
8.029
7.930
7.915
7.238
6.969
6.955
3.868
2.621
O
O
O
MeO
(2ad)
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 ppm
4.01
2.00
2.06
3.07
3.05

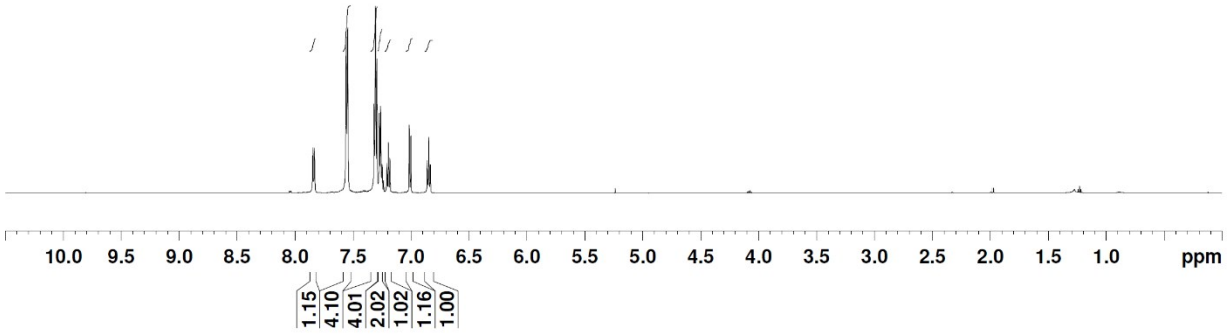

197.26
193.84
192.26
165.20
141.15
136.20
132.45
130.07
128.62
125.72
114.46
77.21
76.99
76.78
55.67
26.92
O
O
O
MeO
(2ad)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

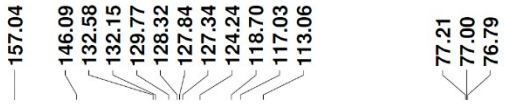

7.340
7.329
7.239
7.167
7.166
7.164
7.160
7.156
7.153
7.149
7.147
7.141
7.140
7.135
7.129
7.127
7.125
7.123
7.120
7.116
6.194
HO COOH
(3)
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 ppm
4.00
6.01
1.21
175.50
142.22
127.46
127.26
127.03
80.15
77.23
77.01
76.80
39.55
39.41
39.27
39.13
38.99
HO COOH
(3)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

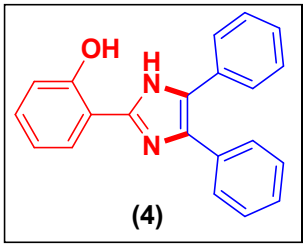

7.846
7.833
7.559
7.547
7.320
7.308
7.306
7.295
7.275
7.263
7.251
7.239
7.208
7.196
7.195
7.185
7.182
7.015
7.001
6.859
6.847
6.834


OH
H
N
N

(4)

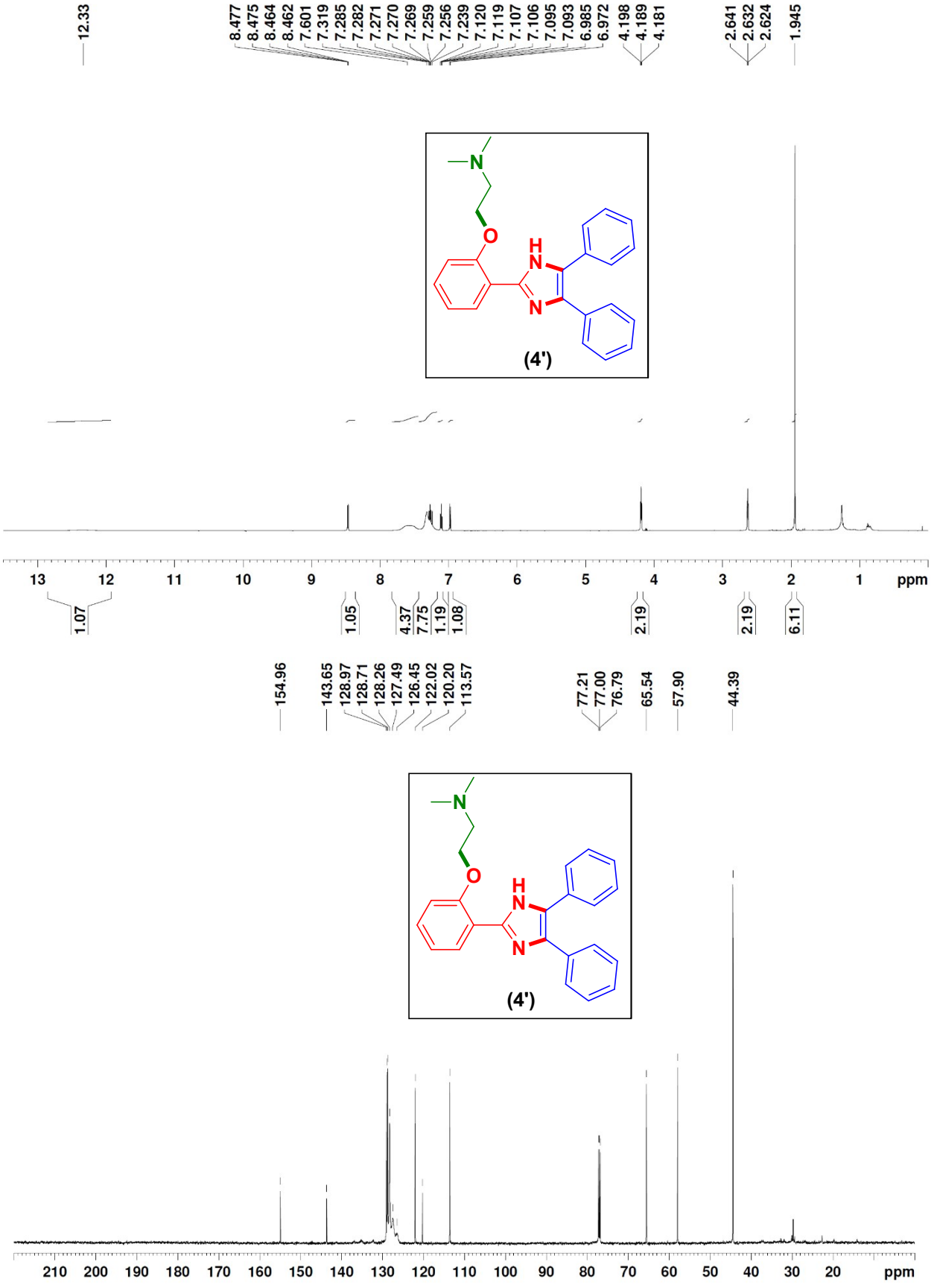

10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 ppm
1.15
4.10
4.01
2.02
1.02
1.16
1.00

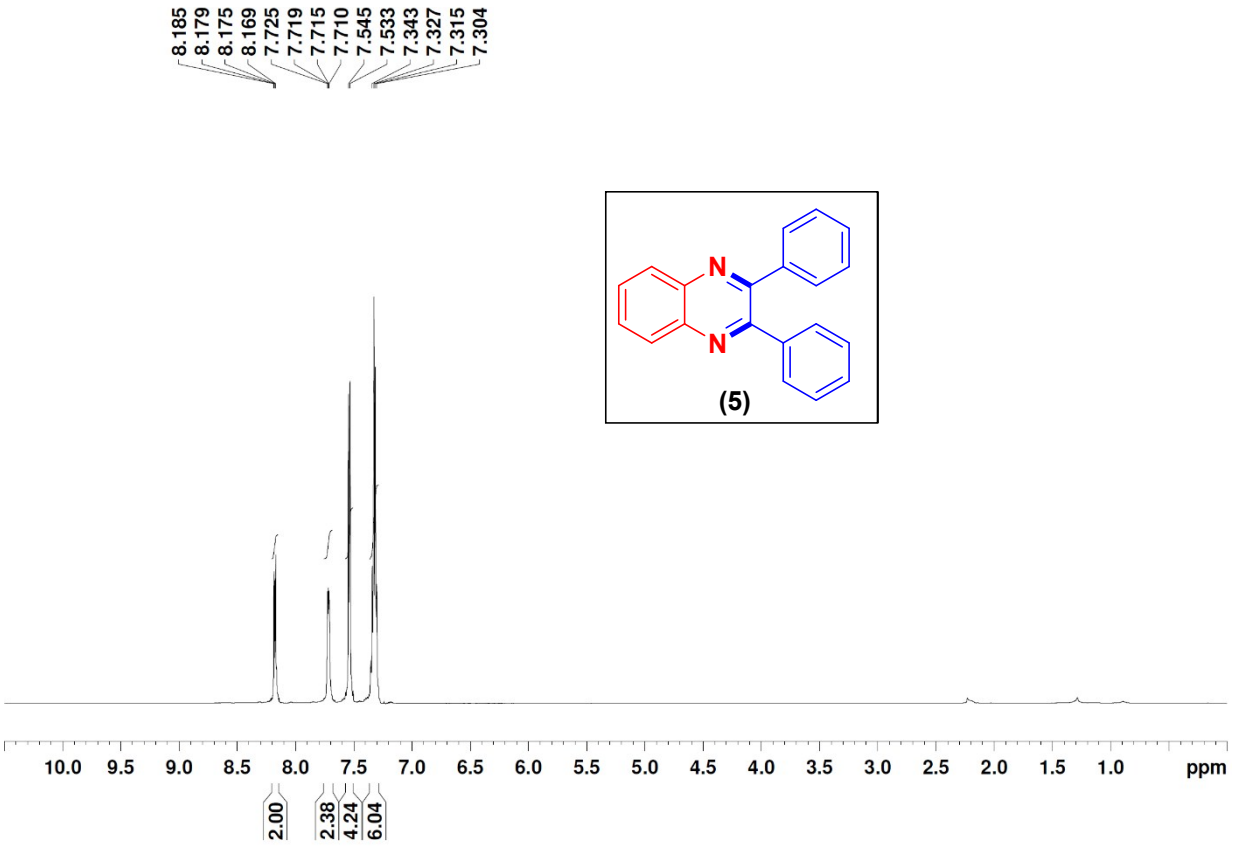

157.04
146.09
132.58
132.15
129.77
128.32
127.84
127.34
124.24
118.70
117.03
113.06
77.21
77.00
76.79

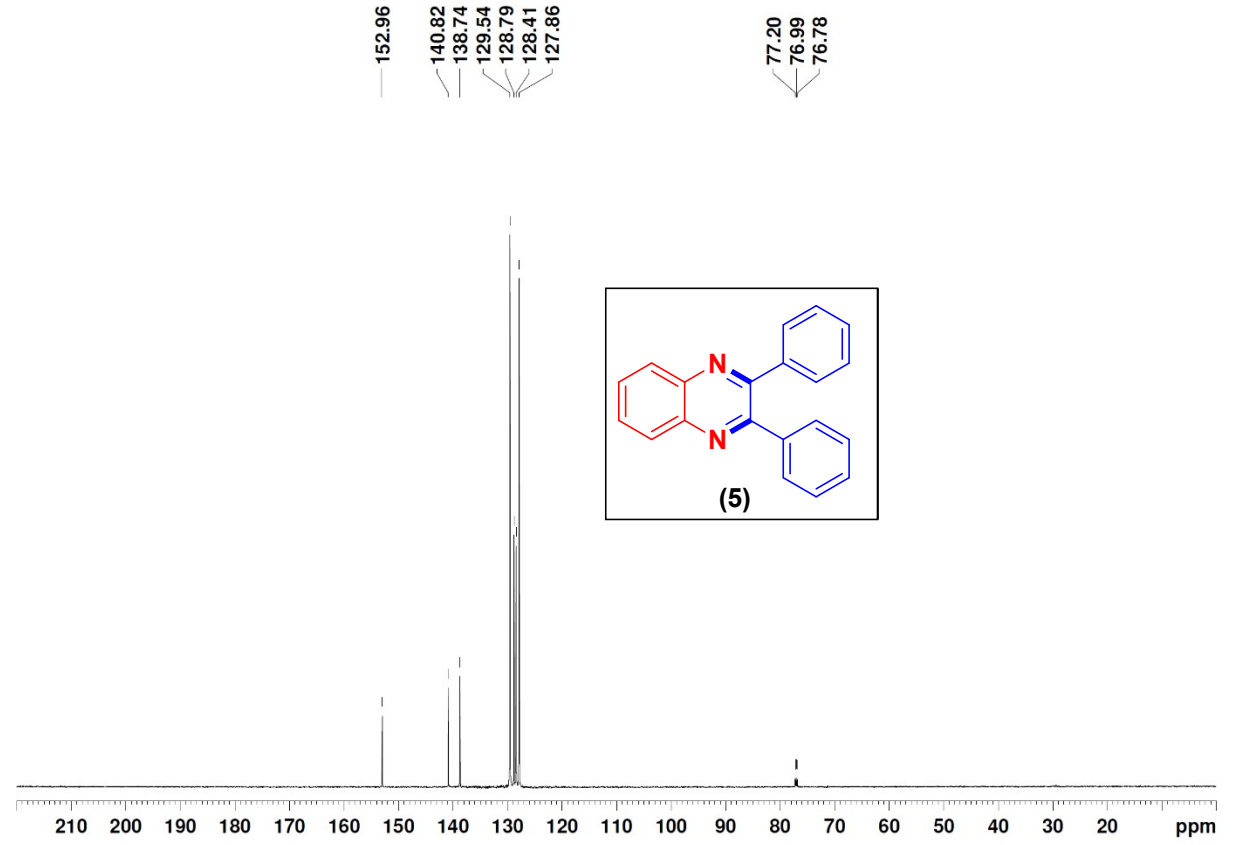

OH
H
N
N

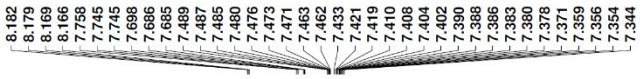
(4)

210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm


12.33
8.477
8.475
8.464
8.462
7.601
7.319
7.285
7.282
7.271
7.270
7.269
7.259
7.256
7.239
7.120
7.119
7.107
7.106
7.095
7.093
6.985
6.972
4.198
4.189
4.181
2.641
2.632
2.624
1.945
(4')
13
12
11
10
9
8
7
6
5
4
3
2
1
ppm
1.07
1.05
4.37
7.75
1.19
1.08
2.19
2.19
6.11
154.96
143.65
128.97
128.71
128.26
127.49
126.45
122.02
120.20
113.57
77.21
77.00
76.79
65.54
57.90
44.39
(4')
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm


8.185
8.179
8.175
8.169
7.725
7.719
7.715
7.710
7.545
7.533
7.343
7.327
7.315
7.304
N
N
(5)
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 ppm
2.00
2.38
4.24
6.04


152.96
140.82
138.74
129.54
128.79
128.41
127.86
77.20
76.99
76.78
N
N
(5)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm


8.182
8.179
8.169
8.166
7.758
7.745
7.745
7.698
7.686
7.685
7.489
7.487
7.485
7.480
7.476
7.473
7.471
7.463
7.462
7.433
7.421
7.419
7.410
7.408
7.404
7.402
7.390
7.388
7.386
7.383
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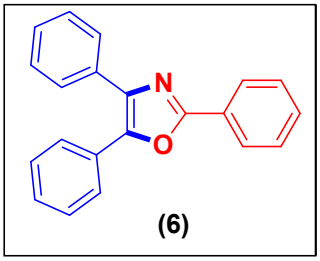
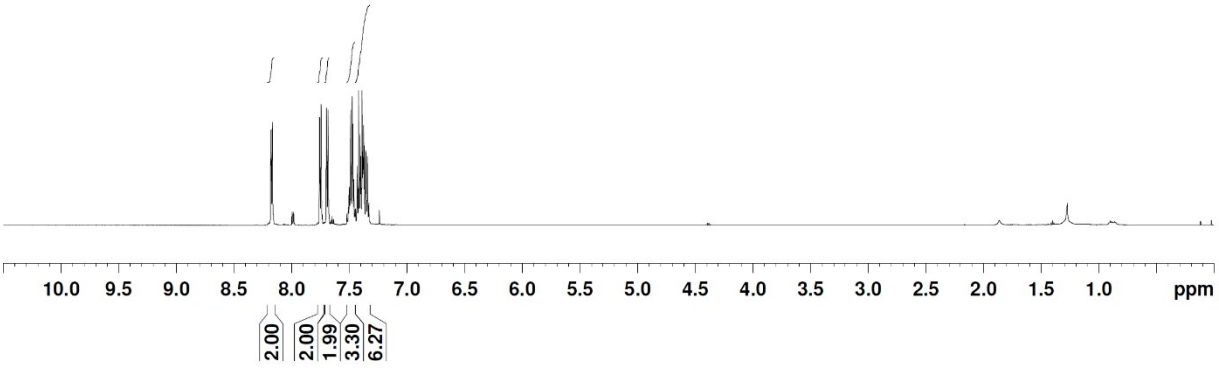
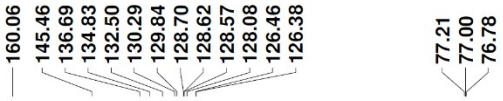
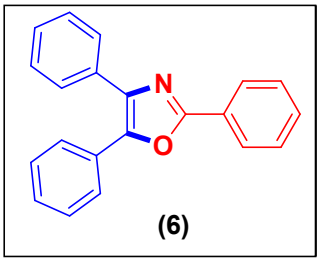
7.378
7.371
7.359
7.356
7.354
7.344


N
O

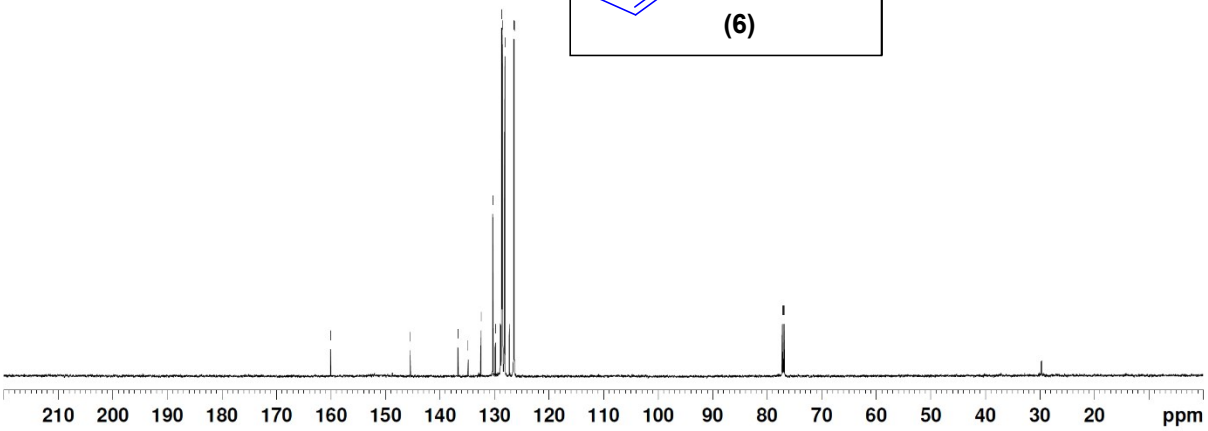
(6)

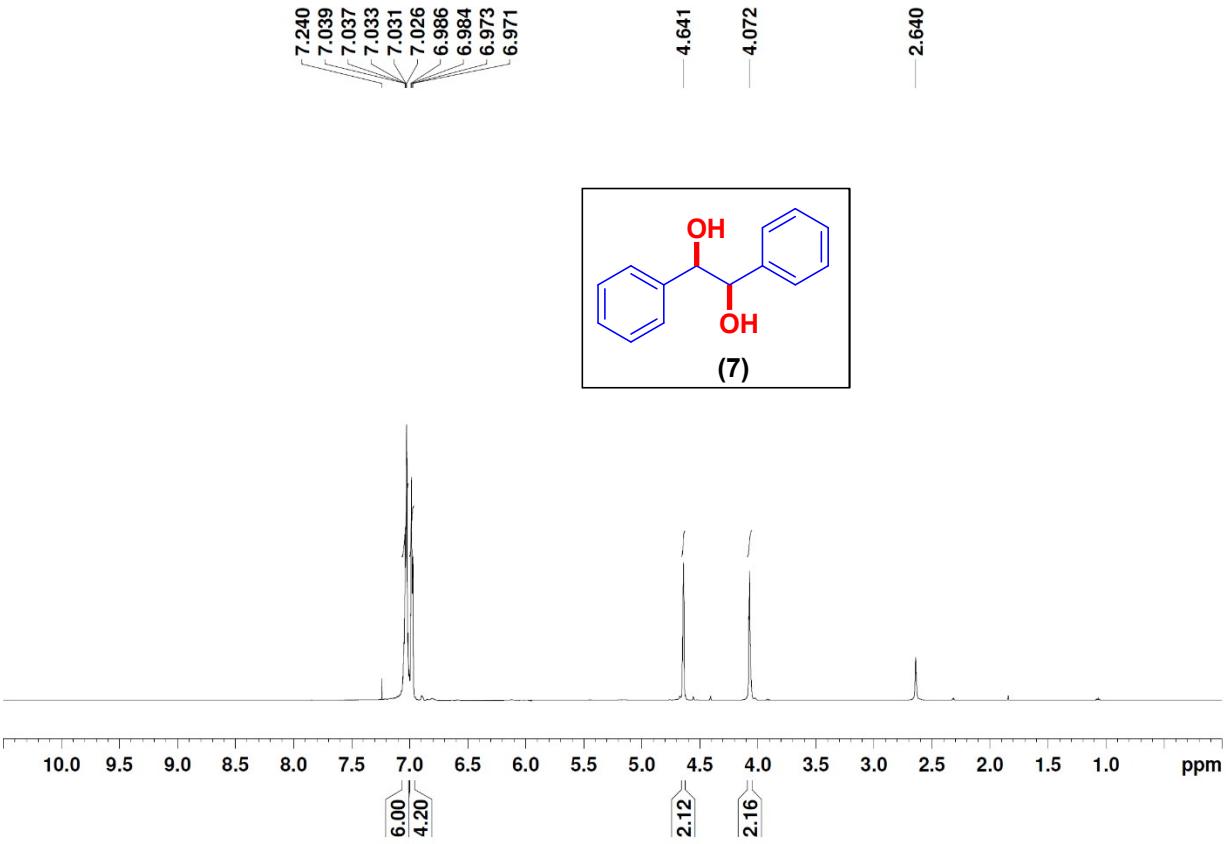

10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 ppm
2.00
2.00
1.99
3.30
6.27

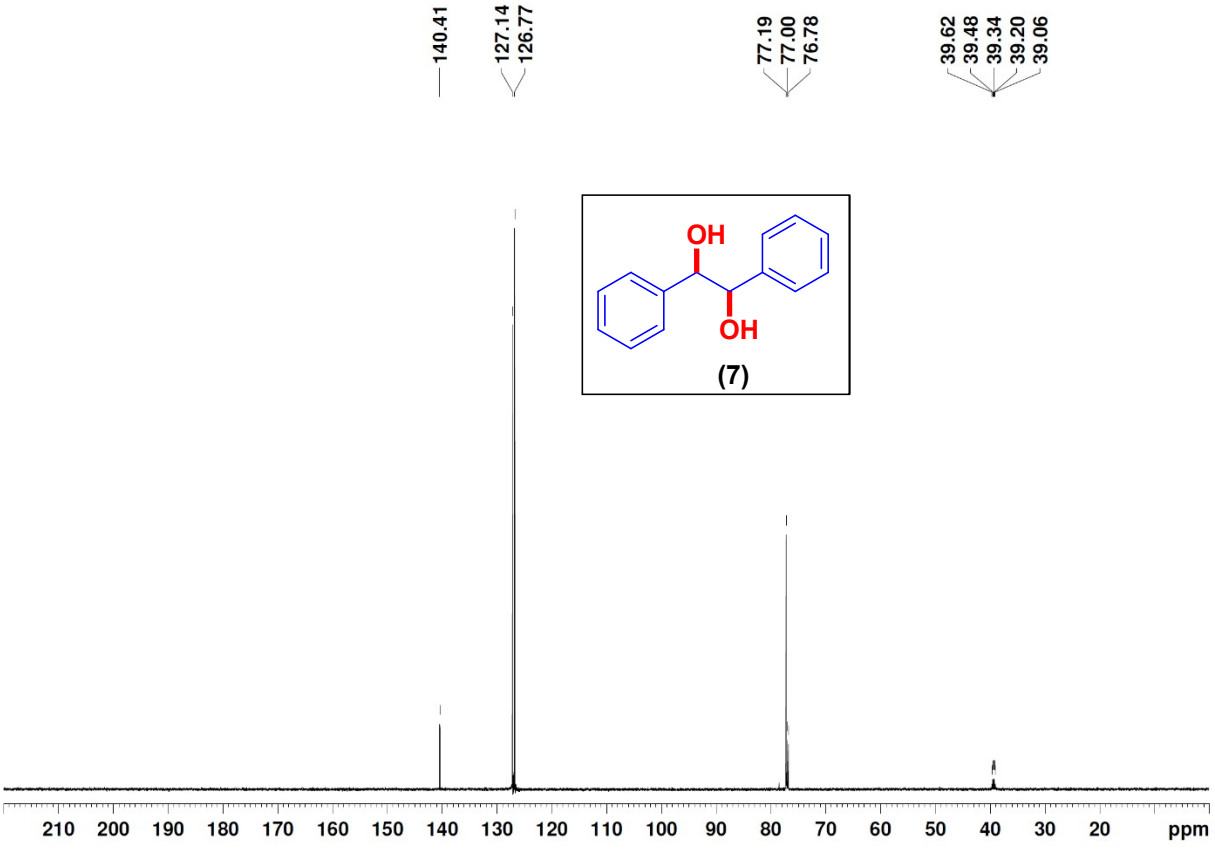

160.06
145.46
136.69
134.83
132.50
130.29
129.84
128.70
128.62
128.57
128.08
126.46
126.38
77.21
77.00
76.78

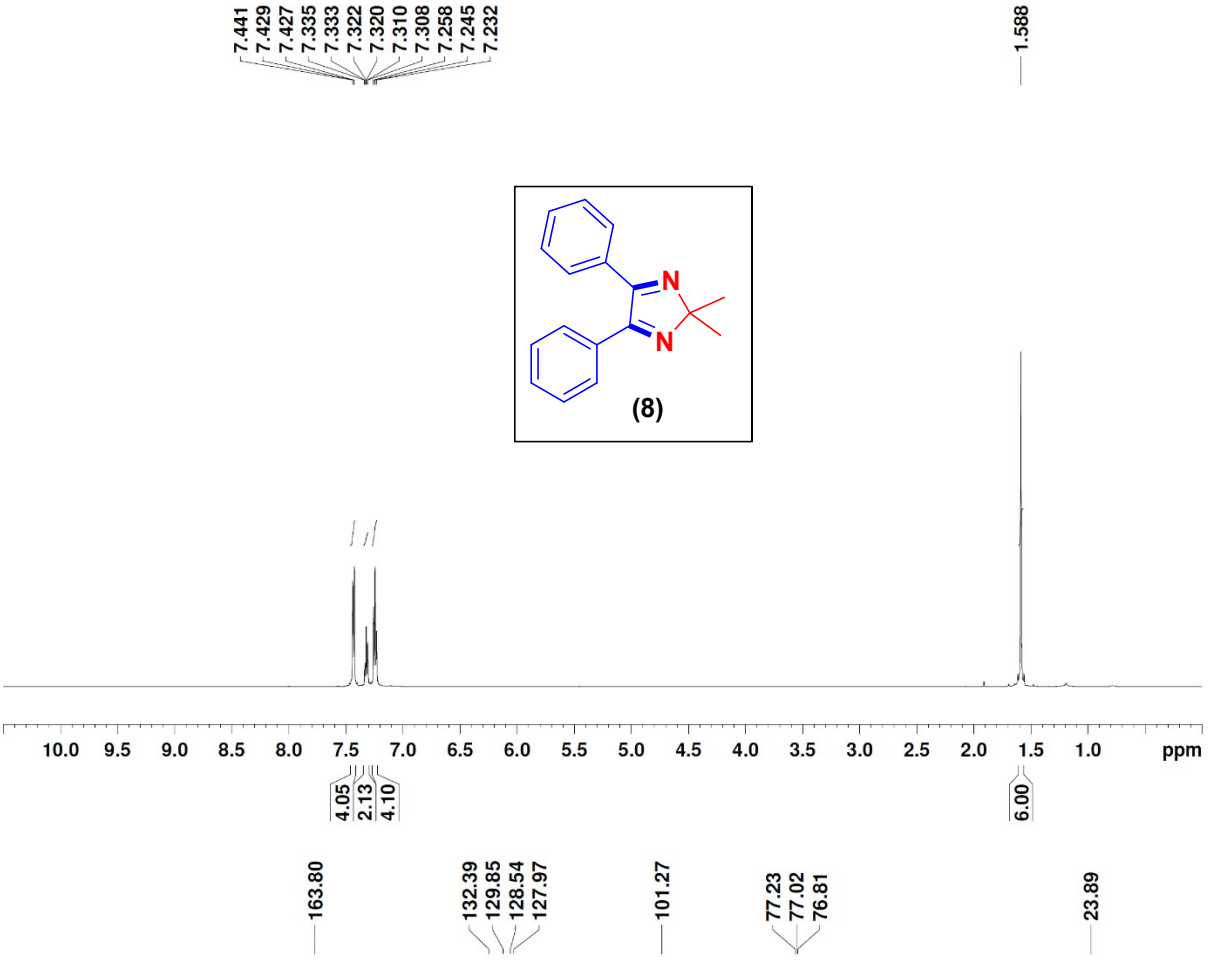

N
O

(6)


210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm


7.240
7.039
7.037
7.033
7.031
7.026
6.986
6.984
6.973
6.971
4.641
4.072
2.640
OH
OH
(7)
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 ppm
6.00
4.20
2.12
2.16


140.41
127.14
126.77
77.19
77.00
76.78
39.62
39.48
39.34
39.20
39.06
OH
OH
(7)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm


7.441
7.429
7.427
7.335
7.333
7.322
7.320
7.310
7.308
7.258
7.245
7.232
1.588
N
N
(8)
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 ppm
4.05
2.13
4.10
6.00

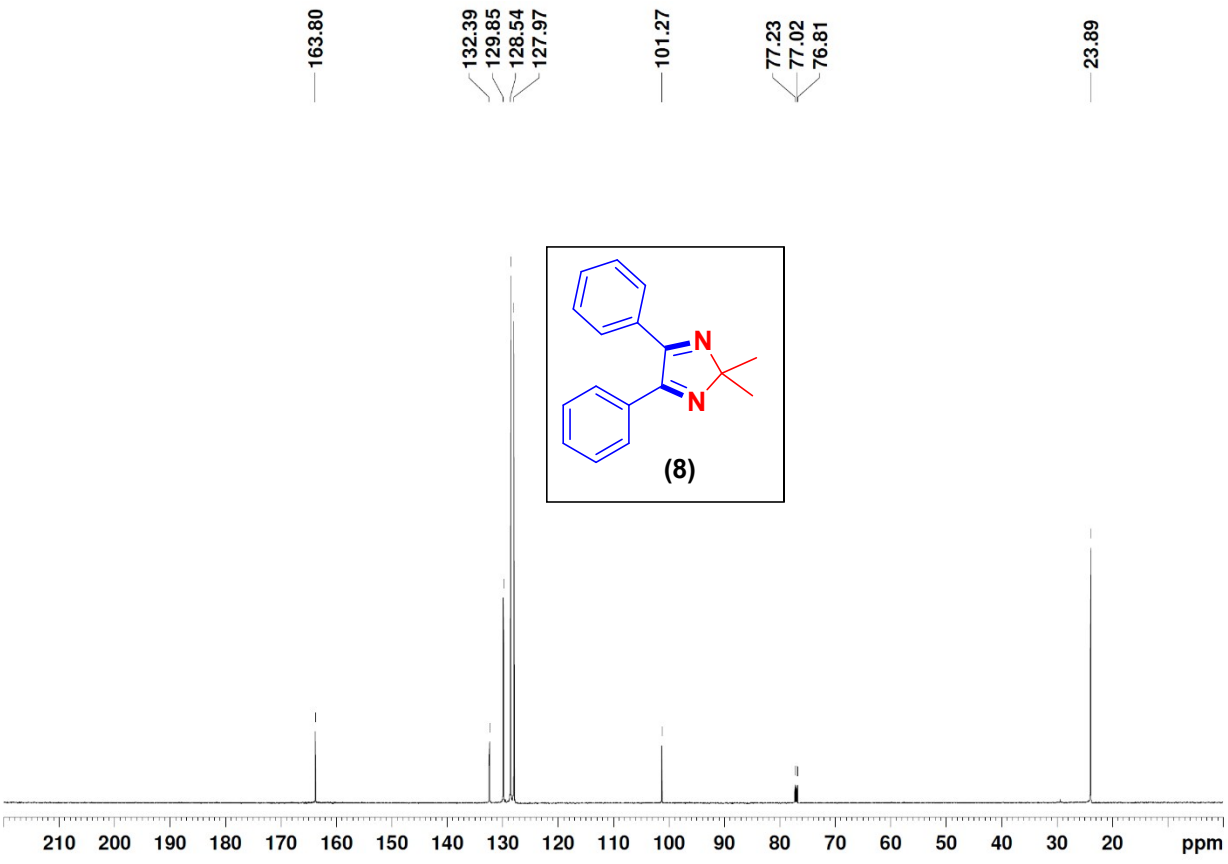
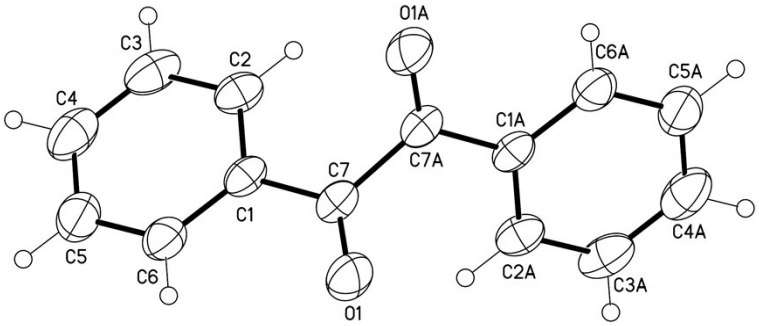

163.80
132.39
129.85
128.54
127.97
101.27
77.23
77.02
76.81
23.89
N
N
(8)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

Figure S3: ORTEP diagram of compound **2a (CCDC No. 1859205)**



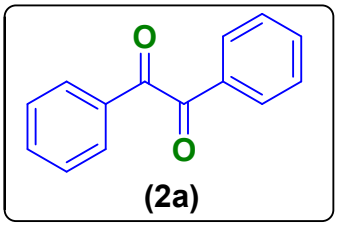


Table S1. Crystal data and structure refinement for 180116LT_0M_a.

Identification code	180116LT_0m_a	
Empirical formula	C14 H10 O2	
Formula weight	210.22	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Trigonal	
Space group	P 32 2 1	
Unit cell dimensions	a = 8.3601(7) Å	a= 90°.
	b = 8.3601(7) Å	b= 90°.
	c = 13.3968(12) Å	g = 120°.
Volume	810.88(15) $Å^3$	
Z	3	
Density (calculated)	1.291 Mg/m^3	
Absorption coefficient	0.086 mm^{-1}	
F(000)	330	
Crystal size	0.18 x 0.16 x 0.16 mm^3	
Theta range for data collection	2.813 to 26.509°.	
Index ranges	-10<=h<=10, -10<=k<=10, -16<=l<=16	
Reflections collected	10682	
Independent reflections	1127 [R(int) = 0.0333]	
Completeness to theta = 25.242°	100.0 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9485 and 0.7698	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	1127 / 0 / 74	

Goodness-of-fit on F^2	1.105
Final R indices [I>2sigma(I)]	R1 = 0.0295, wR2 = 0.0685
R indices (all data)	R1 = 0.0313, wR2 = 0.0695
Absolute structure parameter	0(2)
Extinction coefficient	n/a
Largest diff. peak and hole	0.144 and -0.131 e.$Å^{-3}$

Table S2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for 180116LT_0M_a. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	2346(2)	2085(2)	2450(1)	32(1)
C(2)	1826(2)	2964(2)	1749(1)	37(1)
C(3)	1825(3)	4570(2)	2001(1)	47(1)
C(4)	2361(3)	5303(3)	2948(1)	52(1)
C(5)	2888(3)	4441(3)	3650(1)	48(1)
C(6)	2880(2)	2831(2)	3407(1)	39(1)
C(7)	2305(2)	344(2)	2210(1)	35(1)
O(1)	2623(2)	-553(2)	2811(1)	49(1)

Table S3. Bond lengths [Å] and angles [°] for 180116LT_0M_a.

C(1)-C(2)	1.390(2)
C(1)-C(6)	1.397(2)
C(1)-C(7)	1.474(2)
C(2)-C(3)	1.386(2)
C(2)-H(2)	0.9500
C(3)-C(4)	1.383(3)
C(3)-H(3)	0.9500
C(4)-C(5)	1.384(3)
C(4)-H(4)	0.9500
C(5)-C(6)	1.381(3)
C(5)-H(5)	0.9500
C(6)-H(6)	0.9500
C(7)-O(1)	1.2166(19)

C(7)-C(7)#1	1.539(3)
C(2)-C(1)-C(6)	119.92(16)
C(2)-C(1)-C(7)	121.01(15)
C(6)-C(1)-C(7)	119.06(14)
C(3)-C(2)-C(1)	119.97(17)
C(3)-C(2)-H(2)	120.0
C(1)-C(2)-H(2)	120.0
C(4)-C(3)-C(2)	119.74(17)
C(4)-C(3)-H(3)	120.1
C(2)-C(3)-H(3)	120.1
C(3)-C(4)-C(5)	120.64(17)
C(3)-C(4)-H(4)	119.7
C(5)-C(4)-H(4)	119.7
C(6)-C(5)-C(4)	119.98(17)
C(6)-C(5)-H(5)	120.0
C(4)-C(5)-H(5)	120.0
C(5)-C(6)-C(1)	119.75(16)
C(5)-C(6)-H(6)	120.1
C(1)-C(6)-H(6)	120.1
O(1)-C(7)-C(1)	124.02(14)
O(1)-C(7)-C(7)#1	116.95(15)
C(1)-C(7)-C(7)#1	118.92(14)

Symmetry transformations used to generate equivalent atoms: #1 x-y,-y,-z+1/3

Table S4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for 180116LT_0M_a. The anisotropic displacement factor exponent takes the form: $-2p^2[\ h^2\ a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

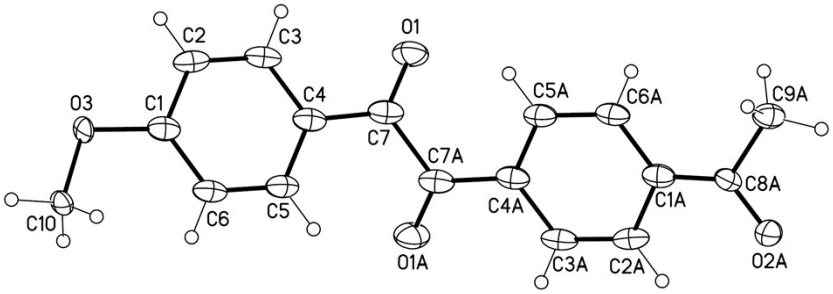
	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	25(1)	26(1)	41(1)	7(1)	7(1)	10(1)
C(2)	31(1)	36(1)	45(1)	10(1)	9(1)	16(1)
C(3)	48(1)	41(1)	60(1)	18(1)	16(1)	28(1)
C(4)	56(1)	35(1)	69(1)	9(1)	24(1)	26(1)
C(5)	51(1)	34(1)	52(1)	-1(1)	11(1)	16(1)

C(6)	37(1)	31(1)	43(1)	5(1)	4(1)	12(1)
C(7)	31(1)	26(1)	43(1)	5(1)	1(1)	11(1)
O(1)	63(1)	36(1)	51(1)	3(1)	-10(1)	27(1)

Table S5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for 180116LT_0M_a.

H(2)	1472	2463	1096	45
H(3)	1458	5167	1525	56
H(4)	2367	6409	3119	62
H(5)	3255	4955	4298	57
H(6)	3236	2234	3888	47

Figure S4: ORTEP diagram of compound **2ad (CCDC No. 1859723)**



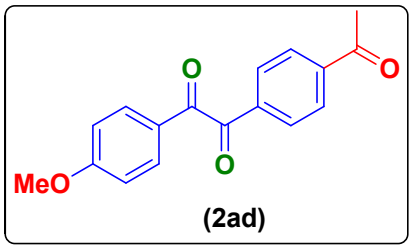


Table S6. Crystal data and structure refinement for twin5.

Identification code	twin5	
Empirical formula	C17 H14 O4	
Formula weight	282.28	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	C 2/c	
Unit cell dimensions	a = 23.502(2) Å	a= 90°.
	b = 3.9358(3) Å	b= 105.082(2)°.
	c = 15.1235(12) Å	g = 90°.
Volume	1350.73(19) $Å^3$	
Z	4	
Density (calculated)	1.388 Mg/m^3	
Absorption coefficient	0.099 mm^{-1}	
F(000)	592	
Crystal size	0.25 x 0.12 x 0.04 mm^3	
Theta range for data collection	1.795 to 26.552°.	
Index ranges	-28<=h<=28, 0<=k<=4, 0<=l<=19	
Reflections collected	1467	
Independent reflections	1467 [R(int) = 0.0370]	
Completeness to theta = 25.242°	99.8 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9485 and 0.7780	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	1467 / 52 / 122	
Goodness-of-fit on F^2	1.044	

Final R indices [I>2sigma(I)]	R1 = 0.0379, wR2 = 0.0865
R indices (all data)	R1 = 0.0537, wR2 = 0.0944
Extinction coefficient	n/a
Largest diff. peak and hole	0.208 and -0.172 e.Å^{-3}

Table S7. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^{2}x 10^3) for twin5. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

C(1)	3512(1)	8295(4)	3835(1)	24(1)
C(2)	3291(1)	6782(4)	2976(1)	27(1)
C(3)	3668(1)	5597(4)	2492(1)	26(1)
C(4)	4279(1)	5884(4)	2846(1)	24(1)
C(5)	4498(1)	7418(4)	3698(1)	27(1)
C(6)	4119(1)	8593(4)	4193(1)	26(1)
C(7)	4663(1)	4563(4)	2299(1)	27(1)
O(1)	4477(1)	3217(3)	1550(1)	34(1)
C(8)	3121(9)	9420(50)	4255(12)	21(2)
O(2)	2592(1)	9116(6)	3950(1)	31(1)
C(9)	3276(7)	10880(50)	5206(12)	27(2)
O(3)	3069(6)	9460(40)	4341(8)	21(2)
C(10)	3354(7)	11120(50)	5222(12)	22(2)

Table S8. Bond lengths [Å] and angles [°] for twin5.

C(1)-C(8)	1.32(2)
C(1)-C(6)	1.3930(19)
C(1)-C(2)	1.401(2)
C(1)-O(3)	1.515(14)
C(2)-C(3)	1.368(2)
C(2)-H(2)	0.9500
C(3)-C(4)	1.4002(19)
C(3)-H(3)	0.9500
C(4)-C(5)	1.3950(19)
C(4)-C(7)	1.469(2)
C(5)-C(6)	1.382(2)
C(5)-H(5)	0.9500
C(6)-H(6)	0.9500
C(7)-O(1)	1.2241(17)
C(7)-C(7)#1	1.542(3)
C(8)-O(2)	1.22(2)
C(8)-C(9)	1.50(2)
C(9)-H(9A)	0.9800
C(9)-H(9B)	0.9800
C(9)-H(9C)	0.9800
O(3)-C(10)	1.48(2)
C(10)-H(10A)	0.9800
C(10)-H(10B)	0.9800
C(10)-H(10C)	0.9800
C(8)-C(1)-C(6)	123.7(7)
C(8)-C(1)-C(2)	116.8(7)
C(6)-C(1)-C(2)	119.40(14)
C(6)-C(1)-O(3)	123.3(5)
C(2)-C(1)-O(3)	117.3(5)
C(3)-C(2)-C(1)	120.39(13)
C(3)-C(2)-H(2)	119.8
C(1)-C(2)-H(2)	119.8
C(2)-C(3)-C(4)	120.62(13)
C(2)-C(3)-H(3)	119.7

C(4)-C(3)-H(3)	119.7
C(5)-C(4)-C(3)	118.91(14)
C(5)-C(4)-C(7)	122.69(13)
C(3)-C(4)-C(7)	118.40(12)
C(6)-C(5)-C(4)	120.67(14)
C(6)-C(5)-H(5)	119.7
C(4)-C(5)-H(5)	119.7
C(5)-C(6)-C(1)	120.01(13)
C(5)-C(6)-H(6)	120.0
C(1)-C(6)-H(6)	120.0
O(1)-C(7)-C(4)	123.38(13)
O(1)-C(7)-C(7)#1	116.58(16)
C(4)-C(7)-C(7)#1	119.85(14)
O(2)-C(8)-C(1)	123.9(14)
O(2)-C(8)-C(9)	111.6(17)
C(1)-C(8)-C(9)	124.3(15)
C(8)-C(9)-H(9A)	109.5
C(8)-C(9)-H(9B)	109.5
H(9A)-C(9)-H(9B)	109.5
C(8)-C(9)-H(9C)	109.5
H(9A)-C(9)-H(9C)	109.5
H(9B)-C(9)-H(9C)	109.5
C(10)-O(3)-C(1)	112.2(11)
O(3)-C(10)-H(10A)	109.5
O(3)-C(10)-H(10B)	109.5
H(10A)-C(10)-H(10B)	109.5
O(3)-C(10)-H(10C)	109.5
H(10A)-C(10)-H(10C)	109.5
H(10B)-C(10)-H(10C)	109.5

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,y,-z+1/2

Table S9. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for twin5. The anisotropic displacement factor exponent takes the form: $-2p^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	30(1)	17(1)	22(1)	5(1)	-1(1)	0(1)
C(2)	27(1)	21(1)	26(1)	4(1)	-7(1)	-2(1)
C(3)	33(1)	18(1)	20(1)	1(1)	-7(1)	-2(1)
C(4)	30(1)	16(1)	20(1)	4(1)	-2(1)	-3(1)
C(5)	27(1)	26(1)	21(1)	1(1)	-3(1)	-6(1)
C(6)	31(1)	23(1)	20(1)	1(1)	-4(1)	-6(1)
C(7)	32(1)	21(1)	23(1)	2(1)	-4(1)	-2(1)
O(1)	34(1)	38(1)	26(1)	-10(1)	-2(1)	-3(1)
C(8)	25(3)	23(2)	15(2)	-1(2)	3(3)	2(2)
O(2)	23(1)	44(1)	24(1)	-5(1)	5(1)	5(1)
C(9)	29(4)	24(3)	24(3)	-1(2)	1(3)	6(3)
O(3)	20(2)	27(2)	19(3)	-2(2)	9(2)	10(2)
C(10)	22(3)	28(4)	16(3)	-5(2)	7(2)	6(3)

Table S10. Hydrogen coordinates ($x\ 10^4$) and isotropic displacement parameters ($Å^2 x\ 10^3$) for twin5.

	x	y	z	U(eq)
H(2)	2878	6577	2727	32
H(3)	3513	4569	1910	32
H(5)	4911	7657	3941	32
H(6)	4273	9605	4776	32
H(9A)	2916	11156	5412	40
H(9B)	3465	13096	5204	40
H(9C)	3546	9340	5623	40
H(10A)	3594	9449	5638	33
H(10B)	3052	12028	5497	33
H(10C)	3606	12974	5116	33

Figure S5: ORTEP diagram of compound **4 (CCDC No. 1859204)**

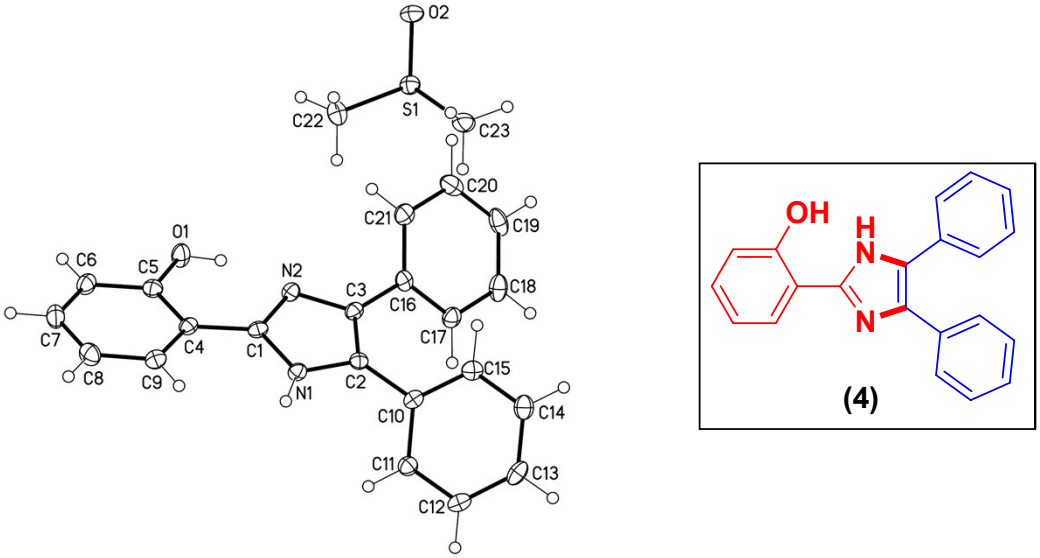


Table S11. Crystal data and structure refinement for mo_180117lt_0m_a.

Identification code	mo_180117lt_0m_a	
Empirical formula	C23 H22 N2 O2 S	
Formula weight	390.48	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P -1	
Unit cell dimensions	a = 9.3322(5) Å	a= 95.845(2)°.
	b = 10.0321(5) Å	b= 105.956(2)°.
	c = 11.8425(6) Å	g = 109.513(2)°.
Volume	981.56(9) $Å^3$	
Z	2	
Density (calculated)	1.321 Mg/m^3	
Absorption coefficient	0.186 mm^{-1}	
F(000)	412	
Crystal size	0.16 x 0.13 x 0.12 mm^3	
Theta range for data collection	1.831 to 26.568°.	
Index ranges	-11<=h<=11, -12<=k<=12, -14<=l<=14	
Reflections collected	28567	
Independent reflections	4075 [R(int) = 0.0443]	

Completeness to theta = 25.242°	99.9 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9485 and 0.8862
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	4075 / 0 / 256
Goodness-of-fit on F^2	1.139
Final R indices [I>2sigma(I)]	R1 = 0.0397, wR2 = 0.1006
R indices (all data)	R1 = 0.0566, wR2 = 0.1081
Extinction coefficient	n/a
Largest diff. peak and hole	0.296 and -0.428 e.$Å^{-3}$

Table S12. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for mo_180117lt_0m_a. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	6025(2)	3360(2)	4578(2)	14(1)
C(2)	5438(2)	3444(2)	6263(2)	14(1)
C(3)	6819(2)	4607(2)	6399(2)	14(1)
C(4)	6005(2)	2873(2)	3368(2)	15(1)
C(5)	7365(2)	3546(2)	3034(2)	16(1)
C(6)	7364(3)	3106(2)	1878(2)	19(1)
C(7)	6025(3)	2017(2)	1056(2)	21(1)
C(8)	4676(3)	1336(2)	1373(2)	21(1)
C(9)	4676(3)	1755(2)	2521(2)	18(1)
C(10)	4551(2)	2980(2)	7095(2)	15(1)
C(11)	3951(2)	1519(2)	7153(2)	17(1)
C(12)	3112(3)	1074(2)	7936(2)	20(1)
C(13)	2870(3)	2085(2)	8676(2)	21(1)
C(14)	3477(3)	3535(2)	8637(2)	21(1)
C(15)	4303(2)	3986(2)	7849(2)	18(1)
C(16)	7889(2)	5766(2)	7463(2)	15(1)
C(17)	8278(2)	5469(2)	8614(2)	17(1)
C(18)	9293(3)	6577(2)	9604(2)	22(1)
C(19)	9924(3)	7988(2)	9467(2)	24(1)

C(20)	9545(3)	8289(2)	8331(2)	22(1)
C(21)	8554(2)	7188(2)	7336(2)	19(1)
C(22)	1042(3)	7558(2)	2964(2)	23(1)
C(23)	259(3)	8251(2)	4897(2)	26(1)
N(1)	4950(2)	2667(2)	5104(2)	14(1)
N(2)	7170(2)	4539(2)	5339(2)	15(1)
O(1)	8705(2)	4624(2)	3804(1)	20(1)
O(2)	2057(2)	10276(2)	4054(1)	20(1)
S(1)	1930(1)	8825(1)	4367(1)	17(1)

Table S13. Bond lengths [Å] and angles [°] for mo_180117lt_0m_a.

C(1)-N(2)	1.328(3)
C(1)-N(1)	1.357(3)
C(1)-C(4)	1.460(3)
C(2)-C(3)	1.376(3)
C(2)-N(1)	1.379(3)
C(2)-C(10)	1.468(3)
C(3)-N(2)	1.382(3)
C(3)-C(16)	1.473(3)
C(4)-C(9)	1.400(3)
C(4)-C(5)	1.408(3)
C(5)-O(1)	1.354(2)
C(5)-C(6)	1.394(3)
C(6)-C(7)	1.380(3)
C(6)-H(6)	0.9500
C(7)-C(8)	1.389(3)
C(7)-H(7)	0.9500
C(8)-C(9)	1.381(3)
C(8)-H(8)	0.9500
C(9)-H(9)	0.9500
C(10)-C(15)	1.398(3)
C(10)-C(11)	1.400(3)
C(11)-C(12)	1.386(3)
C(11)-H(11)	0.9500
C(12)-C(13)	1.389(3)

C(12)-H(12)	0.9500
C(13)-C(14)	1.384(3)
C(13)-H(13)	0.9500
C(14)-C(15)	1.385(3)
C(14)-H(14)	0.9500
C(15)-H(15)	0.9500
C(16)-C(21)	1.395(3)
C(16)-C(17)	1.400(3)
C(17)-C(18)	1.388(3)
C(17)-H(17)	0.9500
C(18)-C(19)	1.385(3)
C(18)-H(18)	0.9500
C(19)-C(20)	1.386(3)
C(19)-H(19)	0.9500
C(20)-C(21)	1.385(3)
C(20)-H(20)	0.9500
C(21)-H(21)	0.9500
C(22)-S(1)	1.780(2)
C(22)-H(22A)	0.9800
C(22)-H(22B)	0.9800
C(22)-H(22C)	0.9800
C(23)-S(1)	1.780(2)
C(23)-H(23A)	0.9800
C(23)-H(23B)	0.9800
C(23)-H(23C)	0.9800
N(1)-H(1)	0.8800
O(1)-H(1A)	0.8400
O(2)-S(1)	1.5132(15)
N(2)-C(1)-N(1)	110.60(18)
N(2)-C(1)-C(4)	123.34(18)
N(1)-C(1)-C(4)	126.00(18)
C(3)-C(2)-N(1)	105.95(17)
C(3)-C(2)-C(10)	131.95(19)
N(1)-C(2)-C(10)	122.10(17)
C(2)-C(3)-N(2)	109.12(18)
C(2)-C(3)-C(16)	129.79(19)

N(2)-C(3)-C(16)	121.04(18)
C(9)-C(4)-C(5)	118.53(19)
C(9)-C(4)-C(1)	122.30(19)
C(5)-C(4)-C(1)	119.17(18)
O(1)-C(5)-C(6)	117.77(19)
O(1)-C(5)-C(4)	122.18(18)
C(6)-C(5)-C(4)	120.05(19)
C(7)-C(6)-C(5)	120.1(2)
C(7)-C(6)-H(6)	120.0
C(5)-C(6)-H(6)	120.0
C(6)-C(7)-C(8)	120.6(2)
C(6)-C(7)-H(7)	119.7
C(8)-C(7)-H(7)	119.7
C(9)-C(8)-C(7)	119.6(2)
C(9)-C(8)-H(8)	120.2
C(7)-C(8)-H(8)	120.2
C(8)-C(9)-C(4)	121.1(2)
C(8)-C(9)-H(9)	119.4
C(4)-C(9)-H(9)	119.4
C(15)-C(10)-C(11)	118.87(19)
C(15)-C(10)-C(2)	120.82(18)
C(11)-C(10)-C(2)	120.30(18)
C(12)-C(11)-C(10)	120.6(2)
C(12)-C(11)-H(11)	119.7
C(10)-C(11)-H(11)	119.7
C(11)-C(12)-C(13)	119.9(2)
C(11)-C(12)-H(12)	120.1
C(13)-C(12)-H(12)	120.1
C(14)-C(13)-C(12)	120.0(2)
C(14)-C(13)-H(13)	120.0
C(12)-C(13)-H(13)	120.0
C(13)-C(14)-C(15)	120.5(2)
C(13)-C(14)-H(14)	119.8
C(15)-C(14)-H(14)	119.8
C(14)-C(15)-C(10)	120.2(2)
C(14)-C(15)-H(15)	119.9

C(10)-C(15)-H(15)	119.9
C(21)-C(16)-C(17)	118.66(19)
C(21)-C(16)-C(3)	120.13(19)
C(17)-C(16)-C(3)	121.21(19)
C(18)-C(17)-C(16)	120.2(2)
C(18)-C(17)-H(17)	119.9
C(16)-C(17)-H(17)	119.9
C(19)-C(18)-C(17)	120.5(2)
C(19)-C(18)-H(18)	119.7
C(17)-C(18)-H(18)	119.7
C(18)-C(19)-C(20)	119.5(2)
C(18)-C(19)-H(19)	120.2
C(20)-C(19)-H(19)	120.2
C(21)-C(20)-C(19)	120.4(2)
C(21)-C(20)-H(20)	119.8
C(19)-C(20)-H(20)	119.8
C(20)-C(21)-C(16)	120.6(2)
C(20)-C(21)-H(21)	119.7
C(16)-C(21)-H(21)	119.7
S(1)-C(22)-H(22A)	109.5
S(1)-C(22)-H(22B)	109.5
H(22A)-C(22)-H(22B)	109.5
S(1)-C(22)-H(22C)	109.5
H(22A)-C(22)-H(22C)	109.5
H(22B)-C(22)-H(22C)	109.5
S(1)-C(23)-H(23A)	109.5
S(1)-C(23)-H(23B)	109.5
H(23A)-C(23)-H(23B)	109.5
S(1)-C(23)-H(23C)	109.5
H(23A)-C(23)-H(23C)	109.5
H(23B)-C(23)-H(23C)	109.5
C(1)-N(1)-C(2)	107.80(16)
C(1)-N(1)-H(1)	126.1
C(2)-N(1)-H(1)	126.1
C(1)-N(2)-C(3)	106.53(17)
C(5)-O(1)-H(1A)	109.5

O(2)-S(1)-C(23)	106.55(10)
O(2)-S(1)-C(22)	105.34(10)
C(23)-S(1)-C(22)	97.70(11)

Symmetry transformations used to generate equivalent atoms:

Table S14. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for mo_180117lt_0m_a. The anisotropic displacement factor exponent takes the form: $-2p^2[\ h^2\ a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

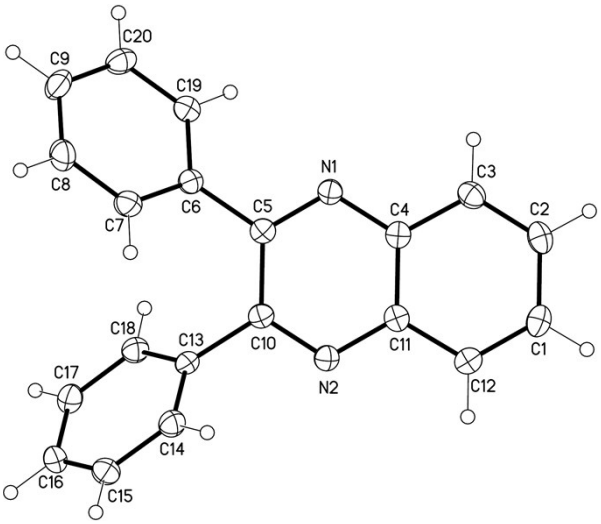
	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	13(1)	14(1)	16(1)	6(1)	4(1)	5(1)
C(2)	13(1)	14(1)	15(1)	4(1)	4(1)	7(1)
C(3)	15(1)	16(1)	15(1)	6(1)	6(1)	7(1)
C(4)	16(1)	16(1)	14(1)	6(1)	5(1)	7(1)
C(5)	16(1)	15(1)	17(1)	4(1)	4(1)	7(1)
C(6)	19(1)	22(1)	19(1)	7(1)	10(1)	10(1)
C(7)	25(1)	24(1)	16(1)	3(1)	8(1)	12(1)
C(8)	20(1)	20(1)	18(1)	0(1)	2(1)	6(1)
C(9)	16(1)	18(1)	19(1)	6(1)	6(1)	6(1)
C(10)	11(1)	17(1)	15(1)	6(1)	3(1)	5(1)
C(11)	17(1)	17(1)	17(1)	4(1)	5(1)	7(1)
C(12)	21(1)	20(1)	21(1)	10(1)	7(1)	7(1)
C(13)	16(1)	30(1)	18(1)	10(1)	9(1)	8(1)
C(14)	18(1)	26(1)	20(1)	3(1)	8(1)	10(1)
C(15)	15(1)	18(1)	21(1)	5(1)	6(1)	6(1)
C(16)	11(1)	18(1)	18(1)	2(1)	7(1)	6(1)
C(17)	16(1)	19(1)	18(1)	4(1)	8(1)	5(1)
C(18)	17(1)	32(1)	18(1)	1(1)	8(1)	9(1)
C(19)	15(1)	24(1)	25(1)	-9(1)	7(1)	1(1)
C(20)	18(1)	16(1)	34(1)	2(1)	14(1)	5(1)
C(21)	15(1)	21(1)	22(1)	4(1)	10(1)	6(1)
C(22)	24(1)	23(1)	18(1)	0(1)	6(1)	9(1)
C(23)	32(1)	16(1)	35(1)	7(1)	22(1)	6(1)
N(1)	11(1)	14(1)	15(1)	3(1)	4(1)	2(1)

N(2)	14(1)	16(1)	14(1)	4(1)	5(1)	5(1)
O(1)	16(1)	22(1)	18(1)	0(1)	8(1)	1(1)
O(2)	20(1)	14(1)	23(1)	6(1)	7(1)	3(1)
S(1)	16(1)	17(1)	16(1)	4(1)	4(1)	6(1)

Table S15. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^{2}x 10^3) for mo_180117lt_0m_a.

H(6)	8286	3556	1656	22
H(7)	6026	1730	267	25
H(8)	3758	586	804	26
H(9)	3758	1277	2739	21
H(11)	4120	826	6651	20
H(12)	2703	80	7965	24
H(13)	2289	1781	9209	25
H(14)	3326	4226	9155	25
H(15)	4703	4981	7821	21
H(17)	7846	4506	8718	21
H(18)	9558	6366	10381	27
H(19)	10611	8743	10148	28
H(20)	9968	9257	8234	27
H(21)	8324	7403	6558	22
H(22A)	89	7700	2481	34
H(22B)	726	6571	3106	34
H(22C)	1822	7704	2533	34
H(23A)	467	8944	5625	39
H(23B)	103	7293	5081	39
H(23C)	-712	8202	4276	39
H(1)	4094	1865	4765	17
H(1A)	8557	4819	4459	31

Figure S6: ORTEP diagram of compound **5 (CCDC No. 1859203)**



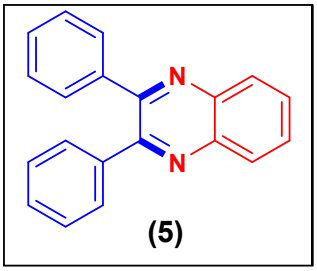


Table S16. Crystal data and structure refinement for mo_170751lt_0m.

Identification code	mo_170751LT_0m	
Empirical formula	C20 H14 N2	
Formula weight	282.33	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 21/n	
Unit cell dimensions	a = 6.0178(13) Å	a= 90°.
	b = 10.934(2) Å	b= 95.035(4)°.
	c = 22.509(5) Å	g = 90°.
Volume	1475.3(6) $Å^3$	
Z	4	
Density (calculated)	1.271 Mg/m^3	
Absorption coefficient	0.075 mm^{-1}	
F(000)	592	
Crystal size	0.25 x 0.20 x 0.20 mm^3	
Theta range for data collection	1.816 to 26.698°.	
Index ranges	-7<=h<=4, -13<=k<=13, -28<=l<=28	
Reflections collected	11963	
Independent reflections	3101 [R(int) = 0.0501]	
Completeness to theta = 25.242°	99.8 %	

Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9485 and 0.6897
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3101 / 0 / 199
Goodness-of-fit on F^2	1.055
Final R indices [I>2sigma(I)]	R1 = 0.0452, wR2 = 0.1197
R indices (all data)	R1 = 0.0571, wR2 = 0.1278
Extinction coefficient	n/a
Largest diff. peak and hole	0.304 and -0.275 e.Å^{-3}

Table S17. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^{2}x 10^3) for mo_170751lt_0m. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

N(1)	5096(2)	132(1)	2411(1)	18(1)
N(2)	7347(2)	2070(1)	1898(1)	19(1)
C(1)	10927(3)	1560(1)	3268(1)	23(1)
C(2)	9732(3)	627(1)	3537(1)	23(1)
C(3)	7782(3)	177(1)	3265(1)	22(1)
C(4)	6956(2)	643(1)	2701(1)	18(1)
C(5)	4407(2)	571(1)	1881(1)	17(1)
C(6)	2513(2)	-96(1)	1556(1)	18(1)
C(7)	2405(3)	-297(1)	940(1)	23(1)
C(8)	630(3)	-947(2)	657(1)	28(1)
C(9)	-1049(3)	-1388(1)	980(1)	27(1)
C(10)	5485(2)	1607(1)	1636(1)	18(1)
C(11)	8143(2)	1579(1)	2433(1)	18(1)
C(12)	10152(2)	2034(1)	2726(1)	20(1)
C(13)	4574(2)	2262(1)	1086(1)	18(1)
C(14)	5951(2)	2474(1)	632(1)	23(1)
C(15)	5191(3)	3147(2)	132(1)	26(1)
C(16)	3056(3)	3628(1)	87(1)	25(1)
C(17)	1677(3)	3418(1)	539(1)	25(1)
C(18)	2417(2)	2731(1)	1035(1)	22(1)
C(19)	853(2)	-585(1)	1879(1)	19(1)

C(20)	-931(3)	-1213(1)	1593(1)	24(1)

Table S18. Bond lengths [Å] and angles [°] for mo_170751lt_0m.

N(1)-C(5)	1.3191(18)
N(1)-C(4)	1.3647(18)
N(2)-C(10)	1.3203(18)
N(2)-C(11)	1.3669(17)
C(1)-C(12)	1.370(2)
C(1)-C(2)	1.414(2)
C(1)-H(1)	0.9500
C(2)-C(3)	1.368(2)
C(2)-H(3)	0.9500
C(3)-C(4)	1.4153(19)
C(3)-H(14)	0.9500
C(4)-C(11)	1.414(2)
C(5)-C(10)	1.440(2)
C(5)-C(6)	1.4901(18)
C(6)-C(19)	1.393(2)
C(6)-C(7)	1.3990(19)
C(7)-C(8)	1.389(2)
C(7)-H(10)	0.9500
C(8)-C(9)	1.382(2)
C(8)-H(11)	0.9500
C(9)-C(20)	1.388(2)
C(9)-H(2)	0.9500
C(10)-C(13)	1.4910(19)
C(11)-C(12)	1.4151(19)
C(12)-H(4)	0.9500
C(13)-C(14)	1.391(2)
C(13)-C(18)	1.391(2)
C(14)-C(15)	1.388(2)
C(14)-H(9)	0.9500
C(15)-C(16)	1.384(2)
C(15)-H(8)	0.9500
C(16)-C(17)	1.387(2)

C(16)-H(7)	0.9500
C(17)-C(18)	1.386(2)
C(17)-H(6)	0.9500
C(18)-H(5)	0.9500
C(19)-C(20)	1.385(2)
C(19)-H(13)	0.9500
C(20)-H(12)	0.9500
C(5)-N(1)-C(4)	117.60(12)
C(10)-N(2)-C(11)	117.46(12)
C(12)-C(1)-C(2)	120.53(13)
C(12)-C(1)-H(1)	119.7
C(2)-C(1)-H(1)	119.7
C(3)-C(2)-C(1)	121.09(13)
C(3)-C(2)-H(3)	119.5
C(1)-C(2)-H(3)	119.5
C(2)-C(3)-C(4)	119.49(14)
C(2)-C(3)-H(14)	120.3
C(4)-C(3)-H(14)	120.3
N(1)-C(4)-C(11)	121.07(12)
N(1)-C(4)-C(3)	119.32(13)
C(11)-C(4)-C(3)	119.50(13)
N(1)-C(5)-C(10)	121.13(12)
N(1)-C(5)-C(6)	115.66(13)
C(10)-C(5)-C(6)	123.18(12)
C(19)-C(6)-C(7)	118.90(13)
C(19)-C(6)-C(5)	118.93(12)
C(7)-C(6)-C(5)	122.10(13)
C(8)-C(7)-C(6)	120.09(14)
C(8)-C(7)-H(10)	120.0
C(6)-C(7)-H(10)	120.0
C(9)-C(8)-C(7)	120.37(14)
C(9)-C(8)-H(11)	119.8
C(7)-C(8)-H(11)	119.8
C(8)-C(9)-C(20)	119.87(14)
C(8)-C(9)-H(2)	120.1
C(20)-C(9)-H(2)	120.1

N(2)-C(10)-C(5)	121.60(12)
N(2)-C(10)-C(13)	114.95(12)
C(5)-C(10)-C(13)	123.42(12)
N(2)-C(11)-C(4)	120.64(12)
N(2)-C(11)-C(12)	119.47(13)
C(4)-C(11)-C(12)	119.87(12)
C(1)-C(12)-C(11)	119.52(14)
C(1)-C(12)-H(4)	120.2
C(11)-C(12)-H(4)	120.2
C(14)-C(13)-C(18)	119.26(13)
C(14)-C(13)-C(10)	119.37(13)
C(18)-C(13)-C(10)	121.26(13)
C(15)-C(14)-C(13)	120.62(14)
C(15)-C(14)-H(9)	119.7
C(13)-C(14)-H(9)	119.7
C(16)-C(15)-C(14)	119.90(14)
C(16)-C(15)-H(8)	120.1
C(14)-C(15)-H(8)	120.1
C(15)-C(16)-C(17)	119.66(13)
C(15)-C(16)-H(7)	120.2
C(17)-C(16)-H(7)	120.2
C(18)-C(17)-C(16)	120.64(14)
C(18)-C(17)-H(6)	119.7
C(16)-C(17)-H(6)	119.7
C(17)-C(18)-C(13)	119.91(14)
C(17)-C(18)-H(5)	120.0
C(13)-C(18)-H(5)	120.0
C(20)-C(19)-C(6)	120.66(13)
C(20)-C(19)-H(13)	119.7
C(6)-C(19)-H(13)	119.7
C(19)-C(20)-C(9)	120.03(14)
C(19)-C(20)-H(12)	120.0
C(9)-C(20)-H(12)	120.0

Symmetry transformations used to generate equivalent atoms:

Table S19. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for mo_170751lt_0m. The

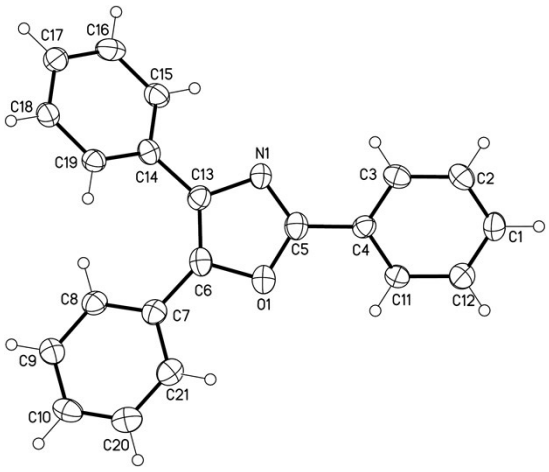
anisotropic displacement factor exponent takes the form: $-2p^2[h^2 a^{*2}U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
N(1)	17(1)	20(1)	17(1)	-1(1)	3(1)	0(1)
N(2)	18(1)	19(1)	19(1)	0(1)	2(1)	1(1)
C(1)	20(1)	24(1)	24(1)	-6(1)	-2(1)	2(1)
C(2)	27(1)	26(1)	17(1)	-2(1)	0(1)	6(1)
C(3)	26(1)	22(1)	19(1)	1(1)	4(1)	1(1)
C(4)	17(1)	19(1)	18(1)	-2(1)	3(1)	3(1)
C(5)	16(1)	19(1)	17(1)	-2(1)	5(1)	2(1)
C(6)	17(1)	16(1)	20(1)	1(1)	2(1)	2(1)
C(7)	26(1)	24(1)	20(1)	1(1)	3(1)	-3(1)
C(8)	33(1)	28(1)	20(1)	-1(1)	-4(1)	-2(1)
C(9)	22(1)	24(1)	33(1)	-3(1)	-5(1)	-4(1)
C(10)	17(1)	18(1)	18(1)	-1(1)	4(1)	0(1)
C(11)	18(1)	18(1)	17(1)	-2(1)	3(1)	3(1)
C(12)	19(1)	20(1)	22(1)	-3(1)	4(1)	0(1)
C(13)	19(1)	18(1)	18(1)	0(1)	0(1)	-4(1)
C(14)	19(1)	27(1)	22(1)	1(1)	2(1)	-2(1)
C(15)	27(1)	33(1)	18(1)	3(1)	4(1)	-6(1)
C(16)	30(1)	26(1)	19(1)	4(1)	-5(1)	-6(1)
C(17)	21(1)	26(1)	27(1)	1(1)	-4(1)	-1(1)
C(18)	19(1)	26(1)	22(1)	1(1)	3(1)	-3(1)
C(19)	19(1)	18(1)	21(1)	1(1)	3(1)	3(1)
C(20)	18(1)	22(1)	32(1)	1(1)	5(1)	-2(1)

Table S20. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^{2}x 10^3) for mo_170751lt_0m.

	x	y	z	U(eq)
H(1)	12277	1862	3466	27
H(3)	10294	309	3913	28
H(14)	6988	-444	3452	26
H(10)	3546	10	715	28
H(11)	571	-1088	240	33
H(2)	-2282	-1810	783	32
H(4)	10957	2662	2548	24
H(9)	7425	2155	664	27
H(8)	6135	3277	-179	31
H(7)	2538	4100	-251	30
H(6)	211	3748	508	30
H(5)	1452	2580	1339	27
H(13)	946	-487	2299	23
H(12)	-2075	-1525	1816	29

Figure S7: ORTEP diagram of compound **6 (CCDC No. 1911059)**



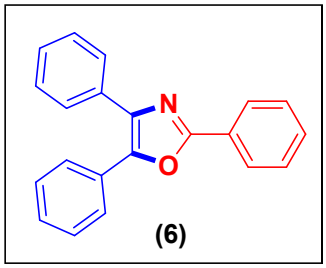


Table S21. Crystal data and structure refinement for 190333lt.

Identification code	190333LT	
Empirical formula	C21 H15 N O	
Formula weight	297.34	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	Pbca	
Unit cell dimensions	a = 19.711(2) Å	a= 90°.
	b = 7.4314(9) Å	b= 90°.
	c = 20.568(2) Å	g = 90°.
Volume	3012.9(6) $Å^3$	
Z	8	
Density (calculated)	1.311 Mg/m^3	
Absorption coefficient	0.080 mm^{-1}	
F(000)	1248	
Crystal size	0.20 x 0.08 x 0.08 mm^3	
Theta range for data collection	1.980 to 26.419°.	
Index ranges	-24<=h<=24, -9<=k<=8, -25<=l<=25	
Reflections collected	16418	
Independent reflections	3037 [R(int) = 0.0457]	
Completeness to theta = 25.242°	97.9 %	

Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.7454 and 0.5925
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3037 / 0 / 209
Goodness-of-fit on F^2	1.156
Final R indices [I>2sigma(I)]	R1 = 0.0611, wR2 = 0.1553
R indices (all data)	R1 = 0.1048, wR2 = 0.2427
Extinction coefficient	0.0030(10)
Largest diff. peak and hole	0.459 and -0.472 e.Å^{-3}

Table S22. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^{2}x 10^3) for 190333lt. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
O(1)	1928(1)	8107(3)	3574(1)	33(1)
N(1)	2587(1)	7639(3)	2723(1)	26(1)
C(1)	4254(2)	8326(5)	4607(2)	32(1)
C(2)	4312(2)	8790(4)	3957(2)	31(1)
C(3)	3764(2)	8659(4)	3546(2)	29(1)
C(4)	3137(2)	8056(4)	3786(1)	25(1)
C(5)	2561(2)	7928(4)	3351(2)	30(1)
C(6)	1508(2)	7927(4)	3032(2)	29(1)
C(7)	777(2)	8018(4)	3145(2)	29(1)
C(8)	316(2)	7142(4)	2735(2)	29(1)
C(9)	-371(2)	7215(4)	2858(2)	29(1)
C(10)	-615(2)	8139(4)	3394(2)	34(1)
C(11)	3080(2)	7600(5)	4436(2)	32(1)
C(12)	3636(2)	7737(5)	4844(2)	33(1)
C(13)	1918(2)	7647(4)	2507(2)	27(1)
C(14)	1792(2)	7372(4)	1817(2)	25(1)
C(15)	2221(2)	6226(4)	1466(2)	30(1)
C(16)	2126(2)	5952(5)	803(2)	34(1)
C(17)	1610(2)	6845(5)	481(2)	34(1)
C(18)	1190(2)	8022(4)	820(2)	30(1)

C(19)	1279(2)	8271(4)	1484(2)	26(1)
C(20)	-163(2)	9008(5)	3805(2)	36(1)
C(21)	523(2)	8952(4)	3688(2)	32(1)

Table S23. Bond lengths [Å] and angles [°] for 190333lt.

O(1)-C(5)	1.337(4)
O(1)-C(6)	1.393(4)
N(1)-C(5)	1.310(4)
N(1)-C(13)	1.391(4)
C(1)-C(12)	1.382(5)
C(1)-C(2)	1.386(5)
C(1)-H(1)	0.9500
C(2)-C(3)	1.374(5)
C(2)-H(15)	0.9500
C(3)-C(4)	1.404(4)
C(3)-H(3)	0.9500
C(4)-C(11)	1.385(4)
C(4)-C(5)	1.448(4)
C(6)-C(13)	1.365(5)
C(6)-C(7)	1.462(5)
C(7)-C(8)	1.400(5)
C(7)-C(21)	1.407(5)
C(8)-C(9)	1.379(5)
C(8)-H(14)	0.9500
C(9)-C(10)	1.385(5)
C(9)-H(13)	0.9500
C(10)-C(20)	1.386(5)
C(10)-H(2)	0.9500
C(11)-C(12)	1.385(5)
C(11)-H(5)	0.9500
C(12)-H(4)	0.9500
C(13)-C(14)	1.455(4)
C(14)-C(19)	1.393(4)
C(14)-C(15)	1.400(4)
C(15)-C(16)	1.391(5)

C(15)-H(10)	0.9500
C(16)-C(17)	1.384(5)
C(16)-H(9)	0.9500
C(17)-C(18)	1.391(5)
C(17)-H(8)	0.9500
C(18)-C(19)	1.389(4)
C(18)-H(7)	0.9500
C(19)-H(6)	0.9500
C(20)-C(21)	1.374(5)
C(20)-H(12)	0.9500
C(21)-H(11)	0.9500

C(5)-O(1)-C(6)	105.7(3)
C(5)-N(1)-C(13)	106.1(3)
C(12)-C(1)-C(2)	119.5(3)
C(12)-C(1)-H(1)	120.2
C(2)-C(1)-H(1)	120.2
C(3)-C(2)-C(1)	120.7(3)
C(3)-C(2)-H(15)	119.7
C(1)-C(2)-H(15)	119.7
C(2)-C(3)-C(4)	119.9(3)
C(2)-C(3)-H(3)	120.0
C(4)-C(3)-H(3)	120.0
C(11)-C(4)-C(3)	119.2(3)
C(11)-C(4)-C(5)	121.2(3)
C(3)-C(4)-C(5)	119.6(3)
N(1)-C(5)-O(1)	112.9(3)
N(1)-C(5)-C(4)	126.1(3)
O(1)-C(5)-C(4)	120.9(3)
C(13)-C(6)-O(1)	107.2(3)
C(13)-C(6)-C(7)	135.7(3)
O(1)-C(6)-C(7)	117.0(3)
C(8)-C(7)-C(21)	118.5(3)
C(8)-C(7)-C(6)	121.5(3)
C(21)-C(7)-C(6)	119.9(3)
C(9)-C(8)-C(7)	120.6(3)

C(9)-C(8)-H(14)	119.7
C(7)-C(8)-H(14)	119.7
C(8)-C(9)-C(10)	120.4(3)
C(8)-C(9)-H(13)	119.8
C(10)-C(9)-H(13)	119.8
C(9)-C(10)-C(20)	119.6(3)
C(9)-C(10)-H(2)	120.2
C(20)-C(10)-H(2)	120.2
C(12)-C(11)-C(4)	120.2(3)
C(12)-C(11)-H(5)	119.9
C(4)-C(11)-H(5)	119.9
C(1)-C(12)-C(11)	120.4(3)
C(1)-C(12)-H(4)	119.8
C(11)-C(12)-H(4)	119.8
C(6)-C(13)-N(1)	108.0(3)
C(6)-C(13)-C(14)	133.8(3)
N(1)-C(13)-C(14)	118.2(3)
C(19)-C(14)-C(15)	118.5(3)
C(19)-C(14)-C(13)	122.4(3)
C(15)-C(14)-C(13)	119.0(3)
C(16)-C(15)-C(14)	120.9(3)
C(16)-C(15)-H(10)	119.6
C(14)-C(15)-H(10)	119.6
C(17)-C(16)-C(15)	119.8(3)
C(17)-C(16)-H(9)	120.1
C(15)-C(16)-H(9)	120.1
C(16)-C(17)-C(18)	120.0(3)
C(16)-C(17)-H(8)	120.0
C(18)-C(17)-H(8)	120.0
C(19)-C(18)-C(17)	120.1(3)
C(19)-C(18)-H(7)	120.0
C(17)-C(18)-H(7)	120.0
C(18)-C(19)-C(14)	120.8(3)
C(18)-C(19)-H(6)	119.6
C(14)-C(19)-H(6)	119.6
C(21)-C(20)-C(10)	120.7(3)

C(21)-C(20)-H(12)	119.6
C(10)-C(20)-H(12)	119.6
C(20)-C(21)-C(7)	120.2(3)
C(20)-C(21)-H(11)	119.9
C(7)-C(21)-H(11)	119.9

Symmetry transformations used to generate equivalent atoms:

Table S24. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for 190333lt. The anisotropic displacement factor exponent takes the form: $-2p^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
O(1)	31(1)	34(1)	33(1)	0(1)	-6(1)	-2(1)
N(1)	25(1)	25(1)	26(1)	2(1)	-4(1)	-1(1)
C(1)	29(2)	35(2)	33(2)	-3(1)	-7(1)	-3(1)
C(2)	25(2)	30(2)	38(2)	4(1)	2(1)	-2(1)
C(3)	28(2)	25(2)	34(2)	1(1)	5(1)	4(1)
C(4)	28(2)	25(2)	22(1)	-1(1)	0(1)	3(1)
C(5)	31(2)	30(2)	31(2)	4(1)	-5(1)	0(1)
C(6)	28(2)	26(2)	34(2)	4(1)	-6(1)	-2(1)
C(7)	31(2)	28(2)	28(2)	2(1)	0(1)	-2(1)
C(8)	32(2)	29(2)	25(2)	3(1)	2(1)	-2(1)
C(9)	28(2)	27(2)	32(2)	7(1)	0(1)	-4(1)
C(10)	31(2)	33(2)	37(2)	9(1)	10(2)	4(1)
C(11)	25(2)	44(2)	27(2)	1(1)	4(1)	-6(1)
C(12)	33(2)	36(2)	31(2)	-1(1)	-1(1)	2(1)
C(13)	29(2)	27(2)	25(2)	1(1)	-2(1)	2(1)
C(14)	23(2)	21(1)	32(2)	1(1)	-2(1)	-3(1)
C(15)	26(2)	32(2)	33(2)	1(1)	2(1)	4(1)
C(16)	32(2)	34(2)	36(2)	-7(1)	10(2)	0(1)
C(17)	28(2)	44(2)	29(2)	-3(1)	2(1)	-10(1)
C(18)	24(2)	37(2)	29(2)	4(1)	-1(1)	1(1)
C(19)	25(2)	27(2)	26(2)	2(1)	2(1)	0(1)
C(20)	42(2)	33(2)	33(2)	0(1)	6(2)	3(2)
C(21)	38(2)	28(2)	31(2)	-1(1)	0(1)	-3(1)

Table S25. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^{2}x 10^3) for 190333lt.

	x	y	z	U(eq)
H(1)	4635	8413	4888	39
H(15)	4735	9202	3793	37
H(3)	3809	8976	3101	35
H(14)	478	6492	2369	34
H(13)	-680	6629	2573	35
H(2)	-1088	8176	3481	40
H(5)	2658	7192	4603	38
H(4)	3594	7424	5290	40
H(10)	2581	5627	1684	36
H(9)	2416	5155	572	41
H(8)	1541	6653	29	40
H(7)	843	8658	597	36
H(6)	986	9063	1713	31
H(12)	-330	9649	4171	43
H(11)	827	9546	3975	39