Supporting Information

Visible-Light Initiated Copper(I)-Catalysed Oxidative C-N Coupling of Anilines with Terminal Alkynes: One-Step Synthesis of α-Ketoamides

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Experimental section

General procedures. All reactions were conducted under an oxygen atmosphere and oven-dried glassware was used. All reactions were conducted using a blue light-emitting diode (LED) as the visible-light source (30 lamps, power density: 40 mW/cm^2 at 460 nm). All solvents were dried and distilled prior to use according to known methods. Starting materials (including for the synthesis of epoxide hydrolase inhibitors) were commercially available (Sigma-Aldrich or Alfa-Aesar or TCI-chemicals) and used as received. NMR spectra were recorded ^{1}H NMR at 400 MHz/ ^{13}C NMR at 100 MHz using deuterated $CDCl_3$ or $CDCl_3$-DMSO 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 solvent (at δ 7.24 and δ 77.00 ppm, respectively) was used as the internal reference. EPR spectra were recorded by a Bruker ESP-300E instrument. Isothermal titration caloriemetry (ITC) experiments were carried out at 25 ^{o}C on a high precision ITC-200 (MicroCal, LLC, and Northampton, MA).

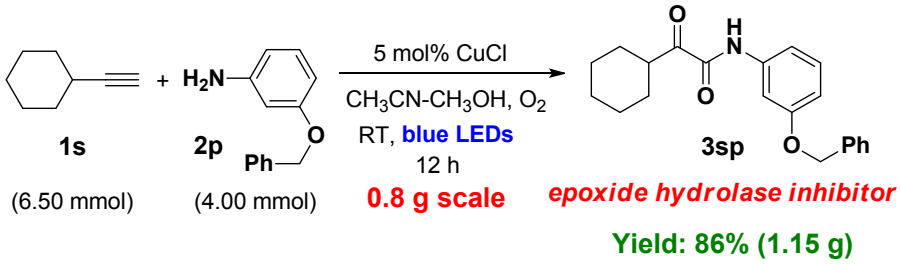
In general, a dry test tube (20 mL) containing 5 mol% CuCl was added 8 mL of dry CH_3CN and CH_3OH (1:1 v/v) via syringe, followed by sequential addition of aniline 0.5 mmol (0.083 M). Finally terminal acetylene 0.6 mmol (0.1 M) was added, which leads to formation of a yellow suspension. The yellow suspension was then irradiated with blue LEDs (40 mW/cm^2 at 460 nm, The distance between the reaction vessel to LEDs light source is 6 cm) at room temperature (25-28 ^{o}C) in the presence of 1 atm oxygen gas balloon for 8-24 h until completion of the reaction (it was 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/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 collect the α-ketoamide product.

Experimental procedure for the synthesis of Epoxide hydrolase inhibitors (3np & 3sp). A dry test tube (20 mL) containing 5 mol% CuCl was added 8 mL of dry CH_3CN and CH_3OH (1:1 v/v) via syringe, followed by sequential addition of 3-benzyloxyaniline (2p) 0.5 mmol (0.083 M). Finally it was added 1-ethynyl-4-(trifluoromethyl)benzene (1n) or ethynylcyclohexane (1s) 0.6 mmol (0.1 M), which results in formation of a suspension of fine yellow precipitate. (Note:

these starting materials were directly purchased from Alfa-Aesar and used as received). The yellow suspension was irradiated with blue LEDs at room temperature in presence of 1 atm. O_2 gas balloon for 12 h. Further procedure same as above mentioned.

*Preparative scale synthesis of epoxide hydrolase inhibitor (**3sp**).*

Scheme S1



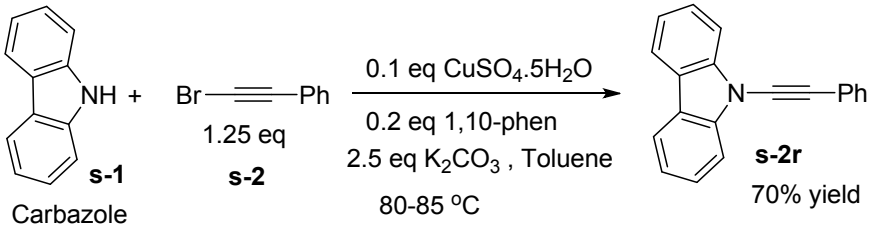
A dry flask (100 mL) containing 5 mol% CuCl was added 70 mL of dry CH_3CN and CH_3OH (1:1 v/v) via syringe, and 3-benzyloxyaniline (**2p**) 0.8 g (4 mmol) and finally added ethynylcyclohexane (**1s**) 0.70 g (6.50 mmol). A yellow suspension was formed. The yellow suspension was irradiated with blue LEDs at room temperature in presence of 1 atm. O_2 (in balloon) for 12 h (it was 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 1.15 g (86% yield) of the desired α-ketoamides product as a yellow solid (see optical picture in Figure **S15** and crystal structure in Figure **S18**).

Preparation of copper(I) phenylacetylide:[S1] CuI (1.0 g, 5.0 mmol) was dissolved in ammonium hydroxide to form a blue solution. While stirring, this solution was added drop wise to the solution of phenylacetylene (0.5g, 5.1 mmol) in 50 mL of ethanol. The system was allowed to stand for 15 min to form a yellow precipitate suspension. The precipitate was filtered out and washed with water, ethanol, and diethyl ether, three times each. The solid was vacuum-dried, and 0.65 g (yield 75%) of a bright yellow solid was obtained. The spectroscopic data for the yellow solid are listed below: IR (KBr, cm^{-1})[S2]: 1931(C≡C), 1596, 1568; UV-Vis λ_{abs} = 476 nm.

Preparation of Starting materials. The starting material, 2-benzyl-1-ethynyl-4-methoxybenzene (**1e**), was synthesized by according to known literature procedure.[S3] The starting material, 1-ethynyl-4-methoxynaphthalene (**1l**), was synthesized from1-bromo-4-methoxynaphthalene by known Sonogashira reaction procedure.[S4]

Preparation of 9-(phenylethynyl)-9H-carbazole (2r).[S5]

Scheme S2



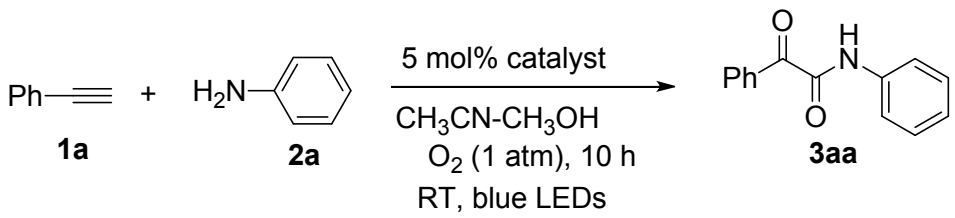
s-1
Carbazole

s-2

s-2r
70% yield

Procedure: To a flame-dried sealed tube was added carbazole (s-1) (350 mg, 2.09 mmol), $CuSO_4 \cdot 5H_2O$ (52.5 mg, 0.208 mmol), 1,10-phenanthroline (75.5 mg, 0.42 mmol) and K_2CO_3 (725 mg, 5.23 mmol), followed by anhydrous toluene (7 mL) and bromoalkyne (s-2) (472 mg, 2.62 mmol). The tube was filled with nitrogen by three vacuum-flush cycles, and the solution was heated to 80-85 °C in an oil bath overnight. When complete, the crude reaction mixture was cooled to RT, filtered through celite and silica gel pads and concentrated in vacuo. Purification of the crude residue using silica gel flash column chromatography (10:1 hexane/EtOAc) gave the pure ynamine **s-2r** as pale yellow solid (391 mg, 70%).

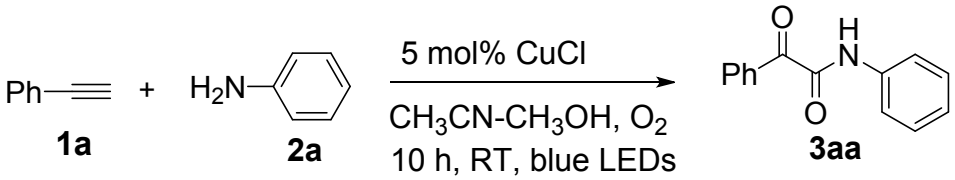
Table S1: Optimization studies on coupling reaction of (**1a**) and (**2a**) under visible light irradiation[a]



Entry	Catalyst	Base	Solvent	Yield [%][b]
1	CuCl	Et_3N (1.5eq)	CH_3CN	35
2	CuCl	K_2CO_3 (1.05 eq)	CH_3CN-MeOH	10
3	CuCl	KOAc (1.2 eq)	CH_3CN-MeOH	78
4	CuCl	NaOAc (1.2 eq)	CH_3CN-MeOH	80
5	CuCl	KOAc (0.25 eq)	CH_3CN-MeOH	84
6	**CuCl**	**no base**	**CH_3CN-MeOH**	**93**
7	$CuCl_2$	no base	CH_3CN-MeOH	trace
8	CuBr	no base	CH_3CN-MeOH	93
9	CuI	no base	CH_3CN-MeOH	93
10	$Cu(OAc)_2$	no base	CH_3CN-MeOH	n.r
11	CuCl	no base	CH_3CN	83
12	CuCl	no base	MeOH	77
13[c]	CuCl	no base	CH_3CN-MeOH	80
14	CuCl	no base	DMF	55
15	CuCl	no base	DMSO	43

[a]0.6 mmol of **1a** (0.1 M), 0.5 mmol of **2a** (0.083 M), and 5 mol% of CuCl in 8 mL of solvent. The solution was irradiated with blue LEDs for 10 h in presence of 1 atm O_2 (in balloon). [b]Yields were determined by the ^1H NMR integration method using mesitylene as an internal standard. [c]0.5 mL of water was added.

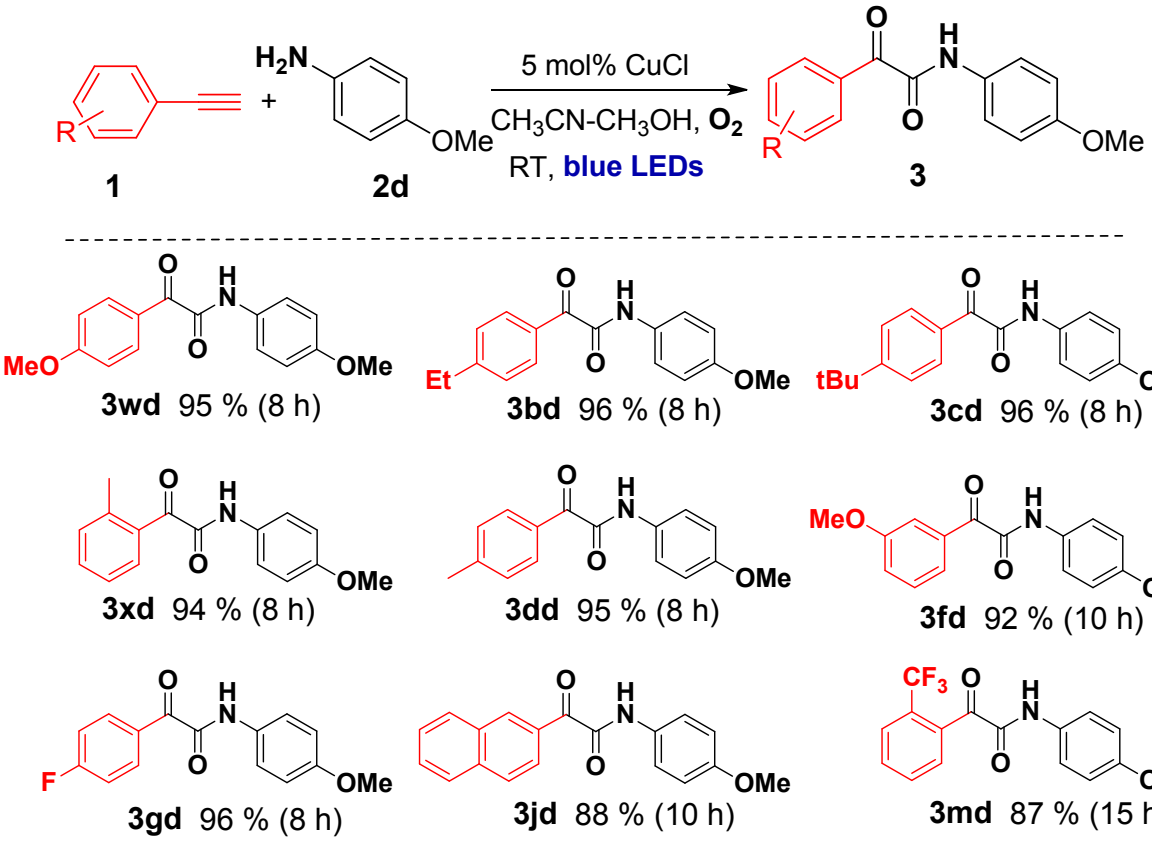
Table S2: Control experiments[a]



Entry	Visible light	Catalyst (CuCl)	O_2	Yield (%)[b]
1	+	+	+	93
2	+	+	–	n.r
3	–	+	+	n.r
4	+	–	+	n.r
5	–	–	+	n.r
6[c]	–	+	+	n.r
7[d]	+	+	+	58

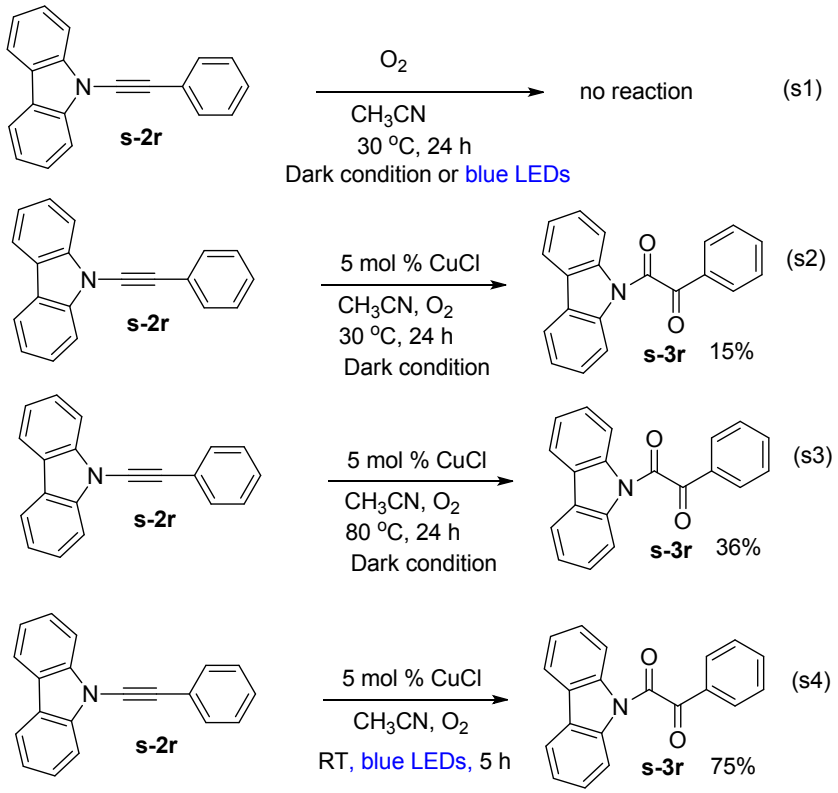
[a]Reaction conditions: 0.6 mmol of **1a** (0.1 M), 0.5 mmol of **2a (**0.083 M), and 5 mol% of CuCl in 8 ml of ACN-MeOH (1:1 v/v). The solution was irradiated with blue LEDs for 10 h in presence of 1 atm O_2 (in balloon).[b]Yields was determined by the ^{1}H NMR integration method using mesitylene as an internal standard. [c]The reaction was carried at 80 ^{o}C, using 10 mol% CuCl for 15 h. [d]The reaction was irradiated under ambient household white light (power density: 8 mW/cm^2 at 460 nm) for 24 h

Table S3: Substrates scope of 4-methoxy-aniline with various terminal alkynes under Cu-catalyzed visible-light-irradiation[a]



[a]Reaction conditions: 0.6 mmol of **1** (0.1 M), 0.5 mmol of **2d (**0.083 M), and 5 mol% of CuCl in 8 ml dry CH_3CN and CH_3OH (1:1). The solution was irradiated with blue LEDs in the presence of 1 atm. O_2 (in balloon). Isolated yield after purification by column chromatography on Silica gel.

Scheme S3: Mechanistic **c**ontrol experiments.



Dark condition (eq. s2-s3): To a flame-dried sealed tube was added **9**-(phenylethynyl)-9H-carbazole **(2r)** 0.187 mmol, 5 mol% of CuCl and added anhydrous CH_3CN (5 mL), the tube was stirring at 30 °C or 80 °C for 24 h under 1 atm. O_2. The crude reaction mixture was filtered through celite and silica gel pads and concentrated in vacuo. Purification of the crude residue using silica gel flash column chromatography (10:1 hexane/EtOAc) gave the yellow solid, 15% for reaction 30 °C and 36% for reaction at 80 °C.

Visible light condition (eq. s4): the above reaction was conducted in blue LEDs under 1 atm. O_2 at room temperature, reaction was monitored by TLC. The resulting reaction provides 75 % yield after 5 h irradiation.

***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= 0 deg; receiver harmonic= 1; field modulation frequency= 100000 Hz; microwave frequency [Hz]= 9.660469 e^{+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**, **2a**, CuCl, 1 atm. O_2) in CH_3CN-CH_3OH mixture was irradiated with blue LEDs for 30 min in the presence of DMPO in an EPR chamber while recording the EPR spectra. The EPR signals shown in Figure S1 is corresponding to DMPO-OO(H). The EPR signals were suppressed upon addition of superoxide dismutase (SOD) (Fig. **S2**). This result indicates that superoxide free radical was formed in the reaction solution. No superoxide EPR signals were observed from the reaction solution under standard condition without CuCl (Fig. S3). Reaction under standard condition without **1a** and **2a** also produces no superoxide EPR signals (Fig. **S4**). Copper(I) phenylacetylide alone was irradiated with blue LEDs in presence of O_2 in CH_3CN-CH_3OH mixture for 30 min in the presence of DMPO in an EPR chamber while recording the EPR spectra. The EPR signals shown in Figure S5 are corresponding to DMPO-OO(H). No EPR signals were observed when copper(I) phenylacetylide alone was stirred in dark condition in presence of O_2 in CH_3CN-CH_3OH (see Fig. **S6**). These results indicate that copper(I) phenylacetylide undergoes single electron transfer to O_2 and generate superoxide free radical upon blue LEDs irradiation.

Finally, the reaction solution was stirred for 30 min in the dark and the presence of DMPO under standard condition (aniline, CuCl, O_2) in CH_3CN-CH_3OH mixture (without phenylacetylene, **1a**) and the EPR spectra were recorded. The EPR signals are corresponding to DMPO-OO(H) (Fig. **S7**). The same reaction was repeated (in the dark) with 4-cyano-aniline (**2m**) instead of aniline (**1a**), no EPR signal was detected (Fig. **S8**). However, the reaction under standard condition containing 4-cyano-aniline (**2m**) phenylacetylene (**1a**), CuCl, O_2 in CH_3CN-CH_3OH mixture was irradiated with blue LEDs for 30 min and DMPO-OO(H) adduct EPR signals were detected (Fig. **S9**). These three results indicates that, electron rich and electron neutral anilines could be produced superoxide compound in presence of CuCl and O_2 in the dark condition (at room temperature), which produces azo compounds products through coupling of

aniline radical-cation.[S6] The electron poor anilines (e.g.,4-cyano-aniline) alone in dark or blue LEDs irradiation do not produce any EPR signals (Fig. **S8**). However, when phenylacetylene was added to the same solution and 30 min blue LEDs irradiation was provided, the DMPO-superoxide adducts EPR signals were generated (see Fig. **S9**). Therefore superoxide free radical is clearly generated in the presence of both copper(I) phenylacetylide and O_2 under blue LEDs irradiation.

EPR spectra of the reaction mixture after blue LEDs irradiation

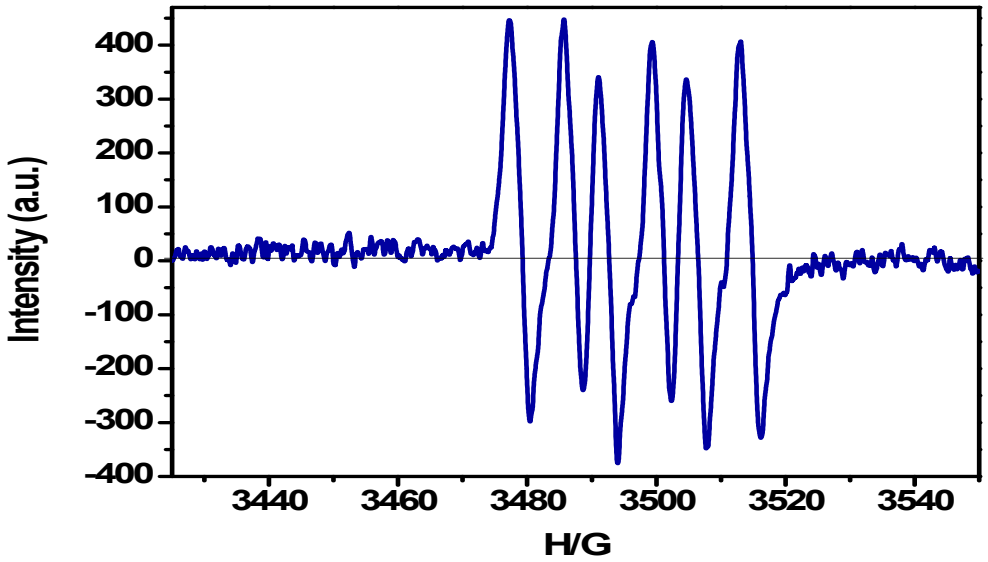


Figure S1: EPR spectra of the reaction mixture: phenylacetylene(**1a)** (0.01 M), aniline (**2a**) (0.0083 M) and 5 mol% of CuCl in CH_3CN: CH_3OH (1:1 v/v), 0.5 mL of this reaction solution was taken out into a small vial, followed by the addition of 0.01 mL of DMPO (5 x 10^{-2} M). The mixture was irradiated with blue LEDs at room temperature under an oxygen atmosphere for 30 minutes. The reaction mixture was then analysed by EPR spectra. There are 6 classical peaks, which are corresponding to the signal from (DMPO-OO(H)). The measured g-values are 2.0162, 2.0113, 2.0083, 2.0035, 2.0004 & 1.9957.

EPR spectra of the reaction mixture + SOD after blue LEDs irradiation

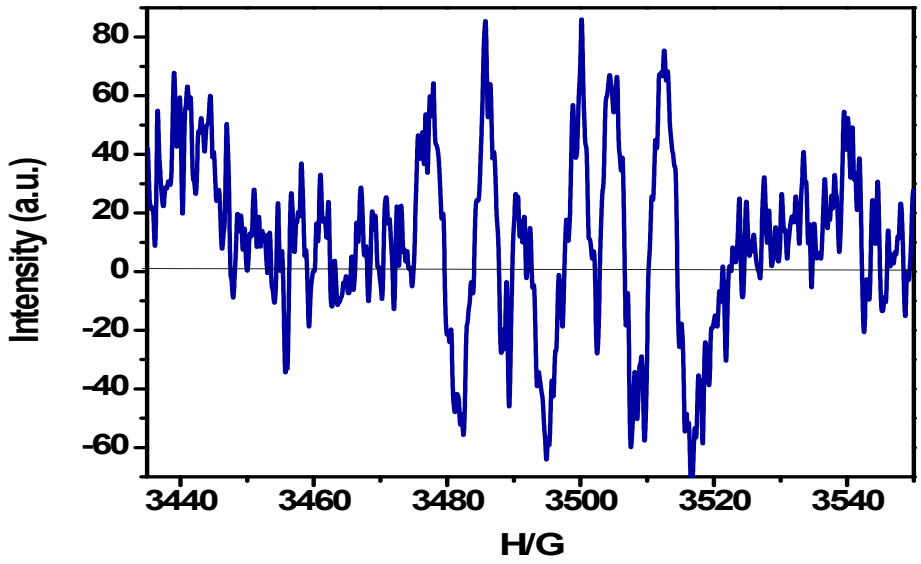


Figure S2: EPR spectra of the reaction mixture: phenylacetylene (**1a)** (0.01 M), aniline (**2a**) (0.0083 M) and 5 mol% of CuCl in CH_3CN: CH_3OH (1:1 v/v). 0.5 ml of this reaction solution was taken out into a small vial, mixed well with 0.01 mL of SOD in CH_3CN solvent ($1x10^{-2}$ M) followed by the addition of 0.01 mL of DMPO (5×10^{-2} M). The mixture was irradiated with blue LEDs at room temperature under an oxygen atmosphere for 30 minutes. The reaction mixtures was analysed by EPR spectra. Signals were suppressed.

EPR spectra of the reaction mixture without CuCl

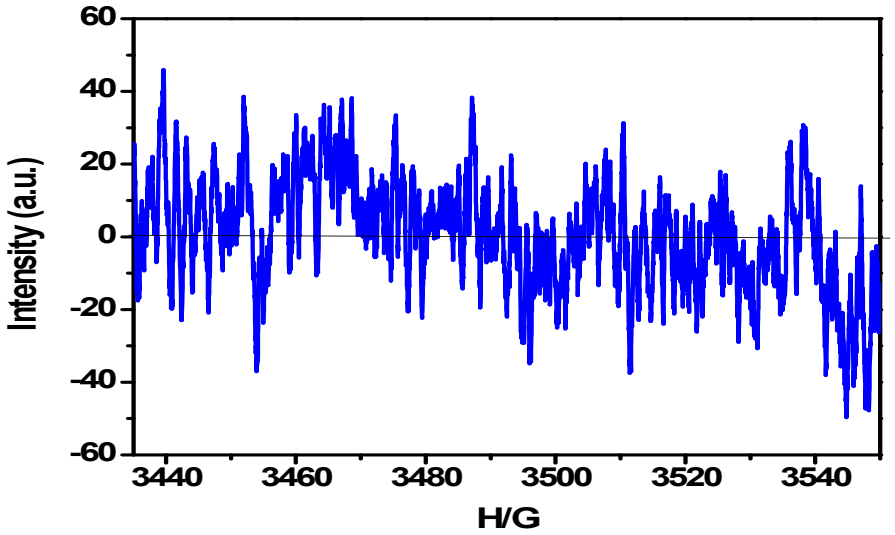


Figure S3: EPR spectra of the reaction mixture: phenylacetylene (**1a)** (0.01 M), aniline (**2a**) (0.0083 M) in CH_3CN: CH_3OH (1:1 v/v). 0.5 mL of this reaction solution was taken out into a small vial, followed by the addition of 0.01 mL of DMPO (5 x 10^{-2} M).The mixture was irradiated with blue LEDs at room temperature under an oxygen atmosphere for 30 minutes. The reaction mixtures was analysed by EPR spectra. No signals were observed.

EPR spectra of the reaction with CuCl and O_2 in ACN-MeOH

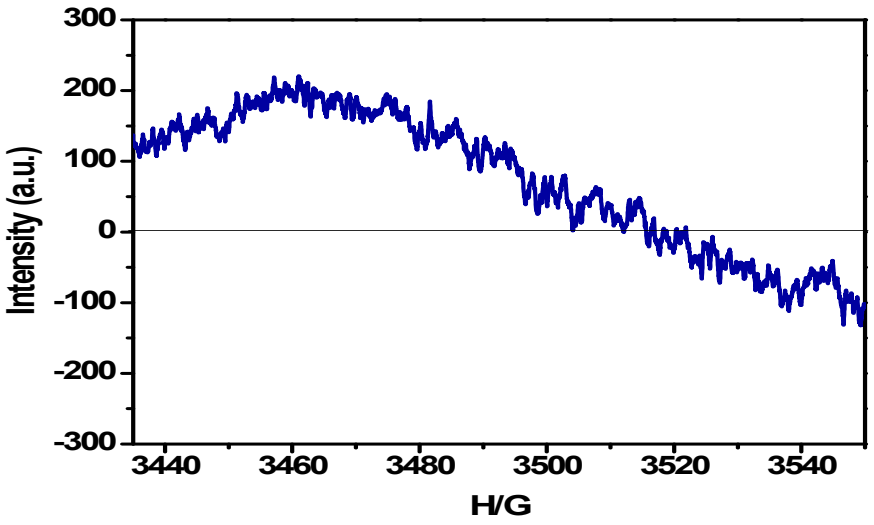


Figure S4: EPR spectra of the reaction mixture: 10 mg of CuCl in 10 mL of CH_3CN-CH_3OH mixture (1:1 v/v). 0.5 ml of this reaction solution was taken out into a small vial, followed by the addition of 0.01 mL of DMPO (5 x 10^{-2} M). The mixture was irradiated with blue LEDs at room temperature under an oxygen atmosphere for 30 minutes. The reaction mixtures was analysed by EPR spectra. No signals were observed.

EPR spectra of the reaction with copper(I) phenylacetylide + blue LEDs

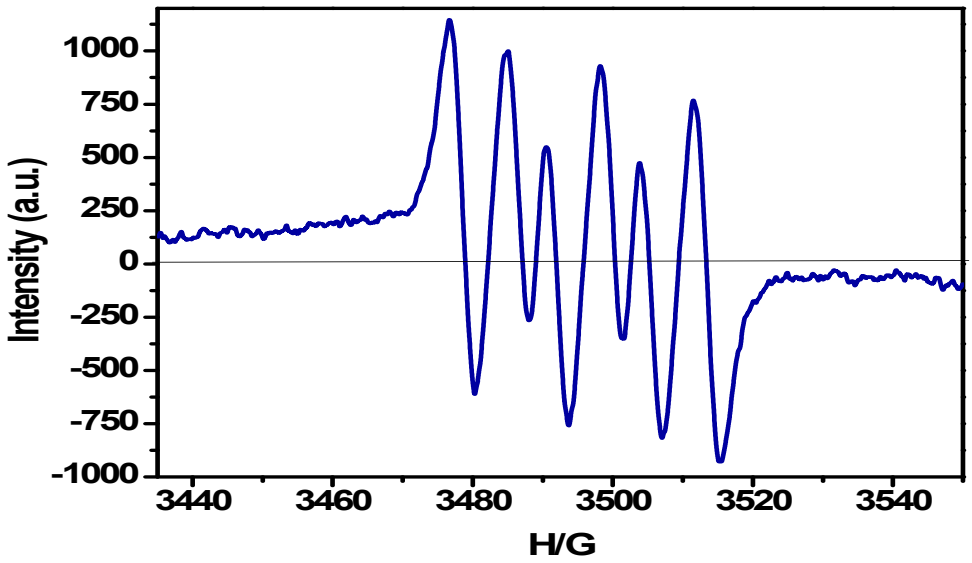


Figure S5: EPR spectra of the reaction mixture: 10 mg of copper(I) phenylacetylide in 8 mL of CH_3CN: CH_3OH (1:1 v/v). 0.5 ml of this reaction solution was taken out into a small vial, followed by the addition of 0.01 ml of DMPO (5 x 10^{-2} M). The mixture was irradiated with blue LEDs at room temperature under an oxygen atmosphere for 30 minutes. The reaction mixtures was analysed by EPR spectra. There are 6 classical peaks, which are corresponding to the signals (DMPO-OO(H)). The calculated g-values are 2.0160, 2.0114, 2.0082, 2.0037, 2.0005 and 1.9959**.**

EPR spectra of the reaction with copper(I) phenylacetylide in dark

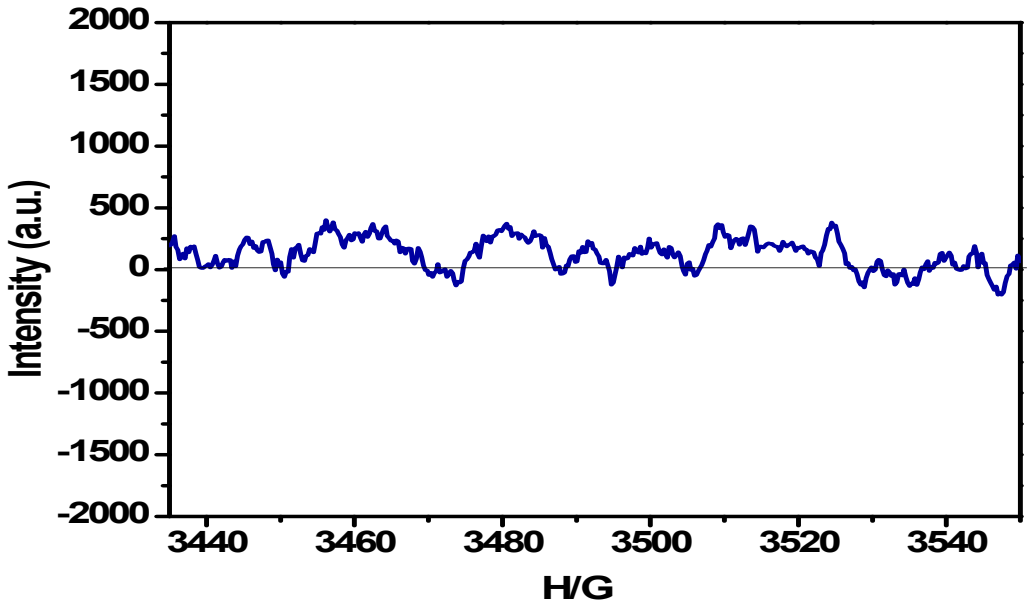


Figure S6: EPR spectra of the reaction mixture: 10 mg of copper(I) phenylacetylide in 8 mL of CH_3CN: CH_3OH (1:1 v/v). 0.5 ml of this reaction solution was taken out into a small vial, followed by the addition of 0.01 mL of DMPO (5 x 10^{-2} M).The mixture was stirred in dark condition (without any light) at room temperature under an oxygen atmosphere for 30 minutes. The reaction mixtures was analysed by EPR spectra. No signals were observed.

EPR spectra of the reaction with aniline + CuCl, without (1a) in dark

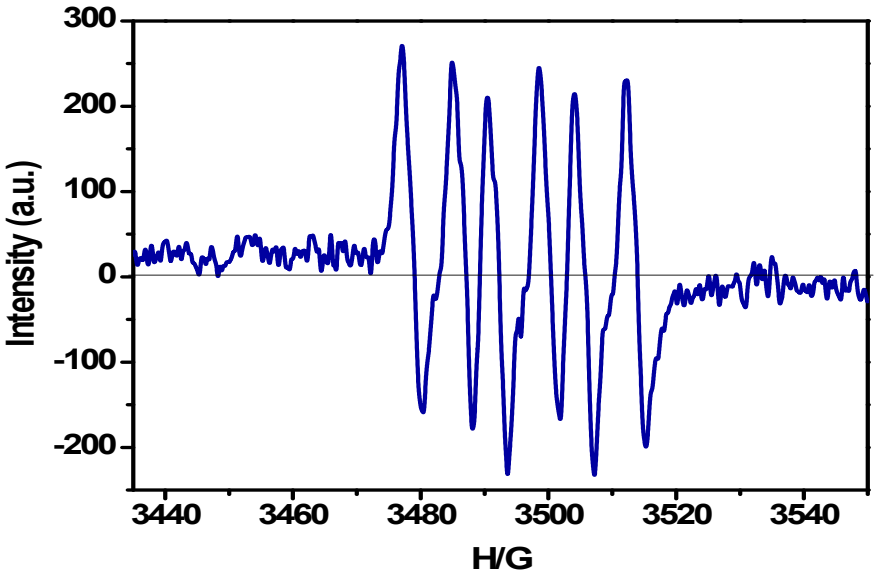


Figure S7: EPR spectra of the reaction mixture: aniline (**2a)** (0.0083 M) and 5 mol% of CuCl in CH_3CN: CH_3OH (1:1 v/v). 0.5 ml of this reaction solution was taken out into a small vial, followed by the addition of 0.01 ml of DMPO (5 x 10^{-2} M). The mixture was stirred in dark condition (without any light) at room temperature under an oxygen atmosphere for 30 minutes. The reaction mixtures was analysed by EPR spectra. There are 6 classical peaks, which are corresponding to the signals from (DMPO-OO(H)). The calculated g-values are 2.0158, 2.0112, 2.0080, 2.0034, 2.0003& 1.9956**.**

EPR spectra of the reaction with 4-cyano-aniline + CuCl, without (1a) in dark

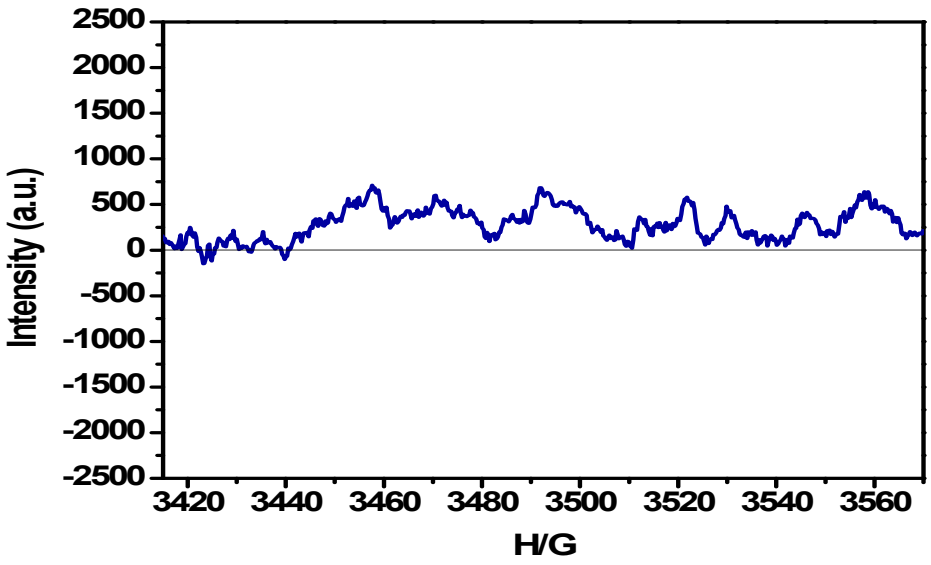


Figure S8: EPR spectra of the reaction mixture: 4-cyano-aniline (**2m)** (0.0083 M) and 5 mol% of CuCl in CH_3CN: CH_3OH (1:1 v/v). 0.5 ml of this reaction solution was taken out into a small vial, followed by the addition of 0.01 ml of DMPO (5×10^{-2} M). The mixture was stirred in dark condition (without any light) at room temperature under an oxygen atmosphere for 30 minutes. The reaction mixtures was analysed by EPR spectra. No signals were observed.

EPR spectra of the reaction mixture with 4-cyano-aniline in blue LEDs

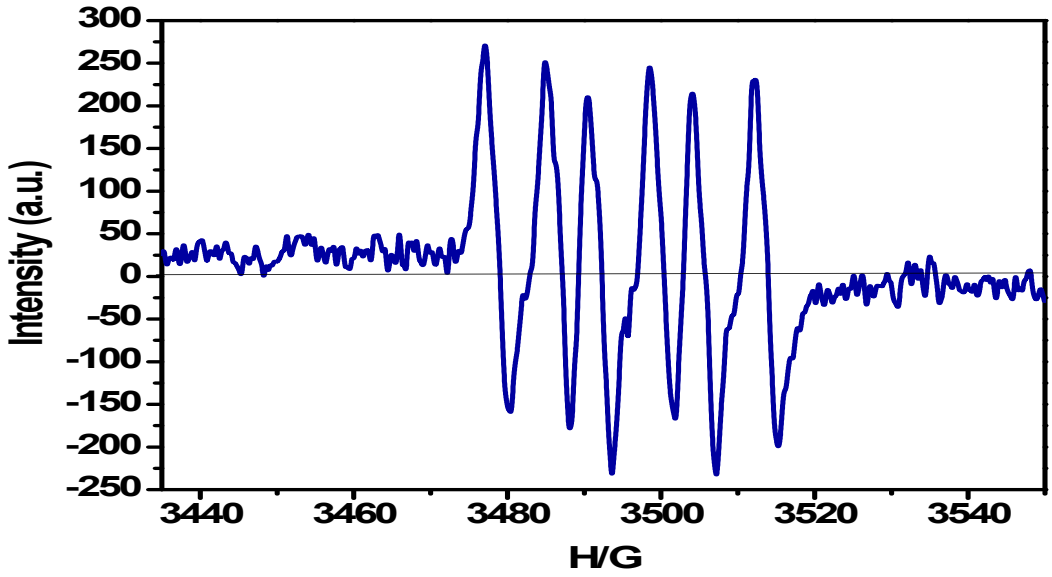


Figure S9: EPR spectra of the reaction mixture: 4-cyano-aniline (**2m)** (0.0083 M), phenylacetylene (**1a**) (0.01 M) and 5 mol% of CuCl in CH_3CN: CH_3OH (1:1 v/v). 0.5 mL of this reaction solution was taken out into a small vial, followed by the addition of 0.01 mL of DMPO (5×10^{-2} M). The mixture was irradiated with blue LEDs at room temperature under an oxygen atmosphere for 30 minutes. The reaction mixtures was analysed by EPR spectra. There are 6 classical peaks, which are corresponding to signals from (DMPO-OO(H)). The calculated g-values are 2.0157, 2.0113, 2.0081, 2.0034, 2.0003 and 1.9957**.**

Excitation and emission spectra of copper(I) phenylacetylide:

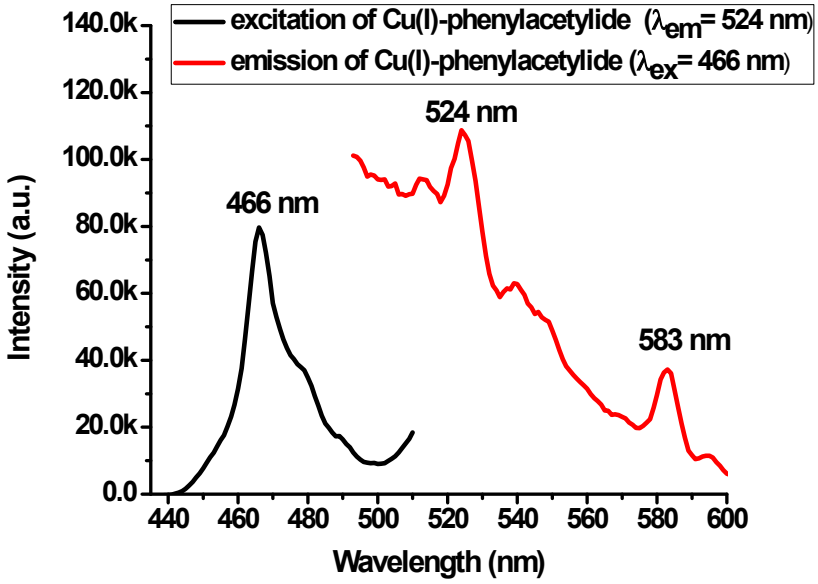


Figure S10: Excitation and emission spectra of in-situ generated copper(I) phenylacetylide in a reaction solution.

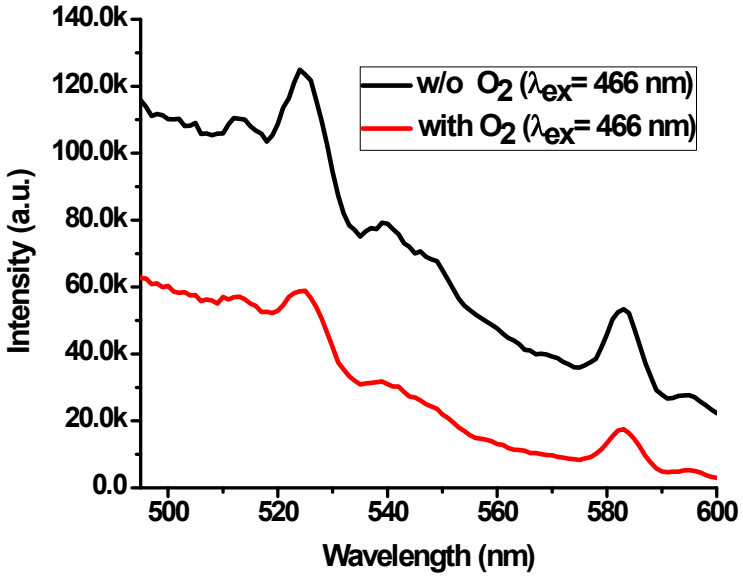


Figure S11: Photoluminescence spectra of copper(I) phenylacetylide (in-situ isolated from a reaction mixture) in the absence (top) and the presence (bottom) of air/oxygen.

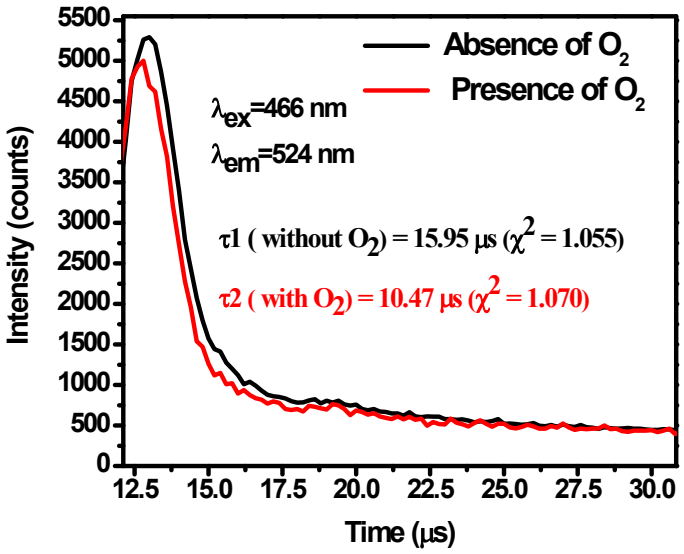
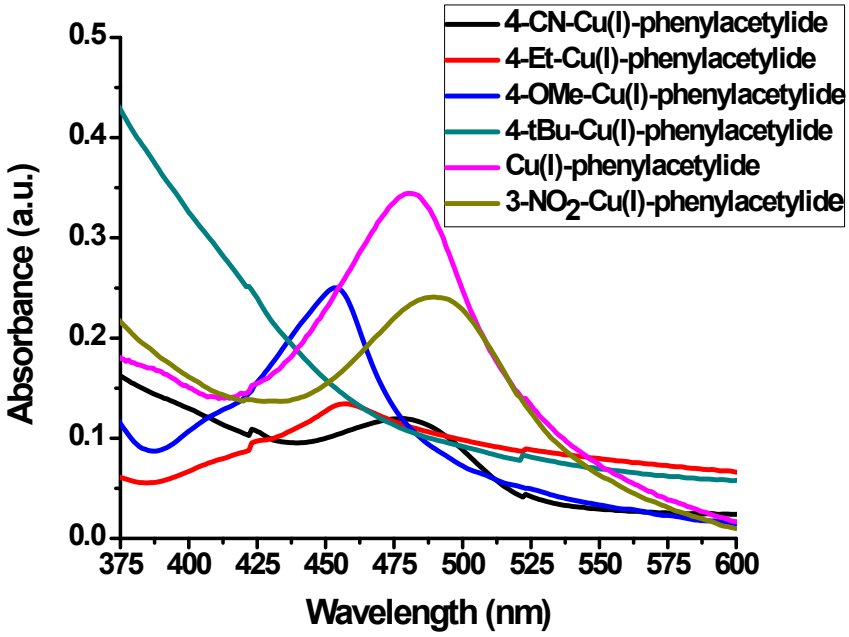


Figure S12: Excited state lifetime measurements of in-situ prepared copper(I) phenylacetylide at 524 nm emission (λ_{ex}= 466 nm) in acetonitrile solution in the absence and presence of oxygen.

a)



b)

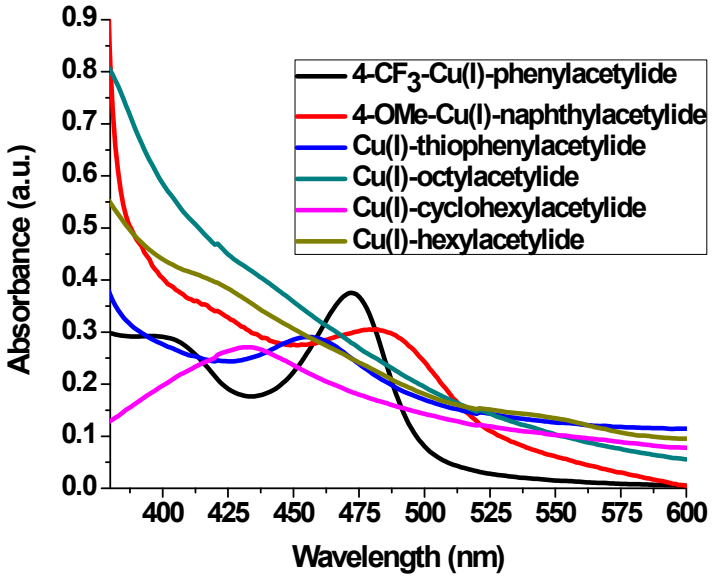


Figure S13: UV-visible spectrum of a) Cu(I)-arylacetylides and b) Cu(I)-alkyl/arylacetylides in CH_3CN and CH_3OH (1:1 v/v).

a) *Reaction mixture before addition of phenylacetylene*

b) *Reaction mixture after addition of phenylacetylene with 10 min stirred*

c) Optical picture of the reaction setup with blue-LEDs

Figure S14: Optical pictures of reaction solution containing aniline (**2a**) (0.083 M), 5 mol% CuCl in CH_3CN-CH_3OH mixture, stirred for 10 min at room temperature (dark condition) (a) before, (b) after addition of phenyl acetylene (**1a**) (0.1 M) in CH_3CN-CH_3OH mixture, and c) Optical picture of the reaction setup with blue-LEDs

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Figure S15: Optical pictures of the large scale prepared 1.15 g (86.0% yield) of *Epoxide hydrolase inhibitor* (3sp).

Estimation of association constant using isothermal titration caloriemetry (ITC). Isothermal titration caloriemetry experiments were carried out at 25 ^{o}C on a high precision ITC-200 (MicroCal, LLC, and Northampton, MA). The solution of copper(I) phenylacetylide (1 mM) and CuCl (2 mM) were prepared by using CH_3CN-CH_3OH mixture (1:1). Before measurements, the samples were degassed for at least 7 minutes. The calorimeter was initially calibrated using water-water titration, in which the reference power of 5 µcal/s was applied. As a set of control experiment, solvent-to-solvent titration was also performed. Then, copper(I) phenylacetylide (**1a'**) was loaded into the cell and CuCl was taken in the syringe. 20 injections were performed with an each titration volume of 2 µL. The reference power of 5µcal/s was applied while the sample contents were stirred at 1000 rpm (rotations per minute).

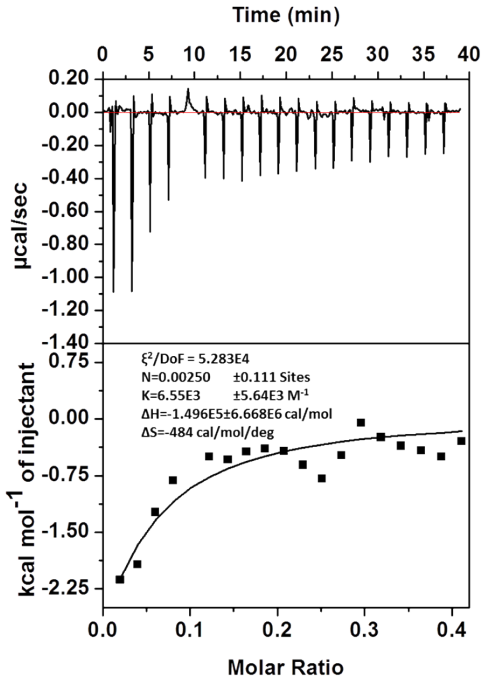

Figure S16. Isothermal titration caloriemetry (ITC) data for the determination of the association constant values. The inset of the bottom panel indicates the peak fitting results of one set of binding sites obtained from the inbuilt Origin Pro software of the Mircrocal ITC-200.

Experimental Results: The binding curve is obtained from a plot of the heat change from each injection against the molar ratio of CuCl (in syringe) and binding partner **1a'** in the cell (Fig.

S18). The binding curve is analyzed with an appropriate binding model to determine the value of K (binding affinity). The isothermal titration reveals the association constant, K_a~ 6550 μM^{-1} and this affinity value suggests a moderate interaction.[S7]

References:

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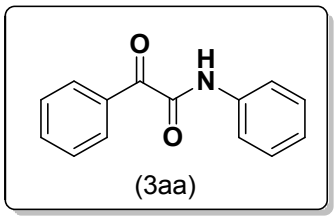
S5. K. A. DeKorver, R. P. Hsung, A. G. Lohse, Y. Zhang, *Org. Lett.* 2010, **12**, 1840-1843.

S6. C. Zhang and N. Jiao, *Angew. Chem. Int. Ed.* 2010, **49**, 6174-6177.

S7. http://www.huck.psu.edu/facilities/calorimetry-up/guides/itc.

Spectroscopic Data:

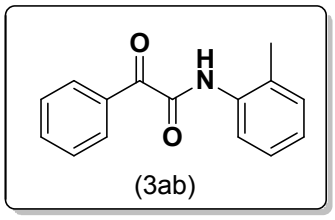
2-oxo-N, 2-diphenylacetamide (3aa)



(3aa)

Pale yellow solid; m.p. 62-66° C; **^{1}H NMR** (400 MHz, $CDCl_3$): **δ** 8.97 (b, 1 H), 8.40-8.38 (m, 2 H), 7.70-7.62 (m, 3 H), 7.49 (t, *J* = 8.0 Hz, 2 H), 7.38 (t, *J* = 8.0 Hz, 2 H), 7.18 (t, *J* = 8.0 Hz, 1 H) ; **^{13}CNMR** (100 MHz, $CDCl_3$): δ 187.4, 158.8, 136.6, 134.5, 133.0, 131.4, 129.1, 128.5, 125.2, 119.9; IR (neat): 3330, 2928, 1691, 1665.0, 1598, 1283 cm^{-1}; **HRMS** calcd for $C_{14}H_{11}NO_2$: 225.0790, found: 225.0793.

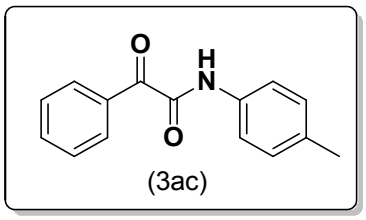
2-oxo-2-phenyl-N-(o-tolyl)acetamidel (3ab)



(3ab)

Pale orange solid; m.p. 91-93° C; **^{1}H NMR** (400 MHz, $CDCl_3$): δ 8.91 (b, 1 H), 8.42 (d, *J* = 8.0 Hz, 2 H), 8.10 (d, *J* = 8.0 Hz, 1 H), 7.67-7.63 (m, 1 H), 7.52-7.48 (m, 2 H), 7.29-7.22 (m, 2 H), 7.12 (t, *J* = 8.0 Hz, 1 H), 2.36 (s, 1 H) ; **^{13}CNMR** (100 MHz, $CDCl_3$): δ 187.5, 158.8, 134.6, 133.1, 131.4, 130.8, 130.6, 128.6, 128.5, 126.9, 125.6, 121.7, 17.5; IR (neat): 3230, 2910, 1672, 1641, 1590, 1280, cm^{-1}; **HRMS** calcd for $C_{15}H_{13}NO_2$: 239.0946, found: 239.0944.

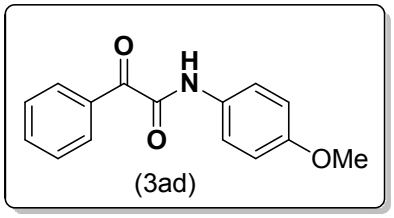
2-oxo-2-phenyl-N-(p-tolyl)acetamide (3ac)



(3ac)

Pale yellow solid; m.p. 112-113° C; **^{1}H NMR** (400 MHz, $CDCl_3$): δ 8.90(b, 1 H), 8.39 (d, *J* = 4.0 Hz, 2 H), 7.65-7.62 (m, 1 H), 7.57 (d, *J* = 8.0 Hz, 2 H), 7.51-7.47 (m, 2 H), 7.18 (d, *J* = 8.0 Hz, 2 H), 2.33 (s, 1 H); **^{13}CNMR** (100 MHz, $CDCl_3$): δ 187.5, 158.7, 135.0, 134.5, 134.0, 133.1, 131.4, 129.7, 128.5, 119.8, 20.9; IR (neat): 3310, 2929, 1673,1646, 1586, 1276 cm^{-1}; **HRMS** calcd for $C_{15}H_{13}NO_2$: 239.0946, found: 239.0951.

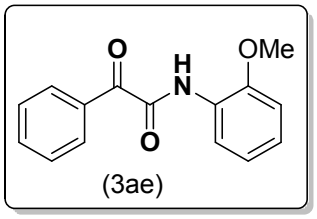
N-(4-methoxyphenyl)-2-oxo-2-phenylacetamide (3ad)



(3ad)

Yellow solid; m.p. 95-97° C; **^{1}H NMR** (400 MHz, $CDCl_3$): δ 8.87(b, 1 H), 8.40-8.38 (m, 2 H), 7.64-7.60 (m, 3 H), 7.49 (t, *J* = 8.0 Hz, 2 H), 6.91 (d, *J* = 8.0 Hz, 2 H), 3.80 (s, 3 H); **^{13}CNMR** (100 MHz, $CDCl_3$): δ 187.5, 158.6, 157.0, 134.5, 133.1, 131.4, 129.7, 128.5, 121.4, 114.3, 55.4; IR (neat): 3346, 2929, 1667, 1634, 1538, 1245 cm^{-1}; **HRMS** calcd for $C_{15}H_{13}NO_3$: 255.0895, found: 255.0891.

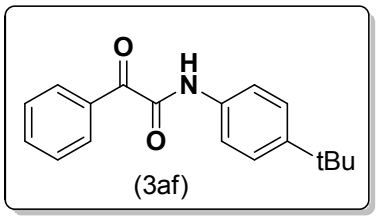
N-(2-methoxyphenyl)-2-oxo-2-phenylacetamide (3ae)



(3ae)

Yellow solid; m.p. 83-85° C; **^{1}H NMR** (400 MHz, $CDCl_3$): δ 9.51(b, 1 H), 8.48 (dd, *J* = 8.0 Hz, 4.0 Hz, 1 H), 8.38 (dd, *J* = 8.0 Hz, 4.0 Hz, 2 H), 7.65-7.61 (m, 1 H), 7.51-7.47(m, 2 H), 7.14-7.10 (m, 1 H), 7.02-6.98 (m, 1 H), 6.92 (d, *J* = 8.0 Hz, 1 H), 3.92 (s, 3 H); **^{13}CNMR** (100 MHz, $CDCl_3$): δ 187.4, 158.9, 148.7, 134.4, 133.2, 131.3, 128.4, 126.3, 125.0, 120.9, 119.7, 110.1, 55.7; IR (neat): 3345, 2943, 1672.0, 1645, 1542, 1249 cm^{-1}; **HRMS** calcd for $C_{15}H_{13}NO_3$: 255.0895, found: 255.0895.

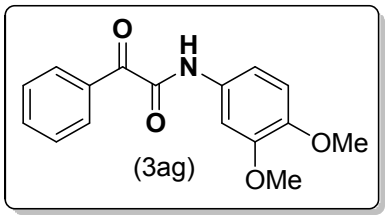
N-(4-(tert-butyl)phenyl)-2-oxo-2-phenylacetamide (3af)



(3af)

Yellow solid; m.p. 92-93° C; **^{1}H NMR** (400 MHz, $CDCl_3$): δ 8.92 (b, 1 H), 8.40 (d, *J* = 8.0 Hz, 2 H), 7.83(d, *J* = 8.0 Hz, 1 H), 7.64-7.60 (m, 2 H), 7.53-7.47(m, 2 H), 7.41-7.39 (m, 2 H); **^{13}CNMR** (100 MHz, $CDCl_3$): δ 187.5, 158.8, 154.1, 148.3, 134.5, 133.9, 131.4, 128.5, 126.0, 119.6, 31.2, 34.48, 31.30; IR (neat): 3339, 2924, 1663, 1642, 1537, 1242 cm^{-1}; **HRMS** calcd for $C_{18}H_{19}NO_2$: 281.1416, found: 281.1421.

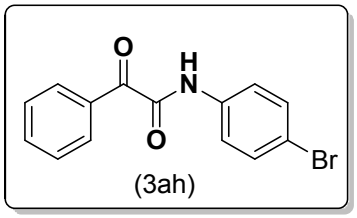
N-(3,4-dimethoxyphenyl)-2-oxo-2-phenylacetamide (3ag)



(3ag)

Yellow solid; m.p. 102-104° C; **^{1}H NMR** (400 MHz, $CDCl_3$): δ 8.93(b, 1 H), 8.38-8.35 (m, 2 H), 7.63-7.59 (m, 1 H), 7.47 (d, *J* = 4.0 Hz, 3 H), 7.10-7.07 (m, 1 H), 6.83 (d, *J* = 8.0 Hz, 1 H), 3.88 (s, 3 H), 3.85 (s, 3 H); **^{13}CNMR** (100 MHz, $CDCl_3$): δ 187.4, 158.6, 149.1, 146.5, 134.4, 133.1, 131.3, 130.2, 128.4, 111.9, 111.3, 104.36, 55.9, 55.8; IR (neat): 3334, 2921, 1695, 1615, 1180 cm-1; **HRMS** calcd for $C_{16}H_{15}NO_4$: 285.1001, found: 285.0991.

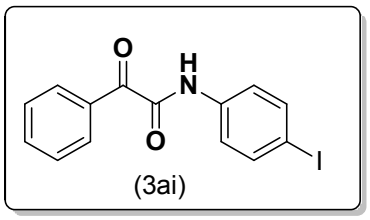
N-(4-bromophenyl)-2-oxo-2-phenylacetamide (3ah)



(3ah)

Yellow solid; m.p. 175-177° C; **^{1}H NMR** (400 MHz, $CDCl_3$): δ 8.99 (b, 1 H), 8.37 (d, *J* = 8.0 Hz, 2 H), 7.66-7.58 (m, 3 H), 7.51-7.47 (m, 4 H); **^{13}CNMR** (100 MHz, $CDCl_3$): δ 187.0, 158.7, 135.7, 134.7, 132.8, 132.2, 131.4, 128.5, 121.4, 118.0; IR (neat): 3342, 2928, 1699, 1663, 1279, 1069 cm^{-1}; **HRMS** calcd for $C_{14}H_{10}BrNO_2$: 302.9895, found: 302.9899.

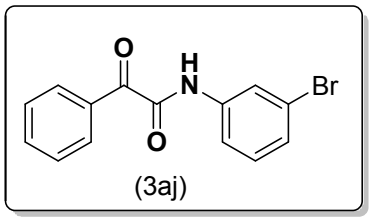
N-(4-iodophenyl)-2-oxo-2-phenylacetamide (3ai)



(3ai)

Yellow solid; m.p. 170-172° C; **^{1}H NMR** (400 MHz, $CDCl_3$): δ 8.96 (b, 1 H), 8.37 (d, *J* = 8.0 Hz, 2 H), 7.69-7.62 (m, 3 H), 7.51-7.45 (m, 4 H); **^{13}CNMR** (100 MHz, $CDCl_3$): δ 186.9, 158.7, 138.1, 136.3, 134.7, 132.8, 131.4, 128.5, 121.6, 88.8; IR (neat): 3344, 2933, 1698, 1666, 1280 cm^{-1}; **HRMS** calcd for $C_{14}H_{10}INO_2$: 350.9756,found: 350.9760.

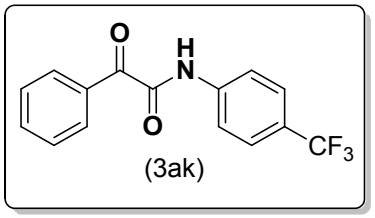
N-(3-bromophenyl)-2-oxo-2-phenylacetamide (3aj)



(3aj)

Yellow solid; m.p. 168-170° C; **^{1}H NMR** (400 MHz, $CDCl_3$): δ 9.05 (b, 1 H), 8.36 (d, *J* = 8.0 Hz, 2 H), 7.97 (s, 1 H), 7.64 (t, *J* = 4.0 Hz, 2 H), 7.61-7.55 (m, 1 H), 7.47 (t, *J* = 8.0 Hz, 2 H), 7.29 (t, *J* = 4.0 Hz, 1 H), 7.21 (t, *J* = 8.0 Hz, 1 H); **^{13}CNMR** (100 MHz, $CDCl_3$): δ 186.9, 158.8, 137.7, 132.7, 131.4, 130.3, 128.5, 128.1, 122.8, 122.7, 118.3; IR (neat): 3340, 2923,1694, 1659, 1275cm^{-1}; **HRMS** calcd for $C_{14}H_{10}BrNO_2$: 302.9895, found: 302.9892.

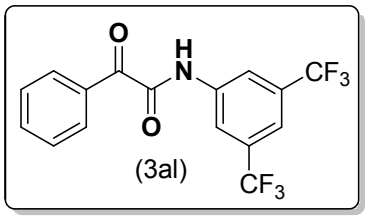
2-oxo-2-phenyl-N-(4-(trifluoromethyl)phenyl)acetamide (3ak)



(3ak)

Yellow solid; m.p. 149-152° C; **^{1}H NMR** (400 MHz, $CDCl_3$): δ 9.10 (b, 1 H), 8.40 (d, *J* = 4.0 Hz, 2 H), 7.82 (d, *J* = 8.0 Hz, 2 H), 7.67-7.64 (m, 2 H), 7.53-7.50 (m, 2 H), 7.33 (t, *J* = 4.0 Hz, 1 H); **^{13}CNMR** (100 MHz, $CDCl_3$): δ 186.7, 158.9, 139.6, 134.9, 132.6 (d, J_{C-F} = 27.0 Hz), 131.5, 129.7, 129.1, 128.1, 128.5 (d, J_{C-F} = 24.0 Hz), 126.3 (d, J_{C-F} = 3.0 Hz), 119.6; IR (neat): 3339, 1709, 1668, 1543, 1330, 1115 cm^{-1}; **HRMS** calcd for $C_{15}H_{10}F_3NO_2$: 293.0664, found: 293.0666.

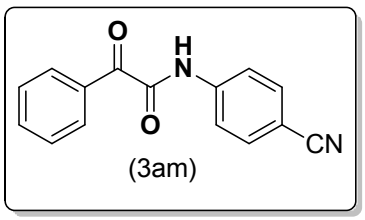
N-(3,5-bis(trifluoromethyl)phenyl)-2-oxo-2-phenylacetamide (3al)



(3al)

Yellow solid; m.p.146-148° C; **^{1}H NMR** (400 MHz, $CDCl_3$): δ 9.26 (b, 1 H), 8.42 (d, *J* = 8.0 Hz, 2 H), 8.21 (s, 2 H), 7.67 (d, *J* = 8.0 Hz, 2 H), 7.54-7.51 (m, 3 H); **^{13}CNMR** (100 MHz, $CDCl_3$): δ 186.0, 158.9, 138.0, 135.1, 132.6 (d, J_{C-F} = 27.0 Hz), 131.5, 130.8, 128.7 (d, J_{C-F} = 1.0 Hz), 119.6 (d, J_{C-F} = 2.0 Hz), 118.5; IR (neat): 3340, 1702, 1666, 1540, 1110 cm^{-1}; **HRMS** calcd for $C_{15}H_9F_6NO_2$: 361.0537, found: 361.0544.

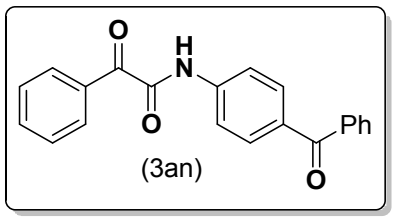
N-(4-cyanophenyl)-2-oxo-2-phenylacetamide (3am)



(3am)

Yellow solid; m.p 143-145° C; **^{1}H NMR** (400 MHz, $CDCl_3$): δ 9.19 (b, 1 H), 8.39 (d, *J* = 8.0 Hz, 2 H), 8.09 (d, *J* = 8.0 Hz, 1 H), 7.83 (d, *J* = 8.0 Hz, 2 H), 7.68 (d, *J* = 8.0 Hz, 2 H), 7.53-7.44 (m, 3 H); **^{13}CNMR** (100 MHz, $CDCl_3$): δ 186.4, 158.9, 140.5, 135.0, 133.4, 132.6, 131.5, 128.7, 119.9, 118.5, 108.4; IR (neat): 3335, 2224, 1708, 1659.2, 1243.2 cm^{-1}; **HRMS** calcd for $C_{15}H_{10}N_2O_2$: 250.0742, found: 250.0739.

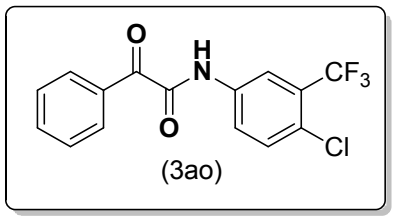
N-(4-benzoylphenyl)-2-oxo-2-phenylacetamide (3an)



(3an)

Yellow solid; m.p. 164-166° C; **^{1}H NMR** (400 MHz, $CDCl_3$): δ 9.15 (b, 1 H), 8.41 (d, *J* = 4.0 Hz, 2 H), 7.88 (d, *J* = 8.0 Hz, 2 H), 7.82 (d, *J* = 8.0 Hz, 2 H), 7.79-7.77 (m, 2 H), 7.67(t, *J* = 4.0 Hz, 1 H), 7.58 (t, *J* = 8.0 Hz, 1 H), 7.53-7.47 (m, 4 H); **^{13}CNMR** (100 MHz, $CDCl_3$): δ 195.4, 186.7, 158.8, 140.3, 137.6, 134.9, 134.0, 132.3, 131.6, 131.5, 129.9, 128.6, 128.3, 119.1; IR (neat): 3339, 1707, 1698, 1665, 1549, 1328 cm^{-1}; **HRMS** calcd for $C_{21}H_{15}NO_3$: 329.1052, found: 329.1055.

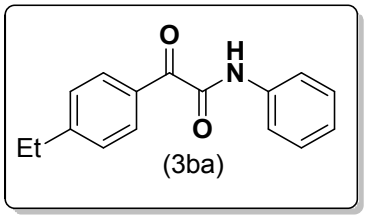
N-(4-chloro-3-(trifluoromethyl)phenyl)-2-oxo-2-phenylacetamide (3ao)



(3ao)

Yellow solid; m.p. 159-161° C; **^{1}H NMR** (400 MHz, $CDCl_3$): δ 9.14 (b, 1 H), 8.38 (d, *J* = 8.0 Hz, 2 H), 8.08 (s, 1 H), 7.84 (d, *J* = 8.0 Hz, 1 H), 7.67 (q, *J* = 8.0 Hz, 1 H), 7.50 (t, *J* = 8.0 Hz, 3 H); **^{13}CNMR** (100 MHz, $CDCl_3$): δ 186.4, 158.8, 135.4, 135.0, 132.4(d, J_{C-F} = 41.0 Hz), 131.5, 129.1 (d, J_{C-F} = 25.0 Hz), 128.6, 128.0, 123.7, 123.4, 121.3, 118.9 (d, J_{C-F} = 4.0 Hz); IR (neat): 3345, 1691, 1663, 1520, 1112 cm^{-1}; **HRMS** calcd for $C_{15}H_9ClF_3NO_2$: 327.0274, found: 327.0265.

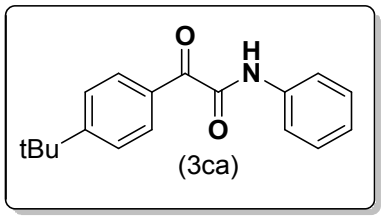
2-(4-ethylphenyl)-2-oxo-N-phenylacetamide (3ba)



(3ba)

Yellow solid; m.p. 136-138° C; **^{1}H NMR** (400 MHz, $CDCl_3$): δ 8.94(b, 1 H), 8.35 (d, *J* = 8.0 Hz, 2 H), 7.68 (d, *J* = 8.0 Hz, 2 H), 7.38 (t, *J* = 8.0 Hz, 2 H), 7.32 (d, *J* = 8.0 Hz, 2 H), 7.18 (t, *J* = 4.0 Hz, 1 H), 2.72 (q, *J* = 8.0 Hz, 2 H), 1.25 (t, *J* = 8.0 Hz, 3 H); **^{13}CNMR** (100 MHz, $CDCl_3$): δ 186.8, 159.1, 152.0, 136.6, 131.7, 130.7, 129.2, 128.1, 125.2, 119.8, 29.1, 15.0; IR (neat): 3331, 1691, 1660, 1589, 1525, 1280 cm^{-1}; **HRMS** calcd for $C_{16}H_{15}NO_2$: 253.1103 found:253.1107.

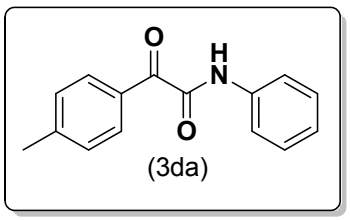
2-(4-(tert-butyl)phenyl)-2-oxo-N-phenylacetamide(3ca)



(3ca)

Yellow solid; m.p. 101-103° C; **^{1}H NMR** (400 MHz, $CDCl_3$): δ 8.97 (b, 1 H), 8.35 (d, *J* = 8.0 Hz, 2 H), 7.69 (d, *J* = 8.0 Hz, 2 H), 7.52-7.50 (m, 2 H), 7.40-7.36 (m, 2 H), 7.18 (t, *J* = 8Hz, 1 H), 1.34 (s, 9 H); **^{13}CNMR** (100 MHz, $CDCl_3$): δ 186.9, 159.1, 158.7, 136.7, 131.4, 130.4, 129.1, 125.5, 125.1, 119.9, 35.3, 30.9; IR (neat): 3329, 1687, 1657, 1584, 1521, 1273 cm^{-1}; **HRMS** calcd for $C_{18}H_{19}NO_2$: 281.1416 found: 281.1418.

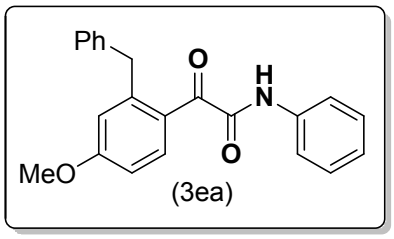
2-oxo-N-phenyl-2-(p-tolyl)acetamide (3da)



(3da)

Yellow solid; m.p. 114-116° C; **^{1}H NMR** (400 MHz, $CDCl_3$): δ 8.96 (b, 1 H), 8.33 (d, *J* = 8.0 Hz, 2 H), 7.68 (d, *J* = 8.0 Hz, 2 H), 7.38 (t, *J* = 8.0 Hz, 2 H), 7.29 (d, *J* = 8.0 Hz, 2 H), 7.17 (t, *J* = 8.0 Hz, 1 H), 2.42 (s, 3 H); **^{13}CNMR** (100 MHz, $CDCl_3$): δ 186.8, 159.1, 145.9, 136.6, 131.6, 130.5, 129.2, 129.1, 125.1, 119.8, 21.8; IR (neat): 3328, 1691, 1660, 1604, 1589, 1525, 1280 cm^{-1}; **HRMS** calcd for $C_{15}H_{13}NO_2$: 239.0946 found: 239.0946.

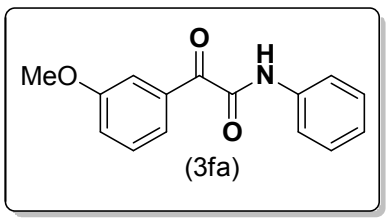
2-(2-benzyl-4-methoxyphenyl)-2-oxo-N-phenylacetamide (3ea)



(3ea)

Yellow solid; m.p.128-130° C; **^{1}H NMR** (400 MHz, $CDCl_3$): δ 8.87 (b, 1 H), 8.24 (d, *J* = 8.0 Hz, 1 H), 7.66 (d, *J* = 8.0 Hz, 2 H), 7.38 (t, *J* = 8.0 Hz, 2 H), 7.28 (t, *J* = 8.0 Hz, 2 H), 7.20-7.15 (m, 4 H), 6.85 (d, *J* = 8.0 Hz, 1 H), 6.78 (s, 1 H), 4.32 (s, 2 H), 3.84 (s, 3 H); **^{13}CNMR** (100 MHz, $CDCl_3$): δ 188.5, 163.3, 159.5, 146.3, 140.2, 136.7, 135.8, 129.1, 128.9, 128.3, 126.1, 125.0, 124.9, 119.7, 118.0, 110.5, 55.3, 39.6; IR (neat): 3338, 1692, 1663, 1608, 1586, 1287 cm^{-1}; **HRMS** calcd for $C_{22}H_{19}NO_3$: 345.1365 found: 345.1371.

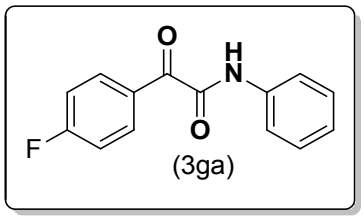
2-(3-methoxyphenyl)-2-oxo-N-phenylacetamide (3fa)



(3fa)

Yellow solid; m.p.117-119° C; **^{1}H NMR** (400 MHz, $CDCl_3$): δ 8.92 (b, 1 H), 8.05 (d, *J* = 8.0 Hz, 1 H), 7.89 (t, *J* = 8.0 Hz, 1 H), 7.68 (d, *J* = 8.0 Hz, 2 H), 7.42-7.36 (m, 2 H), 7.20-7.16 (m, 2 H), 3.86 (s, 3 H); **^{13}CNMR** (100 MHz, $CDCl_3$): δ 187.1, 159.5, 158.8, 136.5, 134.1, 129.5, 129.2, 125.3, 124.3, 121.6, 119.9, 114.9, 55.48; IR (neat): 3341, 1694, 1668, 1606, 1583, 1285 cm^{-1}; **HRMS** calcd for $C_{15}H_{13}NO_3$: 255.0895 found: 255.0897.

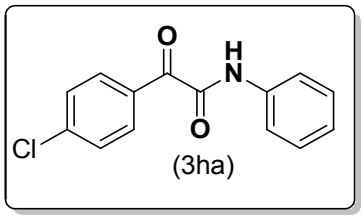
2-(4-fluorophenyl)-2-oxo-N-phenylacetamide (3ga)



(3ga)

Yellow solid; m.p. 128-130° C; **^{1}H NMR** (400 MHz, $CDCl_3$): δ 8.95 (b, 1 H), 8.53-8.50 (m, 2 H), 7.67 (d, *J* = 8.0 Hz, 2H), 7.39 (t, *J* = 4.0 Hz, 2H), 7.20-7.15 (m, 3 H); **^{13}CNMR** (100 MHz, $CDCl_3$): δ 185.5, 167.7, 165.7, 158.6, 136.4, 134.6 (d, J_{C-F} = 7.0 Hz), 129.4 (d, J_{C-F} = 24.0 Hz), 125.4, 119.9, 115.9 (d, J_{C-F} = 17.0 Hz); IR (neat): 3342, 1697,1666, 1590, 1277 cm^{-1}; **HRMS** calcd for $C_{14}H_{10}FNO_2$: 243.0696 found: 243.0700.

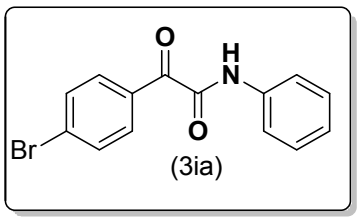
2-(4-chlorophenyl)-2-oxo-N-phenylacetamide (3ha)



(3ha)

Yellow solid; m.p. 131-133° C; **^{1}H NMR** (400 MHz, $CDCl_3$): δ 8.94 (b, 1 H), 8.39 (d, *J* = 8.0 Hz, 2 H), 7.67 (d, *J* = 8.0 Hz, 2 H), 7.47 (d, *J* = 8.0 Hz, 2 H), 7.38 (t, *J* = 8.0 Hz, 2 H), 7.19 (t, *J* = 8.0 Hz, 1 H); **^{13}CNMR** (100 MHz, $CDCl_3$): δ 186.0, 158.5, 141.4, 136.4, 132.9, 131.3, 129.2, 128.9, 125.4, 119.9; IR (neat): 3340, 1691,1660, 1535, 1277 cm^{-1}; **HRMS** calcd for $C_{14}H_{10}ClNO_2$: 259.0400 found: 259.0410.

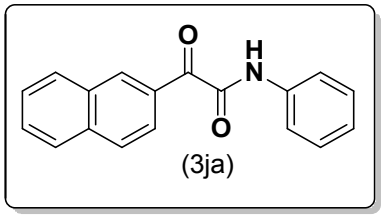
2-(4-bromophenyl)-2-oxo-N-phenylacetamide (3ia)



(3ia)

Yellow solid; m.p. 177-179° C; **^{1}H NMR** (400 MHz, $CDCl_3$): δ 8.93 (b, 1 H), 8.31 (d, *J* = 8.0 Hz, 2 H), 7.68-7.63 (m, 4 H), 7.39 (t, *J* = 8.0 Hz, 2 H), 7.19 (t, *J* = 8.0 Hz, 1 H); **^{13}CNMR** (100 MHz, $CDCl_3$): δ 186.2, 158.4, 136.4, 132.9, 131.9, 131.7, 130.4, 129.2, 125.4, 119.9; IR (neat): ν = 3297.7, 1687.9, 1652.8, 1607.9, 1282.3, 815.3 cm-1; IR (neat): 3342, 1697,1665, 1538, 1279 cm^{-1}; **HRMS** calcd for $C_{14}H_{10}BrNO_2$: 302.9895 found: 302.9899.

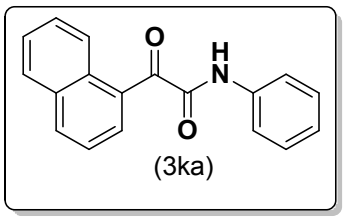
2-(naphthalen-2-yl)-2-oxo-N-phenylacetamide (3ja)



(3ja)

Yellow solid; m.p. 114-116° C; **^{1}H NMR** (400 MHz, $CDCl_3$): δ 9.28 (s, 1 H), 9.03 (b, 1 H), 8.24 (d, *J* = 8.0 Hz, 1 H), 8.01 (d, *J* = 8.0 Hz, 1 H), 7.92-7.86 (m, 2 H), 7.71 (d, *J* = 4.0 Hz, 2 H), 7.64 (t, *J* = 4.0 Hz, 1H), 7.56 (t, *J* = 4.0 Hz, 1 H), 7.41 (t, *J* = 4.0 Hz, 2 H), 7.20 (t, *J* = 8.0 Hz, 1 H); **^{13}CNMR** (100 MHz, $CDCl_3$): δ 186.9, 159.0, 136.6, 136.1, 135.3, 132.3, 130.4, 130.2, 129.5, 129.28, 129.26, 129.25, 129.23, 128.45, 128.43, 127.77, 127.75, 126.92, 126.9, 125.43, 125.41, 125.3, 119.9; IR (neat): 3340, 1690, 1665, 1534, 1274 cm^{-1}; **HRMS** calcd for $C_{18}H_{13}NO_2$: 275.0946 found: 275.0946.

2-(naphthalen-1-yl)-2-oxo-N-phenylacetamide (3ka)

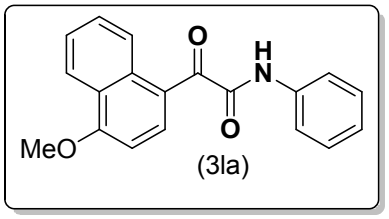


(3ka)

Yellow solid; m.p. 162-164° C; **^{1}H NMR** (400 MHz, $CDCl_3$): δ 9.08 (b, 1 H), 8.55 (d, *J* = 4.0 Hz, 1 H), 8.37 (t, *J* = 8.0 Hz, 1 H), 8.09 (d, *J* = 8.0 Hz, 1 H), 7.91 (d, *J* = 8.0 Hz, 1 H), 7.73 (d, *J* = 8.0 Hz,, 2 H), 7.65-7.61 (m, 1 H), 7.55 (t, *J* = 4.0 Hz, 2 H), 7.40 (t, *J* = 8.0 Hz, 2 H), 7.19 (t, *J*= 8.0 Hz, 1 H); **^{13}CNMR** (100 MHz, $CDCl_3$): δ 190.0, 159.1, 136.7, 134.7, 133.8, 133.2, 131.2,

129.3, 129.2, 128.7, 128.4, 126.6, 125.3, 125.2, 124.2, 119.8; IR (neat): 3339, 1693, 1668, 1536, 1273, cm^{-1}; **HRMS** calcd for $C_{18}H_{13}NO_2$: 275.0946 found: 275.0949.

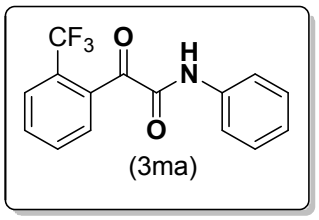
2-(4-methoxynaphthalen-1-yl)-2-oxo-N-phenylacetamide (3la)



(3la)

Yellow solid; m.p. 168-170° C; **^{1}H NMR** (400 MHz, $CDCl_3$): δ 9.23 (s, 1 H), 9.04 (b, 1 H), 8.23 (d, *J* = 4.0 Hz, 1 H), 7.89 (d *J* = 4.0 Hz, 1 H), 7.77 (d, *J* = 8.0 Hz, 1 H), 7.72 (d, *J* = 8.0 Hz, 2 H), 7.39 (t, *J* = 8.0 Hz, 2 H), 7.21-7.18 (m, 2 H), 7.14 (s, 1 H), 3.95 (s, 1 H); **^{13}CNMR** (100 MHz, $CDCl_3$): δ 186.3, 160.6, 159.4, 138.1, 136.7, 135.2, 132.7, 132.1, 129.2, 128.3, 127.7, 127.1, 126.3, 125.2, 119.9, 119.7, 105.8, 55.4; IR (neat): 3337, 1682, 1660, 1529, 1266 cm^{-1}; **HRMS** calcd for $C_{19}H_{15}NO_3$: 305.1052 found: 305.1055.

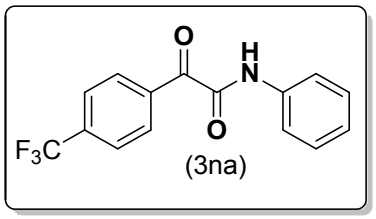
2-oxo-N-phenyl-2-(2-(trifluoromethyl)phenyl)acetamide (3ma)



(3ma)

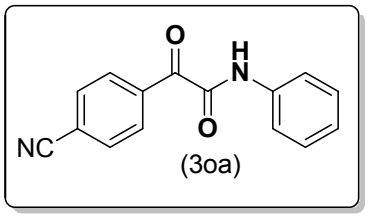
Yellow solid; m.p. 148-150° C; **^{1}H NMR** (400 MHz, $CDCl_3$): δ 8.89 (b, 1 H), 7.80-7.78 (m, 2 H), 7.70-7.68 (m, 4 H), 7.40 (t, *J* = 8.0 Hz, 2 H), 7.21 (t, *J* = 8.0 Hz, 1 H); **^{13}CNMR** (100 MHz, $CDCl_3$): δ 191.0, 157.0, 136.2, 133.4, 131.5, 131.3, 129.4, 129.3, 126.8 (d, J_{C-F} = 4.0 Hz), 125.5, 124.5, 119.7 (d, J_{C-F} = 3.0 Hz); IR (neat): 3345, 1702, 1668, 1544, 1335, 1068 cm^{-1}; **HRMS** calcd for $C_{15}H_{10}F_3NO_2$: 293.0664 found: 293.0664.

2-(4-acetylphenyl)-2-oxo-N-phenylacetamide (3na)



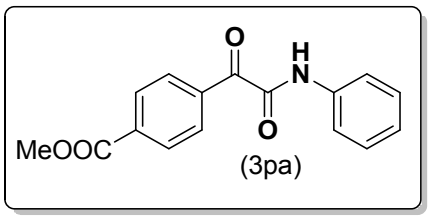
Yellow solid; m.p. 153-156° C; **^{1}H NMR** (400 MHz, $CDCl_3$): δ 8.95 (b, 1 H), 8.50 (d, *J* = 8.0 Hz, 2 H), 7.75-7.67 (m, 4 H), 7.41-7.37 (m, 2 H), 7.20 (t, *J* = 8.0 Hz, 1 H); **^{13}CNMR** (100 MHz, $CDCl_3$): δ 186.5, 158.1, 136.2, 135.7, 135.2, 131.7, 129.2, 125.5 (d, J_{C-F} = 6.0 Hz), 125.45 (d, J_{C-F} = 3.0 Hz), 125.40, 119.9 (d, J_{C-F} = 1.0 Hz); IR (neat): 3345, 1704, 1670, 1545, 1337, 1065 cm^{-1}; **HRMS** calcd for $C_{15}H_{10}F_3NO_2$: 293.0664 found: 293.0663.

2-(4-cyanophenyl)-2-oxo-N-phenylacetamide (3oa)



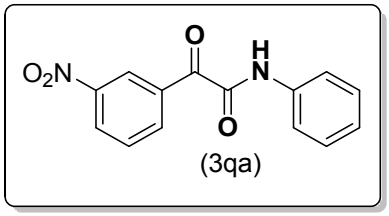
Yellow solid; m.p. 146-148° C; **^{1}H NMR** (400 MHz, $CDCl_3$): δ 8.92 (b, 1 H), 8.49 (d, *J* = 4.0 Hz, 2 H), 7.78 (d, *J* = 8.0 Hz, 2 H), 7.67 (d, *J* = 8.0 Hz, 2 H), 7.39 (t, *J* = 8.0 Hz, 2 H), 7.20 (t, *J* = 4.0 Hz, 1 H); **^{13}CNMR** (100 MHz, $CDCl_3$): δ 186.1, 157.8, 136.15, 136.11, 132.1, 131.7, 129.3, 125.6, 119.9, 117.7, 117.5; IR (neat): 3342, 2253, 1702, 1669, 1545, 1337, 1065 cm^{-1}; **HRMS** calcd for $C_{15}H_{10}N_2O_2$: 250.0742 found: 250.0745.

methyl 4-(2-oxo-2-(phenylamino)acetyl)benzoate (3pa)



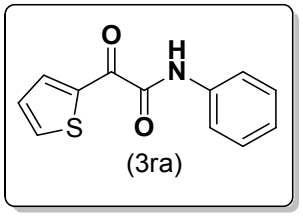
Yellow solid; m.p. 167-169° C; **^{1}H NMR** (400 MHz, $CDCl_3$): δ 8.93 (b, 1 H), 8.44 (d, *J* = 8.0 Hz, 2 H), 8.13 (d, *J* = 8.0 Hz, 2 H), 7.68 (d, *J* = 8.0 Hz, 2 H), 7.38 (t, *J* = 8.0 Hz, 2 H), 7.19 (t, *J* = 8.0 Hz, 1 H), 3.94 (s, 3 H); **^{13}CNMR** (100 MHz, $CDCl_3$): δ 186.9, 166.0, 158.2, 136.3, 136.2, 134.9, 131.3, 129.5, 129.2, 125.4, 119.9; IR (neat): 3330, 2982, 1712, 1701, 1527, 1279 cm^{-1}**;** **HRMS** calcd for $C_{16}H_{13}NO_4$: 283.0845 found: 283.0848.

2-(3-nitrophenyl)-2-oxo-N-phenylacetamide (3qa)



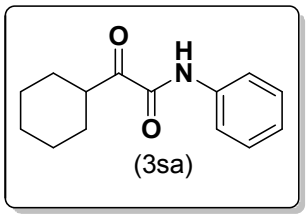
Yellow solid; m.p. 158-160° C; **^{1}H NMR** (400 MHz, $CDCl_3$): δ 9.25 (s, 1 H), 8.95 (b, 1 H), 8.78-8.76 (m, 1 H), 8.49-8.46 (m, 1 H), 7.70-7.67 (m, 3 H), 7.41-7.37 (m, 2 H), 7.22-7.19 (m, 1 H); **^{13}CNMR** (100 MHz, $CDCl_3$): δ 185.3, 157.7, 148.2, 137.0, 136.1, 134.2, 129.8, 129.3, 128.5, 126.3, 125.7, 120.0; IR (neat): 3337, 2919, 1708, 1666, 1511 cm^{-1}; **HRMS** calcd for $C_{14}H_{10}N_2O_4$: 270.0641 found: 270.0641.

2-oxo-N-phenyl-2-(thiophen-2-yl)acetamide (3ra)



Yellow solid; m.p. 133-135° C; **^{1}H NMR** (400 MHz, $CDCl_3$): δ 9.11 (b, 1 H), 8.45 (d, *J* = 4.0 Hz, 1 H), 7.85 (d, *J* = 4.0 Hz, 1 H), 7.68 (t, *J* = 8.0 Hz, 2 H), 7.38 (t, *J* = 8.0 Hz, 2 H), 7.21-7.18 (m, 2 H); **^{13}CNMR** (100 MHz, $CDCl_3$): δ 178.3, 158.2, 139.2, 138.5, 136.3, 129.2, 129.1, 128.3, 125.3, 119.9; IR (neat): 3330, 1690, 1650, 1409, 1283, 1048 cm^{-1}; **HRMS** calcd for $C_{12}H_9NO_2S$: 231.0354 found: 231.0357.

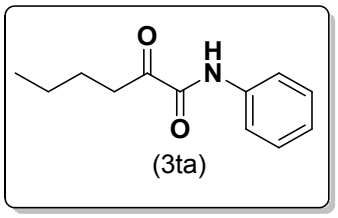
2-cyclohexyl-2-oxo-N-phenylacetamide (3sa)



(3sa)

Yellow solid; m.p. 105-107° C; **^{1}H NMR** (400 MHz, $CDCl_3$): δ 8.75 (b, 1 H), 7.62 (d, *J* = 4.0 Hz, 2 H), 7.34 (t, *J* = 4.0 Hz, 2 H), 7.14 (t, *J* = 4.0 Hz, 1 H), 3.50-3.46 (m, 1 H), 1.92 (d, *J* = 8.0 Hz, 2 H), 1.80 (d, *J* = 12.0 Hz, 2 H), 1.70 (t, *J* = 8.0 Hz, 1 H), 1.40-1.25 (m, 6 H); **^{13}CNMR** (100 MHz, $CDCl_3$): δ 201.6, 157.2, 136.4, 129.1, 125.1, 119.6, 43.1, 28.1, 25.7, 25.3; IR (neat): 3320, 1713, 1668, 1511,1148 cm^{-1}; **HRMS** calcd for $C_{14}H_{17}NO_2$: 231.1259 found: 231.1257.

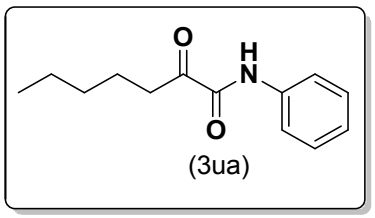
2-oxo-N-phenylhexanamide (3ta)



(3ta)

Yellow solid; m.p. 79-82° C; **^{1}H NMR** (400 MHz, $CDCl_3$): δ 8.72 (b, 1 H), 7.62 (d, *J* = 8.0 Hz, 2 H), 7.35 (t, *J* = 4.0 Hz, 2 H), 7.15 (t, *J* = 4.0 Hz, 1 H), 2.99 (t, *J*= 4.0 Hz, 2 H), 1.66-1.60 (m, 2 H), 1.42-1.34 (m, 2 H), 0.92 (t, *J* = 4 Hz, 3 H); **^{13}CNMR** (100 MHz, $CDCl_3$): δ 199.5, 157.5, 136.3, 129.2, 125.2, 119.7, 36.0, 25.4, 22.2, 13.8; IR (neat): 3325, 2936, 1714, 1670, 1239 cm^{-1} ; **HRMS** calcd for $C_{12}H_{15}NO_2$: 205.1103 found: 205.1098.

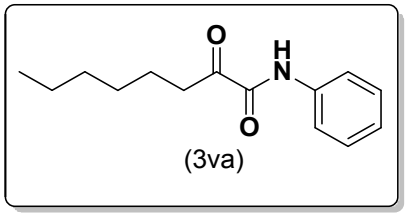
2-oxo-N-phenylheptanamide (3ua)



(3ua)

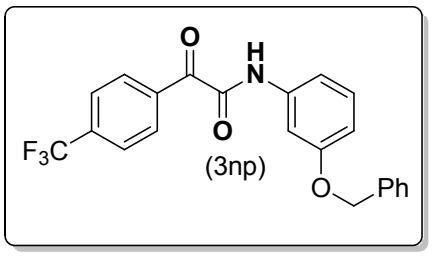
Yellow solid; m.p. 90-92° C; **^{1}H NMR** (400 MHz, $CDCl_3$): δ 8.72 (b, 1 H), 7.62 (d, *J* = 8.0 Hz, 2 H), 7.35 (t, *J* = 4.0 Hz, 2 H), 7.15 (t, *J* = 4.0 Hz, 1 H), 2.98 (t, *J* = 8.0 Hz, 2 H), 1.68-1.62 (m, 2 H), 1.34-1.32 (m, 4 H), 0.89 (t, *J*= 4 Hz, 3 H); **^{13}CNMR** (100 MHz, $CDCl_3$): δ 199.5, 157.5, 136.3, 129.2, 125.2, 119.7, 36.3, 31.2, 23.0, 22.3, 13.8; IR (neat): 3325, 2936, 1713, 1667, 1237 cm^{-1}; **HRMS** calcd for $C_{13}H_{17}NO_2$: 219.1259 found: 219.1260.

2-oxo-N-phenyloctanamide (3va)



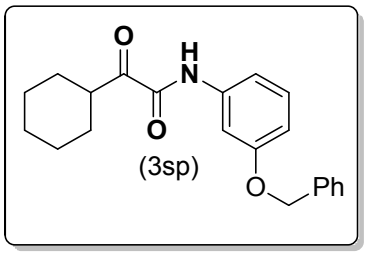
Yellow solid; m.p. 108-111° C; **^{1}H NMR** (400 MHz, $CDCl_3$): δ 8.73 (b, 1 H), 7.62 (d, *J* = 8.0 Hz, 2 H), 7.35 (t, *J* = 8.0 Hz, 2 H), 7.15 (t, *J* = 4.0 Hz, 1 H), 2.98(t, *J* = 4.0 Hz, 2 H), 1.67-1.61 (m, 2 H), 1.36-1.30 (m, 7 H), 0.87 (t, *J* = 8 Hz, 3 H); **^{3}CNMR** (100 MHz, $CDCl_3$): δ 199.5, 157.5, 136.3, 129.2, 125.2, 119.6, 36.3, 31.4, 23.0, 28.7, 23.2, 22.4, 14.0; IR (neat): 3321, 2939, 1715, 1669, 1529, 1235, 1054 cm^{-1}; **HRMS** calcd for $C_{14}H_{19}NO_2$: 233.1416 found: 233.1416.

N-(3-(benzyloxy)phenyl)-2-oxo-2-(4-(trifluoromethyl)phenyl)acetamide (3np)



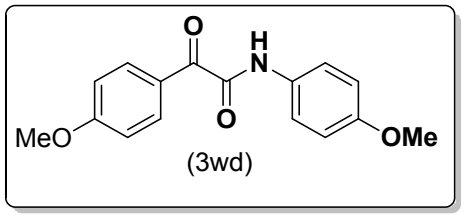
Yellow solid; m.p. 157-160° C; **^{1}H NMR** (400 MHz, $CDCl_3$): δ 8.91 (b, 1 H), 8.51 (d, *J* = 8.0 Hz, 2 H), 7.76 (d, *J* = 8.0 Hz, 2 H), 7.53 (s, 1 H), 7.44 (d, *J* = 8.0 Hz, 2 H), 7.40-7.37 (m, 2 H), 7.34-7.27 (m, 2 H), 7.16 (d, *J* = 4.0 Hz, 1 H), 6.83 (t, *J* = 4.0 Hz, 1 H), 5.09 (s, 2 H); **^{13}CNMR** (100 MHz, $CDCl_3$): δ 186.4, 159.4, 158.0, 137.4, 136.6, 135.8, 135.7 (d, J_{C-F} = 11.0 Hz), 135.1, 132.7, 131.7, 130.0, 28.6, 128.0, 127.5, 125.5 (d, J_{C-F} = 3.0 Hz), 112.4 (d, J_{C-F} = 17.0 Hz), 106.5, 70.0; IR (neat): 3340, 2929,1702, 1680, 1598 cm^{-1}; **HRMS** calcd for $C_{22}H_{16}F_3NO_3$: 399.1082 found: 399.1087.

N-(3-(benzyloxy)phenyl)-2-cyclohexyl-2-oxoacetamide (3sp)



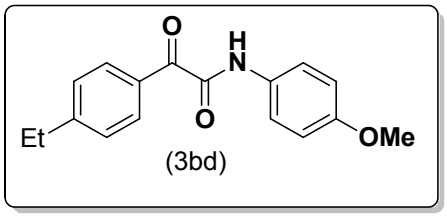
Yellow solid; m.p. 148-152° C; **^{1}H NMR** (400 MHz, $CDCl_3$): δ 8.78 (b, 1 H), 7.54 (s, 1 H), 7.45-7.33 (m, 5 H), 7.27 (d, *J* = 8.0 Hz, 1 H), 7.13 (d, *J* = 8.0 Hz, 1 H), 6.80 (d, *J* = 8.0 Hz, 1 H), 5.08(s, 2 H), 3.51-3.47 (m, 1 H), 1.96-1.72 (m, 5 H), 1.46-1.22 (m, 6 H); **^{13}CNMR** (100 MHz, $CDCl_3$): δ 201.5, 159.3, 157.2, 137.6, 136.6, 129.8, 128.5, 127.9, 127.4, 112.1, 112.0, 106.0, 43.1, 28.1, 25.7, 25.3; IR (neat): 3329, 2933, 1717, 1670, 1539, 1235, 1054 cm-1; **HRMS** calcd for $C_{21}H_{23}NO_3$: 337.1678 found: 337.1679.

N,2-bis(4-methoxyphenyl)-2-oxoacetamide (3wd)



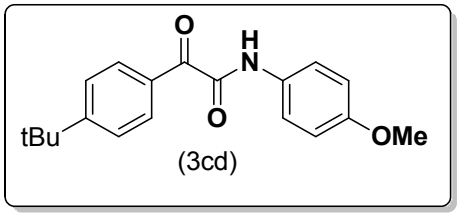
Yellow solid; m.p. 118-120° C; **^{1}H NMR** (400 MHz, $CDCl_3$): δ 8.93 (b, 1 H), 8.48 (d, *J* = 8.0 Hz, 2 H), 7.59 (d, *J* = 8.0 Hz, 2 H), 6.96-6.89 (m, 4 H), 3.88 (s, 3 H), 3.79 (s, 3 H); **^{13}CNMR** (100 MHz, $CDCl_3$): δ 185.3, 164.8, 159.2, 156.9, 134.2, 129.9, 126.2, 121.4, 114.3, 113.8, 55.5, 55.4; IR (neat): 3333, 1689, 1668, 1587, 1258 cm^{-1}; **HRMS** calcd for $C_{16}H_{15}NO_4$: 285.1001, found: 285.1005.

2-(4-ethylphenyl)-N-(4-methoxyphenyl)-2-oxoacetamide (3bd)



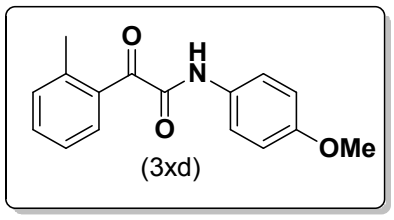
Yellow solid; m.p. 132-134° C; **^{1}H NMR** (400 MHz, $CDCl_3$): δ 8.89 (b, 1 H), 8.34 (d, *J* = 8.0 Hz, 2 H), 7.60 (d, *J* = 4.0 Hz, 2 H), 7.30 (d, *J* = 8.0 Hz, 2 H), 6.90 (d, *J* = 8.0 Hz, 2 H), 3.80 (s, 3 H), 2.71 (q, *J* = 8.0 Hz, 2 H), 1.25 (t, *J* = 8.0 Hz, 3 H); **^{13}CNMR** (100 MHz, $CDCl_3$): δ 187.0, 158.9, 156.9, 151.9, 131.7, 130.8, 129.8, 128.0, 121.4, 114.3, 55.4, 29.1, 15.0; IR (neat): 3335, 1690, 1671, 1580, 1257 cm^{-1}; **HRMS** calcd for $C_{17}H_{17}NO_3$: 283.1208, found: 283.1216.

2-(4-(tert-butyl)phenyl)-N-(4-methoxyphenyl)-2-oxoacetamide (3cd)



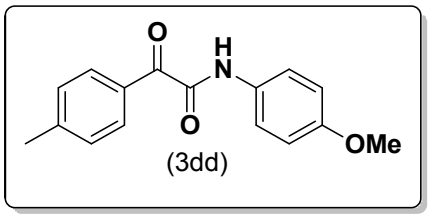
Yellow solid; m.p. 116-118° C; **^{1}H NMR** (400 MHz, $CDCl_3$): δ 8.87 (b, 1 H), 8.34 (d, *J* = 8.0 Hz, 2 H), 7.60 (d, *J* = 12.0 Hz, 2 H), 7.50 (d, *J* = 8.0 Hz, 2 H), 6.90 (d, *J* = 12.0 Hz, 2 H), 3.80 (s, 3 H), 1.34 (s, 9 H); **^{13}CNMR** (100 MHz, $CDCl_3$): δ 187.1, 158.9, 158.5, 156.9, 131.4, 130.5, 129.8, 125.5, 121.4, 114.3, 55.4, 35.2, 30.9; IR (neat): 3340, 1692, 1670, 1585, 1257 cm^{-1}; **HRMS** calcd for $C_{19}H_{21}NO_3$: 311.1521, found: 311.1523.

N-(4-methoxyphenyl)-2-oxo-2-(o-tolyl)acetamide (3xd)



Yellow solid; m.p. 127-129° C; **^{1}H NMR** (400 MHz, $CDCl_3$): δ 8.84 (b, 1 H), 7.97 (d, *J* = 4.0 Hz, 1 H), 7.59 (d, *J* = 4.0 Hz, 2 H), 7.46-7.42 (m, 1 H), 7.30-7.24 (m, 2 H), 6.91-6.88 (m, 2 H), 3.80 (s, 3 H), 2.50 (s, 3 H); **^{13}CNMR** (100 MHz, $CDCl_3$): δ 191.2, 158.6, 157.0, 140.0, 131.9, 131.6, 129.8, 125.3, 121.3, 114.3, 55.4, 20.7; IR (neat): 3340, 1694, 1670, 1584, 1258 cm^{-1} ; **HRMS** calcd for $C_{16}H_{15}NO_3$: 269.1052 found: 269.1039.

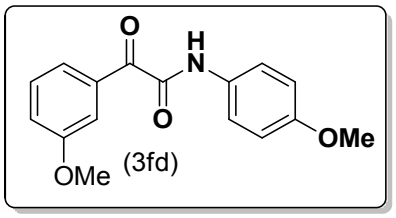
N-(4-methoxyphenyl)-2-oxo-2-(p-tolyl)acetamide (3dd)



(3dd)

Pale yellow solid; m.p. 129-131° C; **^{1}H NMR** (400 MHz, $CDCl_3$): δ 8.87 (b, 1 H), 8.32 (d, *J* = 8.0 Hz, 2 H), 7.61-7.59 (m, 2 H), 7.28 (d, *J* = 8.0 Hz, 2 H), 6.90 (d, *J* = 8.0 Hz, 2 H), 3.80 (s, 3 H), 2.42 (s, 3 H); **^{13}CNMR** (100 MHz, $CDCl_3$): δ 187.0, 158.9, 157.0, 145.84 145.82, 131.6 130.7, 129.8, 129.2, 121.4, 114.3, 55.4, 21.8; IR (neat): 3338, 1689, 1670, 1583, 1256 cm^{-1}; **HRMS** calcd for $C_{16}H_{15}NO_3$: 269.1052 found: 269.1058.

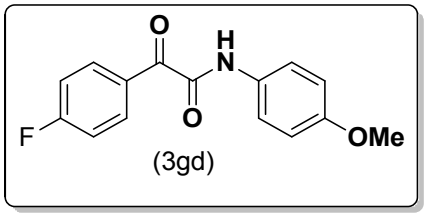
2-(3-methoxyphenyl)-N-(4-methoxyphenyl)-2-oxoacetamide (3fd)



(3fd)

Yellow solid; m.p. 119-122° C; **^{1}H NMR** (400 MHz, $CDCl_3$): δ 8.91 (b, 1 H), 8.01 (d, *J* = 8.0 Hz, 1 H), 7.86 (s, 1 H), 7.59 (d, *J* = 8.0 Hz, 2 H), 7.37 (t, *J* = 8.0 Hz, 1 H), 7.18-7.15 (m, 1 H), 6.88 (d, *J* = 8.0 Hz, 2 H), 3.83 (s, 3 H), 3.78 (s, 3 H); **^{13}CNMR** (100 MHz, $CDCl_3$): δ 187.3, 159.4, 158.7, 157.0, 134.2, 129.7, 129.4, 124.2, 121.5, 121.4, 114.9, 114.2, 55.4, 55.3; IR (neat): 3340, 1693, 1673, 1589, 1263 cm^{-1}; **HRMS** calcd for $C_{16}H_{15}NO_4$: 285.1001, found: 285.1010.

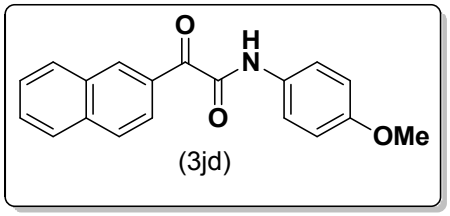
2-(4-fluorophenyl)-N-(4-methoxyphenyl)-2-oxoacetamide (3gd)



(3gd)

Yellow solid; m.p. 132-136° C; **^{1}H NMR** (400 MHz, $CDCl_3$): δ 8.89 (b, 1 H), 8.50 (d, *J* = 8.0 Hz, 2 H), 7.59 (d, *J* = 12.0 Hz, 2 H), 7.15 (t, *J* = 12.0 Hz, 2 H), 6.91 (d, *J* = 8.0 Hz, 2 H), 3.80 (s, 3 H); **^{13}CNMR** (100 MHz, $CDCl_3$): δ 185.7, 167.9, 165.4, 158.4, 157.1, 134.5 (d, J_{C-F} = 10.0 Hz), 129.6, 121.5, 115.8 (d, J_{C-F} = 22.0 Hz), 114.3, 55.4; IR (neat): 3338, 1688, 1667, 1585, 1253 cm^{-1}; **HRMS** calcd for $C_{15}H_{12}FNO_3$: 273.0801, found: 273.0795.

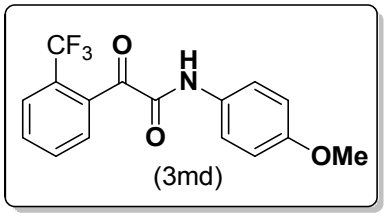
N-(4-methoxyphenyl)-2-(naphthalen-2-yl)-2-oxoacetamide (3jd)



(3jd)

Yellow solid; m.p. 166-168° C; **^{1}H NMR** (400 MHz, $CDCl_3$): δ 9.27 (s, 1 H), 8.97 (b, 1 H), 8.24-8.21 (m, 1 H), 8.00 (d, *J* = 8.0 Hz, 1 H), 7.90-7.85 (m, 2 H), 7.65-7.63 (m, 3 H), 7.56-7.52 (m, 1 H), 6.92 (d, *J* = 8.0 Hz, 2 H), 3.81 (s, 3 H); **^{13}CNMR** (100 MHz, $CDCl_3$): δ 187.1, 158.9, 157.0, 136.1, 135.26, 135.24, 132.3, 130.3, 129.8, 129.4, 128.3, 127.7, 126.8, 125.4, 121.5, 114.3, 55.4; IR (neat): 3340, 1692, 1666, 1580, 1274 cm^{-1}; **HRMS** calcd for $C_{19}H_{15}NO_3$: 305.1052, found: 305.1050.

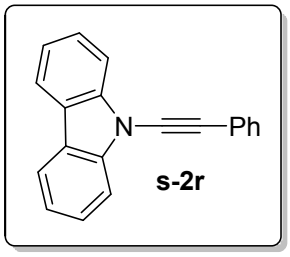
N-(4-methoxyphenyl)-2-oxo-2-(2-(trifluoromethyl)phenyl)acetamide (3md)



(3md)

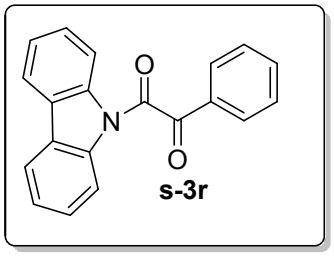
Yellow solid; m.p. 156-159° C; **^{1}H NMR** (400 MHz, $CDCl_3$): δ 8.82 (b, 1 H), 7.76 (t, *J* = 4.0 Hz, 1 H), 7.65-7.58 (m, 5 H), 6.89 (d, *J* = 12.0 Hz, 2 H), 3.79 (s, 3 H); **^{13}CNMR** (100 MHz, $CDCl_3$): δ 191.1, 157.2, 156.8, 131.4, 131.3, 129.4 (d, J_{C-F} = 4.0 Hz), 126.9, 126.8 (d, J_{C-F} = 5.0 Hz), 124.8, 122.1, 121.3, 114.4, 55.4; IR (neat): 3345, 1705, 1672, 1548, 1335 cm^{-1}; **HRMS** calcd for $C_{16}H_{12}F_3NO_3$: 323.0769, found: 323.0771.

9-(phenylethynyl)-9H-carbazole (s-2r)

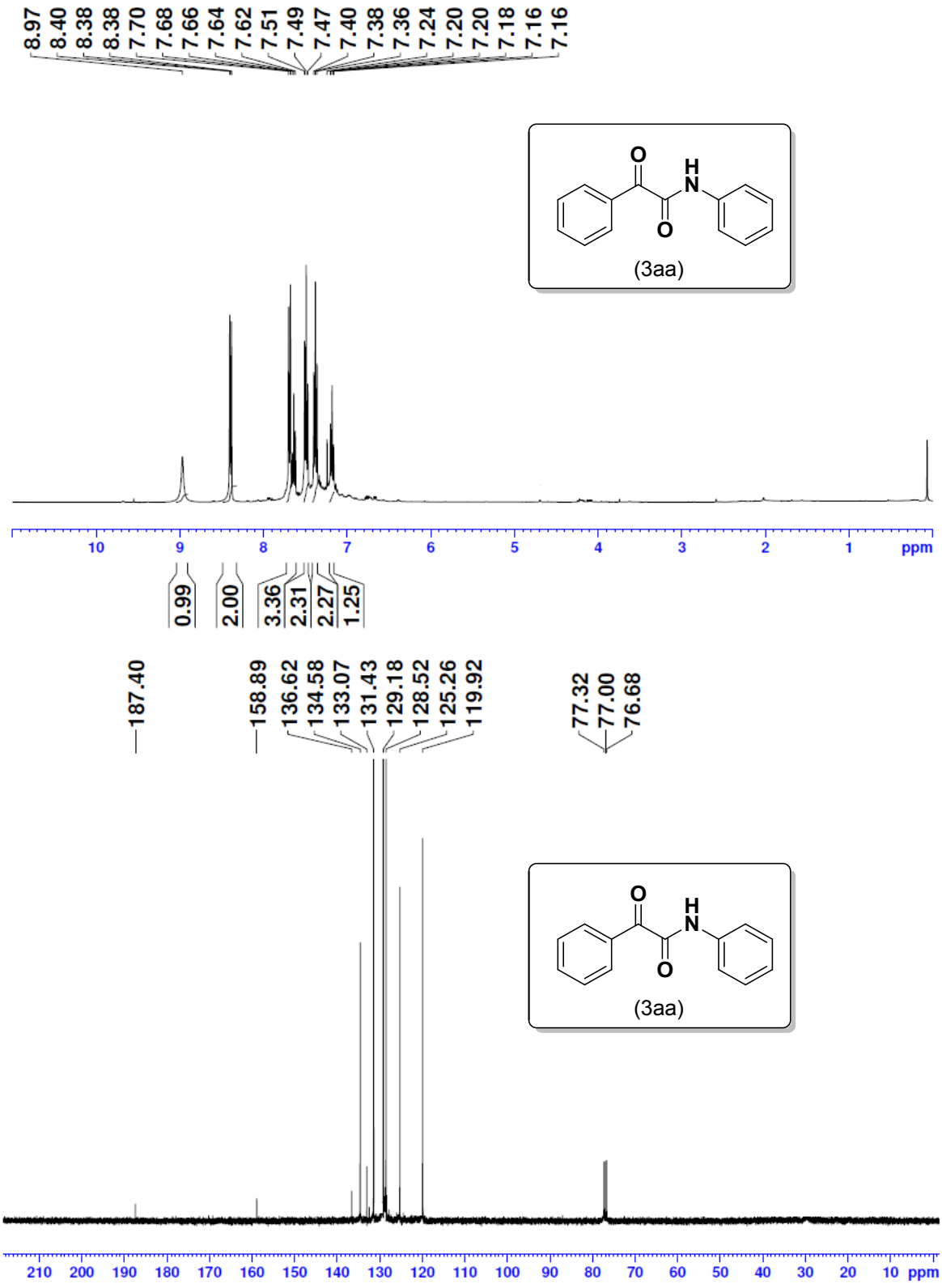


Pale yellow solid; m.p. 127-130° C; **^{1}H NMR** (400 MHz, $CDCl_3$): δ 8.02 (d, , *J* = 4.0 Hz, 2H), 7.71 (d, *J* = 4.0 Hz, 2 H), 7.61 (d, *J* = 4.0 Hz, 2 H), 7.53-7.51 (m, 2 H), 7.39-7.33 (m, 5 H); **^{13}CNMR** (100 MHz, $CDCl_3$): δ 140.4, 131.4, 128.4, 127.9, 126.7, 123.5, 122.9, 122.0, 120.3, 111.2, 78.8, 74.5; IR (neat): 3054, 2984, 2305, 2178, 1274, cm^{-1}; **HRMS** calcd for $C_{20}H_{13}N$: 267.1048, found: 267.1051.

1-(9H-carbazol-9-yl)-2-phenylethane-1,2-dione (s-3r)



Yellow solid; m.p. 139-142° C; **^{1}H NMR** (400 MHz, $CDCl_3$): δ 8.76 (d, *J* = 5.6 Hz, 1 H), 8.09 (d, *J*= 4.8 Hz, 2 H) 7.98 (q, *J* = 5.4 Hz, 2 H) 7.72 (t, *J*= 4.8 Hz, 1 H), 7.56 (t, *J* = 4.8 Hz, 3 H) 7.48 (t, *J* = 4.8 Hz, 1 H) 7.33 (t, *J* = 4.4 Hz, 1 H), 7.22 (q, *J* = 8.8 Hz, 1 H), 7.16 (d, *J* = 5.2 Hz, 1 H); **^{13}CNMR** (100 MHz, $CDCl_3$): δ 188.8, 165.6, 138.0, 136.1, 135.6, 131.9, 130.2, 129.4, 128.0, 127.1, 126.8, 126.4, 125.2, 124.4, 120.5, 119.7, 117.8, 113.5; IR (neat): 3012, 2937, 2635, 2413, 1680, 1628, 1392, 1029 cm^{-1}; **HRMS** calcd for $C_{20}H_{13}NO_2$: 299.0946, found: 299.0950.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8.38
7.70
7.68
7.66
7.64
7.62
7.51
7.49
7.47
7.40
7.38
7.36
7.24
7.20
7.20
7.18
7.16
7.16
O
H
N
O
(3aa)
10
9
8
7
6
5
4
3
2
1
ppm
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2.00
3.36
2.31
2.27
1.25
187.40
158.89
136.62
134.58
133.07
131.43
129.18
128.52
125.26
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77.32
77.00
76.68
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H
N
O
(3aa)
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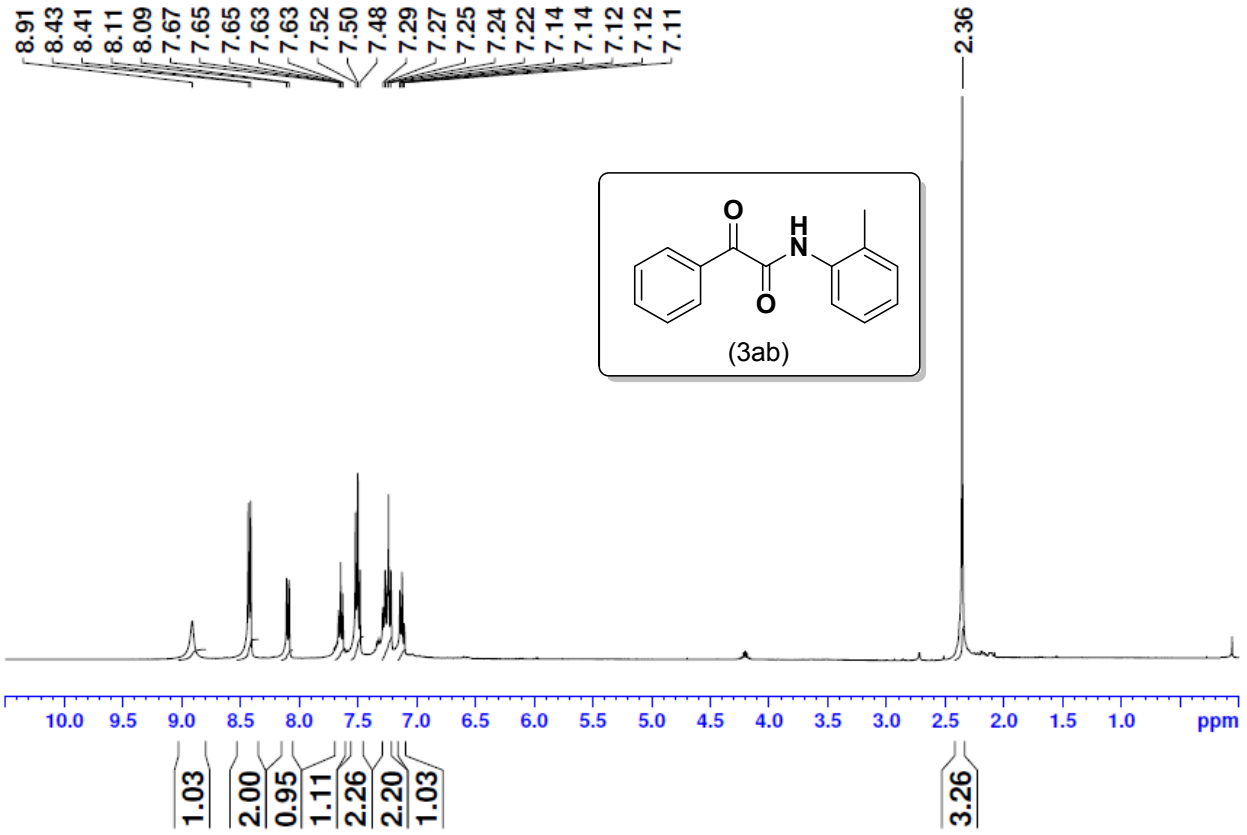
30
20
10
ppm


8.91
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8.11
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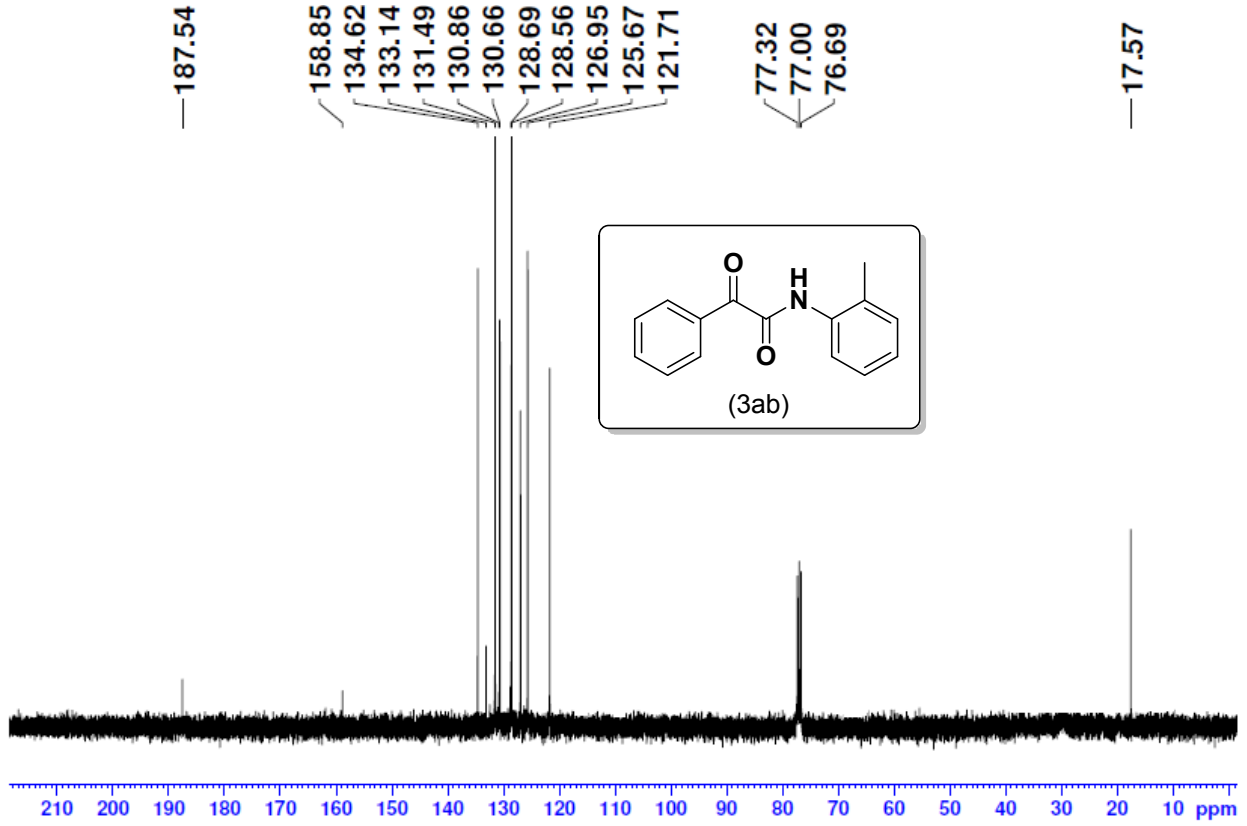
7.65
7.65
7.63
7.63
7.52
7.50
7.48
7.29
7.27
7.25
7.24
7.22
7.14
7.14
7.12
7.12
7.11
2.36
O
H
N
O
(3ab)
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 ppm
1.03
2.00
0.95
1.11
2.26
2.20
1.03
3.26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128.69
128.56
126.95
125.67
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77.00
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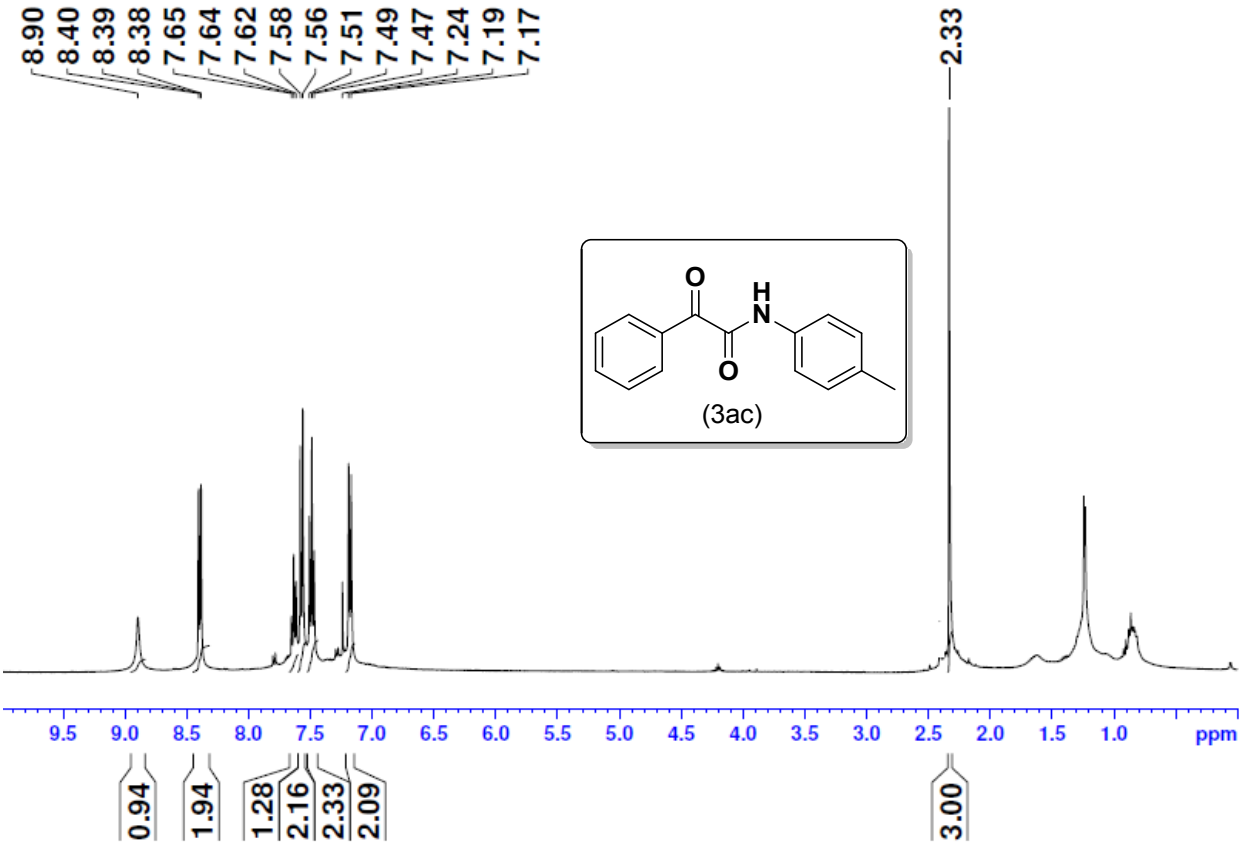
17.57
O
H
N
O
(3ab)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm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7.19
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H
N
O
(3ac)
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 ppm
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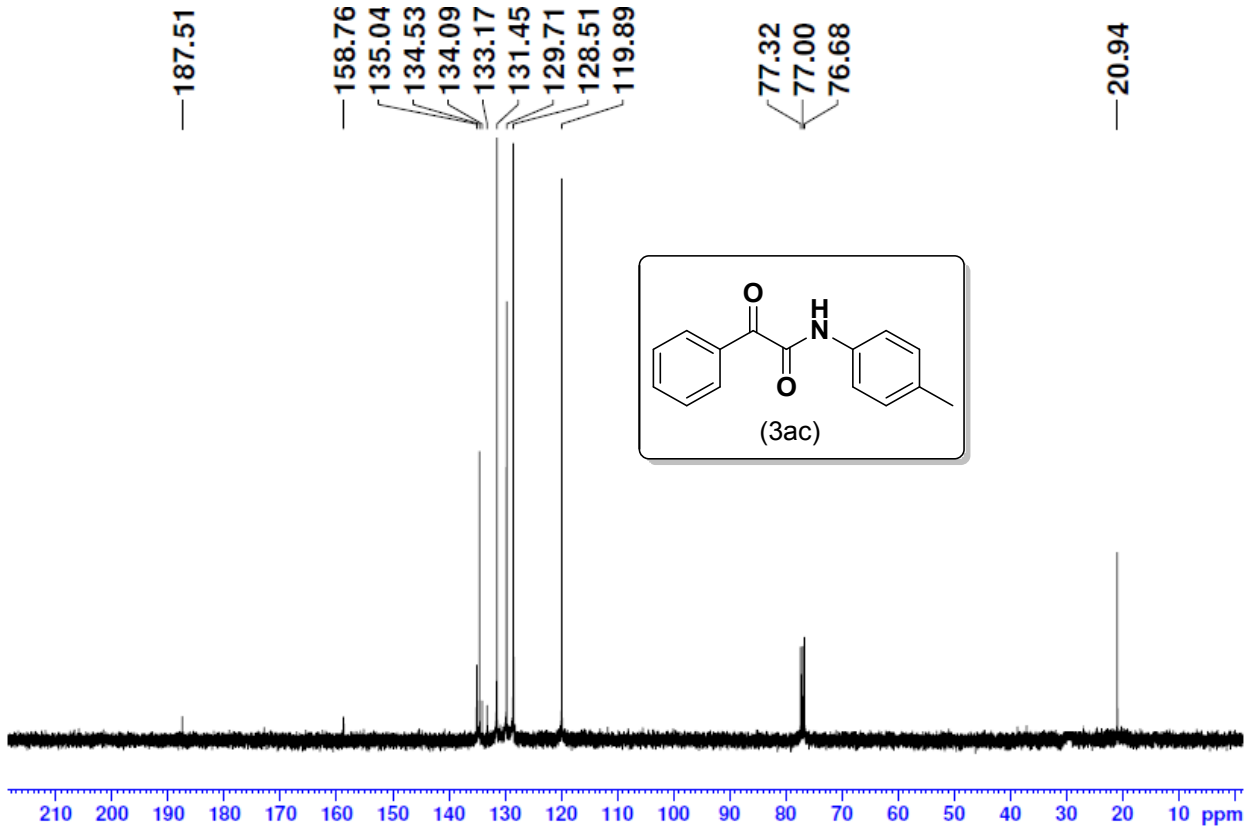
1.94
1.28
2.16
2.33
2.09
3.00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129.71
128.51
119.89
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77.00
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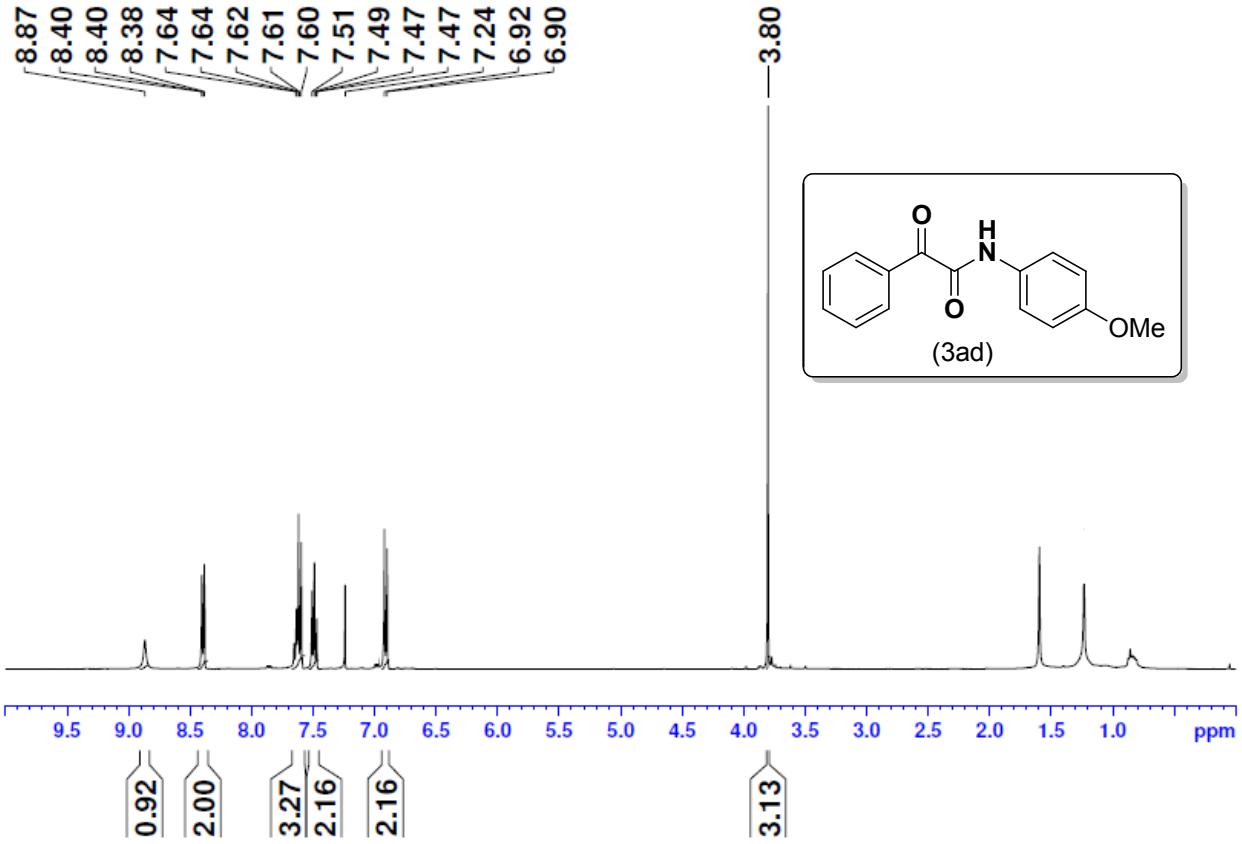
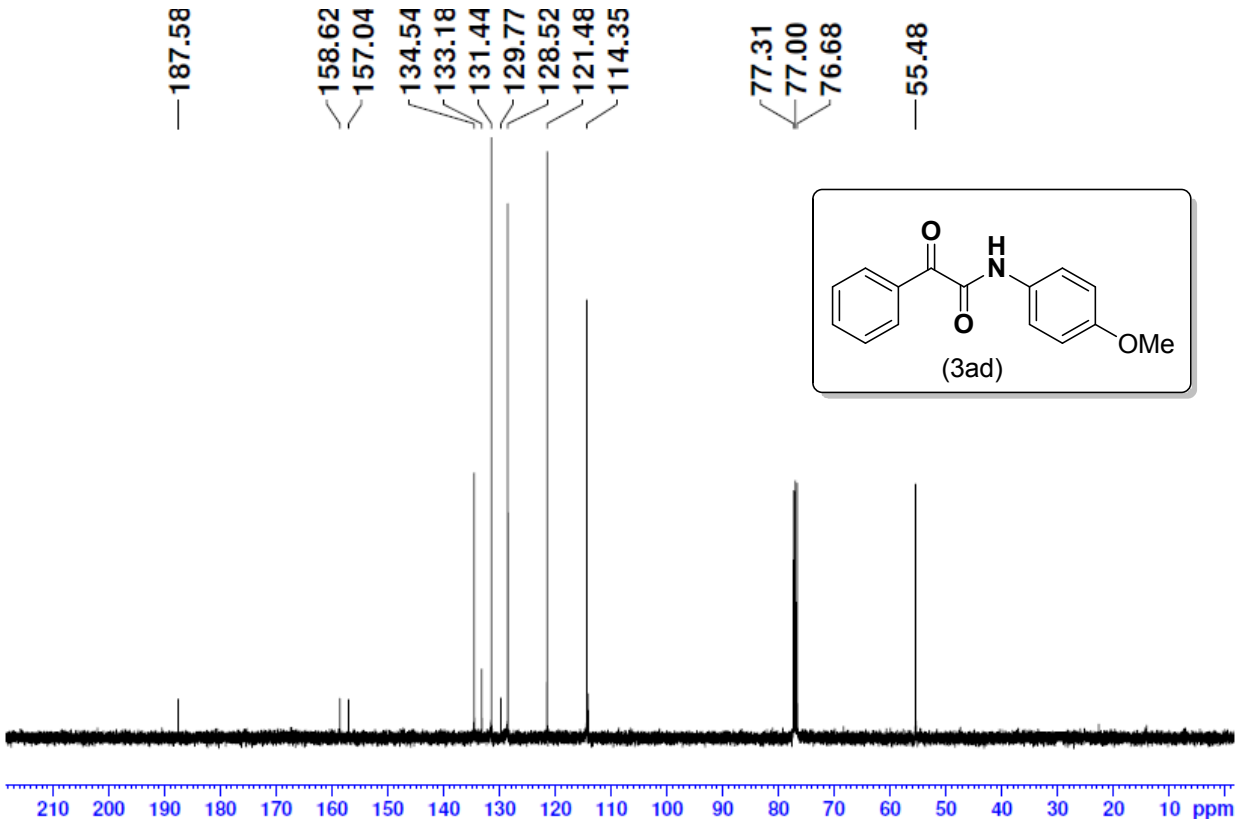
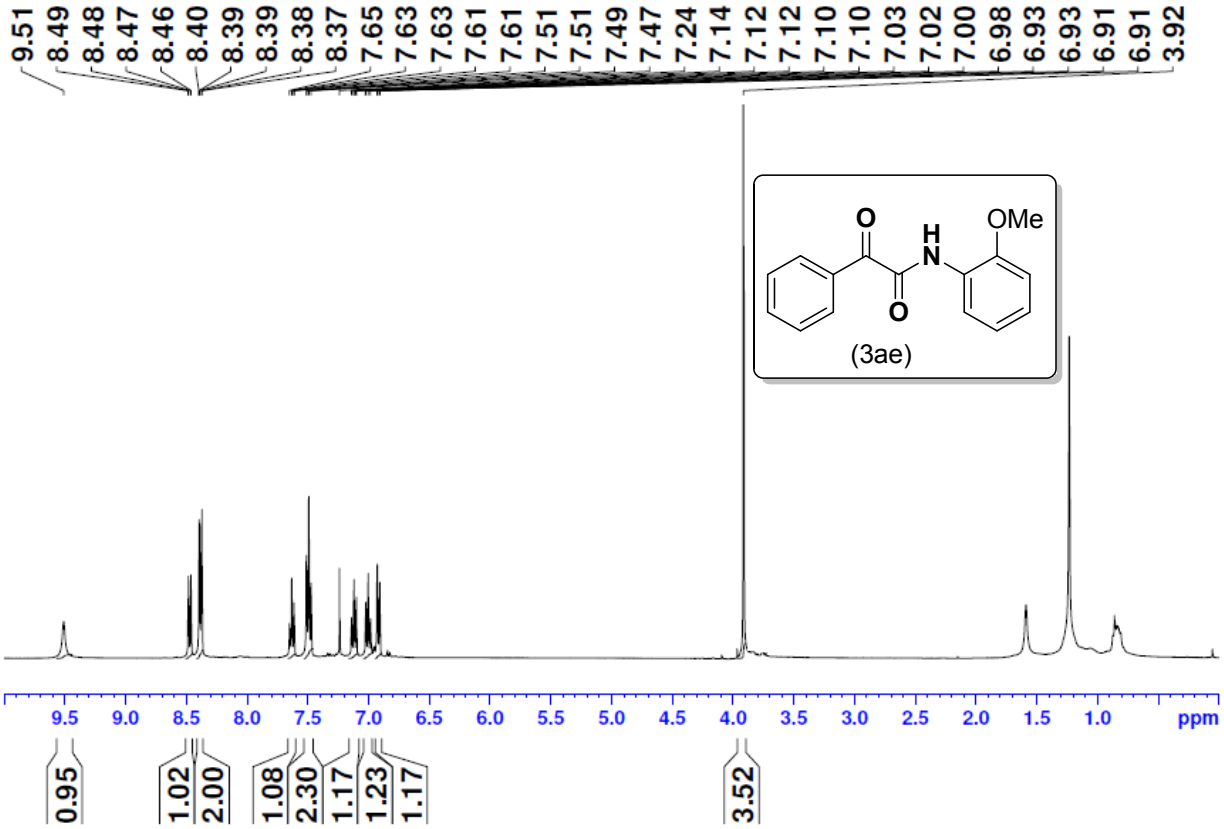
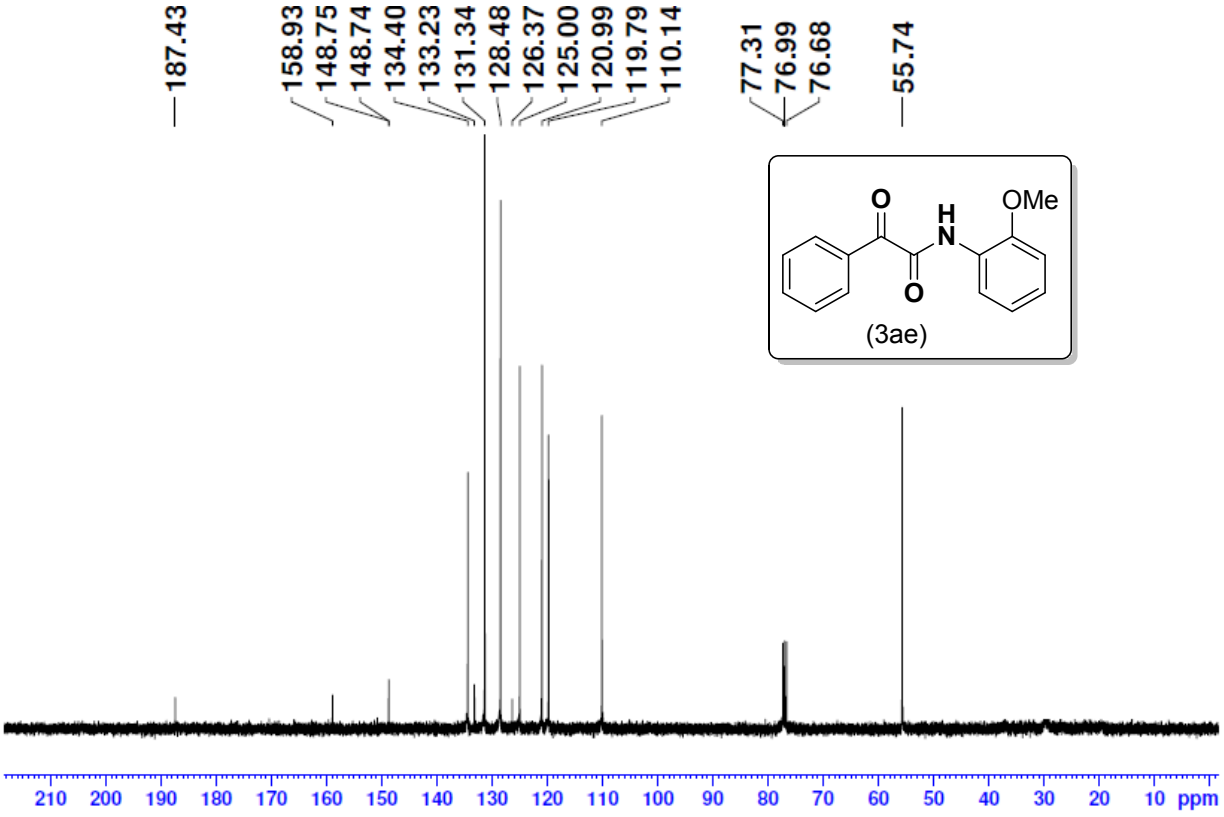
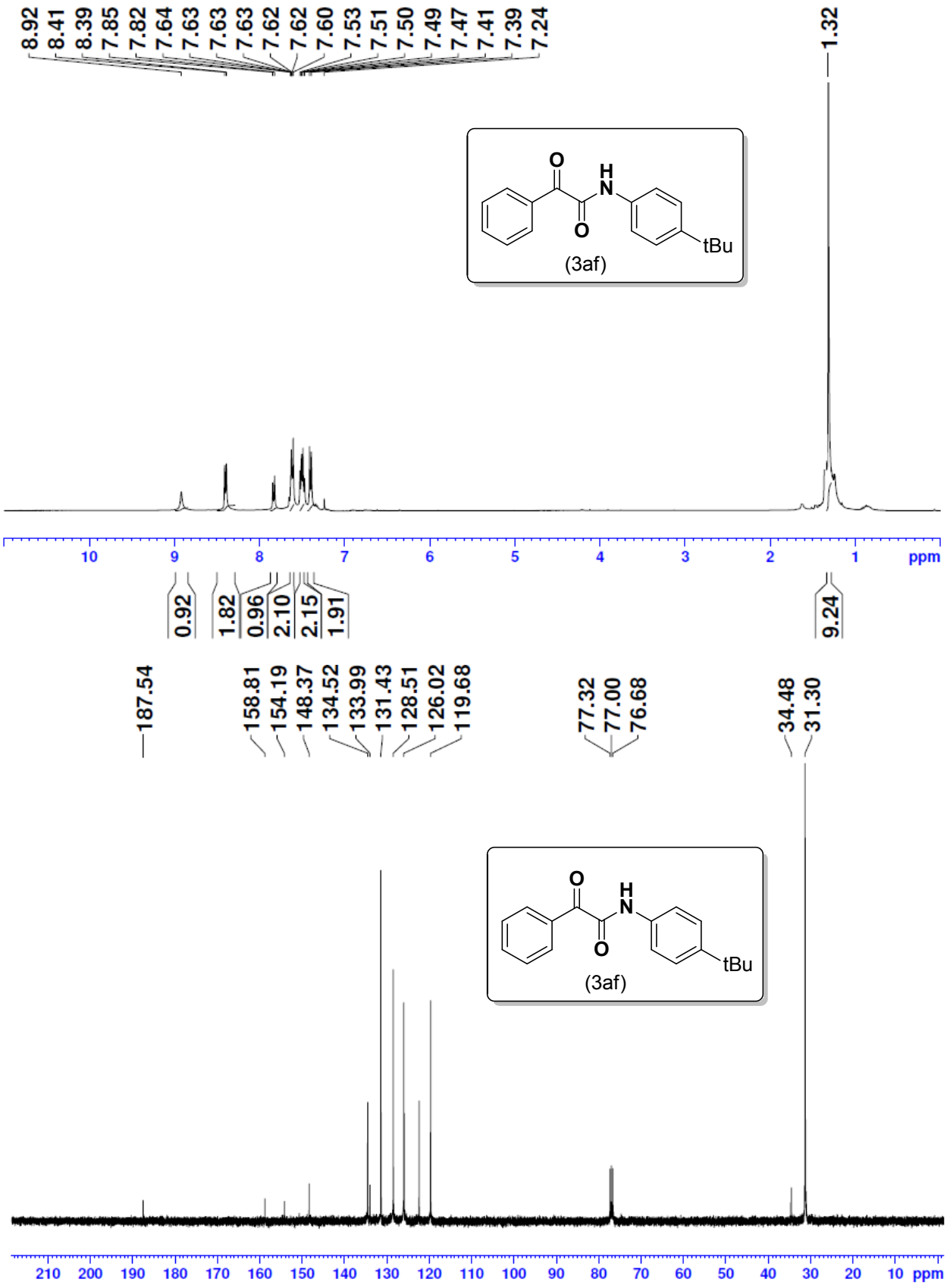
20.94
O
H
N
O
(3ac)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

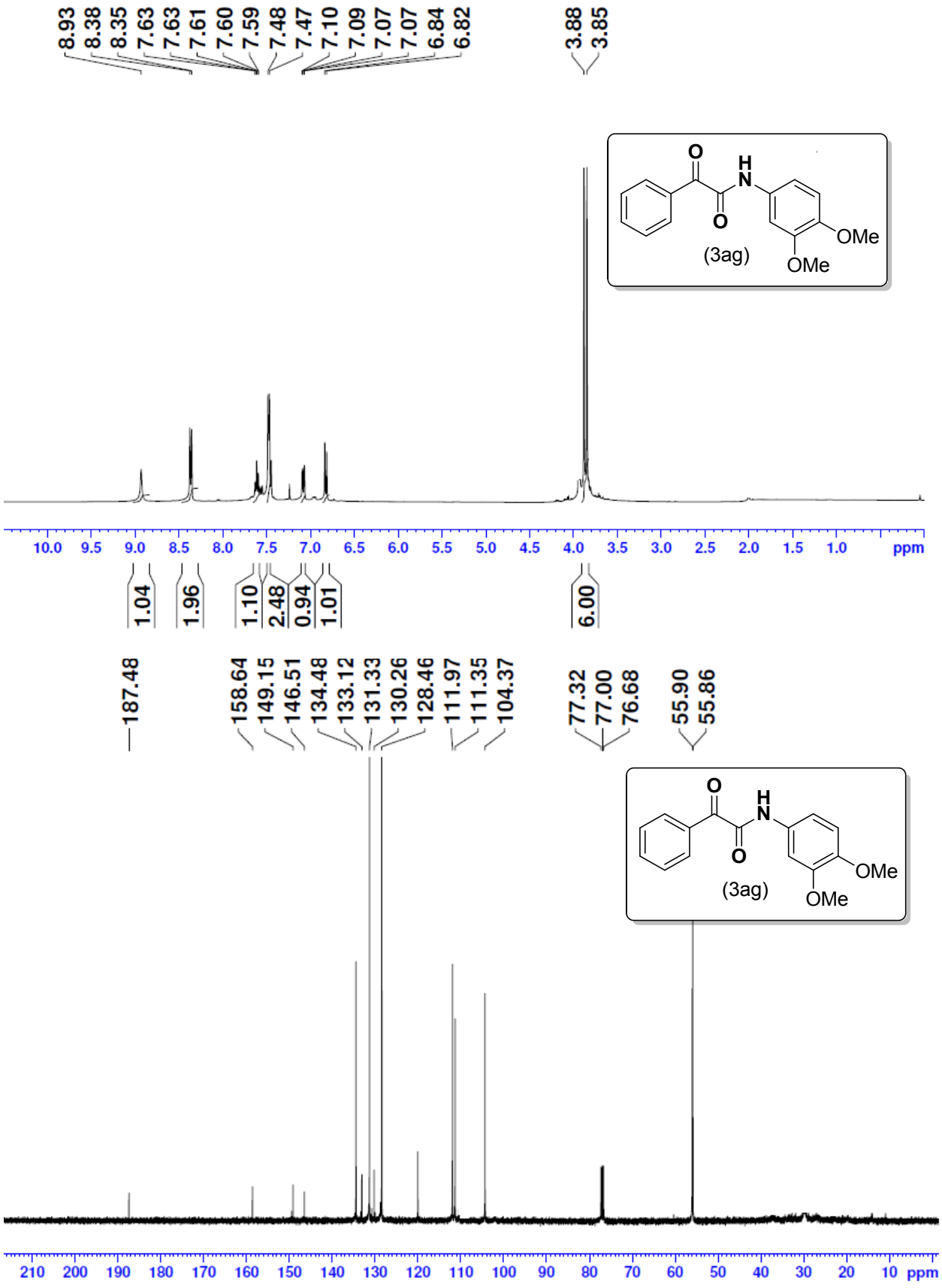

8.87
8.40
8.40
8.38
7.64
7.64
7.62
7.61
7.60
7.51
7.49
7.47
7.47
7.24
6.92
6.90
3.80
O
H
N
O
OMe
(3ad)
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 ppm
0.92
2.00
3.27
2.16
2.16
3.13

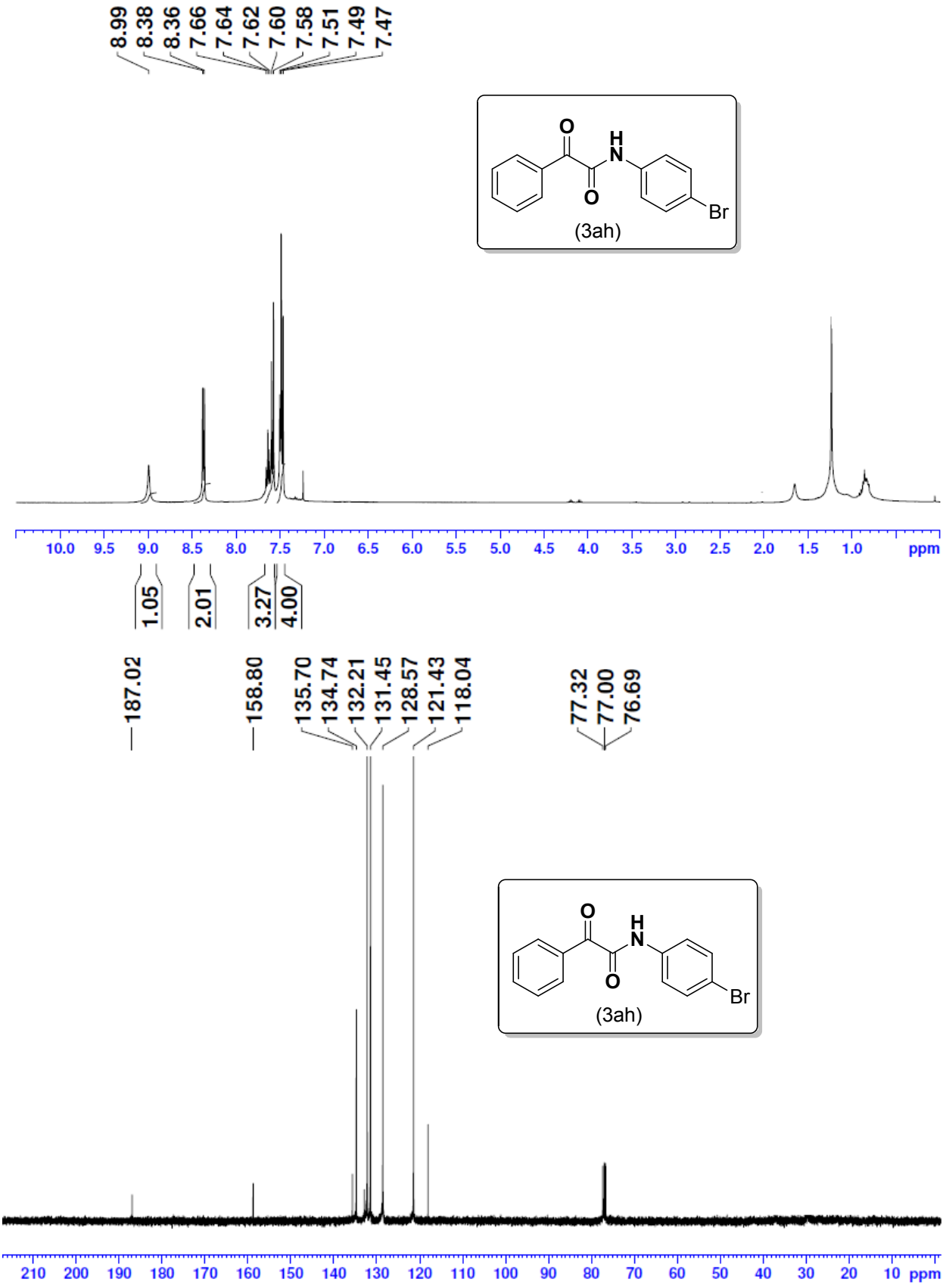

187.58
158.62
157.04
134.54
133.18
131.44
129.77
128.52
121.48
114.35
77.31
77.00
76.68
55.48
O
H
N
O
OMe
(3ad)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

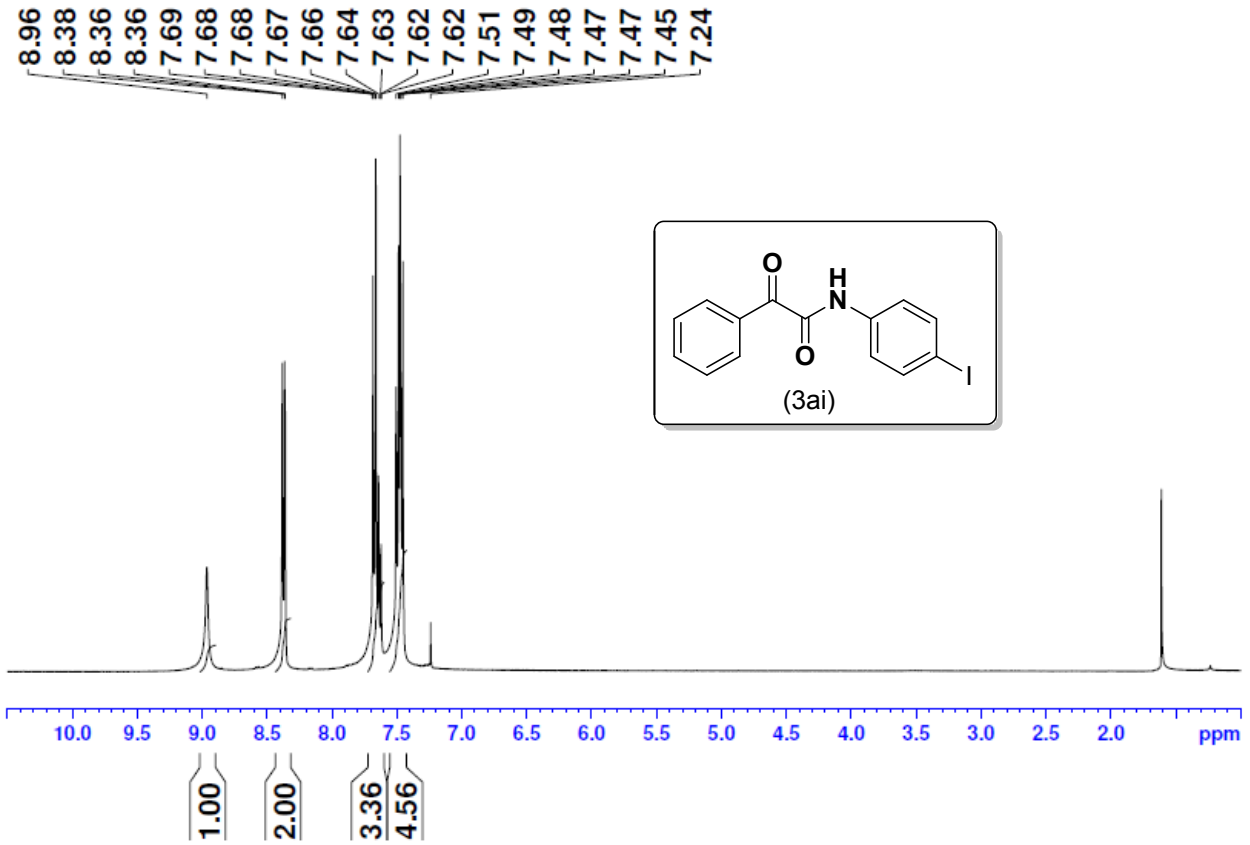

9.51
8.49
8.48
8.47
8.46
8.40
8.39
8.39
8.38
8.37
7.65
7.63
7.63
7.61
7.61
7.51
7.51
7.49
7.47
7.24
7.14
7.12
7.12
7.10
7.10
7.03
7.02
7.00
6.98
6.93
6.93
6.91
6.91
3.92
O
H
N
OMe
O
(3ae)
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 ppm
0.95
1.02
2.00
1.08
2.30
1.17
1.23
1.17
3.52

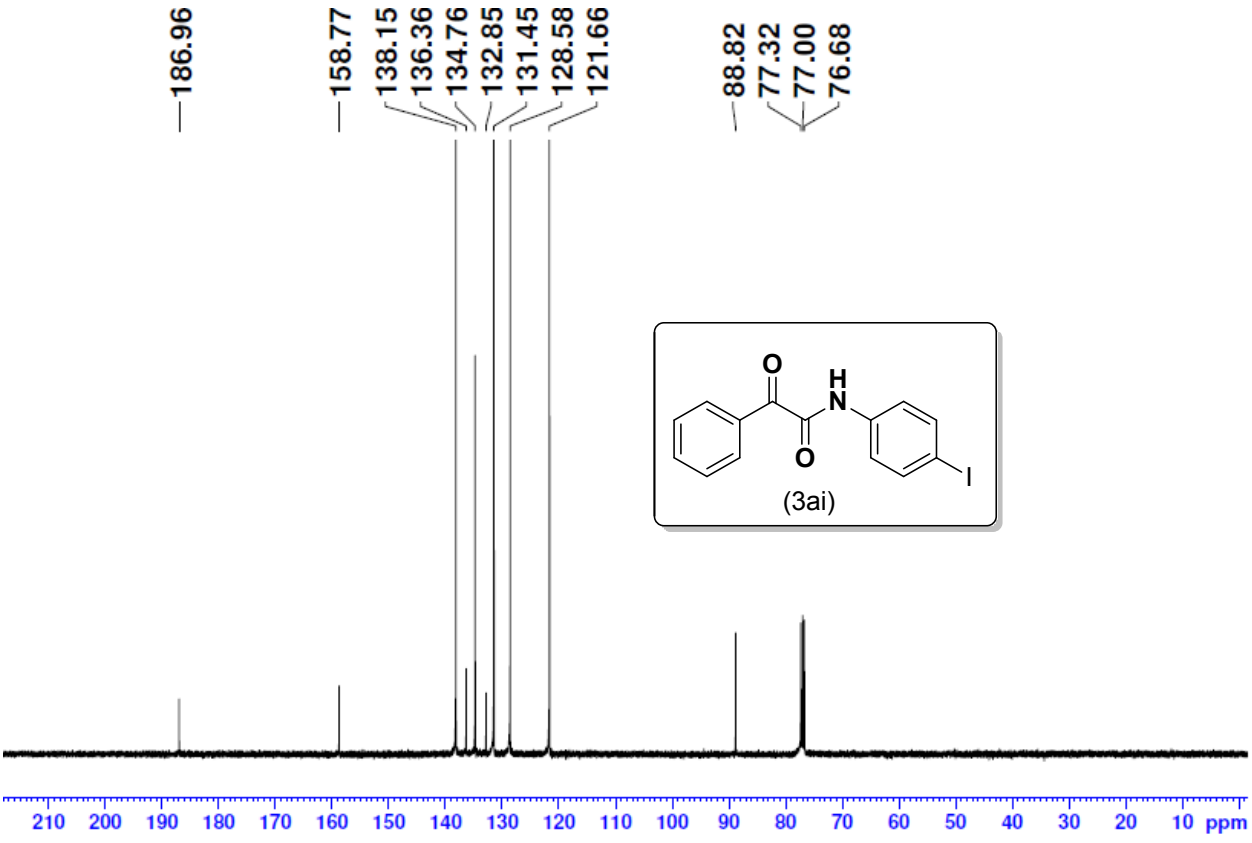

187.43
158.93
148.75
148.74
134.40
133.23
131.34
128.48
126.37
125.00
120.99
119.79
110.14
77.31
76.99
76.68
55.74
O
H
N
OMe
O
(3ae)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

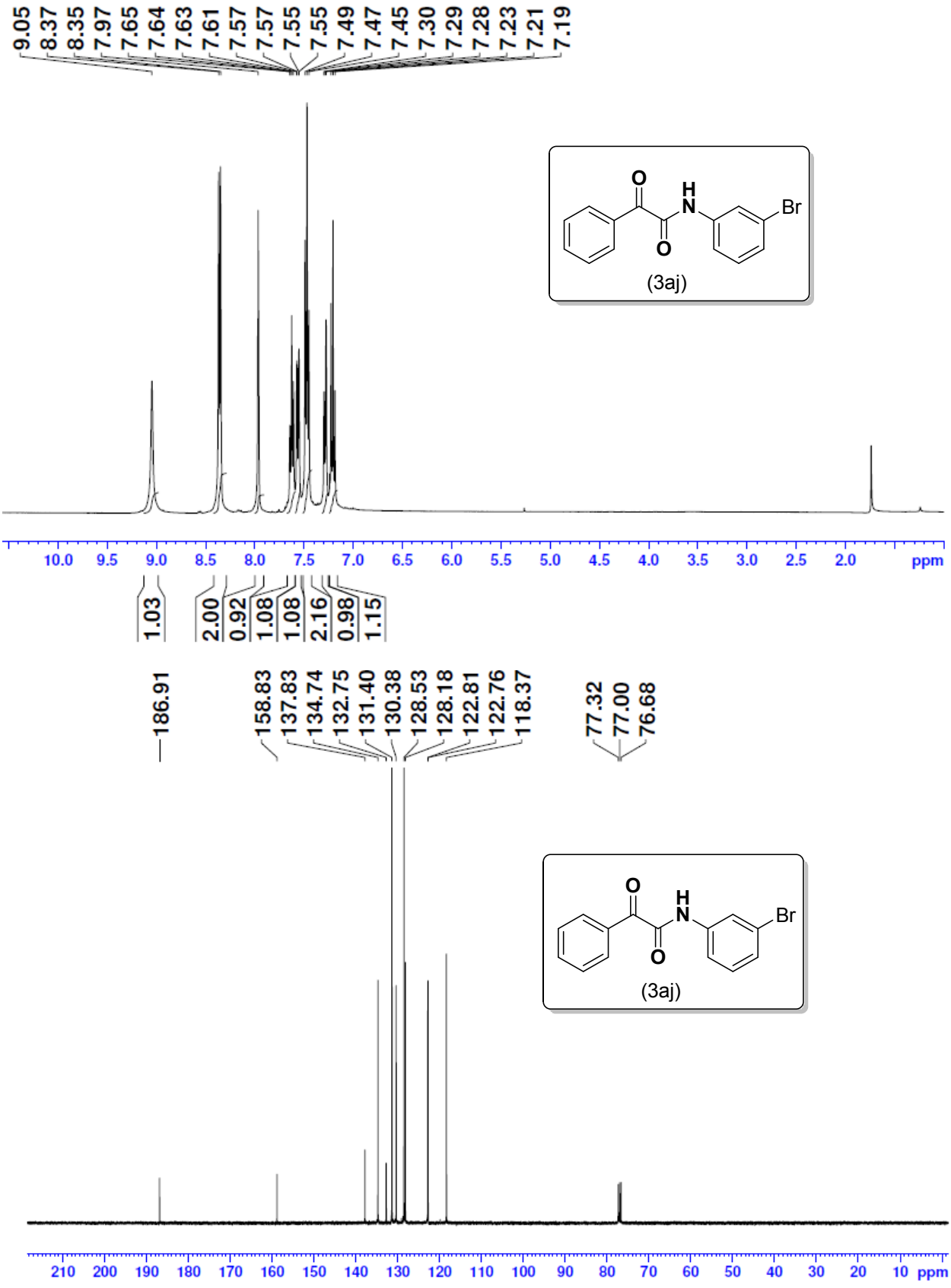

8.92
8.41
8.39
7.85
7.82
7.64
7.63
7.63
7.63
7.62
7.62
7.60
7.53
7.51
7.50
7.49
7.47
7.41
7.39
7.24
1.32
O
H
N
O
tBu
(3af)
10
9
8
7
6
5
4
3
2
1
ppm
0.92
1.82
0.96
2.10
2.15
1.91
9.24
187.54
158.81
154.19
148.37
134.52
133.99
131.43
128.51
126.02
119.68
77.32
77.00
76.68
34.48
31.30
O
H
N
O
tBu
(3af)
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

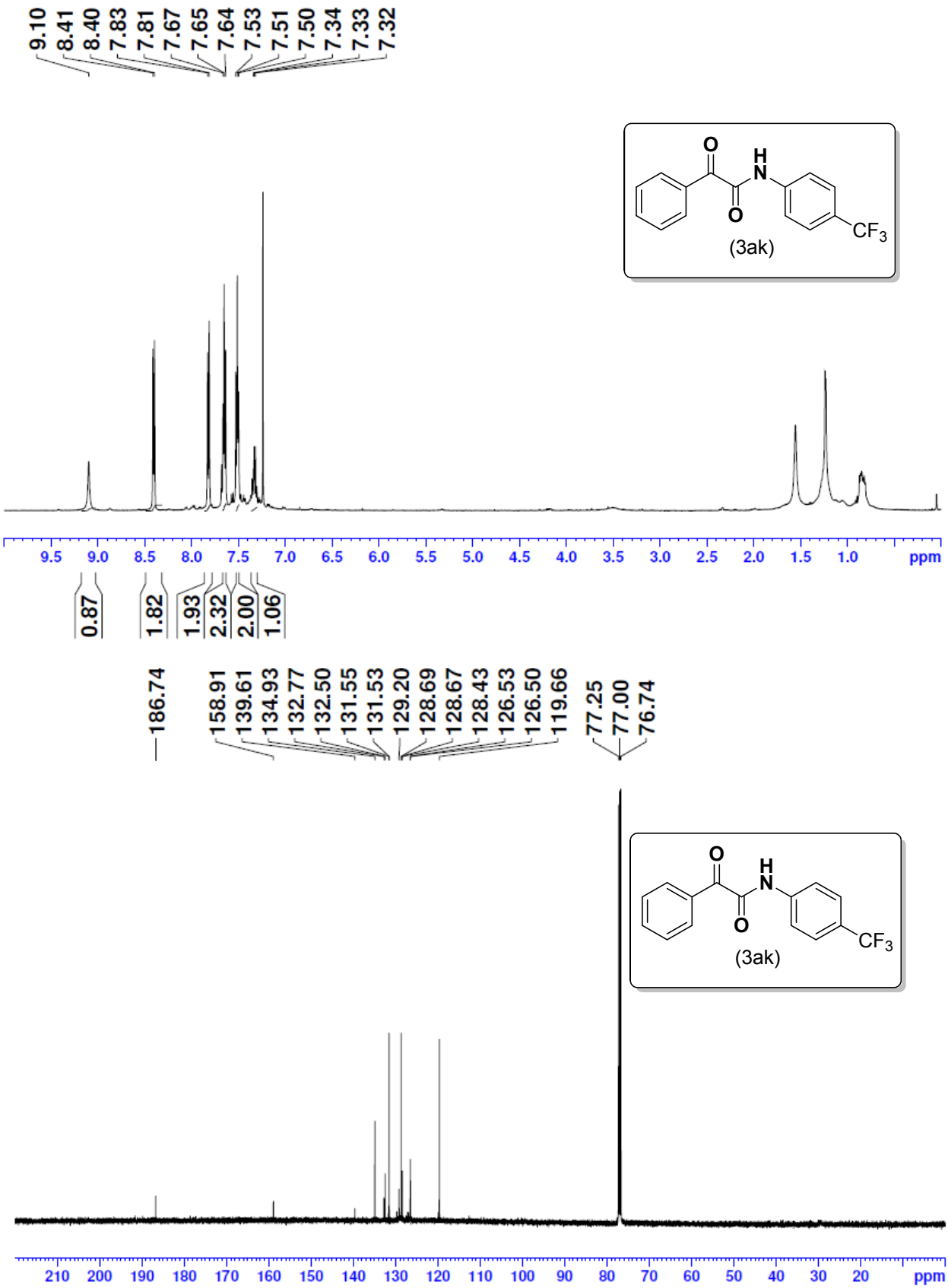

8.93
8.38
8.35
7.63
7.63
7.61
7.60
7.59
7.48
7.47
7.10
7.09
7.07
7.07
6.84
6.82
3.88
3.85
(3ag)
OMe
OMe
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 ppm
1.04
1.96
1.10
2.48
0.94
1.01
6.00
187.48
158.64
149.15
146.51
134.48
133.12
131.33
130.26
128.46
111.97
111.35
104.37
77.32
77.00
76.68
55.90
55.86
(3ag)
OMe
OMe
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

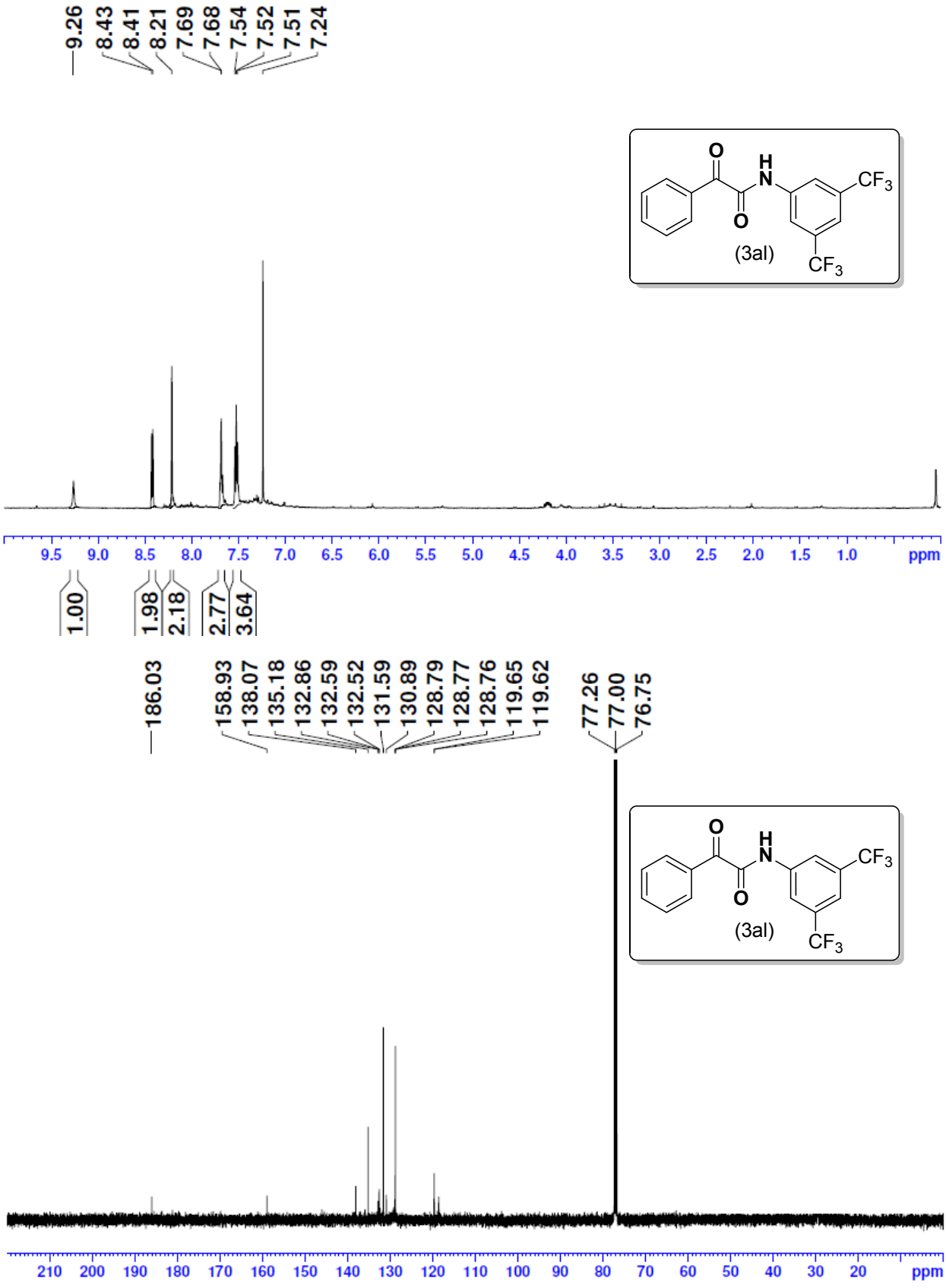

8.99
8.38
8.36
7.66
7.64
7.62
7.60
7.58
7.51
7.49
7.47
O
H
N
O
Br
(3ah)
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 ppm
1.05
2.01
3.27
4.00
187.02
158.80
135.70
134.74
132.21
131.45
128.57
121.43
118.04
77.32
77.00
76.69
O
H
N
O
Br
(3ah)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

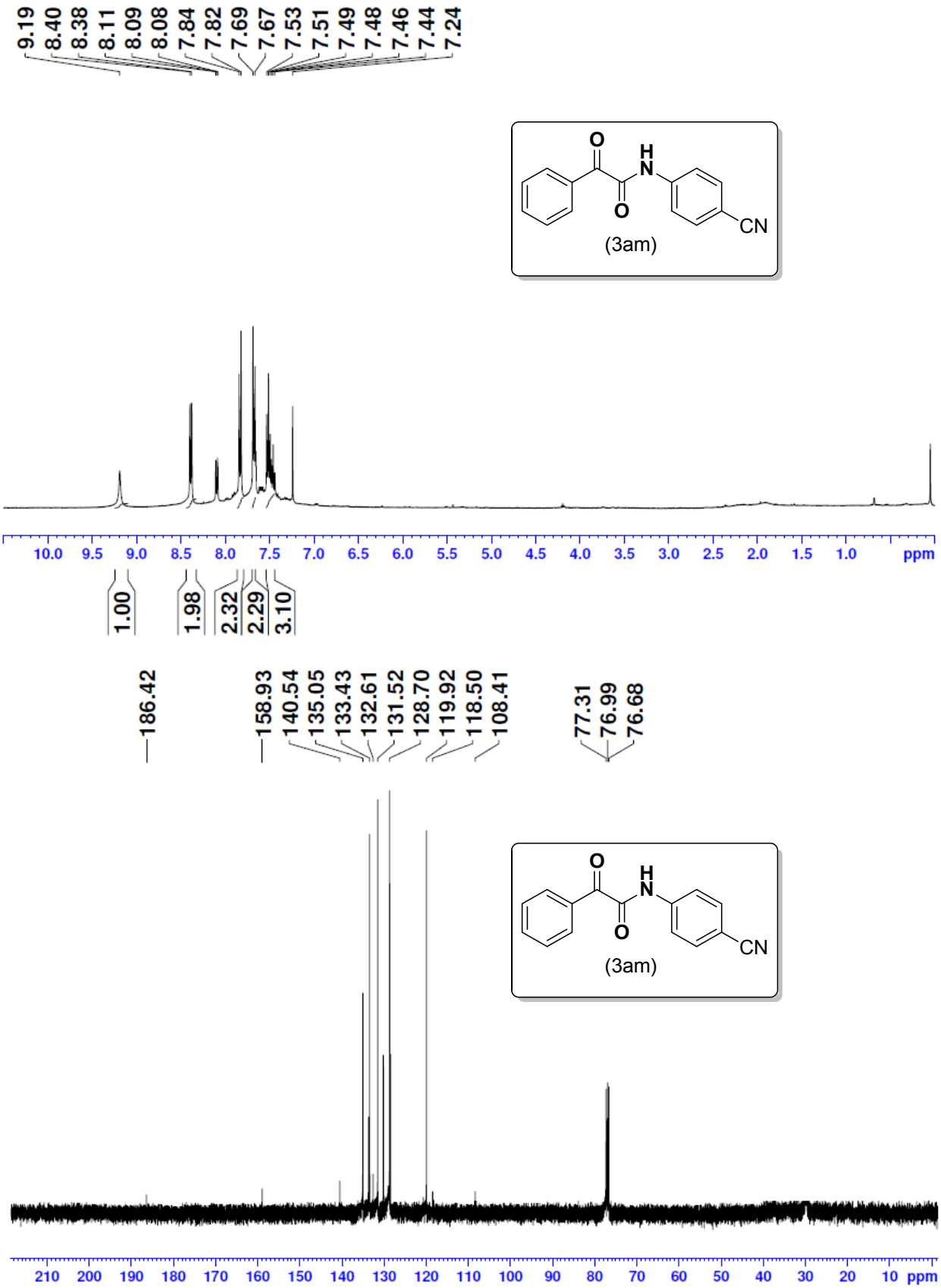

8.96
8.38
8.36
8.36
7.69
7.68
7.68
7.67
7.66
7.64
7.63
7.62
7.62
7.51
7.49
7.48
7.47
7.47
7.45
7.24
O
H
N
O
I
(3ai)
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
ppm
1.00
2.00
3.36
4.56

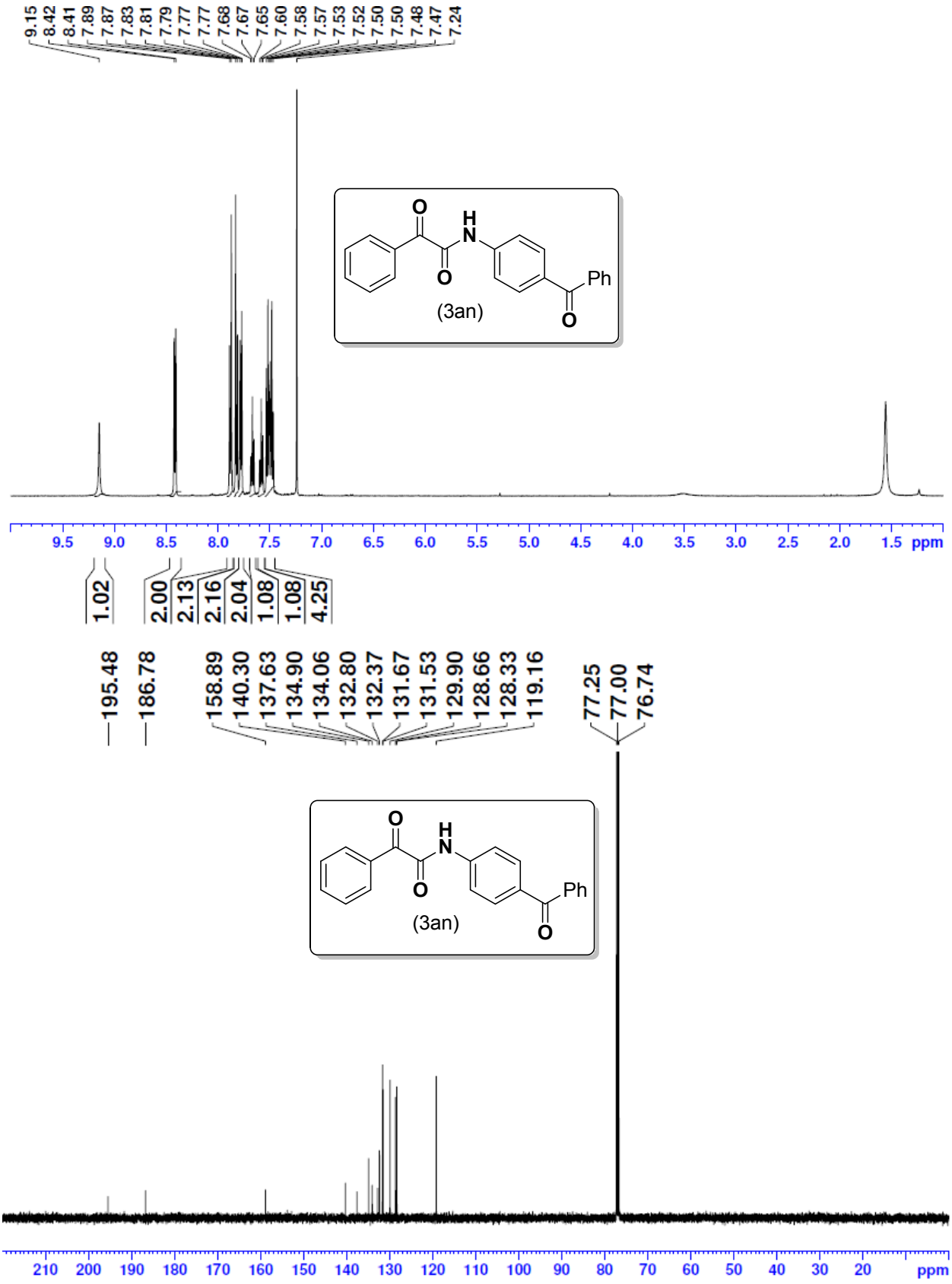

186.96
158.77
138.15
136.36
134.76
132.85
131.45
128.58
121.66
88.82
77.32
77.00
76.68
O
H
N
O
I
(3ai)
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

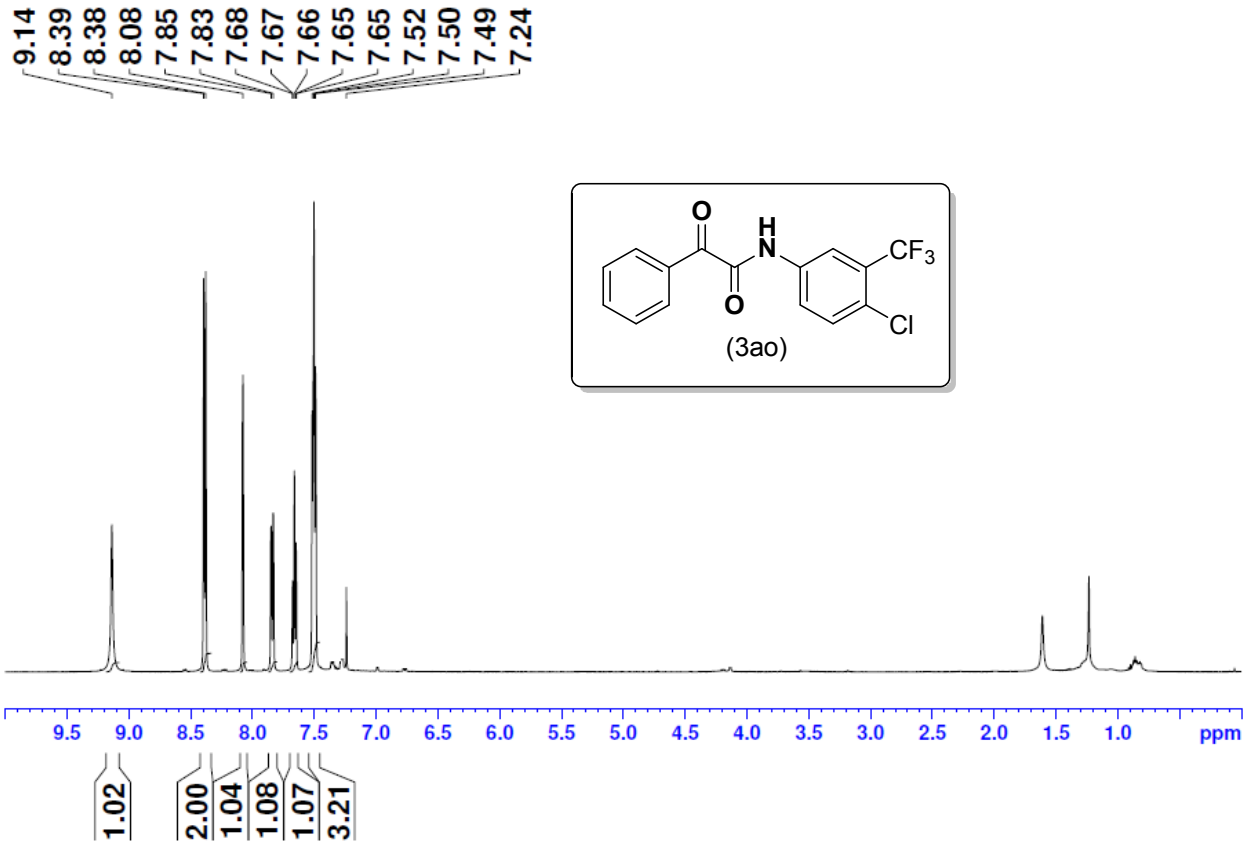

9.05
8.37
8.35
7.97
7.65
7.64
7.63
7.61
7.57
7.57
7.55
7.55
7.49
7.47
7.45
7.30
7.29
7.28
7.23
7.21
7.19
O
H
N
Br
O
(3aj)
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 ppm
1.03
2.00
0.92
1.08
1.08
2.16
0.98
1.15
186.91
158.83
137.83
134.74
132.75
131.40
130.38
128.53
128.18
122.81
122.76
118.37
77.32
77.00
76.68
O
H
N
Br
O
(3aj)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

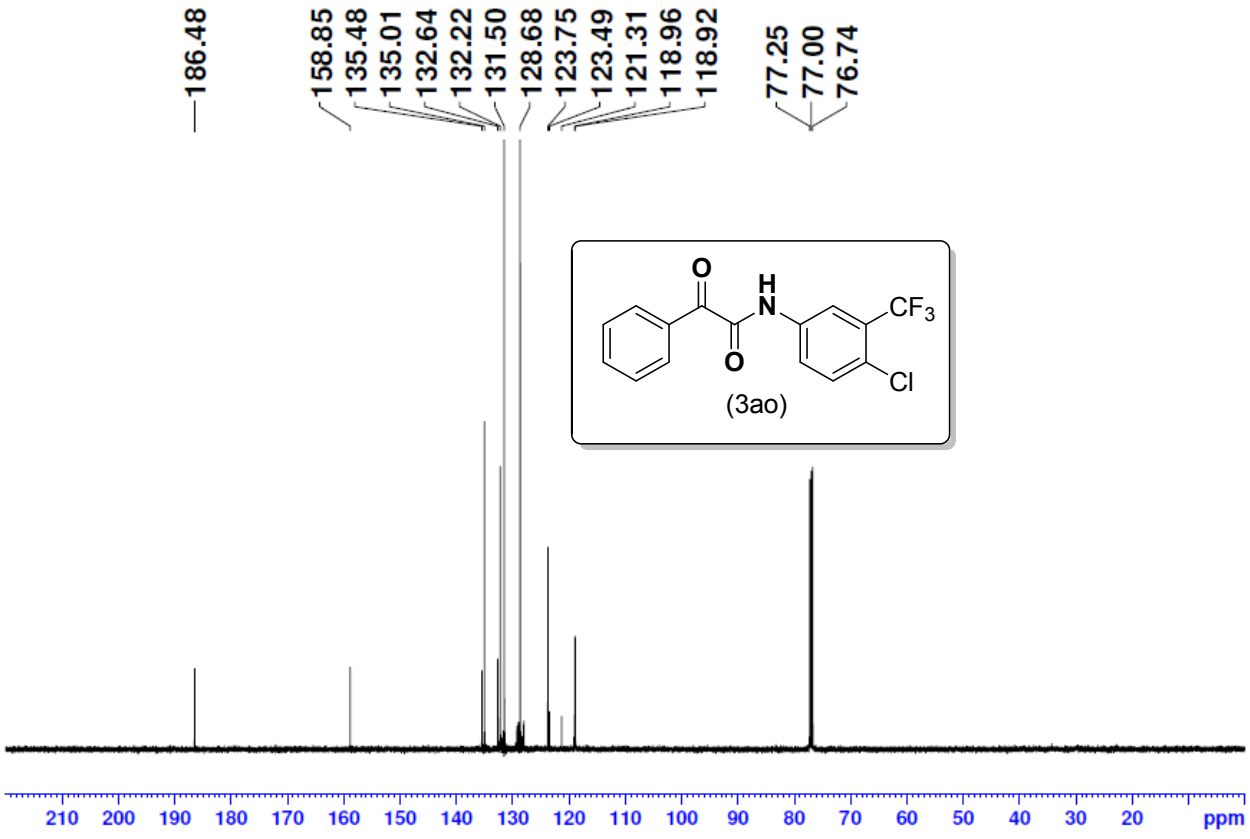

9.10
8.41
8.40
7.83
7.81
7.67
7.65
7.64
7.53
7.51
7.50
7.34
7.33
7.32
O
H
N
O
CF3
(3ak)
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 ppm
0.87
1.82
1.93
2.32
2.00
1.06
186.74
158.91
139.61
134.93
132.77
132.50
131.55
131.53
129.20
128.69
128.67
128.43
126.53
126.50
119.66
77.25
77.00
76.74
O
H
N
O
CF3
(3ak)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

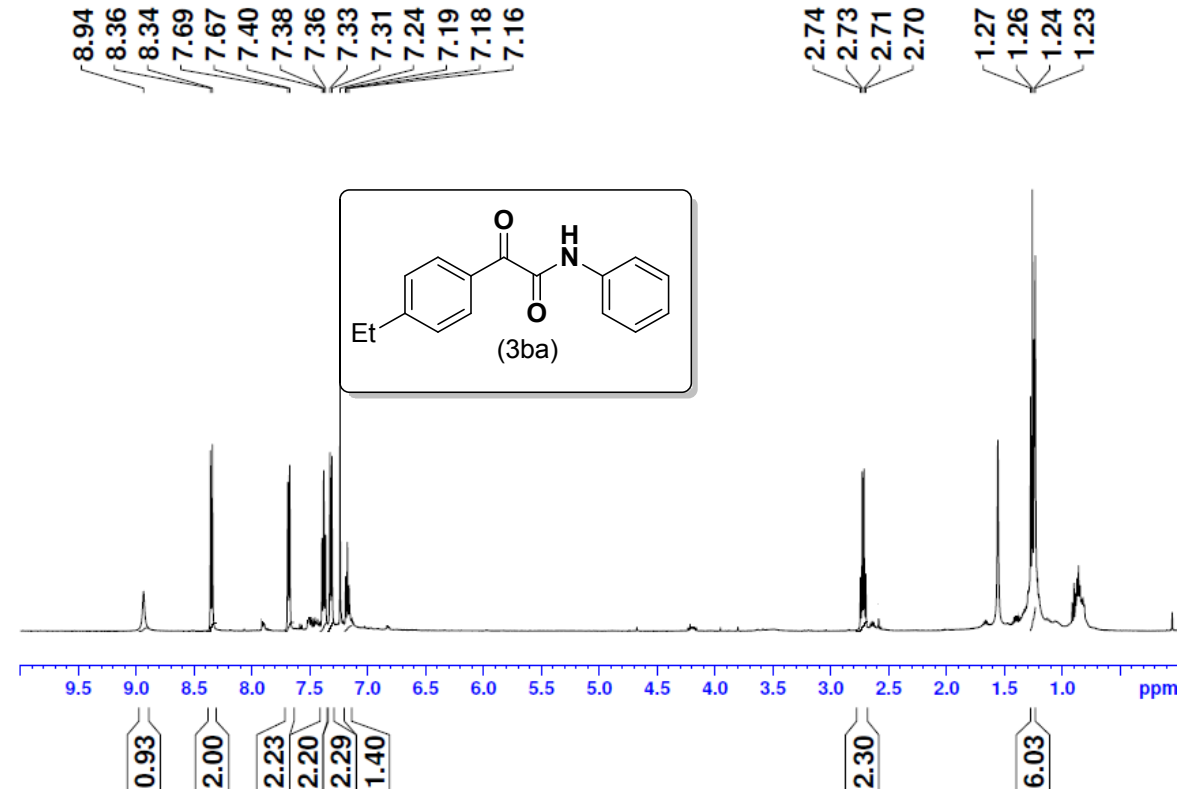

9.26
8.43
8.41
8.21
7.69
7.68
7.54
7.52
7.51
7.24
(3al)
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 ppm
1.00
1.98
2.18
2.77
3.64
186.03
158.93
138.07
135.18
132.86
132.59
132.52
131.59
130.89
128.79
128.77
128.76
119.65
119.62
77.26
77.00
76.75
(3al)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

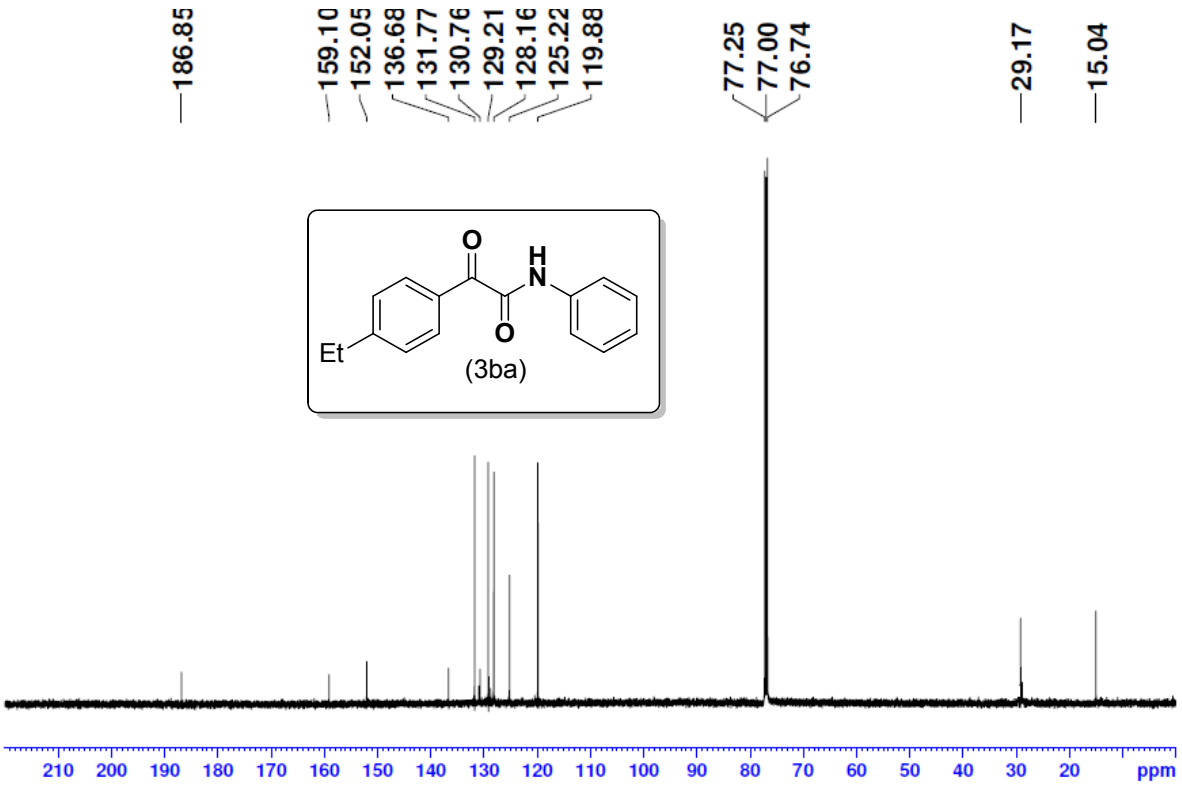

9.19
8.40
8.38
8.11
8.09
8.08
7.84
7.82
7.69
7.67
7.53
7.51
7.49
7.48
7.46
7.44
7.24
O
H
N
O
CN
(3am)
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 ppm
1.00
1.98
2.32
2.29
3.10
186.42
158.93
140.54
135.05
133.43
132.61
131.52
128.70
119.92
118.50
108.41
77.31
76.99
76.68
O
H
N
O
CN
(3am)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

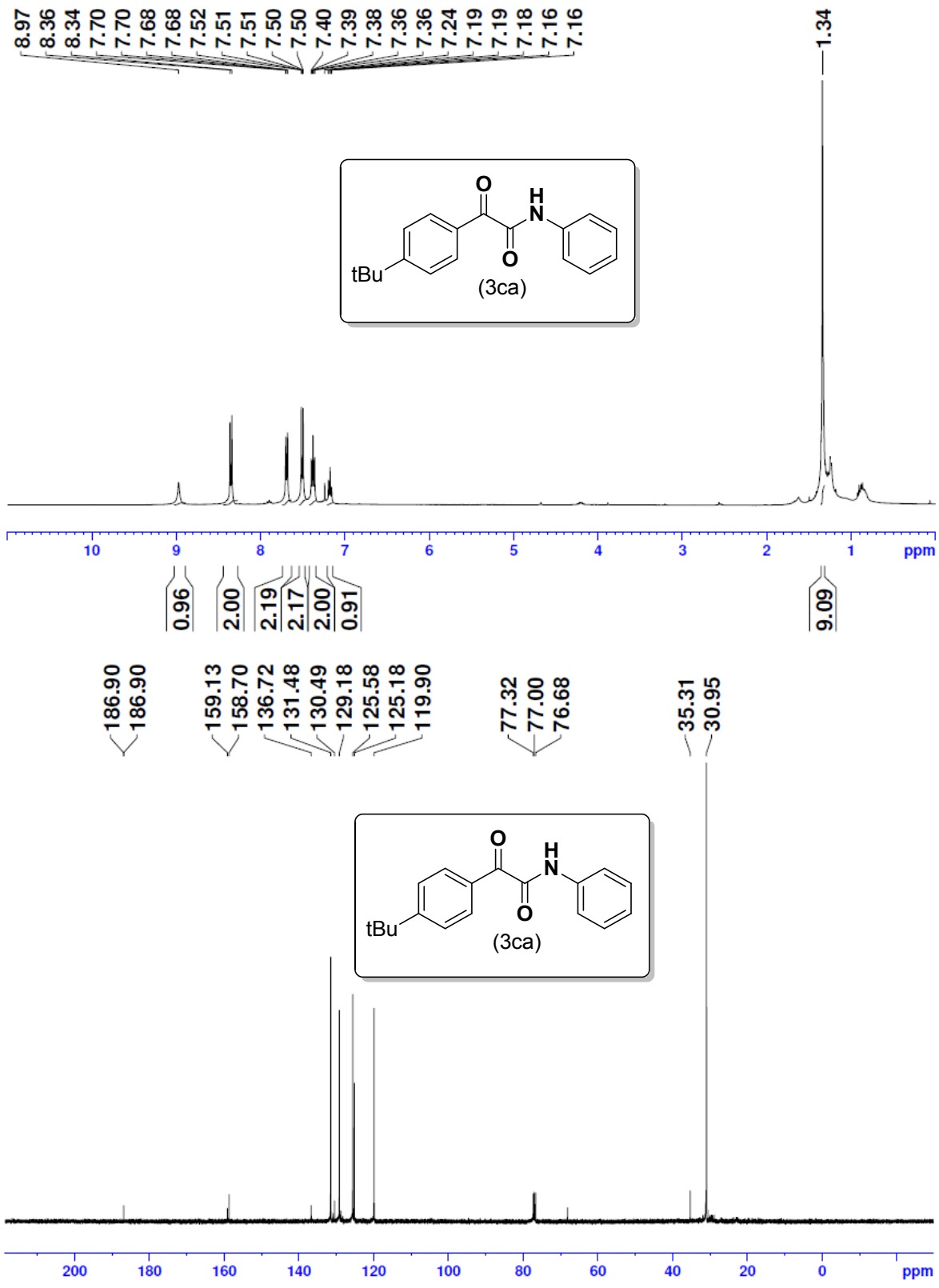

9.15
8.42
8.41
7.89
7.87
7.83
7.81
7.79
7.77
7.77
7.68
7.67
7.65
7.60
7.58
7.57
7.53
7.52
7.50
7.50
7.48
7.47
7.24
O
H
N
O
Ph
O
(3an)
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 ppm
1.02
2.00
2.13
2.16
2.04
1.08
1.08
4.25
195.48
186.78
158.89
140.30
137.63
134.90
134.06
132.80
132.37
131.67
131.53
129.90
128.66
128.33
119.16
77.25
77.00
76.74
O
H
N
O
Ph
O
(3an)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

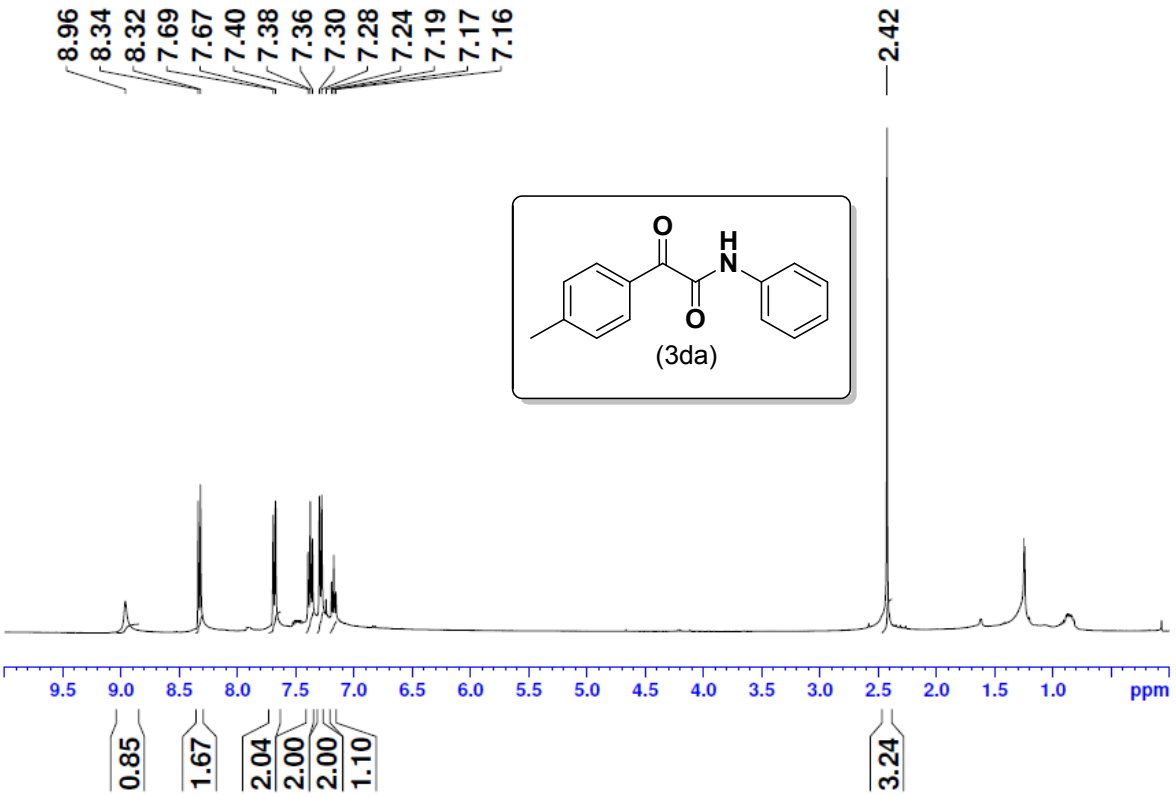

9.14
8.39
8.38
8.08
7.85
7.83
7.68
7.67
7.66
7.65
7.65
7.52
7.50
7.49
7.24
O
H
N
O
CF3
Cl
(3ao)
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
ppm
1.02
2.00
1.04
1.08
1.07
3.21

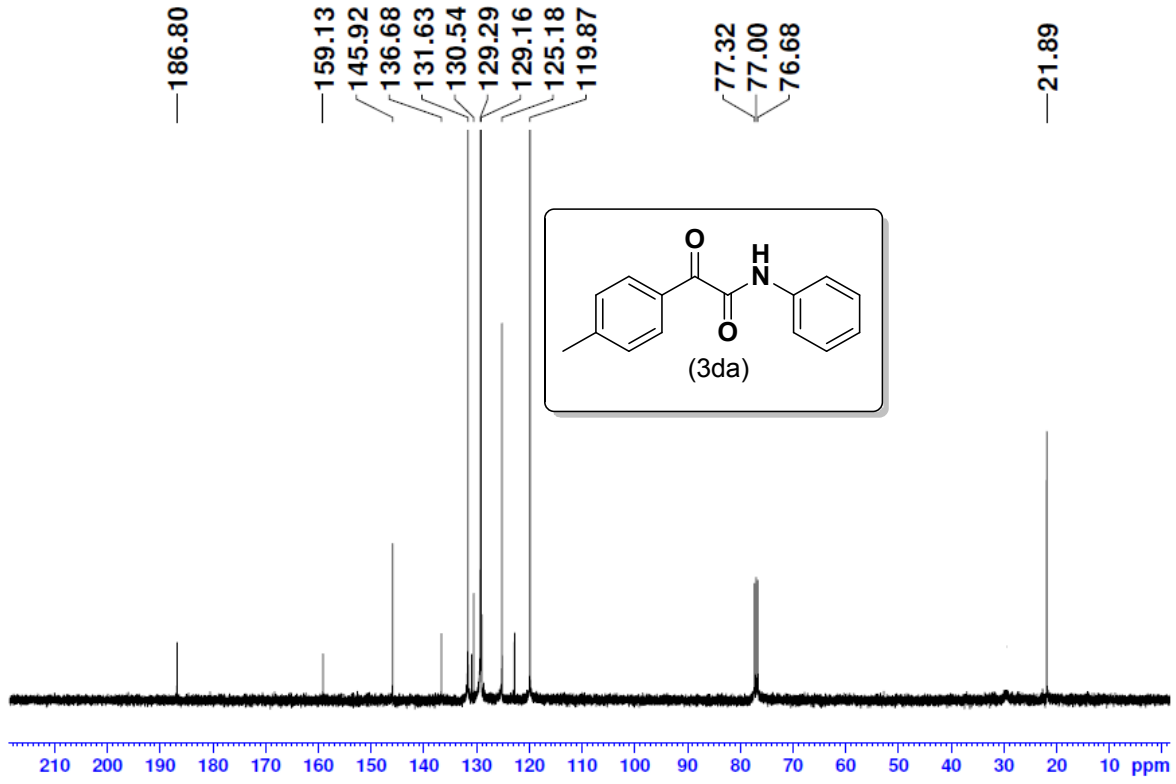

186.48
158.85
135.48
135.01
132.64
132.22
131.50
128.68
123.75
123.49
121.31
118.96
118.92
77.25
77.00
76.74
O
H
N
O
CF3
Cl
(3ao)
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

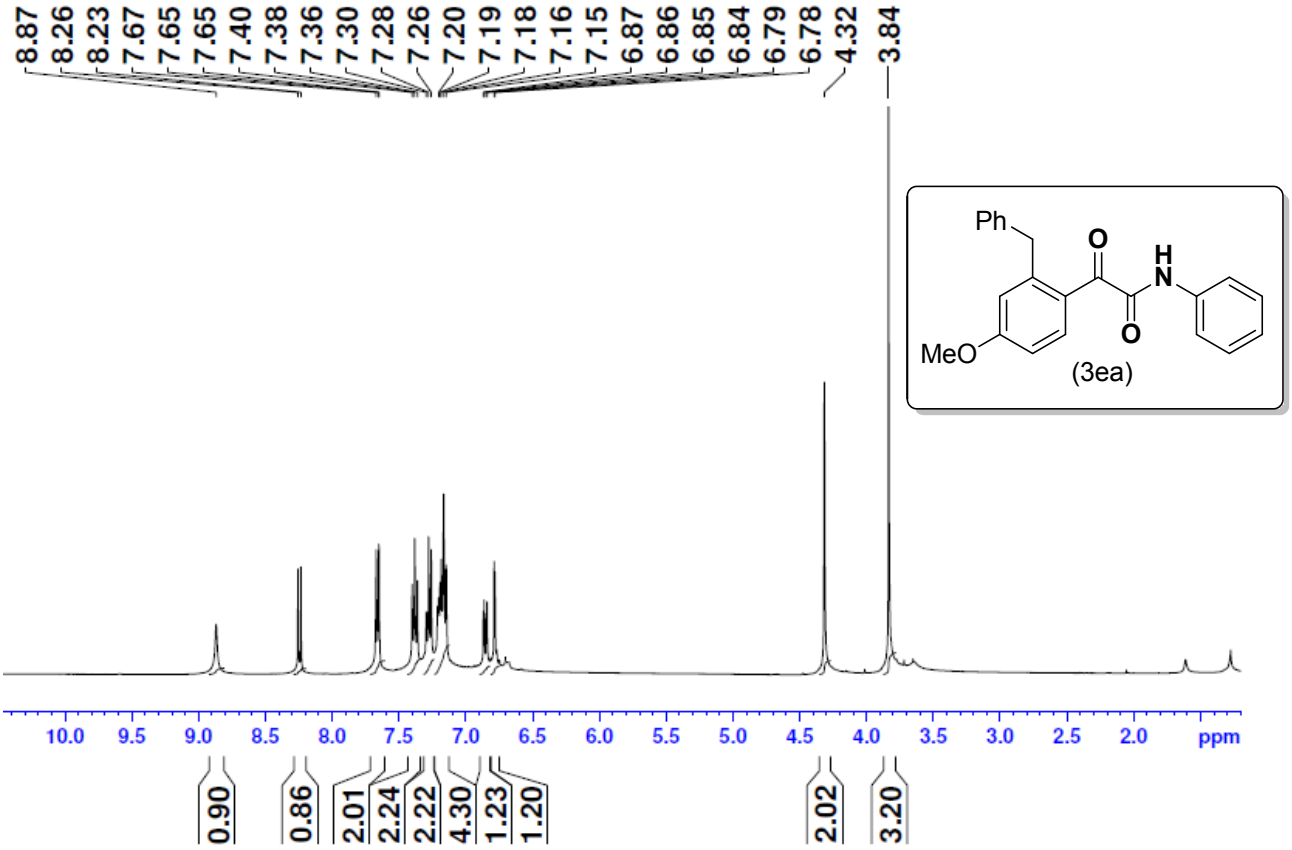

8.94
8.36
8.34
7.69
7.67
7.40
7.38
7.36
7.33
7.31
7.24
7.19
7.18
7.16
2.74
2.73
2.71
2.70
1.27
1.26
1.24
1.23
O
H
N
O
Et
(3ba)
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
ppm
0.93
2.00
2.23
2.20
2.29
1.40
2.30
6.03

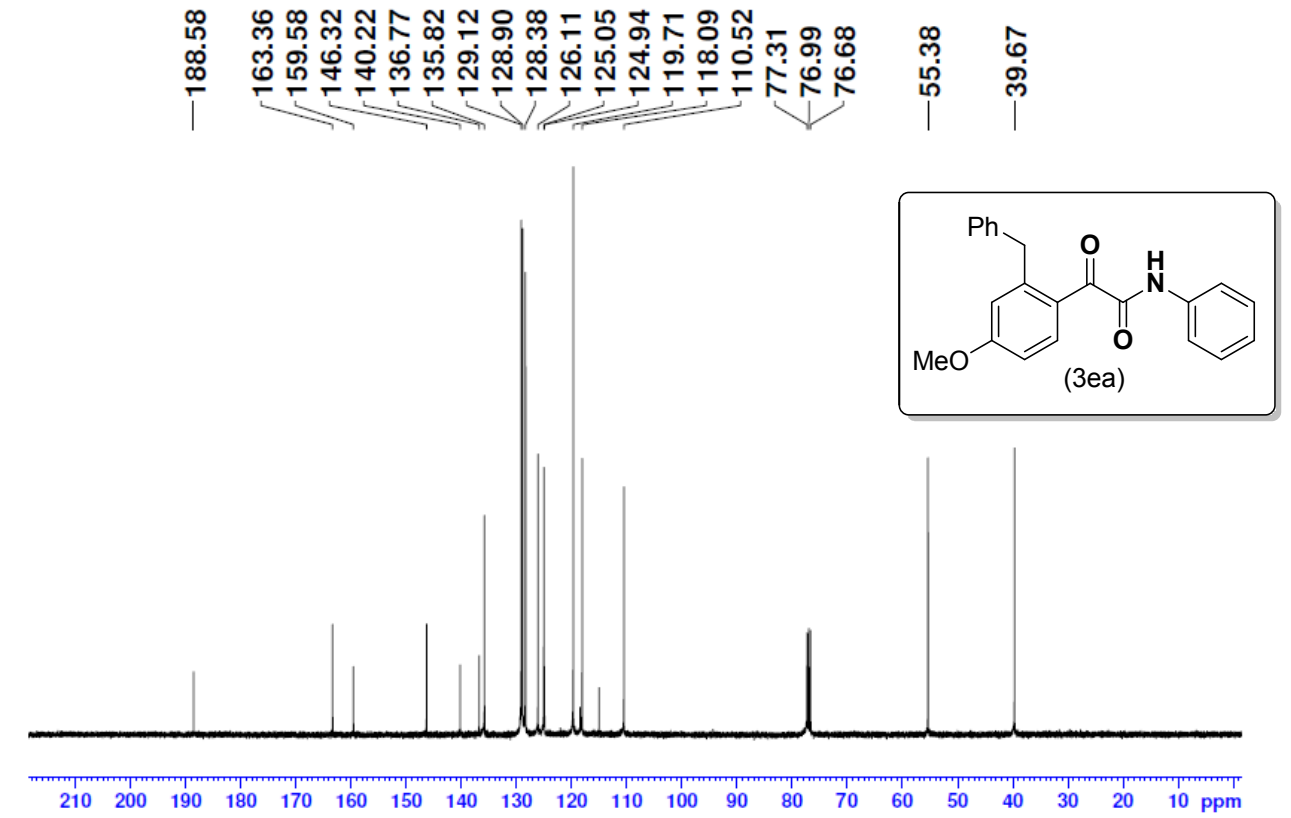

186.85
159.10
152.05
136.68
131.77
130.76
129.21
128.16
125.22
119.88
77.25
77.00
76.74
29.17
15.04
O
H
N
O
Et
(3ba)
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

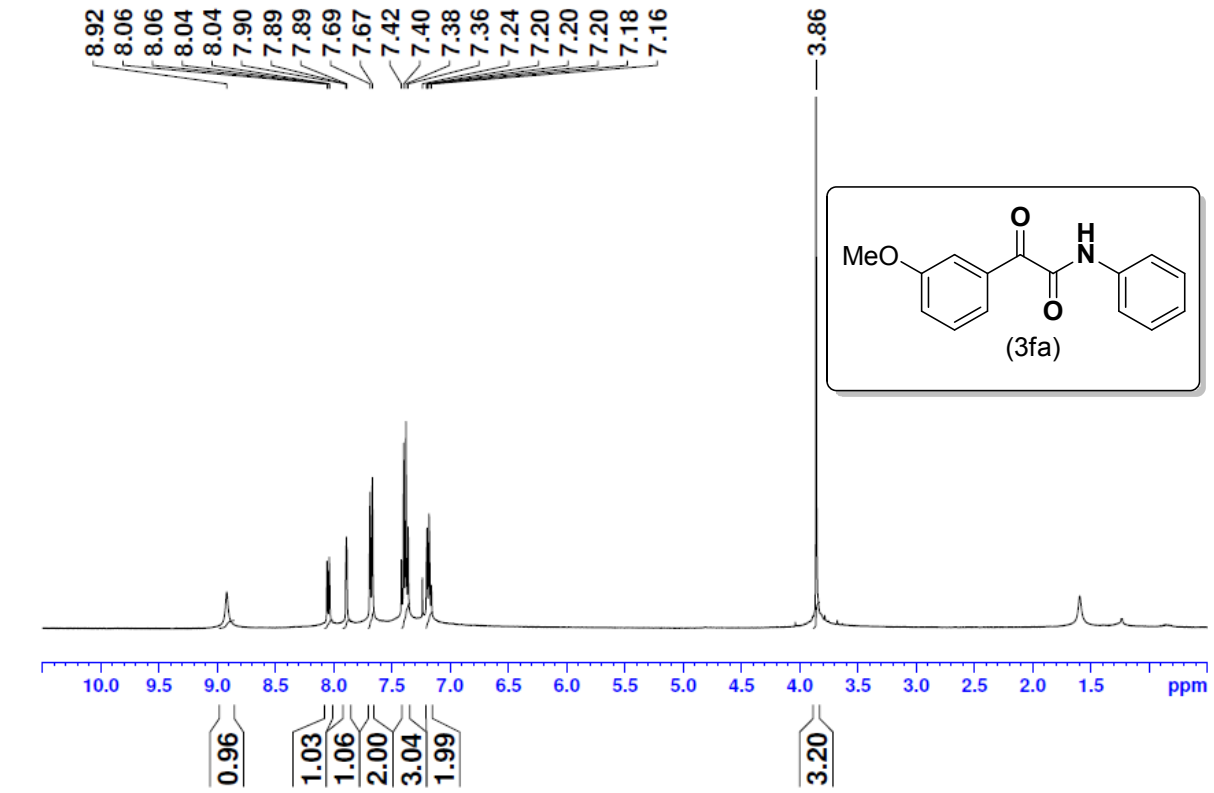

8.97
8.36
8.34
7.70
7.70
7.68
7.68
7.52
7.51
7.51
7.50
7.50
7.40
7.39
7.38
7.36
7.36
7.24
7.19
7.19
7.18
7.16
7.16
1.34
O
H
N
O
tBu
(3ca)
10
9
8
7
6
5
4
3
2
1
ppm
0.96
2.00
2.19
2.17
2.00
0.91
9.09
186.90
186.90
159.13
158.70
136.72
131.48
130.49
129.18
125.58
125.18
119.90
77.32
77.00
76.68
35.31
30.95
O
H
N
O
tBu
(3ca)
200
180
160
140
120
100
80
60
40
20
0
ppm

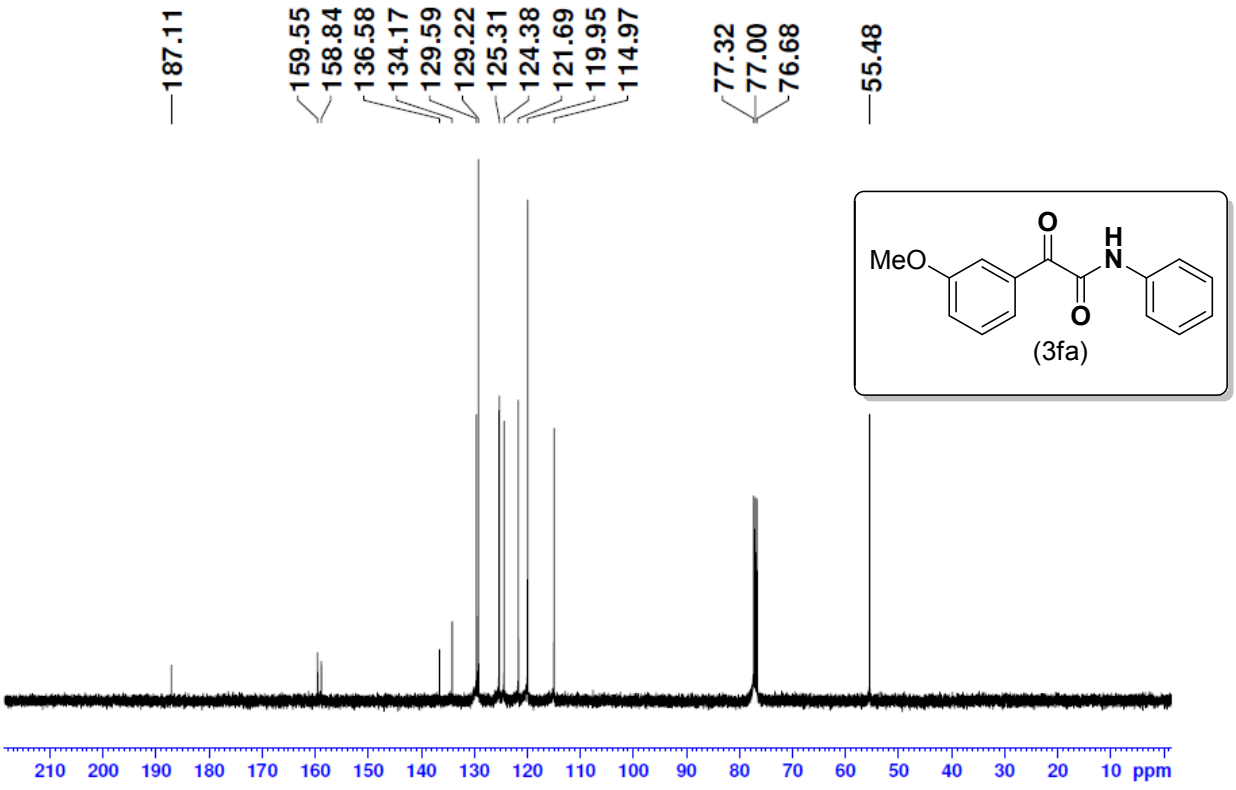

8.96
8.34
8.32
7.69
7.67
7.40
7.38
7.36
7.30
7.28
7.24
7.19
7.17
7.16
2.42
O
H
N
O
(3da)
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 ppm
0.85
1.67
2.04
2.00
2.00
1.10
3.24

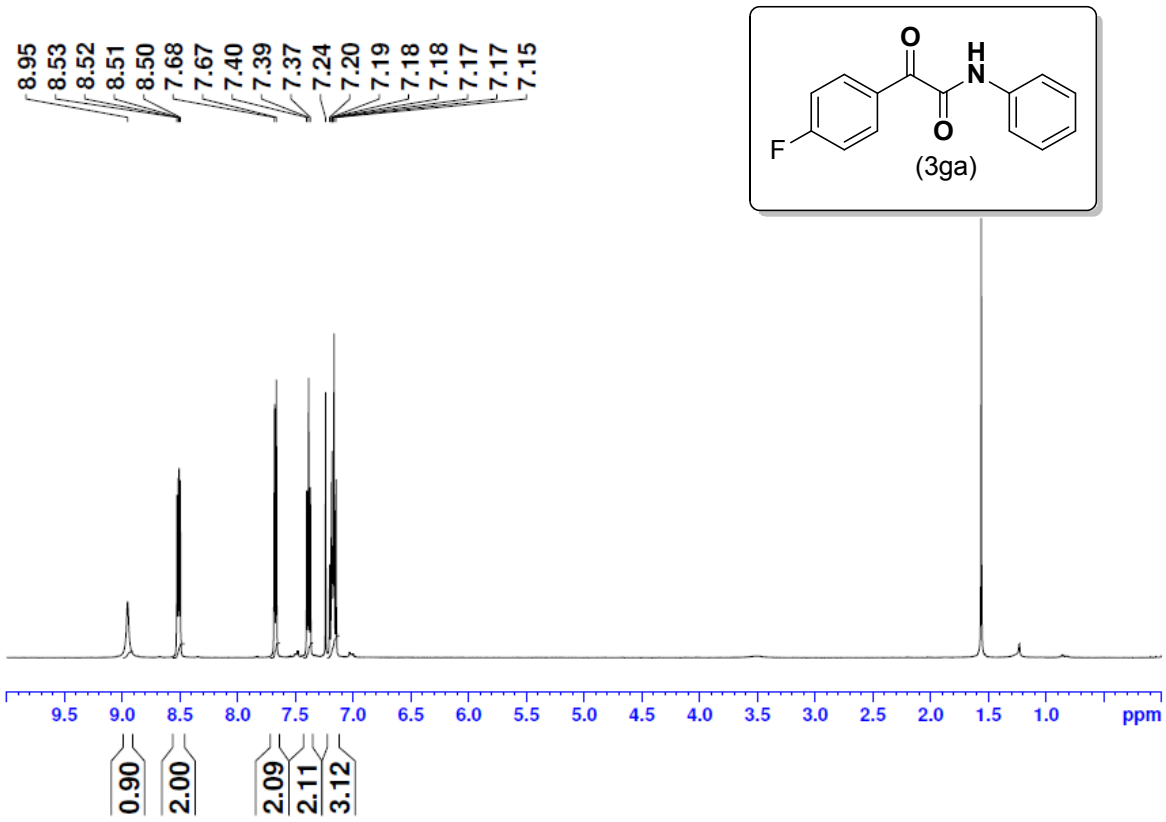

186.80
159.13
145.92
136.68
131.63
130.54
129.29
129.16
125.18
119.87
77.32
77.00
76.68
21.89
O
H
N
O
(3da)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

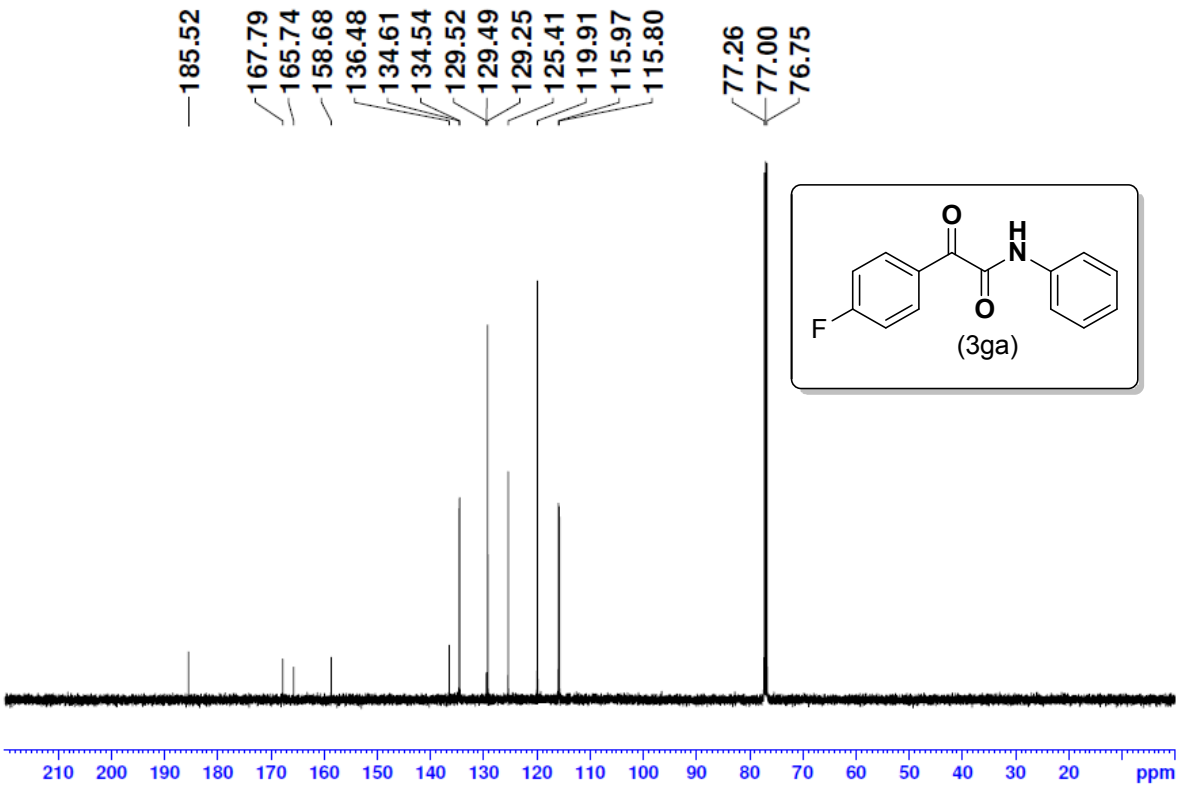

8.87
8.26
8.23
7.67
7.65
7.65
7.40
7.38
7.36
7.30
7.28
7.26
7.20
7.19
7.18
7.16
7.15
6.87
6.86
6.85
6.84
6.79
6.78
4.32
3.84
Ph
O
H
N
O
MeO
(3ea)
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 ppm
0.90
0.86
2.01
2.24
2.22
4.30
1.23
1.20
2.02
3.20

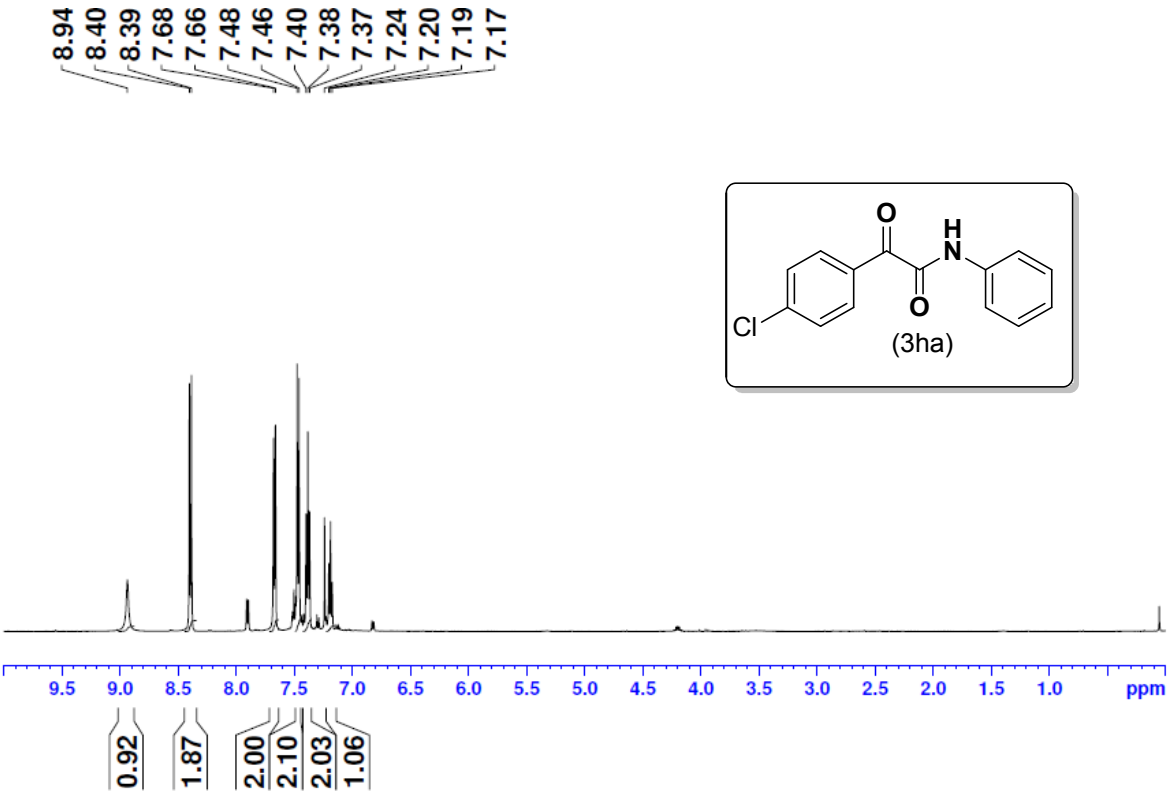

188.58
163.36
159.58
146.32
140.22
136.77
135.82
129.12
128.90
128.38
126.11
125.05
124.94
119.71
118.09
110.52
77.31
76.99
76.68
55.38
39.67
Ph
O
H
N
O
MeO
(3ea)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

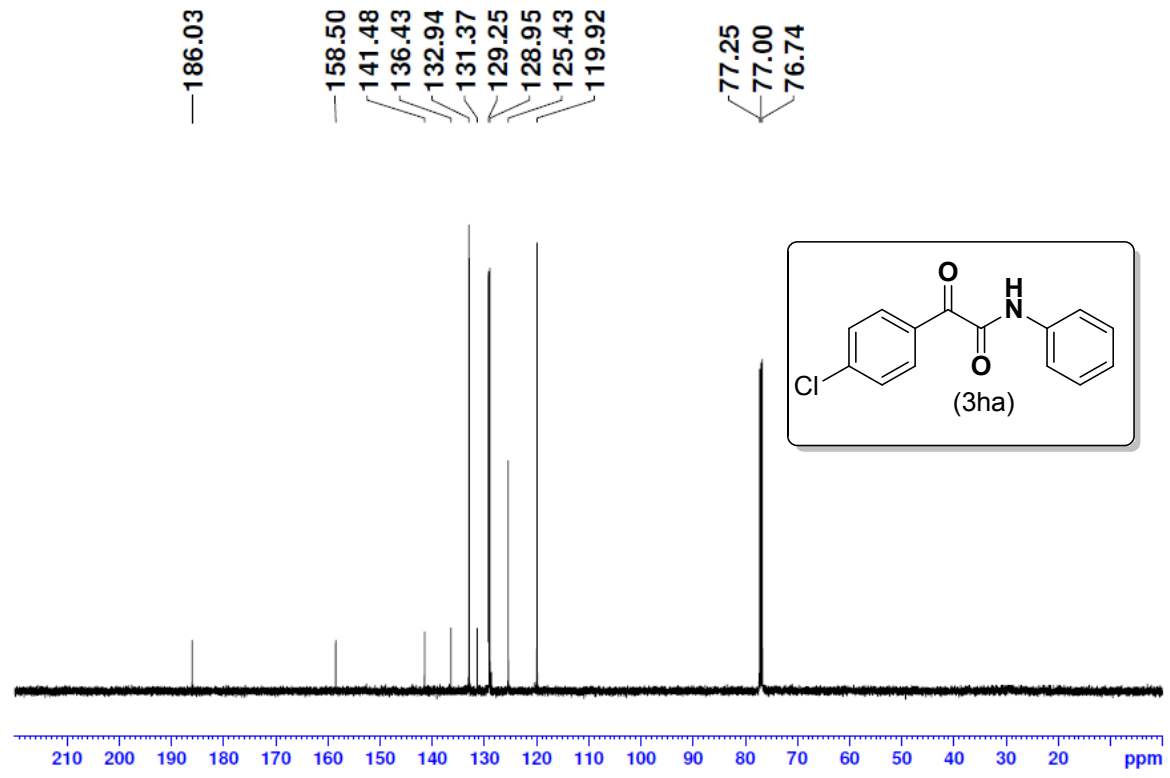

8.92
8.06
8.06
8.04
8.04
7.90
7.89
7.89
7.69
7.67
7.42
7.40
7.38
7.36
7.24
7.20
7.20
7.20
7.18
7.16
3.86
MeO
O
H
N
O
(3fa)
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 ppm
0.96
1.03
1.06
2.00
3.04
1.99
3.20

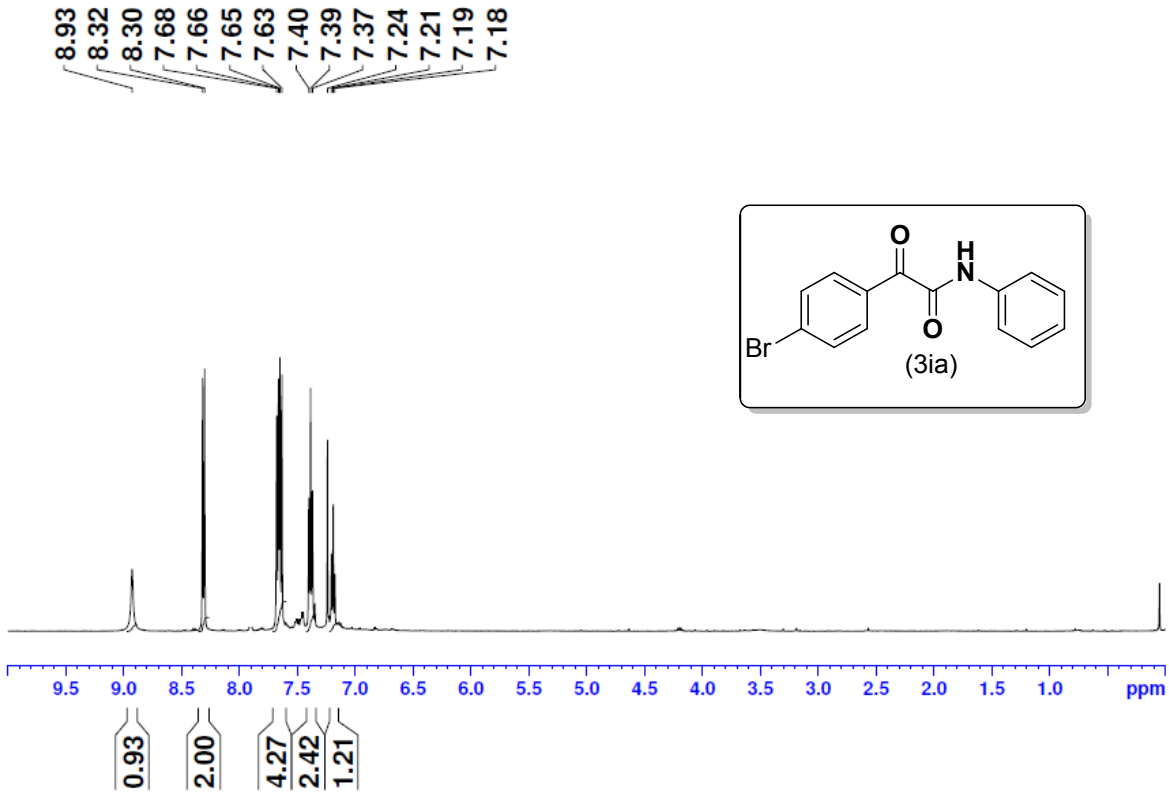

187.11
159.55
158.84
136.58
134.17
129.59
129.22
125.31
124.38
121.69
119.95
114.97
77.32
77.00
76.68
55.48
MeO
O
H
N
O
(3fa)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

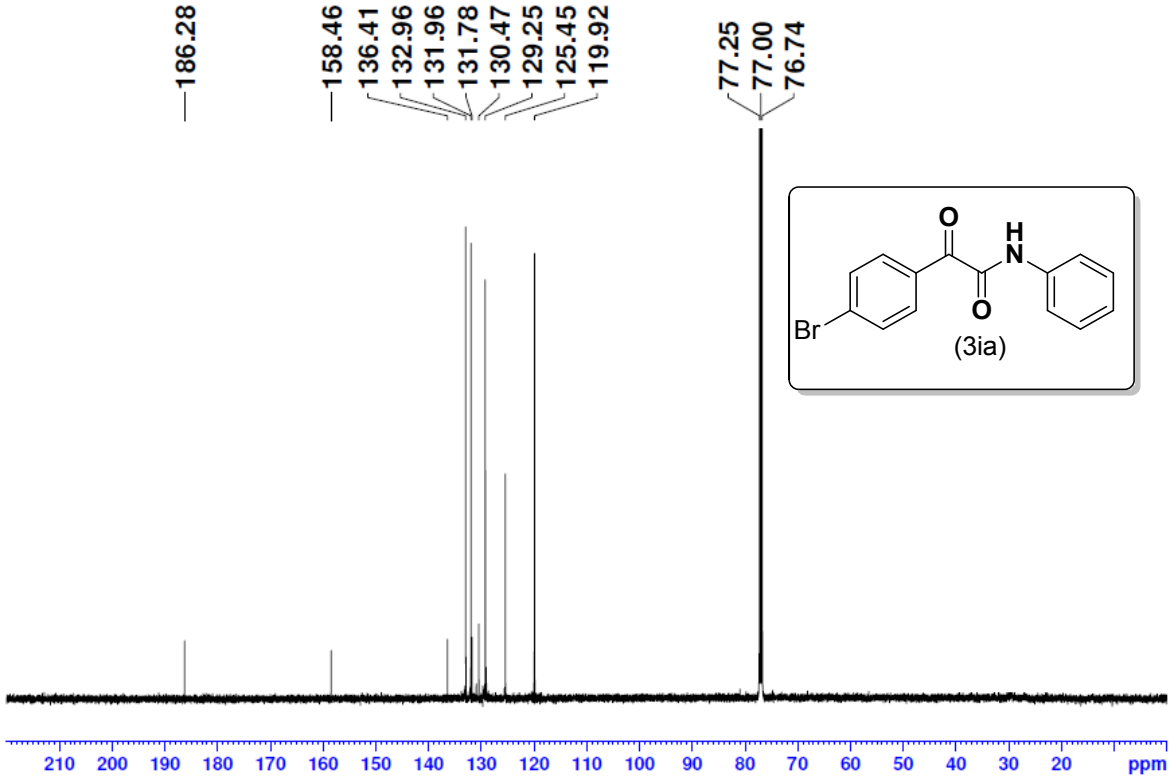

8.95
8.53
8.52
8.51
8.50
7.68
7.67
7.40
7.39
7.37
7.24
7.20
7.19
7.18
7.18
7.17
7.17
7.15
O
H
N
O
F
(3ga)
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
ppm
0.90
2.00
2.09
2.11
3.12

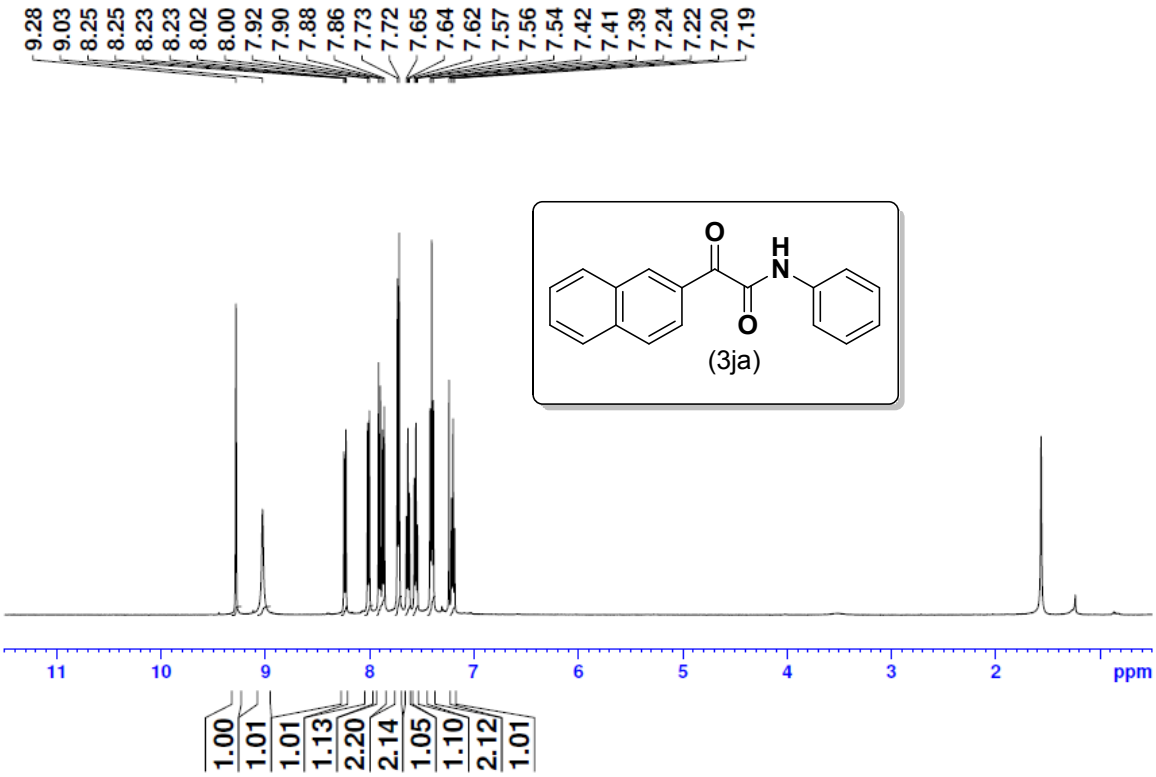

185.52
167.79
165.74
158.68
136.48
134.61
134.54
129.52
129.49
129.25
125.41
119.91
115.97
115.80
77.26
77.00
76.75
O
H
N
O
F
(3ga)
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

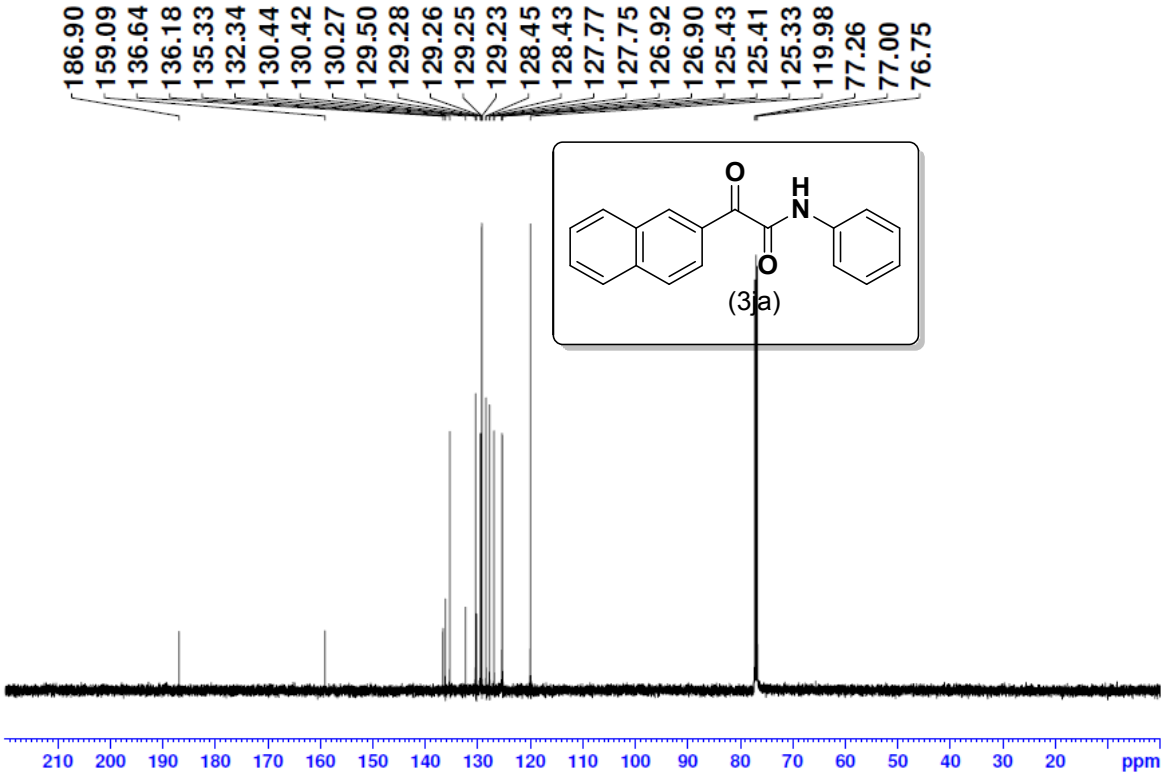

8.94
8.40
8.39
7.68
7.66
7.48
7.46
7.40
7.38
7.37
7.24
7.20
7.19
7.17
O
H
N
O
Cl
(3ha)
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
ppm
0.92
1.87
2.00
2.10
2.03
1.06

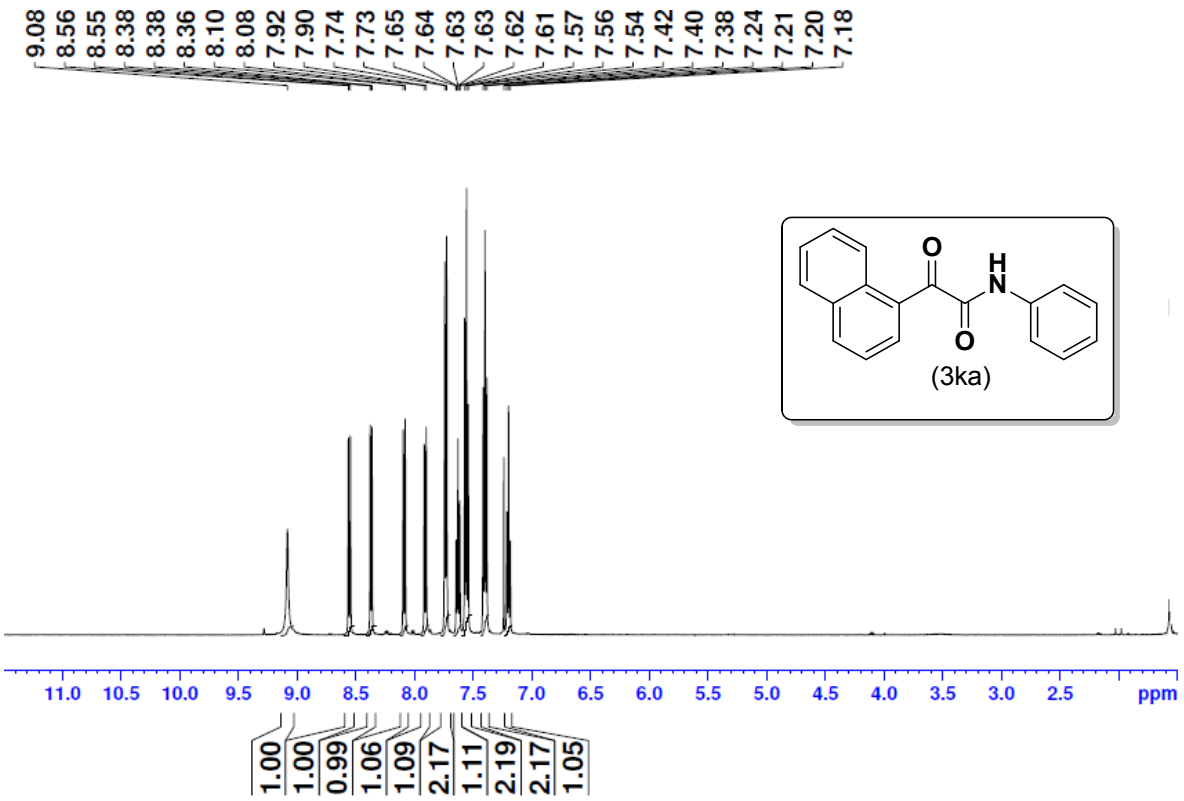

186.03
158.50
141.48
136.43
132.94
131.37
129.25
128.95
125.43
119.92
77.25
77.00
76.74
O
H
N
O
Cl
(3ha)
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

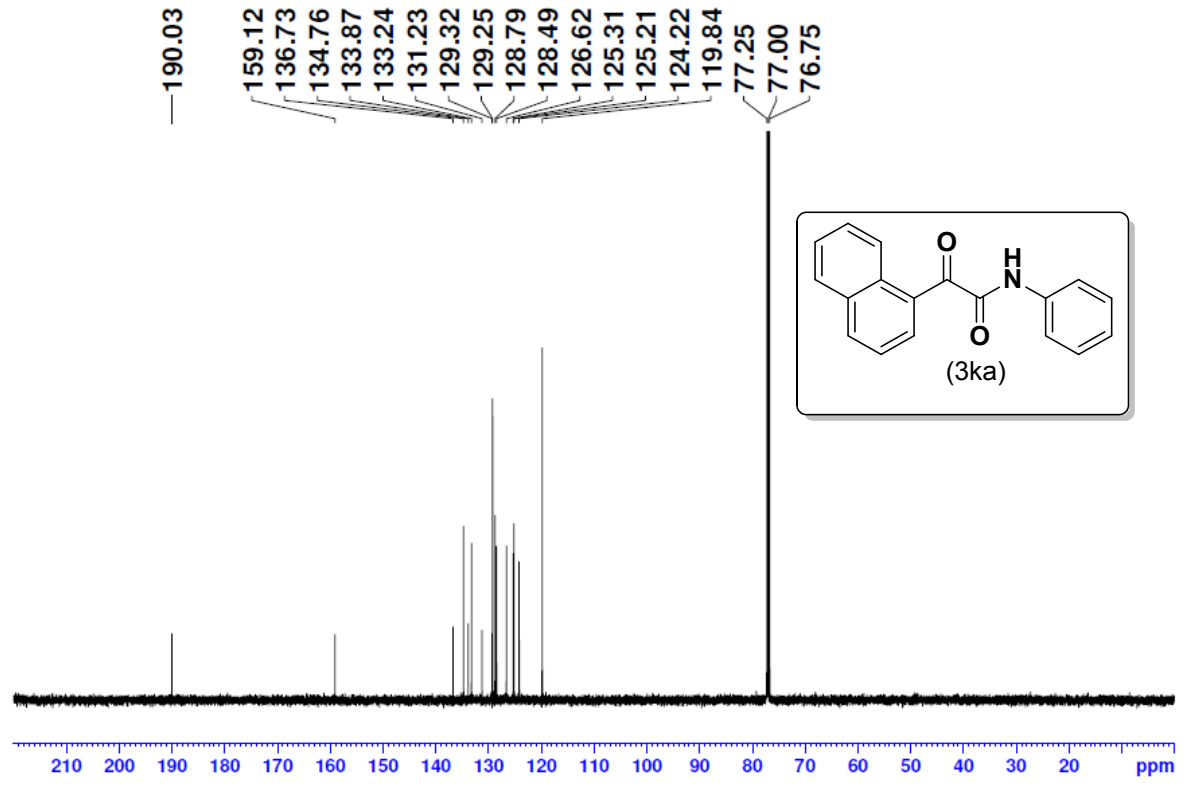

8.93
8.32
8.30
7.68
7.66
7.65
7.63
7.40
7.39
7.37
7.24
7.21
7.19
7.18
O
H
N
O
Br
(3ia)
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 ppm
0.93
2.00
4.27
2.42
1.21

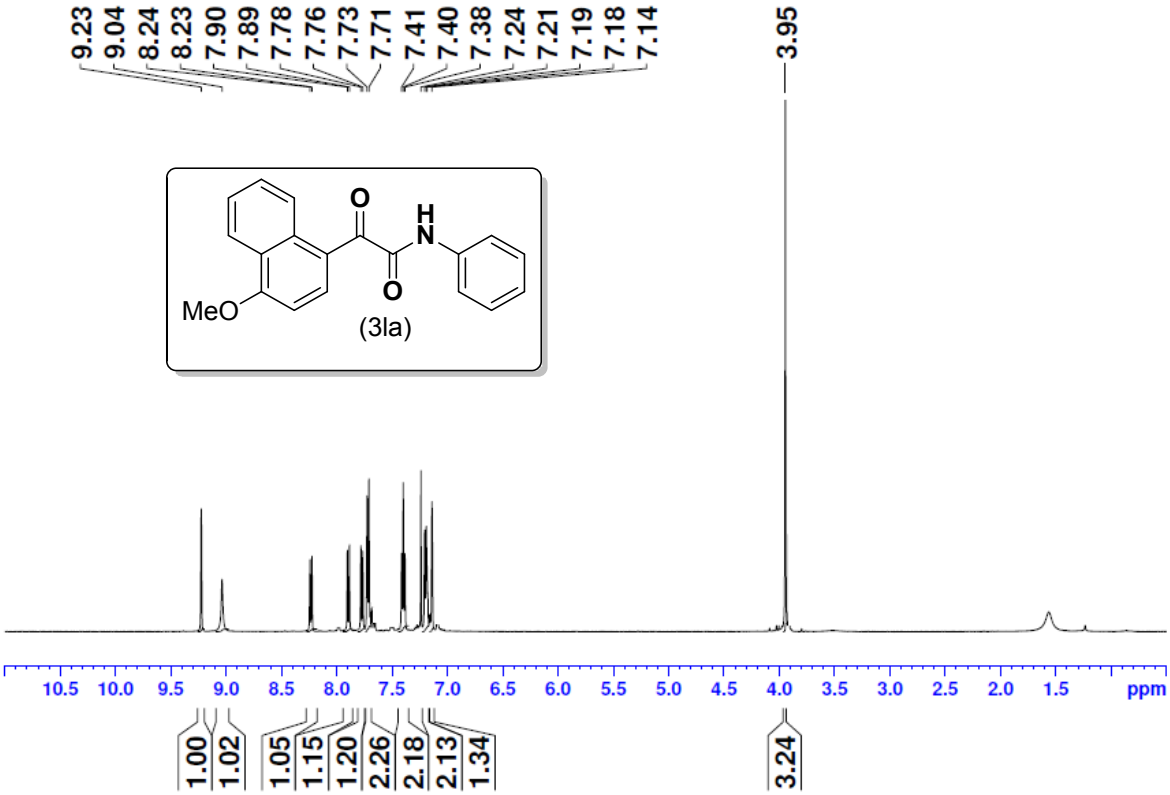

186.28
158.46
136.41
132.96
131.96
131.78
130.47
129.25
125.45
119.92
77.25
77.00
76.74
O
H
N
O
Br
(3ia)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

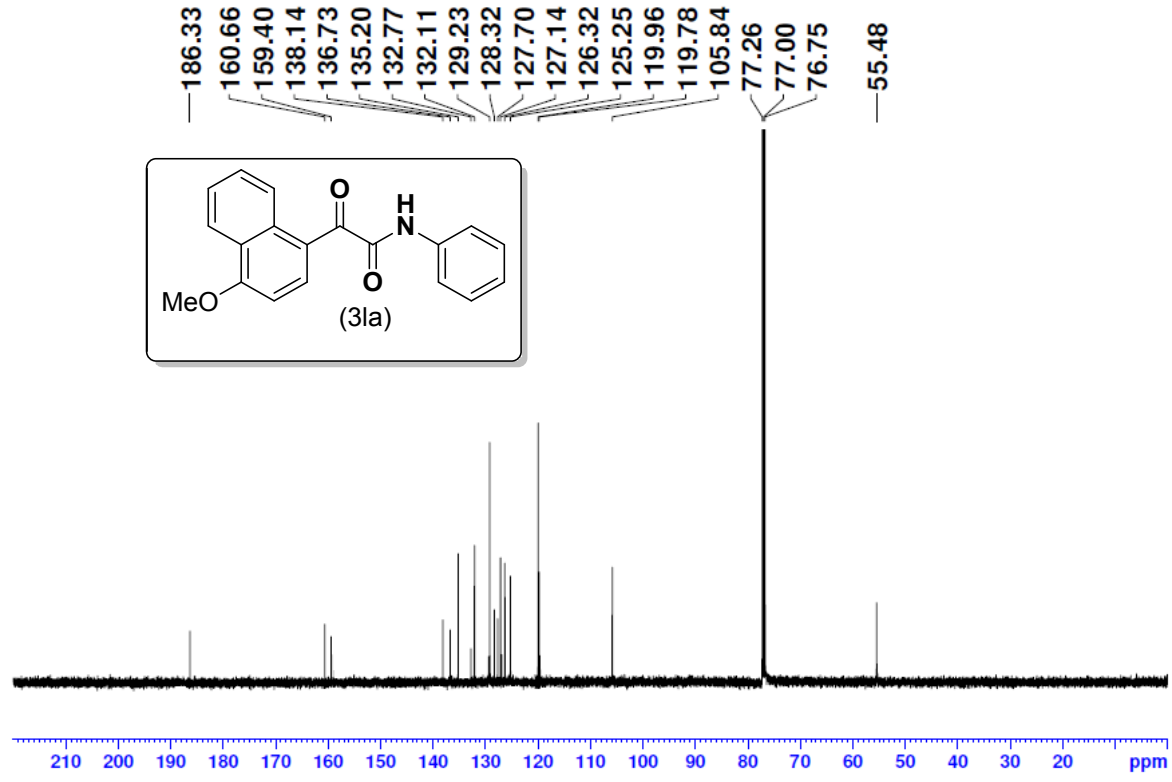

9.28
9.03
8.25
8.25
8.23
8.23
8.02
8.00
7.92
7.90
7.88
7.86
7.73
7.72
7.65
7.64
7.62
7.57
7.56
7.54
7.42
7.41
7.39
7.24
7.22
7.20
7.19
O
H
N
O
(3ja)
11
10
9
8
7
6
5
4
3
2
ppm
1.00
1.01
1.01
1.13
2.20
2.14
1.05
1.10
2.12
1.01

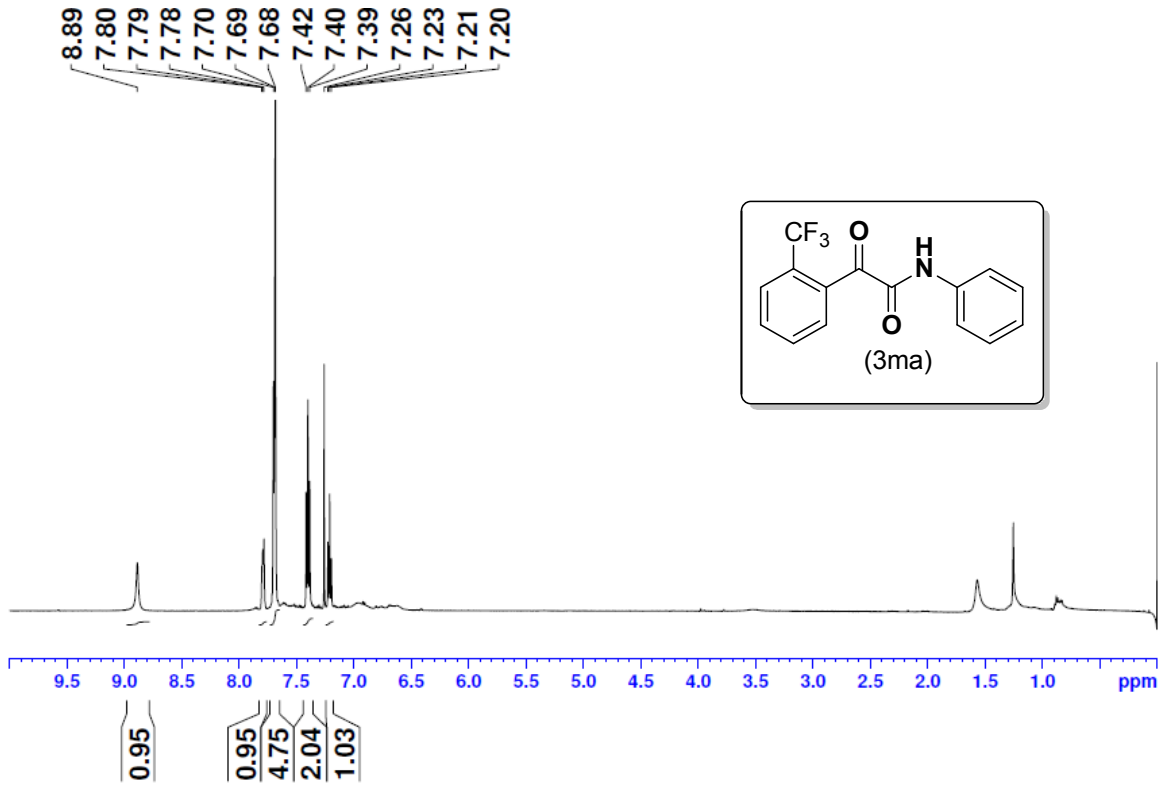

186.90
159.09
136.64
136.18
135.33
132.34
130.44
130.42
130.27
129.50
129.28
129.26
129.25
129.23
128.45
128.43
127.77
127.75
126.92
126.90
125.43
125.41
125.33
119.98
77.26
77.00
76.75
O
H
N
O
(3ja)
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

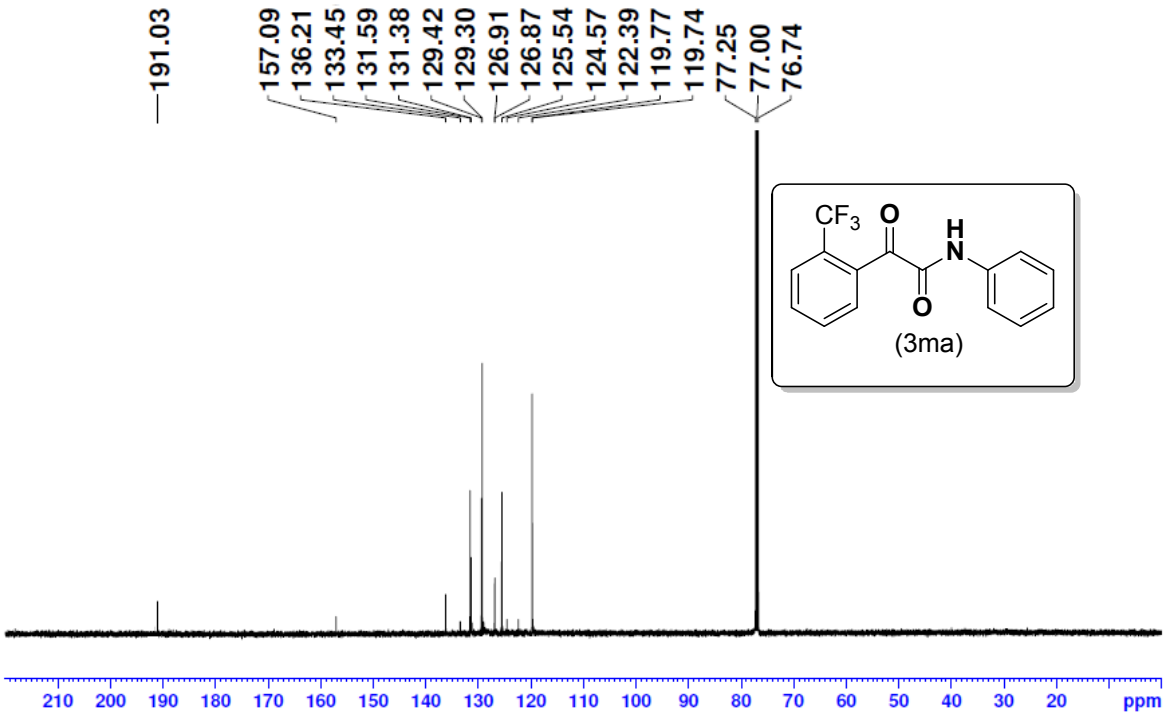

9.08
8.56
8.55
8.38
8.38
8.36
8.10
8.08
7.92
7.90
7.74
7.73
7.65
7.64
7.63
7.63
7.62
7.61
7.57
7.56
7.54
7.42
7.40
7.38
7.24
7.21
7.20
7.18
O
H
N
O
(3ka)
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 ppm
1.00
1.00
0.99
1.06
1.09
2.17
1.11
2.19
2.17
1.05

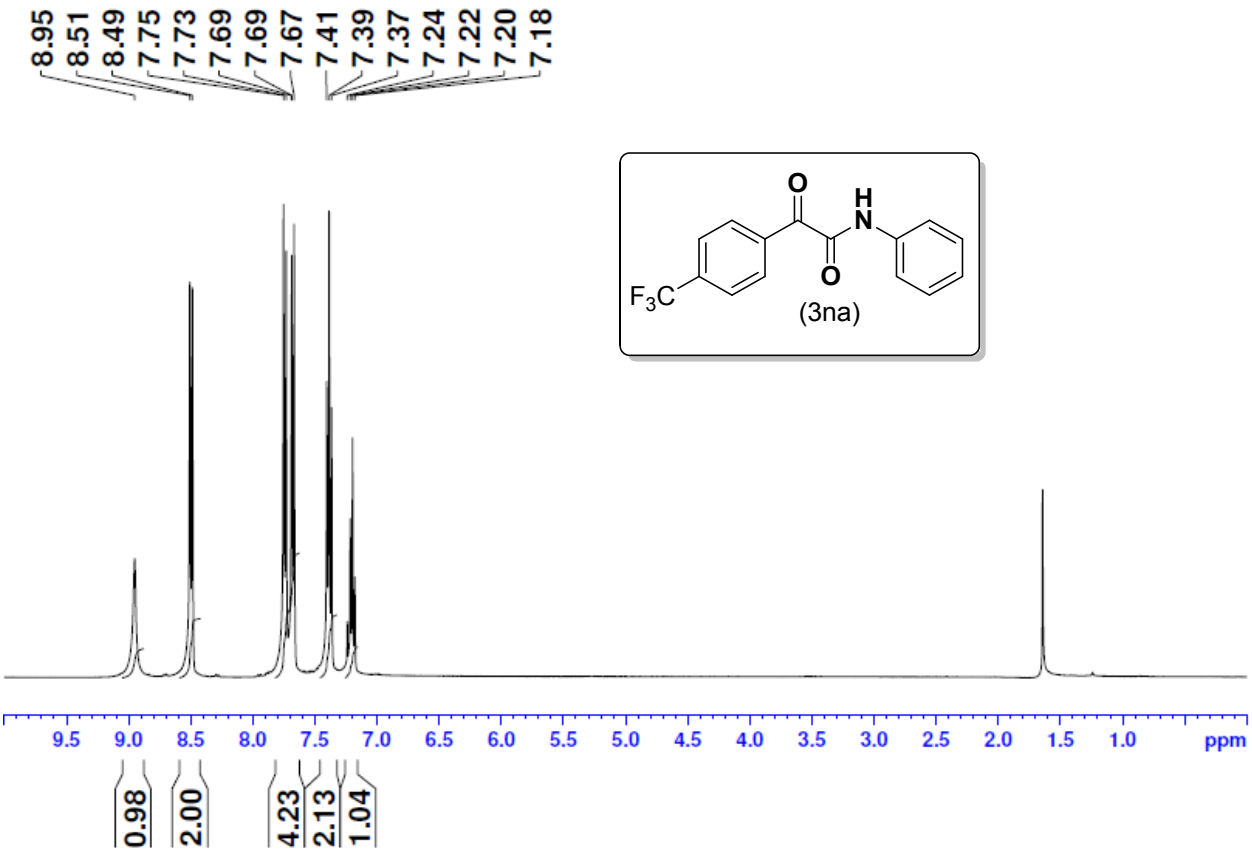

190.03
159.12
136.73
134.76
133.87
133.24
131.23
129.32
129.25
128.79
128.49
126.62
125.31
125.21
124.22
119.84
77.25
77.00
76.75
O
H
N
O
(3ka)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

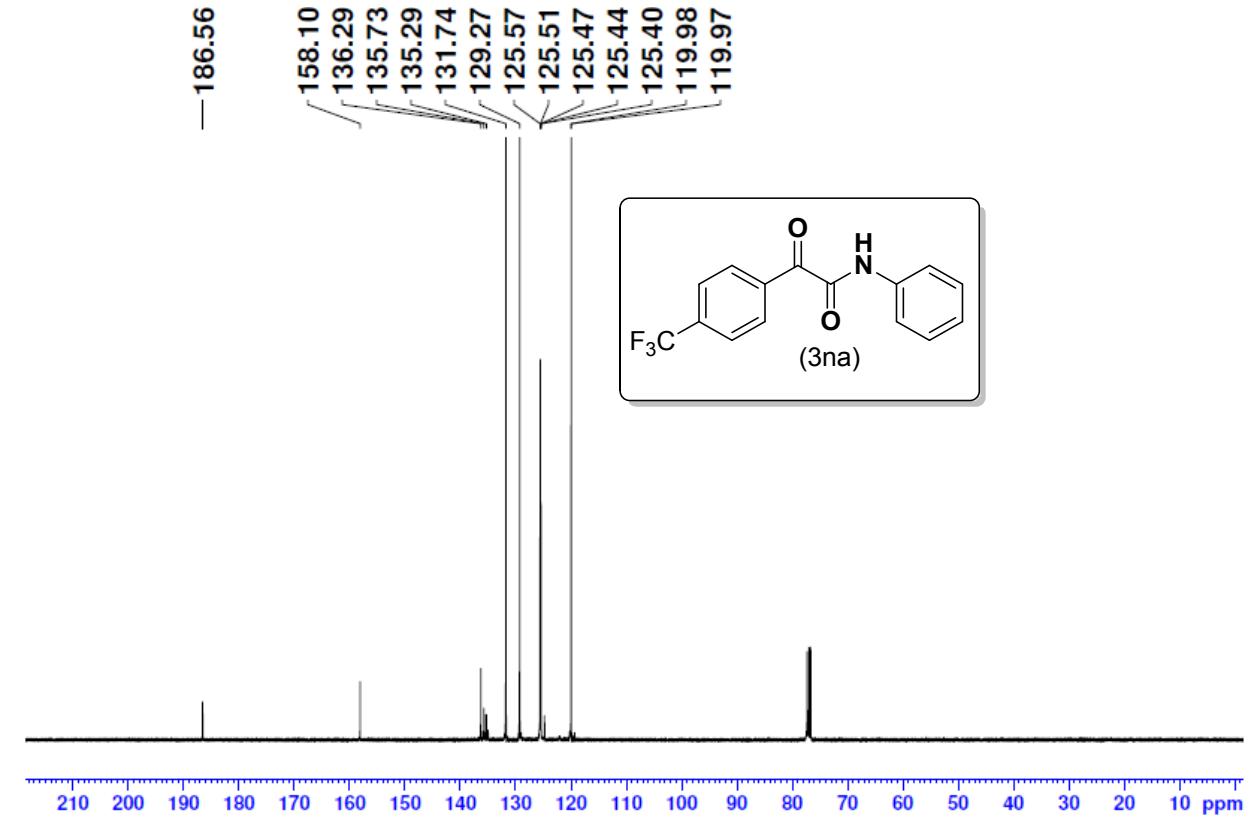

9.23
9.04
8.24
8.23
7.90
7.89
7.78
7.76
7.73
7.71
7.41
7.40
7.38
7.24
7.21
7.19
7.18
7.14
3.95
O
H
N
O
MeO
(3la)
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 ppm
1.00
1.02
1.05
1.15
1.20
2.26
2.18
2.13
1.34
3.24

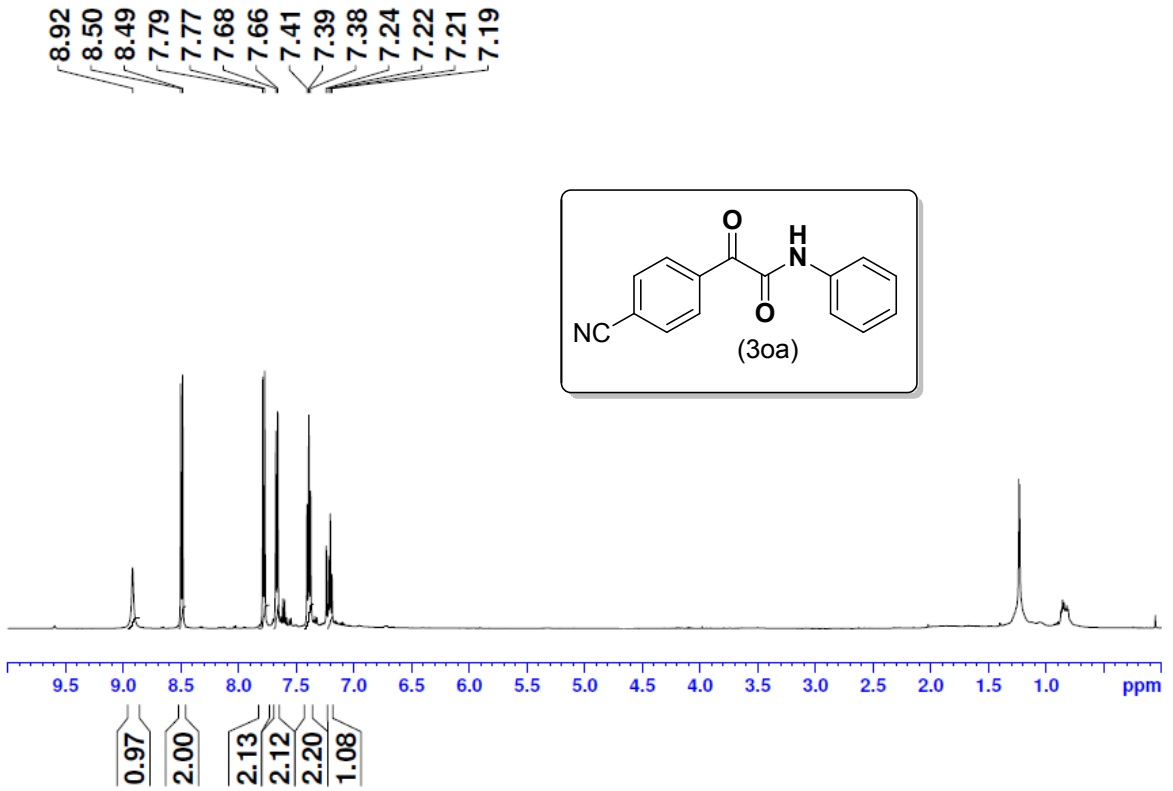

186.33
160.66
159.40
138.14
136.73
135.20
132.77
132.11
129.23
128.32
127.70
127.14
126.32
125.25
119.96
119.78
105.84
77.26
77.00
76.75
55.48
O
H
N
O
MeO
(3la)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

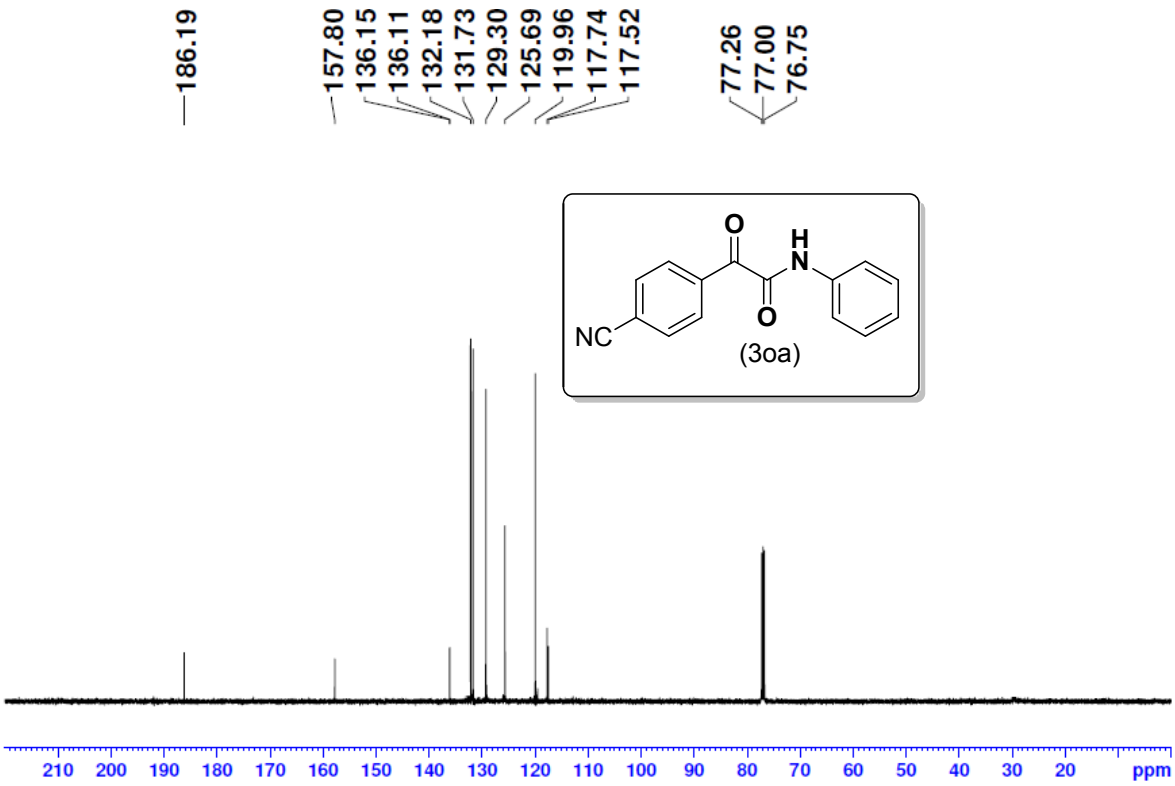

8.89
7.80
7.79
7.78
7.70
7.69
7.68
7.42
7.40
7.39
7.26
7.23
7.21
7.20
CF3
O
H
N
O
(3ma)
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
ppm
0.95
0.95
4.75
2.04
1.03

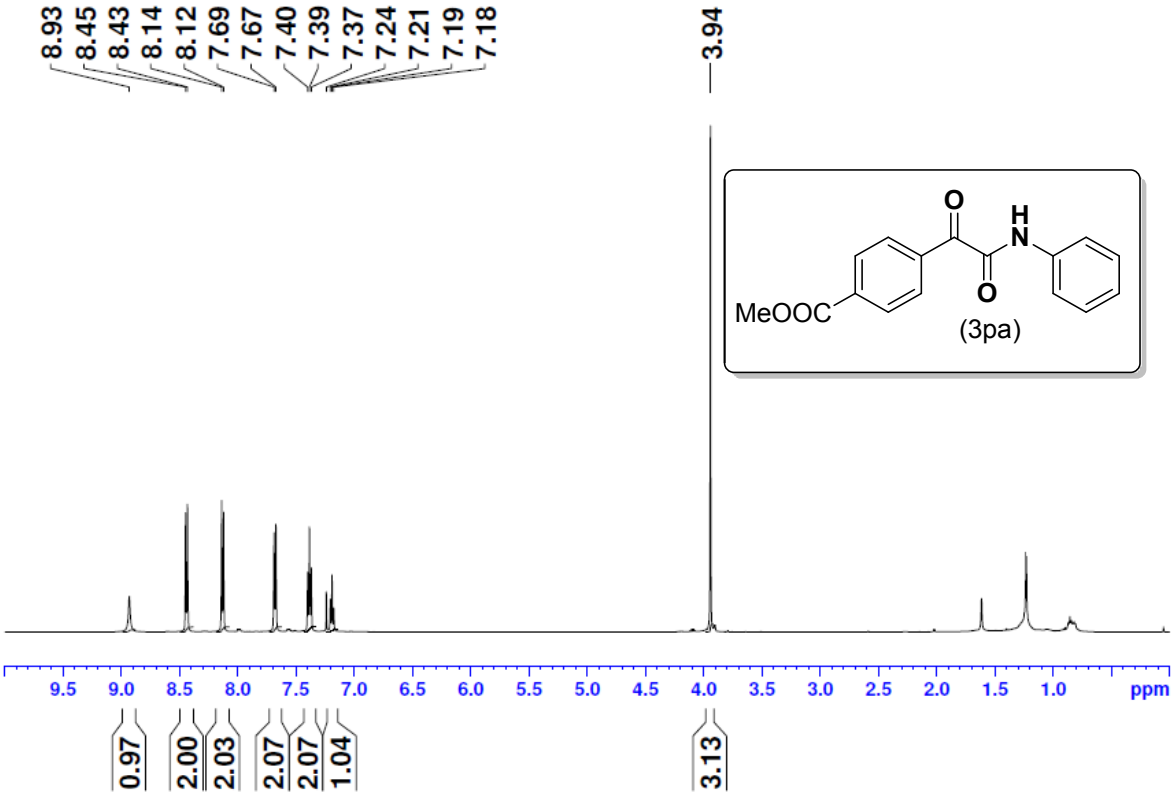

191.03
157.09
136.21
133.45
131.59
131.38
129.42
129.30
126.91
126.87
125.54
124.57
122.39
119.77
119.74
77.25
77.00
76.74
CF3
O
H
N
O
(3ma)
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

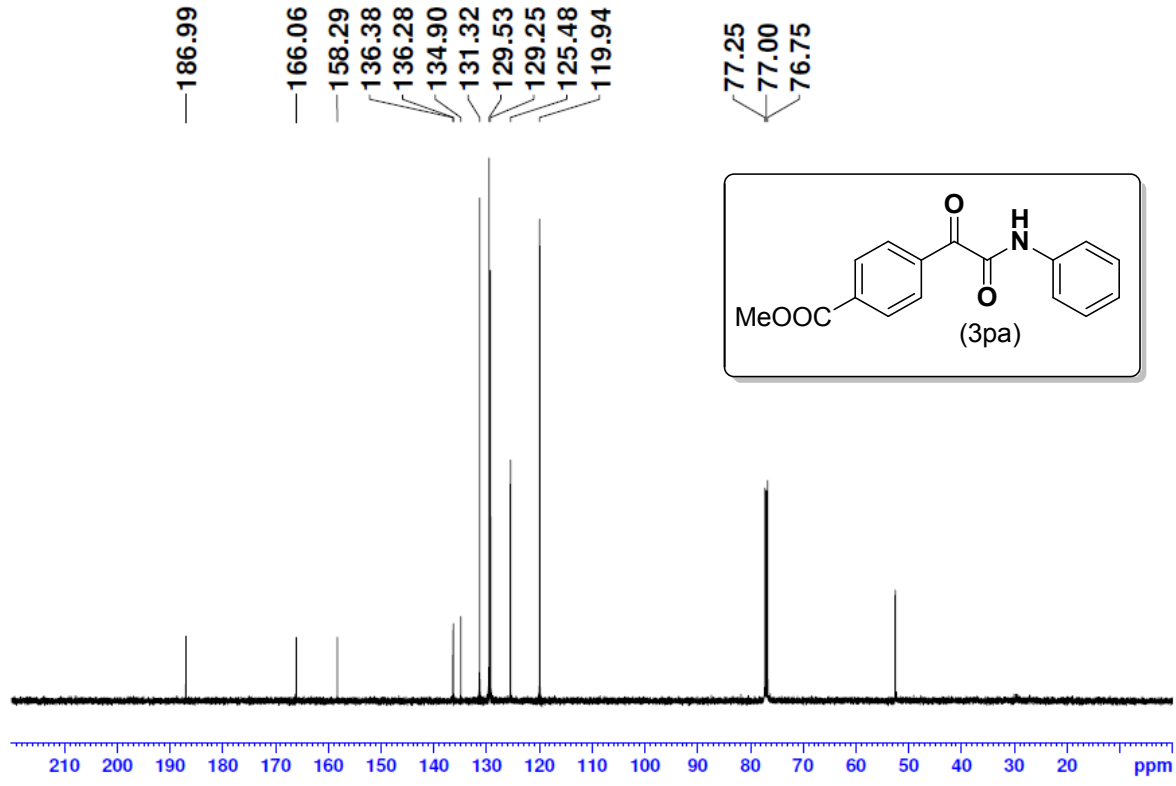

8.95
8.51
8.49
7.75
7.73
7.69
7.69
7.67
7.41
7.39
7.37
7.24
7.22
7.20
7.18
O
H
N
O
F3C
(3na)
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
ppm
0.98
2.00
4.23
2.13
1.04

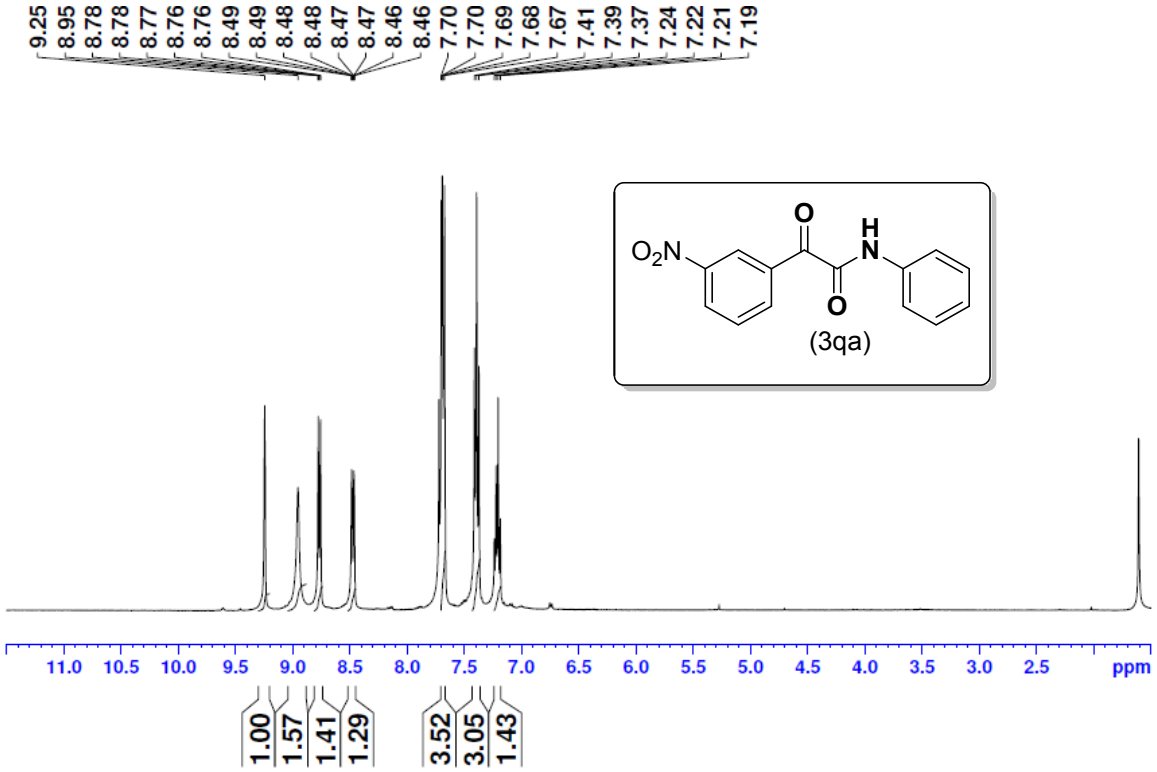

186.56
158.10
136.29
135.73
135.29
131.74
129.27
125.57
125.51
125.47
125.44
125.40
119.98
119.97
O
H
N
O
F3C
(3na)
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

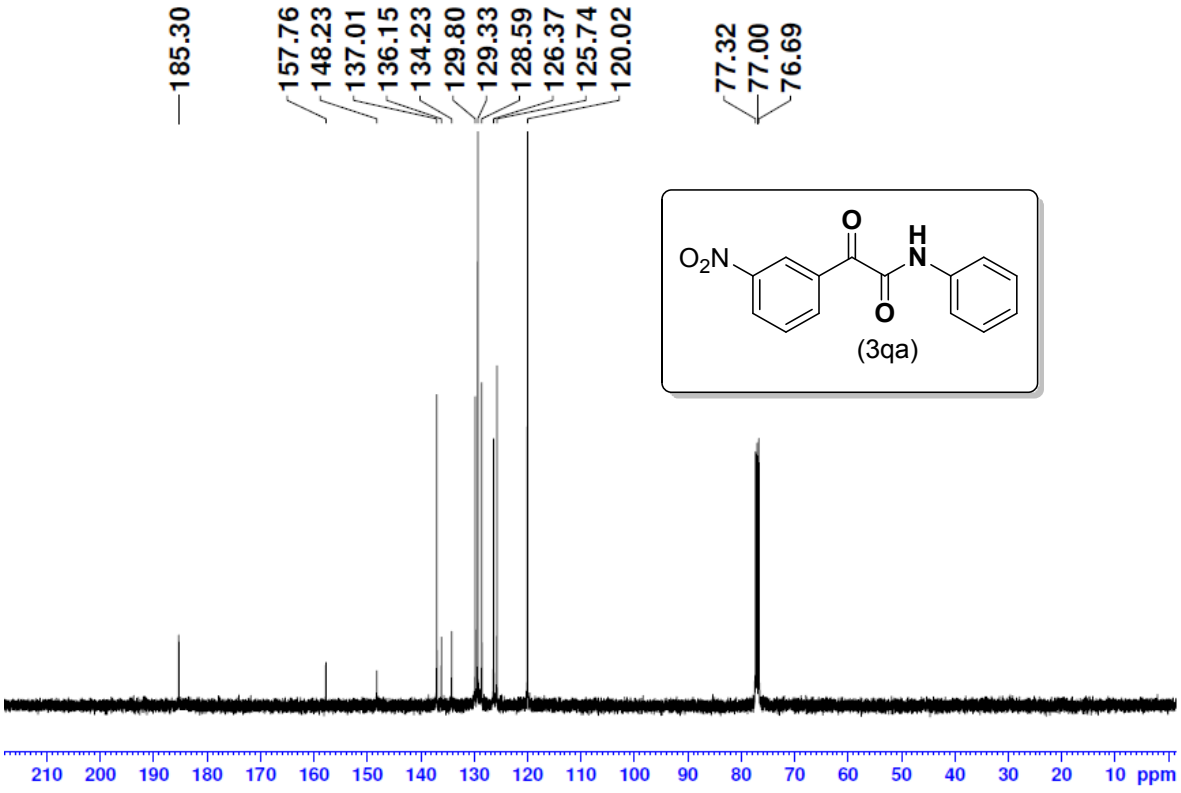

8.92
8.50
8.49
7.79
7.77
7.68
7.66
7.41
7.39
7.38
7.24
7.22
7.21
7.19
O
H
N
O
NC
(3oa)
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
ppm
0.97
2.00
2.13
2.12
2.20
1.08

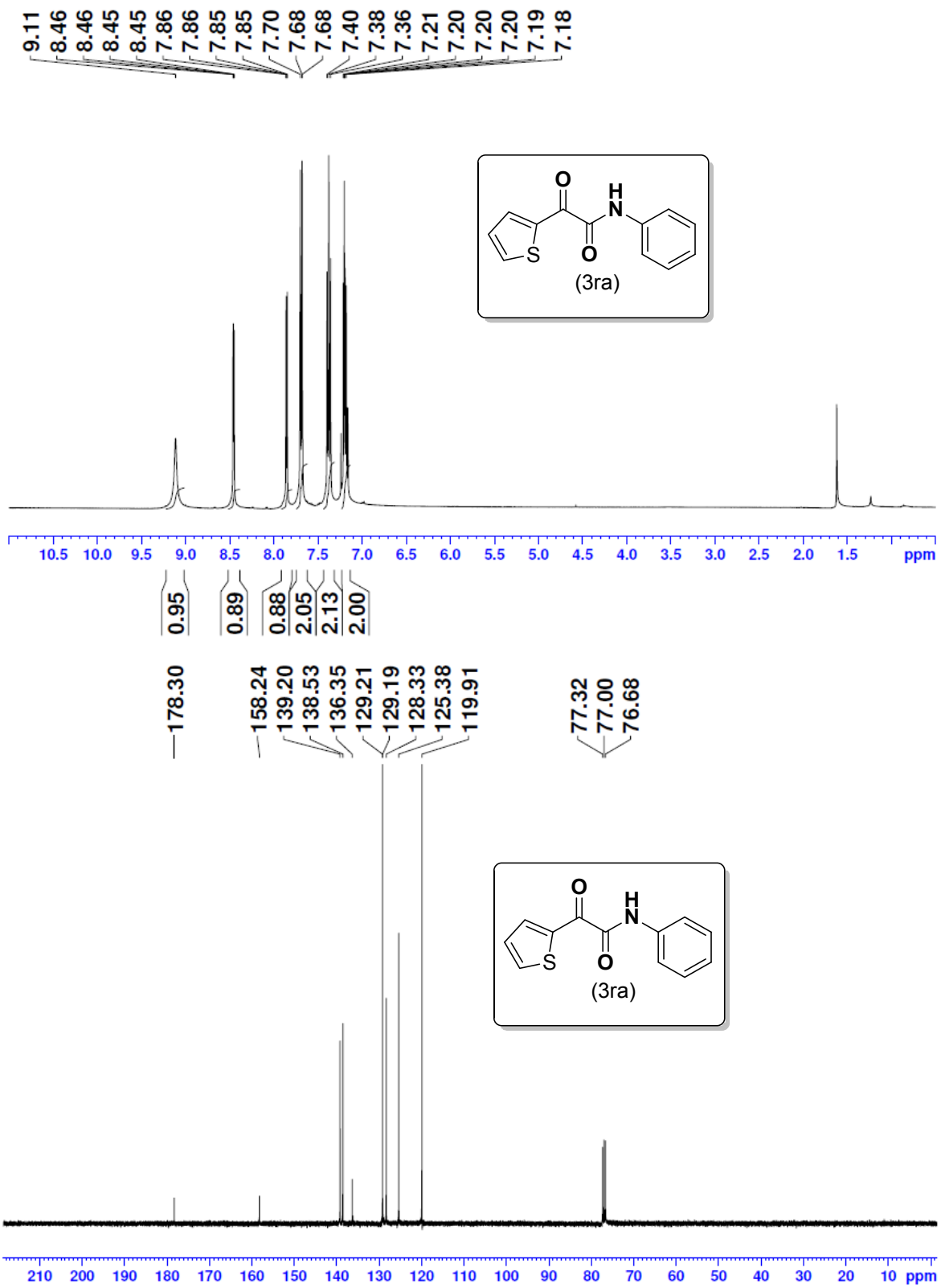

186.19
157.80
136.15
136.11
132.18
131.73
129.30
125.69
119.96
117.74
117.52
77.26
77.00
76.75
O
H
N
O
NC
(3oa)
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

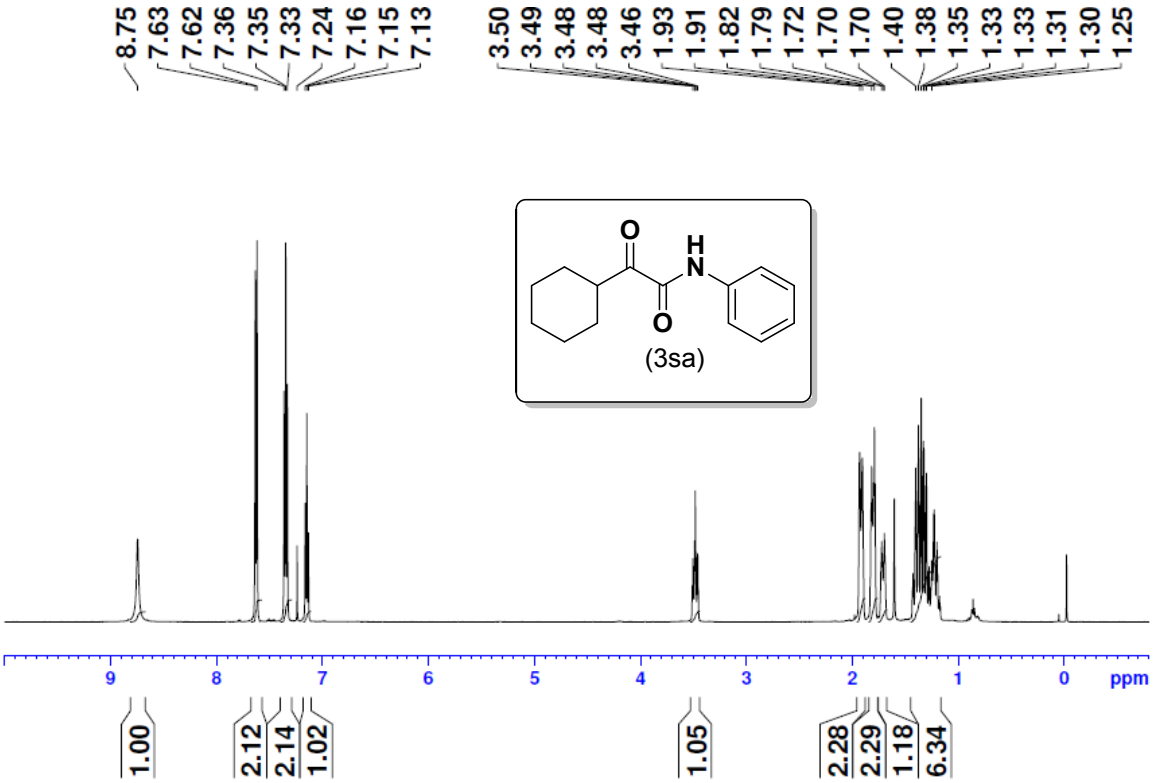

8.93
8.45
8.43
8.14
8.12
7.69
7.67
7.40
7.39
7.37
7.24
7.21
7.19
7.18
3.94
MeOOC
(3pa)
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 ppm
0.97
2.00
2.03
2.07
2.07
1.04
3.13


186.99
166.06
158.29
136.38
136.28
134.90
131.32
129.53
129.25
125.48
119.94
77.25
77.00
76.75
MeOOC
(3pa)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm


9.25
8.95
8.78
8.78
8.77
8.76
8.76
8.49
8.49
8.48
8.48
8.47
8.47
8.46
8.46
7.70
7.70
7.69
7.68
7.67
7.41
7.39
7.37
7.24
7.22
7.21
7.19
O2N
O
H
N
O
(3qa)
11.0 10.5 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 ppm
1.00
1.57
1.41
1.29
3.52
3.05
1.43


185.30
157.76
148.23
137.01
136.15
134.23
129.80
129.33
128.59
126.37
125.74
120.02
77.32
77.00
76.69
O2N
O
H
N
O
(3qa)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm


9.11
8.46
8.46
8.45
8.45
7.86
7.86
7.85
7.85
7.70
7.68
7.68
7.40
7.38
7.36
7.21
7.20
7.20
7.20
7.19
7.18
O
H
N
S
O
(3ra)
10.5 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 ppm
0.95
0.89
0.88
2.05
2.13
2.00
178.30
158.24
139.20
138.53
136.35
129.21
129.19
128.33
125.38
119.91
77.32
77.00
76.68
O
H
N
S
O
(3ra)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm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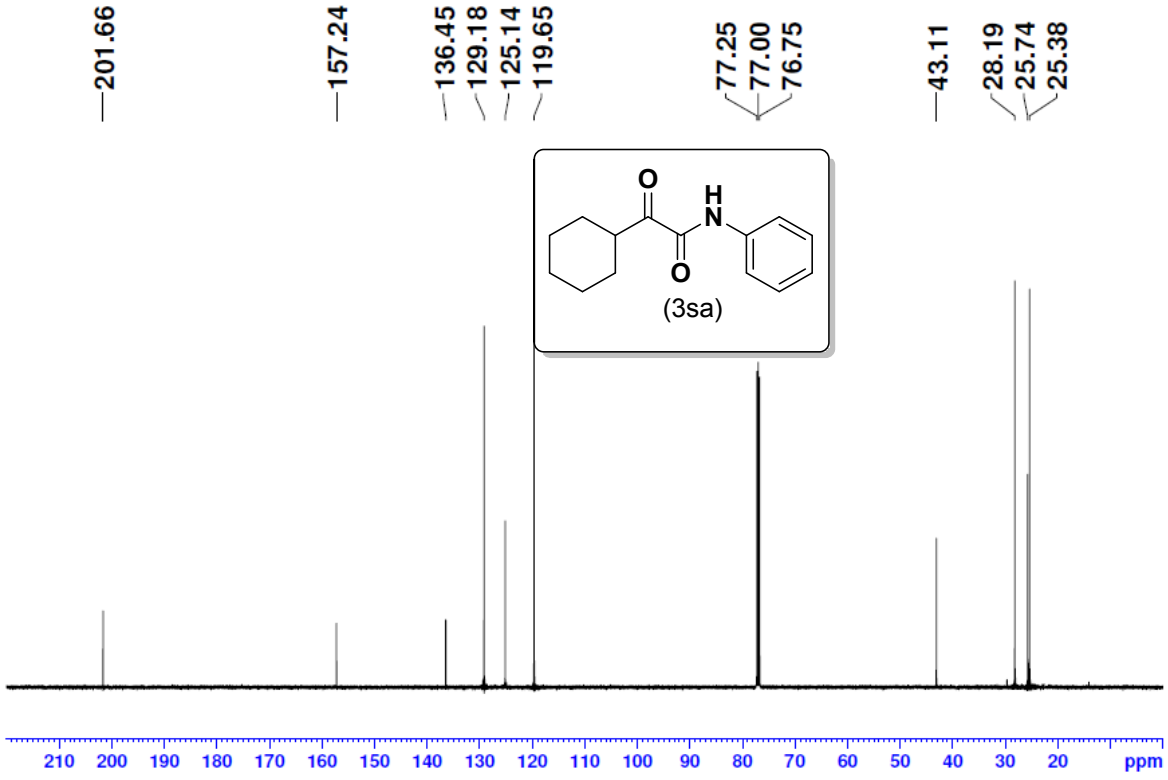
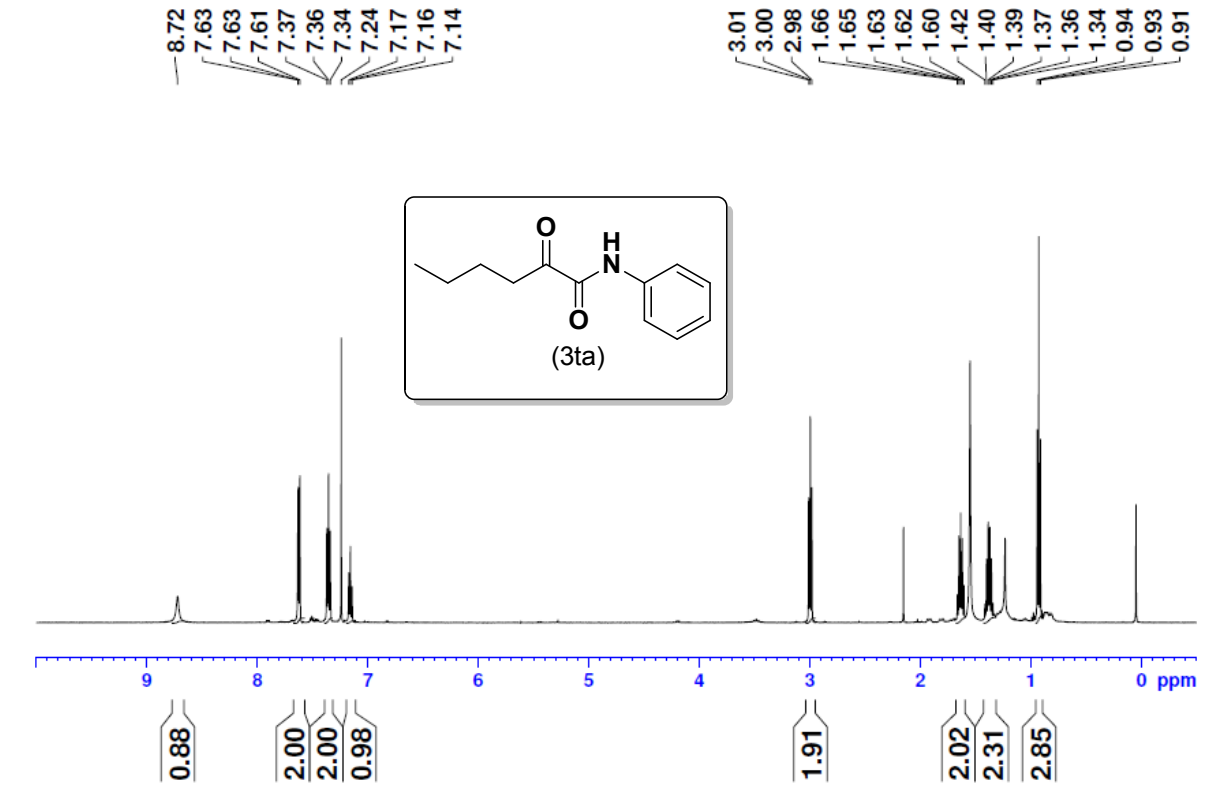
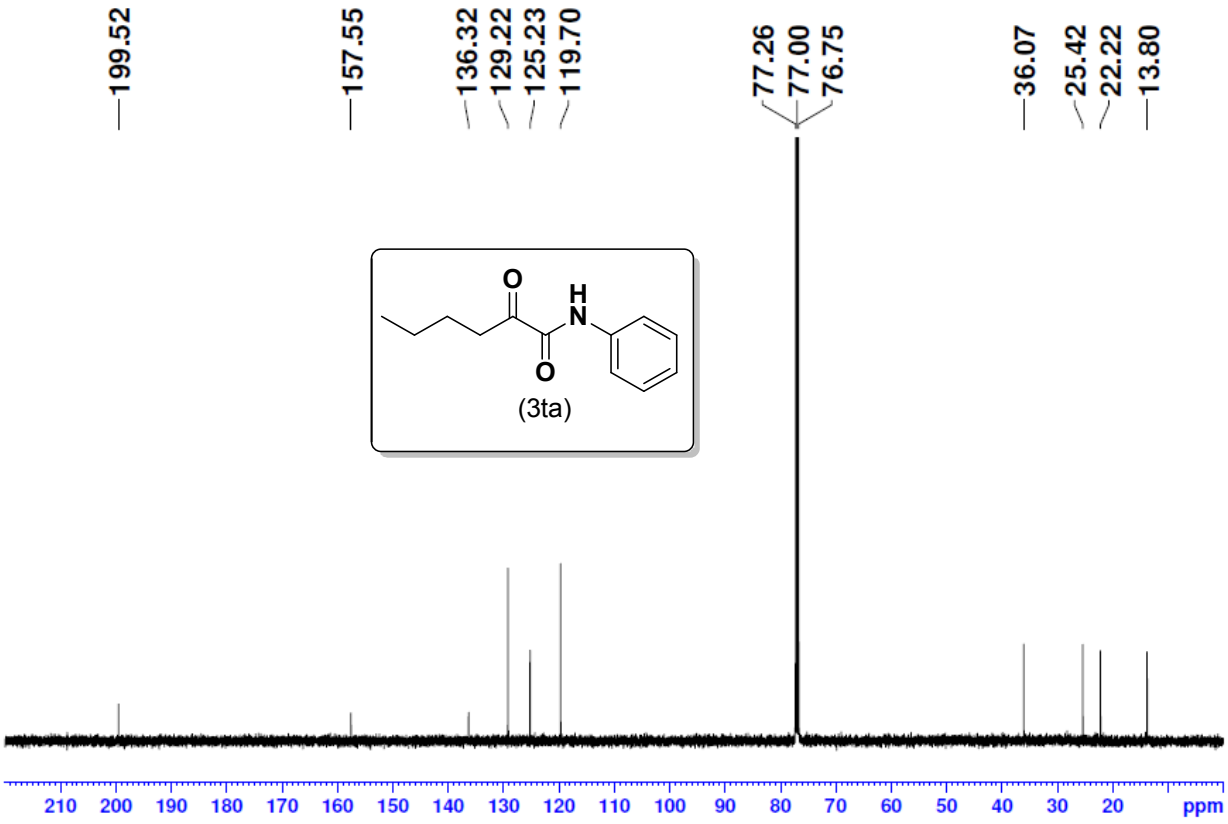
7.63
7.62
7.36
7.35
7.33
7.24
7.16
7.15
7.13
3.50
3.49
3.48
3.48
3.46
1.93
1.91
1.82
1.79
1.72
1.70
1.70
1.40
1.38
1.35
1.33
1.33
1.31
1.30
1.25
O
H
N
O
(3sa)
9
8
7
6
5
4
3
2
1
0
ppm
1.00
2.12
2.14
1.02
1.05
2.28
2.29
1.18
6.34


201.66
157.24
136.45
129.18
125.14
119.65
77.25
77.00
76.75
43.11
28.19
25.74
25.38
O
H
N
O
(3sa)
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm


8.72
7.63
7.63
7.61
7.37
7.36
7.34
7.24
7.17
7.16
7.14
3.01
3.00
2.98
1.66
1.65
1.63
1.62
1.60
1.42
1.40
1.39
1.37
1.36
1.34
0.94
0.93
0.91
O
H
N
O
(3ta)
9
8
7
6
5
4
3
2
1
0 ppm
0.88
2.00
2.00
0.98
1.91
2.02
2.31
2.85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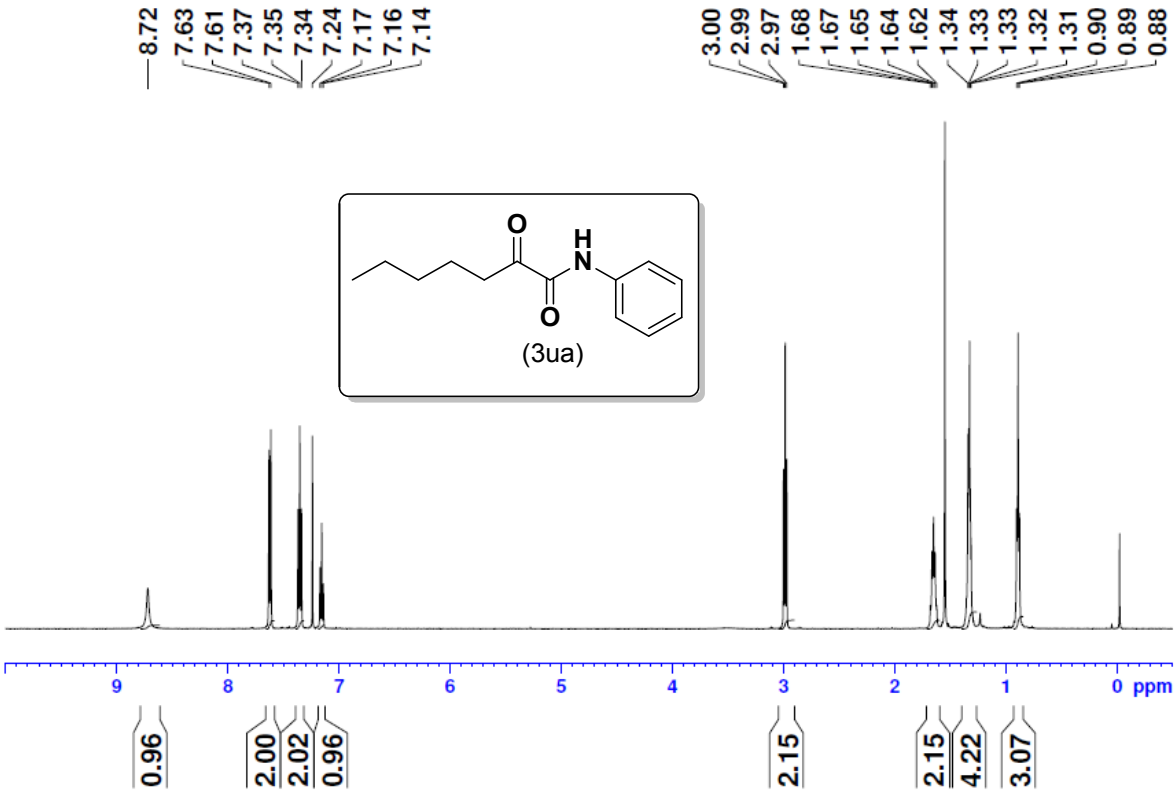
157.55
136.32
129.22
125.23
119.70
77.26
77.00
76.75
36.07
25.42
22.22
13.80
O
H
N
O
(3ta)
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm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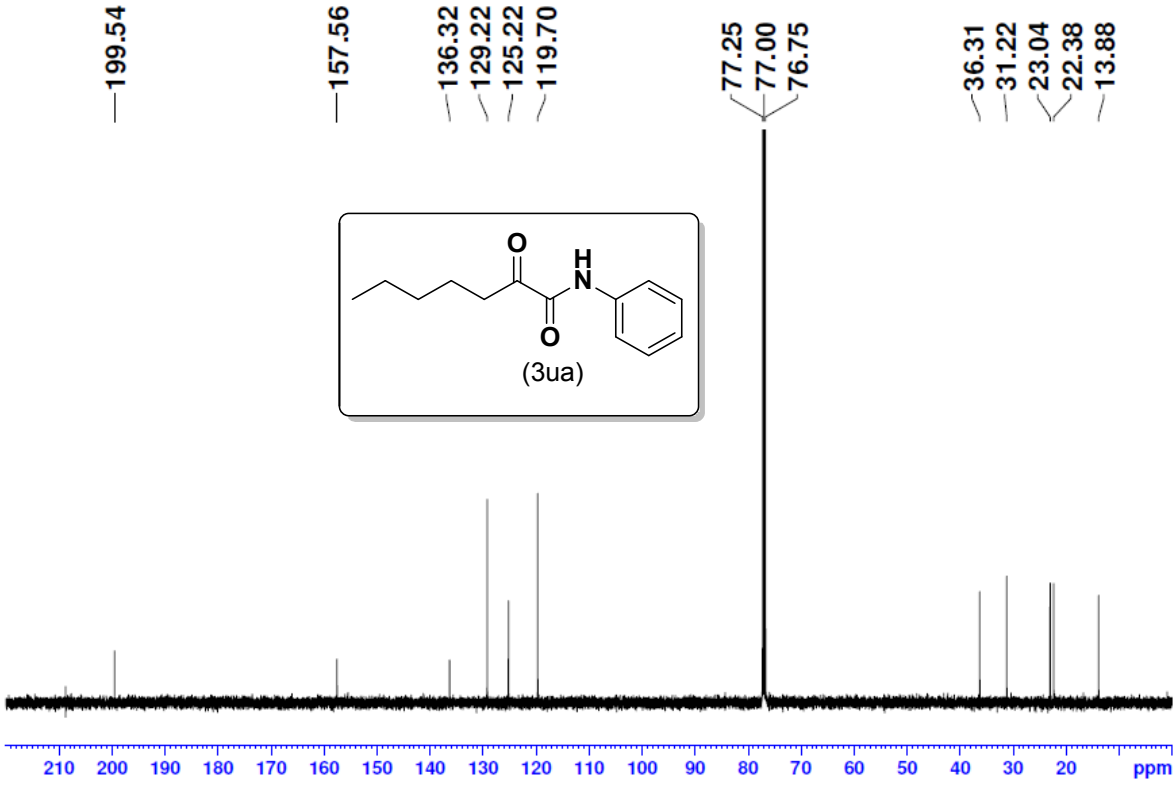
7.63
7.61
7.37
7.35
7.34
7.24
7.17
7.16
7.14
3.00
2.99
2.97
1.68
1.67
1.65
1.64
1.62
1.34
1.33
1.33
1.32
1.31
0.90
0.89
0.88
O
H
N
O
(3ua)
9
8
7
6
5
4
3
2
1
0 ppm
0.96
2.00
2.02
0.96
2.15
2.15
4.22
3.07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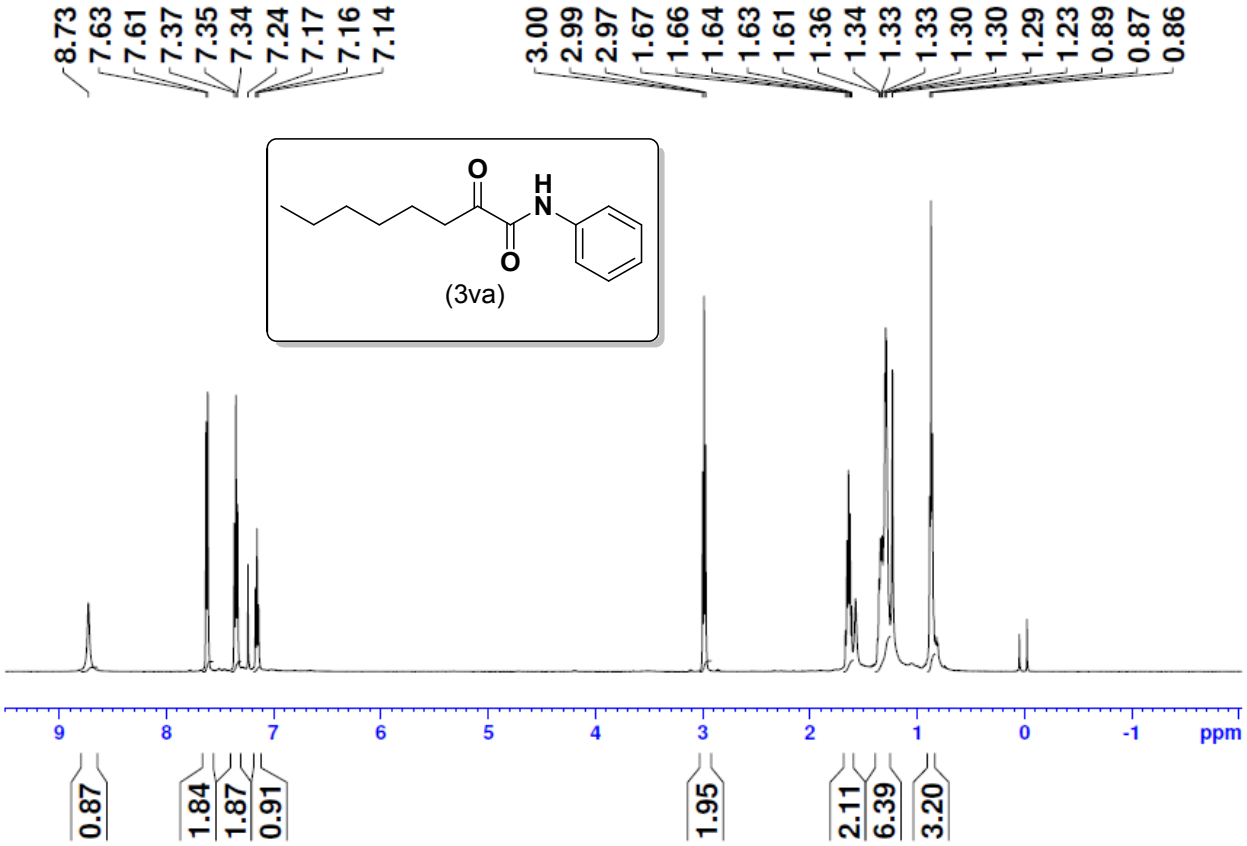
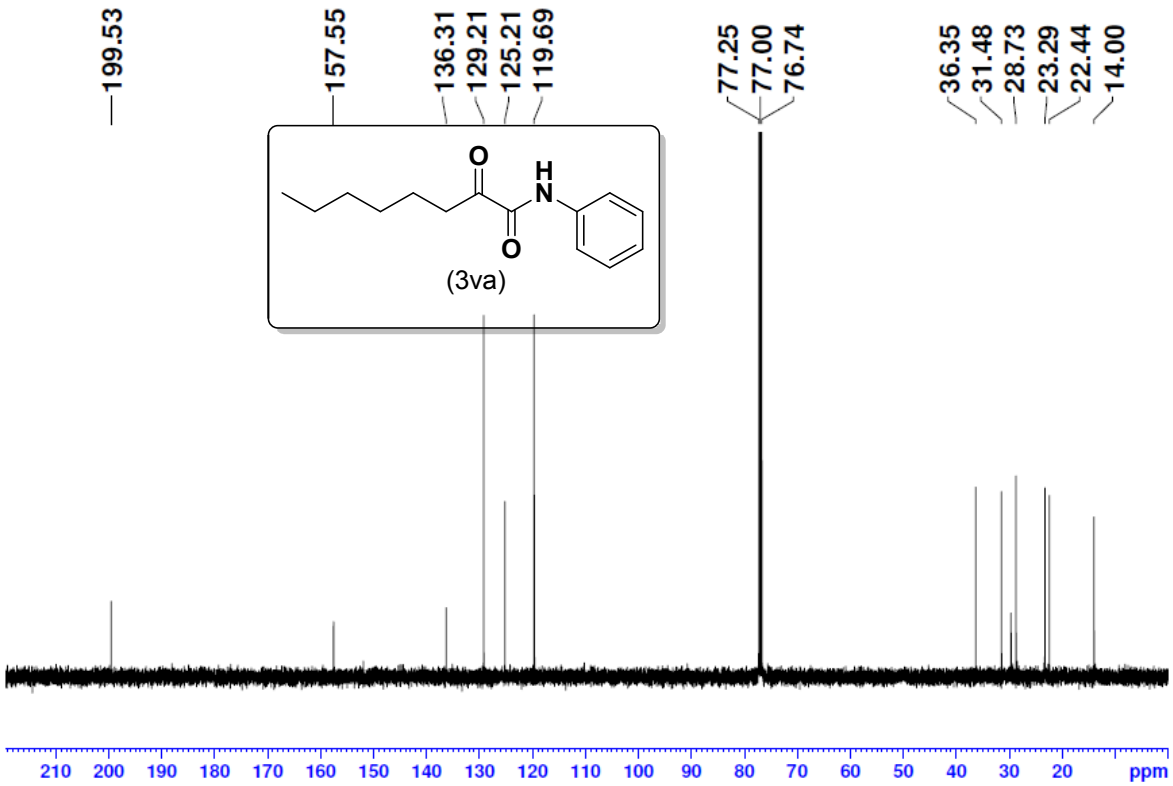
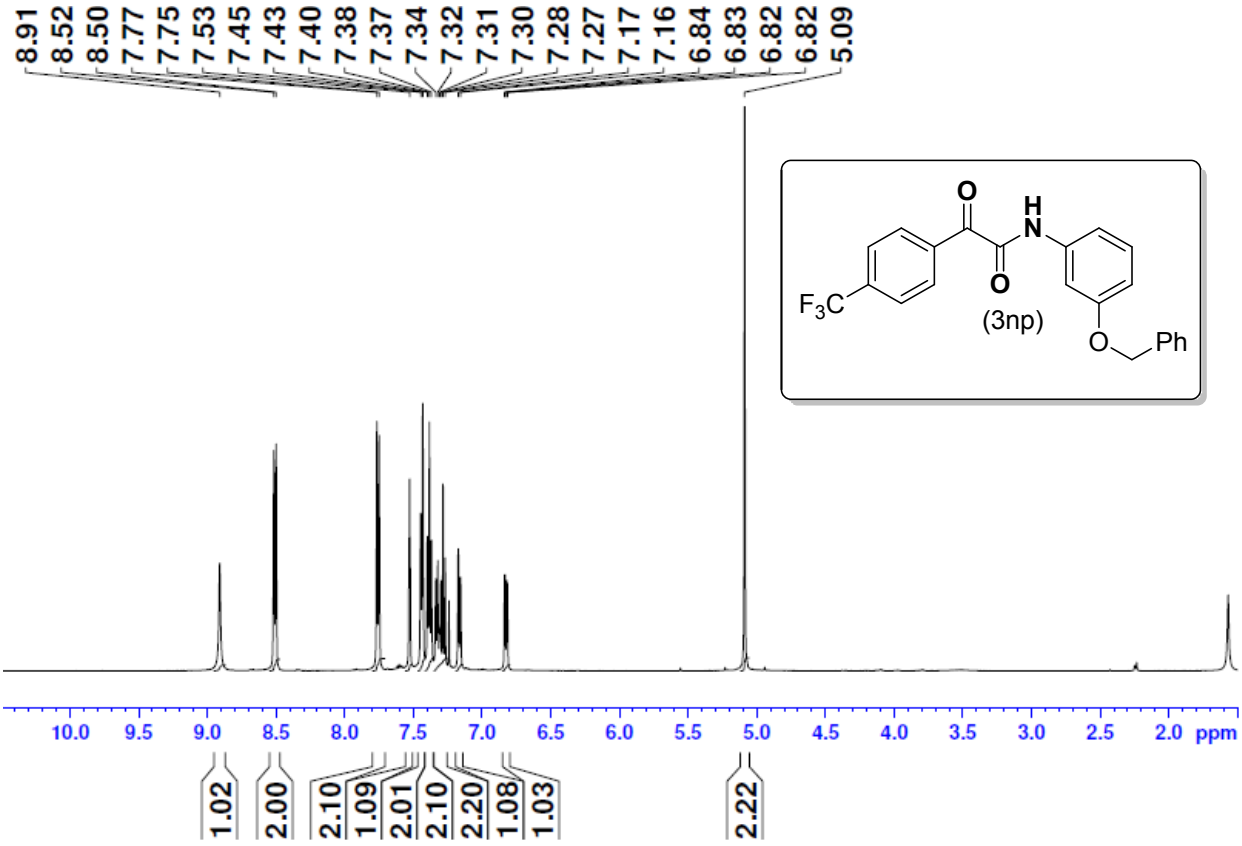
157.56
136.32
129.22
125.22
119.70
77.25
77.00
76.75
36.31
31.22
23.04
22.38
13.88
O
H
N
O
(3ua)
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm


8.73
7.63
7.61
7.37
7.35
7.34
7.24
7.17
7.16
7.14
3.00
2.99
2.97
1.67
1.66
1.64
1.63
1.61
1.36
1.34
1.33
1.33
1.30
1.30
1.29
1.23
0.89
0.87
0.86
O
H
N
O
(3va)
9
8
7
6
5
4
3
2
1
0
-1
ppm
0.87
1.84
1.87
0.91
1.95
2.11
6.39
3.20


199.53
157.55
136.31
129.21
125.21
119.69
77.25
77.00
76.74
36.35
31.48
28.73
23.29
22.44
14.00
O
H
N
O
(3va)
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm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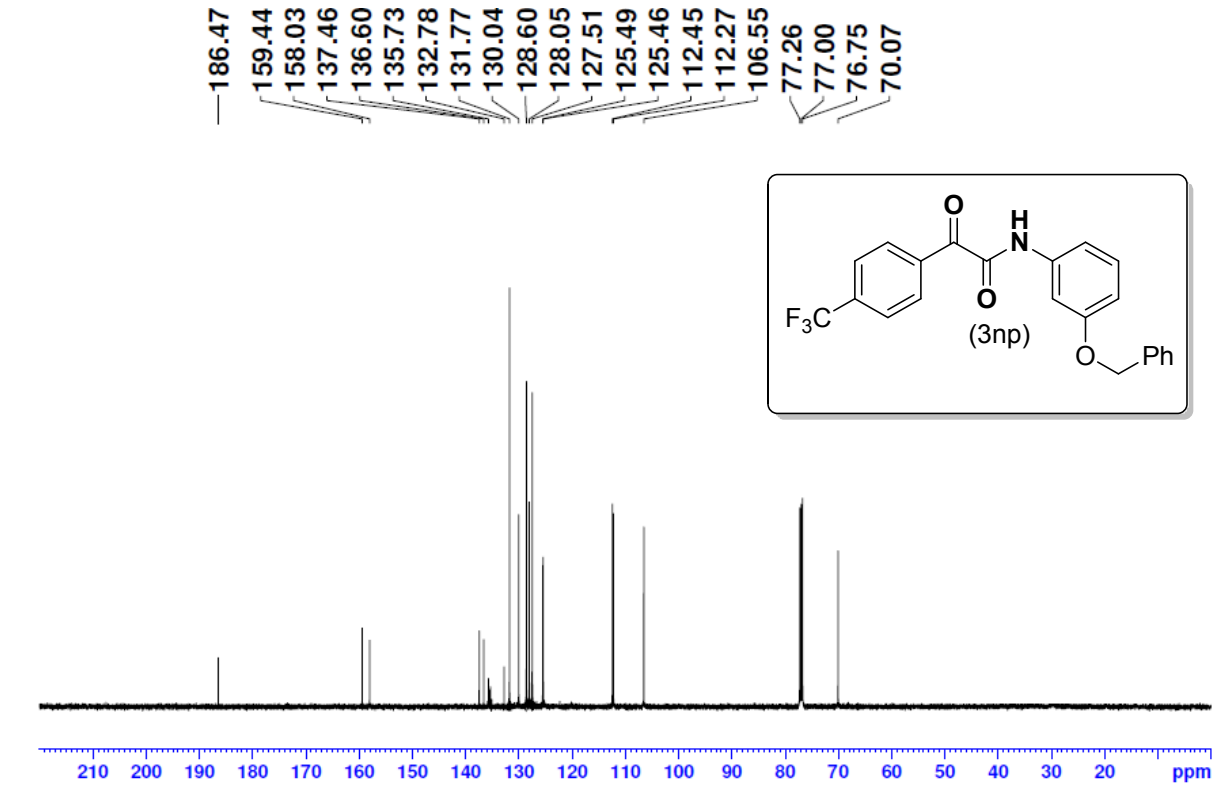
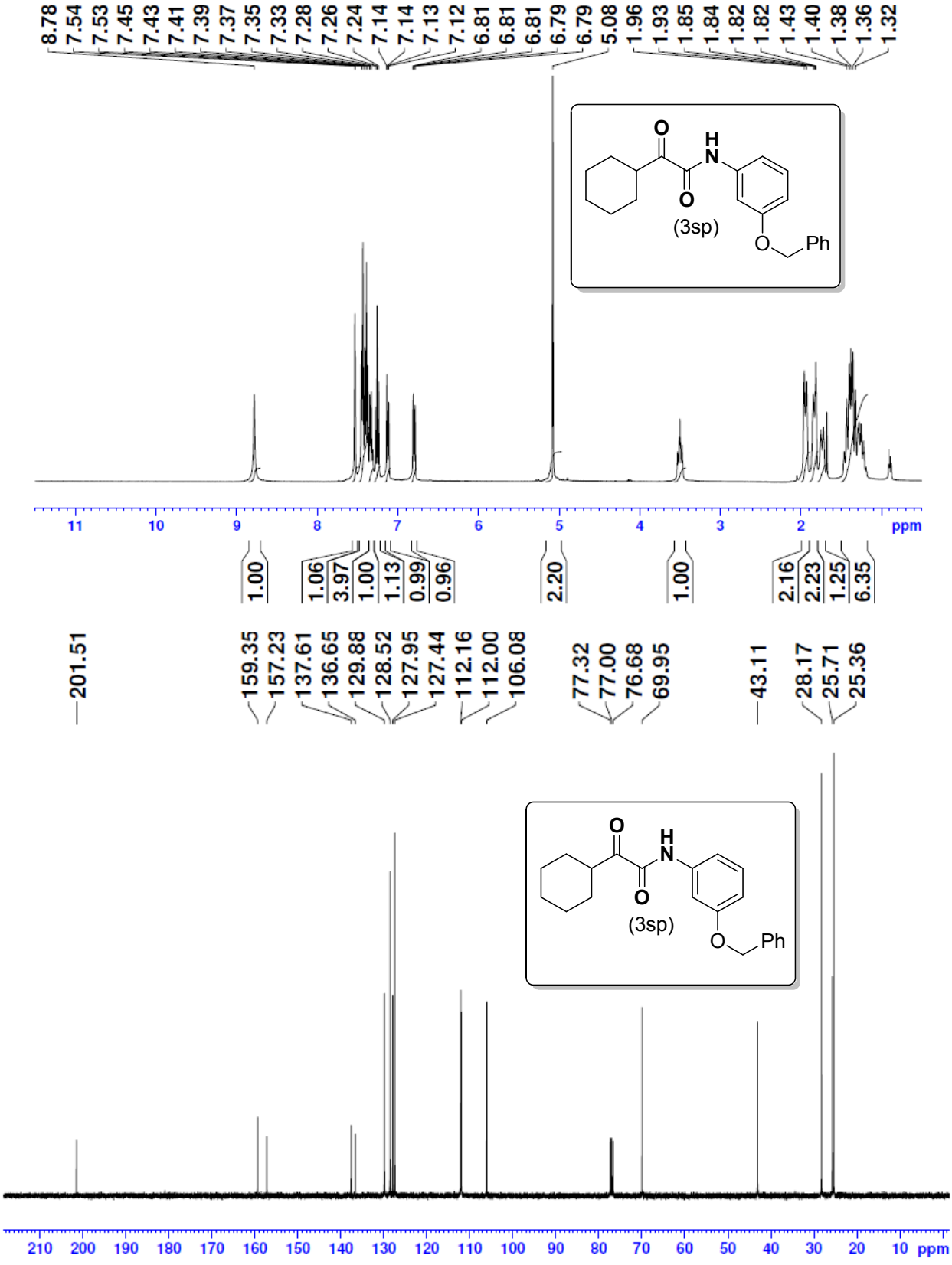
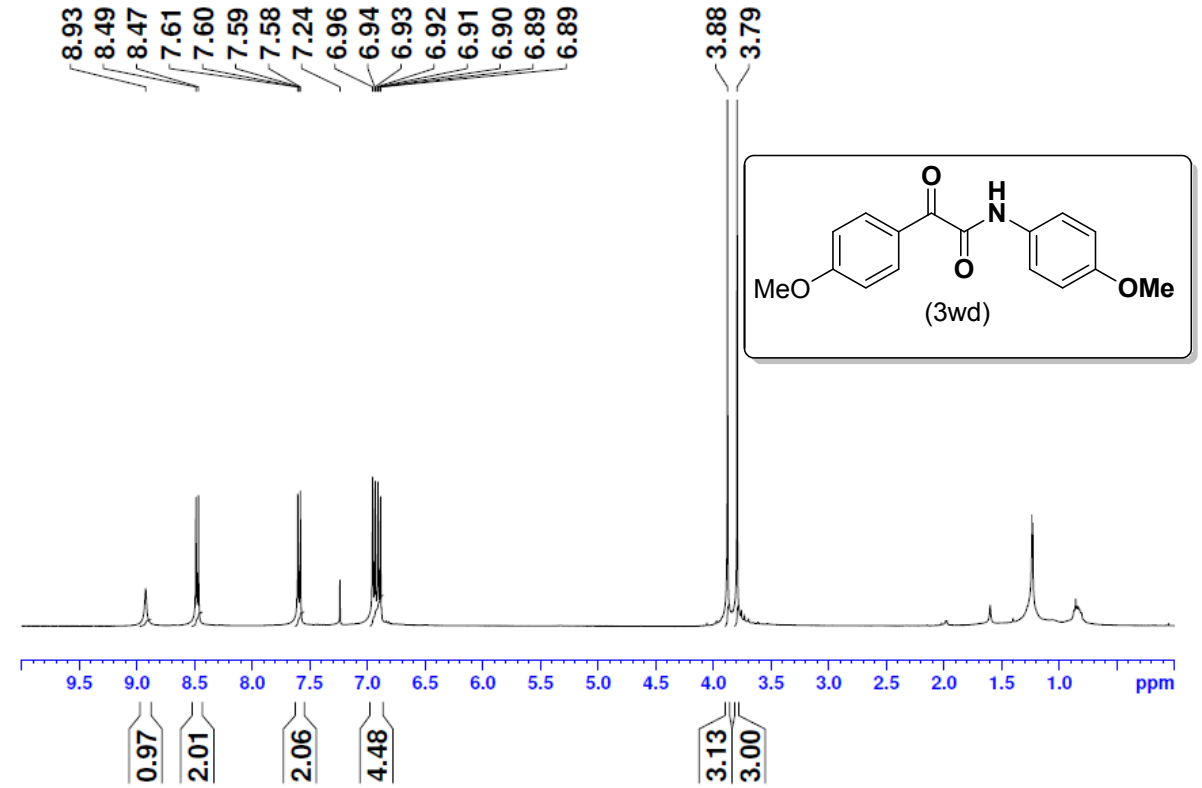
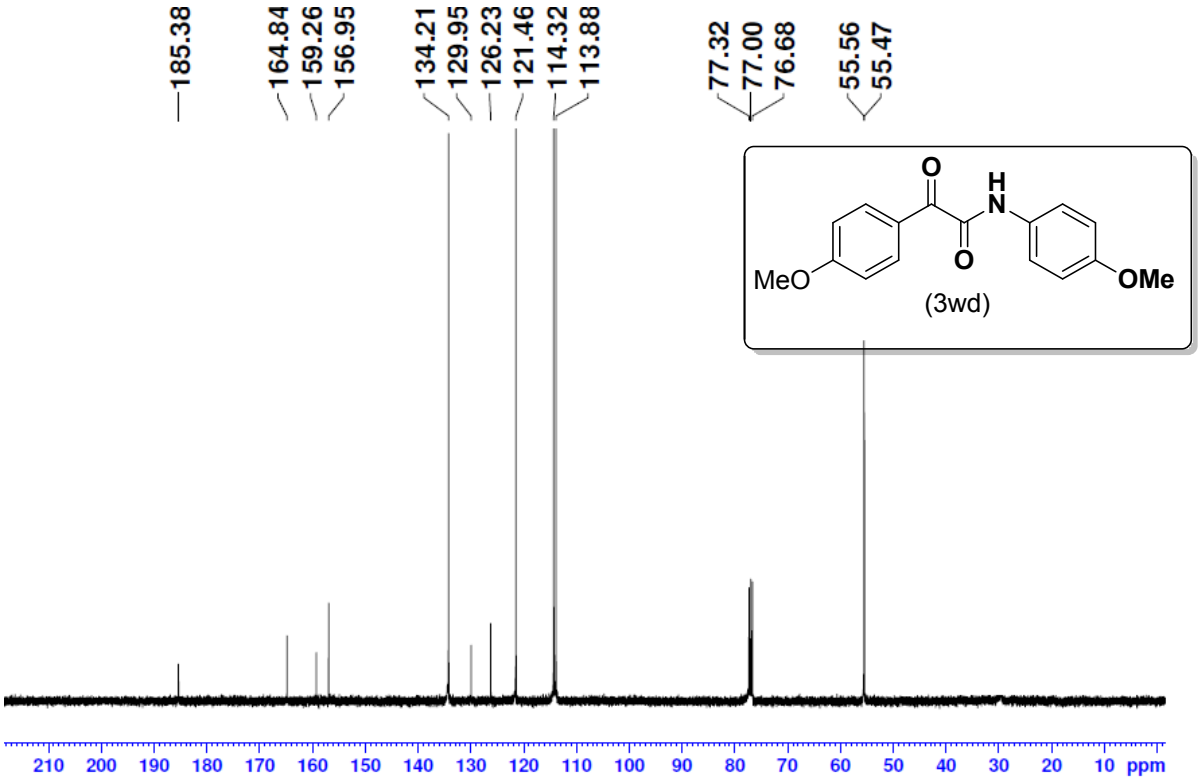
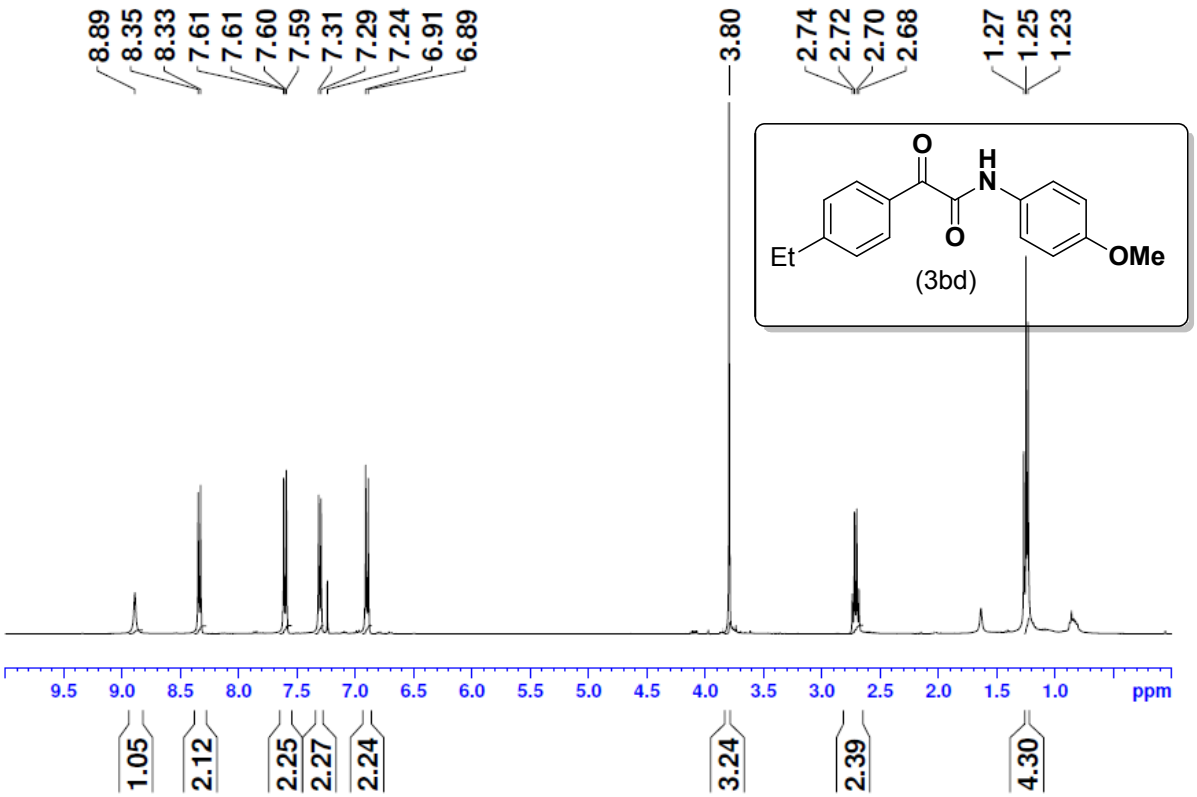
8.52
8.50
7.77
7.75
7.53
7.45
7.43
7.40
7.38
7.37
7.34
7.32
7.31
7.30
7.28
7.27
7.17
7.16
6.84
6.83
6.82
6.82
5.09
O
H
N
O
F3C
(3np)
O
Ph
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
ppm
1.02
2.00
2.10
1.09
2.01
2.10
2.20
1.08
1.03
2.22

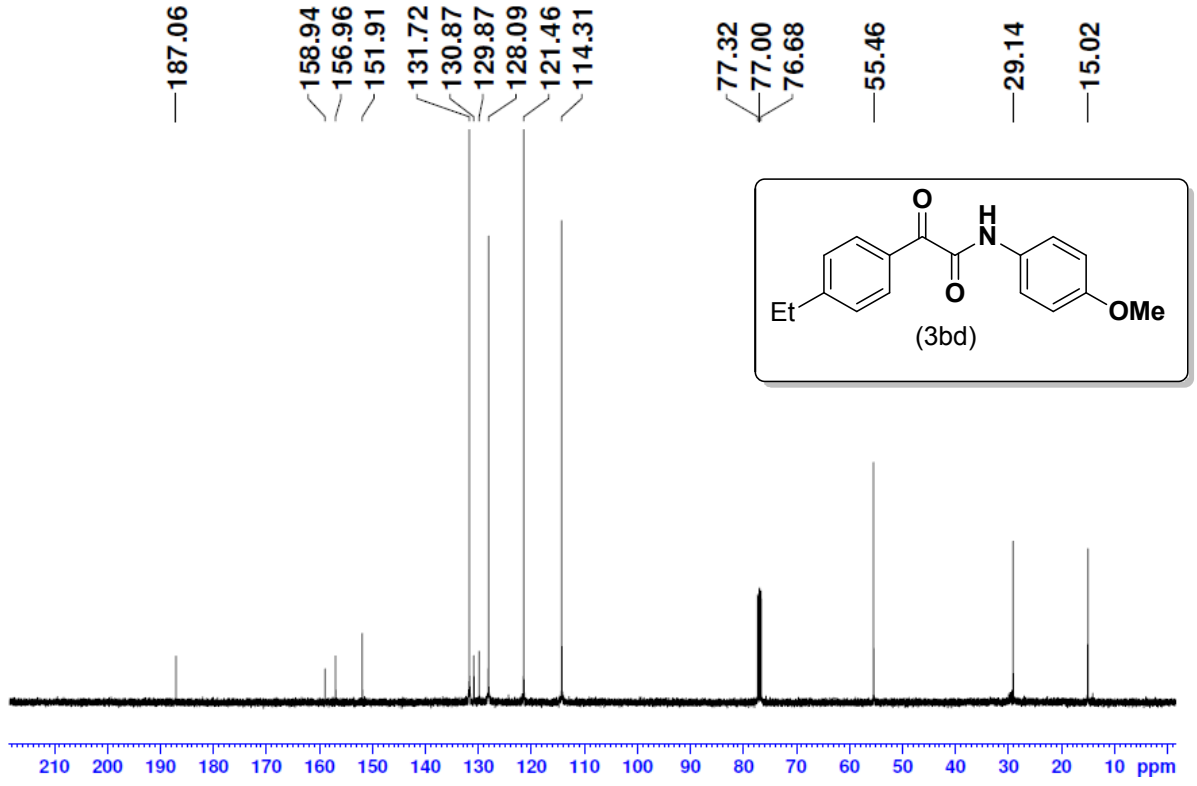

186.47
159.44
158.03
137.46
136.60
135.73
132.78
131.77
130.04
128.60
128.05
127.51
125.49
125.46
112.45
112.27
106.55
77.26
77.00
76.75
70.07
O
H
N
O
F3C
(3np)
O
Ph
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

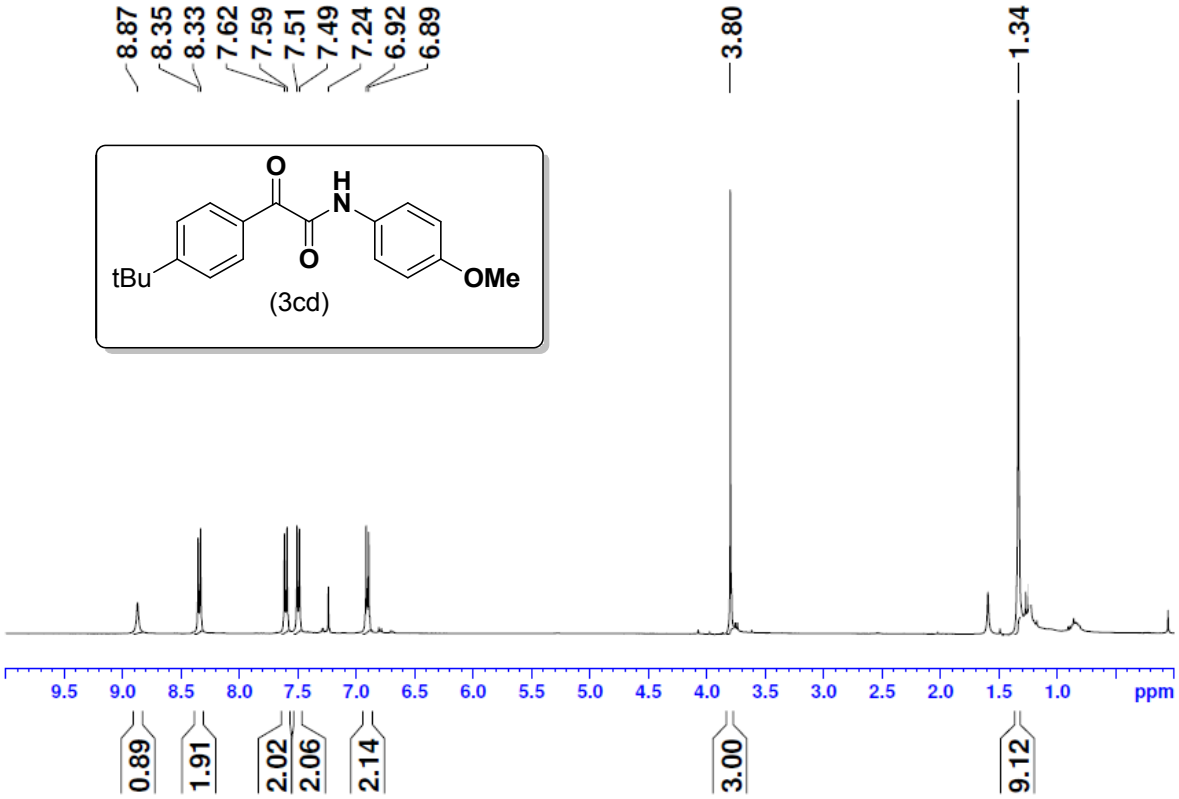

8.78
7.54
7.53
7.45
7.43
7.41
7.39
7.37
7.35
7.33
7.28
7.26
7.24
7.14
7.14
7.13
7.12
6.81
6.81
6.81
6.79
6.79
5.08
1.96
1.93
1.85
1.84
1.82
1.82
1.43
1.40
1.38
1.36
1.32
O
H
N
O
(3sp)
O
Ph
11
10
9
8
7
6
5
4
3
2
ppm
1.00
1.06
3.97
1.00
1.13
0.99
0.96
2.20
1.00
2.16
2.23
1.25
6.35
201.51
159.35
157.23
137.61
136.65
129.88
128.52
127.95
127.44
112.16
112.00
106.08
77.32
77.00
76.68
69.95
43.11
28.17
25.71
25.36
O
H
N
O
(3sp)
O
Ph
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

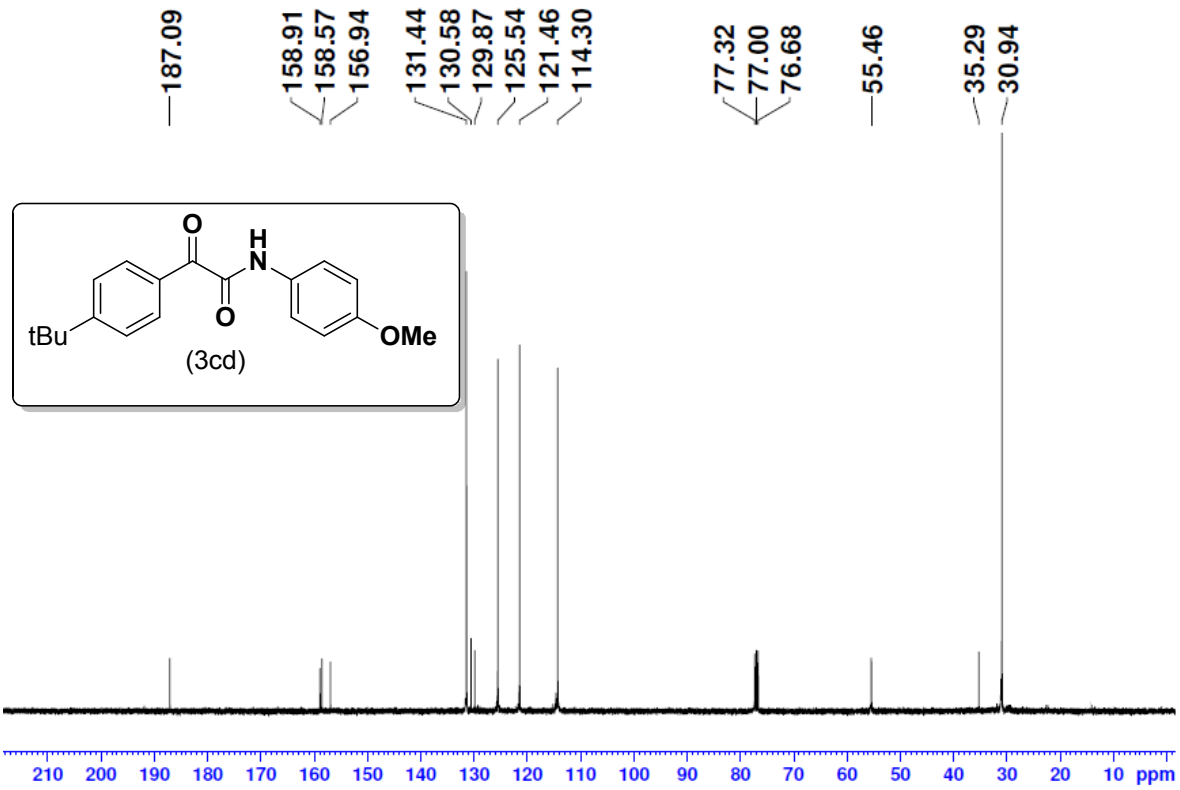

8.93
8.49
8.47
7.61
7.60
7.59
7.58
7.24
6.96
6.94
6.93
6.92
6.91
6.90
6.89
6.89
3.88
3.79
O
H
N
O
MeO
OMe
(3wd)
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
ppm
0.97
2.01
2.06
4.48
3.13
3.00

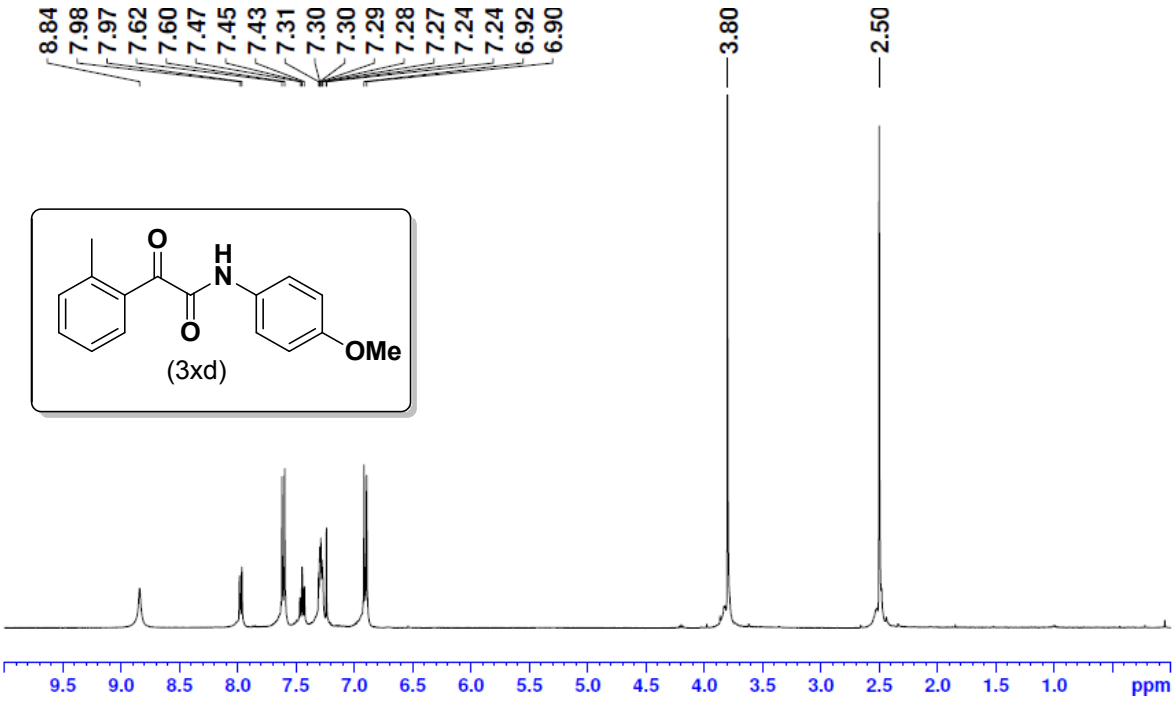

185.38
164.84
159.26
156.95
134.21
129.95
126.23
121.46
114.32
113.88
77.32
77.00
76.68
55.56
55.47
O
H
N
O
MeO
OMe
(3wd)
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

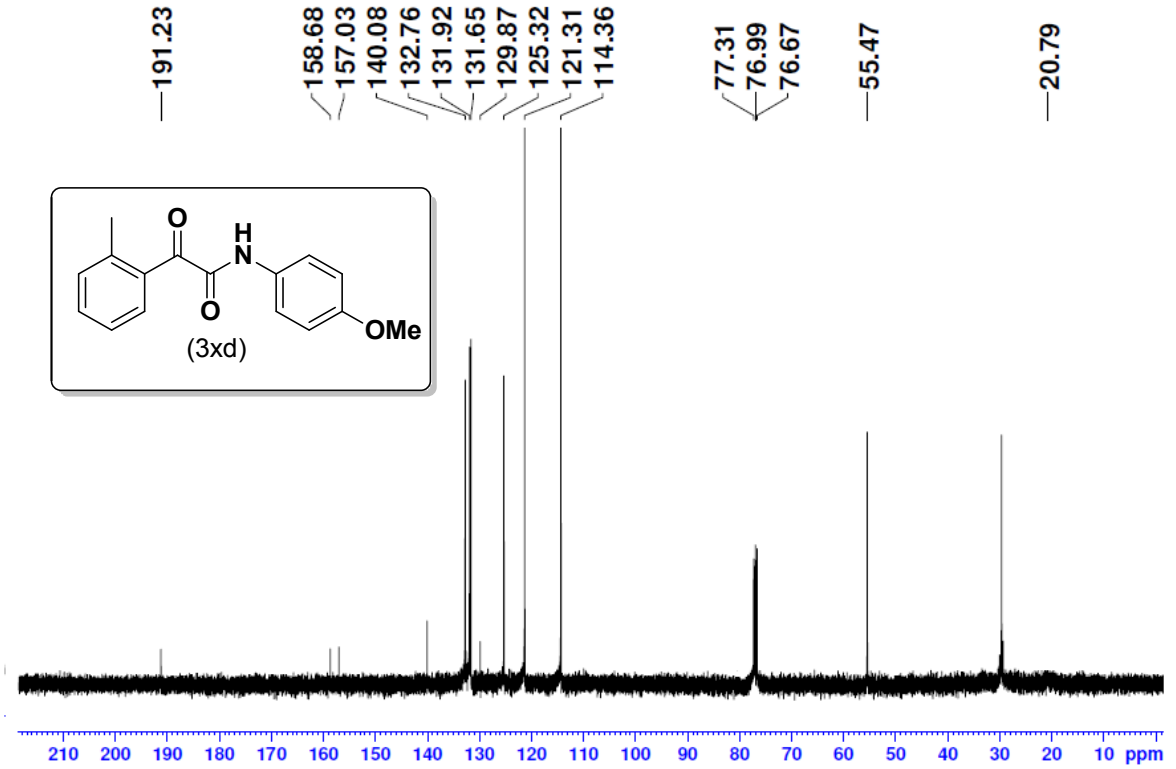

8.89
8.35
8.33
7.61
7.61
7.60
7.59
7.31
7.29
7.24
6.91
6.89
3.80
2.74
2.72
2.70
2.68
1.27
1.25
1.23
O
H
N
O
Et
OMe
(3bd)
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 ppm
1.05
2.12
2.25
2.27
2.24
3.24
2.39
4.30

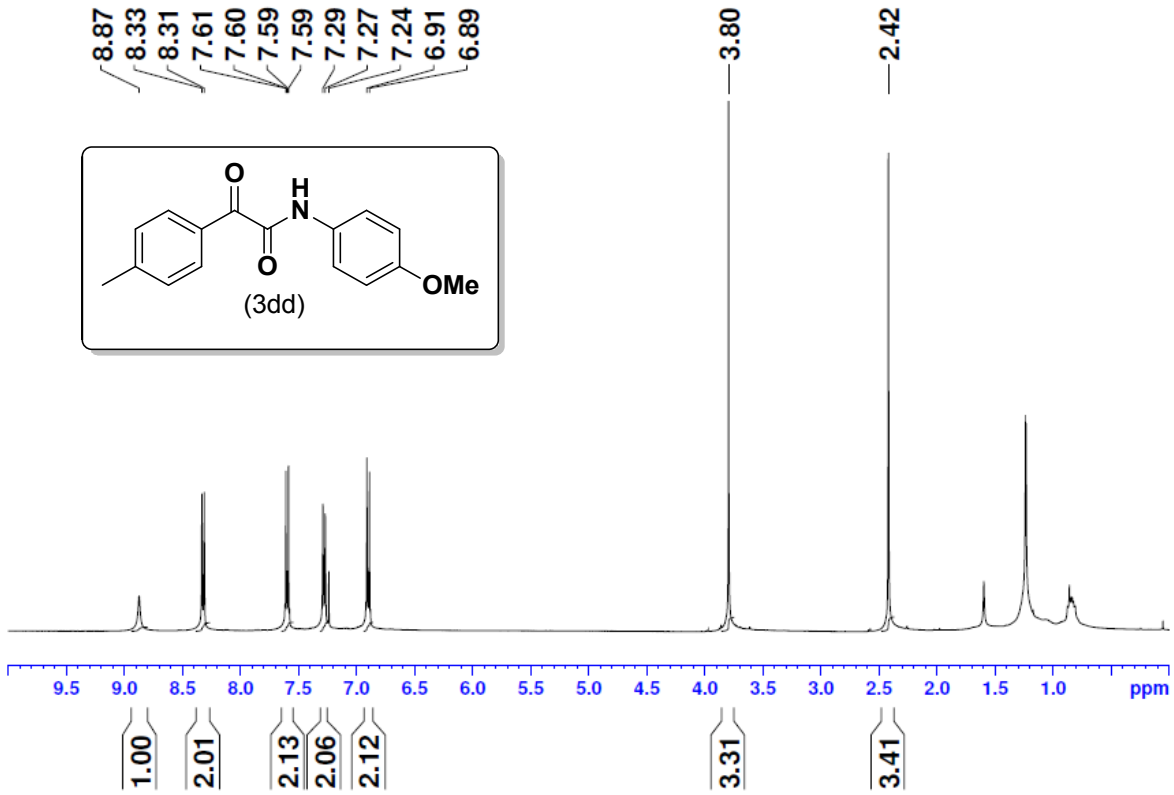

187.06
158.94
156.96
151.91
131.72
130.87
129.87
128.09
121.46
114.31
77.32
77.00
76.68
55.46
29.14
15.02
O
H
N
O
Et
OMe
(3bd)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

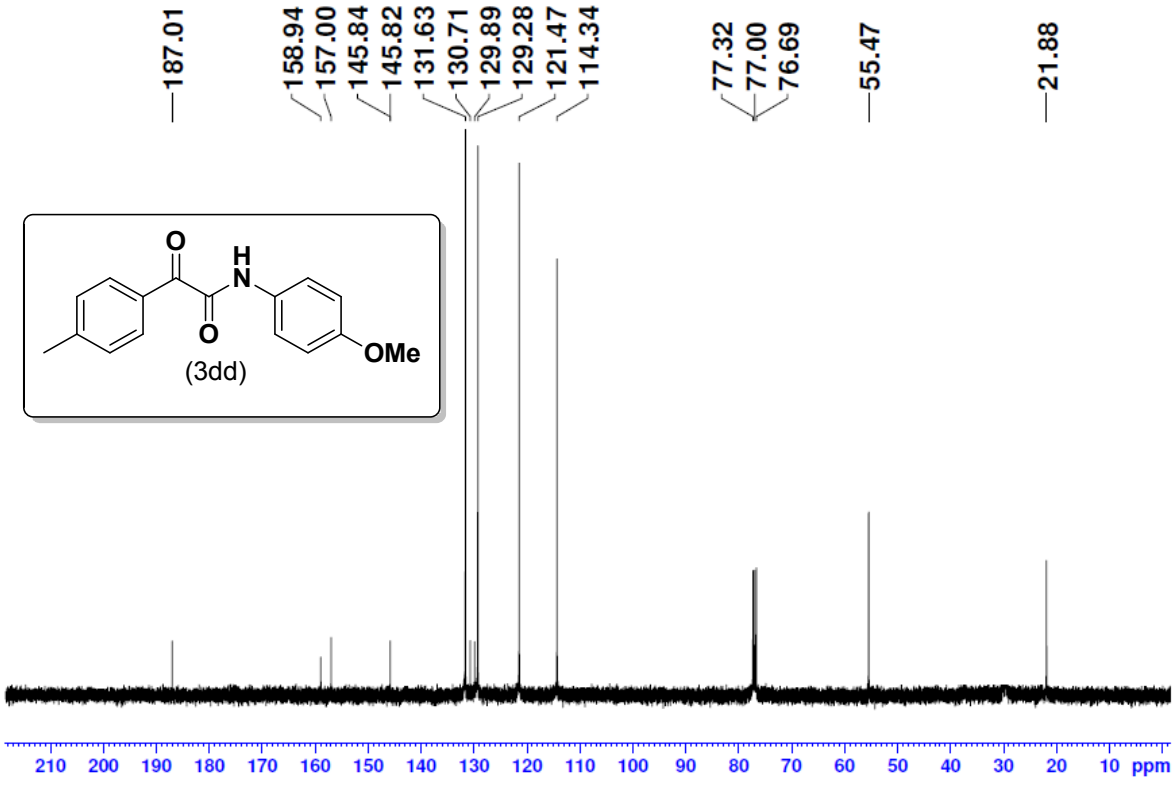

8.87
8.35
8.33
7.62
7.59
7.51
7.49
7.24
6.92
6.89
3.80
1.34
O
H
N
O
tBu
OMe
(3cd)
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 ppm
0.89
1.91
2.02
2.06
2.14
3.00
9.12

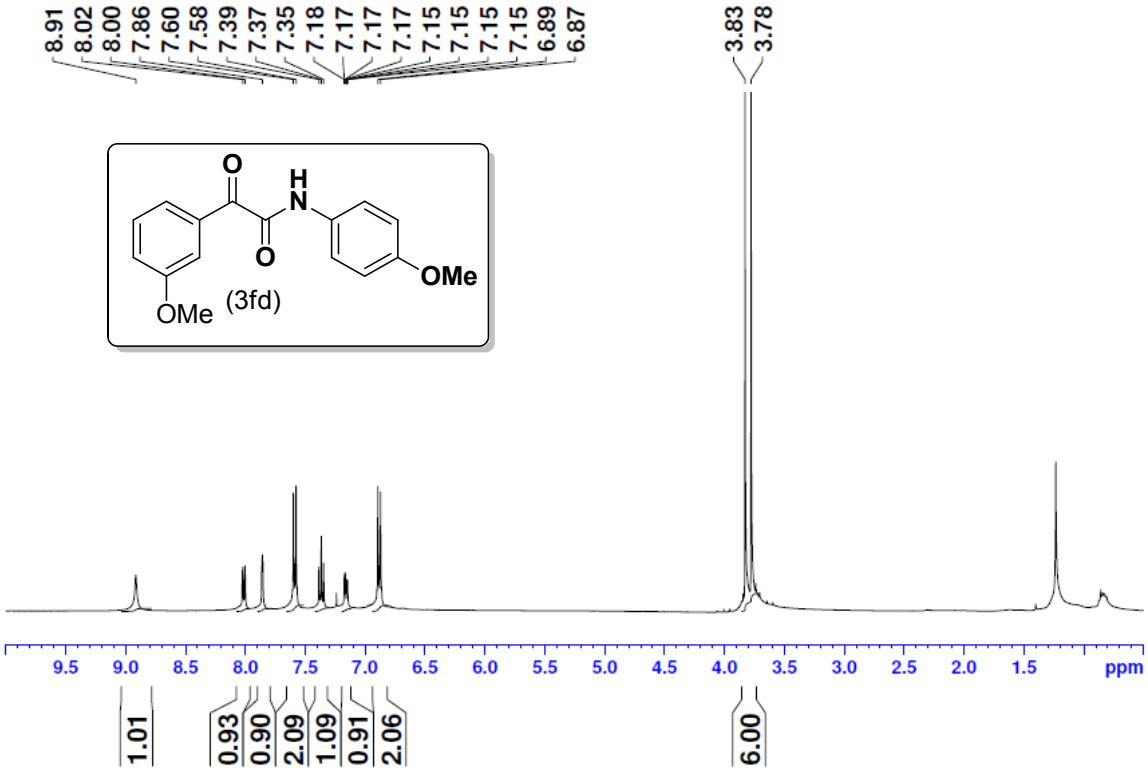

187.09
158.91
158.57
156.94
131.44
130.58
129.87
125.54
121.46
114.30
77.32
77.00
76.68
55.46
35.29
30.94
O
H
N
O
tBu
OMe
(3cd)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

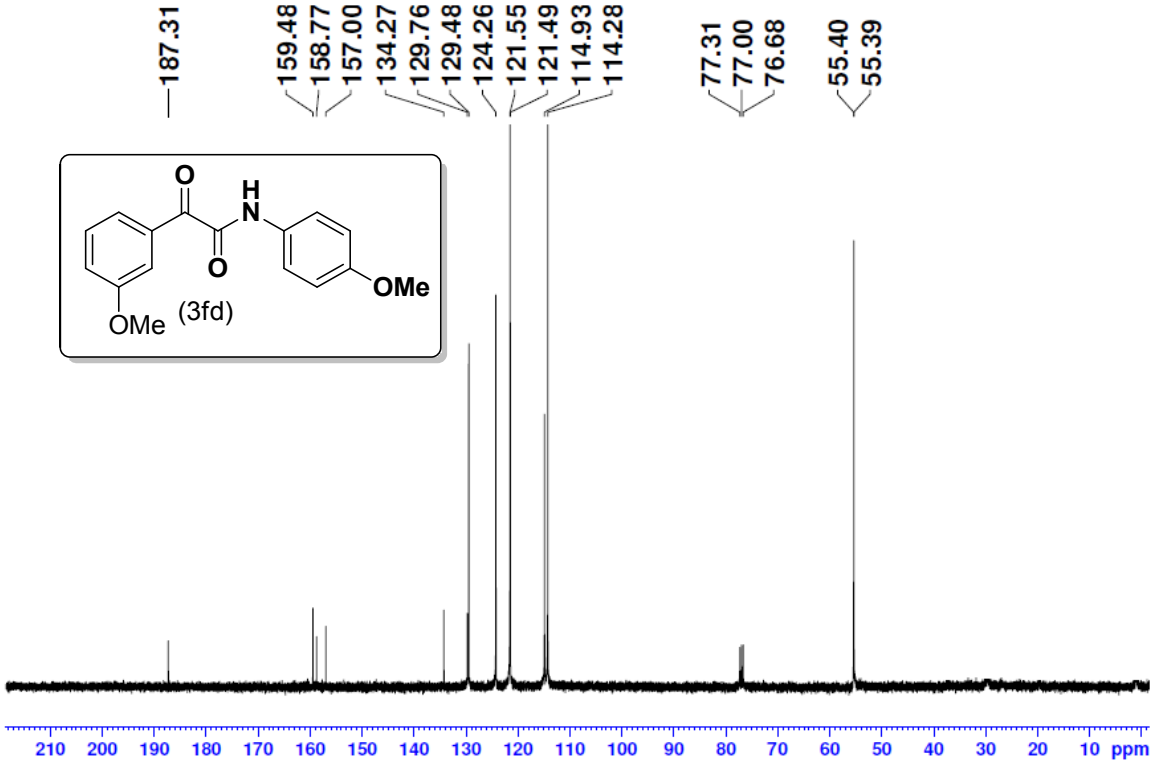

8.84
7.98
7.97
7.62
7.60
7.47
7.45
7.43
7.31
7.30
7.30
7.29
7.28
7.27
7.24
7.24
6.92
6.90
3.80
2.50
O
H
N
O
OMe
(3xd)
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 ppm

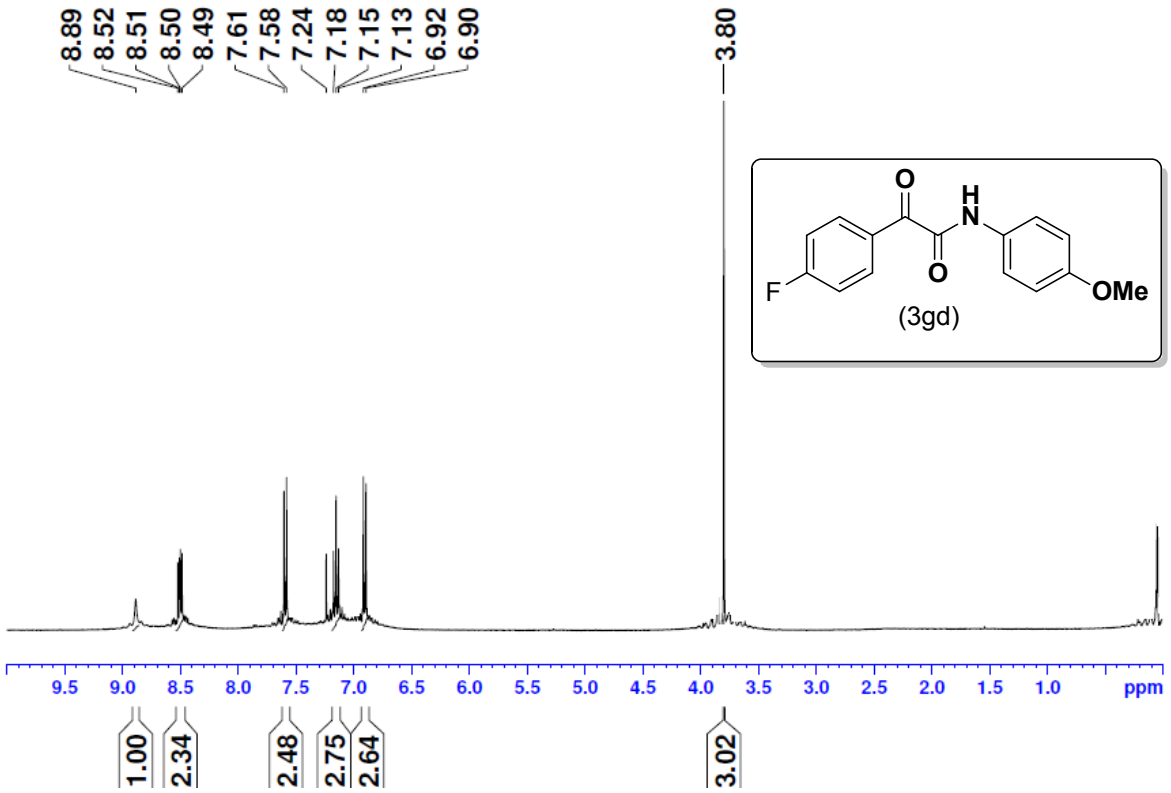

191.23
158.68
157.03
140.08
132.76
131.92
131.65
129.87
125.32
121.31
114.36
77.31
76.99
76.67
55.47
20.79
O
H
N
O
OMe
(3xd)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

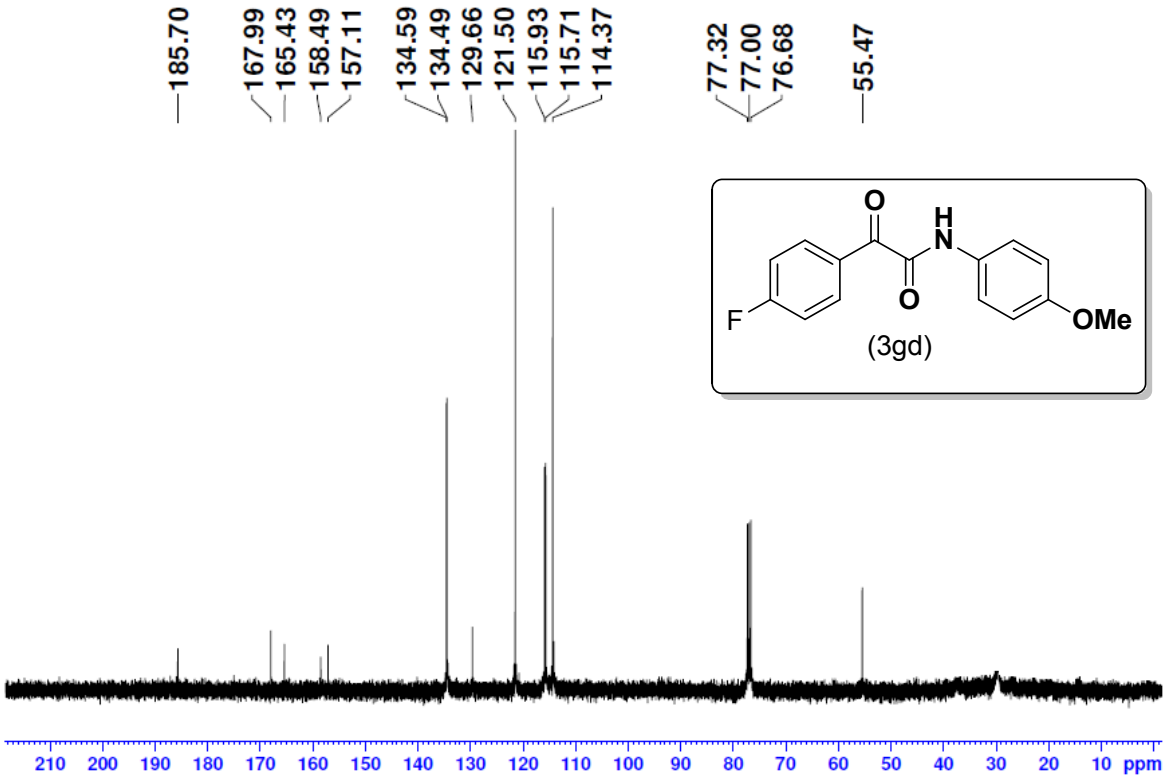

8.87
8.33
8.31
7.61
7.60
7.59
7.59
7.29
7.27
7.24
6.91
6.89
3.80
2.42
O
H
N
O
OMe
(3dd)
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 ppm
1.00
2.01
2.13
2.06
2.12
3.31
3.41


187.01
158.94
157.00
145.84
145.82
131.63
130.71
129.89
129.28
121.47
114.34
77.32
77.00
76.69
55.47
21.88
O
H
N
O
OMe
(3dd)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm


8.91
8.02
8.00
7.86
7.60
7.58
7.39
7.37
7.35
7.18
7.17
7.17
7.17
7.15
7.15
7.15
7.15
6.89
6.87
3.83
3.78
O
H
N
O
OMe
OMe
(3fd)
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
ppm
1.01
0.93
0.90
2.09
1.09
0.91
2.06
6.00


187.31
159.48
158.77
157.00
134.27
129.76
129.48
124.26
121.55
121.49
114.93
114.28
77.31
77.00
76.68
55.40
55.39
O
H
N
O
OMe
OMe
(3fd)
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm


8.89
8.52
8.51
8.50
8.49
7.61
7.58
7.24
7.18
7.15
7.13
6.92
6.90
3.80
O
H
N
O
F
OMe
(3gd)
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
2.34
2.48
2.75
2.64
3.02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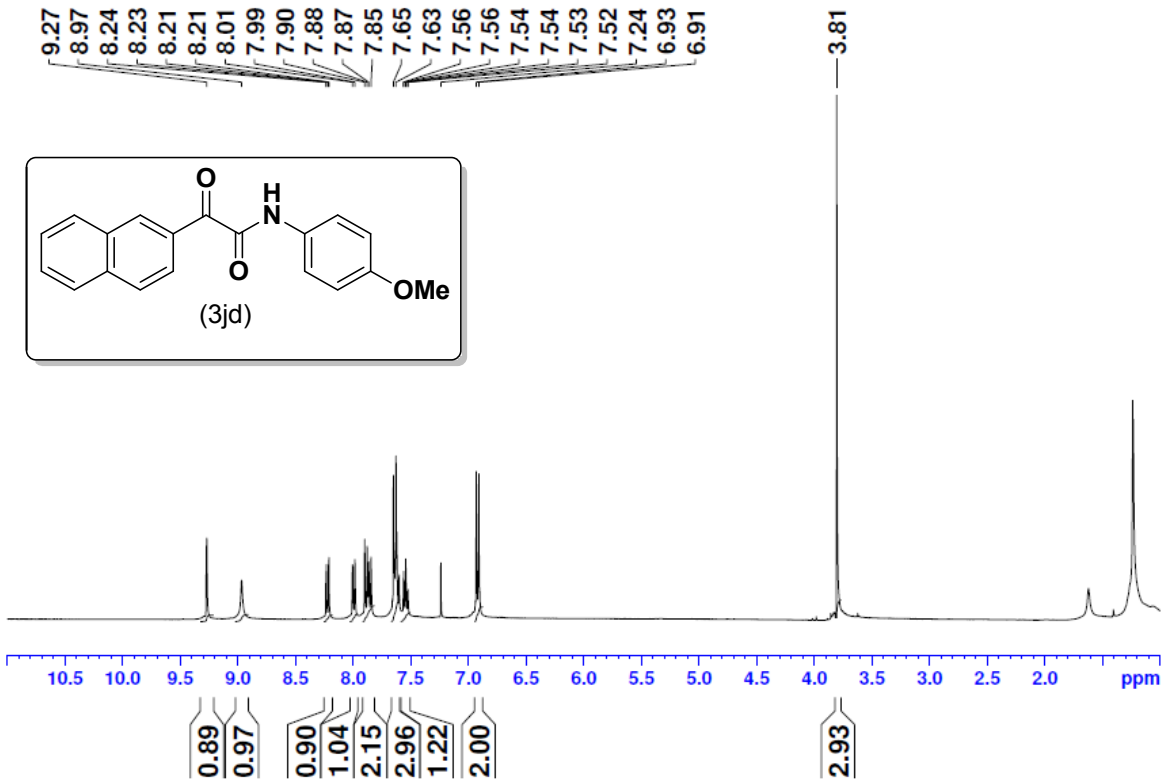
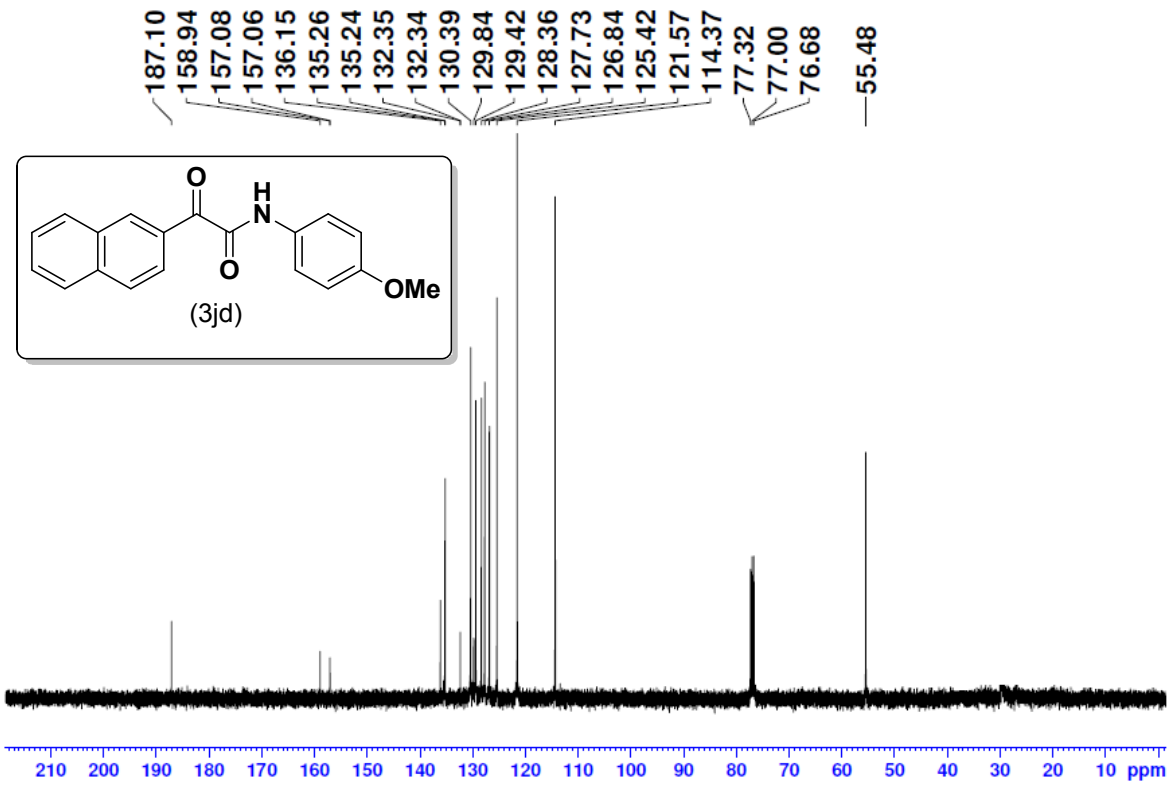
167.99
165.43
158.49
157.11
134.59
134.49
129.66
121.50
115.93
115.71
114.37
77.32
77.00
76.68
55.47
O
H
N
O
F
OMe
(3gd)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm


9.27
8.97
8.24
8.23
8.21
8.21
8.01
7.99
7.90
7.88
7.87
7.85
7.65
7.63
7.56
7.56
7.54
7.54
7.53
7.52
7.24
6.93
6.91
3.81
O
H
N
O
OMe
(3jd)
10.5 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 ppm
0.89
0.97
0.90
1.04
2.15
2.96
1.22
2.00
2.93


187.10
158.94
157.08
157.06
136.15
135.26
135.24
132.35
132.34
130.39
129.84
129.42
128.36
127.73
126.84
125.42
121.57
114.37
77.32
77.00
76.68
55.48
O
H
N
O
OMe
(3jd)
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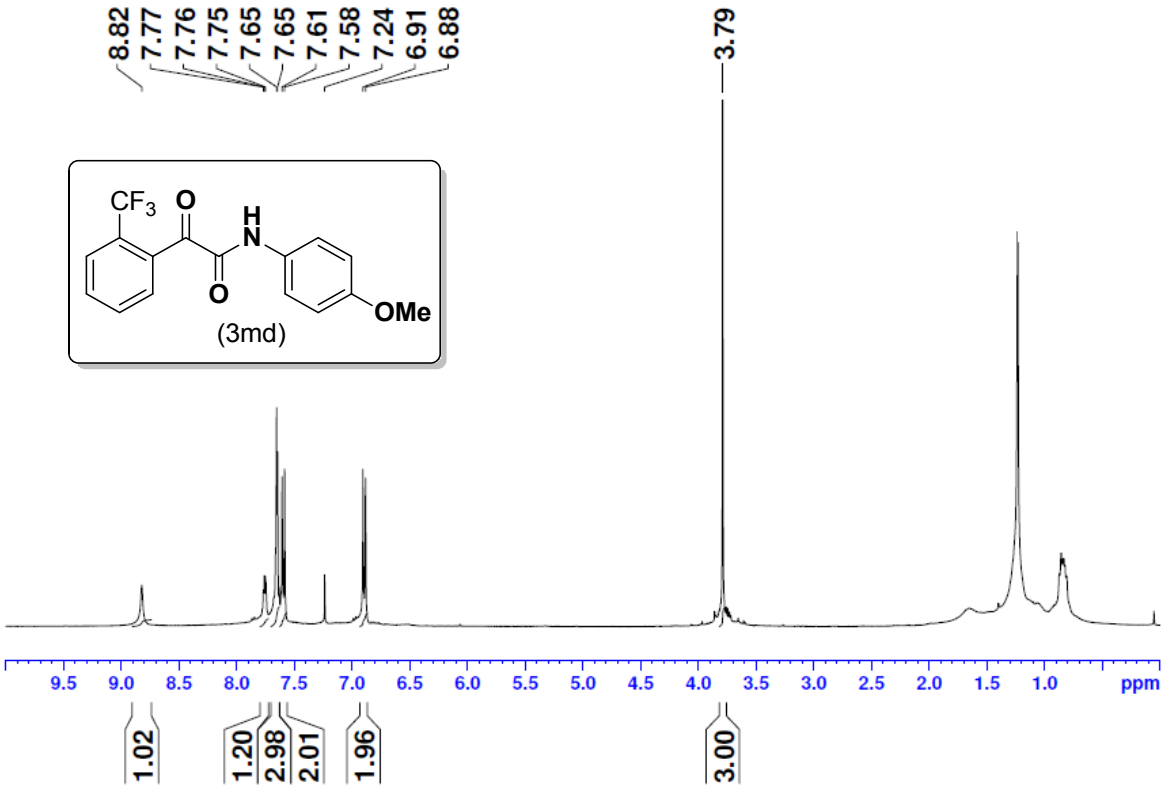
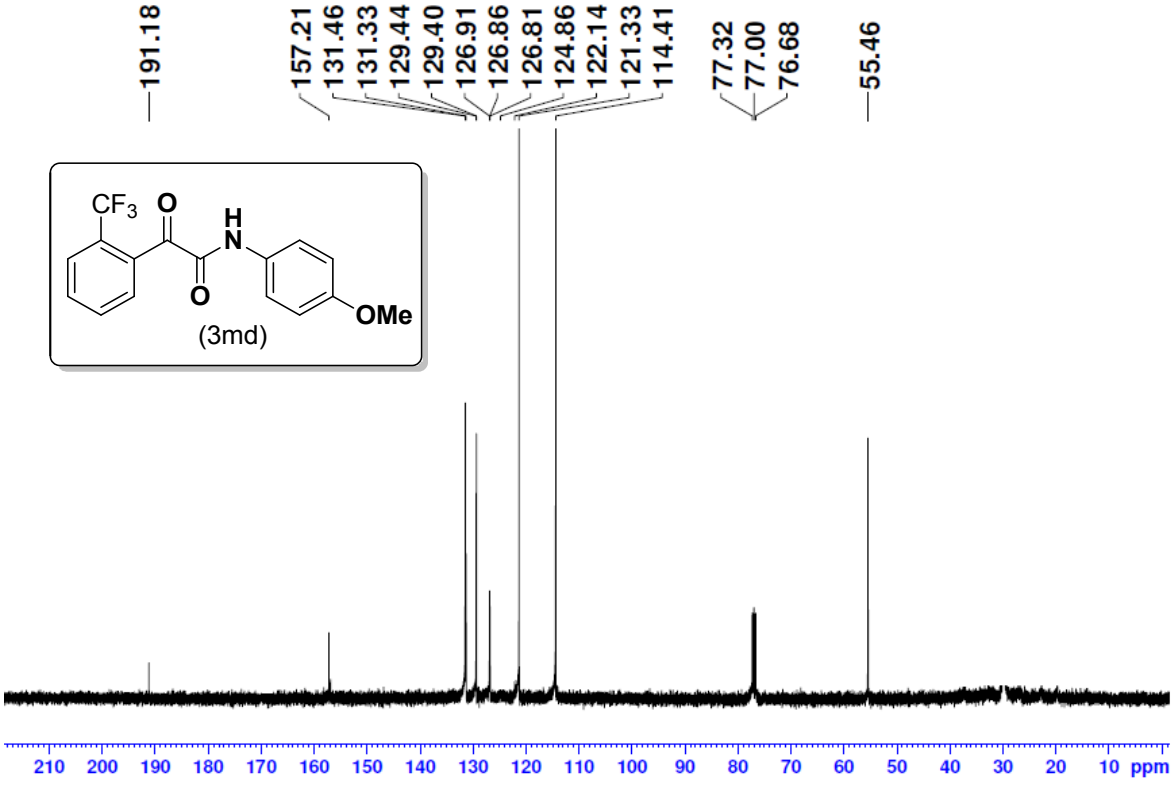
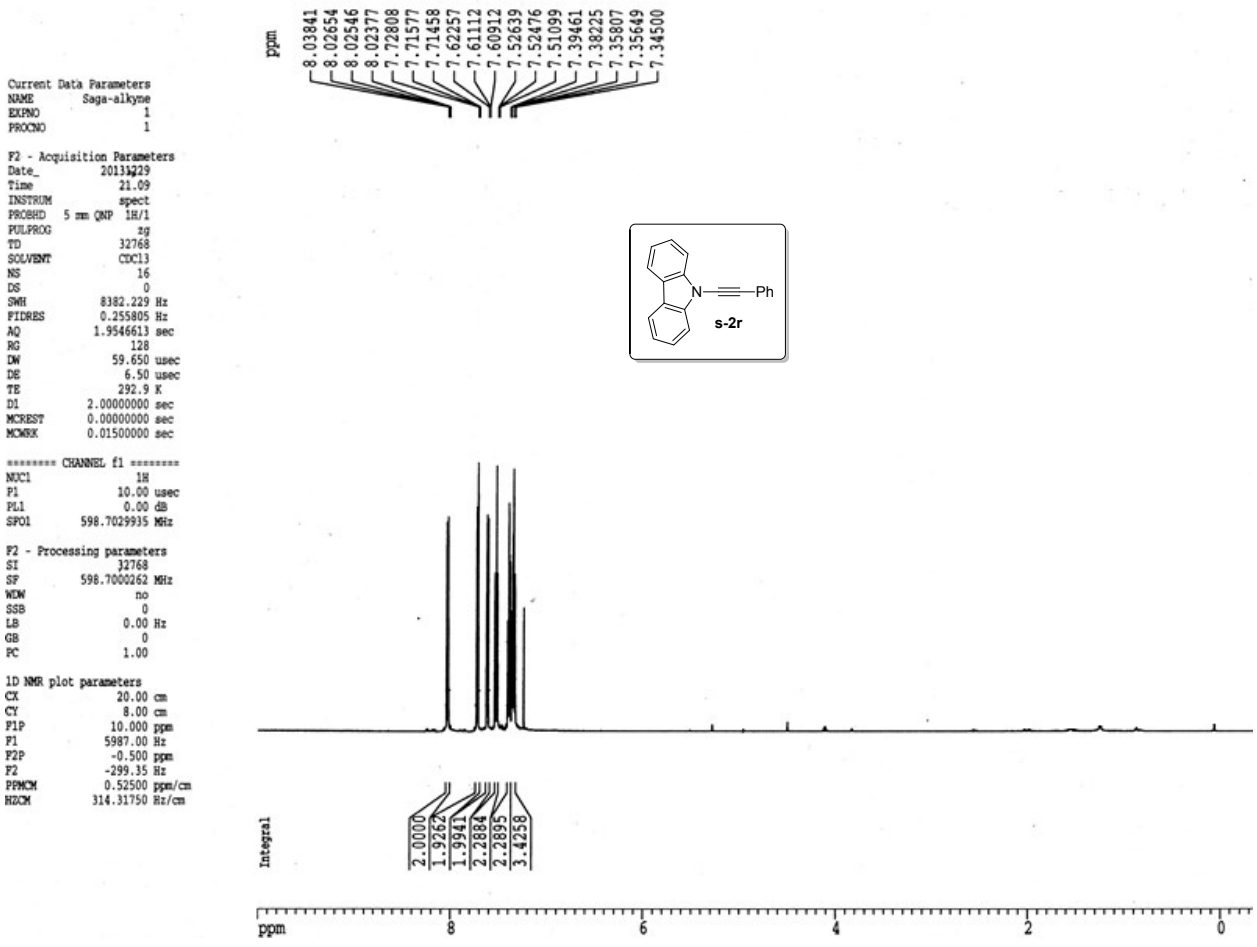

8.82
7.77
7.76
7.75
7.65
7.65
7.61
7.58
7.24
6.91
6.88
3.79
CF3
O
H
N
O
OMe
(3md)
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 ppm
1.02
1.20
2.98
2.01
1.96
3.00


191.18
157.21
131.46
131.33
129.44
129.40
126.91
126.86
126.81
124.86
122.14
121.33
114.41
77.32
77.00
76.68
55.46
CF3
O
H
N
O
OMe
(3md)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm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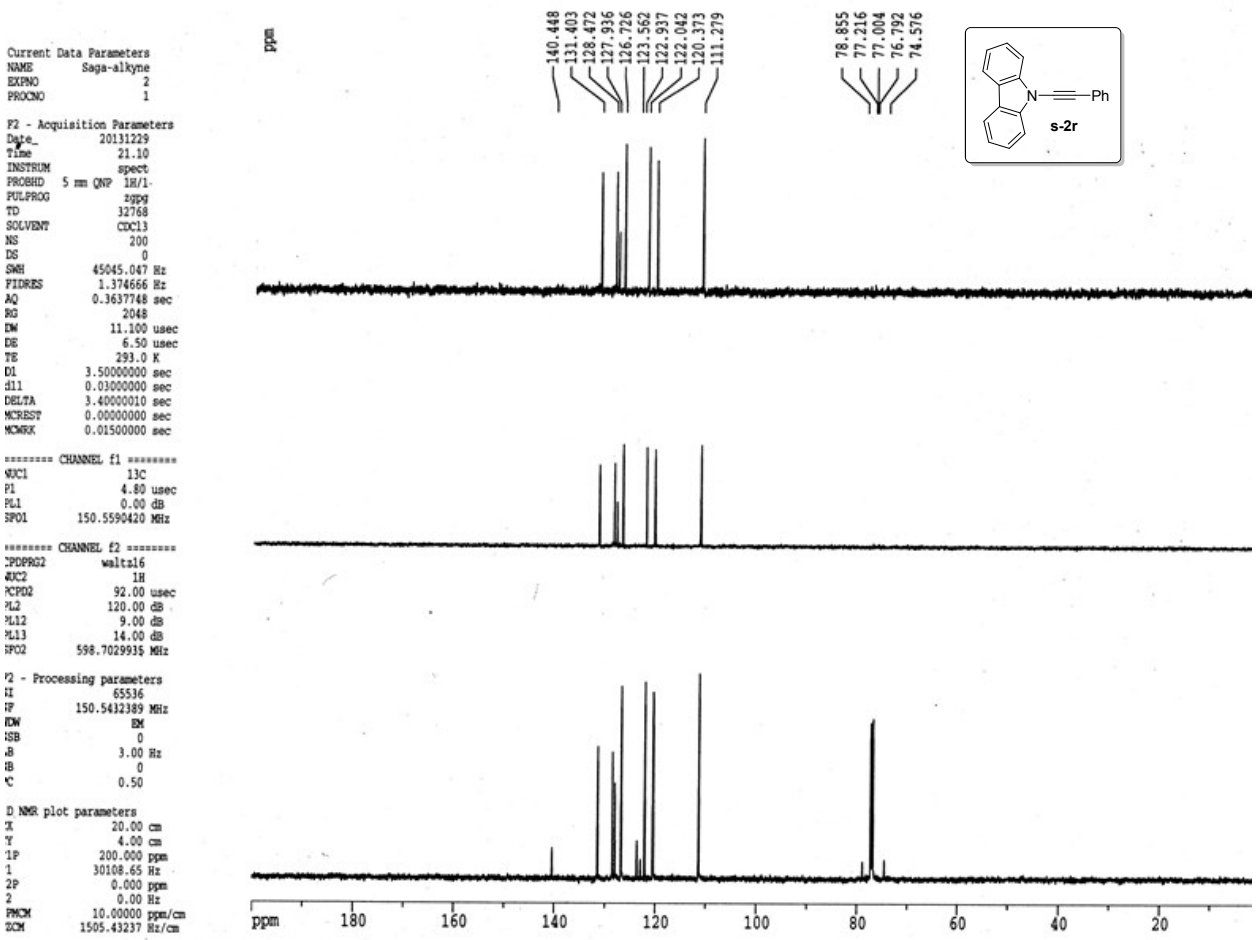
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20131229
Time 21.09
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 8382.229 Hz
FIDRES 0.255805 Hz
AQ 1.9546613 sec
RG 128
DW 59.650 usec
DE 6.50 usec
TE 292.9 K
D1 2.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 10.00 usec
PL1 0.00 dB
SFO1 598.7029935 MHz
F2 - Processing parameters
SI 32768
SF 598.7000262 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 20.00 cm
CY 8.00 cm
F1P 10.000 ppm
F1 5987.00 Hz
F2P -0.500 ppm
F2 -299.35 Hz
PPMCM 0.52500 ppm/cm
HZCM 314.31750 Hz/cm
ppm
8.03841
8.02654
8.02546
8.02377
7.72808
7.71577
7.71458
7.62257
7.61112
7.60912
7.52639
7.52476
7.51099
7.39461
7.38225
7.35807
7.35649
7.34500
N
Ph
s-2r
Integral
2.0000
1.9262
1.9941
2.2884
2.2895
3.4258
ppm
8
6
4
2
0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PROCNO 1
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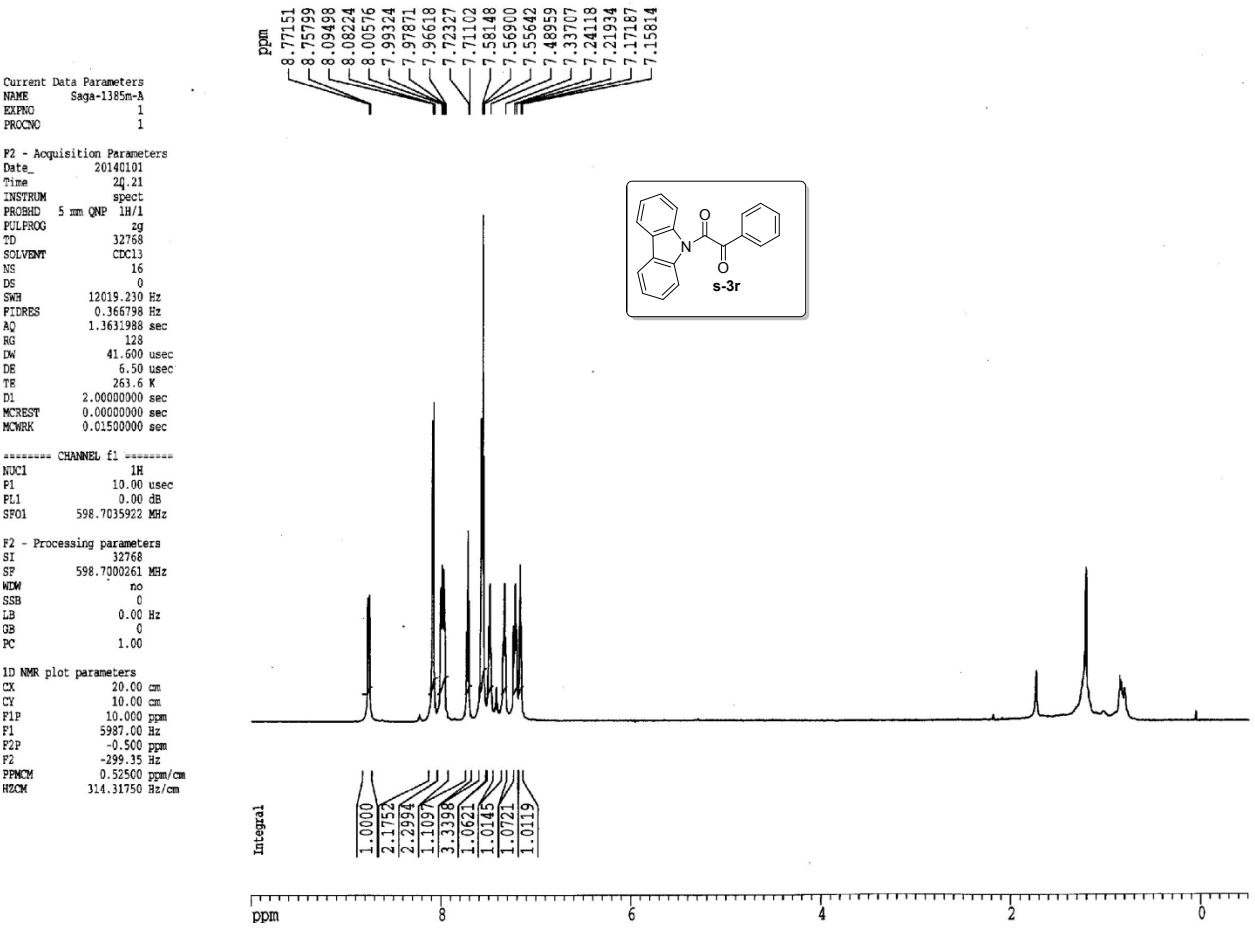
PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 200
DS 0
SWH 45045.047 Hz
FIDRES 1.374666 Hz
AQ 0.3637748 sec
RG 2048
DW 11.100 usec
DE 6.50 usec
TE 293.0 K
D1 3.50000000 sec
d11 0.03000000 sec
DELTA 3.40000010 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 4.80 usec
PL1 0.00 dB
SFO1 150.5590420 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 92.00 usec
PL2 120.00 dB
PL12 9.00 dB
PL13 14.00 dB
SFO2 598.7029935 MHz
F2 - Processing parameters
SI 65536
SF 150.5432389 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 0.50
1D NMR plot parameters
WX 20.00 cm
WY 4.00 cm
F1P 200.000 ppm
F1 30108.65 Hz
F2P 0.000 ppm
F2 0.00 Hz
PPMCM 10.00000 ppm/cm
HZCM 1505.43237 Hz/cm
ppm
140.448
131.403
128.472
127.936
126.726
123.562
122.937
122.042
120.373
111.279
78.855
77.216
77.004
76.792
74.576
N
Ph
s-2r
ppm
180
160
140
120
100
80
60
40
20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PROCNO 1
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Time 2q.21
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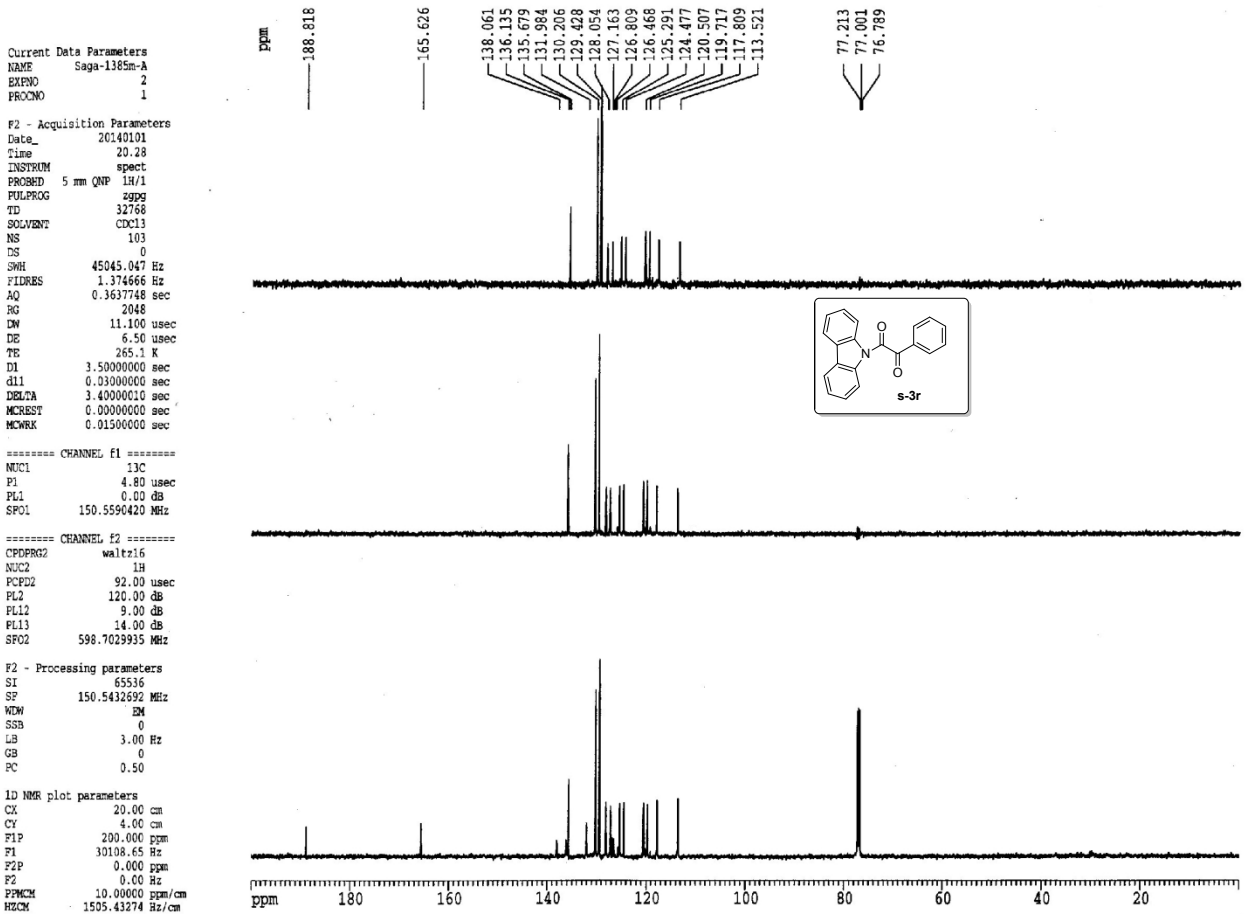
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 12019.230 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 128
DW 41.600 usec
DE 6.50 usec
TE 263.6 K
D1 2.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 10.00 usec
PL1 0.00 dB
SFO1 598.7035922 MHz
F2 - Processing parameters
SI 32768
SF 598.7000261 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 20.00 cm
CY 10.00 cm
F1P 10.000 ppm
F1 5987.00 Hz
F2P -0.500 ppm
F2 -299.35 Hz
PPMCM 0.52500 ppm/cm
HZCM 314.31750 Hz/cm
ppm
8.77151
8.75799
8.09498
8.08224
8.00576
7.99324
7.97871
7.96618
7.72327
7.71102
7.58148
7.56900
7.55642
7.48959
7.33707
7.24118
7.21934
7.17187
7.15814
s-3r
Integral
1.0000
2.1752
2.2994
1.1097
3.3398
1.0621
1.0145
1.0721
1.0119
ppm
8
6
4
2
0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PROCNO 1
F2 - Acquisition Parameters
Date_ 20140101
Time 20.28
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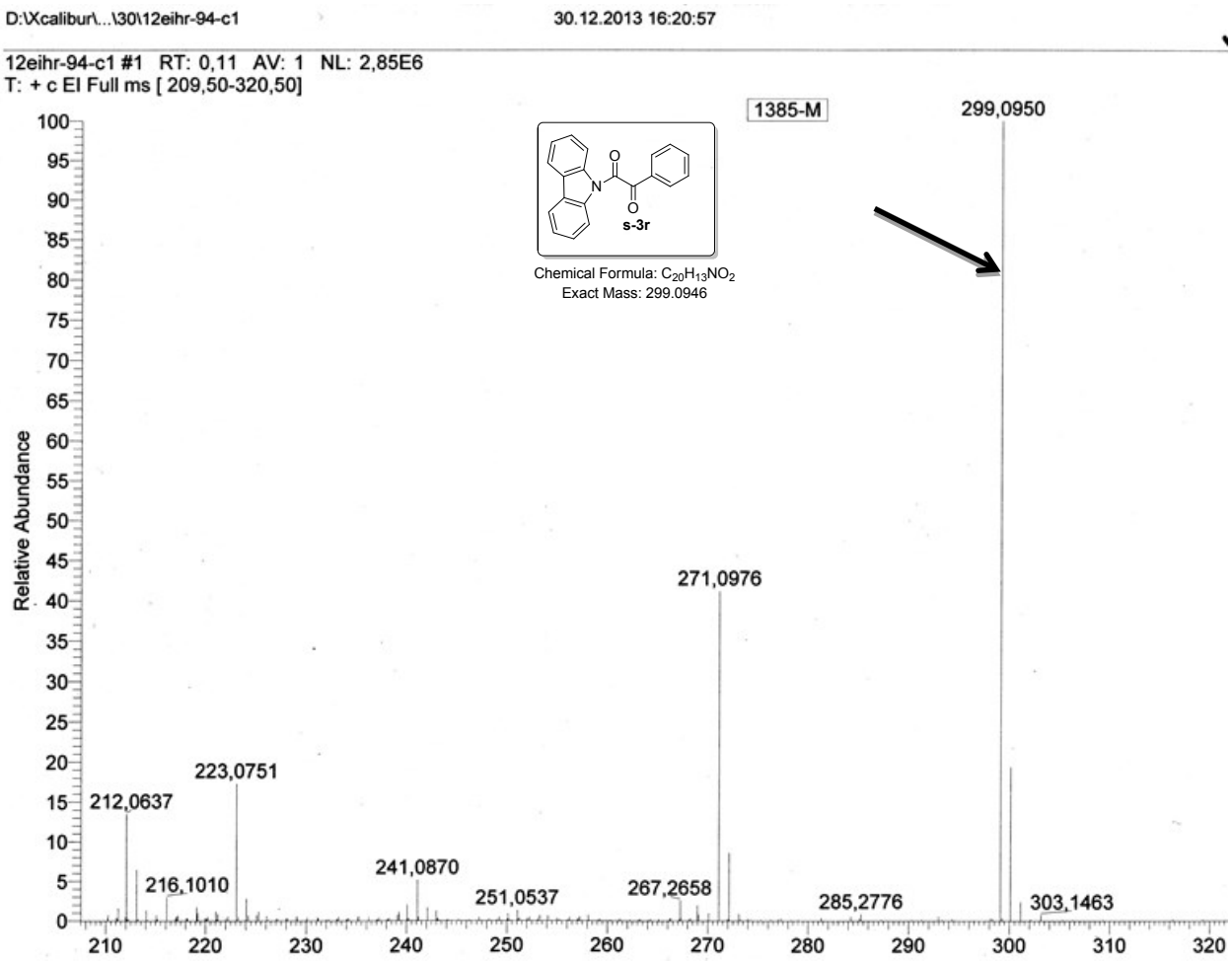
PROBHD 5 mm QNP 1H/1
PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 103
DS 0
SWH 45045.047 Hz
FIDRES 1.374666 Hz
AQ 0.3637748 sec
RG 2048
DW 11.100 usec
DE 6.50 usec
TE 265.1 K
D1 3.50000000 sec
d11 0.03000000 sec
DELTA 3.40000010 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 4.80 usec
PL1 0.00 dB
SFO1 150.5590420 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 92.00 usec
PL2 120.00 dB
PL12 9.00 dB
PL13 14.00 dB
SFO2 598.7029935 MHz
F2 - Processing parameters
SI 65536
SF 150.5432692 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 0.50
1D NMR plot parameters
CX 20.00 cm
CY 4.00 cm
F1P 200.000 ppm
F1 30108.65 Hz
F2P 0.000 ppm
F2 0.00 Hz
PPMCM 10.00000 ppm/cm
HZCM 1505.43274 Hz/cm
ppm
188.818
165.626
138.061
136.135
135.679
131.984
130.206
129.428
128.054
127.163
126.809
126.468
125.291
124.477
120.507
119.717
117.809
113.521
77.213
77.001
76.789
s-3r
ppm
180
160
140
120
100
80
60
40
20


D:\Xcalibur\...\30\12eihr-94-c1
30.12.2013 16:20:57
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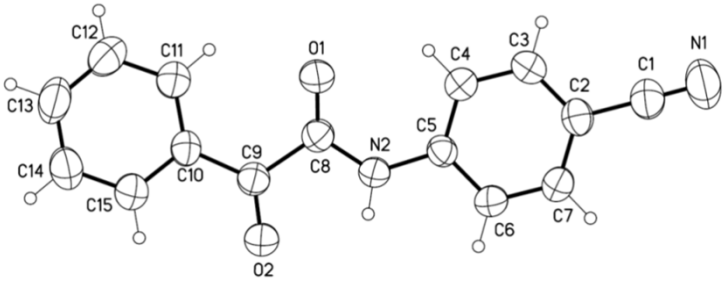
T: + c EI Full ms [209,50-320,50]
1385-M
299,0950
s-3r
Chemical Formula: C20H13NO2
Exact Mass: 299.0946
271,0976
223,0751
212,0637
216,1010
241,0870
251,0537
267,2658
285,2776
303,1463
Relative Abundance

Figure S17. ORTEP diagram of compound 3am**.**



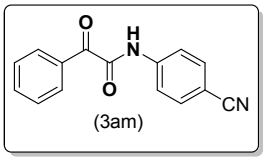


Table S4. Crystal data and structure refinement for 130832.

Identification code	130832	
Empirical formula	C15 H10 N2 O2	
Formula weight	250.25	
Temperature	296(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P -1	
Unit cell dimensions	a = 6.3094(4) Å	□= 80.486(3)°.
	b = 7.4430(5) Å	□= 79.734(3)°.
	c = 13.8773(8) Å	□ = 72.162(2)°.
Volume	606.15(7) $Å^3$	
Z	2	
Density (calculated)	1.371 Mg/m^3	
Absorption coefficient	0.093 mm^{-1}	
F(000)	260	
Crystal size	0.12 x 0.07 x 0.02 mm^3	
Theta range for data collection	1.50 to 26.42°.	
Index ranges	-7<=h<=7, -9<=k<=9, -17<=l<=14	
Reflections collected	9021	
Independent reflections	2464 [R(int) = 0.0563]	
Completeness to theta = 26.42°	99.0 %	

Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9486 and 0.8382
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	2464 / 0 / 172
Goodness-of-fit on F^2	0.996
Final R indices [I>2sigma(I)]	R1 = 0.0537, wR2 = 0.1395
R indices (all data)	R1 = 0.1396, wR2 = 0.1932
Largest diff. peak and hole	0.298 and -0.281 e.$Å^{-3}$

Table S5. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for 130832. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	1240(6)	2910(5)	1739(2)	58(1)
C(2)	2477(5)	2738(4)	2538(2)	47(1)
C(3)	1360(5)	3322(4)	3432(2)	52(1)
C(4)	2529(5)	3110(4)	4216(2)	49(1)
C(5)	4820(5)	2311(4)	4106(2)	40(1)
C(6)	5946(5)	1756(4)	3201(2)	54(1)
C(7)	4787(5)	1966(4)	2429(2)	54(1)
C(8)	5512(5)	2639(4)	5767(2)	46(1)
C(9)	7478(5)	1962(4)	6389(2)	44(1)
C(10)	7149(5)	2325(4)	7426(2)	44(1)
C(11)	5071(5)	2850(5)	7994(2)	63(1)
C(12)	4948(6)	3059(6)	8985(2)	82(1)
C(13)	6857(7)	2769(5)	9393(2)	76(1)
C(14)	8922(6)	2260(5)	8835(2)	68(1)
C(15)	9056(5)	2050(4)	7860(2)	57(1)
N(1)	236(5)	2999(5)	1113(2)	86(1)
N(2)	6122(4)	1981(3)	4878(2)	47(1)
O(1)	3682(4)	3654(3)	6047(2)	70(1)
O(2)	9311(3)	1134(3)	5981(2)	61(1)

Table S6. Bond lengths [Å] and angles [°] for 130832.

C(1)-N(1)	1.146(4)
C(1)-C(2)	1.435(5)
C(2)-C(3)	1.380(4)
C(2)-C(7)	1.383(4)
C(3)-C(4)	1.382(4)
C(3)-H(3)	0.9300
C(4)-C(5)	1.375(4)
C(4)-H(4)	0.9300
C(5)-C(6)	1.388(4)
C(5)-N(2)	1.409(3)
C(6)-C(7)	1.364(4)
C(6)-H(6)	0.9300
C(7)-H(7)	0.9300
C(8)-O(1)	1.208(3)
C(8)-N(2)	1.351(3)
C(8)-C(9)	1.547(4)
C(9)-O(2)	1.218(3)
C(9)-C(10)	1.474(4)
C(10)-C(11)	1.383(4)
C(10)-C(15)	1.385(4)
C(11)-C(12)	1.395(4)
C(11)-H(11)	0.9300
C(12)-C(13)	1.364(5)
C(12)-H(12)	0.9300
C(13)-C(14)	1.369(5)
C(13)-H(13)	0.9300
C(14)-C(15)	1.373(4)
C(14)-H(14)	0.9300
C(15)-H(15)	0.9300
N(2)-H(2)	0.8600
N(1)-C(1)-C(2)	177.9(4)
C(3)-C(2)-C(7)	119.3(3)
C(3)-C(2)-C(1)	120.0(3)

C(7)-C(2)-C(1)	120.7(3)
C(2)-C(3)-C(4)	120.4(3)
C(2)-C(3)-H(3)	119.8
C(4)-C(3)-H(3)	119.8
C(5)-C(4)-C(3)	119.9(3)
C(5)-C(4)-H(4)	120.0
C(3)-C(4)-H(4)	120.0
C(4)-C(5)-C(6)	119.6(3)
C(4)-C(5)-N(2)	123.4(2)
C(6)-C(5)-N(2)	117.0(3)
C(7)-C(6)-C(5)	120.4(3)
C(7)-C(6)-H(6)	119.8
C(5)-C(6)-H(6)	119.8
C(6)-C(7)-C(2)	120.4(3)
C(6)-C(7)-H(7)	119.8
C(2)-C(7)-H(7)	119.8
O(1)-C(8)-N(2)	125.1(3)
O(1)-C(8)-C(9)	123.4(3)
N(2)-C(8)-C(9)	111.5(3)
O(2)-C(9)-C(10)	121.6(3)
O(2)-C(9)-C(8)	117.0(3)
C(10)-C(9)-C(8)	121.4(3)
C(11)-C(10)-C(15)	118.5(3)
C(11)-C(10)-C(9)	124.1(3)
C(15)-C(10)-C(9)	117.3(3)
C(10)-C(11)-C(12)	119.6(3)
C(10)-C(11)-H(11)	120.2
C(12)-C(11)-H(11)	120.2
C(13)-C(12)-C(11)	120.5(3)
C(13)-C(12)-H(12)	119.8
C(11)-C(12)-H(12)	119.8
C(12)-C(13)-C(14)	120.4(3)
C(12)-C(13)-H(13)	119.8
C(14)-C(13)-H(13)	119.8
C(13)-C(14)-C(15)	119.4(3)
C(13)-C(14)-H(14)	120.3

C(15)-C(14)-H(14)	120.3
C(14)-C(15)-C(10)	121.5(3)
C(14)-C(15)-H(15)	119.2
C(10)-C(15)-H(15)	119.2
C(8)-N(2)-C(5)	128.3(3)
C(8)-N(2)-H(2)	115.8
C(5)-N(2)-H(2)	115.8

Symmetry transformations used to generate equivalent atoms:

Table S7. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for 130832. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2} U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	64(2)	60(2)	53(2)	-6(2)	-15(2)	-16(2)
C(2)	54(2)	43(2)	46(2)	-1(1)	-15(2)	-14(2)
C(3)	41(2)	59(2)	55(2)	-8(2)	-11(2)	-8(2)
C(4)	45(2)	56(2)	44(2)	-10(1)	-5(1)	-10(2)
C(5)	40(2)	38(2)	41(2)	-4(1)	-10(1)	-7(1)
C(6)	43(2)	65(2)	45(2)	-13(2)	-6(1)	0(2)
C(7)	53(2)	65(2)	41(2)	-12(2)	-7(2)	-7(2)
C(8)	46(2)	46(2)	43(2)	-7(1)	-7(1)	-9(2)
C(9)	46(2)	40(2)	44(2)	-5(1)	-8(1)	-8(1)
C(10)	51(2)	44(2)	41(2)	-7(1)	-11(1)	-13(1)
C(11)	54(2)	89(3)	50(2)	-18(2)	-6(2)	-22(2)
C(12)	70(3)	126(4)	54(2)	-27(2)	7(2)	-33(2)
C(13)	90(3)	101(3)	46(2)	-18(2)	-11(2)	-36(3)
C(14)	69(2)	81(3)	61(2)	-16(2)	-24(2)	-16(2)
C(15)	54(2)	65(2)	52(2)	-16(2)	-10(2)	-11(2)
N(1)	91(2)	102(3)	73(2)	-12(2)	-36(2)	-24(2)
N(2)	39(1)	52(2)	42(1)	-10(1)	-8(1)	0(1)
O(1)	48(1)	89(2)	62(1)	-34(1)	-13(1)	11(1)
O(2)	47(1)	75(2)	53(1)	-18(1)	-10(1)	2(1)

Table S8. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for 130832.

	x	y	z	U(eq)
H(3)	-190	3862	3508	63
H(4)	1768	3508	4817	59
H(6)	7499	1237	3121	65
H(7)	5554	1589	1825	65
H(11)	3765	3063	7718	75
H(12)	3553	3399	9370	98
H(13)	6755	2917	10053	91
H(14)	10222	2058	9115	82
H(15)	10460	1715	7482	68
H(2)	7480	1268	4769	56

Figure S18. ORTEP diagram of compound 3sp.

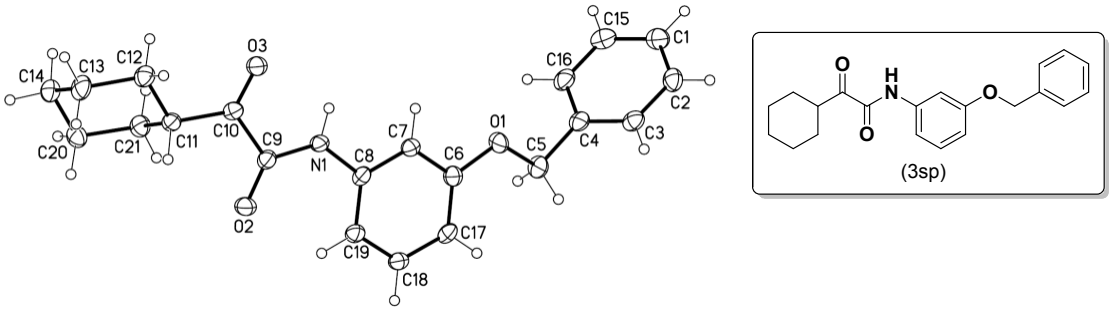


Table S9. Crystal data and structure refinement for 130958lt_0m.

Identification code	130958lt_0m	
Empirical formula	C21 H23 N O3	
Formula weight	337.40	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 1 21/c 1	
Unit cell dimensions	a = 16.806(3) Å	a= 90°.
	b = 5.5338(9) Å	b= 95.944(6)°.
	c = 18.763(3) Å	g = 90°.
Volume	1735.7(5) $Å^3$	
Z	4	
Density (calculated)	1.291 Mg/m^3	
Absorption coefficient	0.086 mm^{-1}	
F(000)	720	
Crystal size	0.30 x 0.05 x 0.03 mm^3	
Theta range for data collection	1.22 to 26.41°.	
Index ranges	-20<=h<=21, -6<=k<=4, -23<=l<=23	
Reflections collected	13422	
Independent reflections	3544 [R(int) = 0.0705]	
Completeness to theta = 26.41°	99.8 %	
Absorption correction	Semi-empirical from equivalents	

Max. and min. transmission	0.9486 and 0.7137
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3544 / 0 / 226
Goodness-of-fit on F^2	0.983
Final R indices [I>2sigma(I)]	R1 = 0.0587, wR2 = 0.1466
R indices (all data)	R1 = 0.1038, wR2 = 0.2059
Largest diff. peak and hole	0.372 and -0.420 e.Å^{-3}

Table S10. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^{2}x 10^3)
for 130958lt_0m. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
O(1)	-1975(1)	9807(3)	2868(1)	27(1)
O(2)	1657(1)	10360(3)	4524(1)	31(1)
O(3)	950(1)	5176(3)	5299(1)	25(1)
N(1)	418(1)	8561(4)	4361(1)	21(1)
C(1)	-4482(2)	6671(5)	1583(1)	29(1)
C(2)	-4551(2)	8797(5)	1959(1)	27(1)
C(3)	-3872(2)	10144(5)	2176(1)	25(1)
C(4)	-3122(2)	9392(5)	2024(1)	24(1)
C(5)	-2398(2)	10908(5)	2245(1)	29(1)
C(6)	-1236(2)	10770(5)	3093(1)	22(1)
C(7)	-784(2)	9381(5)	3604(1)	20(1)
C(8)	-18(2)	10119(4)	3858(1)	20(1)
C(9)	1186(2)	8761(5)	4647(1)	22(1)
C(10)	1445(2)	6652(5)	5158(1)	20(1)
C(11)	2321(1)	6516(5)	5423(1)	22(1)
C(12)	2496(2)	4667(5)	6019(1)	26(1)
C(13)	3395(2)	4498(5)	6248(1)	30(1)
C(14)	3855(2)	3843(5)	5618(2)	30(1)
C(15)	-3732(2)	5893(5)	1429(2)	30(1)
C(16)	-3056(2)	7244(5)	1651(1)	28(1)
C(17)	-939(2)	12922(5)	2855(1)	22(1)
C(18)	-176(2)	13637(5)	3121(1)	22(1)

C(19)	294(2)	12267(4)	3618(1)	23(1)
C(20)	3687(2)	5673(5)	5011(1)	26(1)
C(21)	2793(2)	5889(5)	4781(1)	25(1)

Table S11. Bond lengths [Å] and angles [°] for 130958lt_0m.

O(1)-C(6)	1.377(3)
O(1)-C(5)	1.439(3)
O(2)-C(9)	1.224(3)
O(3)-C(10)	1.214(3)
N(1)-C(9)	1.351(3)
N(1)-C(8)	1.424(3)
N(1)-H(1)	0.8800
C(1)-C(2)	1.383(4)
C(1)-C(15)	1.390(4)
C(1)-H(1A)	0.9500
C(2)-C(3)	1.389(4)
C(2)-H(2)	0.9500
C(3)-C(4)	1.384(4)
C(3)-H(3)	0.9500
C(4)-C(16)	1.391(4)
C(4)-C(5)	1.500(4)
C(5)-H(5A)	0.9900
C(5)-H(5B)	0.9900
C(6)-C(17)	1.383(4)
C(6)-C(7)	1.391(3)
C(7)-C(8)	1.386(3)
C(7)-H(7)	0.9500
C(8)-C(19)	1.393(4)
C(9)-C(10)	1.545(3)
C(10)-C(11)	1.506(3)
C(11)-C(12)	1.521(3)
C(11)-C(21)	1.548(4)
C(11)-H(11)	1.0000

C(12)-C(13)	1.530(3)
C(12)-H(12A)	0.9900
C(12)-H(12B)	0.9900
C(13)-C(14)	1.522(4)
C(13)-H(13A)	0.9900
C(13)-H(13B)	0.9900
C(14)-C(20)	1.528(4)
C(14)-H(14A)	0.9900
C(14)-H(14B)	0.9900
C(15)-C(16)	1.387(4)
C(15)-H(15)	0.9500
C(16)-H(16)	0.9500
C(17)-C(18)	1.384(3)
C(17)-H(17)	0.9500
C(18)-C(19)	1.386(4)
C(18)-H(18)	0.9500
C(19)-H(19)	0.9500
C(20)-C(21)	1.525(3)
C(20)-H(20A)	0.9900
C(20)-H(20B)	0.9900
C(21)-H(21A)	0.9900
C(21)-H(21B)	0.9900

C(6)-O(1)-C(5)	116.1(2)
C(9)-N(1)-C(8)	128.2(2)
C(9)-N(1)-H(1)	115.9
C(8)-N(1)-H(1)	115.9
C(2)-C(1)-C(15)	119.7(3)
C(2)-C(1)-H(1A)	120.1
C(15)-C(1)-H(1A)	120.1
C(1)-C(2)-C(3)	119.7(3)
C(1)-C(2)-H(2)	120.1
C(3)-C(2)-H(2)	120.1
C(4)-C(3)-C(2)	121.1(3)
C(4)-C(3)-H(3)	119.4
C(2)-C(3)-H(3)	119.4

C(3)-C(4)-C(16)	118.9(3)
C(3)-C(4)-C(5)	120.3(3)
C(16)-C(4)-C(5)	120.8(3)
O(1)-C(5)-C(4)	107.8(2)
O(1)-C(5)-H(5A)	110.1
C(4)-C(5)-H(5A)	110.1
O(1)-C(5)-H(5B)	110.1
C(4)-C(5)-H(5B)	110.1
H(5A)-C(5)-H(5B)	108.5
O(1)-C(6)-C(17)	125.3(2)
O(1)-C(6)-C(7)	114.1(2)
C(17)-C(6)-C(7)	120.6(2)
C(8)-C(7)-C(6)	119.7(2)
C(8)-C(7)-H(7)	120.2
C(6)-C(7)-H(7)	120.2
C(7)-C(8)-C(19)	120.6(2)
C(7)-C(8)-N(1)	116.4(2)
C(19)-C(8)-N(1)	123.0(2)
O(2)-C(9)-N(1)	126.4(2)
O(2)-C(9)-C(10)	121.2(2)
N(1)-C(9)-C(10)	112.4(2)
O(3)-C(10)-C(11)	124.3(2)
O(3)-C(10)-C(9)	119.2(2)
C(11)-C(10)-C(9)	116.4(2)
C(10)-C(11)-C(12)	112.6(2)
C(10)-C(11)-C(21)	108.5(2)
C(12)-C(11)-C(21)	110.2(2)
C(10)-C(11)-H(11)	108.5
C(12)-C(11)-H(11)	108.5
C(21)-C(11)-H(11)	108.5
C(11)-C(12)-C(13)	111.0(2)
C(11)-C(12)-H(12A)	109.4
C(13)-C(12)-H(12A)	109.4
C(11)-C(12)-H(12B)	109.4
C(13)-C(12)-H(12B)	109.4
H(12A)-C(12)-H(12B)	108.0

C(14)-C(13)-C(12)	111.2(2)
C(14)-C(13)-H(13A)	109.4
C(12)-C(13)-H(13A)	109.4
C(14)-C(13)-H(13B)	109.4
C(12)-C(13)-H(13B)	109.4
H(13A)-C(13)-H(13B)	108.0
C(13)-C(14)-C(20)	110.6(2)
C(13)-C(14)-H(14A)	109.5
C(20)-C(14)-H(14A)	109.5
C(13)-C(14)-H(14B)	109.5
C(20)-C(14)-H(14B)	109.5
H(14A)-C(14)-H(14B)	108.1
C(16)-C(15)-C(1)	120.2(3)
C(16)-C(15)-H(15)	119.9
C(1)-C(15)-H(15)	119.9
C(15)-C(16)-C(4)	120.4(3)
C(15)-C(16)-H(16)	119.8
C(4)-C(16)-H(16)	119.8
C(6)-C(17)-C(18)	118.7(2)
C(6)-C(17)-H(17)	120.6
C(18)-C(17)-H(17)	120.6
C(17)-C(18)-C(19)	122.0(2)
C(17)-C(18)-H(18)	119.0
C(19)-C(18)-H(18)	119.0
C(18)-C(19)-C(8)	118.4(2)
C(18)-C(19)-H(19)	120.8
C(8)-C(19)-H(19)	120.8
C(21)-C(20)-C(14)	111.3(2)
C(21)-C(20)-H(20A)	109.4
C(14)-C(20)-H(20A)	109.4
C(21)-C(20)-H(20B)	109.4
C(14)-C(20)-H(20B)	109.4
H(20A)-C(20)-H(20B)	108.0
C(20)-C(21)-C(11)	111.5(2)
C(20)-C(21)-H(21A)	109.3
C(11)-C(21)-H(21A)	109.3

C(20)-C(21)-H(21B)	109.3
C(11)-C(21)-H(21B)	109.3
H(21A)-C(21)-H(21B)	108.0

Symmetry transformations used to generate equivalent atoms:

Table S12. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for 130958lt_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}
O(1)	22(1)	29(1)	27(1)	10(1)	-9(1)	-5(1)
O(2)	27(1)	23(1)	39(1)	9(1)	-8(1)	-6(1)
O(3)	25(1)	22(1)	27(1)	3(1)	-3(1)	-2(1)
N(1)	22(1)	17(1)	24(1)	4(1)	-4(1)	-2(1)
C(1)	32(2)	27(2)	26(1)	2(1)	-6(1)	-4(1)
C(2)	24(2)	32(2)	26(1)	3(1)	-2(1)	2(1)
C(3)	30(2)	21(2)	22(1)	0(1)	-4(1)	2(1)
C(4)	26(2)	23(2)	22(1)	8(1)	-5(1)	1(1)
C(5)	26(2)	32(2)	27(2)	12(1)	-10(1)	0(1)
C(6)	22(1)	24(2)	22(1)	0(1)	0(1)	0(1)
C(7)	22(1)	18(1)	21(1)	2(1)	1(1)	0(1)
C(8)	22(1)	18(1)	19(1)	-1(1)	-2(1)	4(1)
C(9)	22(1)	19(1)	23(1)	0(1)	-2(1)	2(1)
C(10)	25(1)	17(1)	17(1)	-1(1)	-2(1)	0(1)
C(11)	22(1)	18(1)	25(1)	-3(1)	-6(1)	-1(1)
C(12)	27(2)	26(2)	24(1)	3(1)	-1(1)	2(1)
C(13)	27(2)	35(2)	26(1)	7(1)	-6(1)	5(1)
C(14)	24(2)	27(2)	37(2)	2(1)	-4(1)	2(1)
C(15)	40(2)	22(2)	28(1)	2(1)	2(1)	1(1)
C(16)	29(2)	25(2)	28(1)	8(1)	1(1)	6(1)
C(17)	26(1)	20(1)	21(1)	2(1)	-2(1)	6(1)
C(18)	24(1)	17(1)	25(1)	2(1)	2(1)	-1(1)
C(19)	24(1)	17(1)	26(1)	-3(1)	-2(1)	0(1)
C(20)	23(1)	29(2)	26(1)	-1(1)	-1(1)	-2(1)

C(21)	25(2)	26(2)	24(1)	-1(1)	-2(1)	0(1)

Table S13. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for 130958lt_0m.

	x	y	z	U(eq)
H(1)	153	7310	4504	26
H(1A)	-4944	5746	1430	35
H(2)	-5062	9333	2068	33
H(3)	-3923	11607	2432	30
H(5A)	-2050	10988	1851	35
H(5B)	-2561	12572	2358	35
H(7)	-998	7934	3778	24
H(11)	2499	8140	5611	26
H(12A)	2293	3065	5850	31
H(12B)	2214	5135	6435	31
H(13A)	3590	6067	6451	36
H(13B)	3494	3257	6627	36
H(14A)	3696	2209	5442	36
H(14B)	4436	3816	5777	36
H(15)	-3682	4432	1172	36
H(16)	-2545	6699	1546	33
H(17)	-1252	13890	2514	27
H(18)	30	15112	2958	27
H(19)	818	12781	3792	27
H(20A)	3901	7271	5172	32
H(20B)	3966	5163	4596	32
H(21A)	2593	4342	4566	31
H(21B)	2701	7163	4411	31