

Supporting Information

Harnessing the Magic Methyl Effect: A Rhodium-Catalyzed Switchable Chemoselective Synthesis of Isocoumarins and Isoquinolines

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1. General Information:

Reactions were performed using borosil sealed tube vial under N₂ atmosphere. Solvents were dehydrated and distilled under nitrogen. Column chromatography was done by using 100-200 mesh silica gel of Acme synthetic chemicals company. A gradient elution was performed by using distilled petroleum ether and ethyl acetate. TLC plates detected under UV light at 254 nm and vanillin. ¹H NMR, ¹³C NMR, recorded on Bruker AV 400 and 700 MHz spectrometer using CDCl₃ as the deuterated solvent.¹ Multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, quint = quintet, sept = septet, m = multiplet, dd = doublet of doublet, dt = doublet of triplet, td = triplet of doublet, br = broad signal), integration, and coupling constants (*J*) in hertz (Hz). HRMS signal analysis was performed using micro TOF Q-II mass spectrometer and Waters LCT Premier XE spectrometer. Reagents and starting materials were purchased from Sigma Aldrich, TCI, Avra, Spectrochem and other commercially available sources, used without further purification unless otherwise noted. *O*-benzoyl oxime and its derivatives,² internal alkynes,^{3,4} and [Cp*RhCl₂]₂,⁵ were prepared according to the literature reported procedure.

Abbreviation:

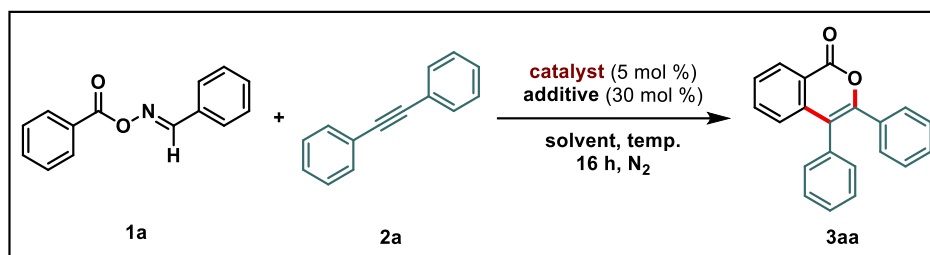
TFE (Trifluoroethanol), **EtOAc** (Ethyl acetate), **DCM** (Dichloromethane), **Et₃N** (Triethyl amine), **EDC.HCl** (*N*-(3-Dimethylaminopropyl)-*N'*-ethylcarbodiimide hydrochloride), **DMAP** (4-(Dimethylamino)pyridine).

2. Experimental details

2.1 Optimization of reaction conditions

We commenced our study for finding the suitable reaction conditions for the rhodium catalyzed chemoselective C(*sp*²)-H activation/annulation of *O*-benzoyl oxime with alkynes. Subsequently, (*E*)-benzaldehyde *O*-benzoyl oxime **1a** and 1,2-diphenylethyne **2a** were chosen as the model substrates in the presence of 5 mol % of a rhodium catalyst. Initially, different solvents were screened with Ag₂CO₃ as an additive at 60 °C (Table S1, entries 1-5). With *t*-amyl alcohol as solvent we were able to get desired annulated product in 8% yield. The use of various other solvents such as 1,4-dioxane, THF, MeCN and TFE produced the annulated product **3aa** in 21%, 33%, 45%, and 49% yields respectively. As TFE gave the better yield among the solvents used, we stuck to TFE and varied different silver additives for further improvement of the yield. Interestingly, the other silver additives such as Ag₂O, AgBF₄, AgOCOCF₃, AgOTf and AgOAc helped significantly to enhance the product yield (Table S1, entries 6-10). It is worthy to mention that AgOAc was found to be most effective among them, affording 67% yield of **3aa**. Intrigued by these results, we next investigated the effect of different acetate additives on the outcome of the reaction (Table S1, entries 11-13). Interestingly, the yield of **3aa** further improved in the cases of KOAc (76%) and NaOAc (89%) (Table S1, entries 12 and 13). However, attempts to carry out the reaction at higher or lower temperatures resulted in lower product yield, affording the desired product in 76% and 5% yield respectively (Table S1, entries 14-15). Efforts to replace the catalyst [Cp**RhCl*₂]₂ with [Rh₂(OAc)₄], and [Rh₂(TFA)₄] had a deleterious effect on the reaction furnishing the desired product in <5% and 5% yields respectively (Table S1, entries 16-17). To check the effect of NaOAc additive and [Cp**RhCl*₂]₂ catalyst we performed two control experiments. In the absence of NaOAc, 42% of **3aa** was obtained while without [Cp**RhCl*₂]₂ catalyst no product was observed. (Table S1, entries 18-19). Hence, the use of 5 mol % of [Cp**RhCl*₂]₂ along with 30 mol % of NaOAc in TFE (0.1 M) at 60 °C gave the best yield of **3aa** (Table S1, entry 13).

Table S1: Optimization of reaction conditions:

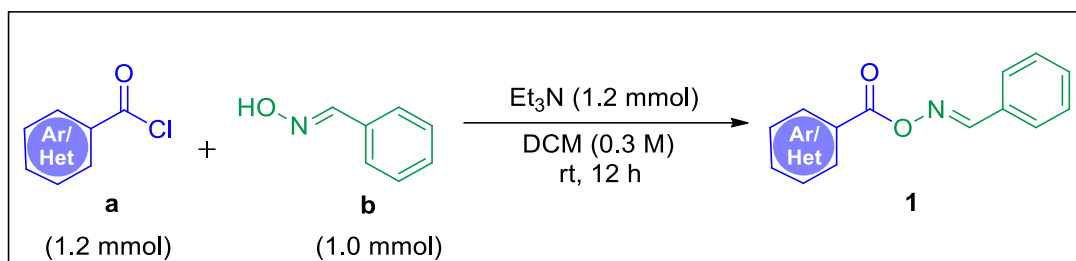


| entry | solvent (0.1 M) | catalyst | additive | yield of 3aa (%) ^b |
|-----------------|-----------------|--|---------------------------------|-------------------------------|
| 1 | t-amyl alcohol | [Cp*RhCl ₂] ₂ | Ag ₂ CO ₃ | 8 |
| 2 | 1,4-Dioxane | [Cp*RhCl ₂] ₂ | Ag ₂ CO ₃ | 21 |
| 3 | THF | [Cp*RhCl ₂] ₂ | Ag ₂ CO ₃ | 33 |
| 4 | MeCN | [Cp*RhCl ₂] ₂ | Ag ₂ CO ₃ | 45 |
| 5 | TFE | [Cp*RhCl ₂] ₂ | Ag ₂ CO ₃ | 49 |
| 6 | TFE | [Cp*RhCl ₂] ₂ | Ag ₂ O | 58 |
| 7 | TFE | [Cp*RhCl ₂] ₂ | AgBF ₄ | 61 |
| 8 | TFE | [Cp*RhCl ₂] ₂ | AgOCOCF ₃ | 65 |
| 9 | TFE | [Cp*RhCl ₂] ₂ | AgOTf | 66 |
| 10 | TFE | [Cp*RhCl ₂] ₂ | AgOAc | 67 |
| 11 | TFE | [Cp*RhCl ₂] ₂ | LiOAc | 36 |
| 12 | TFE | [Cp*RhCl ₂] ₂ | KOAc | 76 |
| 13 | TFE | [Cp*RhCl₂]₂ | NaOAc | 89 (87) |
| 14 ^d | TFE | [Cp*RhCl ₂] ₂ | NaOAc | 76 ^d |
| 15 ^e | TFE | [Cp*RhCl ₂] ₂ | NaOAc | 5 ^e |
| 16 | TFE | [Rh ₂ (OAc) ₄] | NaOAc | <5 |
| 17 | TFE | [Rh ₂ (TFA) ₄] | NaOAc | 5 |
| 18 | TFE | [Cp*RhCl ₂] ₂ | -- | 42 |
| 19 | TFE | -- | NaOAc | nd ^c |

^aUnless otherwise specified, all reactions were carried out using catalyst (5 mol %), additive (0.3 equiv), **1a** (0.10 mmol, 1.0 equiv), **2a** (0.10 mmol, 1.5 equiv) in a solvent (0.10 M) at 60 °C for 16 h. ^bYields determined by NMR, using 1,3,5-trimethoxy benzene as internal reference. ^cnd = not detected. ^dReaction was carried out at 90 °C. ^eReaction was carried out at rt. Isolated yield is mentioned in the parenthesis.

2.2 General procedure for the preparation of *O*-benzoyl oxime

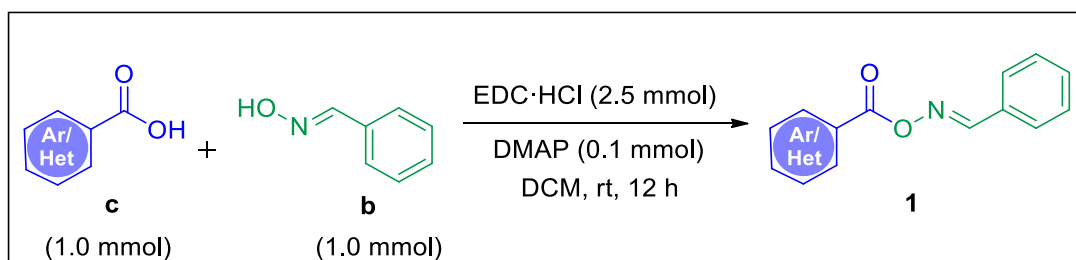
[General Procedure A]



O-benzoyl oximes (**1**) were prepared following the previously reported procedure.¹ The corresponding benzoyl chloride (**a**) (1.2 mmol) was added to a solution of aldoxime (**b**) (1.0 mmol) and Et₃N (1.5 mmol) in DCM (0.30 M) with stirring at ice cold temperature. After addition was complete, the reaction mixture was stirred for 12 h at room temperature. Then saturated NH₄Cl aq. (3 mL) was added to quench the reaction. The organic layer was washed with brine (10 mL) and extracted with DCM (20 mL). The combined organic layer was dried over MgSO₄, filtered, and concentrated in vacuum. The remaining crude mixture was purified by silica gel column chromatography to afford pure *O*-benzoyl oximes (**1**) in pure form.

2.3 General procedure for the preparation of *O*-benzoyl oxime

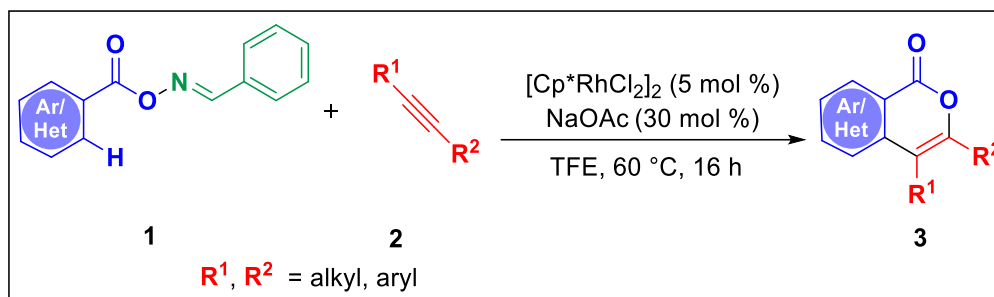
[General Procedure B]



O-benzoyl oximes (**1**) were prepared following the previously reported procedure.¹ To a solution of aldoxime (**b**) (1.0 mmol) in DCM (10 mL) was added aromatic carboxylic acid (**c**) (1.0 mmol) followed by EDC·HCl (2.5 mmol) and DMAP (0.1 mmol). The mixture was magnetically stirred at r.t. under N₂ atmosphere until the reaction was complete (TLC monitoring). The mixture was diluted with H₂O (15 mL) and the CH₂Cl₂ layer was separated. The CH₂Cl₂ layer was dried over anhydrous Na₂SO₄, and concentrated. The crude mass obtained was treated with PE (2–3 mL); separation of a solid occurred when sonicated. The resultant solid was filtered and dried under suction to afford the oxime esters (**1**) in pure form.

2.4 General procedure for chemoselective *ortho*-C(sp²)-H activation/annulation of *O*-benzoyl oxime with alkynes for the synthesis of isocoumarins

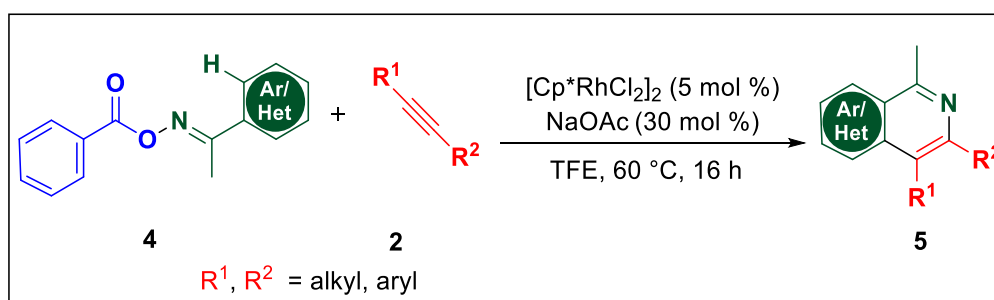
[General Procedure C]



A flame-dried 15 mL screw capped vial equipped with magnetic stir bar was charged with *O*-benzoyl oxime **1** (0.10 mmol, 2 equiv), alkyne **2** (0.13 mmol, 1 equiv), [Cp^{*}RhCl₂]₂ (0.005 mmol), AgOAc (0.03 mmol), and TFE (1.0 mL). Then the contents were allowed to stir at 60 °C in a preheated aluminum block for 16 h. The completion of the reaction was monitored by TLC. Upon completion of the reaction, the tube was cooled down to room temperature, the reaction mixture was diluted with 5 mL of dichloromethane and filtered with a plug Celite bed, followed by washing with 20 mL of dichloromethane. The combined residue was concentrated under reduced pressure, and the resulting crude was purified by silica gel column chromatography using hexane/ethyl acetate to afford the desired product **3**.

2.5 General procedure for chemoselective *ortho*-C(sp²)-H activation/annulation of *O*-benzoyl oxime with alkynes for the synthesis of isoquinolines

[General Procedure D]

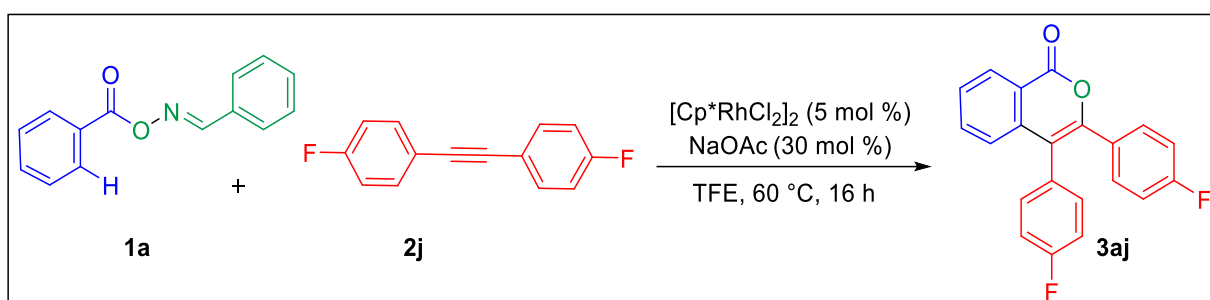


A flame-dried 15 mL screw capped vial equipped with magnetic stir bar was charged with *O*-benzoyl oxime **4** (0.10 mmol, 2 equiv), alkyne **2** (0.13 mmol, 1 equiv), [Cp^{*}RhCl₂]₂ (0.005 mmol), AgOAc (0.03 mmol), and TFE (1.0 mL). Then the contents were allowed to stir at 60

°C in a preheated aluminum block for 16 h. The completion of the reaction was monitored by TLC. Upon completion of the reaction, the tube was cooled down to room temperature, the reaction mixture was diluted with 5 mL of dichloromethane and filtered with a plug Celite bed, followed by washing with 20 mL of dichloromethane. The combined residue was concentrated under reduced pressure, and the resulting crude was purified by silica gel column chromatography using hexane/ethyl acetate to afford the desired product **5**.

2.6 General procedure for chemoselective *ortho*-C(sp²)-H activation/annulation of *O*-benzoyl oxime with alkynes in 1 mmol scale

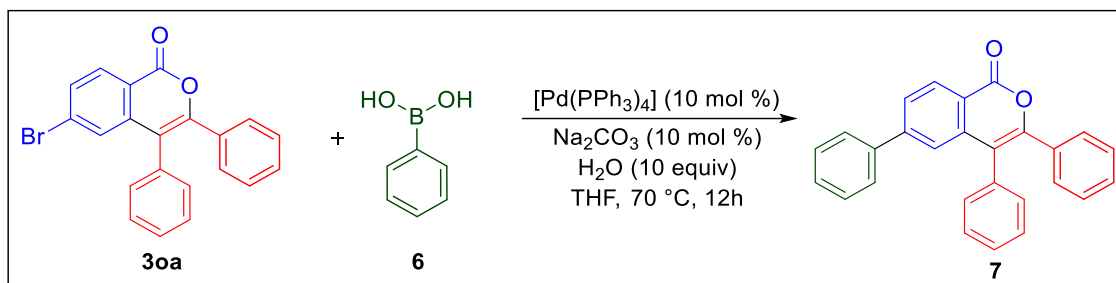
[General Procedure E]



A flame-dried 25 mL screw capped vial equipped with magnetic stir bar was charged with *O*-benzoyl oxime **1a** (1.0 mmol, 1 equiv), alkyne **2j** (1.3 mmol, 1 equiv), $[\text{Cp}^*\text{RhCl}_2]_2$ (0.05 mmol), AgOAc (0.3 mmol), and TFE (10.0 mL). Then the contents were allowed to stir at 60 °C in a preheated aluminum block for 16 h. The completion of the reaction was monitored by TLC. Upon completion of the reaction, the tube was cooled down to room temperature, the reaction mixture was diluted with 50 mL of dichloromethane and filtered with a plug Celite bed, followed by washing with 100 mL of dichloromethane. The combined residue was concentrated under reduced pressure, and the resulting crude was purified by silica gel column chromatography using hexane/ethyl acetate to afford the desired product **3aj** (277 mg) in 83% yield.

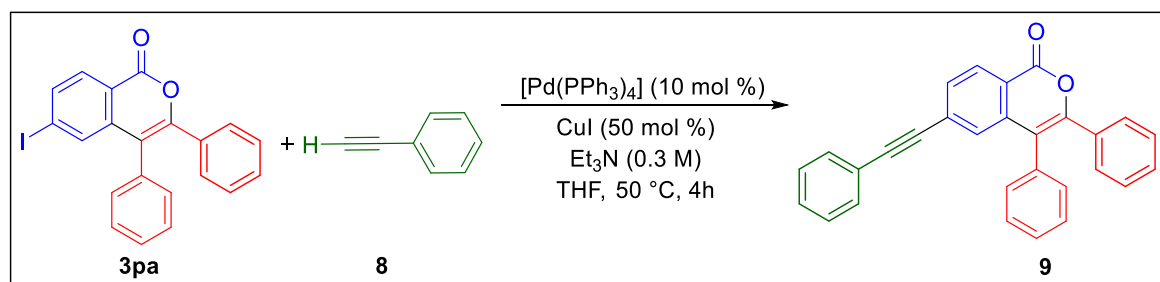
2.7 Synthetic derivatization of the isocoumarin molecules

2.7.1 Procedure for the Arylation of 30a with phenyl boronic acid.



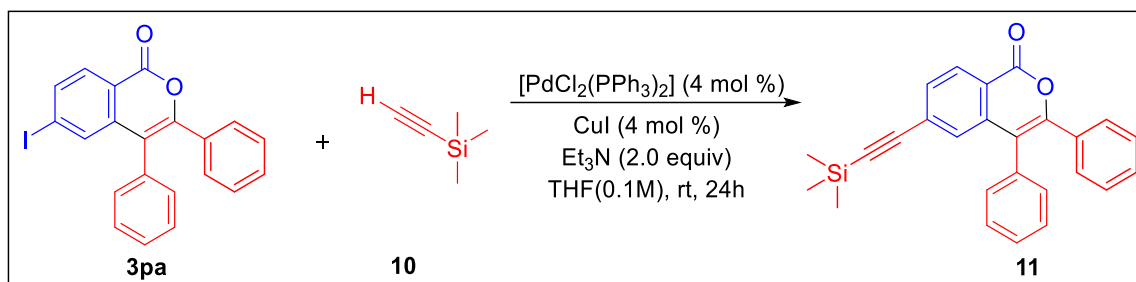
A mixture of **30a** (0.1 mmol, 1.0 equiv), phenylboronic acid **6** (0.15 mmol, 1.5 equiv), Na₂CO₃ (10.0 equiv), and Pd(PPh₃)₄ (10.0 mol %) in THF (1.0 mL) and H₂O (0.25 mL) was stirred at 70 °C for 12 h under N₂ atmosphere. The mixture was added with H₂O (10 mL) and extracted with CH₂Cl₂. The combined organic phase was dried over MgSO₄ and concentrated under reduced pressure. The residue was purified by chromatography on silica gel (EtOAc/hexane) to afford product **7**.

2.7.2 General Procedure for the Alkynylation of 3pa with phenyl acetylene.



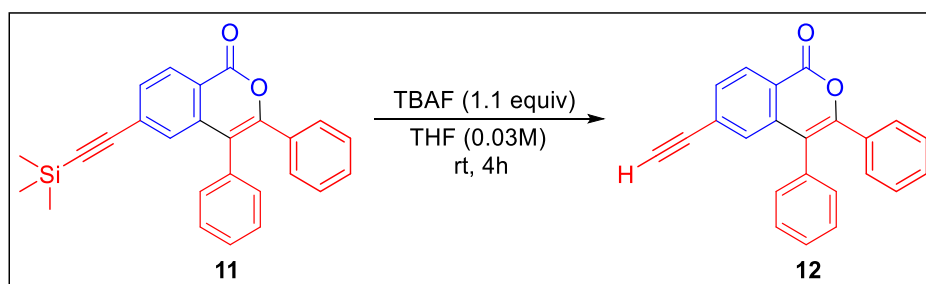
A mixture of **3pa** (0.1 mmol, 1.0 equiv), phenylacetylene **8** (1.5 mmol, 1.5 equiv), CuI (50 mol %), and Pd(PPh₃)₄ (5.0 mol %) in THF (0.5 mL) and Et₃N (0.5 mL) was stirred at 50 °C for 4 h under N₂ atmosphere. The reaction mixture was poured into a sat. NH₄Cl solution and extracted with CH₂Cl₂. The combined organic phase was dried over MgSO₄ and concentrated under reduced pressure. The residue was purified by chromatography on silica gel (EtOAc/hexane) to afford product **9**.

2.7.3 General Procedure for the Alkynylation of **3pa** with trimethylsilyl acetylene.



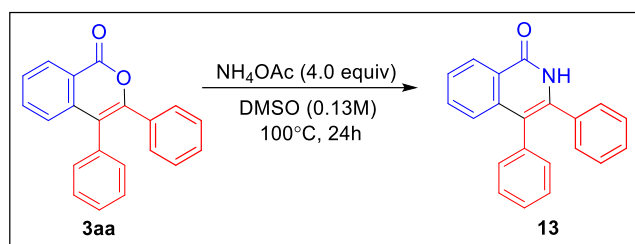
A mixture of **3pa** (0.1 mmol, 1.0 equiv), ethynyltrimethylsilane **10** (0.15 mmol, 1.5 equiv), $\text{PdCl}_2(\text{PPh}_3)_2$ (0.04 mmol) and CuI (0.04 mmol) were mixed in THF (1.0 mL) containing NEt_3 (2 equiv). The resulting solution was stirred at room temperature for 24 h. After the reaction was finished, ethyl acetate (10 mL) was poured into the mixture. The resulting mixture was then washed with brine, extracted with ethyl acetate, and dried over anhydrous Na_2SO_4 . After filtration and removal of the solvents, the residue was subjected to flash column chromatography on silica gel (100-200 mesh) using (EtOAc/hexane) as eluent to afford silylated alkynes **11**.

2.7.4 Procedure for the desilylation of **11**.



The substrate **11** (0.1 mmol) was dissolved in THF (0.03 M) and TBAF (1.0 M in THF, 0.11 mmol) was added slowly at 0 °C. The reaction mixture was stirred for 2 h at room temperature. After complete conversion of starting material, reaction mixture was evaporated *in vacuo*. The crude product, thus obtained, was purified by column chromatography (eluent: pet. ether/EtOAc) to afford the terminal alkyne **12** as a yellow solid.

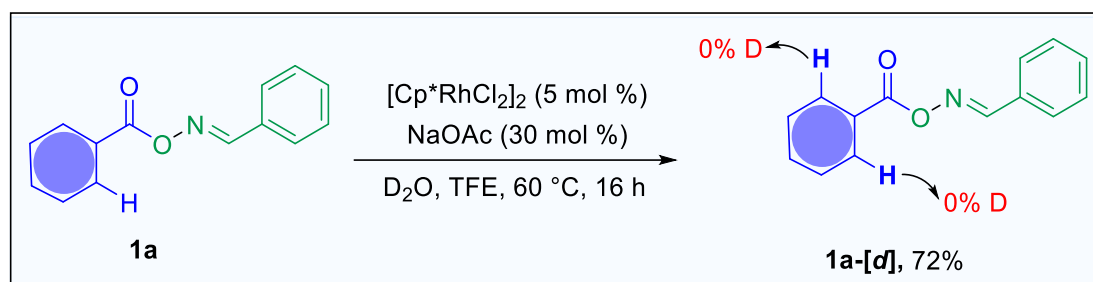
2.7.5 Procedure for the synthesis of isoquinolone **13** from isocoumarin **3aa**.



A mixture of **3aa** (0.1 mmol, 1.0 equiv), NH_4OAc (3.0 equiv) in DMSO (0.1 M, 1 mL) was stirred at 100°C for 4 h. The reaction mixture was poured into water and extracted with CH_2Cl_2 . The combined organic phase was dried over MgSO_4 and concentrated under reduced pressure. The residue was purified by chromatography on silica gel (EtOAc /hexane) to afford product **13**.

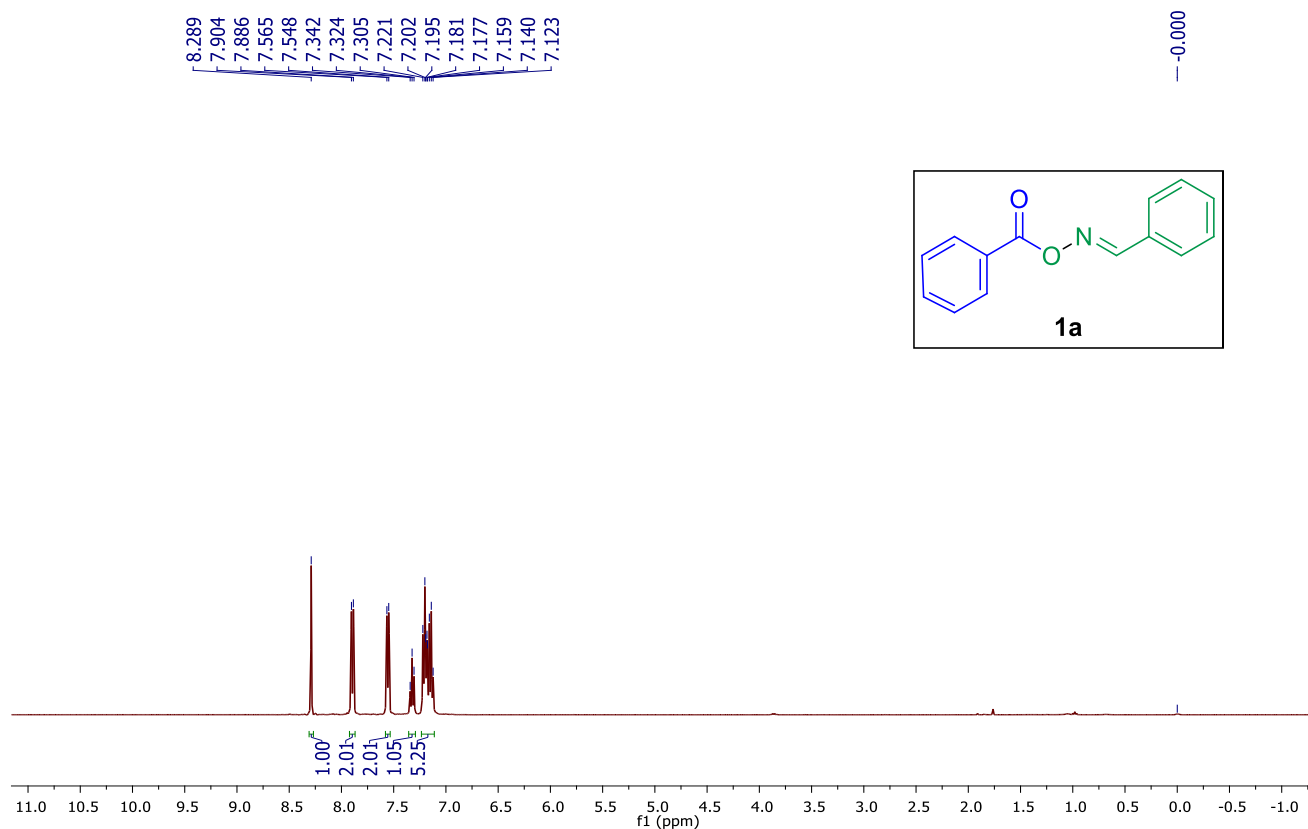
3. Mechanistic Investigation:

3.1 Deuterium labeling experiment

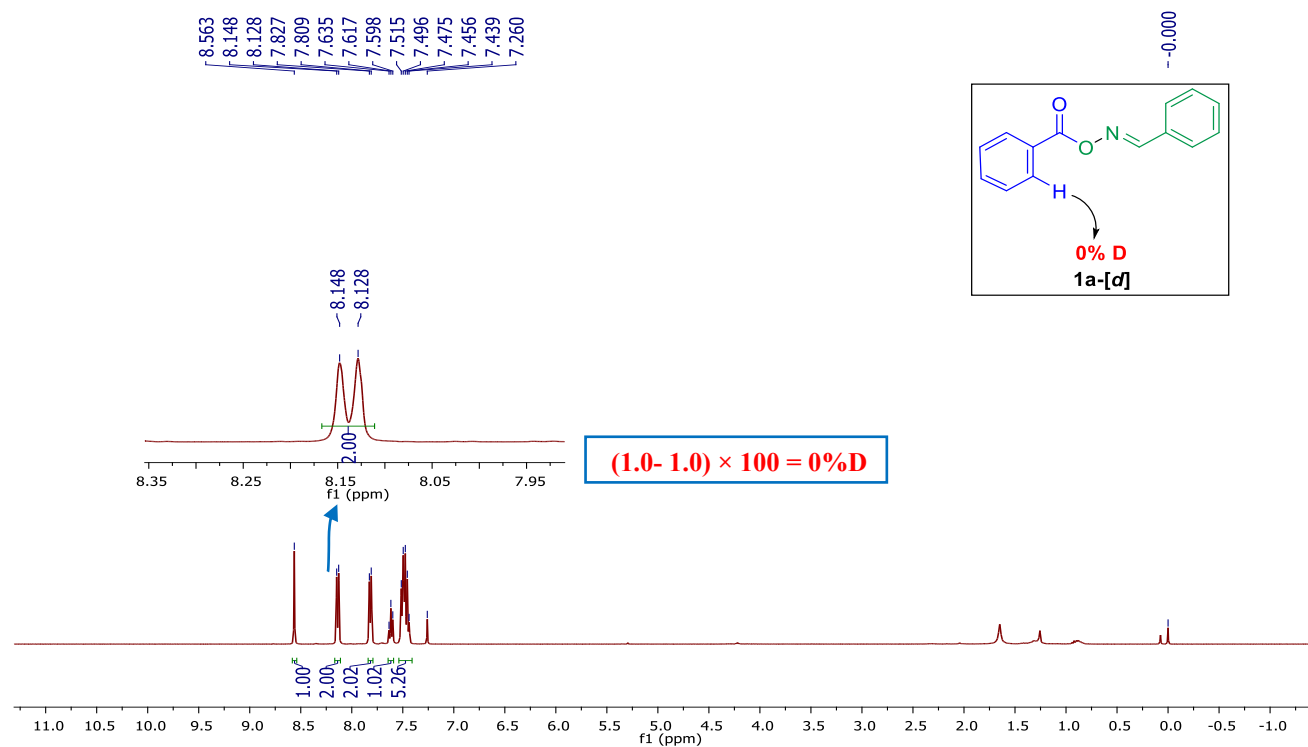


A flame-dried 15 mL screw capped vial equipped with magnetic stir bar was charged with *O*-benzoyl oxime **1a** (0.1 mmol), $[\text{Cp}^*\text{RhCl}_2]_2$ (0.005 mmol), NaOAc (0.03 mmol), D_2O (10 equiv) and TFE ($500\ \mu\text{L}$). The contents were allowed to stir at 60°C in a pre-heated aluminum block for 16 h. Then the contents were allowed to cool down to room temperature. Later, the reaction mixture was diluted with 10 mL of dichloromethane and filtered through a Celite pad. The filtered solution was concentrated under reduced pressure. Then, the residue was purified by column chromatography with EtOAc /Hexane as eluent. The extent H/D exchange was calculated by ^1H NMR (see the following spectra).

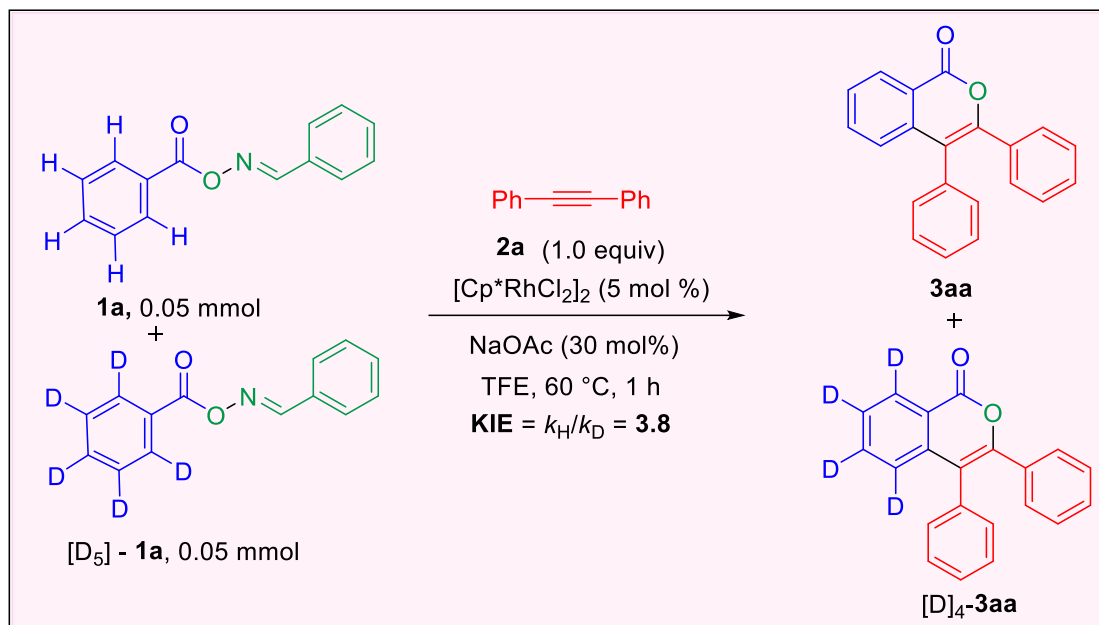
¹H NMR of 1a (400 MHz, CDCl₃)



¹H NMR of 1a-[d] (400 MHz, CDCl₃)

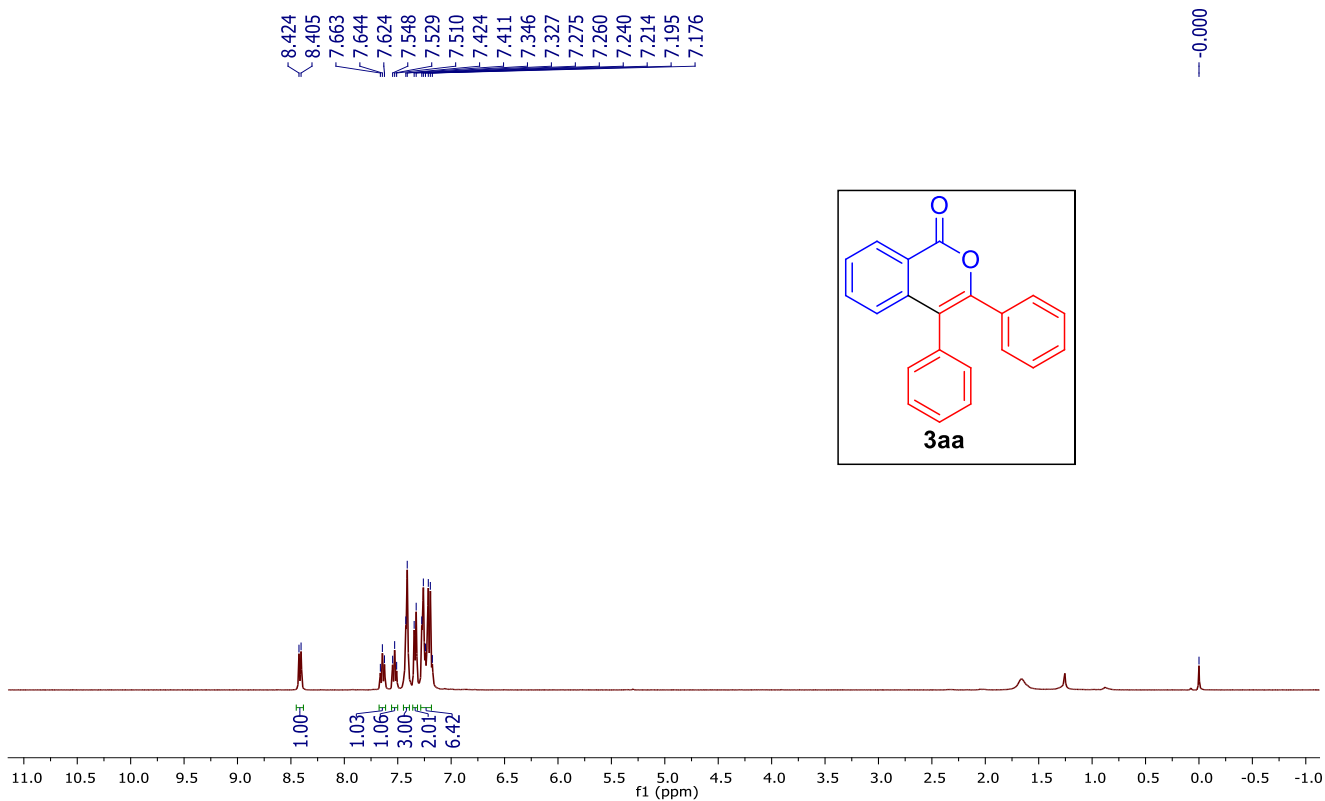


3.2 Intermolecular competition KIE for the reaction

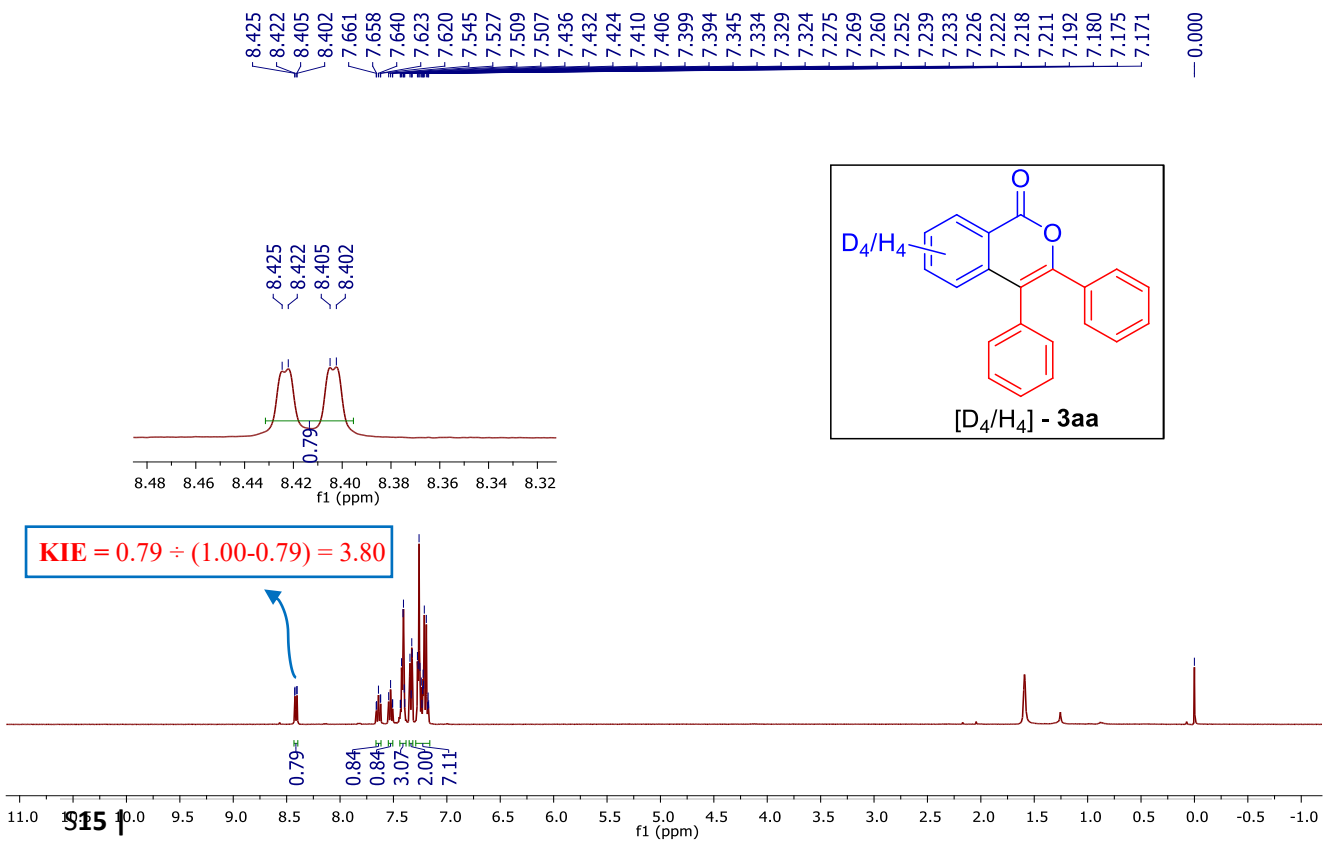


A flame-dried 5 mL screw capped vial equipped with magnetic stir bar was charged with *O*-benzoyl oxime **1a** (0.05 mmol), $[D_5]-\mathbf{1a}$ (0.05 mmol), 1,2-diphenylethyne (**2a**, 0.05 mmol, 1 equiv), $[Cp^*RhCl_2]_2$ (5 mol %), NaOAc (30 mol %), and TFE (0.25 mL). The contents were allowed to stir at 60 °C in a pre-heated aluminum block for 25 minutes. After 25 minutes the reaction tube was cooled down to room temperature and the reaction mixture was diluted with 1 mL of dichloromethane and filtered with a small plug of Celite bed, followed by washing with 3 mL of dichloromethane. Then, the residue was purified by column chromatography with EtOAc/Hexane as eluent to afford the desired product $[D_4/H_4]-\mathbf{3aa}$. The kinetic isotopic value ($k_H/k_D \approx 3.8$) was calculated from the 1H NMR of the mixture $[D_4/H_4]-\mathbf{3aa}$ (see the following spectra).

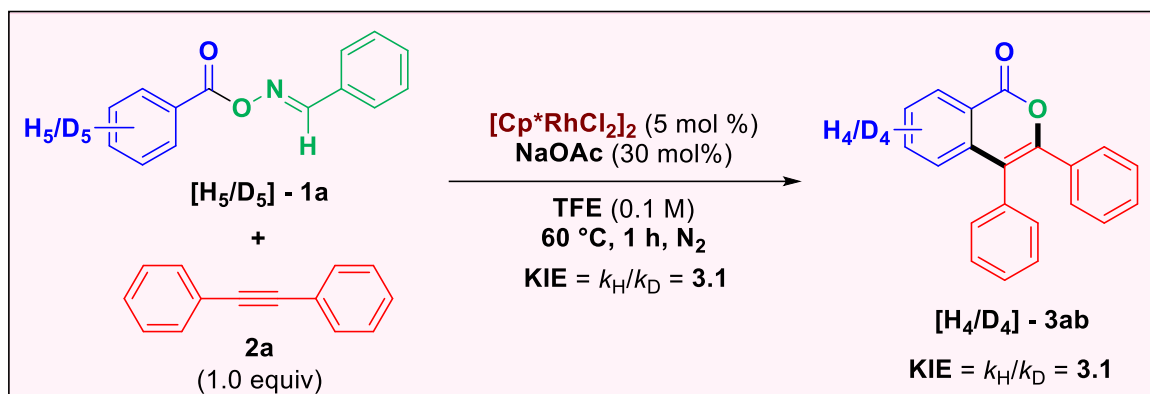
¹H NMR of 3aa (400 MHz, CDCl₃)



¹H NMR of [D₄/H₄]-3aa (400 MHz, CDCl₃)

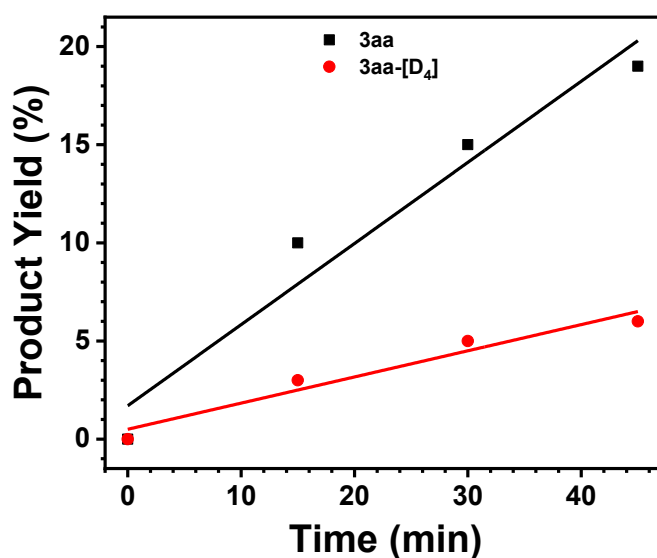


3.3 Kinetic isotope effect: Parallel reactions

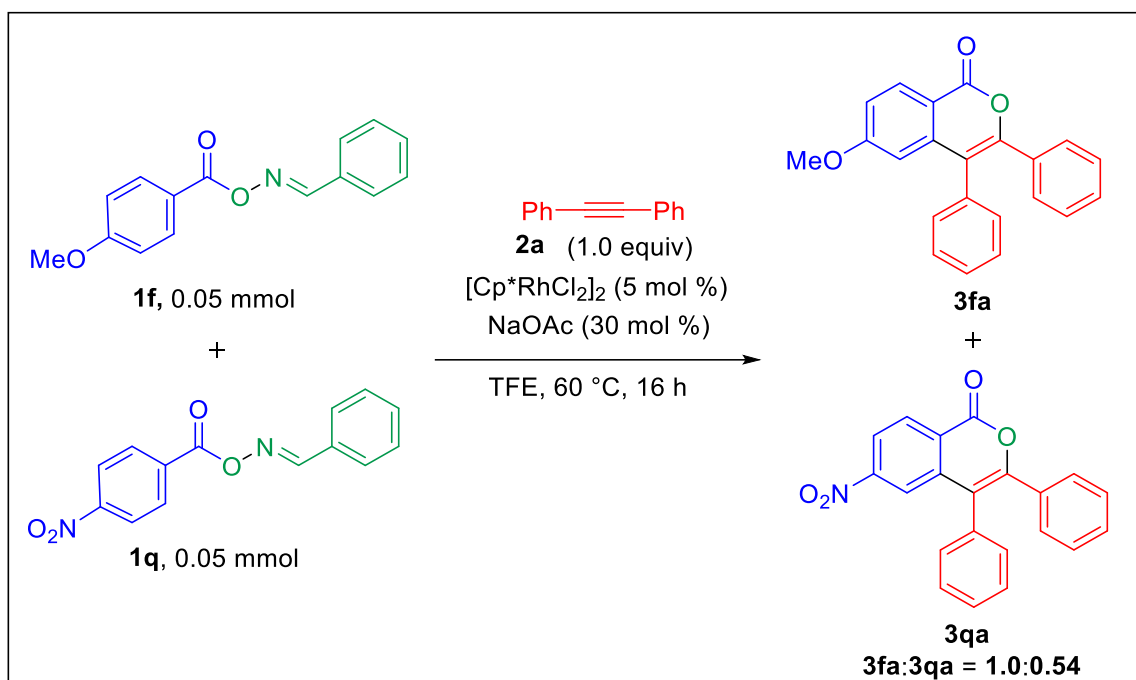


By following the general procedure, 3 sets of parallel experiments were set. To a flame-dried 5.00 mL screw capped vial equipped with magnetic stir bar were charged H₅/[D]5-**1a** (1.00 equiv), 1,4-diphenylbuta-1,3-diyne (**2a**, 0.05 mmol, 1.00 equiv), [Cp*RhCl₂]₂ (5 mol %), NaOAc (30 mol %), and TFE (0.25 mL). The reactions were carried out at 15 min time intervals (15, 30, 45 mins) at 60 °C in a pre-heated aluminum block. The product yields were calculated from the ¹H NMR analysis of the crude reaction mixture using 1,3,5-trimethoxy benzene as an internal standard. The KIE value was calculated from the obtained slopes of two lines.

| Time(min) | 0 | 15 | 30 | 45 |
|--------------------------------|---|----|----|----|
| 3aa (%) | 0 | 10 | 15 | 19 |
| [D]₄-3aa (%) | 0 | 3 | 5 | 6 |

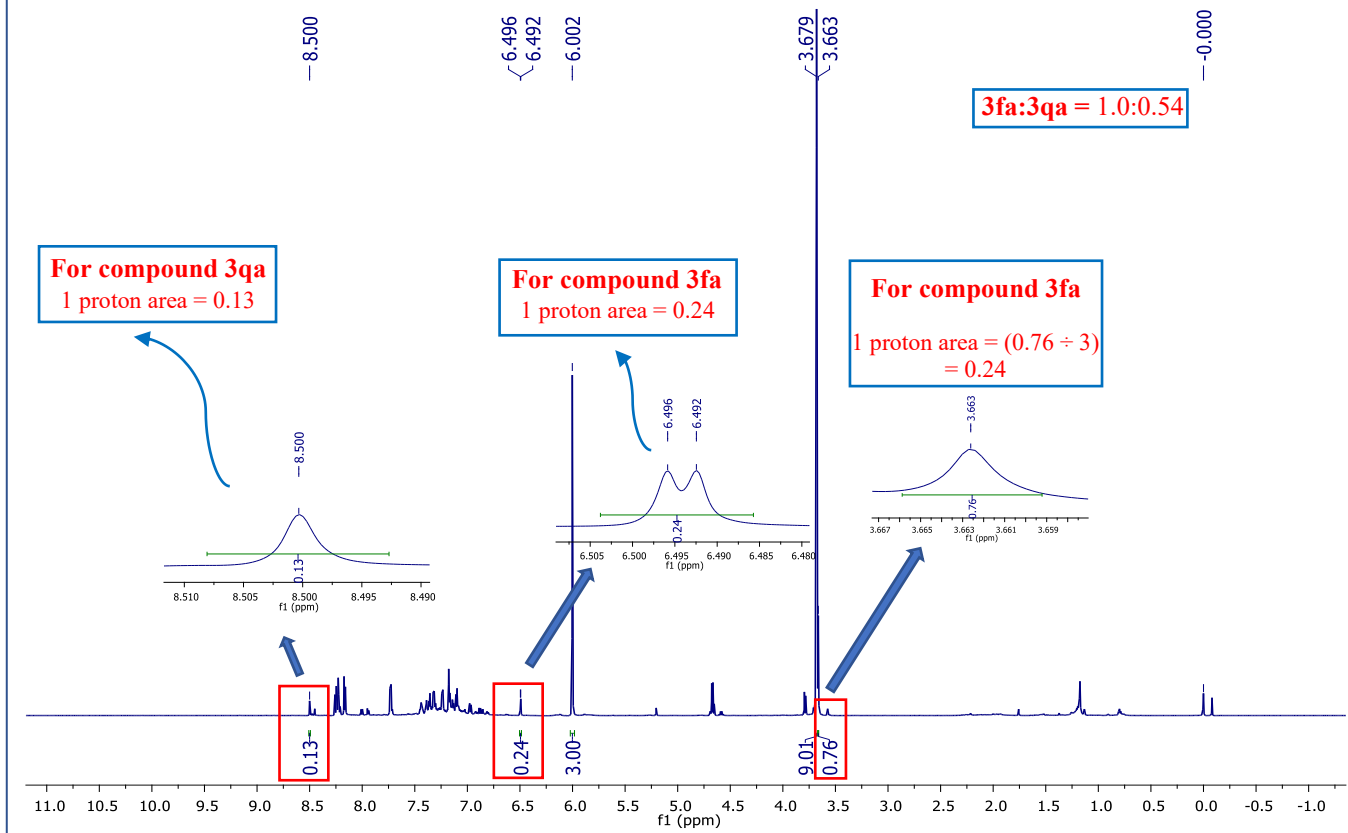


3.4 Intermolecular competitive reaction between two different *O*-benzoyl oximes

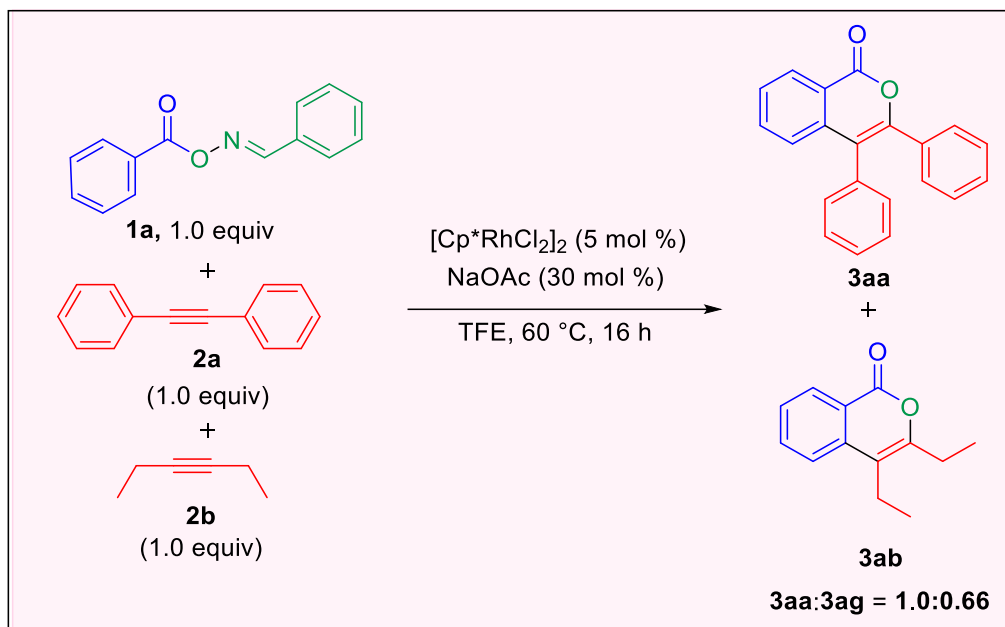


A flame-dried 5 mL screw capped vial equipped with magnetic stir bar was charged with two different *O*-benzoyl oxime (**1f**, 0.10 mmol, 1 equiv), (**1q**, 0.10 mmol, 1 equiv), 1,2-diphenylethyne (**2a**, 0.1 mmol, 1 equiv), $[\text{Cp}^*\text{RhCl}_2]_2$ (5 mol %), (5 mol %), NaOAc (30 mol %) and TFE (0.25 mL). The contents were allowed to stir at 60 °C in a pre-heated aluminum block for 12 h. Upon completion of the standard reaction time the reaction tube was cooled to room temperature, the reaction mixture was diluted with 1 mL of dichloromethane and filtered through Celite bed, followed by washing with 3 mL of dichloromethane. The filtered solution was concentrated under reduced pressure. The ratio of two products **3fa:3qa** (1.0:0.54) was calculated from the ^1H NMR analysis of the crude using 1,3,5-trimethoxy benzene as internal standard (see the following spectra).

¹H NMR of crude mixture of the competition reaction between 2a, 1f and 1q (400 MHz, CDCl₃)

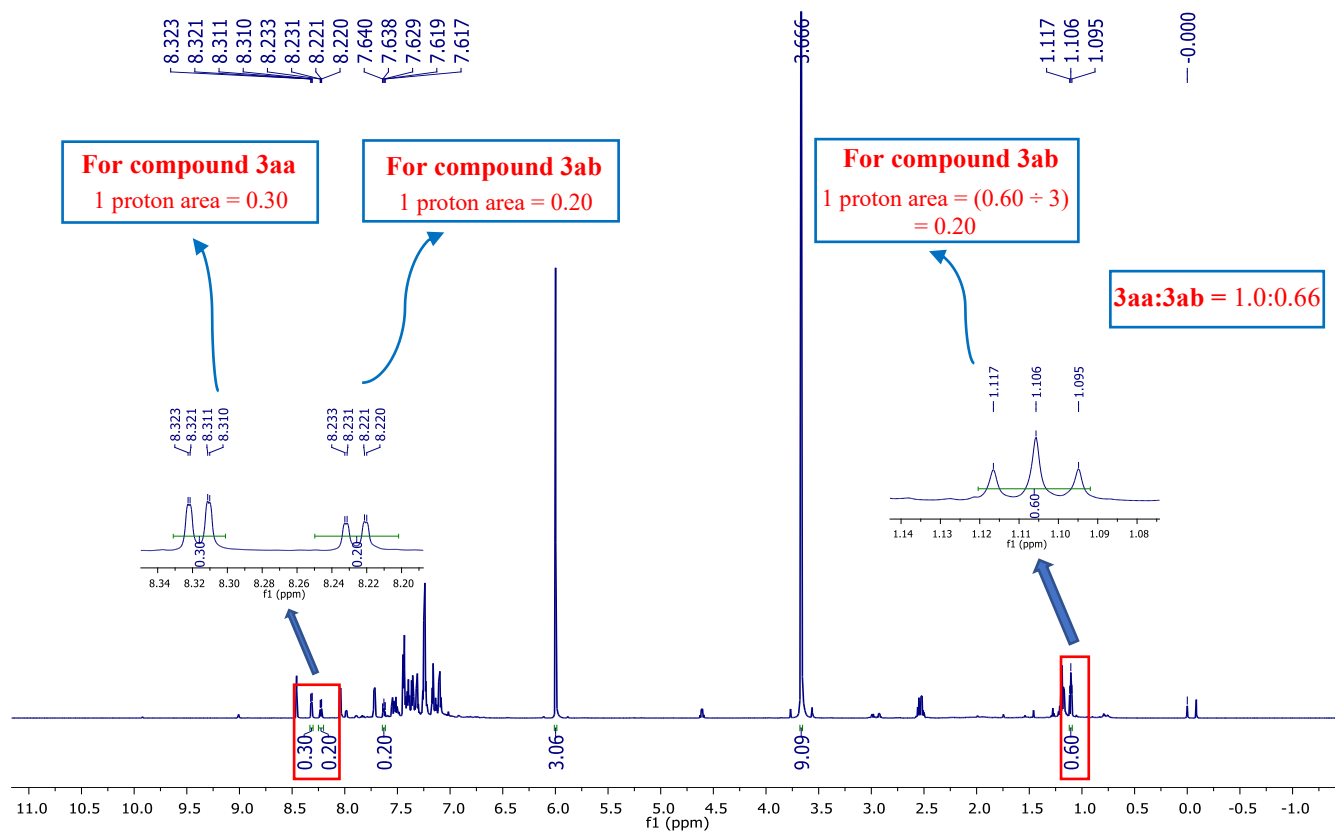


3.5 Intermolecular competitive reaction between two different alkynes

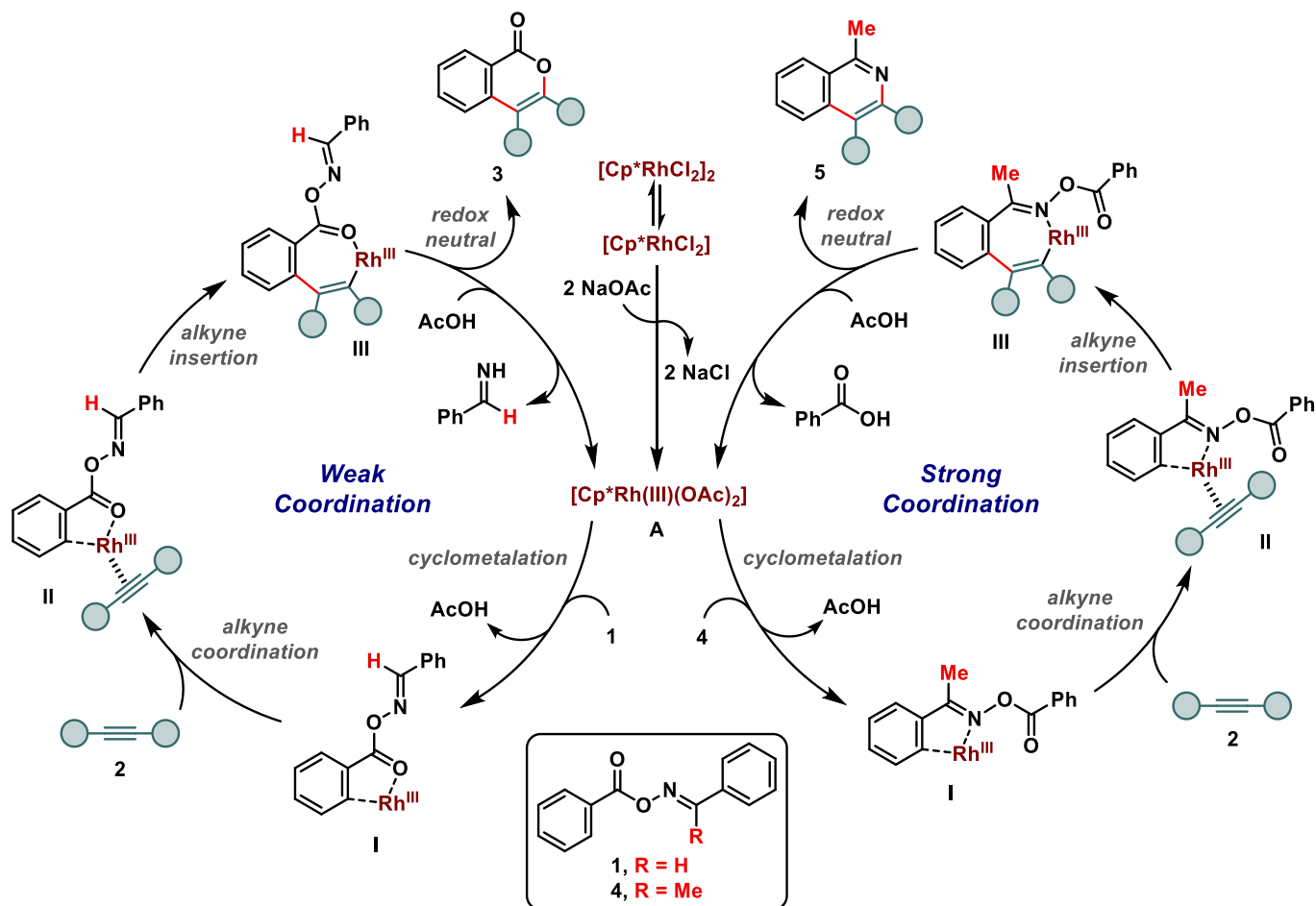


A flame-dried 5 mL screw capped vial equipped with magnetic stir bar was charged with O-benzoyl oxime (**1a**, 0.10 mmol, 1 equiv), two different alkynes (**2a**, 0.05 mmol, 1 equiv), (**2b**, 0.05 mmol, 1 equiv), $[\text{Cp}^*\text{RhCl}_2]_2$ (5 mol %), NaOAc (30 mol %), and TFE (0.25 mL). The contents were allowed to stir at 60 °C in a pre-heated aluminum block for 16 h. Upon completion of the standard reaction time the reaction tube was cooled to room temperature, the reaction mixture was diluted with 1 mL of dichloromethane and filtered through Celite bed, followed by washing with 3 mL of dichloromethane. The filtered solution was concentrated under reduced pressure. The ratio of two products **3aa:3ab** (1:2) was calculated from the ^1H NMR analysis of the crude using 1,3,5-trimethoxy benzene as internal standard (see the following spectra).

^1H NMR of crude mixture of the competition reaction between 1a, 2b and 2f (400 MHz, CDCl_3)



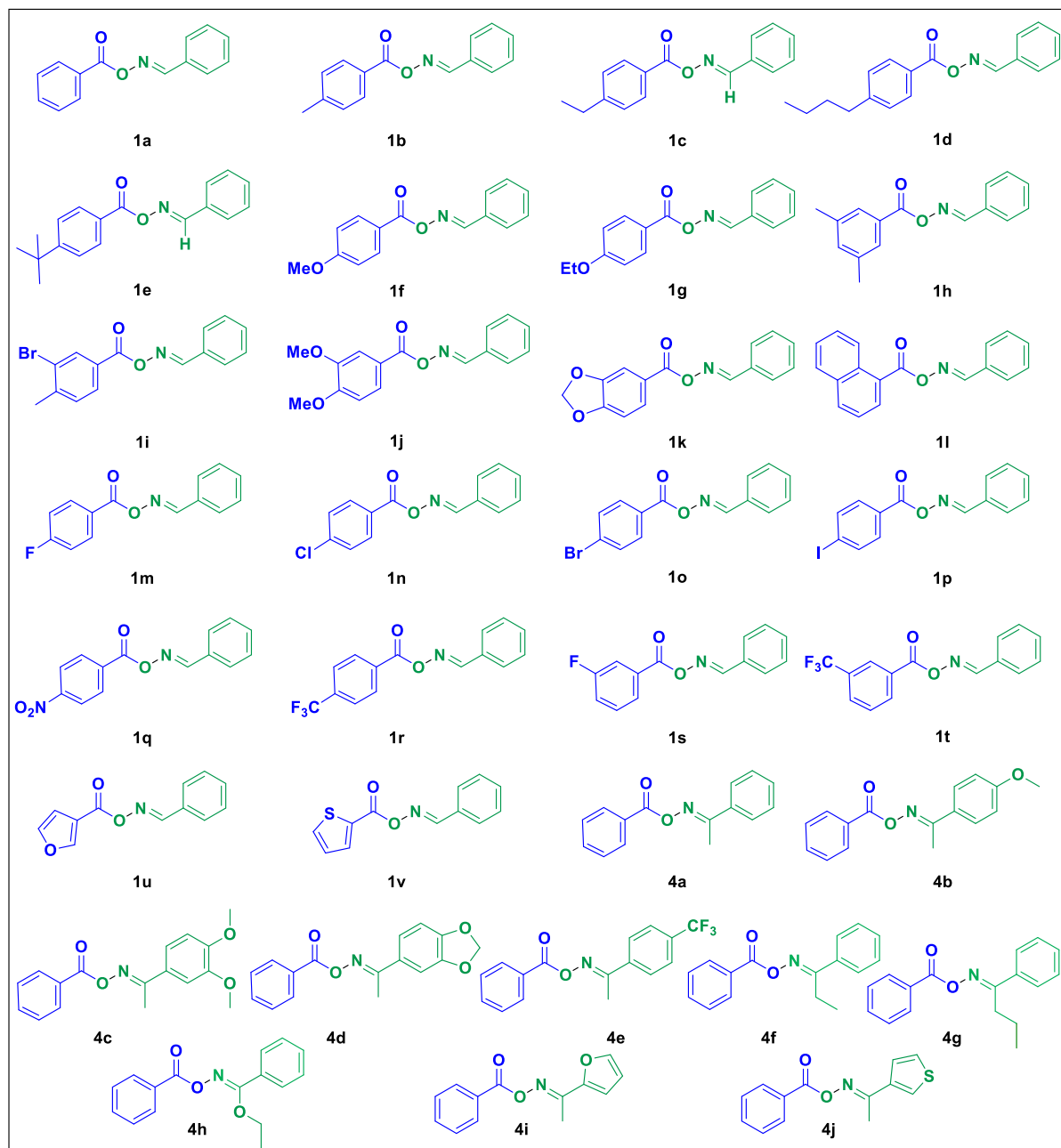
4. Proposed Catalytic Cycle



Based on the above mechanistic findings, and literature precedents, a plausible catalytic cycle is depicted above. The active Rh(III)-species **A** is generated from Rh(III)-dimer in presence of NaOAc. The *O*-benzoyl oxime **1** undergoes cyclometalation with the active catalyst species **A** to form the rhodacyclic intermediate **I**. The intermediate **II** is generated by the coordination of alkyne **2** with the rhodacycle **I**. Subsequently, the 1,2-insertion of the coordinated alkyne in the intermediate **II** leads to the generation of seven-membered rhodacycle intermediate **III**. The isocoumarin product **3** is generated by C–O bond formation, and N–O bond cleavage of intermediate **III** via a redox neutral manner to furnish imine, and active Rh(III) species **A**.

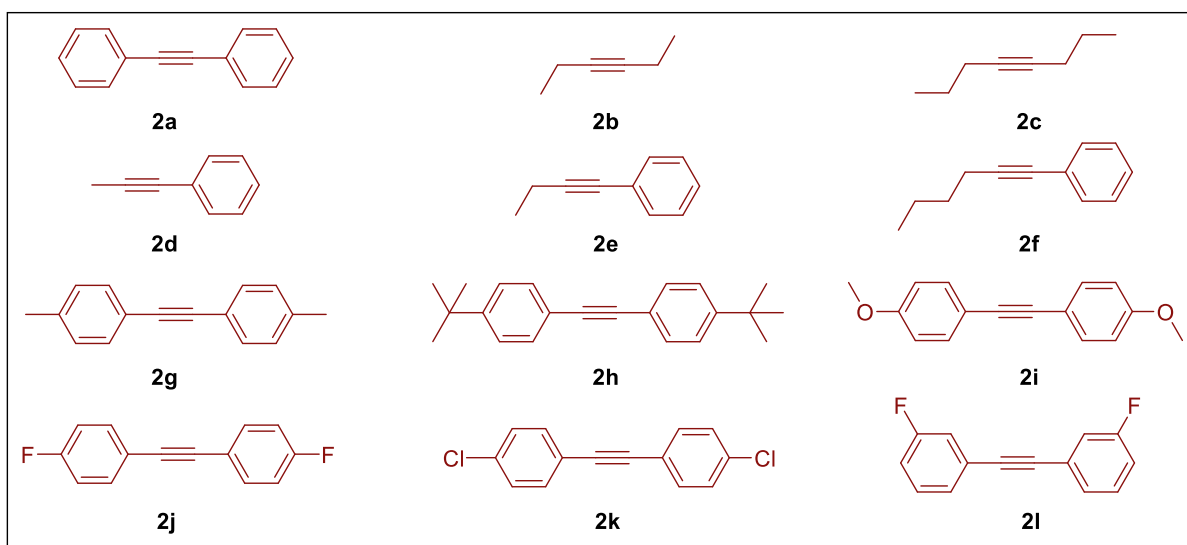
5. Experimental characterization data for the starting materials and products

O-benzoyl oximes used in this study:



O-benzoyl oxime 1a, 1b, 1c, 1d, 1e, 1f, 1g, 1h, 1i, 1j, 1k, 1l, 1m, 1n, 1o, 1p, 1q, 1r, 1s, 1t, 1u, 1v, 4a, 4b, 4c, 4d, 4e, 4f, and 4g, 4h, 4i, 4j were synthesized according to the previously reported procedure¹ (general procedure A and B).

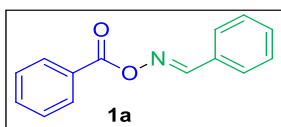
Alkynes used in this study:



Alkynes **2a**, **2b**, **2c**, **2d**, **2e**, **2f**, **2g**, **2h**, **2i**, **2j**, **2k**, and **2l** were synthesized according to the reported literature procedure^{2,3} and spectroscopic data were identical to those.

5.1 Experimental characterization data for the benzoyl oximes:

(*E*)-benzaldehyde *O*-benzoyl oxime (**1a**)



1a was prepared according to general procedure A. The crude reaction mixture was purified by column chromatography using silica gel (100-200 mesh) giving **1a** (207 mg) in 92% yield.

Physical State: Colorless solid

m.p.: 110-112 °C

R_f-value: 0.45 (10% EtOAc/hexane)

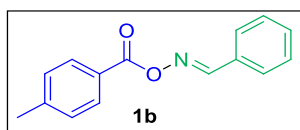
¹H NMR (400 MHz, CDCl₃): δ 8.29 (s, 1H), 7.90 (d, J = 7.2 Hz, 2H), 7.56 (d, J = 6.8 Hz, 2H), 7.32 (t, J = 7.2 Hz, 1H), 7.22-7.12 (m, 5H).

¹³C NMR (100 MHz, CDCl₃): δ 163.6, 156.6, 133.2, 131.4, 129.8, 129.4, 128.6, 128.35, 128.31, 128.2.

IR (KBr, cm⁻¹): 3098, 3068, 2927, 2857, 1736, 1638, 1488, 1447, 1350, 1283, 1217, 1084.

HRMS (ESI) m/z: [M+Na]⁺ Calcd for C₁₄H₁₁NaNO₂ 248.0682; Found 248.0682.

(E)-benzaldehyde O-(4-methylbenzoyl) oxime (1b)



1b was prepared according to general procedure A. The crude reaction mixture was purified by column chromatography using silica gel (100-200 mesh) giving **1b** (215 mg) in 90% yield.

Physical State: Colorless solid

m.p.: 138-140 °C

R_f-value: 0.45 (10% EtOAc/hexane)

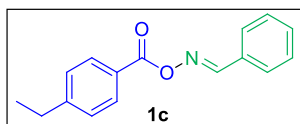
¹H NMR (400 MHz, CDCl₃): δ 8.46 (s, 1H), 7.94 (d, *J* = 8.0 Hz, 2H), 7.72 (d, *J* = 6.8 Hz, 2H), 7.42-7.35 (m, 3H), 7.20 (d, *J* = 8.0 Hz, 2H), 2.34 (s, 3H).

¹³C NMR (100 MHz, CDCl₃): δ 164.3, 156.9, 144.5, 132.0, 130.5, 130.0, 129.6, 129.2, 128.7, 126.1, 22.0.

IR (KBr, cm⁻¹): 3095, 3079, 3037, 2944 2920, 1730, 1684, 1653, 1625, 1589, 1507, 1465.

HRMS (ESI) m/z: [M+Na]⁺ Calcd for C₁₅H₁₃NaNO₂: 262.0838; Found 262.0851.

(E)-benzaldehyde O-(4-ethylbenzoyl) oxime (1c)



1c was prepared according to general procedure A. The crude reaction mixture was purified by column chromatography using silica gel (100-200 mesh) giving **1c** (223 mg) in 88% yield.

Physical State: Colorless solid

m.p.: 122-124 °C

R_f-value: 0.45 (10% EtOAc/hexane)

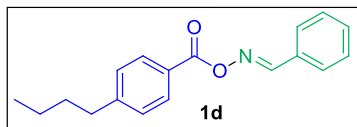
¹H NMR (700 MHz, CDCl₃): δ 8.55 (s, 1H), 8.04 (d, *J* = 8.4 Hz, 2H), 7.82 (d, *J* = 7.7 Hz, 2H), 7.50-7.48 (m, 1H), 7.45 (t, *J* = 7.7 Hz, 2H), 7.32 (d, *J* = 8.4 Hz, 2H), 2.74 (q, *J* = 7.7 Hz, 2H), 1.28 (t, *J* = 7.7 Hz, 3H).

¹³C NMR (176 MHz, CDCl₃): δ 164.2, 156.7, 150.5, 131.8, 130.3, 130.0, 129.0, 128.6, 128.2, 126.1, 29.1, 15.3.

IR (KBr, cm⁻¹): 3061, 3034, 2972, 2905, 2876, 1732, 1688, 1610, 1572, 1509, 1448.

HRMS (ESI) m/z: [M+Na]⁺ Calcd for C₁₆H₁₅NaNO₂: 276.0995; Found 276.0987.

(E)-benzaldehyde O-(4-butylbenzoyl) oxime (1d)



1d was prepared according to general procedure A. The crude reaction mixture was purified by column chromatography using silica gel (100-200 mesh) giving **1d** (236 mg) in 84% yield.

Physical State: Colorless solid

m.p.: 94-96 °C

R_f-value: 0.50 (10% EtOAc/hexane)

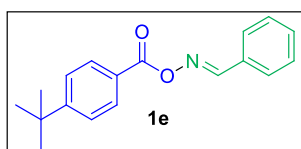
¹H NMR (400 MHz, CDCl₃): δ 8.46 (s, 1H), 7.96 (d, *J* = 8.0 Hz, 2H), 7.73 (d, *J* = 6.4 Hz, 2H), 7.41-7.34 (m, 3H), 7.21 (d, *J* = 8.0 Hz, 2H), 2.60 (t, *J* = 7.6 Hz, 2H), 1.52 (quint, *J* = 7.2 Hz, 2H), 1.33-1.24 (m, 2H), 0.86 (t, *J* = 7.2 Hz, 3H).

¹³C NMR (100 MHz, CDCl₃): δ 164.3, 156.8, 149.4, 132.0, 130.5, 130.1, 129.2, 128.9, 128.8, 126.3, 36.0, 33.5, 22.6, 14.2.

IR (KBr, cm⁻¹): 3084, 3018, 2957, 2926, 2870, 2846, 1736, 1682, 1653, 1614, 1575, 1506, 1488.

HRMS (ESI) m/z: [M+Na]⁺ Calcd for C₁₈H₁₉NaNO₂: 304.1308; Found 304.1312.

(E)-benzaldehyde O-(4-(tert-butyl)benzoyl) oxime (1e)



1e was prepared according to general procedure A. The crude reaction mixture was purified by column chromatography using silica gel (100-200 mesh) giving **1e** (234 mg) in 83% yield.

Physical State: Colorless solid

m.p.: 123-125 °C

R_f-value: 0.45 (10% EtOAc/hexane)

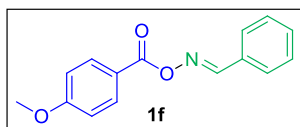
¹H NMR (400 MHz, CDCl₃): δ 8.42 (s, 1H), 7.94 (d, *J* = 8.4 Hz, 2H), 7.67 (d, *J* = 7.2 Hz, 2H), 7.36 (d, *J* = 8.4 Hz, 2H), 7.33-7.27 (m, 3H), 1.21 (s, 9H).

¹³C NMR (100 MHz, CDCl₃): δ 164.0, 157.2, 156.7, 131.8, 130.3, 129.7, 129.0, 128.6, 125.9, 125.6, 35.2, 31.2.

IR (KBr, cm⁻¹): 3057, 3022, 2963, 2910, 2869, 1735, 1678, 1638, 1610, 1537, 1463.

HRMS (ESI) m/z: [M+Na]⁺ Calcd for C₁₈H₁₉NaNO₂: 304.1308; Found 304.1319.

(E)-benzaldehyde O-(4-methoxybenzoyl) oxime (1f)



1f was prepared according to general procedure A. The crude reaction mixture was purified by column chromatography using silica gel (100-200 mesh) giving **1f** (205 mg) in 91% yield.

Physical State: Colorless solid

m.p.: 104-106 °C

R_f-value: 0.45 (20% EtOAc/hexane)

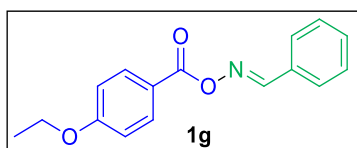
¹H NMR (400 MHz, CDCl₃): δ 8.38 (s, 1H), 7.95 (d, *J* = 8.8 Hz, 2H), 7.66 (d, *J* = 6.8 Hz, 2H), 7.34-7.27 (m, 3H), 6.81 (d, *J* = 8.8 Hz, 2H), 3.70 (s, 3H).

¹³C NMR (100 MHz, CDCl₃): δ 163.9, 163.8, 156.5, 131.9, 131.7, 130.4, 129.0, 128.5, 120.8, 114.0, 55.5.

IR (KBr, cm⁻¹): 3069, 3021, 2935, 2843, 1727, 1684, 1652, 1604, 1558, 1512, 1455, 1250, 1167.

HRMS (ESI) m/z: [M+Na]⁺ Calcd for C₁₅H₁₃NaNO₃: 278.0788; Found 278.0805.

(E)-benzaldehyde O-(4-ethoxybenzoyl) oxime (1g)



1g was prepared according to general procedure A. The crude reaction mixture was purified by column chromatography using silica gel (100-200 mesh) giving **1g** (240 mg) in 89% yield.

Physical State: Colorless solid

m.p.: 113-115 °C

R_f-value: 0.45 (20% EtOAc/hexane)

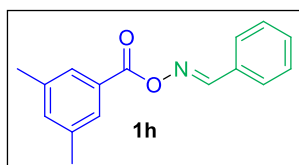
¹H NMR (400 MHz, CDCl₃): δ 8.38 (s, 1H), 7.93 (d, *J* = 8.8 Hz, 2H), 7.66 (d, *J* = 6.8 Hz, 2H), 7.35-7.26 (m, 3H), 6.79 (d, *J* = 8.8 Hz, 2H), 3.93 (q, *J* = 6.8 Hz, 2H), 1.29 (t, *J* = 6.8 Hz, 3H).

¹³C NMR (100 MHz, CDCl₃): δ 163.8, 163.3, 156.5, 131.9, 131.7, 130.4, 129.0, 128.5, 120.6, 114.4, 63.8, 14.7.

IR (KBr, cm⁻¹): 3097, 3049, 3008, 2982, 2925, 2813, 1733, 1684, 1627, 1608, 1576, 1511, 1449, 1266, 1248.

HRMS (ESI) m/z: [M+Na]⁺ Calcd for C₁₆H₁₅NaNO₃ 292.0944; Found 292.0956.

(E)-benzaldehyde O-(3,5-dimethylbenzoyl) oxime (1h)



1h was prepared according to general procedure A. The crude reaction mixture was purified by column chromatography using silica gel (100-200 mesh), giving **1h** (208 mg) in 82% yield.

Physical State: Colorless semi-solid

m.p.: 154-157 °C

R_f-value: 0.45 (10% EtOAc/hexane)

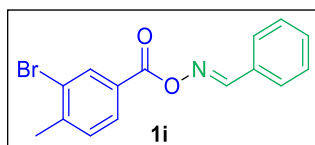
¹H NMR (400 MHz, CDCl₃): δ 8.46 (s, 1H), 7.71 (d, *J* = 7.2 Hz, 2H), 7.65 (s, 2H), 7.41-7.33 (m, 3H), 7.13 (s, 1H), 2.29 (s, 6H).

¹³C NMR (100 MHz, CDCl₃): δ 164.5, 156.9, 138.5, 135.4, 132.0, 130.4, 129.1, 128.76, 128.72, 127.7, 21.4.

IR (KBr, cm⁻¹): 3065, 3010, 2919, 2863, 1742, 1688, 1609, 1575, 1475, 1447, 1381, 1305, 1191.

HRMS (ESI) m/z: [M+Na]⁺ Calcd for C₁₆H₁₅NaNO₂: 276.0955; Found 276.0985.

(E)-benzaldehyde O-(3-bromo-4-methylbenzoyl) oxime (1i)



1i was prepared according to general procedure A. The crude reaction mixture was purified by column chromatography using silica gel (100-200 mesh) giving **1i** (258 mg) in 81% yield.

Physical State: Colorless solid

m.p.: 92-94 °C

R_f-value: 0.40 (10% EtOAc/hexane)

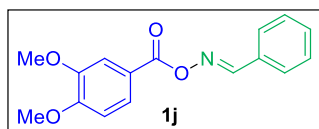
¹H NMR (400 MHz, CDCl₃): δ 8.42 (s, 1H), 8.15 (d, *J* = 1.2 Hz, 1H), 7.83 (dd, *J* = 8.0, 1.6 Hz, 1H), 7.68 (d, *J* = 7.2 Hz, 2H), 7.39-7.30 (m, 3H), 7.20 (d, *J* = 8.0 Hz, 1H), 2.34 (s, 3H).

¹³C NMR (100 MHz, CDCl₃): δ 162.8, 157.1, 144.1, 133.6, 132.0, 131.1, 130.1, 129.1, 128.7, 128.0, 125.1, 23.4.

IR (KBr, cm⁻¹): 3097, 3077, 3049, 2996, 2918, 2847, 1751, 1686, 1624, 1603, 1556, 1485, 1384, 1279.

HRMS (ESI) m/z: [M+Na]⁺ Calcd for C₁₅H₁₂BrNaNO₂ 339.9944; Found 339.9931.

(E)-benzaldehyde O-(3,4-dimethoxybenzoyl) oxime (1j)



1j was prepared according to general procedure A. The crude reaction mixture was purified by column chromatography using silica gel (100-200 mesh) giving **1j** (248 mg) in 87% yield.

Physical State: Colorless solid

m.p.: 99-101 °C

R_f-value: 0.40 (30% EtOAc/hexane)

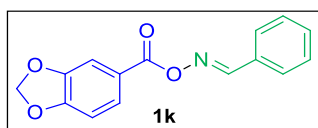
¹H NMR (400 MHz, CDCl₃): δ 8.41 (s, 1H), 7.66-7.61 (m, 3H), 7.47 (d, *J* = 1.6 Hz, 1H), 7.36-7.27 (m, 3H), 6.77 (d, *J* = 8.8 Hz, 1H), 3.80 (s, 3H), 3.79 (s, 3H).

¹³C NMR (100 MHz, CDCl₃): δ 163.7, 156.5, 153.4, 148.8, 131.7, 130.2, 128.9, 128.4, 123.8, 120.8, 112.1, 110.4, 56.0.

IR (KBr, cm⁻¹): 3086, 3065, 3005, 2964, 2934, 2834, 1736, 1598, 1514, 1462, 1417, 1345, 1270, 1213, 1172.

HRMS (ESI) m/z: [M+Na]⁺ Calcd for C₁₆H₁₅NaNO₄: 308.0893; Found 308.0899.

(E)-benzaldehyde O-(benzo[d][1,3]dioxole-5-carbonyl) oxime (1k)



1k was prepared according to general procedure A. The crude reaction mixture was purified by column chromatography using silica gel (100-200 mesh) giving **1k** (226 mg) in 84% yield.

Physical State: Colorless solid

m.p.: 128-130 °C

R_f-value: 0.44 (20% EtOAc/hexane)

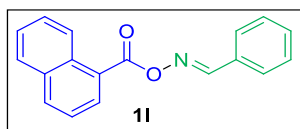
¹H NMR (400 MHz, CDCl₃): δ 8.51 (s, 1H), 7.80 (dd, *J* = 8.0, 1.2 Hz, 2H), 7.75 (dd, *J* = 8.4, 2.0 Hz, 1H), 7.55 (d, *J* = 1.6 Hz, 1), 7.50-7.43 (m, 3H), 6.89 (d, *J* = 8.4 Hz, 1H), 6.07 (s, 2H).

¹³C NMR (176 MHz, CDCl₃): δ 163.5, 156.6, 152.2, 148.0, 131.8, 130.3, 129.0, 128.6, 125.7, 122.4, 109.6, 108.3, 102.1.

IR (KBr, cm⁻¹): 3078, 3056, 3011, 2904, 2843, 1729, 1683, 1653, 1607, 1559, 1503, 1365, 1263, 1216, 1151.

HRMS (ESI) m/z: [M+Na]⁺ Calcd for C₁₅H₁₁NaNO₄: 292.0580; Found 292.0581.

(E)-benzaldehyde O-(1-naphthoyl) oxime (1l)



1l was prepared according to general procedure A. The crude reaction mixture was purified by column chromatography using silica gel (100-200 mesh) giving **1l** (223 mg) in 81% yield.

Physical State: Colorless solid

m.p.: 69-71 °C

R_f-value: 0.40 (10% EtOAc/hexane)

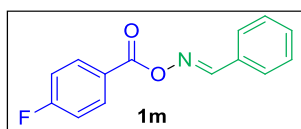
¹H NMR (400 MHz, CDCl₃): δ 8.76 (d, *J* = 8.8 Hz, 1H), 8.38 (s, 1H), 8.05 (dd, *J* = 7.6, 0.8 Hz, 1H), 7.87 (d, *J* = 8.4 Hz, 1H), 7.72 (d, *J* = 8.0 Hz, 1H), 7.66 (dd, *J* = 6.8, 1.2 Hz, 2H), 7.48 (td, *J* = 7.6, 1.2 Hz, 1H), 7.39 (d, *J* = 0.8 Hz, 1H), 7.37-7.35 (m, 4H).

¹³C NMR (100 MHz, CDCl₃): δ 165.0, 157.0, 134.0, 133.9, 131.9, 131.5, 130.3, 130.1, 129.1, 128.8, 128.6, 128.2, 126.6, 125.8, 125.7, 124.6.

IR (KBr, cm⁻¹): 3054, 3032, 3001, 2934, 2906, 2853, 2810, 1732, 1652, 1613, 1574, 1509, 1461, 1371.

HRMS (ESI) m/z: [M+Na]⁺ Calcd for C₁₈H₁₃NaNO₂: 298.0838; Found 298.0843.

(E)-benzaldehyde O-(4-fluorobenzoyl) oxime (1m)



1m was prepared according to general procedure A. The crude reaction mixture was purified by column chromatography using silica gel (100-200 mesh) giving **1m** (195 mg) in 80% yield.

Physical State: Colorless solid

m.p.: 117-119 °C

R_f-value: 0.40 (10% EtOAc/hexane)

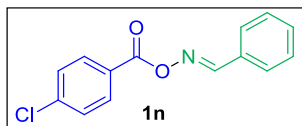
¹H NMR (400 MHz, CDCl₃): δ 8.45 (s, 1H), 8.06 (td, *J* = 7.2, 1.2 Hz, 2H), 7.71 (d, *J* = 6.8 Hz, 2H), 7.42-7.33 (m, 3H), 7.07 (td, *J* = 8.8, 2.0 Hz, 2H).

¹³C NMR (100 MHz, CDCl₃): δ 166.2 (d, *J*_{C-F} = 254 Hz), 163.2, 157.1, 132.6 (d, *J*_{C-F} = 10 Hz), 132.1, 130.0, 129.2, 128.8, 125.1 (d, *J*_{C-F} = 3 Hz), 116.1 (d, *J*_{C-F} = 22 Hz).

IR (KBr, cm⁻¹): 3117, 3098, 3048, 3016, 1741, 1684, 1625, 1589, 1506, 1474, 1408, 1351, 1293.

HRMS (ESI) m/z: [M+Na]⁺ Calcd for C₁₄H₁₀FNANO₂: 266.0588; Found 266.0587.

(E)-benzaldehyde O-(4-chlorobenzoyl) oxime (1n)



1n was prepared according to general procedure A. The crude reaction mixture was purified by column chromatography using silica gel (100-200 mesh) giving **1n** (216 mg) in 83% yield.

Physical State: Colorless solid

m.p.: 125-127 °C

R_f-value: 0.40 (10% EtOAc/hexane)

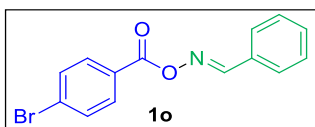
¹H NMR (400 MHz, CDCl₃): δ 8.44 (s, 1H), 7.96 (d, *J* = 8.8 Hz, 2H), 7.70 (d, *J* = 7.2 Hz, 2H), 7.42-7.33 (m, 5H).

¹³C NMR (100 MHz, CDCl₃): δ 163.3, 157.2, 140.2, 132.1, 131.3, 130.2, 129.2, 128.7, 127.3.

IR (KBr, cm⁻¹): 3101, 3077, 3052, 3013, 2945, 2916, 1742, 1630, 1607, 1580, 1530, 1469, 1399, 1351, 1295.

HRMS (ESI) m/z: [M+Na]⁺ Calcd for C₁₄H₁₀ClNaNO₂ 282.0292; Found 282.0296.

(E)-benzaldehyde O-(4-bromobenzoyl) oxime (1o)



1o was prepared according to general procedure A. The crude reaction mixture was purified by column chromatography using silica gel (100-200 mesh) giving **1o** (237 mg) in 78% yield.

Physical State: Colorless solid

m.p.: 132-134 °C

R_f-value: 0.40 (10% EtOAc/hexane)

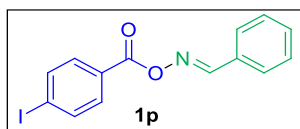
¹H NMR (400 MHz, CDCl₃): δ 8.44 (s, 1H), 7.87 (d, *J* = 8.4 Hz, 2H), 7.69 (d, *J* = 6.8 Hz, 2H), 7.51 (d, *J* = 8.4 Hz, 2H), 7.41-7.32 (m, 3H).

¹³C NMR (100 MHz, CDCl₃): δ 163.4, 157.2, 132.19, 132.15, 131.4, 130.1, 129.2, 128.8, 128.7, 127.7.

IR (KBr, cm⁻¹): 3087, 3064, 3028, 2948, 2917, 1746, 1651, 1613, 1572, 1536, 1483, 1398, 1356, 1296.

HRMS (ESI) m/z: [M+Na]⁺ Calcd for C₁₄H₁₀BrNaNO₂ 325.9787; Found 325.9785.

(E)-benzaldehyde O-(4-iodobenzoyl) oxime (1p)



1p was prepared according to general procedure A. The crude reaction mixture was purified by column chromatography using silica gel (100-200 mesh) giving **1p** (253 mg) in 72% yield.

Physical State: Colorless solid

m.p.: 140-142 °C

R_f-value: 0.40 (10% EtOAc/hexane)

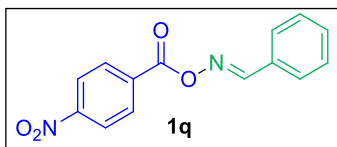
¹H NMR (400 MHz, CDCl₃): δ 8.44 (s, 1H), 7.76-7.68 (m, 6H), 7.43-7.32 (m, 3H).

¹³C NMR (100 MHz, CDCl₃): δ 163.7, 157.3, 138.2, 132.1, 131.3, 130.2, 129.2, 128.8, 128.3, 101.6.

IR (KBr, cm⁻¹): 3084, 3058, 3012, 2943, 2917, 2848, 1752, 1683, 1653, 1606, 1576, 1540, 1473, 1457.

HRMS (ESI) m/z: [M+Na]⁺ Calcd for C₁₄H₁₀INaNO₂ 373.9648; Found 373.9651.

(E)-benzaldehyde O-(4-nitrobenzoyl) oxime (1q)



1q was prepared according to general procedure A. The crude reaction mixture was purified by column chromatography using silica gel (100-200 mesh) giving **1q** (208 mg) in 77% yield.

Physical State: Colorless solid

m.p.: 166-168 °C

R_f-value: 0.40 (20% EtOAc/hexane)

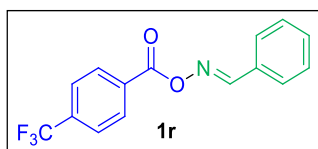
¹H NMR (400 MHz, CDCl₃): δ 8.50 (s, 1H), 8.23 (q, *J* = 9.2 Hz, 4H), 8.72 (d, *J* = 6.8 Hz, 2H), 7.46-7.37 (m, 3H).

¹³C NMR (100 MHz, CDCl₃): δ 162.4, 157.9, 151.0, 134.4, 132.5, 131.1, 129.9, 129.3, 128.9, 124.0.

IR (KBr, cm⁻¹): 3114, 3077, 3056, 3020, 2986, 2936, 2875, 1729, 1684, 1636, 1576, 1508, 1472, 1457, 1419, 1242.

HRMS (ESI) m/z: [M+Na]⁺ Calcd for C₁₄H₁₀NaN₂O₄ 293.0533; Found 293.0528.

(E)-benzaldehyde O-(4-(trifluoromethyl)benzoyl) oxime (1r)



1r was prepared according to general procedure A. The crude reaction mixture was purified by column chromatography using silica gel (100-200 mesh) giving **1r** (220 mg) in 75% yield.

Physical State: Colorless solid

m.p.: 141-143 °C

R_f-value: 0.40 (10% EtOAc/hexane)

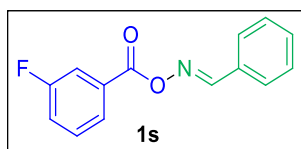
¹H NMR (400 MHz, CDCl₃): δ 8.47 (s, 1H), 8.14 (d, *J* = 8.0 Hz, 2H), 7.71 (d, *J* = 7.6 Hz, 2H), 7.65 (d, *J* = 7.2 Hz, 2H), 7.43-7.34 (m, 3H).

¹³C NMR (100 MHz, CDCl₃): δ 163.0, 157.6, 135.1 (q, *J*_{C-F} = 33.0 Hz), 132.3, 132.2, 130.4, 130.1, 129.8, 128.8, 125.8 (q, *J*_{C-F} = 4.0 Hz), 123.8 (q, *J*_{C-F} = 271.0 Hz).

IR (KBr, cm⁻¹): 3097, 3054, 3015, 2949, 2924, 1754, 1652, 1621, 1588, 1513, 1470, 1409, 1359, 1297, 1170, 1157.

HRMS (ESI) m/z: [M+Na]⁺ Calcd for C₁₅H₁₀F₃NaNO₂: 316.0556; Found 316.0563.

(E)-benzaldehyde O-(3-fluorobenzoyl) oxime (1s)



1s was prepared according to general procedure A. The crude reaction mixture was purified by column chromatography using silica gel (100-200 mesh) giving **1s** (175 mg) in 72% yield.

Physical State: Colorless solid

m.p.: 107-109 °C

R_f-value: 0.40 (10% EtOAc/hexane)

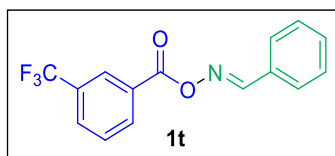
¹H NMR (400 MHz, CDCl₃): δ 8.44 (s, 1H), 7.81 (d, *J* = 7.6 Hz, 1H), 7.69 (d, *J* = 7.2 Hz, 3H), 7.40-7.31 (m, 4H), 7.20 (td, *J* = 8.4, 4.0 Hz, 1H).

¹³C NMR (100 MHz, CDCl₃): δ 163.0 (d, *J*_{C-F} = 3 Hz), 162.8 (d, *J*_{C-F} = 246 Hz), 157.3, 132.1, 130.9 (d, *J*_{C-F} = 7 Hz), 130.5 (d, *J*_{C-F} = 8 Hz), 130.1, 129.2, 128.7, 125.7 (d, *J*_{C-F} = 3 Hz), 120.2 (d, *J*_{C-F} = 21 Hz), 116.8 (d, *J*_{C-F} = 23 Hz).

IR (KBr, cm⁻¹): 3064, 3011, 2917, 2850, 1732, 1614, 1590, 1575, 1484, 1444, 1349, 1286, 1270, 1185, 1057.

HRMS (ESI) m/z: [M+Na]⁺ Calcd for C₁₄H₁₀FNANO₂: 266.0588; Found 266.0593.

(E)-benzaldehyde O-(3-(trifluoromethyl)benzoyl) oxime (1t)



1t was prepared according to general procedure A. The crude reaction mixture was purified by column chromatography using silica gel (100-200 mesh) giving **1t** (226 mg) in 77% yield.

Physical State: Colorless solid

m.p.: 75-77 °C

R_f-value: 0.40 (10% EtOAc/hexane)

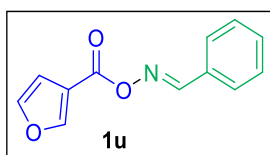
¹H NMR (400 MHz, CDCl₃): δ 8.48 (s, 1H), 8.27 (s, 1H), 8.21 (d, *J* = 7.6 Hz, 1H), 7.75 (d, *J* = 7.6 Hz, 1H), 7.70 (d, *J* = 7.2 Hz, 2H), 7.52 (t, *J* = 8.0 Hz, 1H), 7.41-7.32 (m, 3H).

¹³C NMR (100 MHz, CDCl₃): δ 162.9, 157.6, 133.2, 132.2, 131.5 (q, *J*_{C-F} = 33.0 Hz), 130.1 (q, *J*_{C-F} = 4.0 Hz), 130.0, 129.8, 129.6, 129.2, 128.8, 126.7 (q, *J*_{C-F} = 4.0 Hz), 123.8 (q, *J*_{C-F} = 271.0 Hz).

IR (KBr, cm⁻¹): 3098, 3052, 3027, 2996, 1755, 1616, 1589, 1575, 1488, 1447, 1334, 1296.

HRMS (ESI) m/z: [M+Na]⁺ Calcd for C₁₅H₁₀F₃NaNO₂: 316.0556; Found 316.0558.

(E)-benzaldehyde O-furan-3-carbonyl oxime (1u)



1u was prepared according to general procedure A. The crude reaction mixture was purified by column chromatography using silica gel (100-200 mesh) giving **1u** (146 mg) in 68% yield.

Physical State: Brown gel

R_f-value: 0.60 (20% EtOAc/hexane)

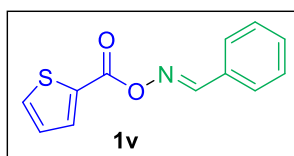
¹H NMR (700 MHz, CDCl₃): δ 8.47 (s, 1H), 8.14 (s, 1H), 7.78 (d, *J* = 7.0 Hz, 2H), 7.48-7.47 (m, 2H), 7.43 (t, *J* = 7.7 Hz, 2H), 6.85 (d, *J* = 1.4 Hz, 1H).

¹³C NMR (100 MHz, CDCl₃): δ 160.7, 156.8, 148.4, 144.3, 132.0, 130.3, 129.2, 128.7, 117.6, 110.1.

IR (KBr, cm⁻¹): 3151, 3134, 3061, 3002, 2956, 2916, 2810, 1754, 1652, 1575, 1507, 1473, 1448.

HRMS (ESI) m/z: [M+Na]⁺ Calcd for C₁₂H₉NO₃Na 238.0475; Found 238.0489.

(E)-benzaldehyde O-thiophene-2-carbonyl oxime (1v)



1v was prepared according to general procedure A. The crude reaction mixture was purified by column chromatography using silica gel (100-200 mesh) giving **1v** (146 mg) in 63% yield.

Physical State: Colorless semi-solid

R_f-value: 0.60 (20% EtOAc/hexane)

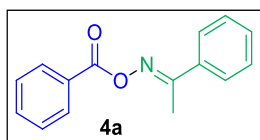
¹H NMR (700 MHz, CDCl₃): δ 8.51 (s, 1H), 7.94 (dd, J = 3.5, 1.4 Hz, 1H), 7.79 (d, J = 7.0 Hz, 2H), 7.63 (dd, J = 4.9, 1.4 Hz, 1H), 7.48 (t, J = 7.7 Hz, 1H), 7.44 (t, J = 7.7 Hz, 2H), 7.15 (t, J = 4.2 Hz, 1H).

¹³C NMR (176 MHz, CDCl₃): δ 159.9, 156.9, 134.6, 133.4, 132.1, 131.4, 130.2, 129.2, 128.8, 128.2.

IR (KBr, cm⁻¹): 3123, 3048, 2942, 2860, 1721, 1671, 1626, 1574, 1522, 1446, 1414, 1358, 1256.

HRMS (ESI) m/z: [M+Na]⁺ Calcd for C₁₂H₉NO₂SNa 254.0252; Found 254.0254.

(E)-1-phenylethan-1-one O-benzoyl oxime (4a)



4a was prepared according to general procedure C. The crude reaction mixture was purified by column chromatography using silica gel (100-200 mesh) giving **4a** (187 mg) in 78 % yield.

Physical State: white solid, **m.p.:** 103-105 °C.

R_f-value: 0.50 (15% EtOAc/hexane).

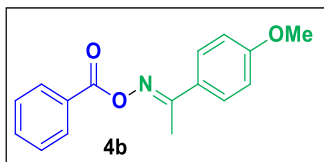
¹H NMR (400 MHz, CDCl₃): δ 8.14 (d, J = 7.2 Hz, 2H), 7.83 (dd, J = 8.0, 1.6 Hz, 2H), 7.62 (tt, J = 7.2, 1.2 Hz, 1H), 7.52-7.41 (m, 5H), 2.53 (s, 3H).

¹³C NMR (100 MHz, CDCl₃): δ 164.1, 163.9, 135.1, 133.6, 131.0, 129.9, 129.4, 128.93, 128.91, 127.4, 15.0.

IR (KBr, cm⁻¹): 3058, 2956, 2919, 2850, 1741, 1598, 1449, 1374, 1240, 1175.

HRMS (ESI) m/z: [M+Na]⁺ Calcd for C₁₅H₁₃NO₂Na: 262.0844; Found 262.0854.

(E)-1-(4-methoxyphenyl)ethanone *O*-benzoyl oxime (4b)



4b was prepared according to general procedure C. The crude reaction mixture was purified by column chromatography using silica gel (100-200 mesh) giving **4b** (199 mg) in 74 % yield.

Physical State: white flake solid, **m.p.:** 111-114 °C.

R_f-value: 0.40 (15% EtOAc/hexane).

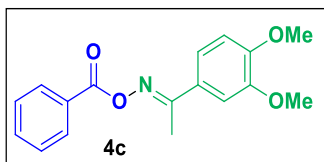
¹H NMR (400 MHz, CDCl₃): δ 8.13 (d, *J* = 7.2 Hz, 2H), 7.80 (d, *J* = 8.8 Hz, 2H), 7.61 (t, *J* = 7.2 Hz, 1H), 7.49 (t, *J* = 8.0 Hz, 2H), 6.94 (d, *J* = 6.8 Hz, 2H), 3.85 (s, 3H), 2.49 (s, 3H).

¹³C NMR (176 MHz, CDCl₃): δ 164.2, 163.3, 162.0, 133.5, 129.9, 129.7, 129.0, 128.9, 127.4, 114.2, 55.7, 14.7.

IR (KBr, cm⁻¹): 3008, 2969, 2933, 2838, 1729, 1594, 1448, 1248, 1176, 1092.

HRMS (ESI) m/z: [M+Na]⁺ Calcd for C₁₆H₁₅NO₃Na: 292.0950; Found 292.0970.

(E)-1-(3,4-dimethoxyphenyl)ethanone *O*-benzoyl oxime (4c)



4c was prepared according to general procedure C. The crude reaction mixture was purified by column chromatography using silica gel (100-200 mesh) giving **4c** (165 mg) in 55 % yield.

Physical State: pale yellow solid, **m.p.:** 125-127 °C.

R_f-value: 0.40 (30% EtOAc/hexane).

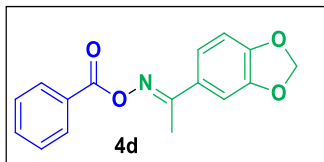
¹H NMR (400 MHz, CDCl₃): δ 8.13 (dd, *J* = 7.2, 1.2 Hz, 2H), 7.62 (tt, *J* = 7.2, 1.2 Hz, 1H), 7.50 (t, *J* = 7.6 Hz, 3H), 7.32 (dd, *J* = 8.4, 2.4 Hz, 1H), 6.89 (d, *J* = 8.4 Hz, 1H), 3.96 (s, 3H), 3.92 (s, 3H), 2.50 (s, 3H).

¹³C NMR (100 MHz, CDCl₃): δ 164.2, 163.4, 151.6, 149.2, 133.6, 129.9, 129.5, 128.9, 127.6, 121.0, 110.7, 109.7, 56.3, 56.2, 14.7.

IR (KBr, cm⁻¹): 3064, 3005, 2956, 2837, 1731, 1597, 1516, 1444, 1338, 1269, 1172, 1077.

HRMS (ESI) m/z: [M+Na]⁺ Calcd for C₁₇H₁₇NO₄Na: 322.1055; Found 322.1076.

(E)-1-(benzo[d][1,3]dioxol-5-yl)ethanone *O*-benzoyl oxime (4d)



4d was prepared according to general procedure C. The crude reaction mixture was purified by column chromatography using silica gel (100-200 mesh) giving **4d** (235 mg) in 83 % yield.

Physical State: white solid, **m.p.:** 133-135 °C.

R_f-value: 0.55 (15% EtOAc/hexane).

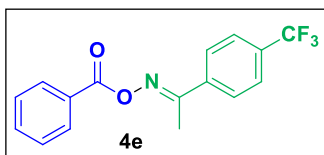
¹H NMR (400 MHz, CDCl₃): δ 8.12 (d, *J* = 7.2 Hz, 2H), 7.61 (t, *J* = 7.6 Hz, 1H), 7.49 (t, *J* = 7.6 Hz, 2H), 7.41 (s, 1H), 7.30 (d, *J* = 8.0 Hz, 1H), 6.84 (d, *J* = 8.4 Hz, 1H), 6.01 (s, 2H), 2.47 (s, 3H).

¹³C NMR (176 MHz, CDCl₃): δ 164.1, 163.2, 150.2, 148.4, 133.6, 129.9, 129.6, 129.1, 128.9, 122.2, 120.6, 108.4, 108.3, 107.5, 106.5, 101.9, 101.6, 14.9.

IR (KBr, cm⁻¹): 3058, 2895, 2792, 1728, 1589, 1504, 1313, 1227.

HRMS (ESI) m/z: [M+Na]⁺ Calcd for C₁₆H₁₃NO₄Na: 306.0742; Found 306.0767.

(E)-1-(4-(trifluoromethyl)phenyl)ethanone *O*-benzoyl oxime (4e)



4e was prepared according to general procedure C. The crude reaction mixture was purified by column chromatography using silica gel (100-200 mesh) giving **4e** (187 mg) in 61% yield.

Physical State: white solid, **m.p.:** 121-123 °C,

R_f-value: 0.50 (15% EtOAc/hexane).

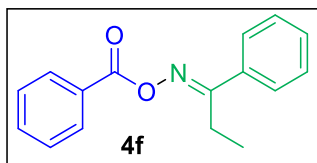
¹H NMR (400 MHz, CDCl₃): δ 8.14 (dd, *J* = 8.0, 1.2 Hz, 2H), 7.95 (d, *J* = 8.0 Hz, 2H), 7.70 (d, *J* = 8.0 Hz, 2H), 7.62 (d, *J* = 7.6 Hz, 1H), 7.51 (t, *J* = 8.0 Hz, 2H), 2.55 (s, 3H).

¹³C NMR (176 MHz, CDCl₃): δ 163.9, 162.6, 138.5, 133.9, 132.7 (q, *J*_{C-F} = 33.0 Hz), 130.0, 129.0, 127.8, 125.9 (q, *J*_{C-F} = 4.0 Hz), 125.6 (q, *J*_{C-F} = 4.0 Hz), 124.2 (q, *J*_{C-F} = 272.3 Hz), 15.0.

IR (KBr, cm⁻¹): 3071, 2931, 1741, 1619, 1452, 1403, 1327, 1242, 1153, 1112.

HRMS (ESI) m/z: [M+H]⁺ Calcd for C₁₆H₁₃F₃NO₂: 308.0898; Found 308.0894.

(E)-1-phenylpropan-1-one O-benzoyl oxime (4f)



4f was prepared according to general procedure C. The crude reaction mixture was purified by column chromatography using silica gel (100-200 mesh) giving **4f** (185 mg) in 73 % yield.

Physical State: white solid, **m.p:** 105-107 °C.

R_f-value: 0.50 (15% EtOAc/hexane).

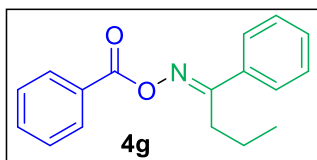
¹H NMR (400 MHz, CDCl₃): δ 8.12 (d, *J* = 6.8 Hz, 2H), 7.79 (d, *J* = 6.4 Hz, 2H), 7.61 (t, *J* = 7.6 Hz, 1H), 7.49 (t, *J* = 8.0 Hz, 2H), 7.46-7.40 (m, 3H), 2.98 (q, *J* = 7.6 Hz, 2H), 1.29 (t, *J* = 8.0 Hz, 3H).

¹³C NMR (176 MHz, CDCl₃): δ 168.6, 164.0, 133.9, 133.4, 130.7, 129.7, 129.3, 128.8, 128.7, 127.4, 22.3, 11.5.

IR (KBr, cm⁻¹): 3056, 2958, 2922, 2851, 1742, 1599, 1447, 1373, 1241, 1176.

HRMS (ESI) m/z: [M+Na]⁺ Calcd for C₁₆H₁₅NO₂Na: 276.1000; Found 276.1005.

(E)-1-phenylbutan-1-one O-benzoyl oxime (4g)



4g was prepared according to general procedure C. The crude reaction mixture was purified by column chromatography using silica gel (100-200 mesh) giving **4g** (187 mg) in 70 % yield.

Physical State: white solid, **m.p:** 106-108 °C.

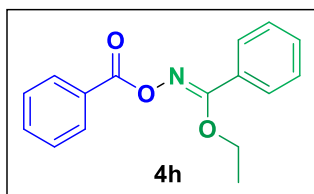
R_f-value: 0.50 (15% EtOAc/hexane).

¹H NMR (400 MHz, CDCl₃): δ 8.11 (d, *J* = 6.8 Hz, 2H), 7.78 (d, *J* = 6.4 Hz, 2H), 7.61 (t, *J* = 7.2 Hz, 1H), 7.49 (t, *J* = 8.0 Hz, 2H), 7.45-7.40 (m, 3H), 2.96 (t, *J* = 7.6 Hz, 2H), 1.70 (sextet, *J* = 7.6 Hz, 2H), 1.03 (t, *J* = 7.6 Hz, 3H).

¹³C NMR (176 MHz, CDCl₃): δ 167.5, 164.0, 134.2, 133.4, 130.7, 129.7, 129.3, 128.77, 128.75, 127.5, 30.6, 20.4, 14.4. **IR (KBr, cm⁻¹):** 3058, 2959, 2923, 2852, 1741, 1596, 1446, 1374, 1243, 1175.

HRMS (ESI) m/z: [M+Na]⁺ Calcd for C₁₇H₁₇NO₂Na: 290.1157; Found 290.1165.

Ethyl (*E*)-*N*-(benzyloxy)benzimidate (**4h**)



4h was prepared according to general procedure C. The crude reaction mixture was purified by column chromatography using silica gel (100-200 mesh) giving **4h** (199 mg) in 74 % yield.

Physical State: white solid, **m.p:** 111-113 °C.

R_f-value: 0.50 (15% EtOAc/hexane).

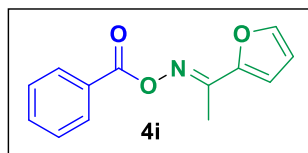
¹H NMR (400 MHz, CDCl₃): δ 7.92 – 7.84 (m, 2H), 7.69 – 7.62 (m, 2H), 7.55 – 7.42 (m, 4H), 7.38 (t, *J* = 7.8 Hz, 2H), 4.48 (q, *J* = 7.1 Hz, 2H), 1.45 (t, *J* = 7.1 Hz, 3H).

¹³C NMR (100 MHz, CDCl₃): δ 167.30, 164.08, 133.15, 130.96, 129.66, 129.60, 129.04, 128.72, 128.55, 128.27, 64.73, 14.45.

IR (KBr, cm⁻¹): 3057, 2956, 2921, 2852, 1743, 1598, 1446, 1375, 1242, 1175.

HRMS (ESI) m/z: [M+Na]⁺ Calcd for C₁₆H₁₆NO₃: 270.1130; Found 270.1125.

(*E*)-1-(furan-2-yl)ethan-1-one *O*-benzoyl oxime (**4i**)



4i was prepared according to general procedure C. The crude reaction mixture was purified by column chromatography using silica gel (100-200 mesh) giving **4i** (156 mg) in 68 % yield.

Physical State: white solid, **m.p:** 76-78 °C.

R_f-value: 0.45 (20% EtOAc/hexane).

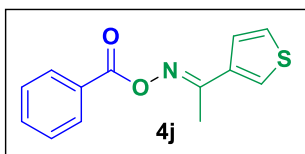
¹H NMR (400 MHz, CDCl₃): δ 8.15 – 8.05 (m, 2H), 7.64 – 7.53 (m, 2H), 7.54 – 7.42 (m, 2H), 6.98 (d, *J* = 3.5 Hz, 1H), 6.51 (dd, *J* = 3.5, 1.8 Hz, 1H), 2.44 (s, 3H).

¹³C NMR (100 MHz, CDCl₃): δ 163.57, 154.99, 148.35, 145.23, 133.47, 129.75, 129.06, 128.68, 113.53, 111.92, 13.41.

IR (KBr, cm⁻¹): 3153, 3135, 3058, 3003, 2954, 2914, 2812, 1756, 1653, 1576, 1506, 1474, 1447.

HRMS (ESI) m/z: [M+Na]⁺ Calcd for C₁₃H₁₁NO₃Na: 252.0637; Found 252.0628.

(*E*)-1-(thiophen-3-yl)ethan-1-one O-benzoyl oxime (**4j**)



4j was prepared according to general procedure C. The crude reaction mixture was purified by column chromatography using silica gel (100-200 mesh) giving **4j** (152 mg) in 62 % yield.

Physical State: white solid, **m.p.:** 83-85 °C.

R_f-value: 0.45 (20% EtOAc/hexane).

¹H NMR (400 MHz, CDCl₃): δ 8.14 – 8.08 (m, 2H), 7.73 (dd, *J* = 3.0, 1.3 Hz, 1H), 7.66 (dd, *J* = 5.1, 1.3 Hz, 1H), 7.64 – 7.57 (m, 1H), 7.49 (t, *J* = 7.8 Hz, 2H), 7.36 (dd, *J* = 5.1, 2.9 Hz, 1H), 2.50 (s, 3H).

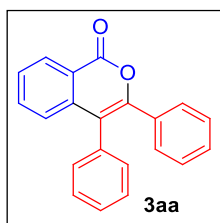
¹³C NMR (100 MHz, CDCl₃): δ 163.86, 159.35, 136.91, 133.42, 129.73, 129.28, 128.68, 127.03, 126.55, 125.97, 14.92.

IR (KBr, cm⁻¹): 3121, 3049, 2944, 2862, 1722, 1673, 1628, 1573, 1525, 1443, 1416, 1356, 1259.

HRMS (ESI) m/z: [M+Na]⁺ Calcd for C₁₃H₁₁NO₂SNa: 268.0408; Found 268.0409.

5.2 Experimental characterization data for the compounds

3,4-diphenyl-1*H*-isochromen-1-one (**3aa**)



3aa was prepared according to general procedure C. The crude reaction mixture was purified by column chromatography using silica gel (100-200 mesh) giving **3aa** (26 mg) in 87 % yield.

Physical State: pale yellow solid, **m.p.:** 170-173 °C,

R_f-value: 0.45 (10% EtOAc/hexane).

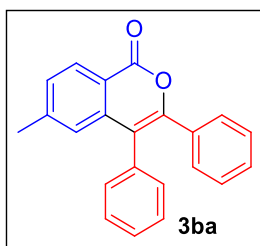
¹H NMR (400 MHz, CDCl₃): δ 8.33 (d, *J* = 8.0 Hz, 1H), 7.56 (t, *J* = 7.2 Hz, 1H), 7.45 (t, *J* = 7.2 Hz, 1H), 7.34-7.30 (m, 3H), 7.26 (d, *J* = 8.0 Hz, 2H), 7.19-7.10 (m, 6H).

¹³C NMR (100 MHz, CDCl₃): δ 162.6, 151.2, 139.2, 134.9, 134.6, 133.2, 131.5, 129.9, 129.5, 129.4, 129.2, 128.46, 128.43, 128.2, 125.6, 120.7, 117.2.

IR (KBr, cm⁻¹): 3074, 3019, 2923, 2852, 1737, 1614, 1559, 1489, 1443, 1317, 1243, 1195.

HRMS (ESI) m/z: [M+Na]⁺ Calcd for C₂₁H₁₄NaO₂: 321.0886; Found 321.0886.

6-methyl-3,4-diphenyl-1*H*-isochromen-1-one (3ba)



3ba was prepared according to general procedure C. The crude reaction mixture was purified by column chromatography using silica gel (100-200 mesh) giving **3ba** (26 mg) in 84% yield.

Physical State: colorless solid, **m.p.:** 162-164 °C,

R_f-value: 0.55 (10% EtOAc/hexane).

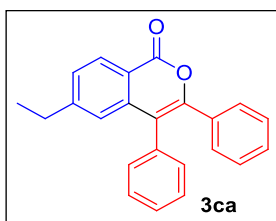
¹H NMR (400 MHz, CDCl₃): δ 8.21 (d, *J* = 8.0 Hz, 1H), 7.35-7.32 (m, 3H), 7.24 (td, *J* = 8.0, 0.8 Hz, 3H), 7.18-7.07 (m, 5H), 6.88 (s, 1H), 2.88 (s, 3H).

¹³C NMR (100 MHz, CDCl₃): δ 162.6, 151.3, 146.0, 139.2, 134.7, 133.3, 131.5, 129.9, 129.8, 129.5, 129.3, 129.1, 128.3, 128.1, 125.6, 118.3, 117.1, 22.5.

IR (KBr, cm⁻¹): 3082, 3053, 2986, 2933, 2875, 1734, 1622, 1574, 1481, 1443, 1209, 1172, 1072.

HRMS (ESI) m/z: [M+Na]⁺ Calcd for C₂₂H₁₆NaO₂: 335.1043; Found 335.1054.

6-ethyl-3,4-diphenyl-1*H*-isochromen-1-one (3ca)



3ca was prepared according to general procedure C. The crude reaction mixture was purified by column chromatography using silica gel (100-200 mesh) giving **3ca** (27 mg) in 83 % yield.

Physical State: off-white solid, **m.p.:** 153-154 °C,

R_f-value: 0.55 (10% EtOAc/hexane).

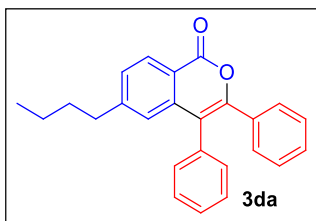
¹H NMR (400 MHz, CDCl₃): δ 8.32 (d, *J* = 8.0 Hz, 1H), 7.43-7.36 (m, 4H), 7.32-7.30 (m, 2H), 7.27-7.24 (m, 3H), 7.22-7.16 (m, 3H), 6.98 (d, *J* = 0.8 Hz, 1H), 2.65 (q, *J* = 7.6 Hz, 2H), 1.18 (t, *J* = 7.6 Hz, 3H).

¹³C NMR (100 MHz, CDCl₃): δ 162.6, 152.2, 151.3, 139.3, 134.8, 133.4, 131.6, 130.0, 129.5, 129.3, 129.1, 128.6, 128.3, 128.1, 124.5, 118.6, 117.3, 29.7, 15.5.

IR (KBr, cm⁻¹): 3085, 3055, 2981, 2936, 2875, 1733, 1621, 1574, 1485, 1323, 1264, 1172.

HRMS (ESI) m/z: [M+Na]⁺ Calcd for C₂₃H₁₈NaO₂: 349.1205; Found 349.1205.

6-butyl-3,4-diphenyl-1*H*-isochromen-1-one (3da)



3da was prepared according to general procedure C. The crude reaction mixture was purified by column chromatography using silica gel (100-200 mesh) giving **3da** (28 mg) in 79 % yield.

Physical State: off-white solid, **m.p.:** 132-134 °C,

R_f-value: 0.65 (10% EtOAc/hexane).

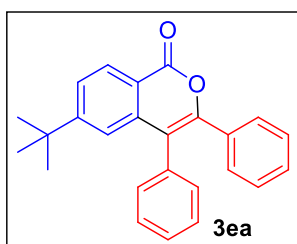
¹H NMR (400 MHz, CDCl₃): δ 8.24 (d, *J* = 8.0 Hz, 1H), 7.36-7.33 (m, 3H), 7.27 (dd, *J* = 8.0, 1.2 Hz, 1H), 7.23 (dd, *J* = 8.0, 1.2 Hz, 2H), 7.19-7.16 (m, 2H), 7.14-7.08 (m, 3H), 6.88 (s, 1H), 2.53 (t, *J* = 7.6 Hz, 2H), 1.45 (quint, *J* = 7.2 Hz, 2H), 1.27-1.18 (m, 2H), 0.80 (t, *J* = 7.2 Hz, 3H),

¹³C NMR (100 MHz, CDCl₃): δ 162.6, 151.3, 150.9, 139.2, 134.8, 133.4, 131.6, 129.9, 129.5, 129.3, 129.15, 129.10, 128.3, 128.1, 125.0, 118.5, 117.2, 36.4, 33.4, 22.5, 14.1.

IR (KBr, cm⁻¹): 3062, 3020, 2927, 2855, 1732, 1615, 1573, 1558, 1481, 1442, 1293, 1247.

HRMS (ESI) m/z: [M+H]⁺ Calcd for C₂₅H₂₃O₂: 355.1693; Found 355.1693.

6-(tert-butyl)-3,4-diphenyl-1*H*-isochromen-1-one (3ea)



3ea was prepared according to general procedure C. The crude reaction mixture was purified by column chromatography using silica gel (100-200 mesh) giving **3ea** (29 mg) in 82% yield.

Physical State: light yellow solid, **m.p.:** 161-163 °C,

R_f-value: 0.55 (10% EtOAc/hexane).

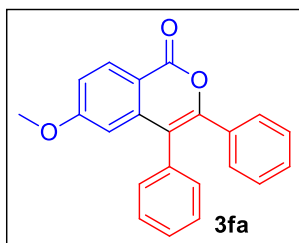
¹H NMR (400 MHz, CDCl₃): δ 8.25 (d, *J* = 8.4 Hz, 1H), 7.50 (dd, *J* = 8.4, 1.6 Hz, 1H), 7.35-7.31 (m, 3H), 7.25 (dd, *J* = 7.6, 0.8 Hz, 2H), 7.19 (dd, *J* = 7.6, 2.4 Hz, 2H), 7.15-7.08 (m, 4H), 1.16 (s, 9H).

¹³C NMR (100 MHz, CDCl₃): δ 162.6, 158.9, 151.2, 139.0, 134.7, 133.4, 131.5, 129.6, 129.5, 129.2, 129.1, 128.3, 128.1, 126.3, 122.0, 118.3, 117.5, 35.8, 31.2.

IR (KBr, cm⁻¹): 3052, 2967, 2927, 2865, 1728, 1698, 1619, 1574, 1483, 1296, 1252.

HRMS (ESI) m/z: [M+H]⁺ Calcd for C₂₅H₂₃O₂: 355.1693; Found 355.1705.

6-methoxy-3,4-diphenyl-1*H*-isochromen-1-one (3fa)



3fa was prepared according to general procedure C. The crude reaction mixture was purified by column chromatography using silica gel (100-200 mesh) giving **3fa** (28 mg) in 85% yield.

Physical State: light brown solid, **m.p.:** 178-180 °C,

R_f-value: 0.40 (10% EtOAc/hexane).

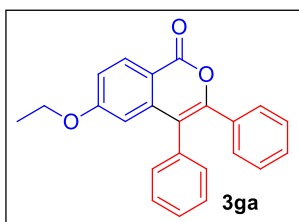
¹H NMR (400 MHz, CDCl₃): δ 8.26 (d, *J* = 8.8 Hz, 1H), 7.33-7.31 (m, 3H), 7.24 (d, *J* = 6.8 Hz, 2H), 7.18-7.08 (m, 5H), 6.98 (dd, *J* = 8.4, 2.0 Hz, 1H), 6.50 (d, *J* = 2.0 Hz, 1H), 3.67 (s, 3H).

¹³C NMR (100 MHz, CDCl₃): δ 164.9, 162.3, 151.8, 141.5, 134.7, 133.3, 132.2, 131.5, 129.5, 129.3, 129.2, 128.4, 128.1, 117.1, 115.9, 114.0, 108.8, 55.8.

IR (KBr, cm⁻¹): 3079, 3054, 2997, 2952, 2847, 1731, 1661, 1574, 1531, 1485, 1262, 1192.

HRMS (ESI) m/z: [M+H]⁺ Calcd for C₂₂H₁₇O₃: 329.1172; Found 329.1172.

6-ethoxy-3,4-diphenyl-1*H*-isochromen-1-one (3ga)



3ga was prepared according to general procedure C. The crude reaction mixture was purified by column chromatography using silica gel (100-200 mesh) giving **3ga** (28 mg) in 81 % yield.

Physical State: off white solid, **m.p.:** 171-173 °C,

R_f-value: 0.40 (10% EtOAc/hexane).

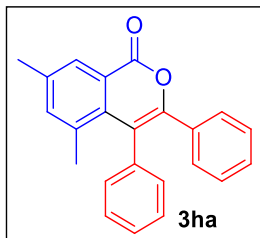
¹H NMR (400 MHz, CDCl₃): δ 8.25 (d, *J* = 8.8 Hz, 1H), 7.33-7.31 (m, 3H), 7.24 (d, *J* = 7.6 Hz, 2H), 7.18-7.08 (m, 5H), 6.96 (dd, *J* = 8.8, 2.0 Hz, 1H), 6.48 (d, *J* = 2.0 Hz, 1H), 3.88 (q, *J* = 7.2 Hz, 2H), 1.28 (t, *J* = 6.8 Hz, 3H).

¹³C NMR (100 MHz, CDCl₃): δ 164.3, 162.3, 151.7, 141.4, 134.7, 133.3, 132.2, 131.5, 129.5, 129.3, 129.2, 128.4, 128.1, 117.1, 116.2, 113.8, 109.3, 64.1, 14.8.

IR (KBr, cm⁻¹): 3073, 3022, 2970, 2927, 2849, 1741, 1698, 1650, 1605, 1538, 1485, 1202.

HRMS (ESI) m/z: [M+H]⁺ Calcd for C₂₃H₁₉O₃: 343.1329; Found 343.1322.

5,7-dimethyl-3,4-diphenyl-1*H*-isochromen-1-one (**3ha**)



3ha was prepared according to general procedure C. The crude reaction mixture was purified by column chromatography using silica gel (100-200 mesh) giving **3ha** (23 mg) in 70% yield.

Physical State: pale yellow solid, **m.p.:** 165-167 °C,

R_f-value: 0.50 (10% EtOAc/hexane).

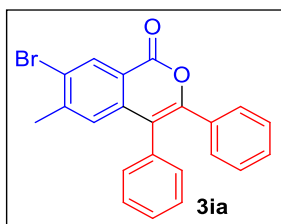
¹H NMR (400 MHz, CDCl₃): δ 8.10 (s, 1H), 7.22-7.18 (m, 4H), 7.15-7.06 (m, 7H), 2.35 (s, 3H), 1.64 (s, 3H).

¹³C NMR (100 MHz, CDCl₃): δ 163.3, 151.0, 140.7, 138.5, 137.6, 135.8, 134.1, 133.8, 132.1, 129.8, 128.6, 128.5, 128.1, 127.9, 121.9, 117.6, 23.5, 21.2.

IR (KBr, cm⁻¹): 3078, 3051, 2977, 2851, 1733, 1682, 1650, 1634, 1575, 1488, 1267, 1216.

HRMS (ESI) m/z: [M+H]⁺ Calcd for C₂₃H₁₉O₂: 327.1380; Found 327.1370.

7-bromo-6-methyl-3,4-diphenyl-1*H*-isochromen-1-one (**3ia**)



3ia was prepared according to general procedure C. The crude reaction mixture was purified by column chromatography using silica gel (100-200 mesh) giving **3ia** (26 mg) in 67 % yield.

Physical State: white solid, **m.p.:** 207-209 °C,

R_f-value: 0.55 (10% EtOAc/hexane).

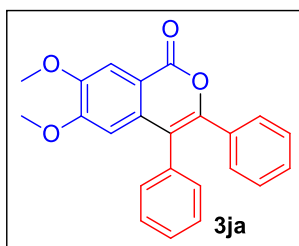
¹H NMR (400 MHz, CDCl₃): δ 8.47 (s, 1H), 7.36-7.34 (m, 3H), 7.22 (d, *J* = 6.8 Hz, 2H), 7.18-7.08 (m, 6H), 6.94 (s, 1H), 2.32 (s, 3H).

¹³C NMR (100 MHz, CDCl₃): δ 161.3, 151.7, 145.8, 138.1, 134.2, 133.2, 133.0, 131.4, 129.5, 129.4, 128.6, 128.2, 127.4, 125.1, 119.9, 116.6, 24.1.

IR (KBr, cm⁻¹): 3053, 3024, 2924, 2852, 1734, 1695, 1652, 1627, 1576, 1489, 1264.

HRMS (ESI) m/z: [M+H]⁺ Calcd for C₂₂H₁₆BrO₂: 391.0328; Found 391.0344.

6,7-dimethoxy-3,4-diphenyl-1*H*-isochromen-1-one (3ja)



3ja was prepared according to general procedure C. The crude reaction mixture was purified by column chromatography using silica gel (100-200 mesh) giving **3ja** (29 mg) in 80% yield.

Physical State: brown solid, **m.p.:** 197-199 °C,

R_f-value: 0.45 (30% EtOAc/hexane).

¹H NMR (400 MHz, CDCl₃): δ 7.70 (s, 1H), 7.37-7.33 (m, 3H), 7.24-7.19 (m, 4H), 7.14-7.08 (m, 3H), 6.48 (s, 1H), 3.94 (s, 3H),

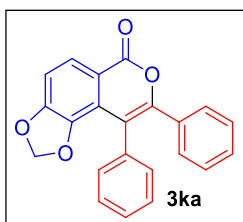
3.66 (s, 3H).

¹³C NMR (100 MHz, CDCl₃): δ 162.4, 155.2, 150.4, 149.9, 134.9, 134.8, 133.3, 131.4, 129.44, 129.40, 129.0, 128.4, 128.1, 117.0, 114.0, 109.7, 106.5, 56.71, 56.27.

IR (KBr, cm⁻¹): 3092, 3056, 2964, 2856, 1726, 1607, 1574, 1510, 1463, 1280, 1193.

HRMS (ESI) m/z: [M+H]⁺ Calcd for C₂₃H₁₉O₄: 359.1278; Found 359.1281.

8,9-diphenyl-6*H*-[1,3]dioxolo[4,5-*f*]isochromen-6-one (3ka)



3ka was prepared according to general procedure C. The crude reaction mixture was purified by column chromatography using silica gel (100-200 mesh) giving **3ka** (28 mg) in 81 % yield.

Physical State: light-brown solid, **m.p.:** 207-210 °C,

R_f-value: 0.45 (30% EtOAc/hexane).

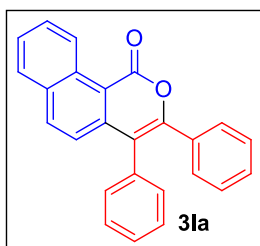
¹H NMR (400 MHz, CDCl₃): δ 8.08 (d, *J* = 8.4 Hz, 1H), 7.32-7.25 (m, 8H), 7.21-7.13 (m, 3H), 7.02 (d, *J* = 8.4 Hz, 1H), 5.81 (s, 2H).

¹³C NMR (100 MHz, CDCl₃): δ 161.9, 153.5, 151.5, 142.9, 135.3, 133.2, 131.4, 129.6, 129.1, 128.3, 128.1, 128.0, 126.5, 122.2, 115.2, 113.7, 109.8, 102.3.

IR (KBr, cm⁻¹): 3087, 3031, 2919, 2834, 1739, 1698, 1614, 1574, 1493, 1456, 1275, 1223.

HRMS (ESI) m/z: [M+Na]⁺ Calcd for C₂₂H₁₄NaO₄: 365.0790; Found 365.0804.

3,4-diphenyl-1*H*-benzo[*h*]isochromen-1-one (3la)



3la was prepared according to general procedure C. The crude reaction mixture was purified by column chromatography using silica gel (100-200 mesh) giving **3la** (26 mg) in 75% yield.

Physical State: pale yellow solid, **m.p.:** 170-172 °C,

R_f-value: 0.50 (10% EtOAc/hexane).

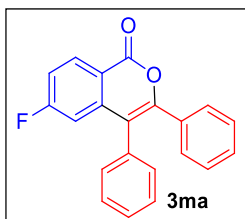
¹H NMR (400 MHz, CDCl₃): δ 9.77 (d, *J* = 8.8 Hz, 1H), 7.92 (d, *J* = 9.2 Hz, 1H), 7.79 (d, *J* = 8.0 Hz, 1H), 7.71 (td, *J* = 7.2, 1.2 Hz, 1H), 7.55 (t, *J* = 7.2 Hz, 1H), 7.40-7.36 (m, 3H), 7.30 (d, *J* = 6.8 Hz, 2H), 7.23-7.20 (m, 2H), 7.18-7.10 (m, 4H).

¹³C NMR (100 MHz, CDCl₃): δ 161.7, 152.8, 141.1, 136.2, 135.1, 133.1, 132.9, 131.9, 131.8, 129.8, 129.56, 129.51, 129.4, 128.8, 128.5, 128.2, 127.4, 123.0, 117.6, 114.3.

IR (KBr, cm⁻¹): 3132, 3055, 2932, 2834, 1713, 1673, 1611, 1549, 1495, 1445, 1230.

HRMS (ESI) m/z: [M+Na]⁺ Calcd for C₂₅H₁₆NaO₂: 371.1043; Found 371.1055.

6-fluoro-3,4-diphenyl-1*H*-isochromen-1-one (3ma)



3ma was prepared according to general procedure C. The crude reaction mixture was purified by column chromatography using silica gel (100-200 mesh) giving **3ma** (22 mg) in 69 % yield.

Physical State: off-white solid, **m.p.:** 130-132 °C,

R_f-value: 0.50 (10% EtOAc/hexane).

¹H NMR (400 MHz, CDCl₃): δ 8.35 (dd, *J* = 8.8, 5.6 Hz, 1H), 7.38-7.34 (m, 3H), 7.25 (d, *J* = 6.8 Hz, 2H), 7.19-7.10 (m, 6H), 6.76 (dd, *J* = 10.0, 2.4 Hz, 1H).

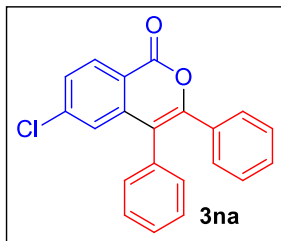
¹³C NMR (100 MHz, CDCl₃): δ 167.1 (d, *J*_{C-F} = 254 Hz), 161.5, 152.3, 142.2 (d, *J*_{C-F} = 11 Hz), 134.1, 133.2, 133.1, 132.8, 131.4, 129.6, 129.5, 128.7, 128.2, 117.2 (d, *J*_{C-F} = 2 Hz), 116.6 (d, *J*_{C-F} = 23 Hz), 116.7 (d, *J*_{C-F} = 3 Hz), 111.6 (d, *J*_{C-F} = 24 Hz).

¹⁹F NMR (376 MHz, CDCl₃): δ -101.0.

IR (KBr, cm⁻¹): 3057, 3024, 2986, 2929, 2851, 1732, 1680, 1626, 1574, 1557, 1472, 1227.

HRMS (ESI) m/z: [M+H]⁺ Calcd for C₂₁H₁₄FO₂: 317.0972; Found 317.0978.

6-chloro-3,4-diphenyl-1*H*-isochromen-1-one (3na)



3na was prepared according to general procedure C. The crude reaction mixture was purified by column chromatography using silica gel (100-200 mesh) giving **3na** (23 mg) in 70% yield.

Physical State: light-brown solid, **m.p.:** 164-166 °C,

R_f-value: 0.50 (10% EtOAc/hexane).

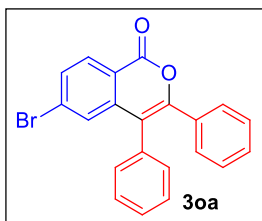
¹H NMR (400 MHz, CDCl₃): δ 8.25 (d, *J* = 8.4 Hz, 1H), 7.40-7.35 (m, 4H), 7.24 (d, *J* = 7.6 Hz, 2H), 7.17-7.08 (m, 6H).

¹³C NMR (100 MHz, CDCl₃): δ 161.7, 152.5, 141.9, 140.7, 133.9, 132.8, 131.5, 131.4, 129.63, 129.60, 129.5, 128.91, 128.7, 128.2, 125.3, 119.0, 116.3.

IR (KBr, cm⁻¹): 3058, 3030, 2958, 2851, 1737, 1682, 1633, 1574, 1494, 1262, 1193.

HRMS (ESI) m/z: [M+H]⁺ Calcd for C₂₁H₁₄ClO₂: 333.0677; Found 333.0673.

6-bromo-3,4-diphenyl-1*H*-isochromen-1-one (3oa)



3oa was prepared according to general procedure C. The crude reaction mixture was purified by column chromatography using silica gel (100-200 mesh) giving **3oa** (26 mg) in 68 % yield.

Physical State: pale yellow solid, **m.p.:** 197-200 °C,

R_f-value: 0.55 (10% EtOAc/hexane).

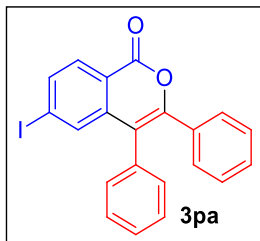
¹H NMR (400 MHz, CDCl₃): δ 8.17 (d, *J* = 8.4 Hz, 1H), 7.56 (dd, *J* = 8.4, 1.6 Hz, 1H), 7.37-7.35 (m, 3H), 7.25-7.22 (m, 3H), 7.19-7.09 (m, 5H).

¹³C NMR (100 MHz, CDCl₃): δ 161.9, 152.5, 140.7, 133.9, 132.8, 131.8, 131.5, 131.4, 130.8, 129.64, 129.61, 129.5, 128.8, 128.3, 128.2, 119.4, 116.2.

IR (KBr, cm⁻¹): 3059, 2988, 2826, 1731, 1673, 1621, 1574, 1444, 1264, 1192.

HRMS (ESI) m/z: [M+Na]⁺ Calcd for C₂₁H₁₃BrNaO₂: 398.9991; Found 399.0004.

6-iodo-3,4-diphenyl-1*H*-isochromen-1-one (3pa)



3pa was prepared according to general procedure C. The crude reaction mixture was purified by column chromatography using silica gel (100-200 mesh) giving **3pa** (25 mg) in 59% yield.

Physical State: off-white solid, **m.p.:** 228-230 °C,

R_f-value: 0.55 (10% EtOAc/hexane).

¹H NMR (400 MHz, CDCl₃): δ 8.00 (d, *J* = 8.4 Hz, 1H), 7.78 (dd, *J* = 8.4, 1.2 Hz, 1H), 7.47 (d, *J* = 1.2 Hz, 1H), 7.37-7.35 (m, 3H),

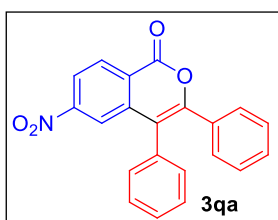
7.23 (d, *J* = 7.2 Hz, 2H), 7.18-7.09 (m, 5H).

¹³C NMR (100 MHz, CDCl₃): δ 162.2, 152.4, 140.4, 137.6, 134.5, 133.8, 132.9, 131.4, 131.1, 129.6, 129.5, 128.7, 128.2, 119.9, 116.0, 103.8.

IR (KBr, cm⁻¹): 3069, 2926, 2855, 1729, 1650, 1581, 1488, 1278, 1190.

HRMS (ESI) m/z: [M+H]⁺ Calcd for C₂₁H₁₄IO₂: 425.0033; Found 425.0028.

6-nitro-3,4-diphenyl-1*H*-isochromen-1-one (3qa)



3qa was prepared according to general procedure C. The crude reaction mixture was purified by column chromatography using silica gel (100-200 mesh) giving **3qa** (22 mg) in 64 % yield.

Physical State: yellow solid, **m.p.:** 155-156 °C,

R_f-value: 0.55 (20% EtOAc/hexane).

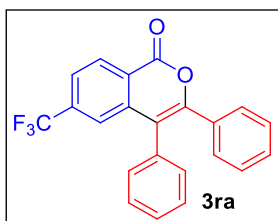
¹H NMR (700 MHz, CDCl₃): δ 8.50 (d, *J* = 9.1 Hz, 1H), 8.20 (dd, *J* = 9.1, 2.1 Hz, 1H), 7.96 (d, *J* = 2.1 Hz, 1H), 7.40-7.39 (m, 3H), 7.27 (d, *J* = 7.0 Hz, 2H), 7.22-7.18 (m, 3H), 7.15 (t, *J* = 7.7 Hz, 2H).

¹³C NMR (176 MHz, CDCl₃): δ 160.8, 153.4, 152.1, 140.6, 133.1, 132.3, 131.9, 131.31, 130.0, 129.9, 129.6, 129.2, 128.4, 124.5, 122.2, 120.8, 116.5.

IR (KBr, cm⁻¹): 3056, 2984, 2923, 2849, 1736, 1611, 1566, 1490, 1445, 1264, 1191.

HRMS (ESI) m/z: [M+H]⁺ Calcd for C₂₁H₁₄NO₄: 344.0917; Found 344.0910.

3,4-diphenyl-6-(trifluoromethyl)-1*H*-isochromen-1-one (3ra)



3ra was prepared according to general procedure C. The crude reaction mixture was purified by column chromatography using silica gel (100-200 mesh) giving **3ra** (25 mg) in 68% yield.

Physical State: pale-yellow solid, **m.p.:** 165-167 °C,

R_f-value: 0.55 (10% EtOAc/hexane).

¹H NMR (400 MHz, CDCl₃): δ 8.45 (d, *J* = 8.0 Hz, 1H), 7.66 (d, *J* = 8.0 Hz, 1H), 7.38 (d, *J* = 4.4 Hz, 4H), 7.25 (d, *J* = 7.2 Hz, 2H), 7.19-7.11 (m, 5H).

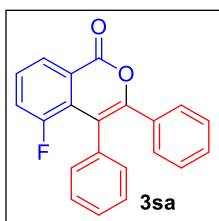
¹³C NMR (100 MHz, CDCl₃): δ 161.4, 152.7, 139.7, 136.6, 136.3, 133.6, 132.7, 131.4, 130.9, 129.7, 129.5, 128.9, 128.3, 124.2 (q, *J*_{C-F} = 3.1 Hz), 123.1, 123.2 (q, *J*_{C-F} = 272 Hz), 122.7 (q, *J*_{C-F} = 3 Hz), 116.7.

¹⁹F NMR (376 MHz, CDCl₃): δ -63.3.

IR (KBr, cm⁻¹): 3060, 2968, 2855, 1737, 1682, 1632, 1599, 1556, 1494, 1446, 1261, 1168.

HRMS (ESI) m/z: [M+H]⁺ Calcd for C₂₂H₁₄F₃O₂: 367.0940; Found 367.0965.

5-fluoro-3,4-diphenyl-1*H*-isochromen-1-one (3sa)



3sa was prepared according to general procedure C. The crude reaction mixture was purified by column chromatography using silica gel (100-200 mesh) giving **3sa** (26 mg) in 82 % yield.

Physical State: light-brown solid, **m.p.:** 188-191 °C,

R_f-value: 0.50 (10% EtOAc/hexane).

¹H NMR (400 MHz, CDCl₃): δ 8.18 (d, *J* = 8.0 Hz, 1H), 7.44-7.39 (m, 1H), 7.25-7.22 (m, 4H), 7.19-7.18 (m, 4H), 7.14-7.07 (m, 3H).

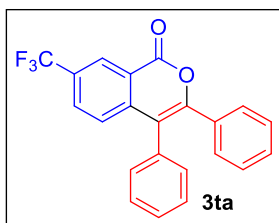
¹³C NMR (100 MHz, CDCl₃): δ 161.4 (d, *J*_{C-F} = 3 Hz), 158.4 (d, *J*_{C-F} = 256 Hz), 152.3, 136.0 (d, *J*_{C-F} = 4 Hz), 133.1, 130.9 (d, *J*_{C-F} = 3 Hz), 129.7, 129.4 (d, *J*_{C-F} = 8 Hz), 129.3, 128.5, 128.1, 128.0, 127.1 (d, *J*_{C-F} = 6 Hz), 126.2 (d, *J*_{C-F} = 4 Hz), 122.7, 122.6 (d, *J*_{C-F} = 22 Hz), 113.6 (d, *J*_{C-F} = 2 Hz).

¹⁹F NMR (376 MHz, CDCl₃): δ -107.5.

IR (KBr, cm⁻¹): 3077, 3021, 2927, 2849, 1734, 1631, 1576, 1495, 1455, 1383, 1275, 1173.

HRMS (ESI) m/z: [M+Na]⁺ Calcd for C₂₁H₁₃FNaO₂: 339.0792; Found 339.0817.

3,4-diphenyl-7-(trifluoromethyl)-1*H*-isochromen-1-one (3ta)



3ta was prepared according to general procedure C. The crude reaction mixture was purified by column chromatography using silica gel (100-200 mesh) giving **3ta** (21 mg) in 57% yield.

Physical State: light-brown solid, **m.p.:** 118-120 °C,

R_f-value: 0.50 (10% EtOAc/hexane).

¹H NMR (400 MHz, CDCl₃): δ 8.60 (s, 1H), 7.75 (dd, *J* = 8.4, 1.6 Hz, 1H), 7.38-7.36 (m, 3H), 7.26 (t, *J* = 6.8 Hz, 3H), 7.20-7.11 (m, 5H).

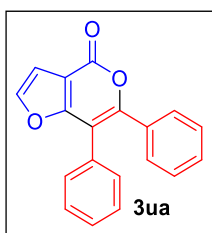
¹³C NMR (100 MHz, CDCl₃): δ 162.5, 153.3, 141.9, 133.9, 132.6, 131.4, 131.1 (q, *J*_{C-F} = 3.0 Hz), 130.4 (q, *J*_{C-F} = 33.0 Hz), 129.8, 129.67, 129.62, 128.8, 128.3, 127.4 (q, *J*_{C-F} = 4.0 Hz), 126.5, 123.7 (q, *J*_{C-F} = 271 Hz), 120.8, 116.6.

¹⁹F NMR (376 MHz, CDCl₃): δ -62.7.

IR (KBr, cm⁻¹): 3067, 3034, 2957, 2928, 2852, 1738, 1621, 1602, 1575, 1500, 1445, 1224, 1190.

HRMS (ESI) m/z: [M+H]⁺ Calcd for C₂₂H₁₄F₃O₂: 367.0946; Found 367.0911.

6,7-diphenyl-4*H*-furo[3,2-*c*]pyran-4-one (3ua)



3ua was prepared according to general procedure C. The crude reaction mixture was purified by column chromatography using silica gel (100-200 mesh) giving **3ua** (18 mg) in 62 % yield.

Physical State: brown solid, **m.p.:** 168-170 °C,

R_f-value: 0.35 (10% EtOAc/hexane).

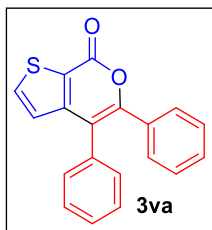
¹H NMR (400 MHz, CDCl₃): δ 7.53 (d, *J* = 2.4 Hz, 1H), 7.41-7.37 (m, 5H), 7.34-7.28 (m, 3H), 7.26-7.21 (m, 2H), 7.00 (d, *J* = 2.0 Hz, 1H).

¹³C NMR (100 MHz, CDCl₃): δ 161.7, 159.3, 158.2, 155.6, 144.9, 132.2, 131.0, 130.7, 130.0, 129.7, 129.2, 128.9, 128.4, 109.9, 108.2.

IR (KBr, cm⁻¹): 3146, 3124, 3055, 2986, 1741, 1698, 1651, 1574, 1494, 1368, 1274, 1263.

HRMS (ESI) m/z: [M+Na]⁺ Calcd for C₁₉H₁₂NaO₃: 311.0679; Found 311.0691.

4,5-diphenyl-7H-thieno[2,3-c]pyran-7-one (3va)



3va was prepared according to general procedure C. The crude reaction mixture was purified by column chromatography using silica gel (100-200 mesh) giving **3va** (17 mg) in 56 % yield.

Physical State: dark-brown solid, **m.p.:** 146-148 °C,

R_f-value: 0.40 (10% EtOAc/hexane).

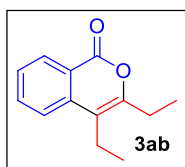
¹H NMR (700 MHz, CDCl₃): δ 7.77 (d, J = 4.90 Hz, 1H), 7.40-7.37 (m, 3H), 7.36 (d, J = 7.0 Hz, 2H), 7.28-7.25 (m, 3H), 7.21 (t, J = 7.7 Hz, 2H), 6.96 (d, J = 4.9 Hz, 1H).

¹³C NMR (176 MHz, CDCl₃): δ 158.5, 153.7, 149.8, 136.5, 135.2, 132.6, 130.6, 129.6, 129.5, 129.4, 128.5, 128.3, 125.5, 123.1, 116.1.

IR (KBr, cm⁻¹): 3103, 3055, 3022, 2962, 2926, 2855, 1718, 1616, 1573, 1515, 1491, 1261.

HRMS (ESI) m/z: [M+Na]⁺ Calcd for C₁₉H₁₂NaSO₂: 327.0456; Found 327.0471.

3,4-diethyl-1H-isochromen-1-one (3ab)



3ab was prepared according to general procedure C. The crude reaction mixture was purified by column chromatography using silica gel (100-200 mesh) giving **3ab** (13 mg) in 64 % yield.

Physical State: colorless solid, **m.p.:** 62-65 °C,

R_f-value: 0.55 (10% EtOAc/hexane).

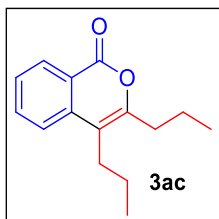
¹H NMR (400 MHz, CDCl₃): δ 8.24 (dd, J = 8.0, 1.2 Hz, 1H), 7.66 (td, J = 8.4, 1.2 Hz, 1H), 7.47 (d, J = 8.0 Hz, 1H), 7.38 (t, J = 8.0 Hz, 1H), 2.61-7.52 (m, 4H), 1.21 (t, J = 7.6 Hz, 3H), 1.13 (t, J = 7.6 Hz, 3H).

¹³C NMR (100 MHz, CDCl₃): δ 163.3, 155.3, 138.1, 134.9, 130.2, 127.4, 122.7, 121.2, 113.3, 24.4, 19.6, 14.6, 12.8.

IR (KBr, cm⁻¹): 3070, 2972, 2934, 2856, 1716, 1644, 1605, 1566, 1488, 1454, 1256, 1183.

HRMS (ESI) m/z: [M+H]⁺ Calcd for C₁₃H₁₅O₂: 203.1067; Found 203.1050.

3,4-dipropyl-1*H*-isochromen-1-one (3ac)



3ac was prepared according to general procedure C. The crude reaction mixture was purified by column chromatography using silica gel (100-200 mesh) giving **3ac** (16 mg) in 69 % yield.

Physical State: colorless oil.

R_f-value: 0.55 (10% EtOAc/hexane).

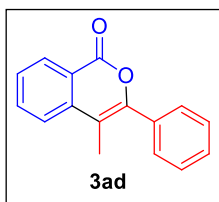
¹H NMR (400 MHz, CDCl₃): δ 8.24 (d, J = 0.8 Hz, 1H), 7.65 (td, J = 8.4, 1.6 Hz, 1H), 7.45 (d, J = 8.4 Hz, 1H), 7.38 (t, J = 8.0 Hz, 1H), 2.25 (q, J = 8.0 Hz, 4H), 1.72-1.63 (m, 2H), 1.57-1.47 (m, 2H), 0.94 (quint, J = 7.2 Hz, 6H).

¹³C NMR (100 MHz, CDCl₃): δ 163.2, 154.4, 138.3, 134.8, 130.1, 127.3, 122.9, 121.6, 112.5, 33.0, 28.5, 23.2, 21.5, 14.4, 14.1.

IR (KBr, cm⁻¹): 3073, 2961, 2931, 2874, 1734, 1640, 1607, 1563, 1486, 1457, 1319, 1246, 1182.

HRMS (ESI) m/z: [M+Na]⁺ Calcd for C₁₅H₁₈NaO₂: 253.1199; Found 253.1183.

4-methyl-3-phenyl-1*H*-isochromen-1-one (3ad)



3ad was prepared according to general procedure C. The crude reaction mixture was purified by column chromatography using silica gel (100-200 mesh) giving **3ad** (14 mg) in 59 % yield.

Physical State: off-white solid, **m.p.:** 92-94 °C,

R_f-value: 0.50 (10% EtOAc/hexane).

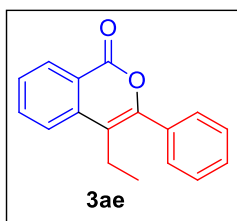
¹H NMR (400 MHz, CDCl₃): δ 8.38 (d, J = 8.0 Hz, 1H), 7.81 (t, J = 7.6 Hz, 1H), 7.64 (d, J = 8.0 Hz, 1H), 7.60-7.53 (m, 3H), 7.48-7.43 (m, 3H), 2.32 (s, 3H).

¹³C NMR (100 MHz, CDCl₃): δ 162.8, 151.5, 139.1, 135.1, 133.5, 130.0, 129.8, 129.6, 128.5, 128.2, 123.7, 121.1, 109.4, 13.9.

IR (KBr, cm⁻¹): 3058, 2994, 2952, 2864, 2849, 1736, 1698, 1617, 1651, 1606, 1577, 1495, 1470, 1443, 1285, 1244.

HRMS (ESI) m/z: [M+Na]⁺ Calcd for C₁₆H₁₂NaO₂: 259.0730; Found 259.0709

4-ethyl-3-phenyl-1*H*-isochromen-1-one (3ae)



3ae was prepared according to general procedure C. The crude reaction mixture was purified by column chromatography using silica gel (100-200 mesh) giving **3ae** (15 mg) in 60% yield.

Physical State: off-white solid, **m.p.:** 138-140 °C,

R_f-value: 0.50 (10% EtOAc/hexane).

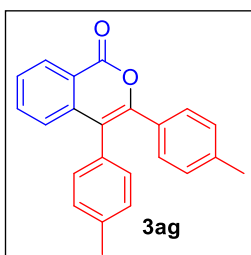
¹H NMR (400 MHz, CDCl₃): δ 8.32 (d, *J* = 7.6 Hz, 1H), 7.72 (td, *J* = 8.0, 0.8 Hz, 1H), 7.60 (d, *J* = 8.0 Hz, 1H), 7.50-7.45 (m, 3H), 7.40-7.38 (m, 3H), 2.65 (q, *J* = 7.2 Hz, 2H), 1.21 (t, *J* = 7.6 Hz, 3H).

¹³C NMR (100 MHz, CDCl₃): δ 162.8, 151.6, 138.0, 135.0, 133.7, 130.3, 129.7, 129.2, 128.6, 128.1, 123.7, 121.6, 115.5, 20.4, 15.0.

IR (KBr, cm⁻¹): 3052, 2988, 2955, 2862, 2848, 1732, 1697, 1652, 1604, 1579, 1493, 1472, 1441, 1288, 1247.

HRMS (ESI) m/z: [M+Na]⁺ Calcd for C₁₇H₁₄NaO₂: 273.0886; Found 273.0891.

3,4-di-*p*-tolyl-1*H*-isochromen-1-one (3ag)



3ag was prepared according to general procedure C. The crude reaction mixture was purified by column chromatography using silica gel (100-200 mesh) giving **3ag** (27 mg) in 83 % yield.

Physical State: brown solid, **m.p.:** 153-155 °C,

R_f-value: 0.55 (10% EtOAc/hexane).

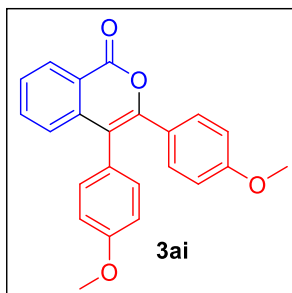
¹H NMR (400 MHz, CDCl₃): δ 8.38 (d, *J* = 7.6 Hz, 1H), 7.60 (t, *J* = 7.2 Hz, 1H), 7.48 (t, *J* = 7.2 Hz, 1H), 7.25-7.17 (m, 5H), 7.13 (d, *J* = 8.0 Hz, 2H), 7.00 (d, *J* = 8.0 Hz, 2H), 2.41 (s, 3H), 2.28 (s, 3H).

¹³C NMR (176 MHz, CDCl₃): δ 162.7, 151.2, 139.5, 139.2, 138.1, 134.8, 131.7, 131.3, 130.4, 130.1, 129.7, 129.3, 128.9, 128.1, 125.6, 120.6, 116.6, 21.67, 21.61.

IR (KBr, cm⁻¹): 3060, 3021, 2991, 2943, 2867, 1732, 1697, 1682, 1652, 1597, 1555, 1478, 1319, 1264, 1182.

HRMS (ESI) m/z: [M+H]⁺ Calcd for C₂₃H₁₉O₂: 327.1380; Found 327.1357.

3,4-bis(4-methoxyphenyl)-1*H*-isochromen-1-one (**3ai**)



3ai was prepared according to general procedure C. The crude reaction mixture was purified by column chromatography using silica gel (100-200 mesh) giving **3ai** (26 mg) in 72% yield.

Physical State: off-white solid, **m.p.:** 159-161 °C,

R_f-value: 0.55 (20% EtOAc/hexane).

¹H NMR (400 MHz, CDCl₃): δ 8.37 (d, *J* = 8.0 Hz, 1H), 7.61 (t, *J* = 7.6 Hz, 1H), 7.48 (t, *J* = 7.2 Hz, 1H), 7.29 (d, *J* = 8.8 Hz, 2H), 7.21-7.15 (m, 3H), 6.96 (d, *J* = 8.4 Hz, 2H), 6.72 (d, *J* = 8.8 Hz,

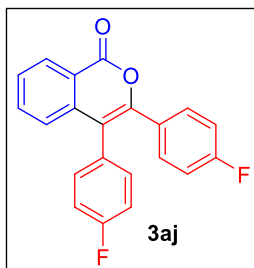
2H), 3.86 (s, 3H), 3.76 (s, 3H).

¹³C NMR (176 MHz, CDCl₃): δ 162.7, 160.1, 159.6, 151.2, 139.8, 134.8, 132.6, 130.9, 129.7, 127.9, 126.9, 125.7, 125.4, 120.5, 115.6, 114.9, 113.6, 55.6, 55.5.

IR (KBr, cm⁻¹): 3073, 3058, 2950, 2835, 1744, 1654, 1612, 1570, 1507, 1480, 1446, 1299, 1238.

HRMS (ESI) m/z: [M+H]⁺ Calcd for C₂₃H₁₉O₄: 359.1278; Found 359.1253.

3,4-bis(4-fluorophenyl)-1*H*-isochromen-1-one (**3aj**)



3aj was prepared according to general procedure C. The crude reaction mixture was purified by column chromatography using silica gel (100-200 mesh) giving **3aj** (29 mg) in 87 % yield.

Physical State: pale-yellow solid, **m.p.:** 161-164 °C,

R_f-value: 0.50 (10% EtOAc/hexane).

¹H NMR (400 MHz, CDCl₃): δ 8.40 (d, *J* = 7.6 Hz, 1H), 7.66 (t, *J* = 7.6 Hz, 1H), 7.54 (t, *J* = 7.6 Hz, 1H), 7.30 (t, *J* = 5.6 Hz, 2H), 7.26-

7.21 (m, 2H), 7.14 (q, *J* = 7.6 Hz, 3H), 6.91 (t, *J* = 8.4 Hz, 2H),

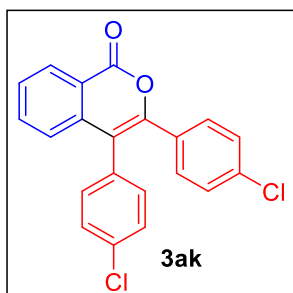
¹³C NMR (100 MHz, CDCl₃): δ 163.2 (d, *J*_{C-F} = 249 Hz), 162.9 (d, *J*_{C-F} = 247 Hz), 162.1, 150.7, 138.9, 135.1, 133.3 (d, *J*_{C-F} = 8 Hz), 131.5 (d, *J*_{C-F} = 9 Hz), 130.4 (d, *J*_{C-F} = 4 Hz), 130.0, 129.3 (d, *J*_{C-F} = 8 Hz), 128.6, 125.4, 120.8, 116.7 (d, *J*_{C-F} = 21 Hz), 116.1, 115.5 (d, *J*_{C-F} = 22 Hz).

¹⁹F NMR (376 MHz, CDCl₃): δ -108.6, δ -113.1.

IR (KBr, cm⁻¹): 3114, 3071, 2957, 2854, 1738, 1624, 1601, 1504, 1481, 1454, 1319, 1233, 1195.

HRMS (ESI) m/z: [M+Na]⁺ Calcd for C₂₁H₁₂F₂NaO₂: 357.0698; Found 357.0669.

3,4-bis(4-chlorophenyl)-1*H*-isochromen-1-one (3ak)



3ak was prepared according to general procedure C. The crude reaction mixture was purified by column chromatography using silica gel (100-200 mesh) giving **3ak** (28 mg) in 76 % yield.

Physical State: yellow solid, **m.p.:** 172-173 °C,

R_f-value: 0.50 (10% EtOAc/hexane).

¹H NMR (700 MHz, CDCl₃): δ 8.40 (d, *J* = 7.7 Hz, 1H), 7.66 (t, *J* = 7.7 Hz, 1H), 7.55 (t, *J* = 7.7 Hz, 1H), 7.43 (d, *J* = 7.7 Hz, 2H), 7.26 (d, *J* = 8.4 Hz, 2H), 7.20 (t, *J* = 6.3 Hz, 4H), 7.16 (d, *J* = 7.7

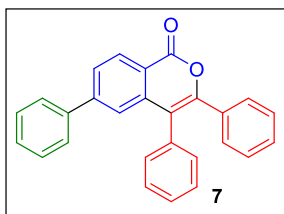
Hz, 1H),

¹³C NMR (176 MHz, CDCl₃): δ 162.1, 150.3, 138.5, 135.6, 135.2, 134.8, 132.8, 131.4, 130.8, 130.1, 129.9, 128.8, 128.7, 125.4, 120.7, 116.4.

IR (KBr, cm⁻¹): 3071, 2925, 2849, 1732, 1620, 1590, 1564, 1488, 1453, 1400, 1263.

HRMS (ESI) m/z: [M+H]⁺ Calcd for C₂₁H₁₃Cl₂O₂: 367.0287; Found 367.0288.

3,4,6-triphenyl-1*H*-isochromen-1-one (7)



7 was prepared according to the procedure in section 2.6.1. The crude reaction mixture was purified by column chromatography using silica gel (100-200 mesh) giving **7** (34 mg) in 91 % yield.

Physical State: colorless solid, **m.p.:** 205-206 °C,

R_f-value: 0.50 (10% EtOAc/hexane).

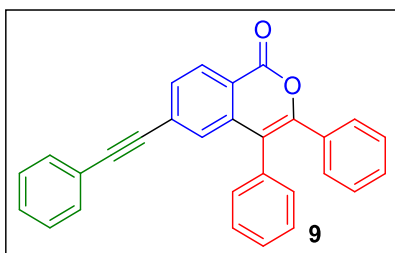
¹H NMR (400 MHz, CDCl₃): δ 8.46 (d, *J* = 8.0 Hz, 1H), 7.74 (d, *J* = 8.0 Hz, 1H), 7.49 (d, *J* = 7.2 Hz, 2H), 7.41-7.37 (m, 7H), 7.34 (d, *J* = 7.6 Hz, 2H), 7.29 (d, *J* = 7.2 Hz, 2H), 7.24-7.19 (m, 3H).

¹³C NMR (100 MHz, CDCl₃): δ 162.4, 151.7, 147.8, 140.0, 139.6, 134.6, 133.3, 131.6, 130.5, 129.6, 129.4, 129.33, 129.30, 128.8, 128.5, 128.2, 127.7, 127.4, 123.9, 119.6, 117.3.

IR (KBr, cm⁻¹): 3106, 3053, 3019, 2955, 2922, 2850, 1737, 1698, 1682, 1651, 1611, 1578, 1556, 1488, 1477, 1444, 1407, 1298, 1220, 1156.

HRMS (ESI) m/z: [M+H]⁺ Calcd for C₂₇H₁₉O₂: 375.1385; Found 375.1375.

3,4-diphenyl-6-(phenylethynyl)-1*H*-isochromen-1-one (9)



9 was prepared according to the procedure in section 2.6.2. The crude reaction mixture was purified by column chromatography using silica gel (100-200 mesh) giving **9** (32 mg) in 80% yield.

Physical State: pale brown solid, **m.p.:** 198-200 °C,
R_f-value: 0.50 (10% EtOAc/hexane).

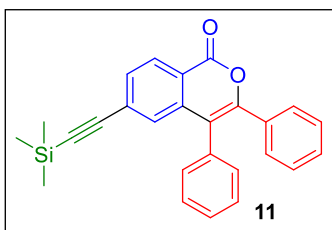
¹H NMR (400 MHz, CDCl₃): δ 8.37 (d, *J* = 8.4 Hz, 1H), 7.63 (dd, *J* = 8.0, 1.2 Hz, 1H), 7.51-7.49 (m, 2H), 7.46-7.42 (m, 3H), 7.35-7.31 (m, 5H), 7.29-7.17 (m, 6H).

¹³C NMR (100 MHz, CDCl₃): δ 162.1, 152.0, 139.2, 134.2, 133.1, 132.1, 131.6, 131.3, 130.2, 129.9, 129.6, 129.5, 129.43, 129.40, 128.7, 128.6, 128.3, 128.2, 122.6, 119.8, 116.7, 93.8, 88.7.

IR (KBr, cm⁻¹): 3081, 3057, 3019, 2206, 1731, 1667, 1625, 1562, 1519, 1441, 1296, 1195.

HRMS (ESI) m/z: [M+H]⁺ Calcd for C₂₉H₁₉O₂: 399.1385; Found 399.1409.

3,4-diphenyl-6-((trimethylsilyl)ethynyl)-1*H*-isochromen-1-one (11)



11 was prepared according to the procedure in section 2.6.3. The crude reaction mixture was purified by column chromatography using silica gel (100-200 mesh) giving **11** (32 mg) in 81 % yield.

Physical State: off-white solid, **m.p.:** 202-205°C,

R_f-value: 0.55 (10% EtOAc/hexane).

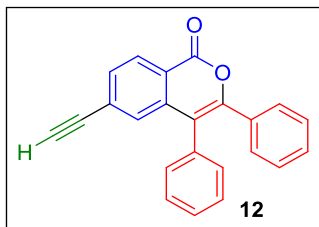
¹H NMR (400 MHz, CDCl₃): δ 8.32 (d, *J* = 8.0 Hz, 1H), 7.57 (dd, *J* = 8.4, 1.6 Hz, 1H), 7.46-7.41 (m, 3H), 7.31-7.28 (m, 2H), 7.26-7.16 (m, 6H), 0.22 (s, 9H).

¹³C NMR (100 MHz, CDCl₃): δ 162.0, 151.9, 139.0, 134.2, 133.1, 131.8, 131.6, 130.0, 129.8, 129.58, 129.51, 129.4, 128.5, 128.2, 120.0, 116.7, 103.9, 99.5, 0.07.

IR (KBr, cm⁻¹): 3129, 3078, 3017, 2156, 1732, 1698, 1661, 1634, 1584, 1557, 1494, 1243.

HRMS (ESI) m/z: [M+Na]⁺ Calcd for C₂₆H₂₂SiNaO₂: 417.1287; Found 417.1290.

6-ethynyl-3,4-diphenyl-1*H*-isochromen-1-one (**12**)



12 was prepared according to the procedure in section 2.6.4. The crude reaction mixture was purified by column chromatography using silica gel (100-200 mesh) giving **12** (27 mg) in 84% yield.

Physical State: yellow solid, **m.p.:** 185-187 °C,

R_f-value: 0.50 (10% EtOAc/hexane).

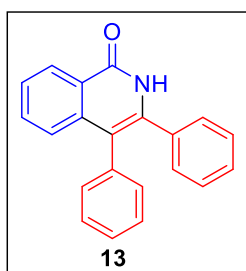
¹H NMR (400 MHz, CDCl₃): δ 8.35 (d, *J* = 8.4 Hz, 1H), 7.58 (d, *J* = 8.0 Hz, 1H), 7.43-7.41 (m, 3H), 7.32-7.30 (m, 3H), 7.26-7.17 (m, 5H), 3.22 (s, 1H).

¹³C NMR (100 MHz, CDCl₃): δ 161.9, 152.0, 139.2, 134.1, 133.0, 131.6, 131.5, 129.9, 129.5, 129.4, 129.2, 128.9, 128.6, 128.2, 120.4, 116.6, 82.8, 81.5.

IR (KBr, cm⁻¹): 3290, 3060, 2921, 2849, 2104, 1727, 1693, 1681, 1599, 1555, 1492, 1476, 1265.

HRMS (ESI) m/z: [M+H]⁺ Calcd for C₂₃H₁₅O₂: 323.1072; Found 323.1094.

3,4-diphenylisoquinolin-1(2*H*)-one (**13**)



13 was prepared according to the procedure in section 2.6.5. The crude reaction mixture was purified by column chromatography using silica gel (100-200 mesh) giving **13** (26 mg) in 87 % yield.

Physical State: off-white solid,

m.p.: 258-260 °C,

R_f-value: 0.40 (30% EtOAc/hexane).

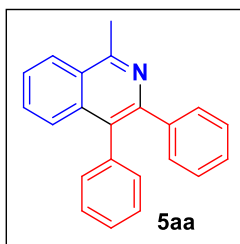
¹H NMR (400 MHz, CDCl₃): δ 9.23 (s, 1H), 8.47 (d, *J* = 7.6 Hz, 1H), 7.58 (t, *J* = 7.6 Hz, 1H), 7.50 (t, *J* = 8.0 Hz, 1H), 7.35 (d, *J* = 8.0 Hz, 1H), 7.33-7.28 (m, 3H), 7.25-7.24 (m, 5H), 7.19-7.17 (m, 2H),

¹³C NMR (100 MHz, CDCl₃): δ 163.0, 139.0, 137.3, 136.0, 135.4, 133.0, 132.1, 129.5, 129.0, 128.7, 127.8, 127.6, 126.9, 126.0, 125.4, 117.6.

IR (KBr, cm⁻¹): 3044, 3025, 2985, 1650, 1576, 1536, 1515, 1471, 1346, 1267, 1156.

HRMS (ESI) m/z: [M+H]⁺ Calcd for C₂₁H₁₆NO: 398.1232; Found 398.1235.

1-methyl-3,4-diphenylisoquinoline (5aa)



5aa was prepared according to general procedure D. The crude reaction mixture was purified by column chromatography using silica gel (100-200 mesh) giving **5aa** (25 mg) in 85% yield.

Physical State: white solid, **m.p.:** 151-153 °C,

R_f-value: 0.45 (10% EtOAc/hexane).

¹H NMR (400 MHz, CDCl₃): δ 8.21-8.19 (m, 1H), 7.67-7.64 (m, 1H), 7.61-7.57 (m, 2H), 7.37-7.31 (m, 5H), 7.23-7.16 (m, 5H), 3.08

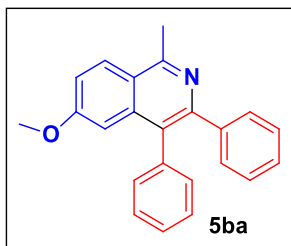
(s, 3H).

¹³C NMR (100 MHz, CDCl₃): δ 158.0, 149.7, 141.3, 137.9, 136.3, 131.7, 130.6, 130.2, 129.5, 128.5, 127.9, 127.4, 127.2, 126.8, 126.5, 126.4, 125.8, 23.0.

IR (KBr, cm⁻¹): 3055, 2952, 2918, 2852, 1610, 1566, 1503, 1431, 1334, 1267, 1156, 1073.

HRMS (ESI) m/z: [M+H]⁺ Calcd for C₂₂H₁₈N: 296.1439; Found 296.1459.

6-methoxy-1-methyl-3,4-diphenylisoquinoline (5ba)



5ba was prepared according to general procedure D. The crude reaction mixture was purified by column chromatography using silica gel (100-200 mesh) giving **5ba** (18 mg) in 55% yield.

Physical State: pale brown solid, **m.p.:** 177-180 °C,

R_f-value: 0.45 (15% EtOAc/hexane).

¹H NMR (400 MHz, CDCl₃): δ 8.11 (d, *J* = 9.2 Hz, 1H), 7.35-7.29 (m, 5H), 7.23-7.16 (m, 6H), 6.91 (d, *J* = 2.8 Hz, 1H), 3.72

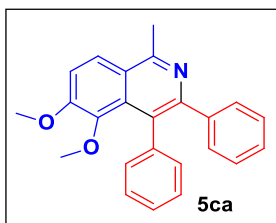
(s, 3H), 3.02 (s, 3H).

¹³C NMR (100 MHz, CDCl₃): δ 160.8, 157.3, 150.4, 141.4, 138.4, 138.1, 131.6, 130.5, 128.9, 128.6, 127.9, 127.8, 127.4, 127.2, 122.2, 119.0, 104.8, 55.5, 22.9.

IR (KBr, cm⁻¹): 3058, 2957, 2854, 1617, 1573, 1500, 1409, 1345, 1260, 1176, 1070.

HRMS (ESI) m/z: [M+H]⁺ Calcd for C₂₃H₂₀NO: 326.1545; Found 326.1532.

5,6-dimethoxy-1-methyl-3,4-diphenylisoquinoline (**5ca**)



5ca was prepared according to general procedure D. The crude reaction mixture was purified by column chromatography using silica gel (100-200 mesh) giving **5ca** (22 mg) in 62 % yield.

Physical State: pale yellow solid, **m.p.:** 162-164 °C,

R_f-value: 0.5 (30% EtOAc/hexane).

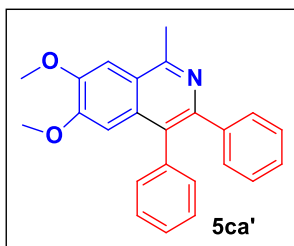
¹H NMR (400 MHz, CDCl₃): δ 8.02 (d, J = 9.2 Hz, 1H), 7.39 (d, J = 9.2 Hz, 1H), 7.22 (dd, J = 8.4, 2.0 Hz, 2H), 7.19-7.10 (m, 8H), 3.98 (s, 3H), 3.07 (s, 3H), 3.01 (s, 3H).

¹³C NMR (100 MHz, CDCl₃): δ 157.7, 153.6, 151.9, 144.2, 141.9, 140.7, 131.4, 131.2, 130.5, 127.6, 126.89, 126.85, 126.1, 123.3, 123.1, 114.7, 60.7, 56.6, 23.3.

IR (KBr, cm⁻¹): 3058, 3007, 2961, 1619, 1573, 1504, 1462, 1381, 1253, 1167, 1062.

HRMS (ESI) m/z: [M+Na]⁺ Calcd for C₂₄H₂₁NO₂Na: 378.1470; Found 378.1450.

6,7-dimethoxy-1-methyl-3,4-diphenylisoquinoline (**5ca'**)



5ca' was prepared according to general procedure D. The crude reaction mixture was purified by column chromatography using silica gel (100-200 mesh) giving **5ca'** (8 mg) in 22% yield.

Physical State: white solid, **m.p.:** 159-161 °C,

R_f-value: 0.45 (30% EtOAc/hexane).

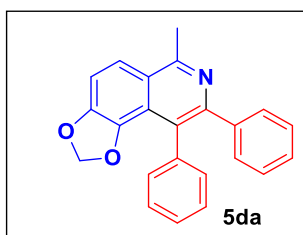
¹H NMR (400 MHz, CDCl₃): δ 7.38-7.30 (m, 6H), 7.23 (d, J = 1.6 Hz, 1H), 7.21-7.14 (m, 4H), 6.92 (s, 1H), 4.07 (s, 3H), 3.77 (s, 3H), 3.00 (s, 3H).

¹³C NMR (176 MHz, CDCl₃): δ 155.3, 152.6, 149.8, 149.0, 141.5, 138.3, 132.9, 131.5, 130.5, 128.7, 128.6, 127.8, 127.4, 127.04, 122.4, 104.9, 104.1, 56.3, 56.0, 23.1.

IR (KBr, cm⁻¹): 3044, 2965, 2853, 1606, 1546, 1499, 1454, 1388, 1273, 1151, 1068.

HRMS (ESI) m/z: [M+Na]⁺ Calcd for C₂₄H₂₁NO₂Na: 378.1470; Found 378.1497.

6-methyl-8,9-diphenyl-[1,3]dioxolo[4,5-f]isoquinoline (**5da**)



5da was prepared according to general procedure D. The crude reaction mixture was purified by column chromatography using silica gel (100-200 mesh) giving **5da** (22 mg) in 65 % yield.

Physical State: pale yellow solid, **m.p.:** 253-256 °C,

R_f-value: 0.45 (15% EtOAc/hexane).

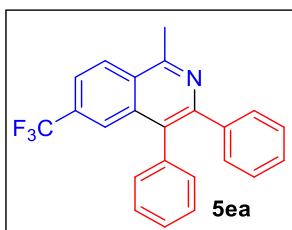
¹H NMR (400 MHz, CDCl₃): δ 7.83 (d, *J* = 8.8 Hz, 1H), 7.29-7.27 (m, 3H), 7.24-7.14 (m, 8H), 5.84 (s, 2H), 3.00 (s, 3H).

¹³C NMR (100 MHz, CDCl₃): δ 158.1, 150.5, 147.9, 142.0, 141.1, 138.7, 131.5, 130.5, 127.8, 127.4, 127.17, 127.12, 125.1, 123.5, 122.8, 121.2, 111.2, 110.7, 23.7.

IR (KBr, cm⁻¹): 3083, 2993, 2903, 2853, 1625, 1576, 1513, 1451, 1353, 1278, 1177, 1036.

HRMS (ESI) m/z: [M+Na]⁺ Calcd for C₂₃H₁₇NO₂Na: 362.1157; Found 362.1167.

3,4-diphenyl-6-(trifluoromethyl)-1*H*-isochromen-1-one (**5ea**)



5ea was prepared according to general procedure D. The crude reaction mixture was purified by column chromatography using silica gel (100-200 mesh) giving **5ea** (16 mg) in 44% yield.

Physical State: white solid, **m.p.:** 105-107 °C,

R_f-value: 0.40 (10% EtOAc/hexane).

¹H NMR (400 MHz, CDCl₃): δ 8.32 (d, *J* = 8.4 Hz, 1H), 7.97 (s, 1H), 7.76 (dd, *J* = 8.4, 1.2 Hz, 1H), 7.38-7.34 (m, 5H), 7.28-7.19 (m, 5H), 3.11 (s, 3H).

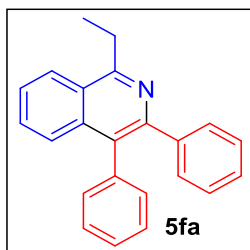
¹³C NMR (176 MHz, CDCl₃): δ 158.2, 151.2, 140.7, 136.8, 135.8, 131.8 (q, *J*_{C-F} = 31.6 Hz), 131.6, 130.5, 130.0, 128.8, 128.08, 128.03, 127.6, 127.3, 127.2, 124.2 (q, *J*_{C-F} = 5.2 Hz), 124.1 (q, *J*_{C-F} = 272.9 Hz), 122.5, 23.1.

¹⁹F NMR (376 MHz, CDCl₃): δ -62.8.

IR (KBr, cm⁻¹): 3087, 3036, 2924, 2854, 1574, 1504, 1434, 1385, 1306, 1256, 1176, 1081.

HRMS (ESI) m/z: [M+H]⁺ Calcd for C₂₃H₁₇F₃N: 364.1313; Found 364.1277.

1-ethyl-3,4-diphenylisoquinoline (5fa)



5fa was prepared according to general procedure D. The crude reaction mixture was purified by column chromatography using silica gel (100-200 mesh) giving **5fa** (25 mg) in 82% yield.

Physical State: white solid, **m.p.:** 152-154 °C.

R_f-value: 0.45 (10% EtOAc/hexane).

¹H NMR (400 MHz, CDCl₃): δ 8.24 (d, *J* = 10.0 Hz, 1H), 7.67-7.65 (m, 1H), 7.58-7.56 (m, 2H), 7.39-7.33 (m, 5H), 7.24-7.17 (m, 5H),

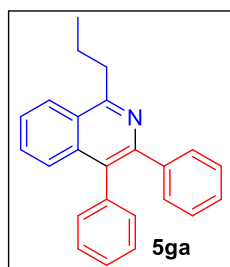
3.44 (t, *J* = 7.6 Hz, 2H), 1.53 (t, *J* = 7.6 Hz, 3H).

¹³C NMR (100 MHz, CDCl₃): δ 162.4, 149.4, 141.2, 137.8, 136.4, 131.5, 130.4, 129.8, 129.0, 128.3, 127.7, 127.2, 127.0, 126.57, 126.54, 125.4, 125.2, 28.9, 14.1.

IR (KBr, cm⁻¹): 3053, 2954, 2917, 2853, 1611, 1564, 1504, 1434, 1335, 1262, 1158, 1076.

HRMS (ESI) m/z: [M+H]⁺ Calcd for C₂₃H₂₀N: 310.1596; Found 310.1606.

3,4-diphenyl-1-propylisoquinoline (5ga)



5ga was prepared according to general procedure D. The crude reaction mixture was purified by column chromatography using silica gel (100-200 mesh) giving **5ga** (26 mg) in 80% yield.

Physical State: white solid, **m.p.:** 155-157 °C.

R_f-value: 0.45 (10% EtOAc/hexane).

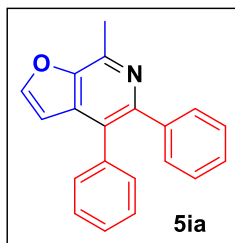
¹H NMR (400 MHz, CDCl₃): δ 8.25-8.22 (m, 1H), 7.67-7.64 (m, 1H), 7.58-7.55 (m, 2H), 7.37-7.33 (m, 5H), 7.24-7.17 (m, 5H), 3.38 (t, *J* = 7.6 Hz, 2H), 2.00 (sextet, *J* = 7.6 Hz, 2H), 1.14 (t, *J* = 7.6 Hz, 3H).

¹³C NMR (100 MHz, CDCl₃): δ 161.4, 149.4, 141.2, 137.8, 136.4, 131.5, 130.4, 129.8, 129.0, 128.3, 127.7, 127.2, 127.0, 126.5, 126.4, 125.6, 125.4, 37.8, 23.3, 14.6.

IR (KBr, cm⁻¹): 3056, 2951, 2916, 2853, 1612, 1562, 1501, 1433, 1331, 1264, 1152, 1071.

HRMS (ESI) m/z: [M+H]⁺ Calcd for C₂₄H₂₁N: 324.1752; Found 324.1761.

7-methyl-4,5-diphenylfuro[2,3-c]pyridine (**5ia**)



5ia was prepared according to general procedure D. The crude reaction mixture was purified by column chromatography using silica gel (100-200 mesh) giving **5ia** (10 mg) in 35% yield.

Physical State: white solid, **m.p.:** 172-174 °C.

R_f-value: 0.50 (10% EtOAc/hexane).

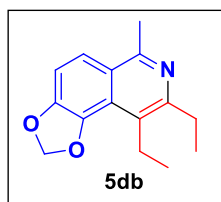
¹H NMR (400 MHz, CDCl₃): δ 7.73 (d, *J* = 2.3 Hz, 1H), 7.33 (dd, *J* = 6.6, 2.9 Hz, 2H), 7.27 (t, *J* = 9.7 Hz, 3H), 7.23 – 7.17 (m, 5H), 6.72 (d, *J* = 2.2 Hz, 1H), 2.85 (s, 3H).

¹³C NMR (100 MHz, CDCl₃): δ 150.04, 149.69, 147.95, 141.40, 140.58, 137.75, 134.37, 130.43, 130.28, 128.40, 127.88, 127.18, 127.14, 126.82, 106.58, 18.79.

IR (KBr, cm⁻¹): 3058, 2950, 2918, 2852, 1614, 1563, 1505, 1431, 1335, 1263, 1151, 1073.

HRMS (ESI) m/z: [M+H]⁺ Calcd for C₂₀H₁₆NO: 287.1310; Found 287.1308.

8,9-diethyl-6-methyl-[1,3]dioxolo[4,5-f]isoquinoline (**5db**)



5db was prepared according to general procedure D. The crude reaction mixture was purified by column chromatography using silica gel (100-200 mesh) giving **5db** (23 mg) in 94 % yield.

Physical State: brown solid, **m.p.:** 79-81 °C,

R_f-value: 0.45 (15% EtOAc/hexane).

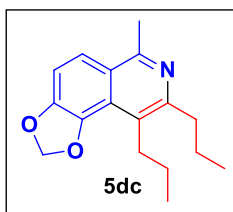
¹H NMR (400 MHz, CDCl₃): δ 7.68 (d, *J* = 8.8 Hz, 1H), 7.17 (d, *J* = 8.8 Hz, 1H), 6.13 (s, 2H), 3.10 (q, *J* = 7.6 Hz, 2H), 2.90 (q, *J* = 7.6 Hz, 2H), 2.84 (s, 3H), 1.32 (t, *J* = 7.6 Hz, 3H), 1.23 (t, *J* = 7.6 Hz, 3H).

¹³C NMR (176 MHz, CDCl₃): δ 156.0, 153.1, 147.1, 141.2, 125.0, 123.9, 123.5, 121.5, 110.2, 101.4, 28.0, 23.2, 22.6, 16.3, 15.2.

IR (KBr, cm⁻¹): 2979, 2955, 2927, 2867, 1629, 1575, 1514, 1445, 1350, 1276, 1185, 1043.

HRMS (ESI) m/z: [M+H]⁺ Calcd for C₁₅H₁₈NO₂: 244.1338; Found 244.1316.

6-methyl-8,9-dipropyl-[1,3]dioxolo[4,5-*f*]isoquinoline (**5dc**)



5dc was prepared according to general procedure D. The crude reaction mixture was purified by column chromatography using silica gel (100-200 mesh) giving **5dc** (24 mg) in 88 % yield.

Physical State: brown solid, **m.p.:** 94-96 °C.

R_f-value: 0.5 (20% EtOAc/hexane).

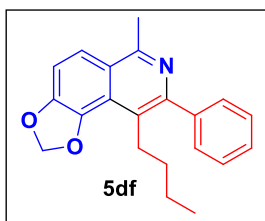
¹H NMR (400 MHz, CDCl₃): δ 7.68 (d, J = 8.8 Hz, 1H), 7.16 (d, J = 8.8 Hz, 1H), 6.12 (s, 2H), 3.02 (t, J = 8.4 Hz, 2H), 2.85-2.81 (m, 5H), 1.76 (sextet, J = 7.6 Hz, 2H), 1.60 (sextet, J = 7.2 Hz, 2H), 1.03 (t, J = 7.2 Hz, 6H).

¹³C NMR (100 MHz, CDCl₃): δ 155.8, 152.1, 147.0, 141.3, 124.0, 123.8, 123.7, 121.5, 110.1, 101.4, 37.0, 31.5, 25.4, 24.4, 23.2, 14.77, 14.72.

IR (KBr, cm⁻¹): 2962, 2931, 2873, 2857, 1629, 1567, 1493, 1443, 1352, 1266, 1180, 1046.

HRMS (ESI) m/z: [M+H]⁺ Calcd for C₁₇H₂₂NO₂: 272.1650; Found 272.1662.

9-butyl-6-methyl-8-phenyl-[1,3]dioxolo[4,5-*f*]isoquinoline (**5df**)



5df was prepared according to general procedure D. The crude reaction mixture was purified by column chromatography using silica gel (100-200 mesh) giving **5df** (13 mg) in 41 % yield.

Physical State: brown solid, **m.p.:** 114-116 °C.

R_f-value: 0.5 (20% EtOAc/hexane).

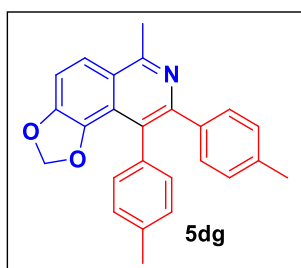
¹H NMR (400 MHz, CDCl₃): δ 7.77 (d, J = 8.8 Hz, 1H), 7.48-7.41 (m, 4H), 7.39-7.35 (m, 1H), 7.26 (d, J = 8.8 Hz, 1H), 6.16 (s, 2H), 2.97 (t, J = 8.0 Hz, 2H), 2.89 (s, 3H), 1.56-1.48 (m, 2H), 1.24 (sextet, J = 7.6 Hz, 2H), 0.78 (t, J = 7.2 Hz, 3H).

¹³C NMR (176 MHz, CDCl₃): δ 155.8, 151.4, 147.4, 141.89, 141.82, 129.7, 128.4, 127.7, 125.3, 124.3, 123.5, 121.7, 110.9, 101.6, 34.6, 30.0, 23.4, 23.0, 14.1.

IR (KBr, cm⁻¹): 3063, 2958, 2928, 2868, 1625, 1563, 1513, 1443, 1352, 1275, 1182, 1118, 1073.

HRMS (ESI) m/z: [M+H]⁺ Calcd for C₂₁H₂₂NO₂: 320.1650; Found 320.1631.

6-methyl-8,9-di-*p*-tolyl-[1,3]dioxolo[4,5-*f*]isoquinoline (**5dg**)



5dg was prepared according to general procedure D. The crude reaction mixture was purified by column chromatography using silica gel (100-200 mesh) giving **5dg** (28 mg) in 76 % yield.

Physical State: white solid, **m.p.:** 179-181 °C,

R_f-value: 0.50 (15% EtOAc/hexane).

¹H NMR (400 MHz, CDCl₃): δ 7.72 (d, *J* = 8.8 Hz, 1H), 7.16 (d, *J* = 8.8 Hz, 1H), 7.11 (d, *J* = 8.0 Hz, 2H), 7.00 (d, *J* = 8.0 Hz,

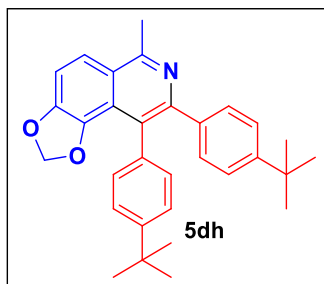
2H), 6.95 (d, *J* = 7.6 Hz, 2H), 6.89 (d, *J* = 8.0 Hz, 2H), 5.76 (s, 2H), 2.91 (s, 3H), 2.27 (s, 3H), 2.18 (s, 3H).

¹³C NMR (100 MHz, CDCl₃): δ 157.8, 150.3, 147.9, 142.0, 138.2, 136.7, 136.5, 135.7, 131.2, 130.4, 128.5, 128.2, 124.9, 123.5, 123.1, 121.2, 111.0, 101.6, 23.6, 21.7, 21.5.

IR (KBr, cm⁻¹): 3025, 2991, 2919, 2854, 1624, 1573, 1551, 1438, 1355, 1276, 1183, 1045.

HRMS (ESI) m/z: [M+Na]⁺ Calcd for C₂₅H₂₁NO₂Na: 390.1470; Found 390.1432.

8,9-bis(4-(*tert*-butyl)phenyl)-6-methyl-[1,3]dioxolo[4,5-*f*]isoquinoline (**5dh**)



5dh was prepared according to general procedure D. The crude reaction mixture was purified by column chromatography using silica gel (100-200 mesh) giving **5dh** (33 mg) in 73% yield.

Physical State: yellow solid, **m.p.:** 134-137 °C,

R_f-value: 0.50 (10% EtOAc/hexane).

¹H NMR (400 MHz, CDCl₃): δ 7.80 (d, *J* = 8.8 Hz, 1H), 7.25-7.21 (m, 3H), 7.18-7.10 (m, 6H), 5.85 (s, 2H), 2.98 (s, 3H), 1.31

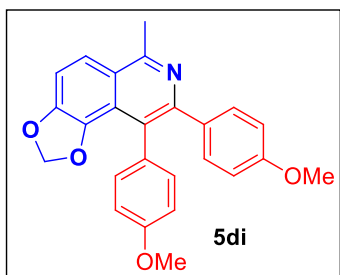
(s, 9H), 1.23 (s, 9H).

¹³C NMR (100 MHz, CDCl₃): δ 157.7, 150.7, 149.9, 149.7, 147.8, 142.0, 138.3, 131.1, 130.0, 124.9, 124.6, 124.2, 123.5, 123.0, 121.1, 110.9, 101.6, 34.8, 34.6, 31.7, 31.5, 23.7.

IR (KBr, cm⁻¹): 2953, 2921, 2857, 1627, 1566, 1519, 1434, 1354, 1278, 1127, 1047.

HRMS (ESI) m/z: [M+H]⁺ Calcd for C₃₁H₃₄NO₂: 452.2589; Found 452.2560.

8,9-bis(4-methoxyphenyl)-6-methyl-[1,3]dioxolo[4,5-f]isoquinoline (**5di**)



5di was prepared according to general procedure D. The crude reaction mixture was purified by column chromatography using silica gel (100-200 mesh) giving **5di** (36 mg) in 90% yield.

Physical State: light brown solid, **m.p.:** 219-220 °C,

R_f-value: 0.50 (30% EtOAc/hexane).

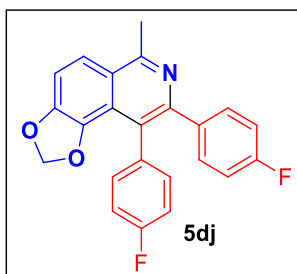
¹H NMR (400 MHz, CDCl₃): δ 7.79 (d, J = 8.8 Hz, 1H), 7.24 (dd, J = 7.2, 1.6 Hz, 3H), 7.10 (d, J = 8.4 Hz, 2H), 6.79 (d, J = 8.8 Hz, 2H), 6.72 (d, J = 8.8 Hz, 2H), 5.85 (s, 2H), 3.81 (s, 3H), 3.75 (s, 3H), 2.98 (s, 3H).

¹³C NMR (176 MHz, CDCl₃): δ 158.7, 157.7, 150.2, 147.8, 141.9, 133.8, 132.5, 131.8, 131.2, 124.3, 123.5, 123.4, 121.2, 113.3, 113.0, 110.9, 101.6, 55.5, 55.4, 23.7.

IR (KBr, cm⁻¹): 3016, 2959, 2918, 2839, 1606, 1578, 1514, 1448, 1354, 1288, 1180, 1048.

HRMS (ESI) m/z: [M+Na]⁺ Calcd for C₂₅H₂₁NO₄Na: 422.1368; Found 422.1354.

8,9-bis(4-fluorophenyl)-6-methyl-[1,3]dioxolo[4,5-f]isoquinoline (**5dj**)



5dj was prepared according to general procedure D. The crude reaction mixture was purified by column chromatography using silica gel (100-200 mesh) giving **5dj** (34 mg) in 91% yield.

Physical State: brown solid, **m.p.:** 194-196 °C,

R_f-value: 0.50 (15% EtOAc/hexane).

¹H NMR (400 MHz, CDCl₃): δ 7.75 (d, J = 8.8 Hz, 1H), 7.20-7.16 (m, 3H), 7.06 (td, J = 5.6, 2.4 Hz, 2H), 6.86 (t, J = 8.8 Hz, 2H), 6.80 (t, J = 8.8 Hz, 2H), 5.78 (s, 2H), 2.91 (s, 3H).

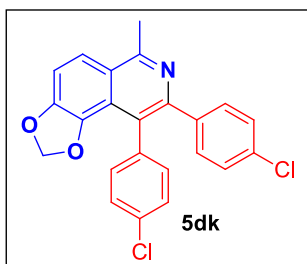
¹³C NMR (100 MHz, CDCl₃): δ 162.3 (d, J_{C-F} = 245 Hz), 162.2 (d, J_{C-F} = 246 Hz), 158.4, 149.4, 148.1, 141.9, 136.8 (d, J_{C-F} = 3 Hz), 134.4 (d, J_{C-F} = 4 Hz), 132.9 (d, J_{C-F} = 8 Hz), 132.2 (d, J_{C-F} = 8 Hz), 124.1, 123.5, 122.8, 121.4, 114.9 (d, J_{C-F} = 22 Hz), 114.6 (d, J_{C-F} = 21 Hz), 111.4, 101.8, 23.6.

¹⁹F NMR (376 MHz, CDCl₃): δ -115.1, δ -115.2.

IR (KBr, cm⁻¹): 3051, 2960, 2921, 2873, 1624, 1599, 1518, 1444, 1347, 1275, 1155, 1044.

HRMS (ESI) m/z: [M+H]⁺ Calcd for C₂₃H₁₆F₂NO₂: 376.1149; Found 376.1163.

8,9-bis(4-chlorophenyl)-6-methyl-[1,3]dioxolo[4,5-f]isoquinoline (**5dk**)



5dk was prepared according to general procedure D. The crude reaction mixture was purified by column chromatography using silica gel (100-200 mesh) giving **5dk** (32 mg) in 78 % yield.

Physical State: white solid, **m.p.:** 231-233 °C,

R_f-value: 0.50 (15% EtOAc/hexane).

¹H NMR (400 MHz, CDCl₃): δ 7.83 (d, *J* = 8.8 Hz, 1H), 7.29-7.21 (m, 5H), 7.17 (d, *J* = 8.4 Hz, 2H), 7.11 (d, *J* = 8.4 Hz, 2H),

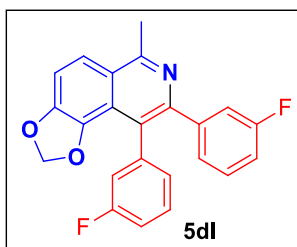
5.87 (s, 2H), 2.98 (s, 3H).

¹³C NMR (100 MHz, CDCl₃): δ 158.7, 149.2, 148.2, 141.9, 139.3, 136.9, 133.49, 133.41, 132.7, 131.8, 128.2, 127.9, 124.0, 123.5, 122.5, 121.4, 111.5, 101.9, 23.7.

IR (KBr, cm⁻¹): 2993, 2921, 2895, 2856, 1625, 1552, 1513, 1448, 1354, 1278, 1119, 1046.

HRMS (ESI) m/z: [M+H]⁺ Calcd for C₂₃H₁₆Cl₂NO₂: 408.0558; Found 408.0546.

8,9-bis(3-fluorophenyl)-6-methyl-[1,3]dioxolo[4,5-f]isoquinoline (**5dl**)



5dl was prepared according to general procedure D. The crude reaction mixture was purified by column chromatography using silica gel (100-200 mesh) giving **5dl** (33 mg) in 87% yield.

Physical State: white solid, **m.p.:** 187-190 °C,

R_f-value: 0.50 (15% EtOAc/hexane).

¹H NMR (400 MHz, CDCl₃): δ 7.83 (d, *J* = 8.8 Hz, 1H), 7.28 (d, *J* = 8.8 Hz, 1H), 7.22-6.94 (m, 7H), 6.86 (td, *J* = 7.2, 2.4 Hz,

1H), 5.87 (d, *J* = 8.8 Hz, 2H), 2.99 (s, 3H).

¹³C NMR (100 MHz, CDCl₃): δ 162.6 (d, *J*_{C-F} = 243 Hz), 162.3 (d, *J*_{C-F} = 244 Hz), 158.7, 149.0 (d, *J*_{C-F} = 2 Hz), 148.2, 143.0 (d, *J*_{C-F} = 8 Hz), 141.9, 140.5 (d, *J*_{C-F} = 8 Hz), 129.3 (d, *J*_{C-F} = 8 Hz), 129.0 (d, *J*_{C-F} = 8 Hz), 127.2 (d, *J*_{C-F} = 3 Hz), 126.1 (d, *J*_{C-F} = 3 Hz), 124.1 (d, *J*_{C-F} = 2 Hz), 123.5, 122.3, 121.4, 118.4 (d, *J*_{C-F} = 21 Hz), 117.4 (d, *J*_{C-F} = 22 Hz), 114.4 (d, *J*_{C-F} = 21 Hz), 111.6, 101.9, 23.7.

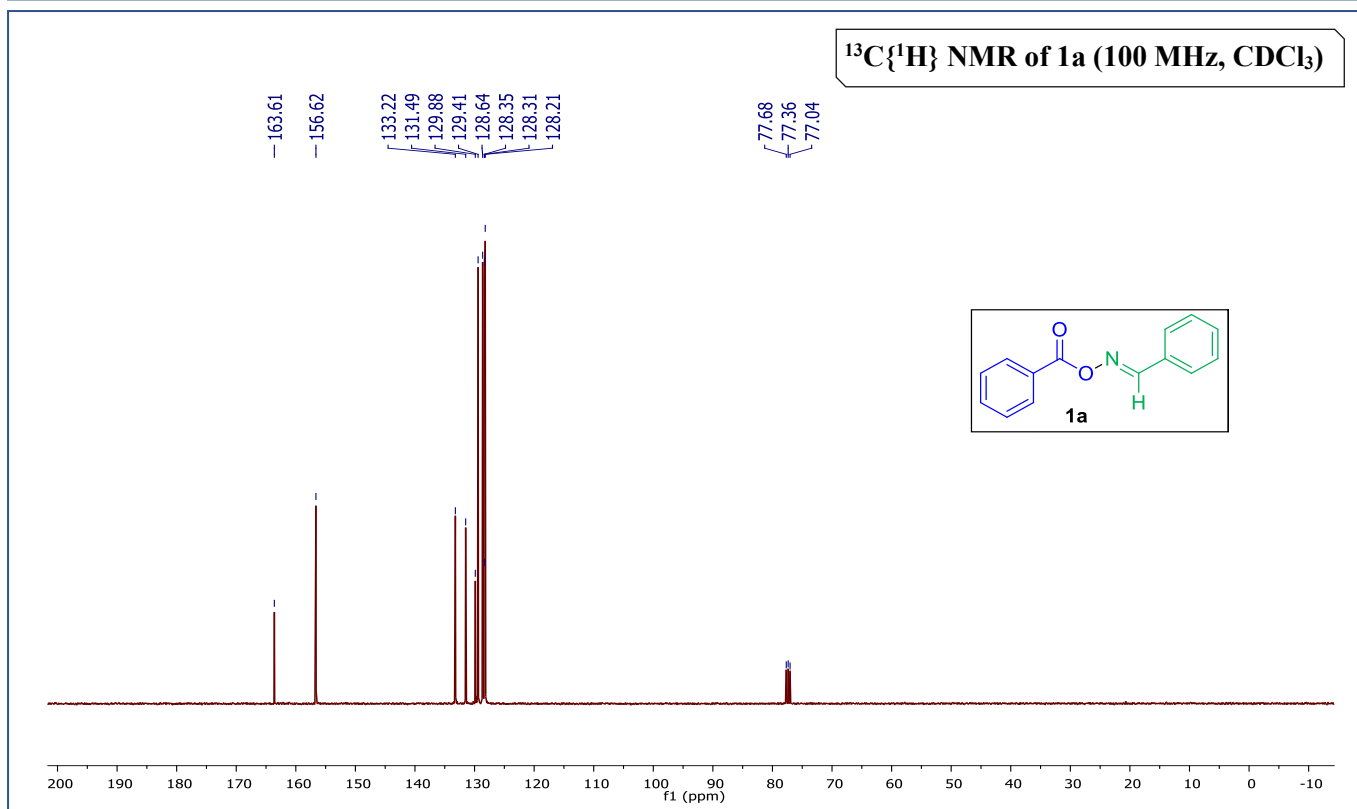
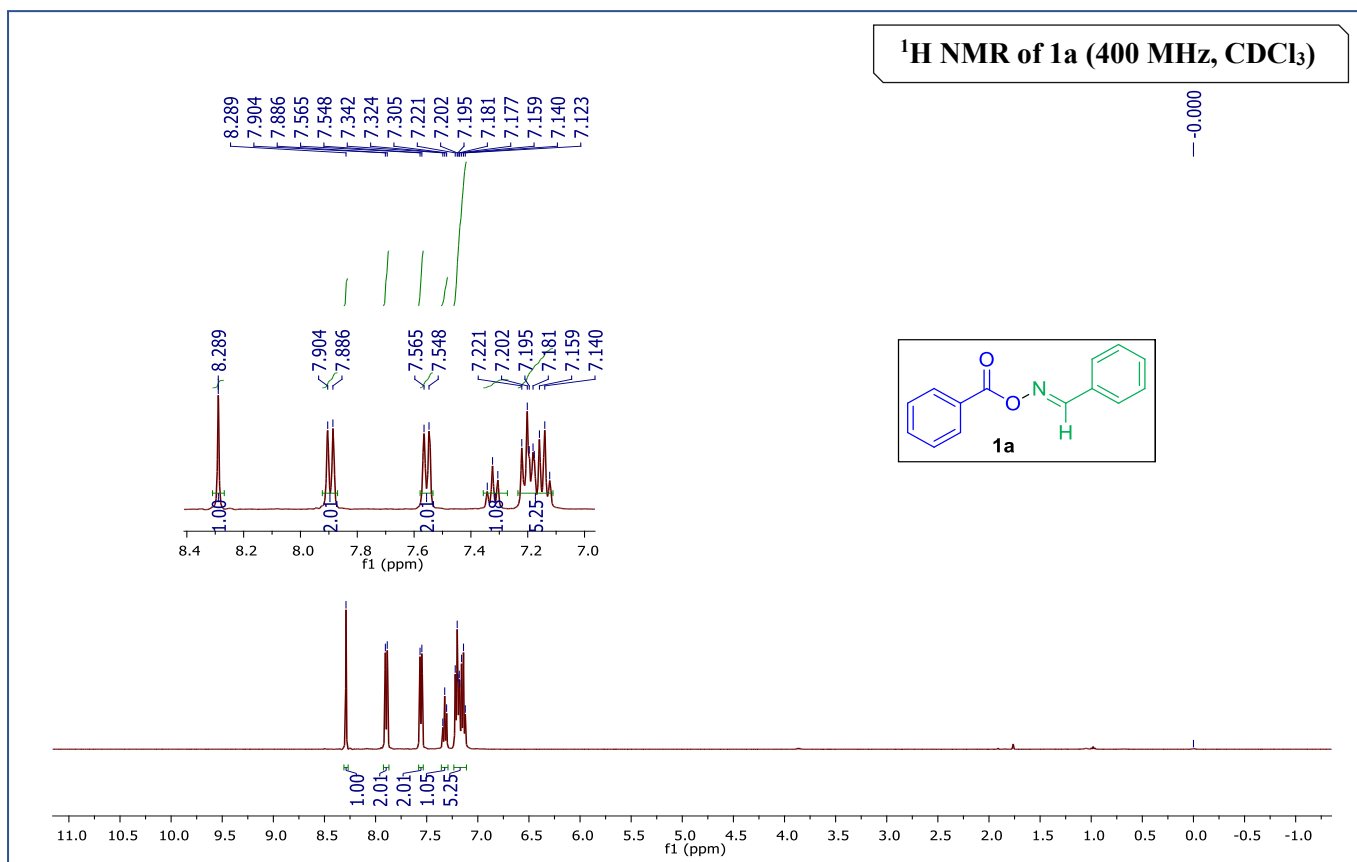
¹⁹F NMR (376 MHz, CDCl₃): δ -114.0, δ -114.5.

IR (KBr, cm⁻¹): 2956, 2924, 2884, 2855, 1612, 1581, 1513, 1440, 1348, 1278, 1181, 1072.

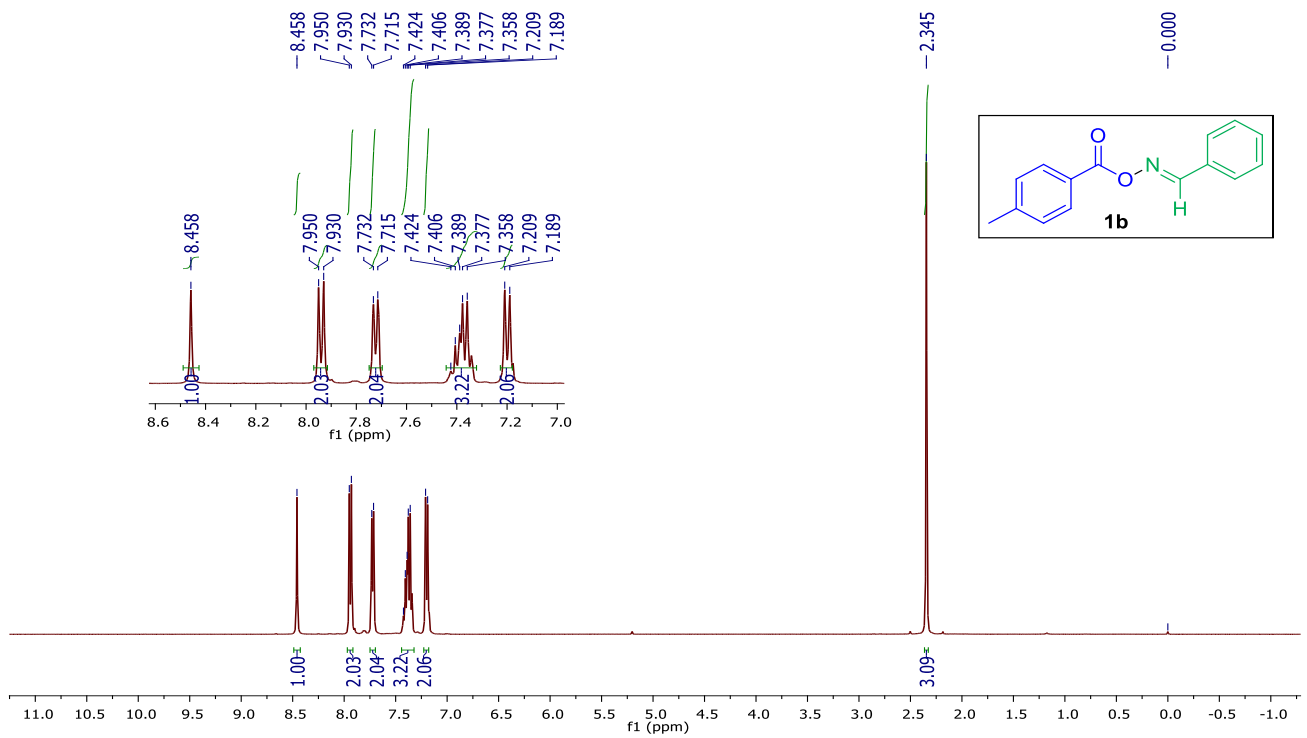
HRMS (ESI) m/z: [M+H]⁺ Calcd for C₂₃H₁₆F₂NO₂: 376.1149; Found 376.1152.

6. Copies of NMR spectra of the starting materials and products:

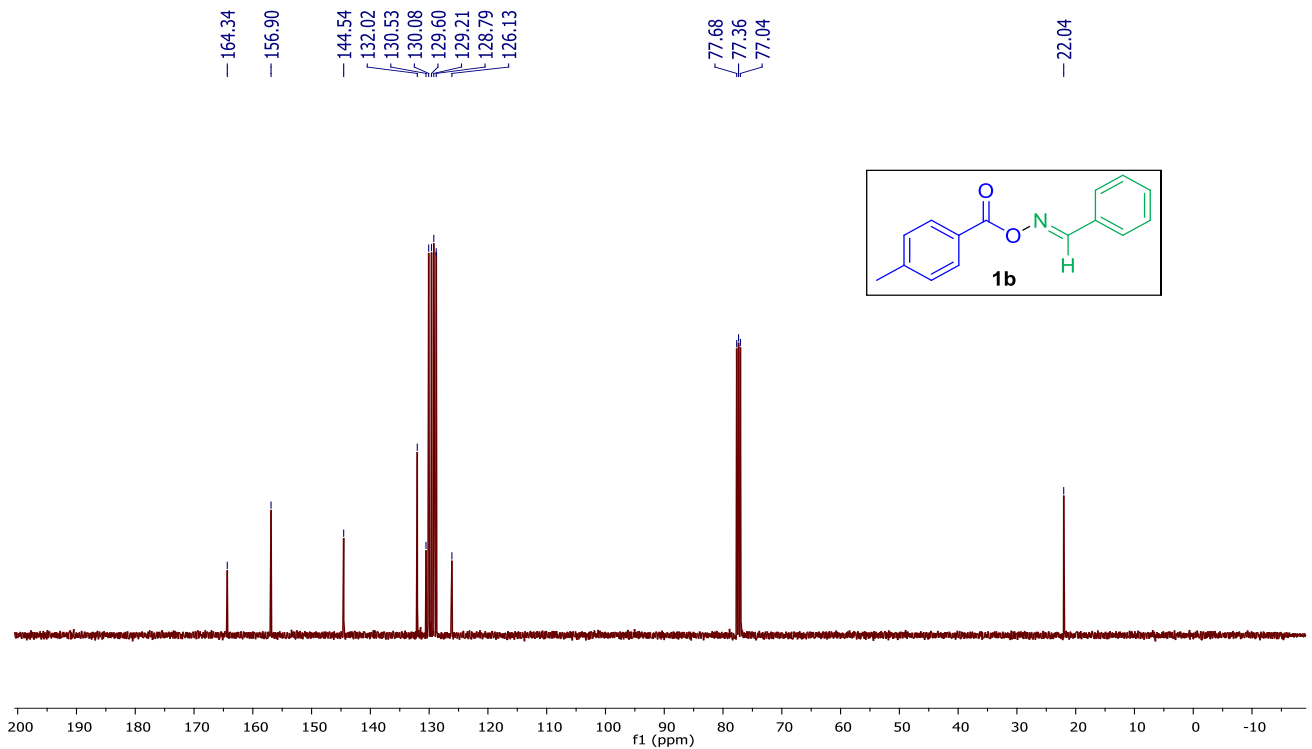
6.1 Copies of NMR spectra of the *O*-benzoyl oximes



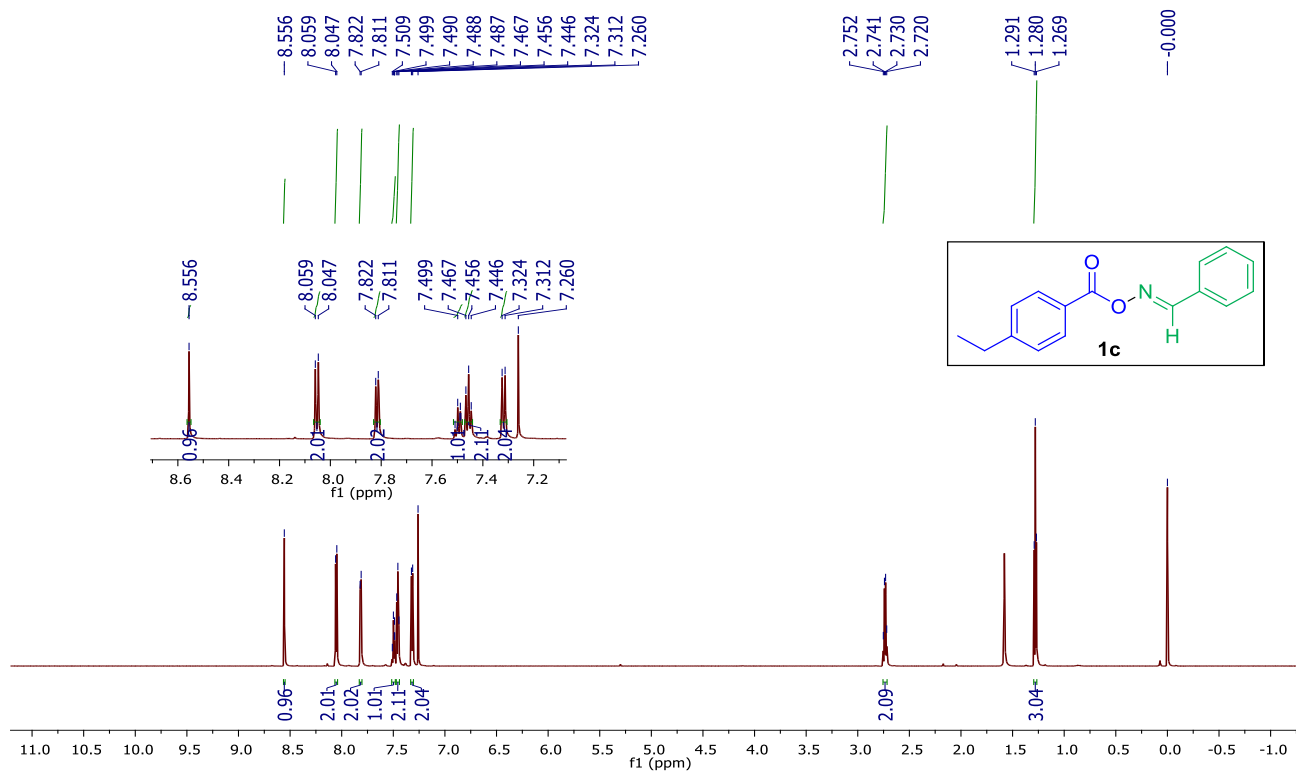
¹H NMR of 1b (400 MHz, CDCl₃)



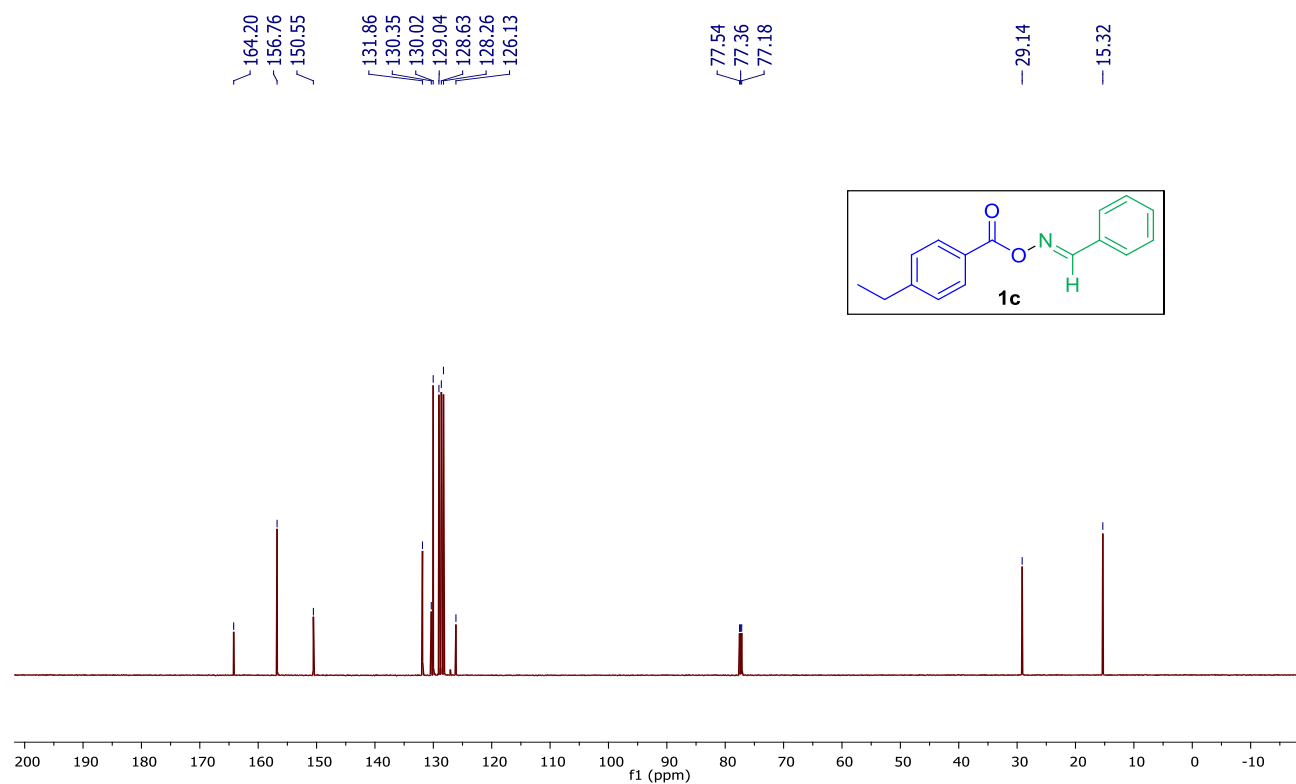
¹³C{¹H} NMR of 1b (100 MHz, CDCl₃)



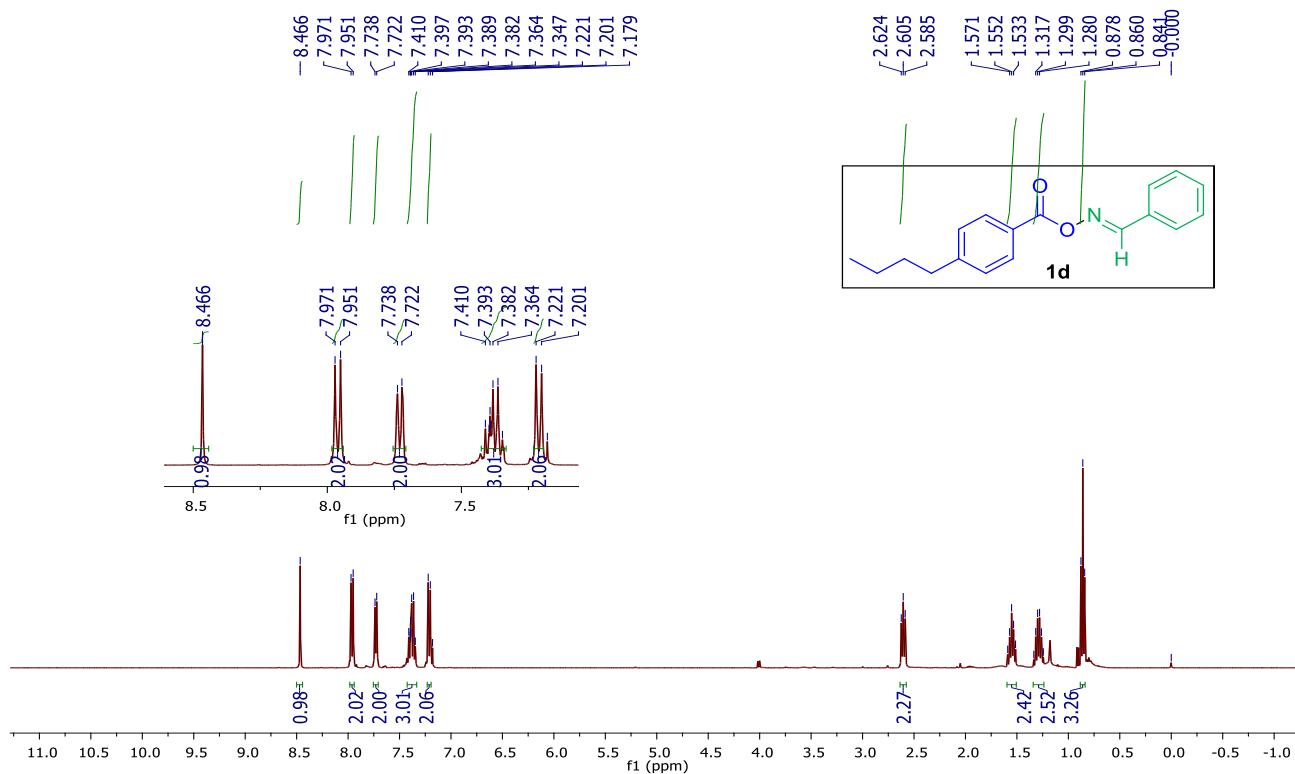
¹H NMR of 1c (700 MHz, CDCl₃)



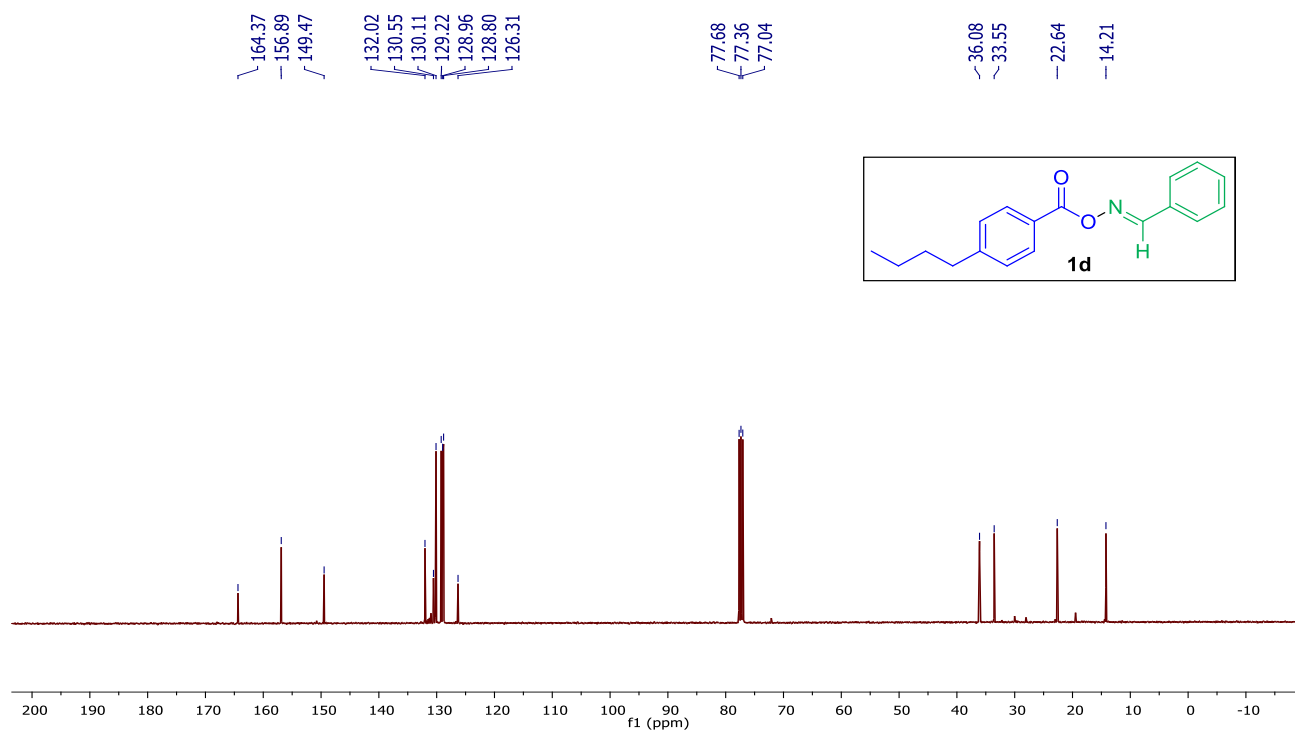
¹³C{¹H} NMR of 1c (176 MHz, CDCl₃)



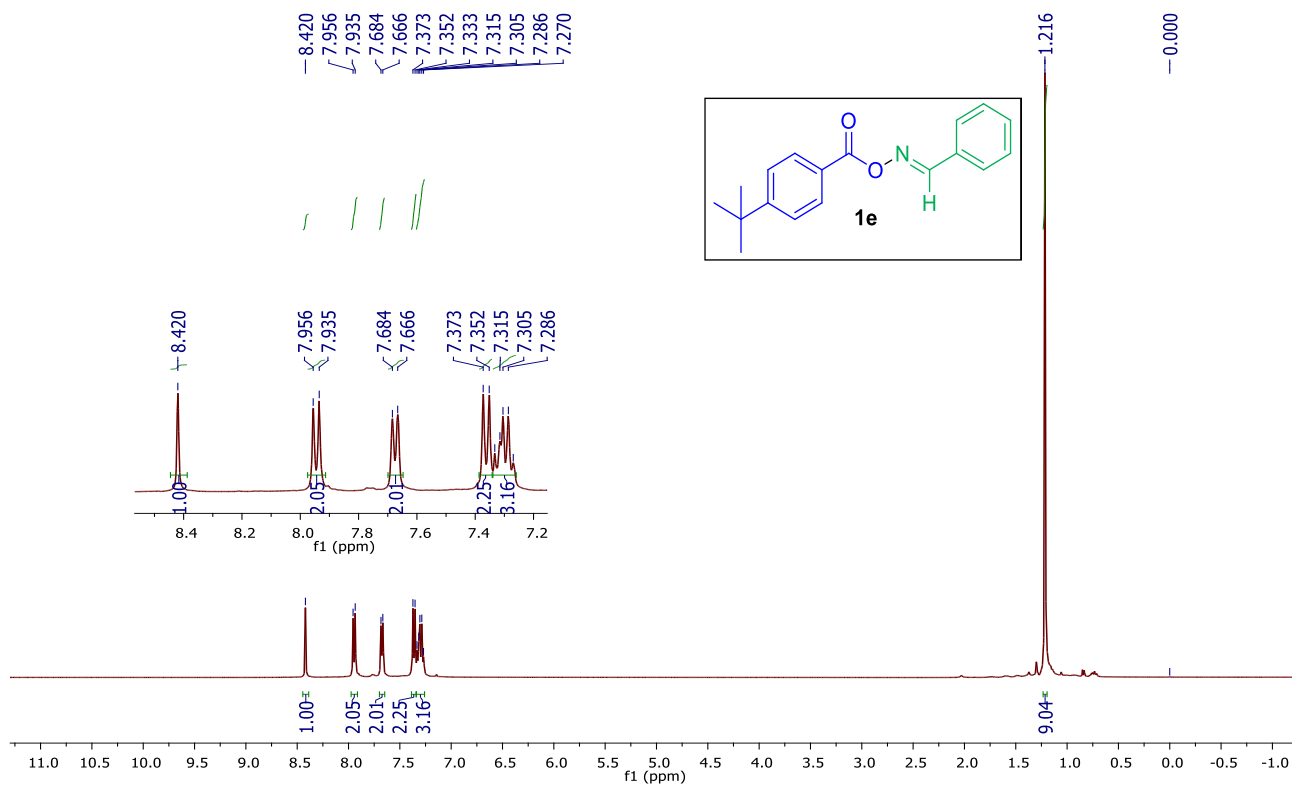
¹H NMR of 1d (400 MHz, CDCl₃)



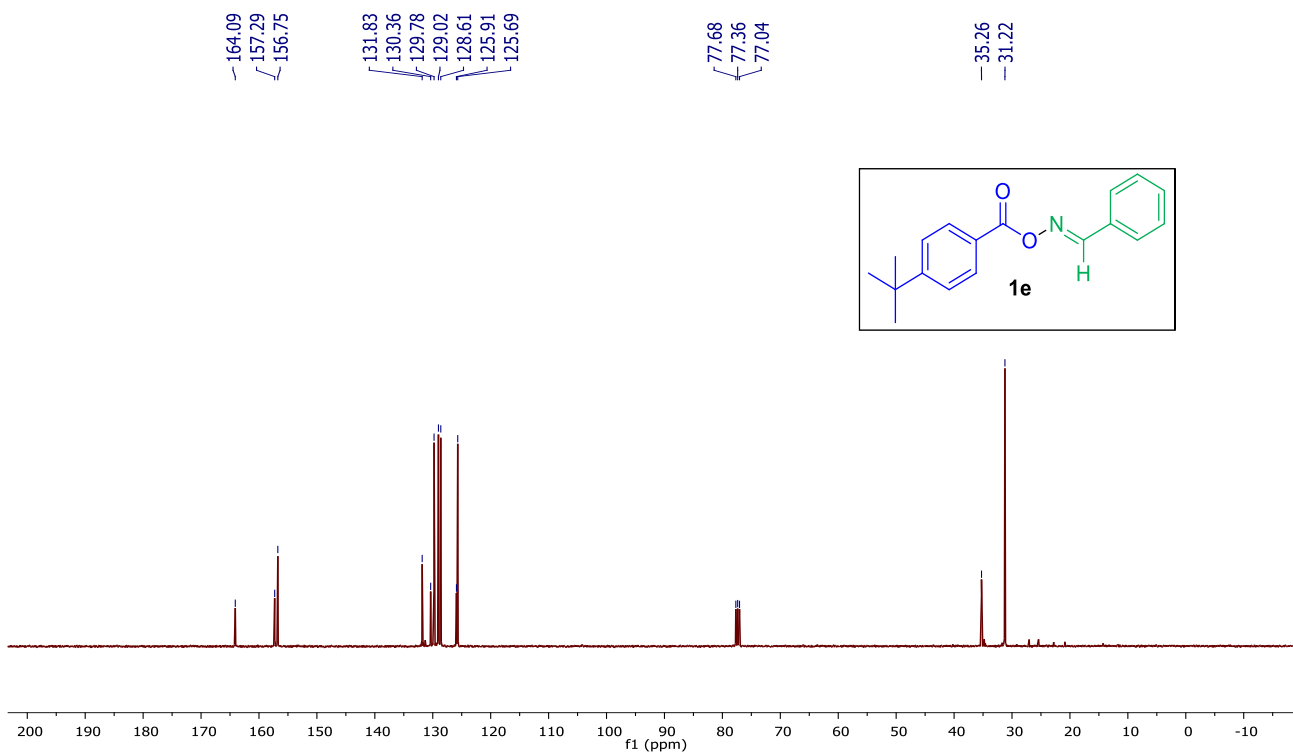
¹³C{¹H} NMR of 1d (100 MHz, CDCl₃)



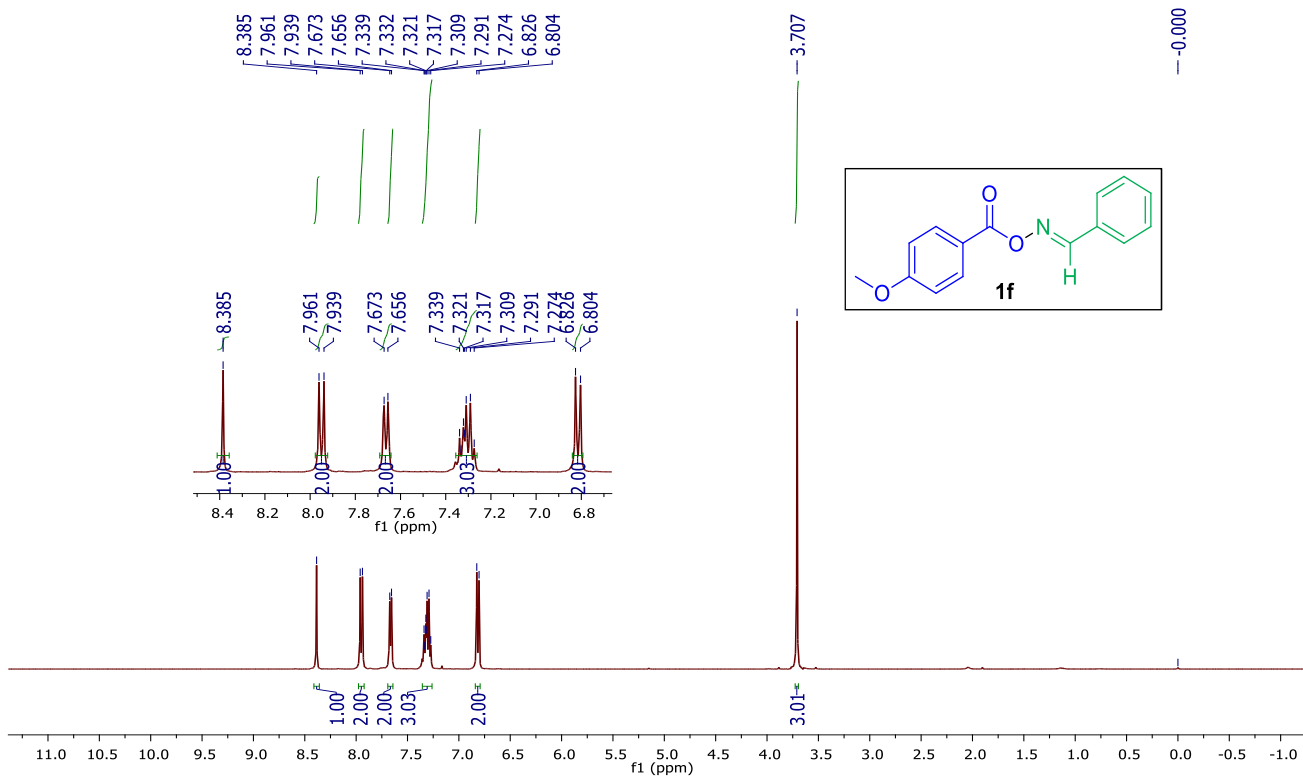
¹H NMR of 1e (400 MHz, CDCl₃)



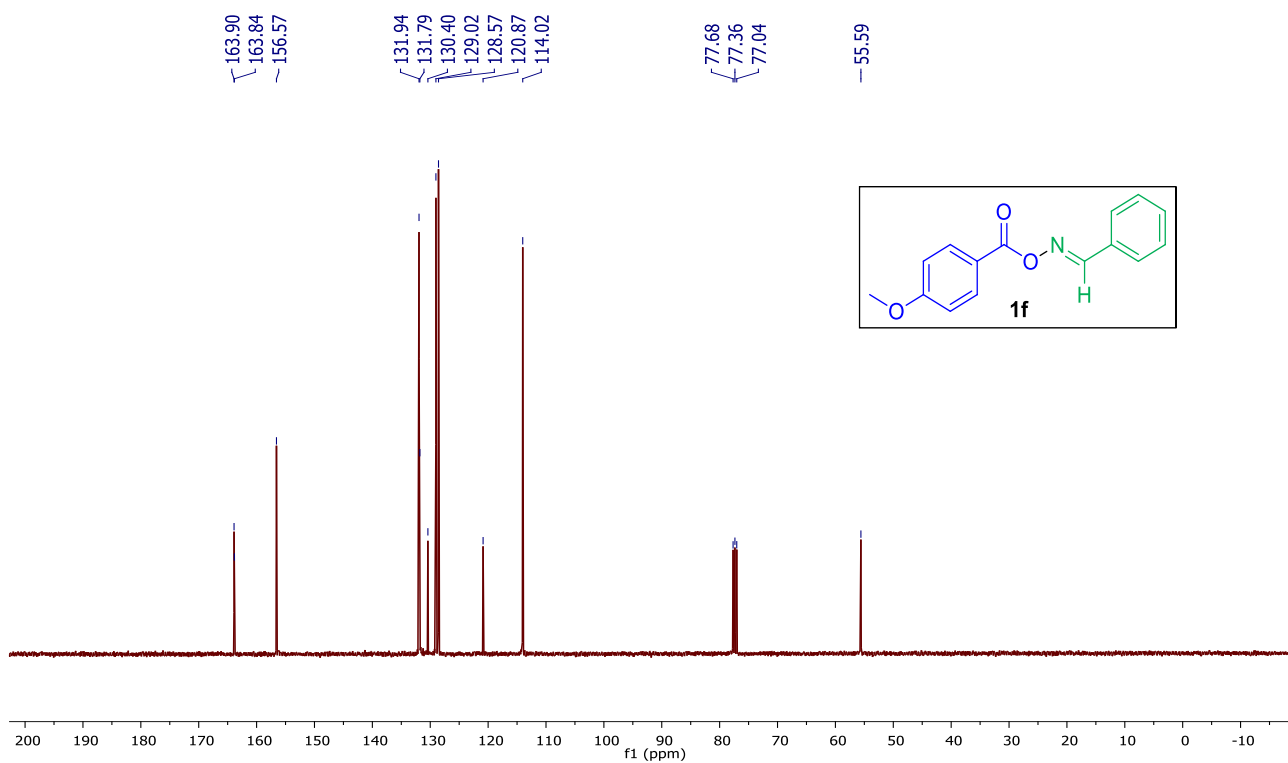
¹³C{¹H} NMR of 1e (100 MHz, CDCl₃)



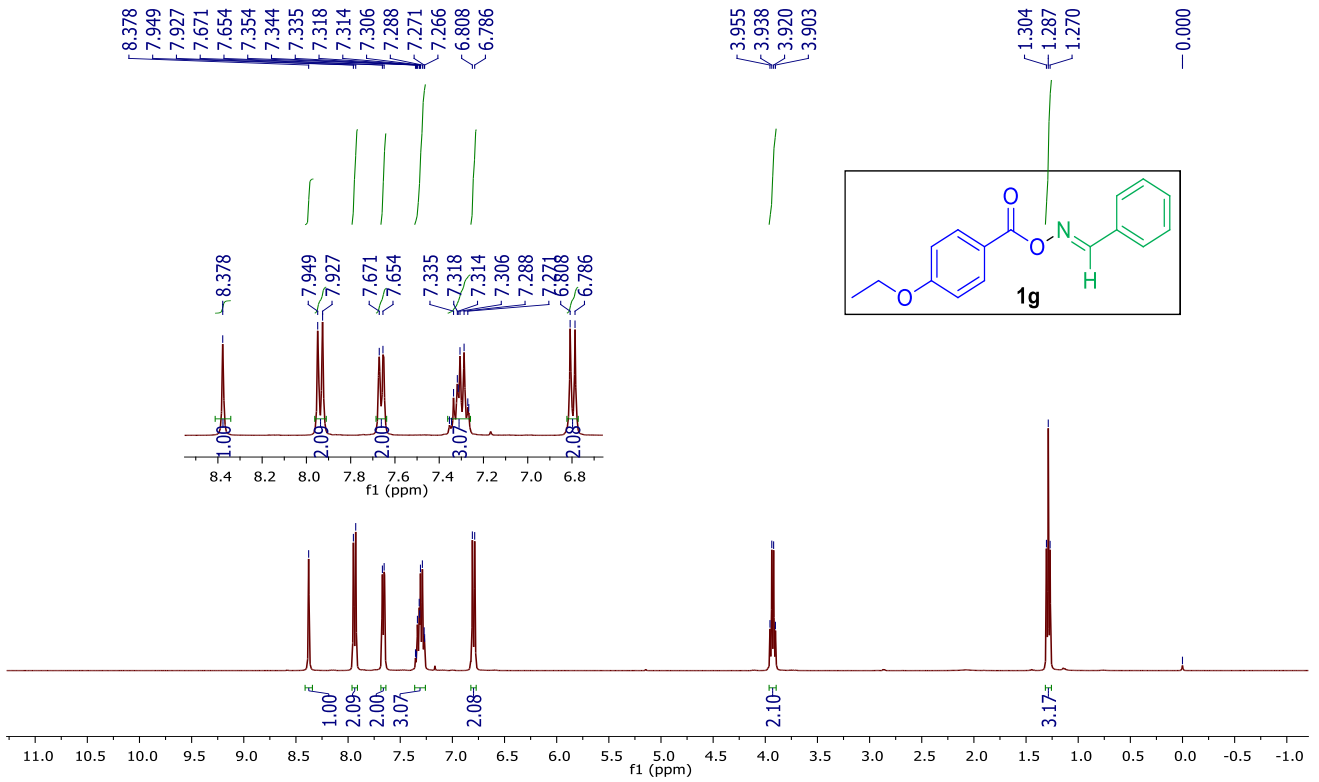
¹H NMR of 1f (400 MHz, CDCl₃)



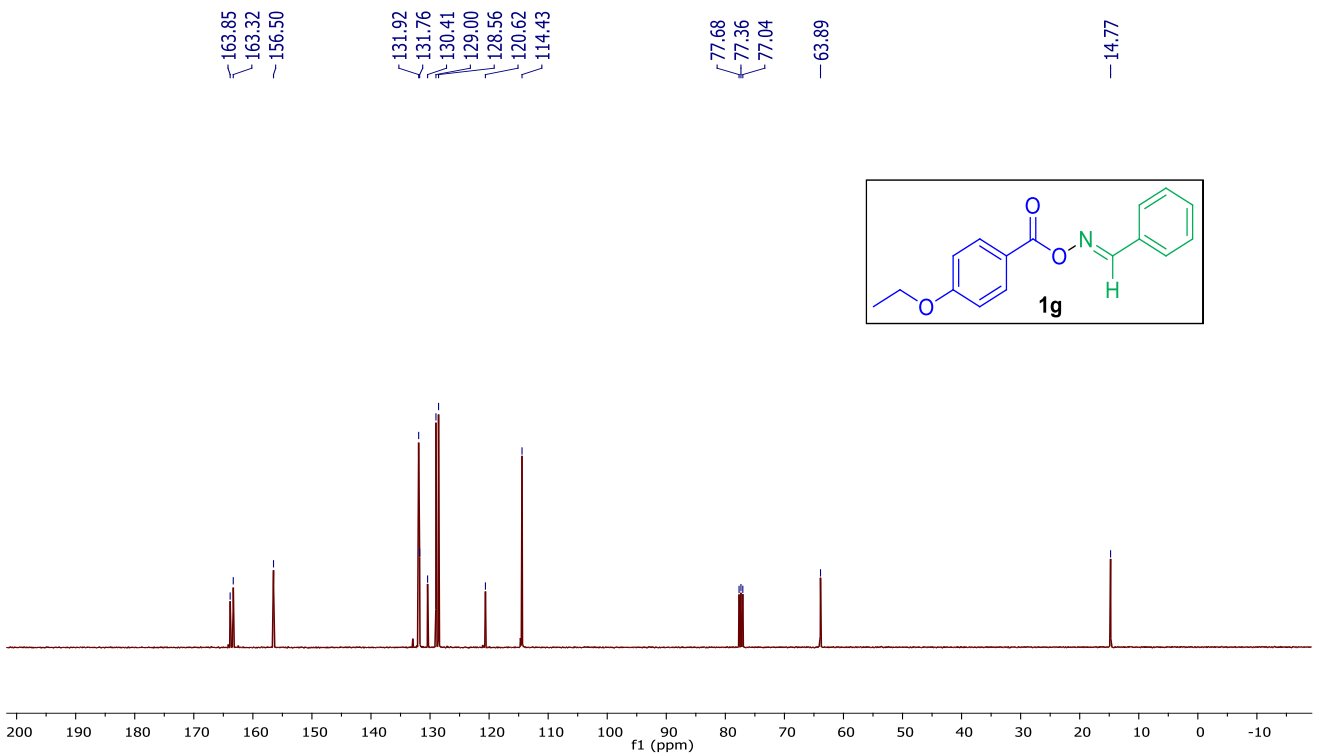
¹³C{¹H} NMR of 1f (100 MHz, CDCl₃)



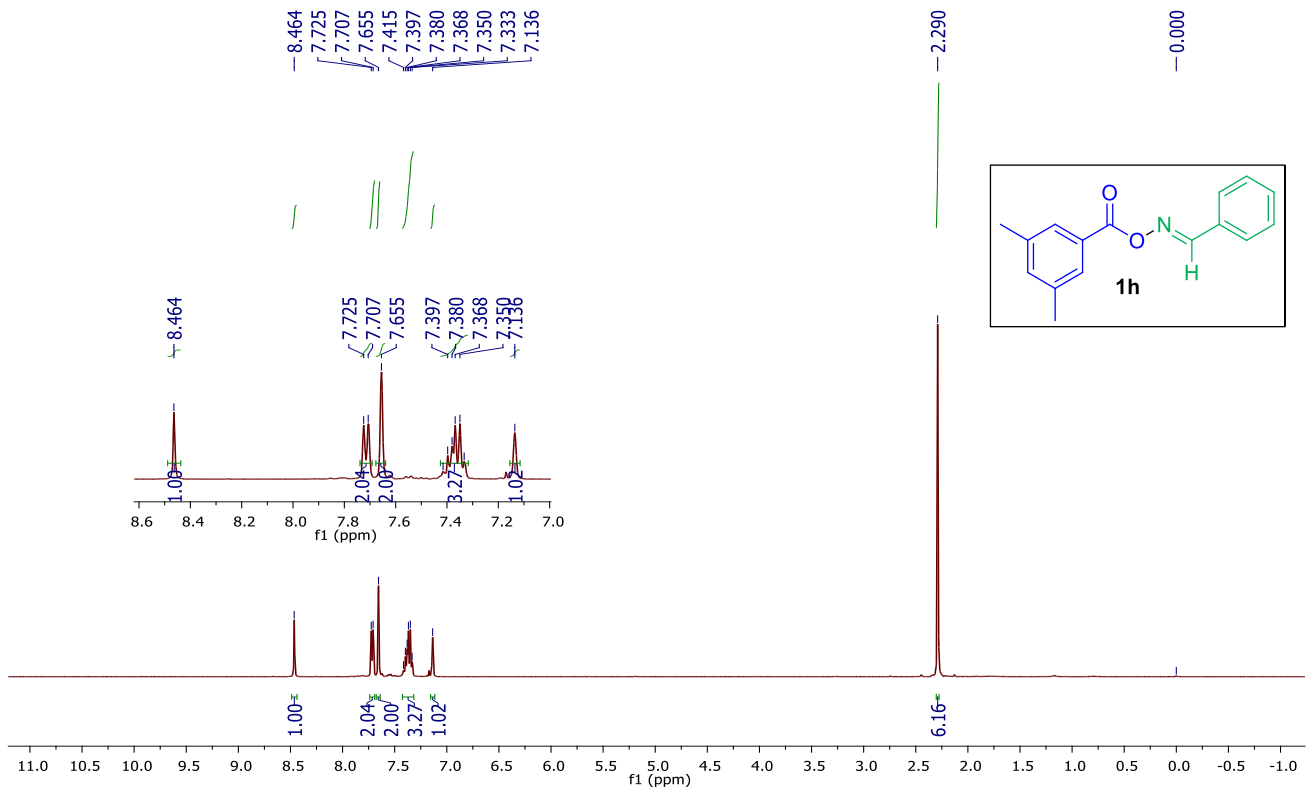
¹H NMR of 1g (400 MHz, CDCl₃)



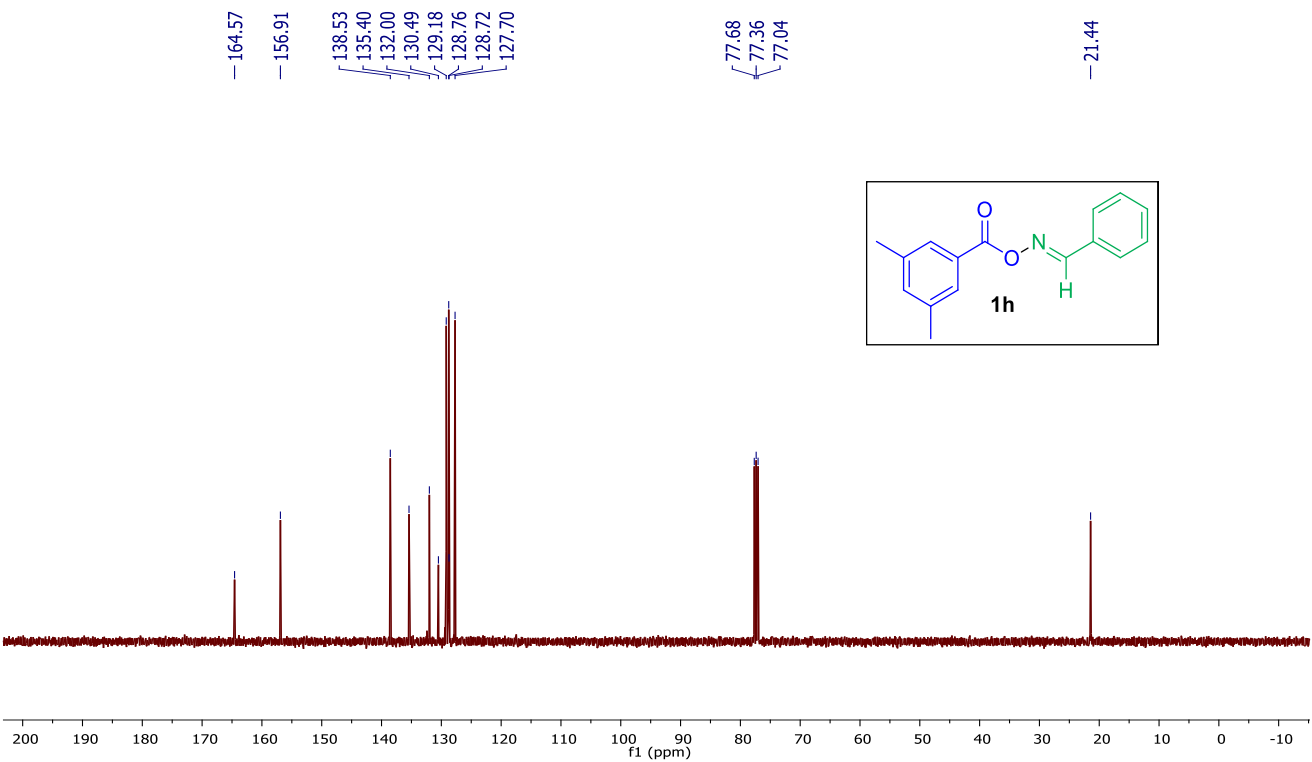
¹³C{¹H} NMR of 1g (100 MHz, CDCl₃)



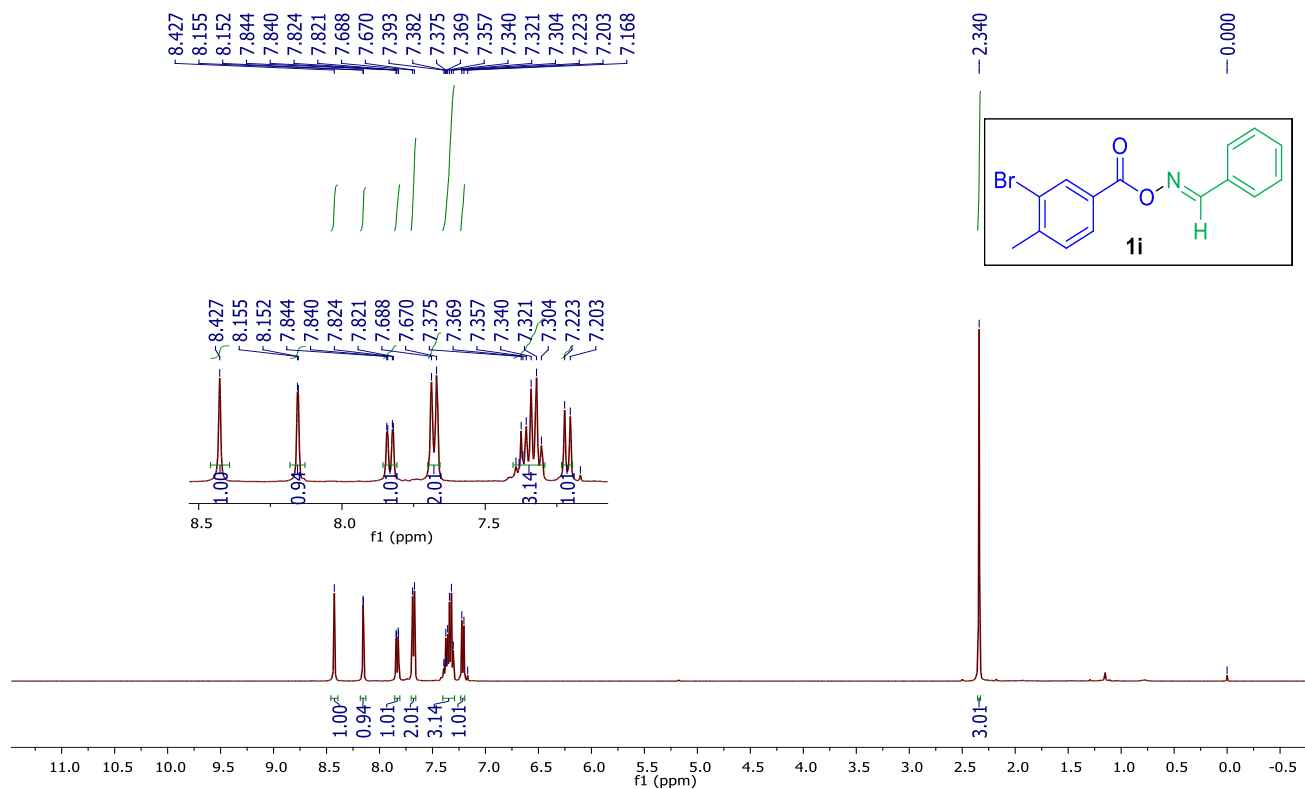
¹H NMR of 1h (400 MHz, CDCl₃)



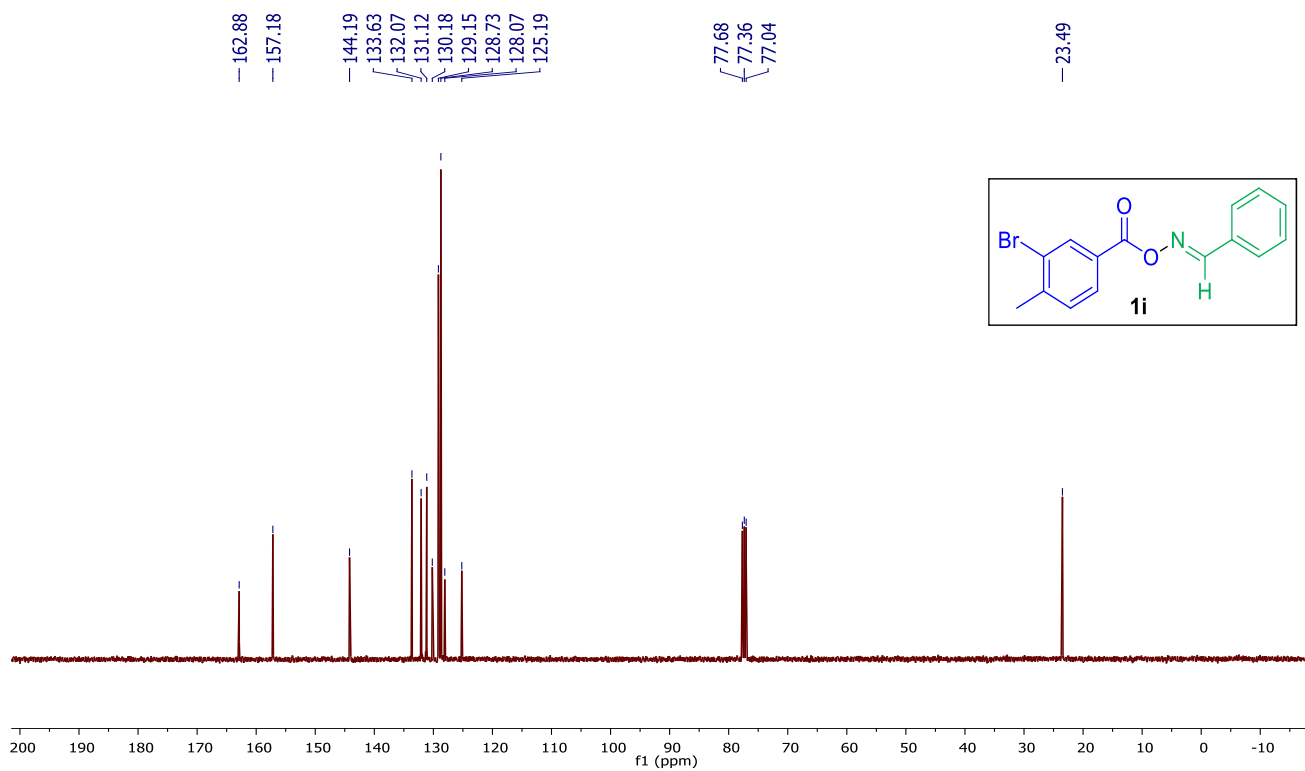
¹³C{¹H} NMR of 1h (100 MHz, CDCl₃)



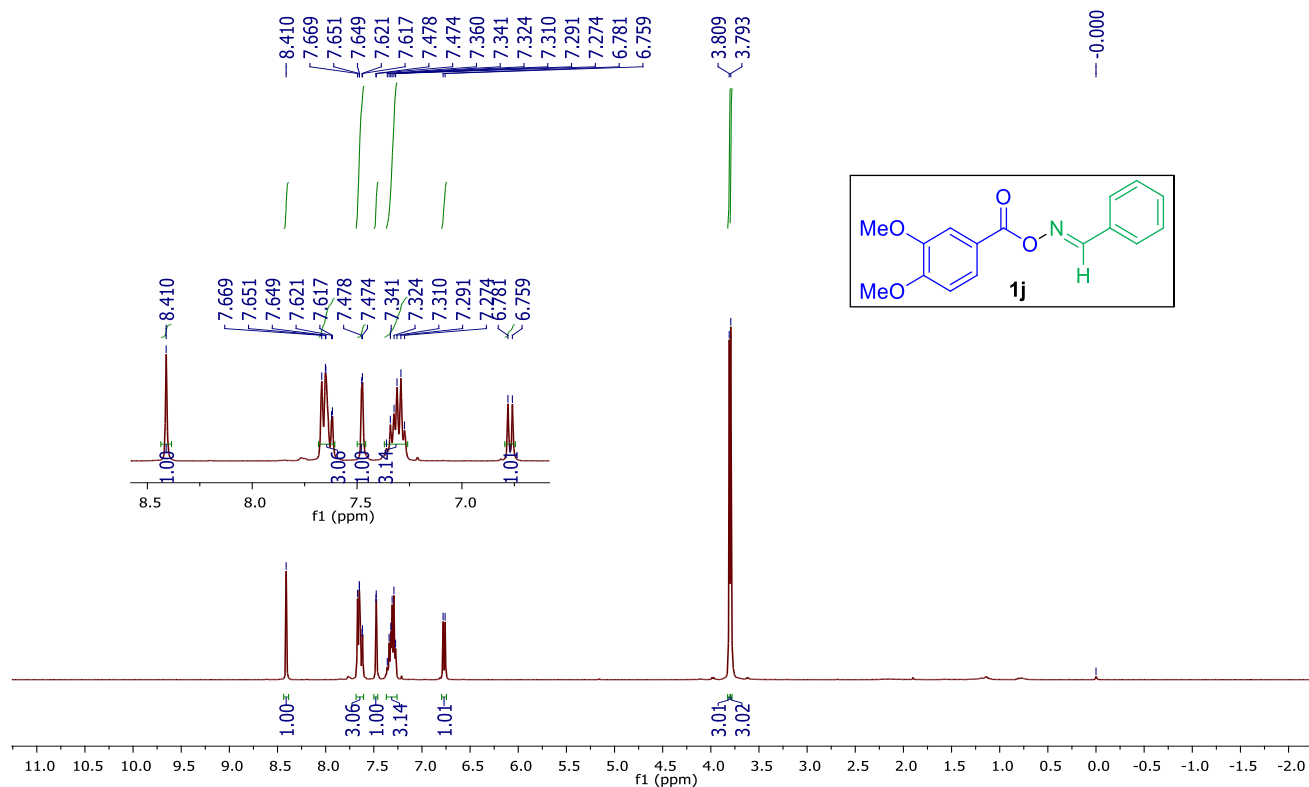
¹H NMR of **1i** (400 MHz, CDCl₃)



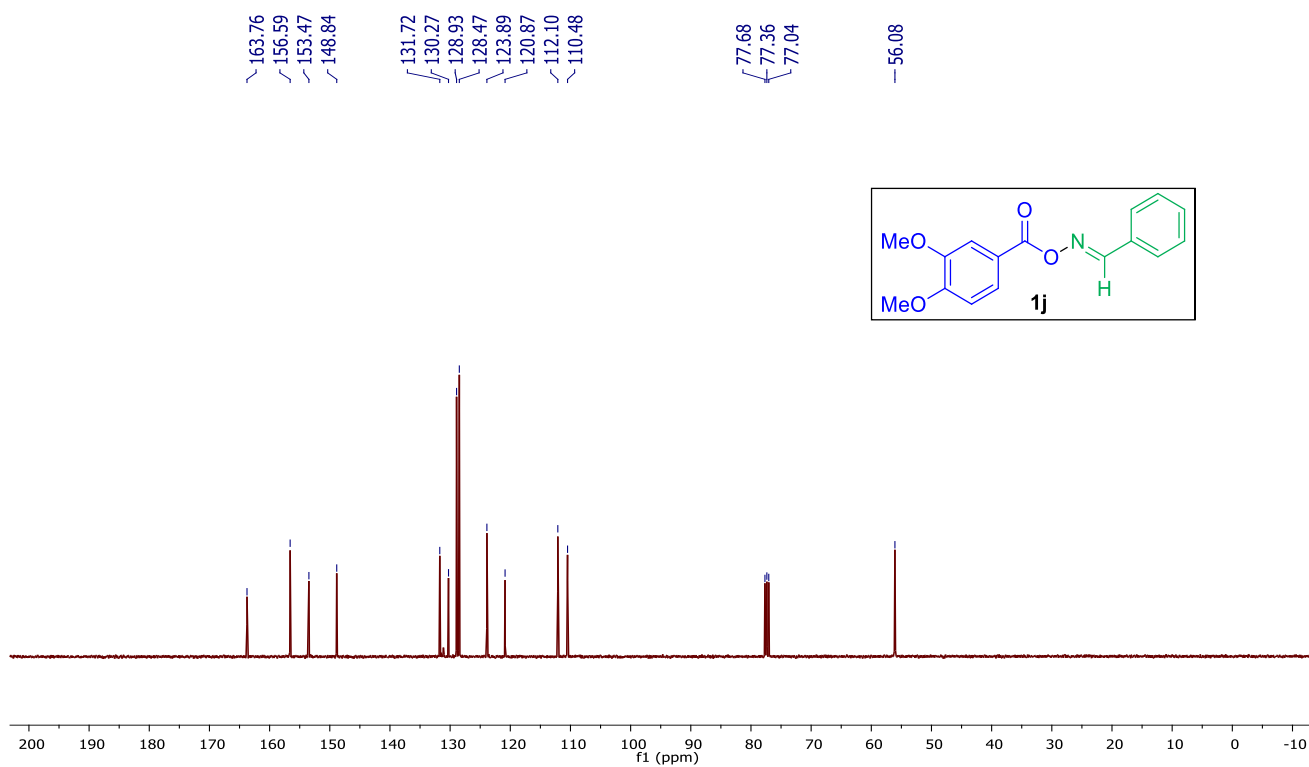
¹³C{¹H} NMR of **1i** (100 MHz, CDCl₃)



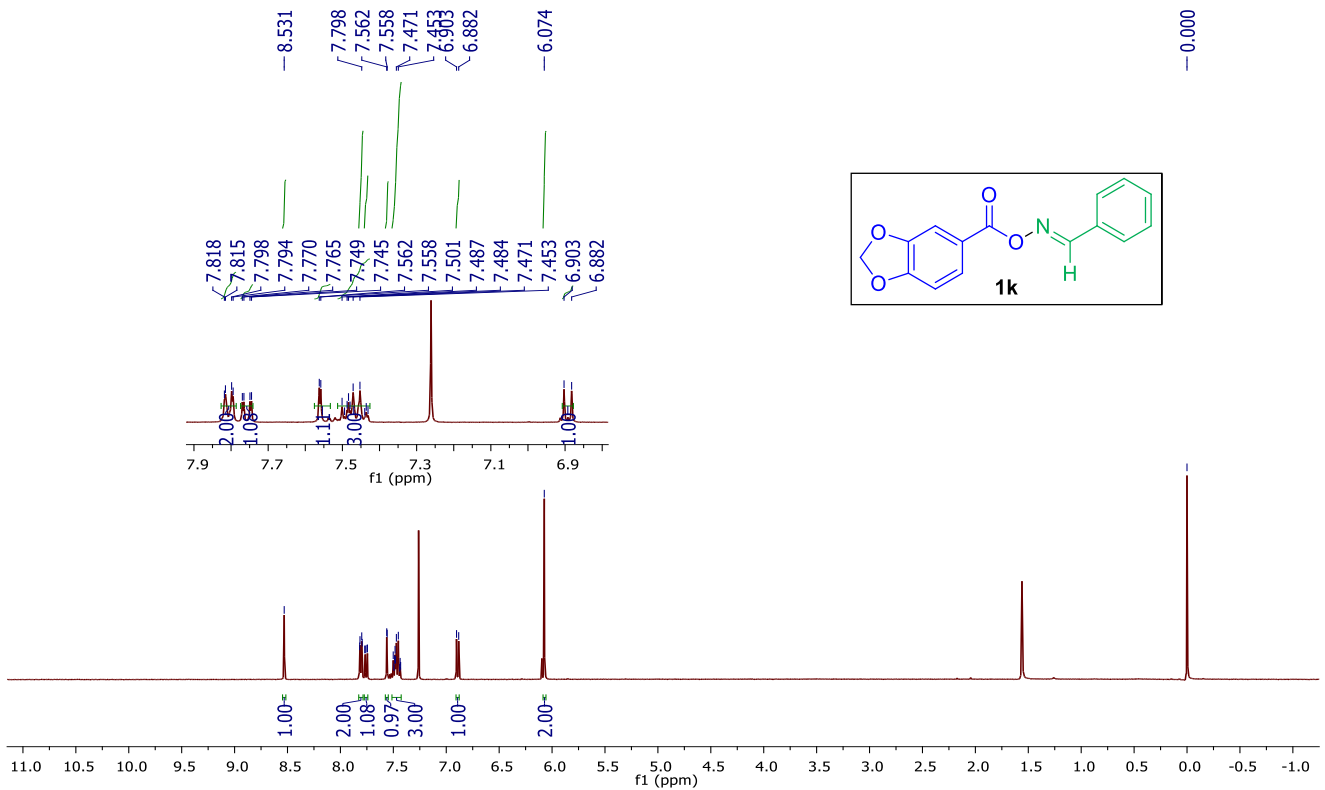
¹H NMR of 1j (400 MHz, CDCl₃)



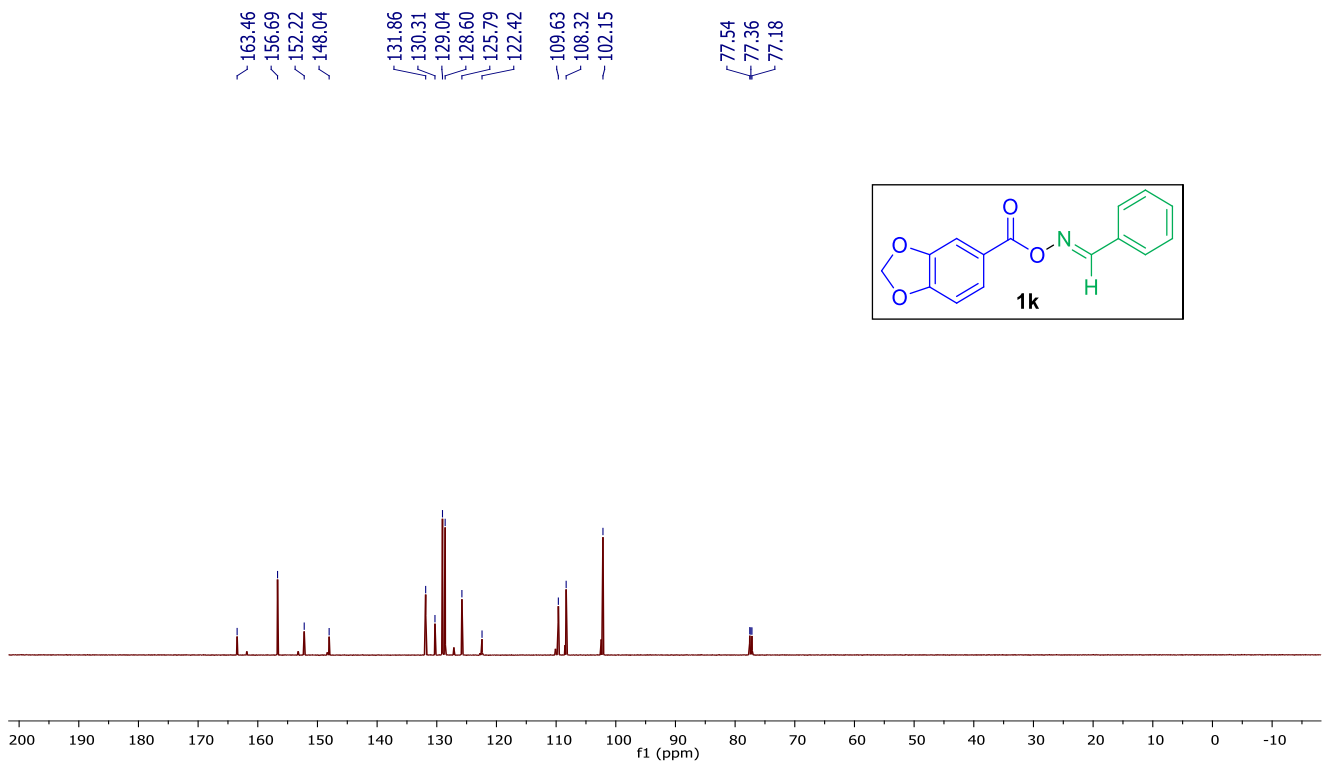
¹³C{¹H} NMR of 1j (100 MHz, CDCl₃)



¹H NMR of 1k (400 MHz, CDCl₃)



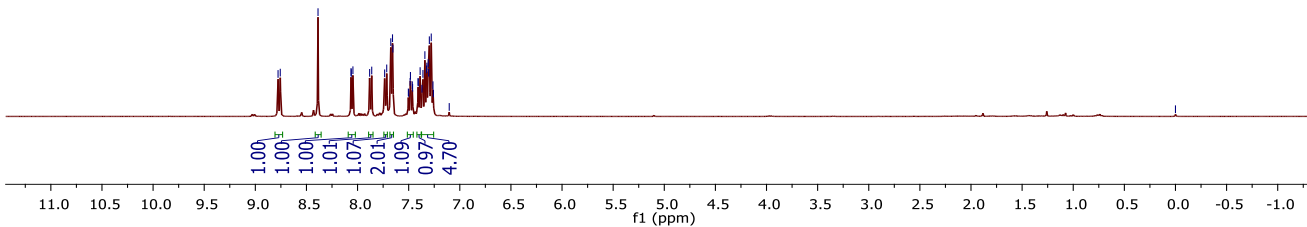
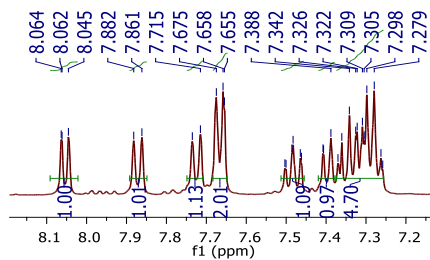
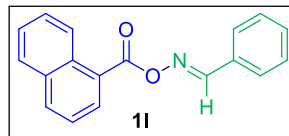
¹³C{¹H} NMR of 1k (176 MHz, CDCl₃)



¹H NMR of 11 (400 MHz, CDCl₃)

8.778
8.756
8.387
8.064
8.062
8.045
7.882
7.861
7.735
7.715
7.675
7.658
7.655
7.503
7.500
7.486
7.483
7.465
7.462
7.408
7.406
7.388
7.370
7.361
7.342
7.326
7.322
7.309
7.305
7.298
7.279
7.263
7.258
7.103

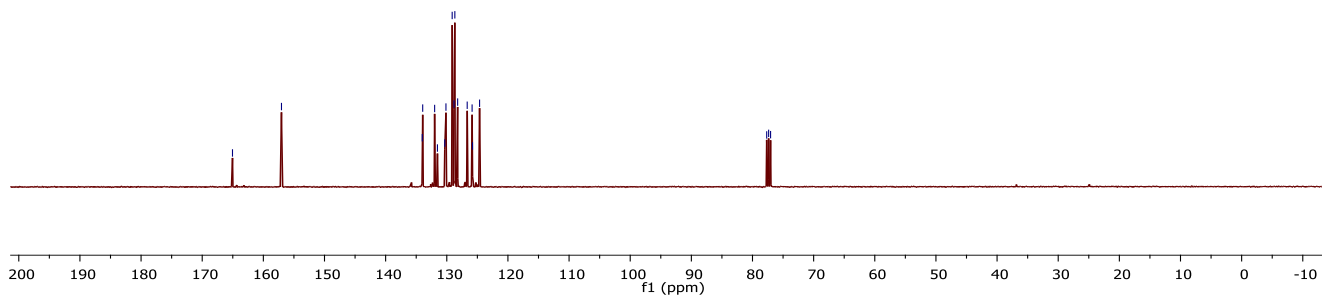
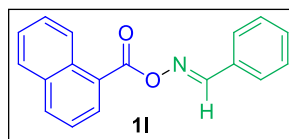
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¹³C{¹H} NMR of 11 (100 MHz, CDCl₃)

165.05
157.04
134.01
133.94
131.99
131.53
130.33
130.14
129.12
128.82
128.68
128.22
126.66
125.86
125.79
124.64

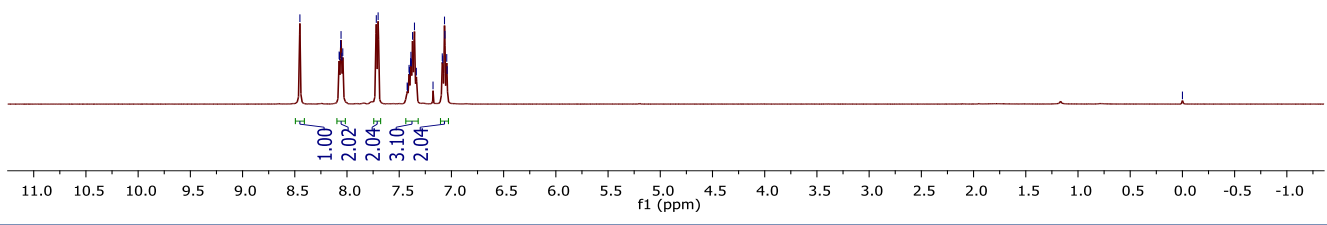
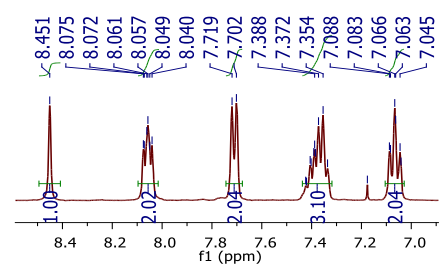
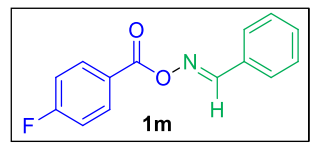
77.68
77.36
77.04



¹H NMR of 1m (400 MHz, CDCl₃)

8.451
8.075
8.072
8.061
8.057
8.049
8.040
7.719
7.702
7.424
7.406
7.402
7.391
7.388
7.384
7.372
7.354
7.336
7.176
7.088
7.083
7.066
7.063
7.045
7.041

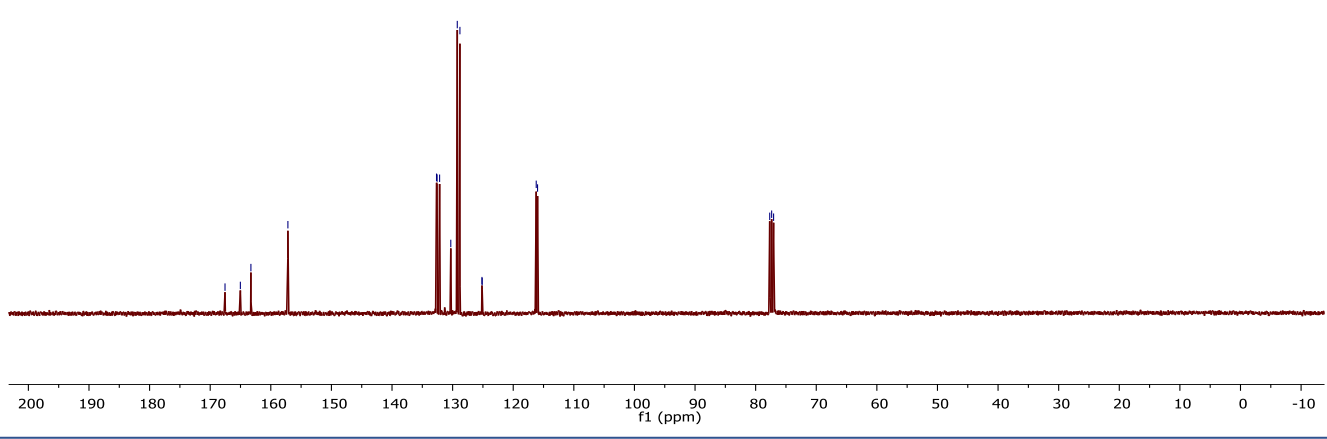
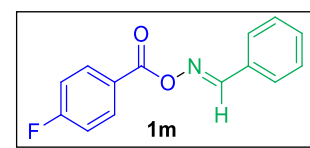
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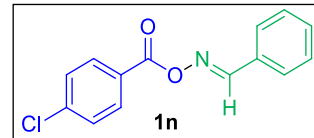
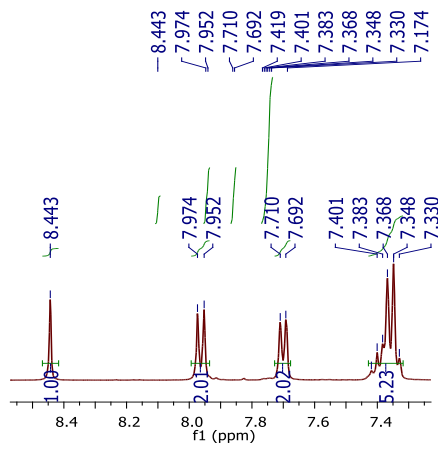
¹³C{¹H} NMR of 1m (100 MHz, CDCl₃)

167.56
165.02
163.28
157.18
132.66
132.56
132.15
130.30
129.23
128.80
125.16
125.13
116.21
115.99

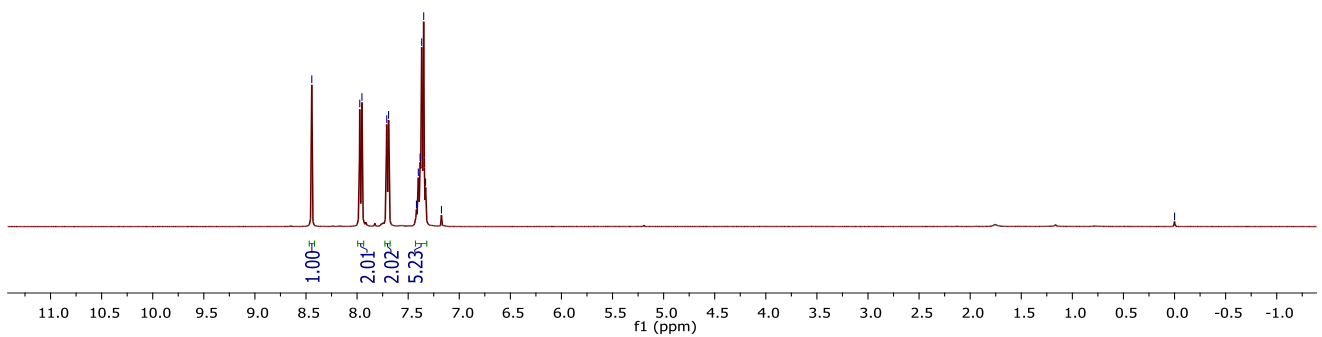
77.68
77.36
77.04



¹H NMR of 1n (400 MHz, CDCl₃)



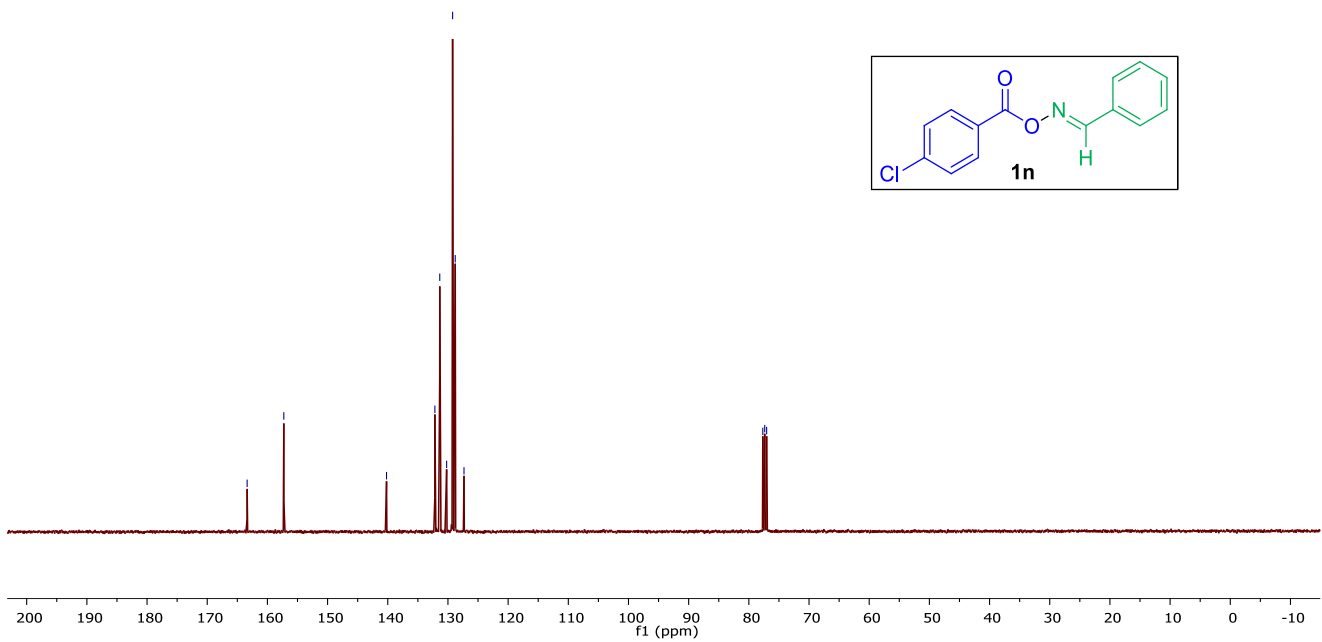
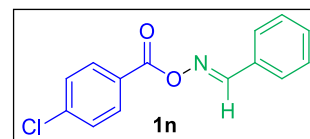
-0.000



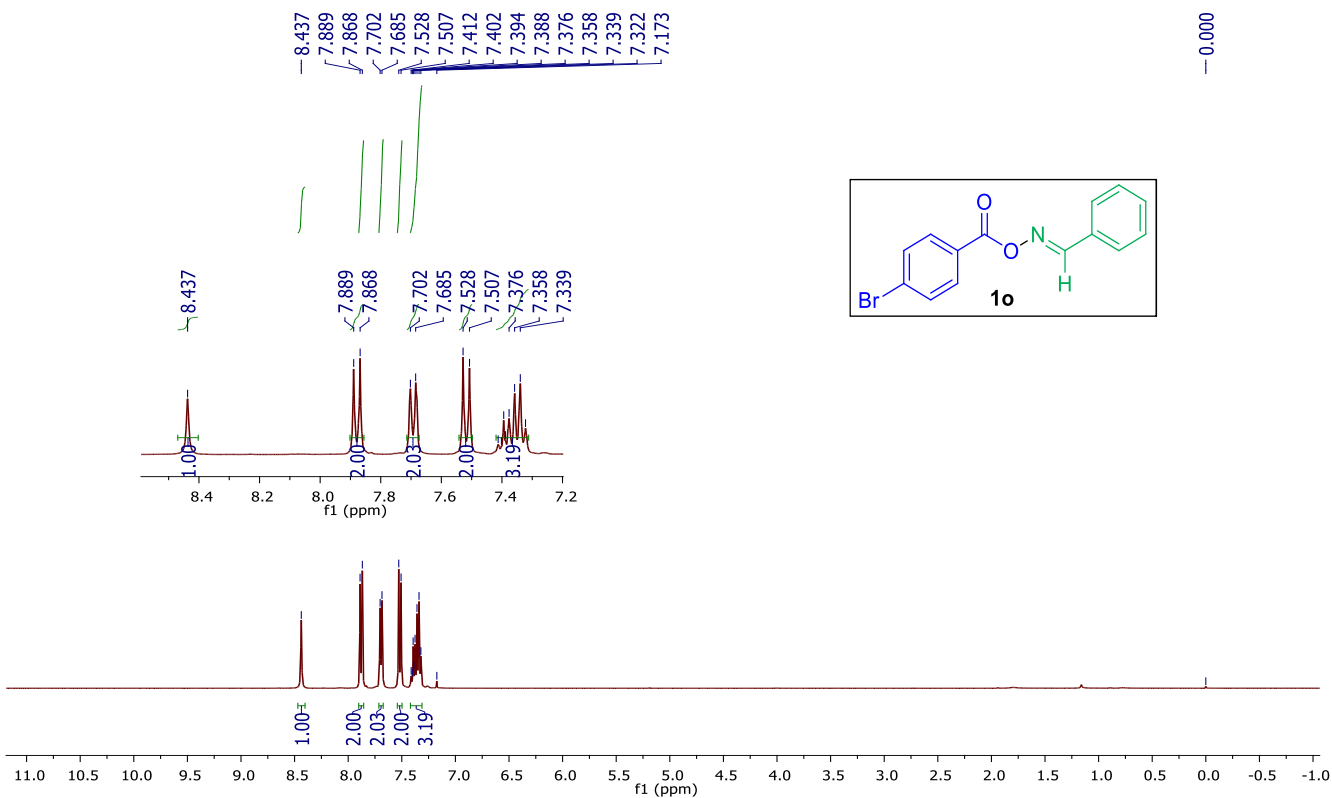
¹³C{¹H} NMR of 1n (100 MHz, CDCl₃)

163.37
157.28
140.20
132.17
131.36
130.22
129.22
128.79
127.33

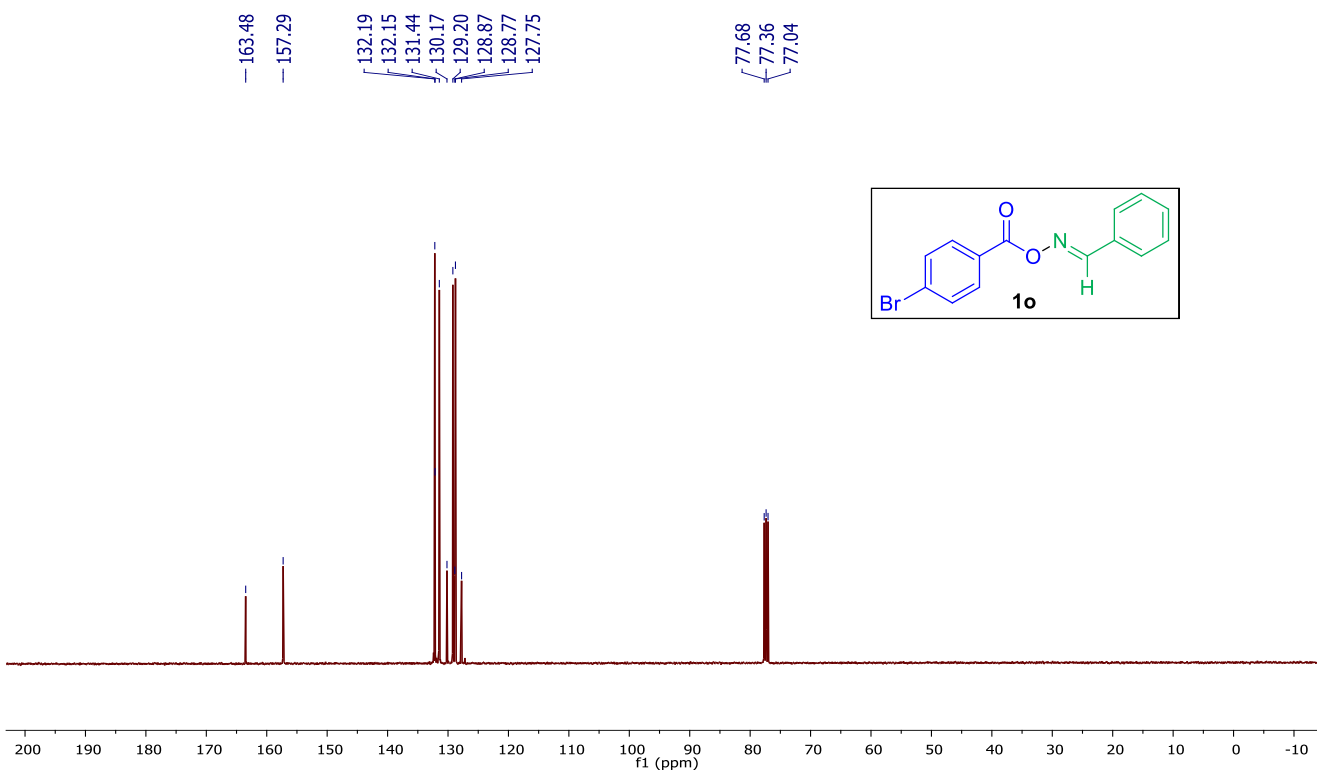
77.68
77.36
77.04



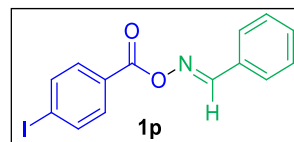
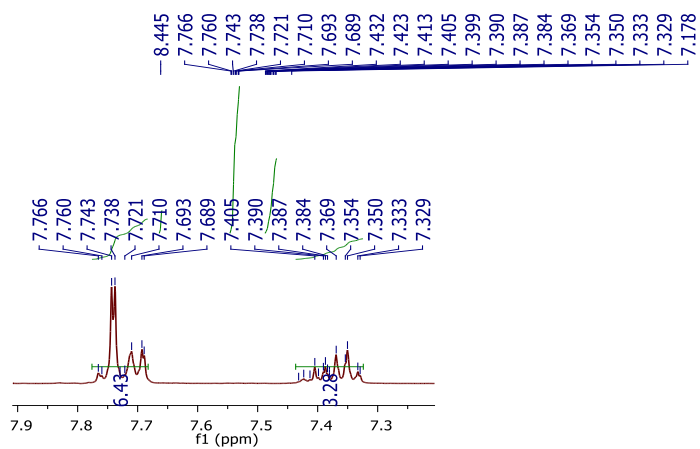
¹H NMR of 1o (400 MHz, CDCl₃)



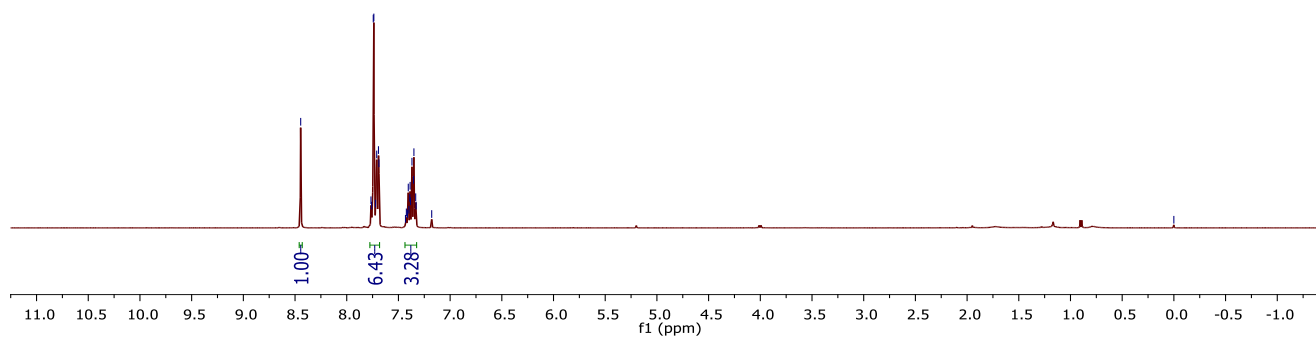
¹³C{¹H} NMR of 1o (100 MHz, CDCl₃)



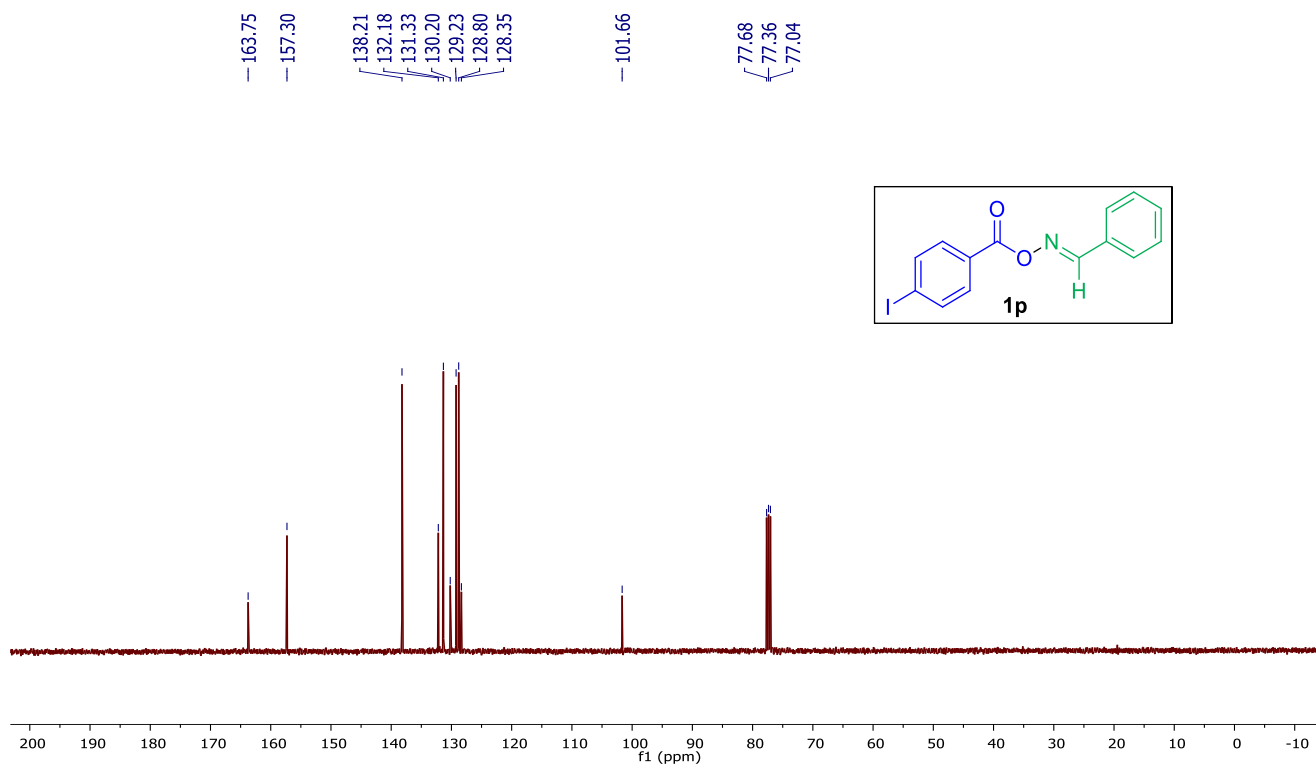
¹H NMR of 1p (400 MHz, CDCl₃)



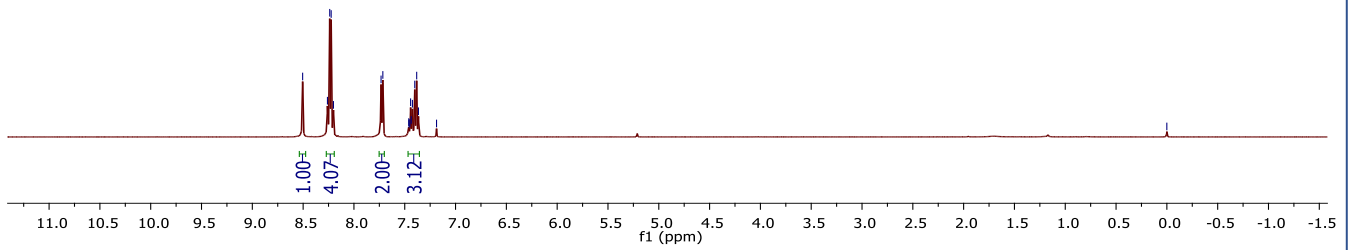
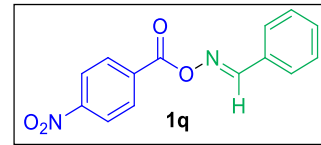
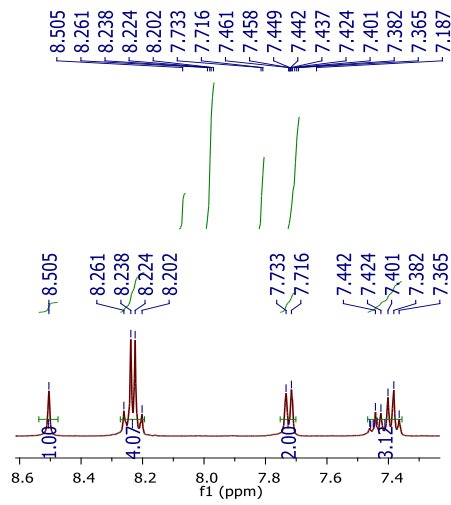
— 0.000



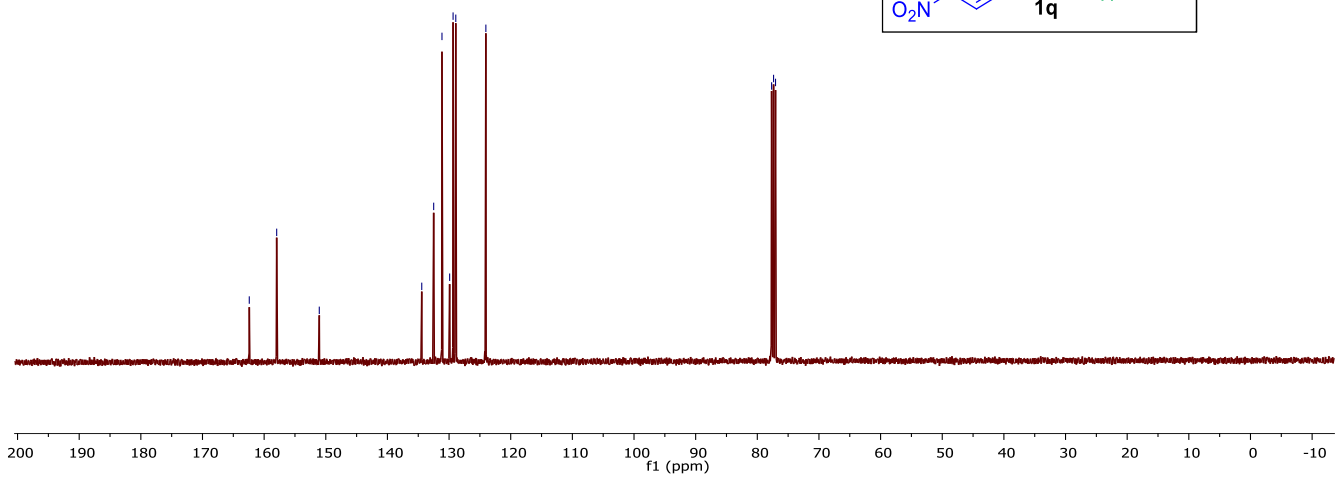
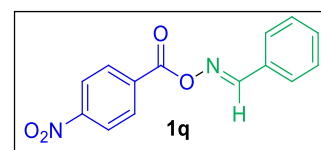
¹³C{¹H} NMR of 1p (100 MHz, CDCl₃)



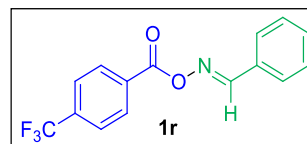
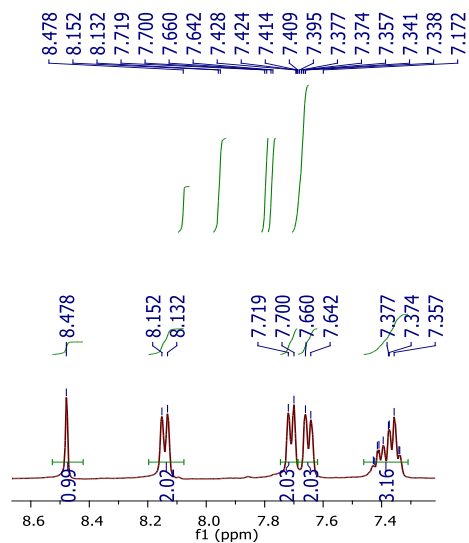
¹H NMR of 1q (400 MHz, CDCl₃)



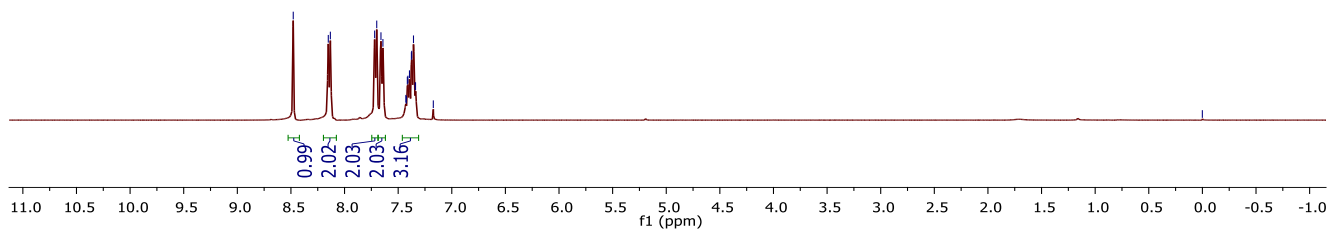
¹³C{¹H} NMR of 1q (100 MHz, CDCl₃)



¹H NMR of 1r (400 MHz, CDCl₃)

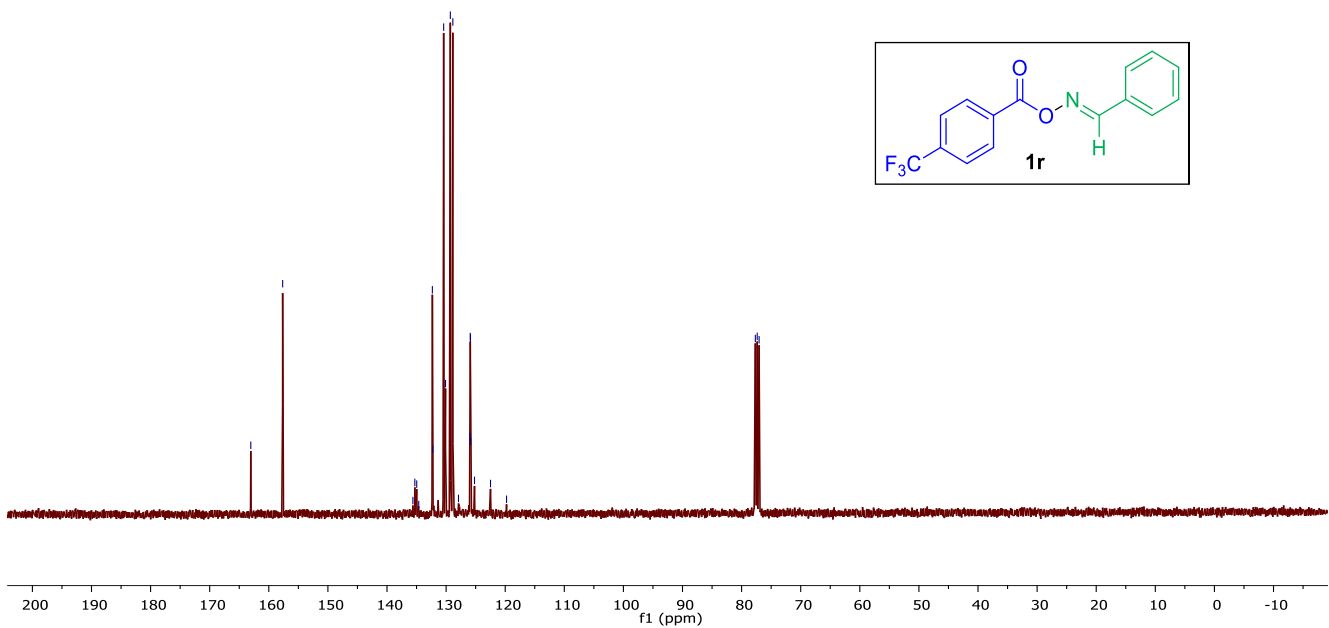
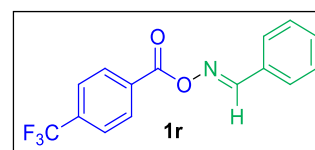


0.000

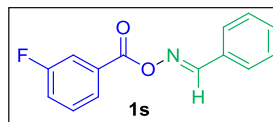
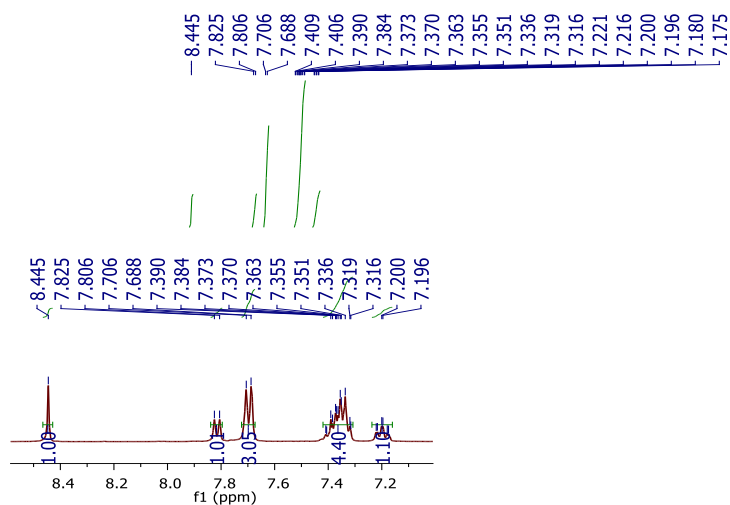


¹³C{¹H} NMR of 1r (100 MHz, CDCl₃)

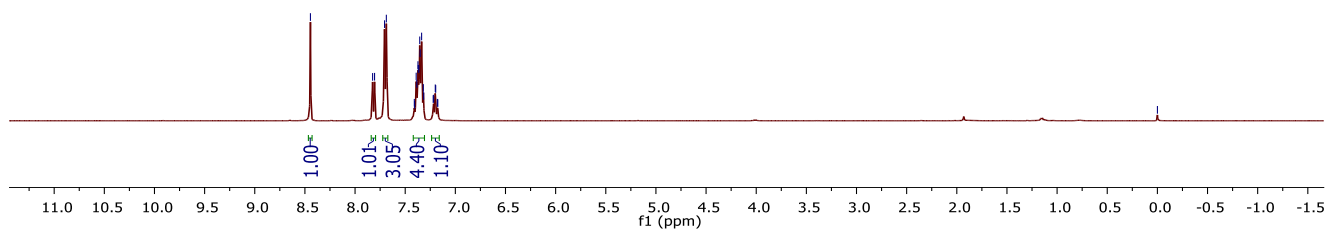
Peak list (ppm): 163.05, 157.65, 135.62, 135.29, 134.97, 132.32, 132.26, 130.41, 130.10, 129.28, 128.86, 127.91, 125.95, 125.91, 125.87, 125.84, 125.19, 122.48, 119.77, 117.88, 77.36, 77.04.



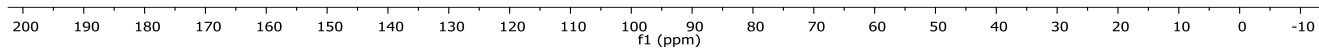
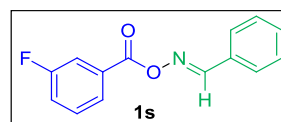
¹H NMR of 1s (400 MHz, CDCl₃)



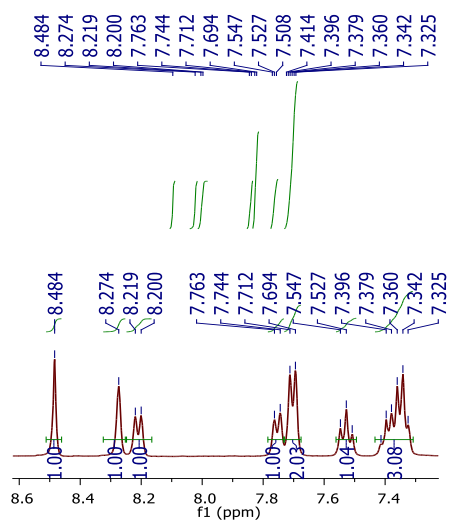
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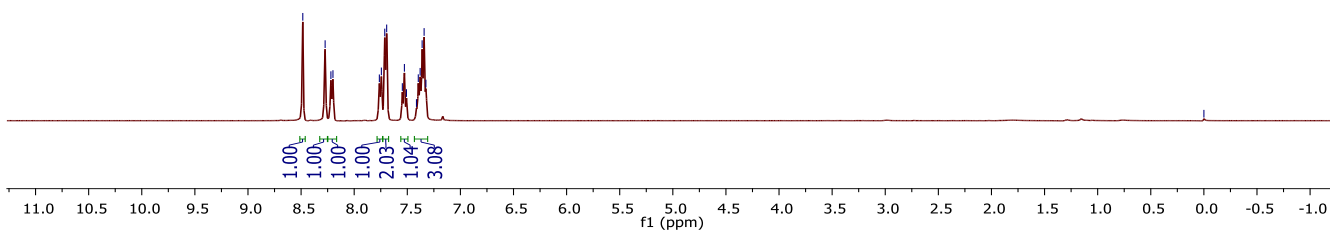
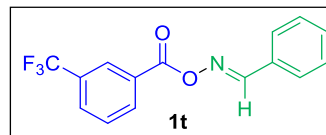
¹³C{¹H} NMR of 1s (100 MHz, CDCl₃)



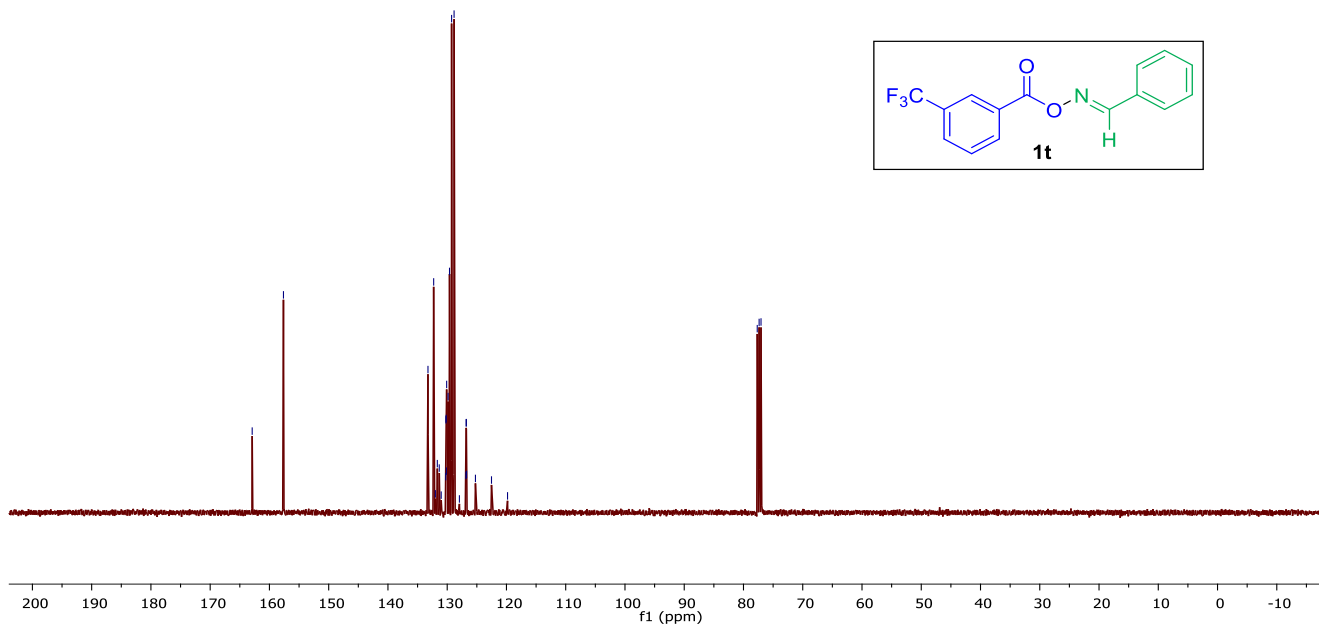
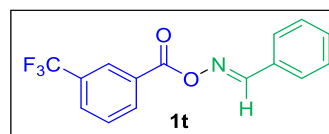
¹H NMR of 1t (400 MHz, CDCl₃)



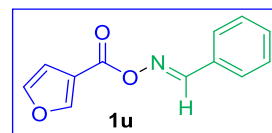
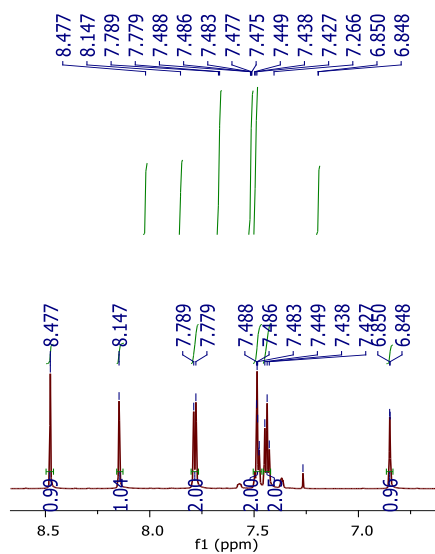
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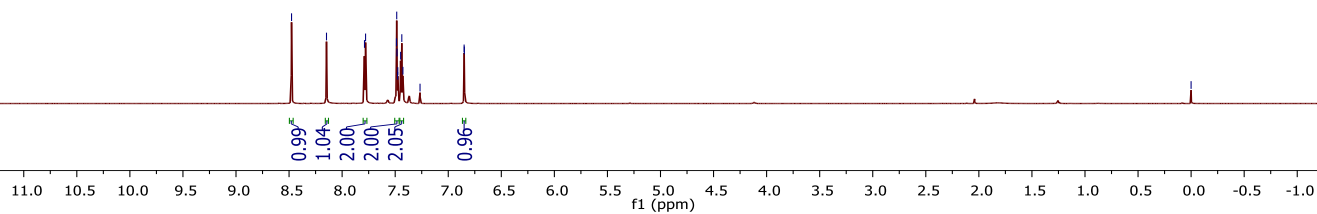
¹³C{¹H} NMR of 1t (100 MHz, CDCl₃)



¹H NMR of 1u (700 MHz, CDCl₃)



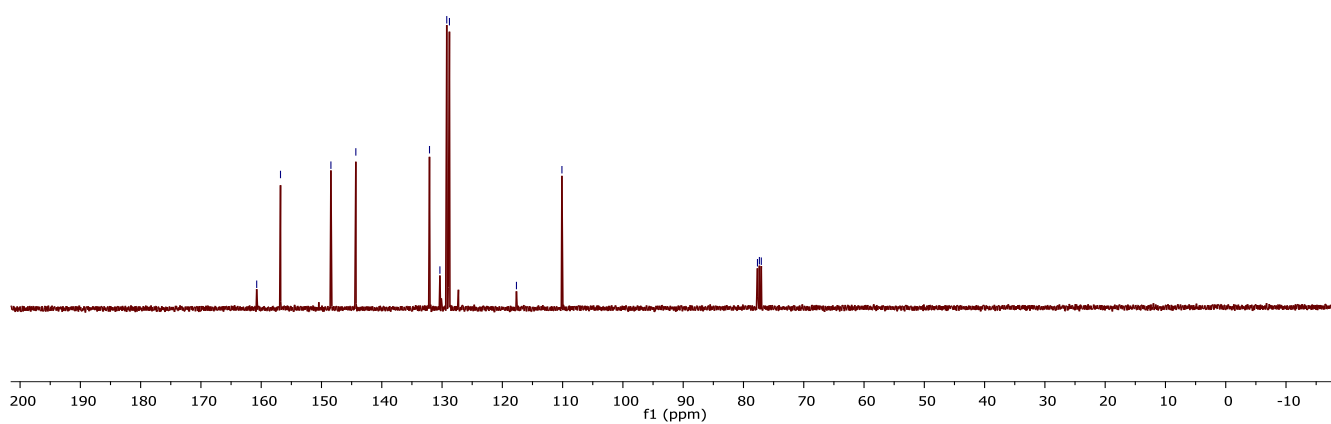
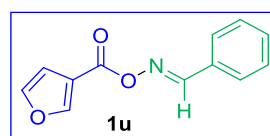
— 0.000



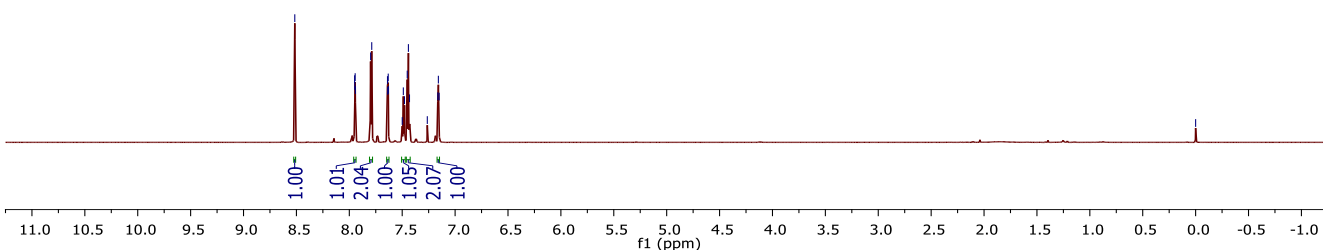
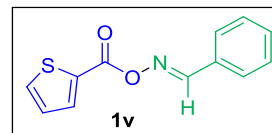
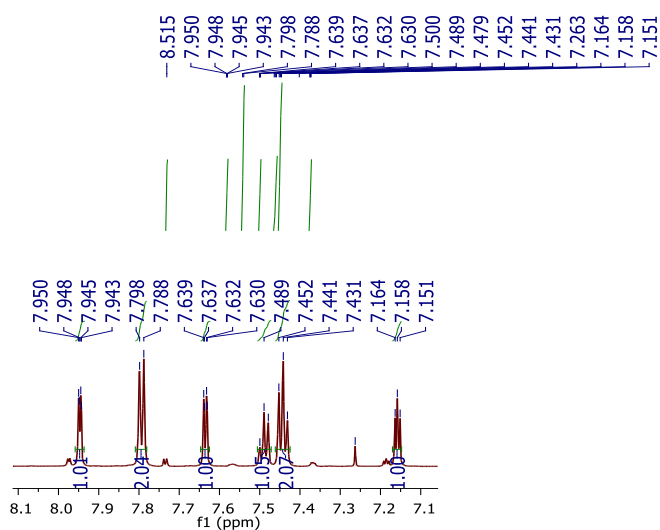
¹³C{¹H} NMR of 1u (100 MHz, CDCl₃)

— 160.75
— 156.80
— 148.44
— 144.30
— 132.08
— 130.36
— 129.22
— 128.78
— 117.66
— 110.12

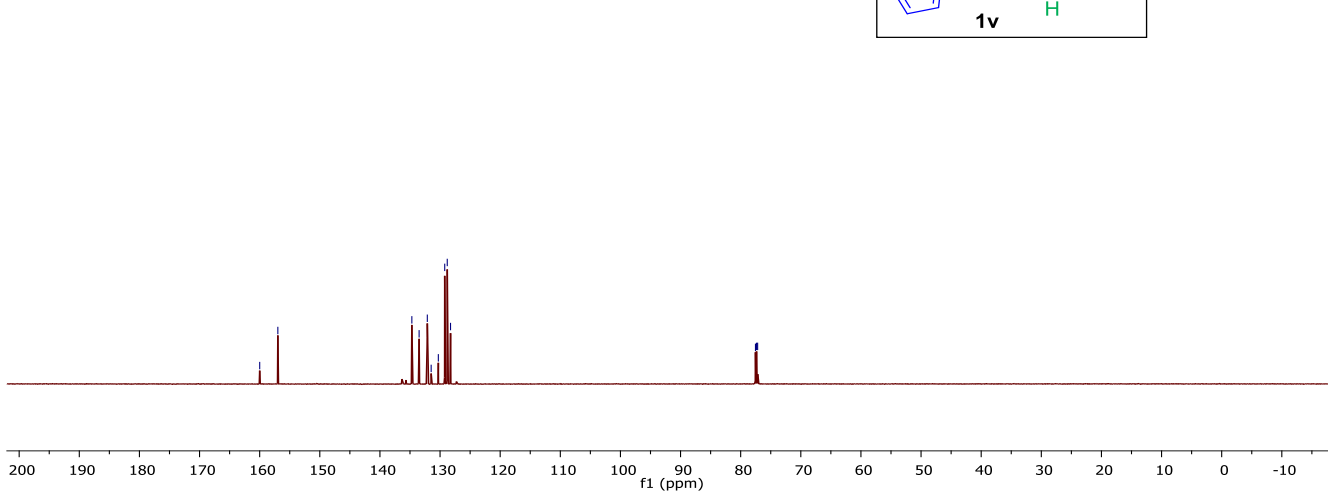
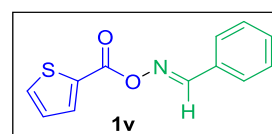
— 77.68
— 77.36
— 77.04



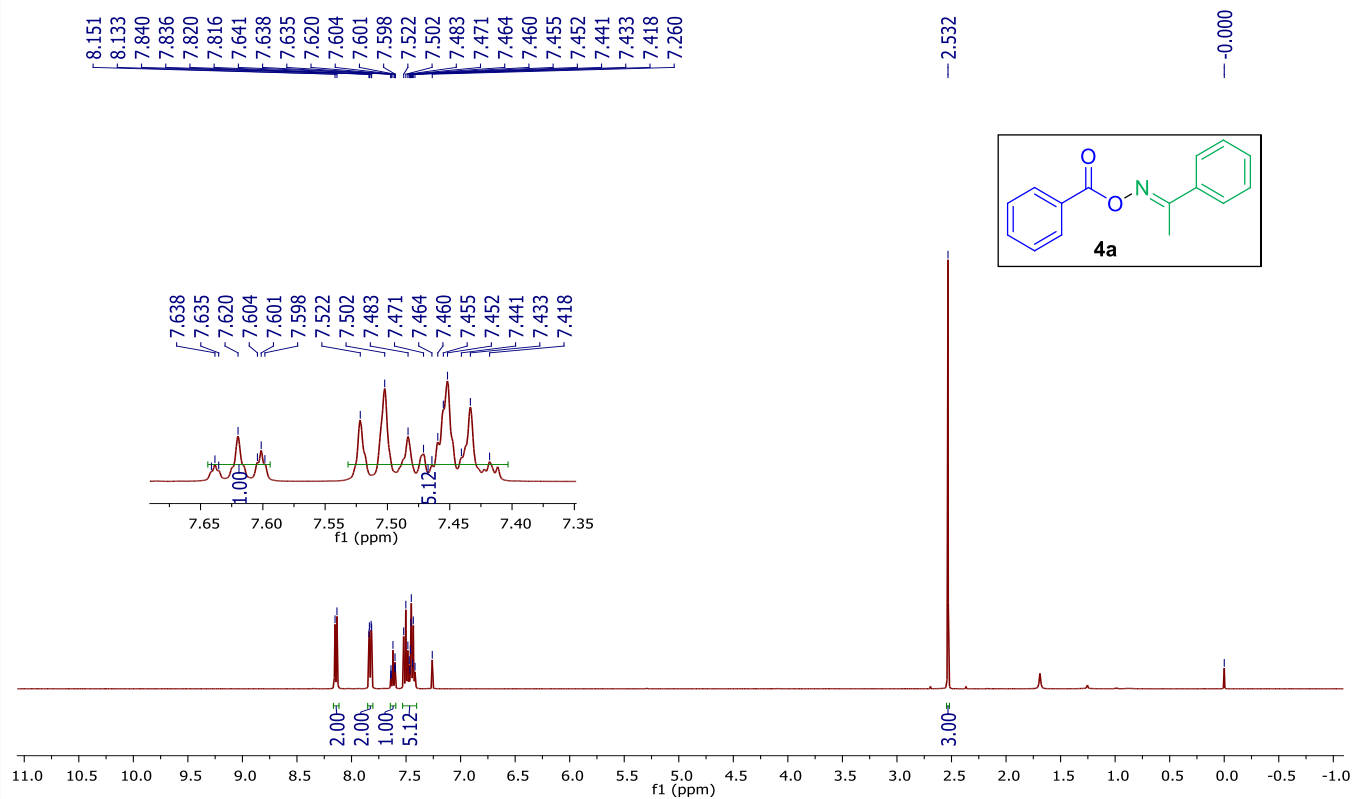
¹H NMR of 1v (700 MHz, CDCl₃)



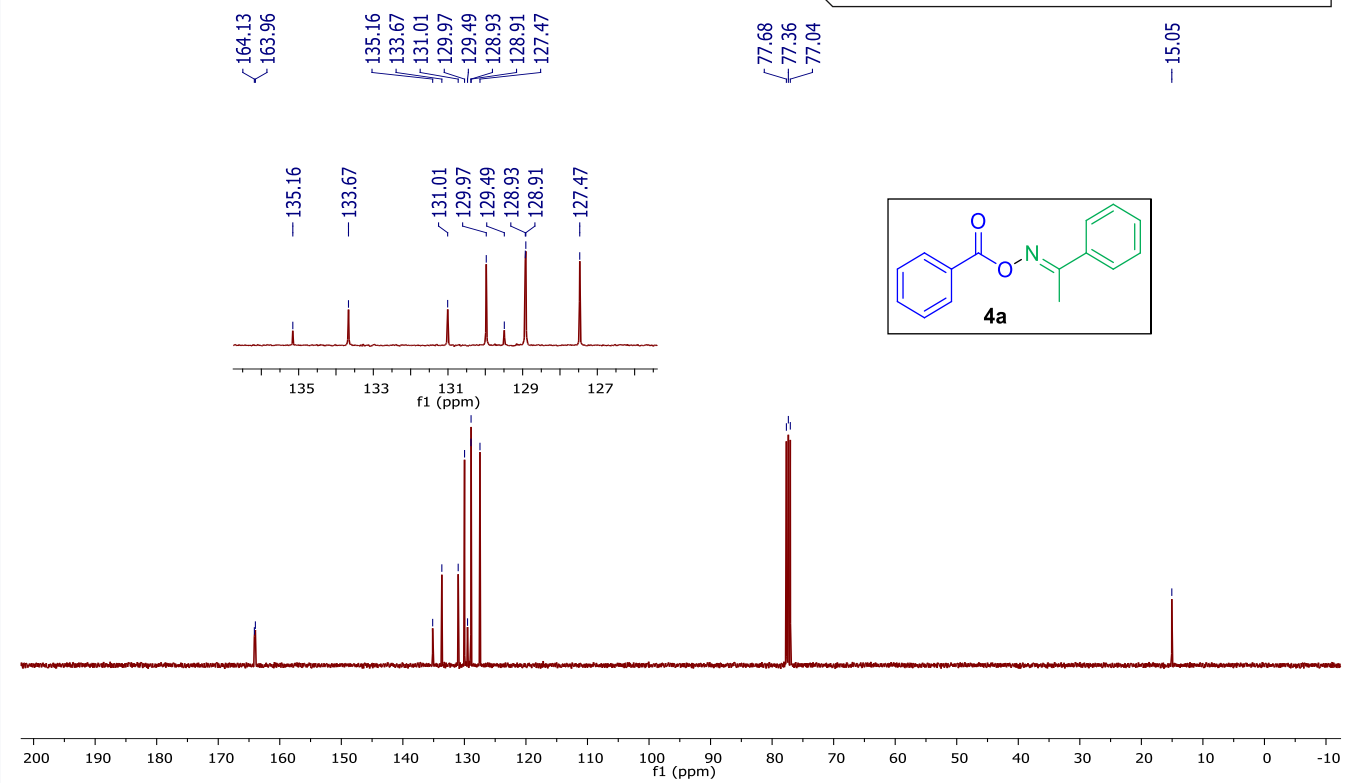
¹³C{¹H} NMR of 1v (176 MHz, CDCl₃)



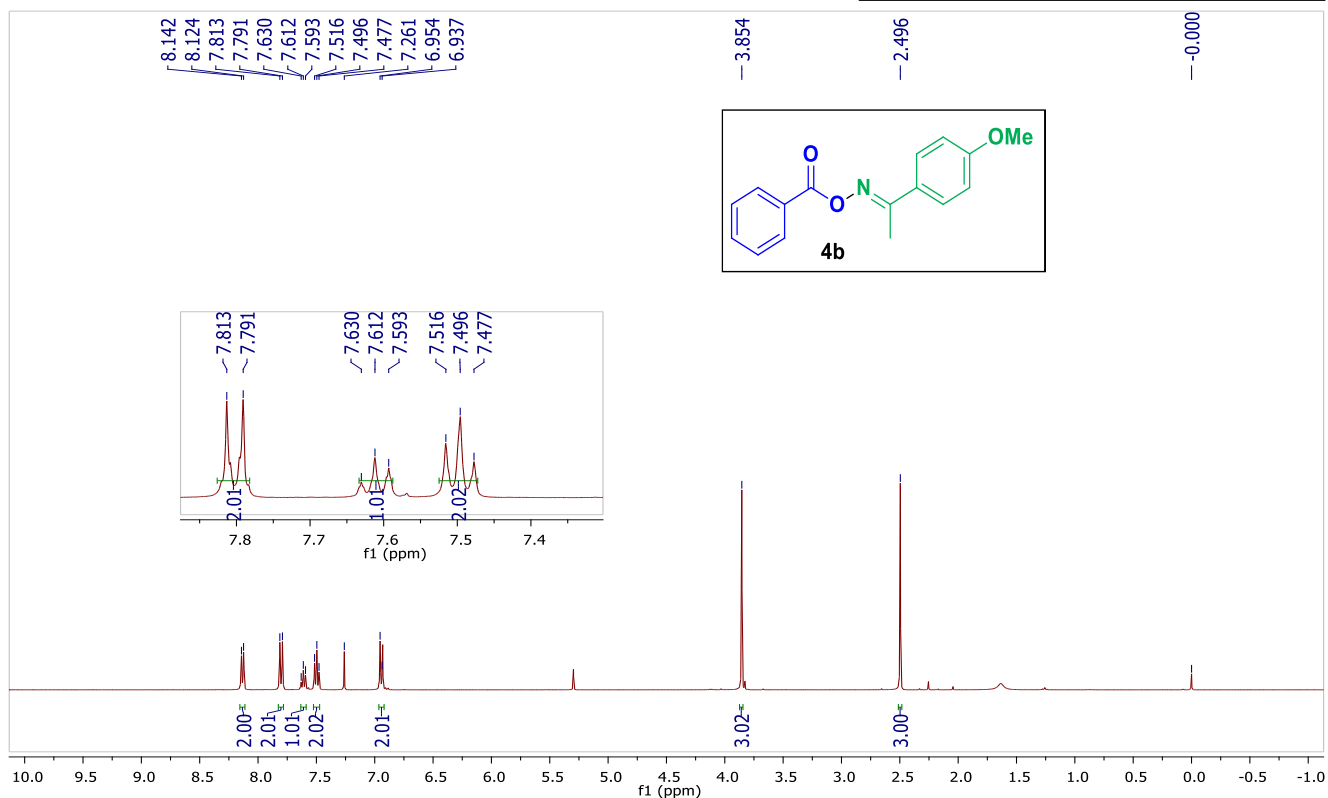
¹H NMR of 4a (400 MHz, CDCl₃)



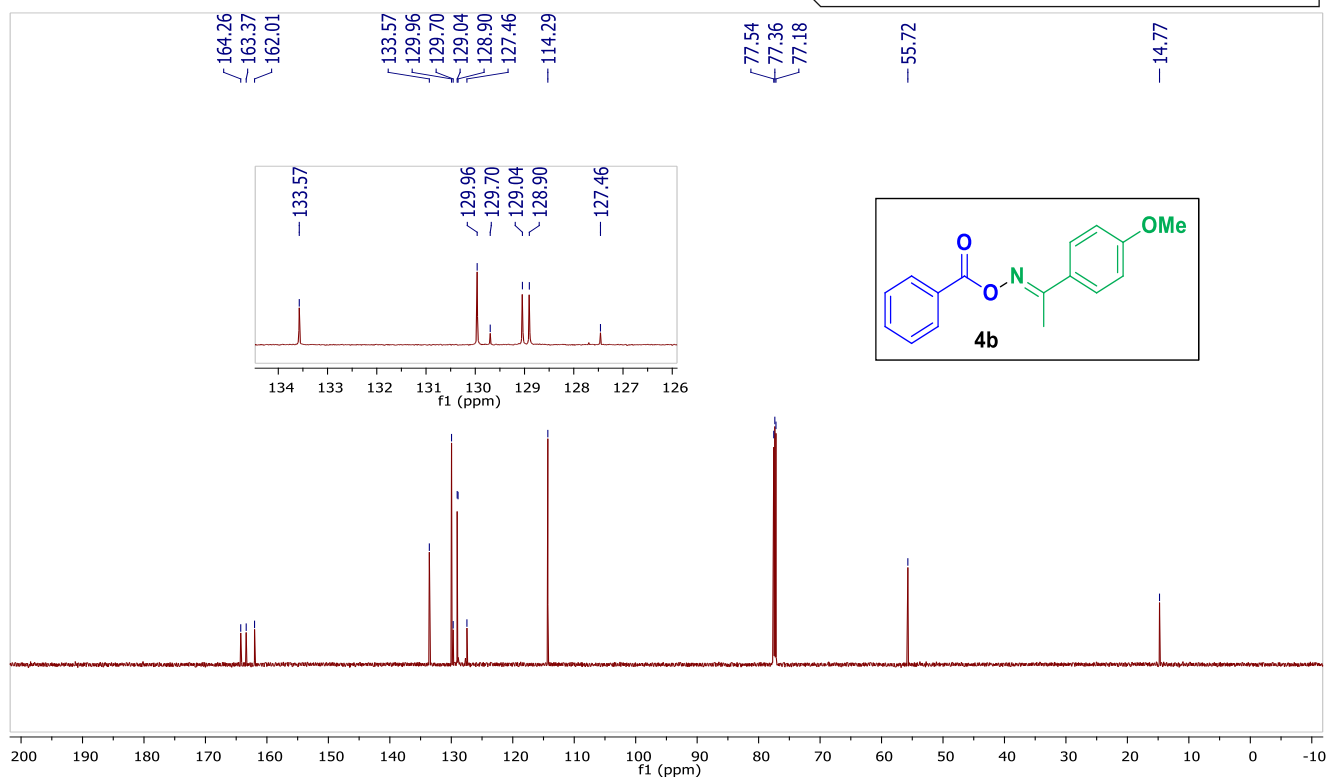
¹³C{¹H} NMR of 4a (100 MHz, CDCl₃)



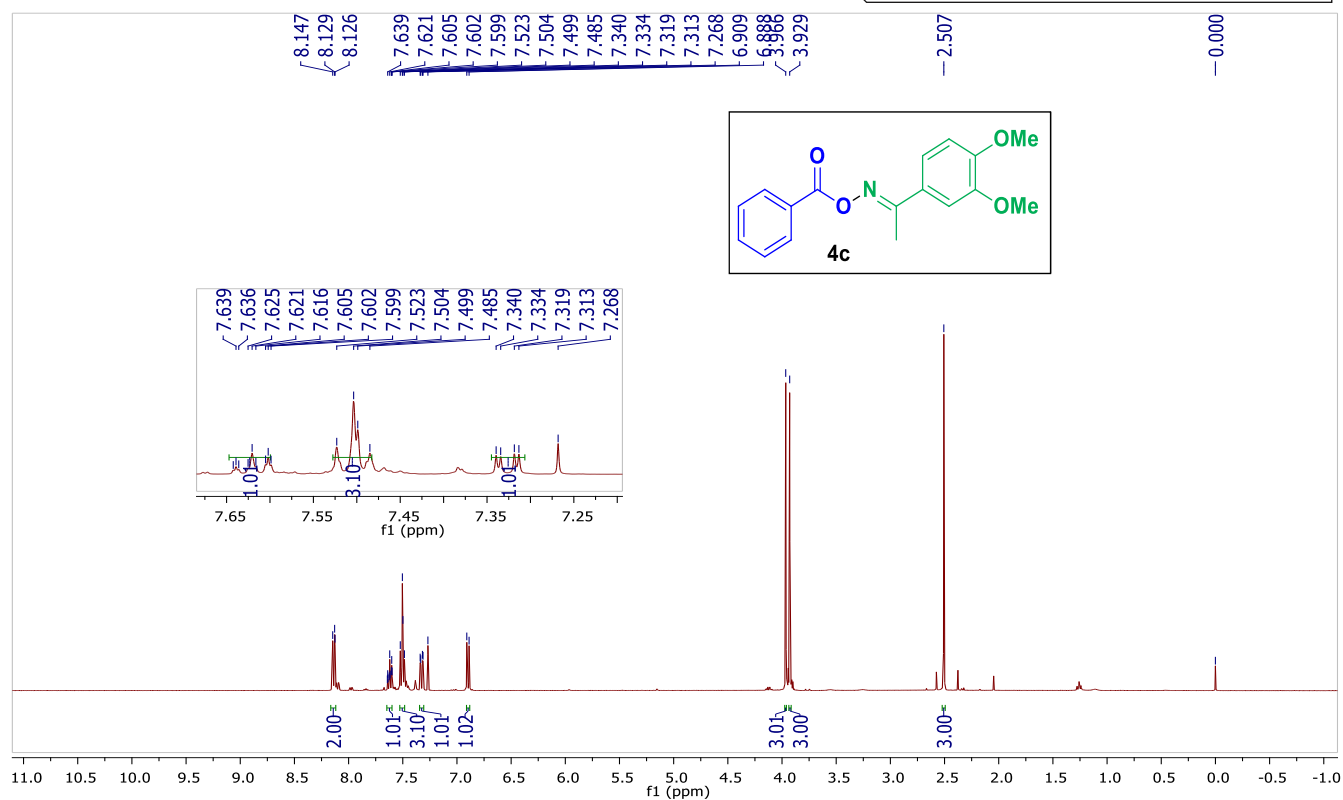
¹H NMR of 4b (400 MHz, CDCl₃)



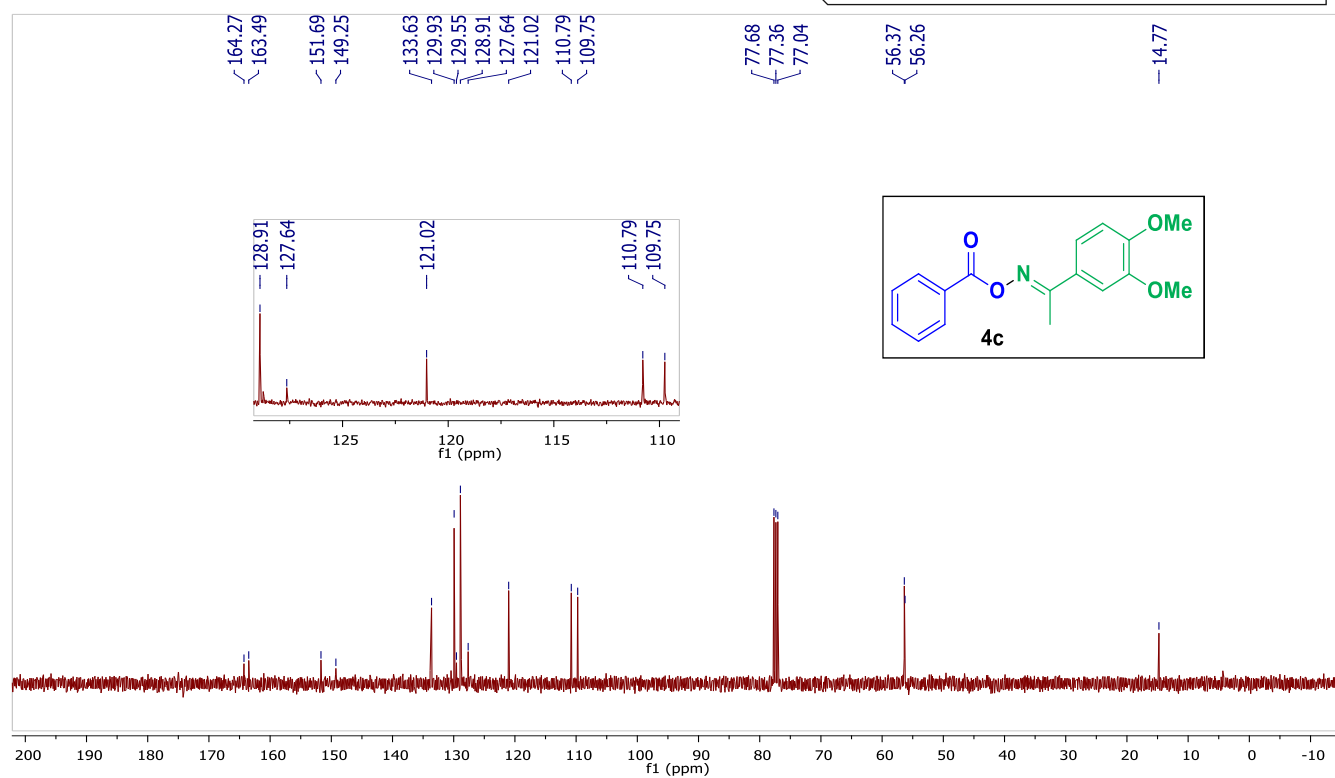
¹³C{¹H} NMR of 4b (176 MHz, CDCl₃)



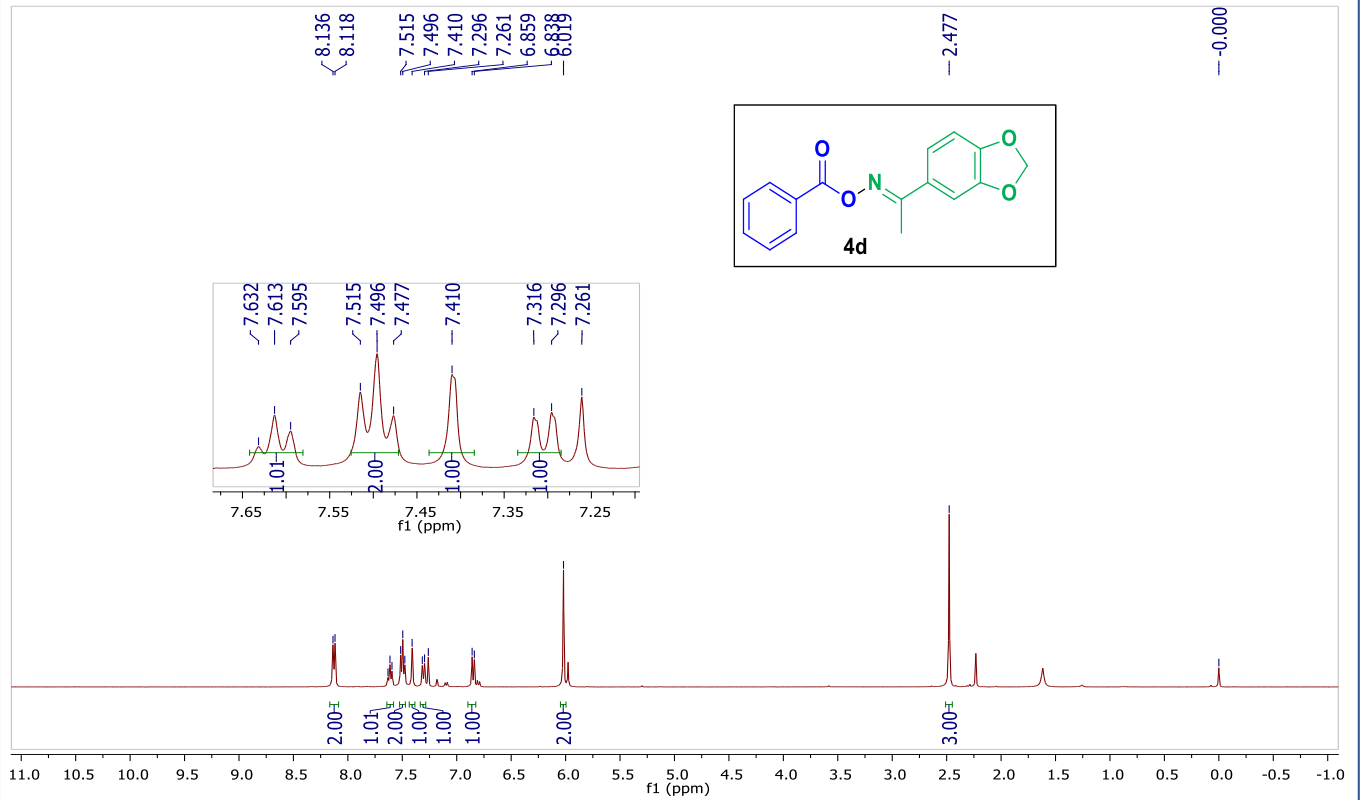
¹H NMR of 4c (400 MHz, CDCl₃)



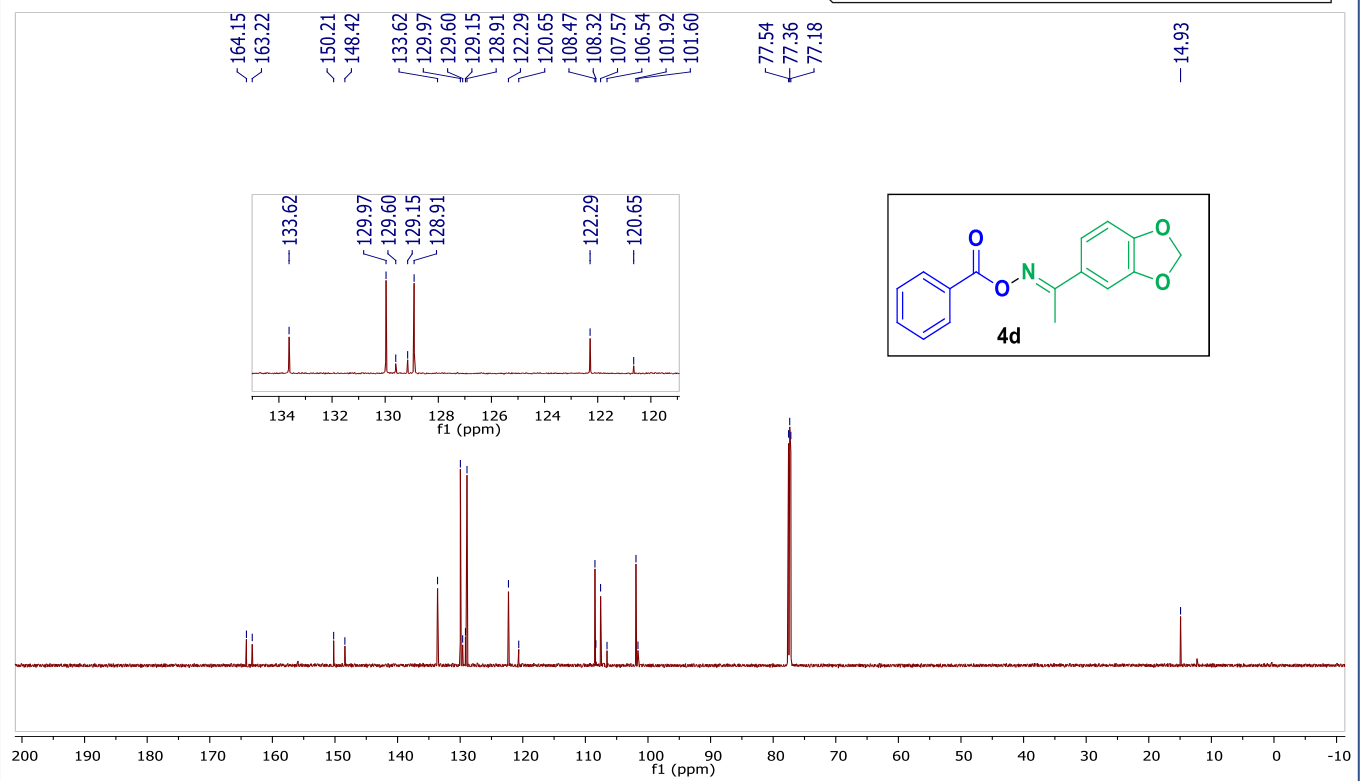
¹³C{¹H} NMR of 4c (100 MHz, CDCl₃)



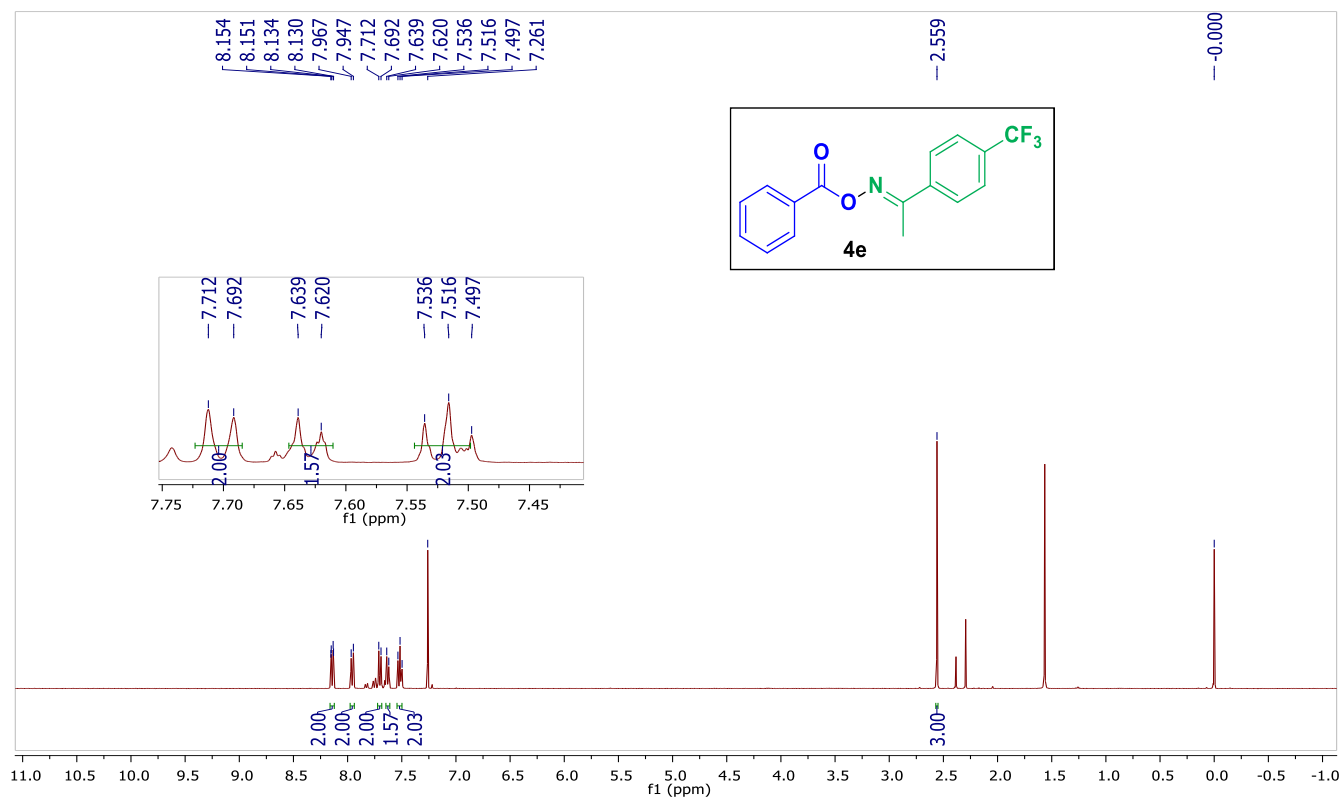
¹H NMR of 4d (400 MHz, CDCl₃)



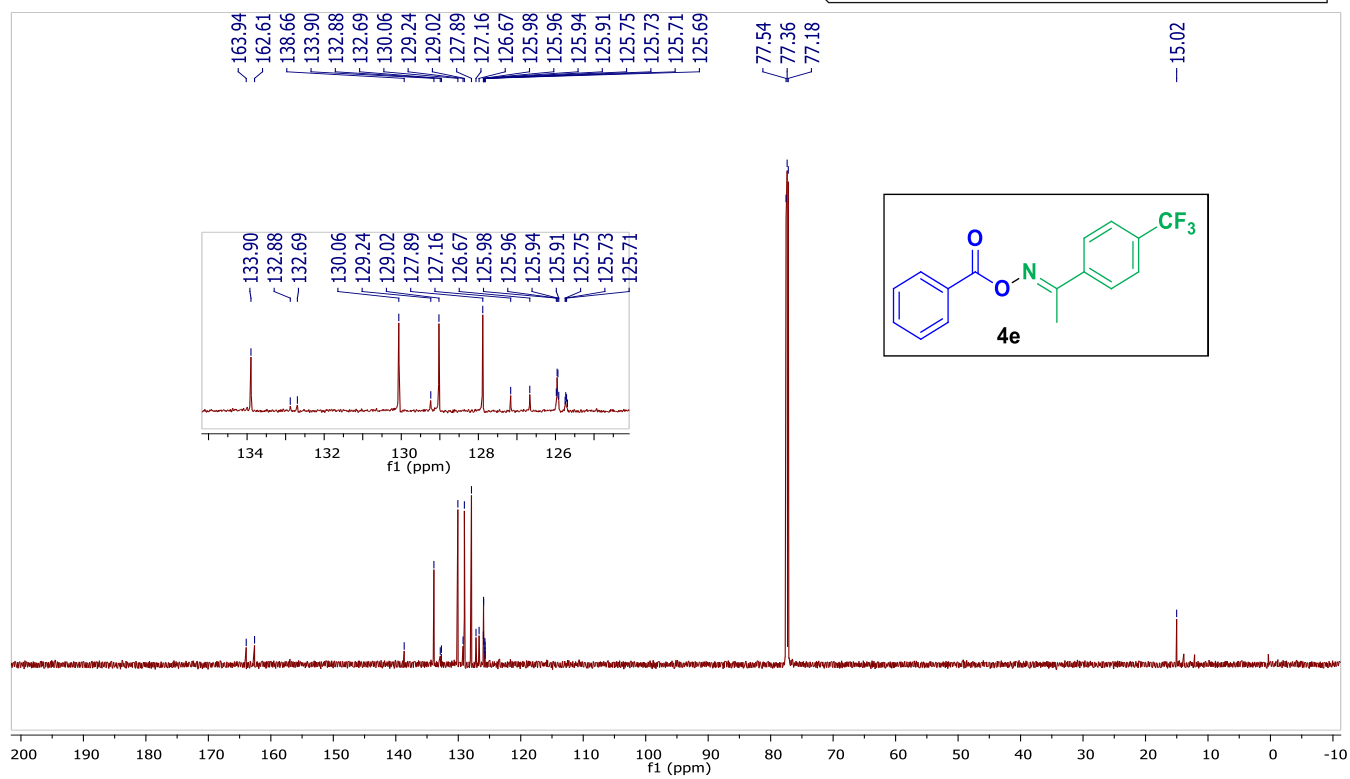
¹³C{¹H} NMR of 4d (176 MHz, CDCl₃)



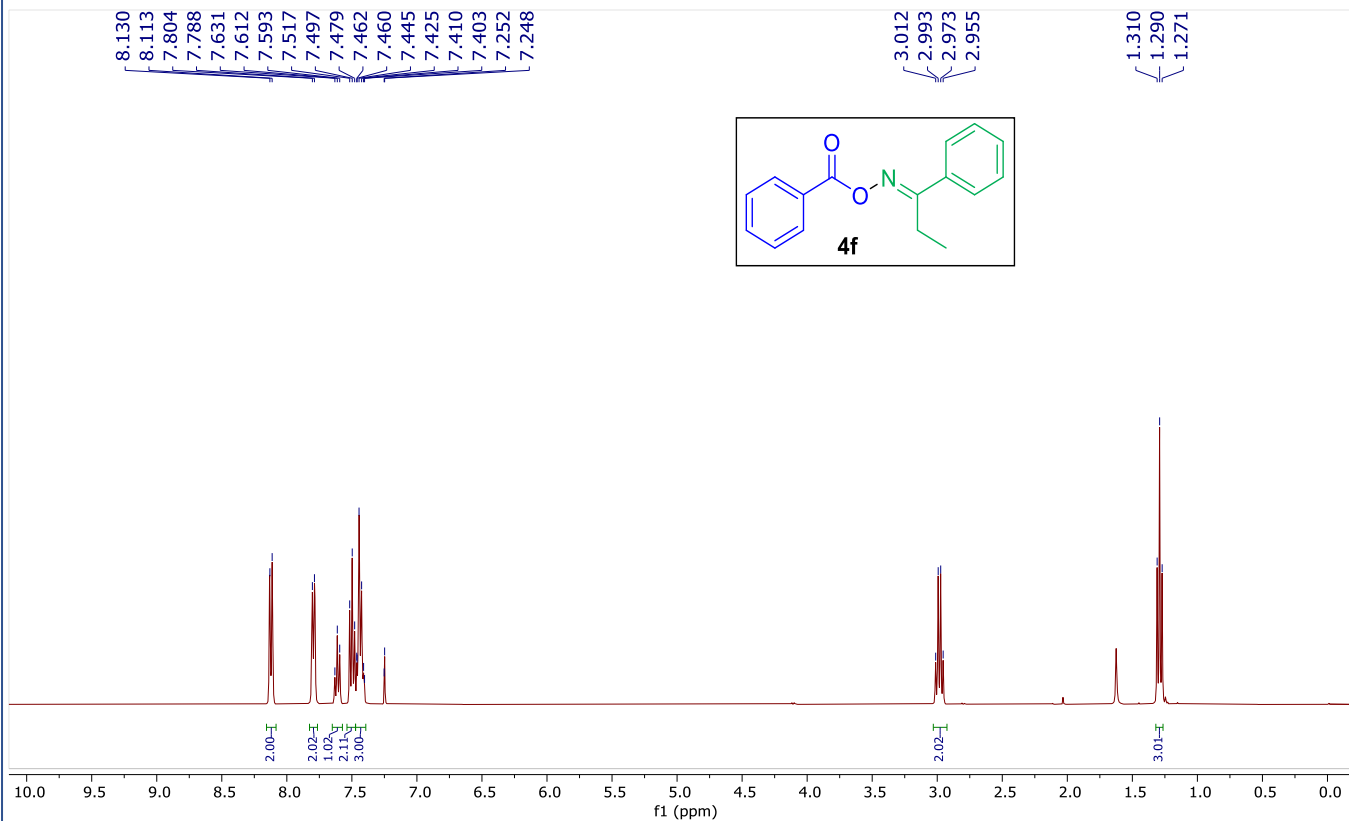
¹H NMR of 4e (400 MHz, CDCl₃)



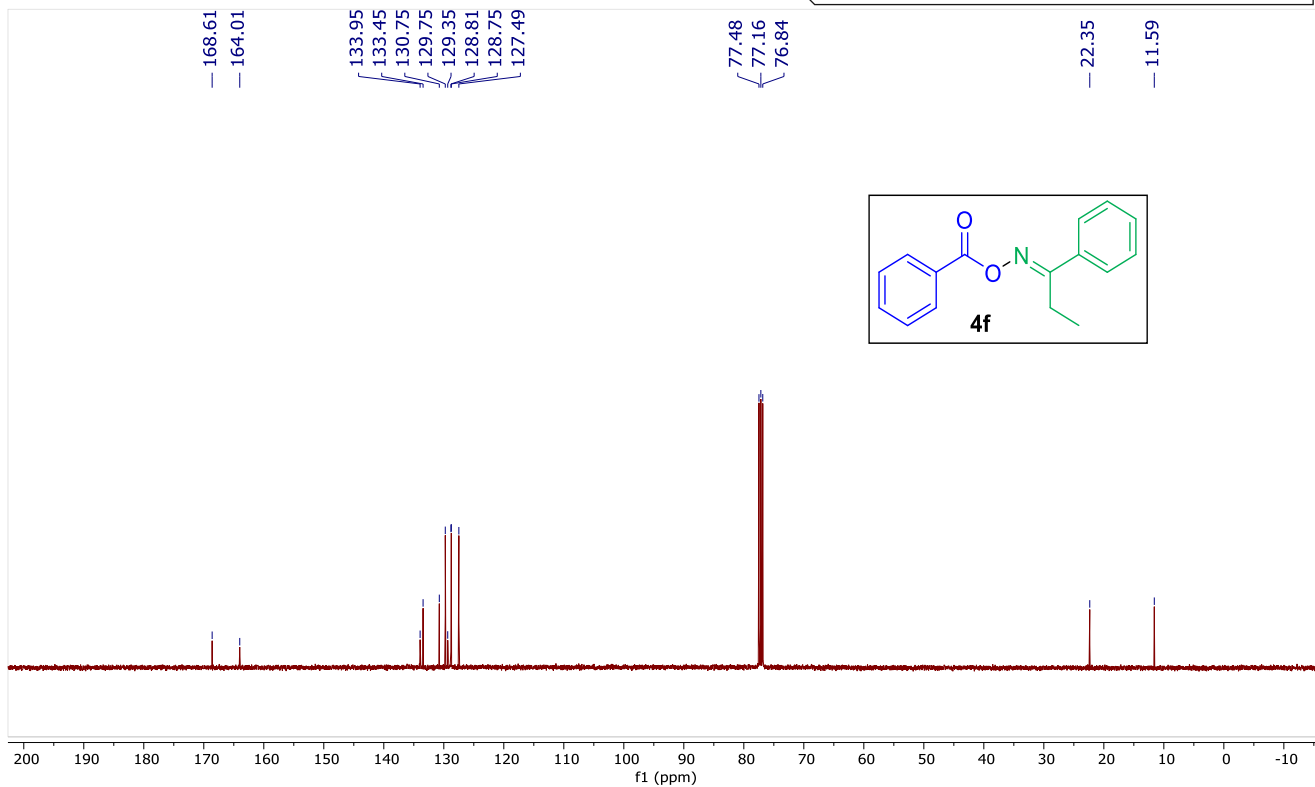
¹³C{¹H} NMR of 4e (176 MHz, CDCl₃)



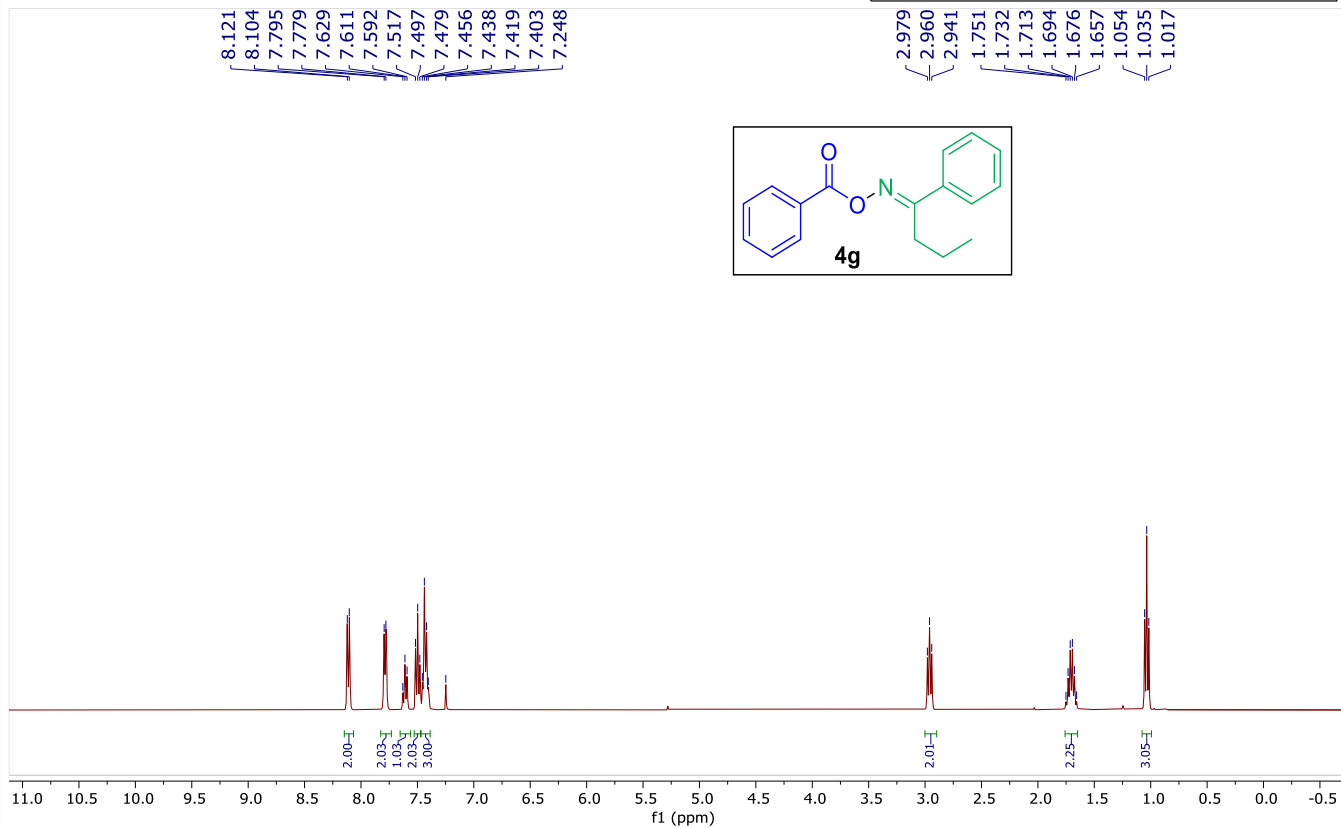
¹H NMR of 4f (400 MHz, CDCl₃)



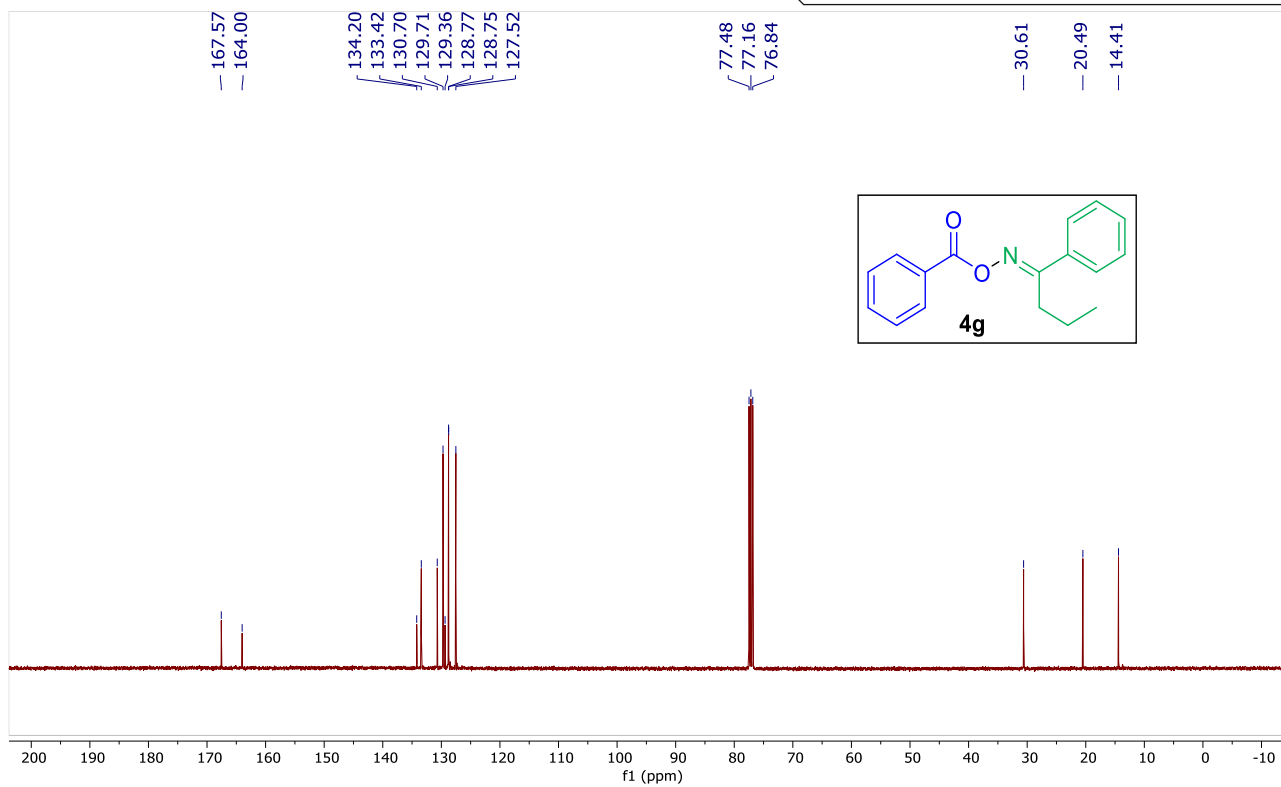
¹³C{¹H} NMR of 4f (100 MHz, CDCl₃)



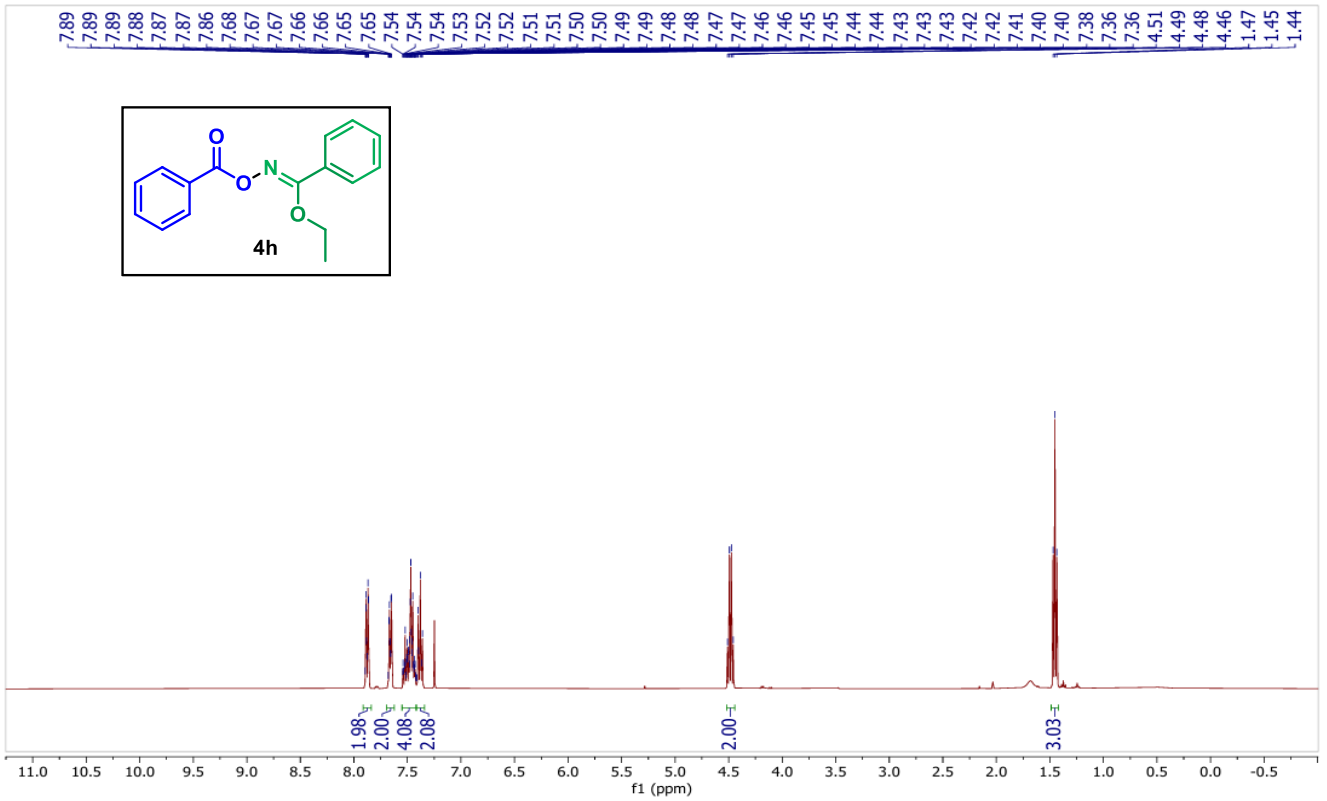
¹H NMR of 4g (400 MHz, CDCl₃)



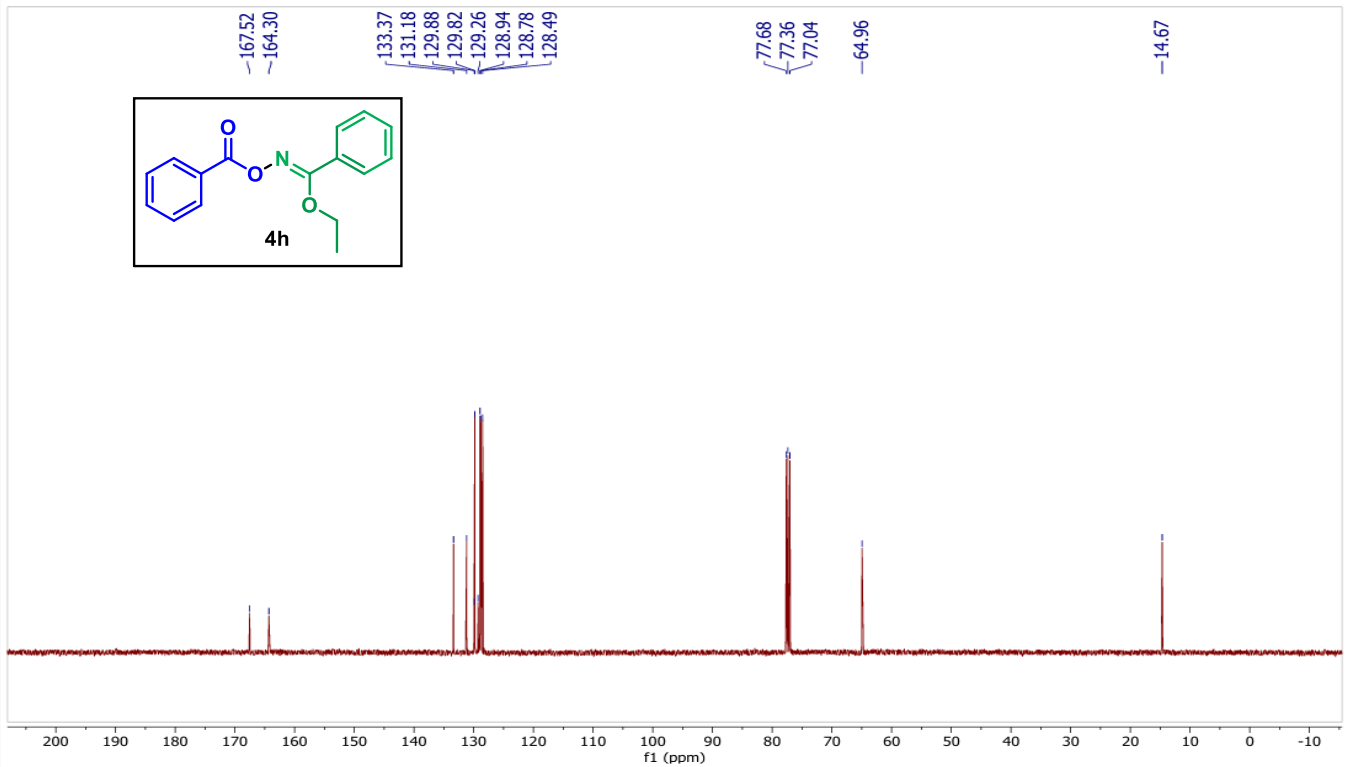
¹³C{¹H} NMR of 4g (100 MHz, CDCl₃)



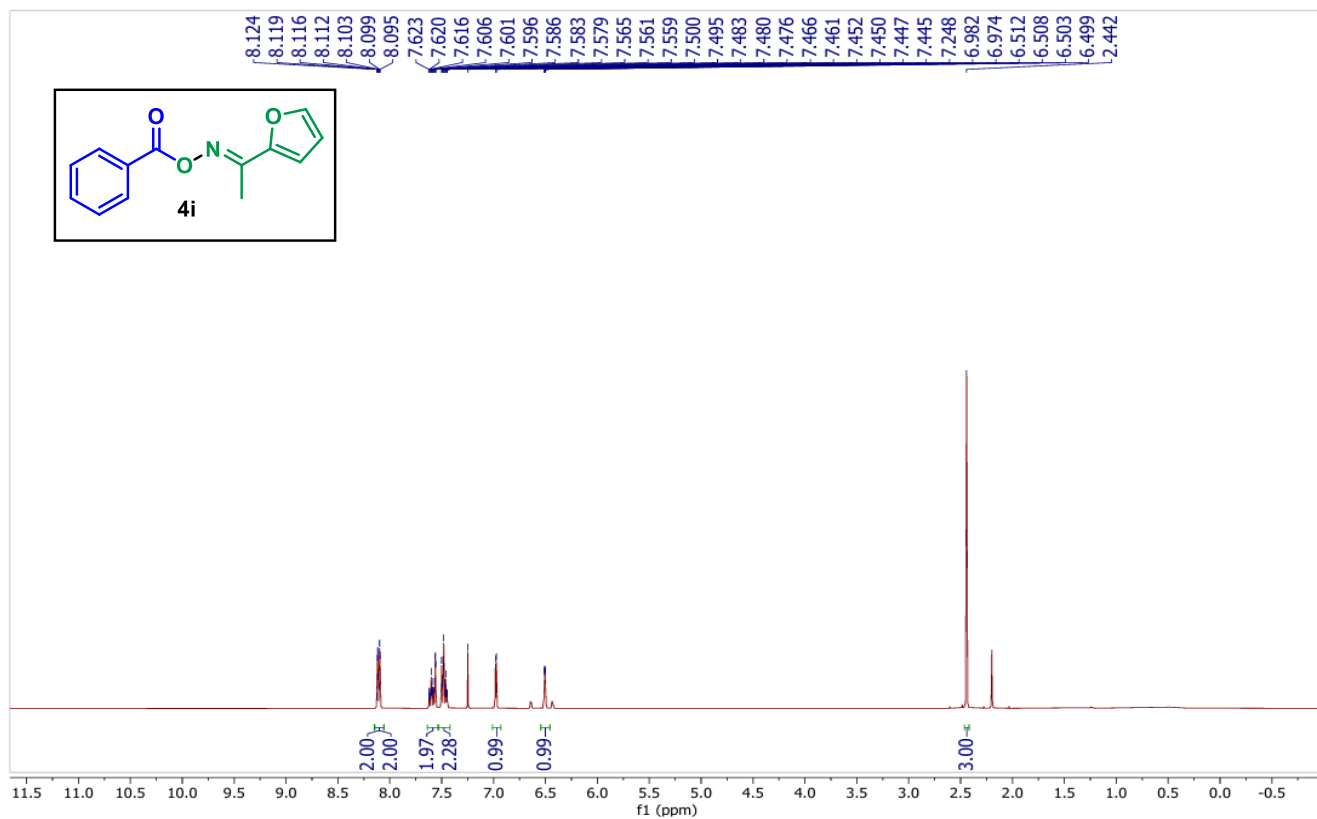
¹H NMR of 4h (400 MHz, CDCl₃)



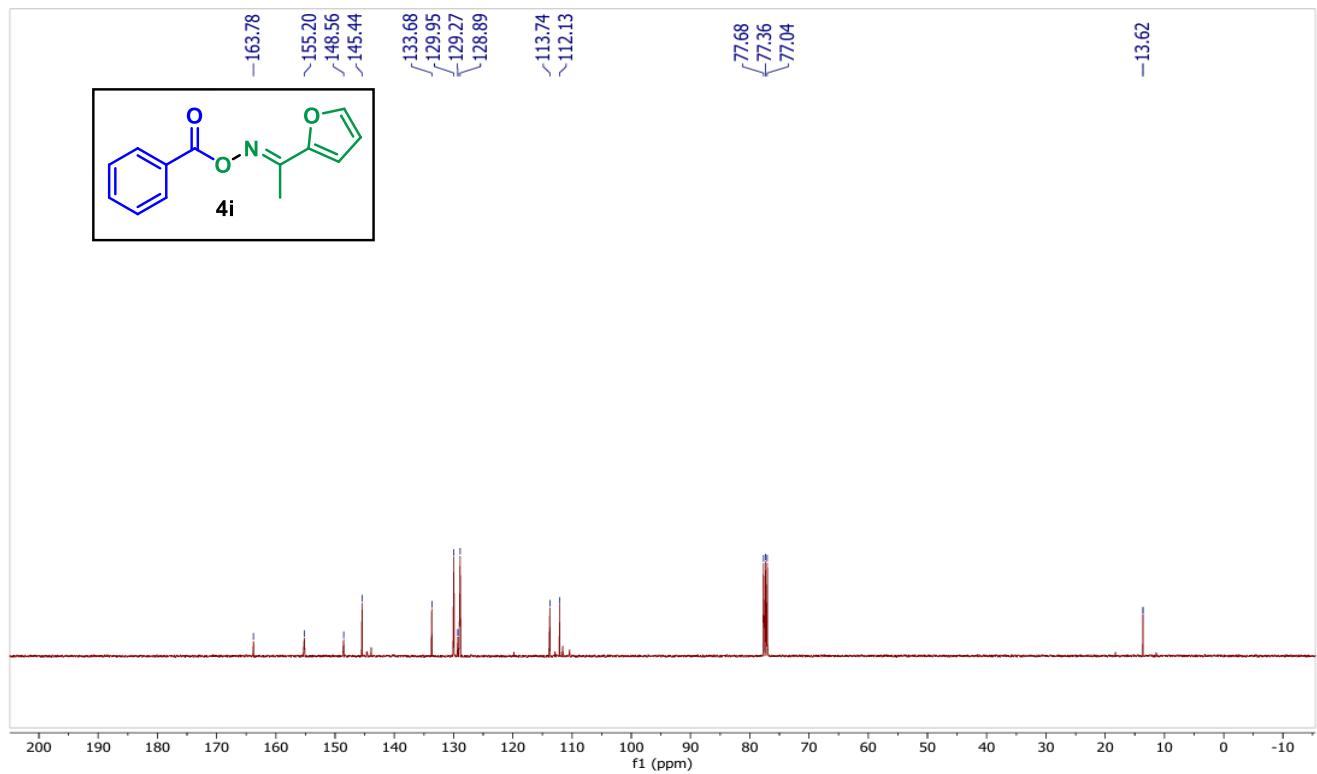
¹³C{¹H} NMR of 4h (100 MHz, CDCl₃)



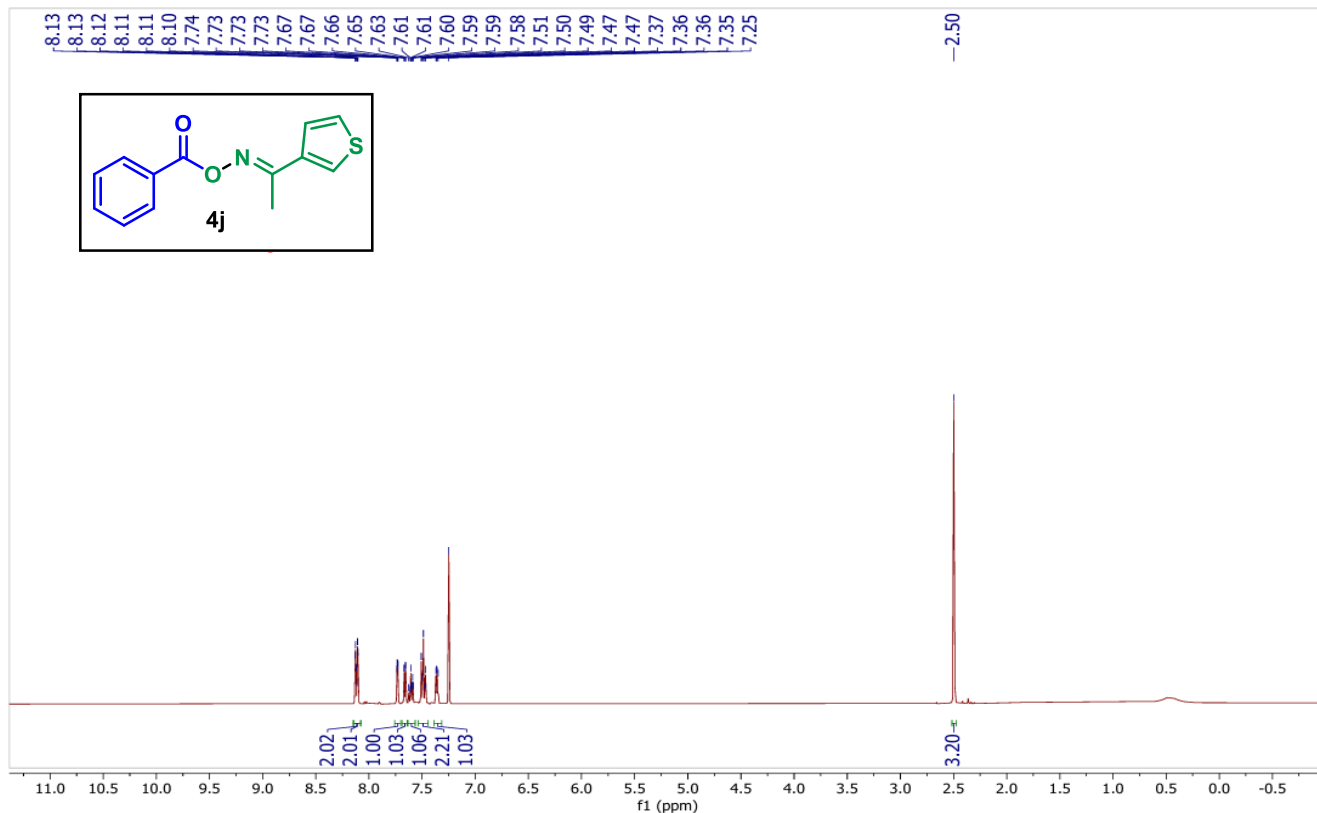
¹H NMR of 4i (400 MHz, CDCl₃)



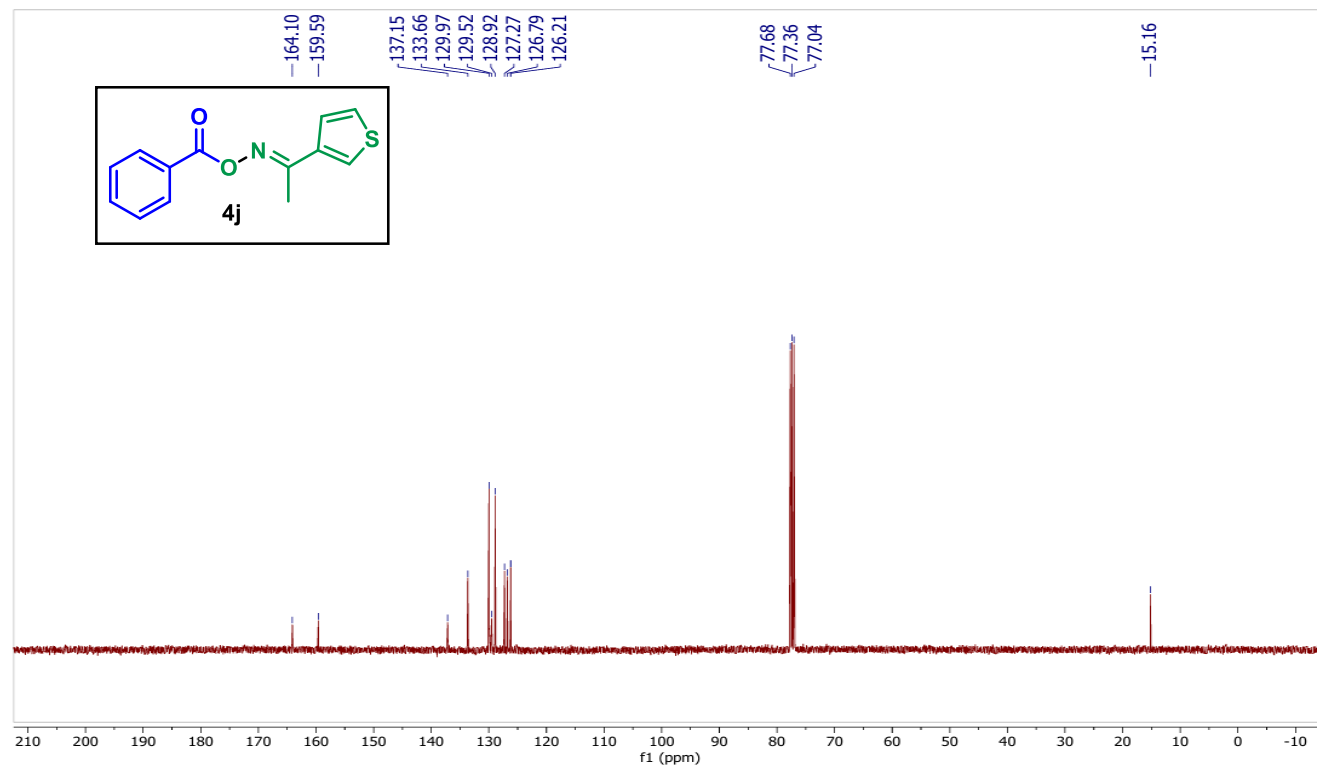
¹³C{¹H} NMR of 4i (100 MHz, CDCl₃)



¹H NMR of 4j (400 MHz, CDCl₃)

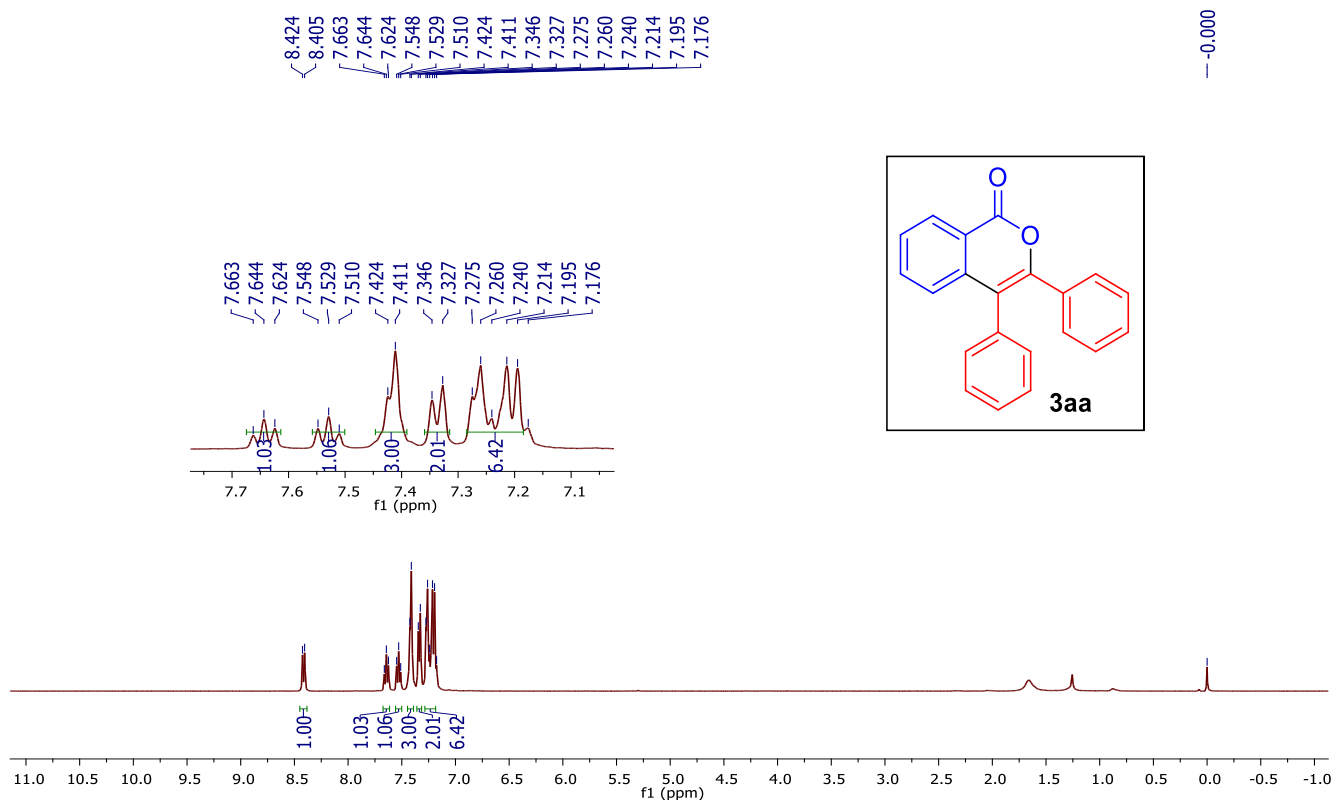


¹³C{¹H} NMR of 4j (100 MHz, CDCl₃)

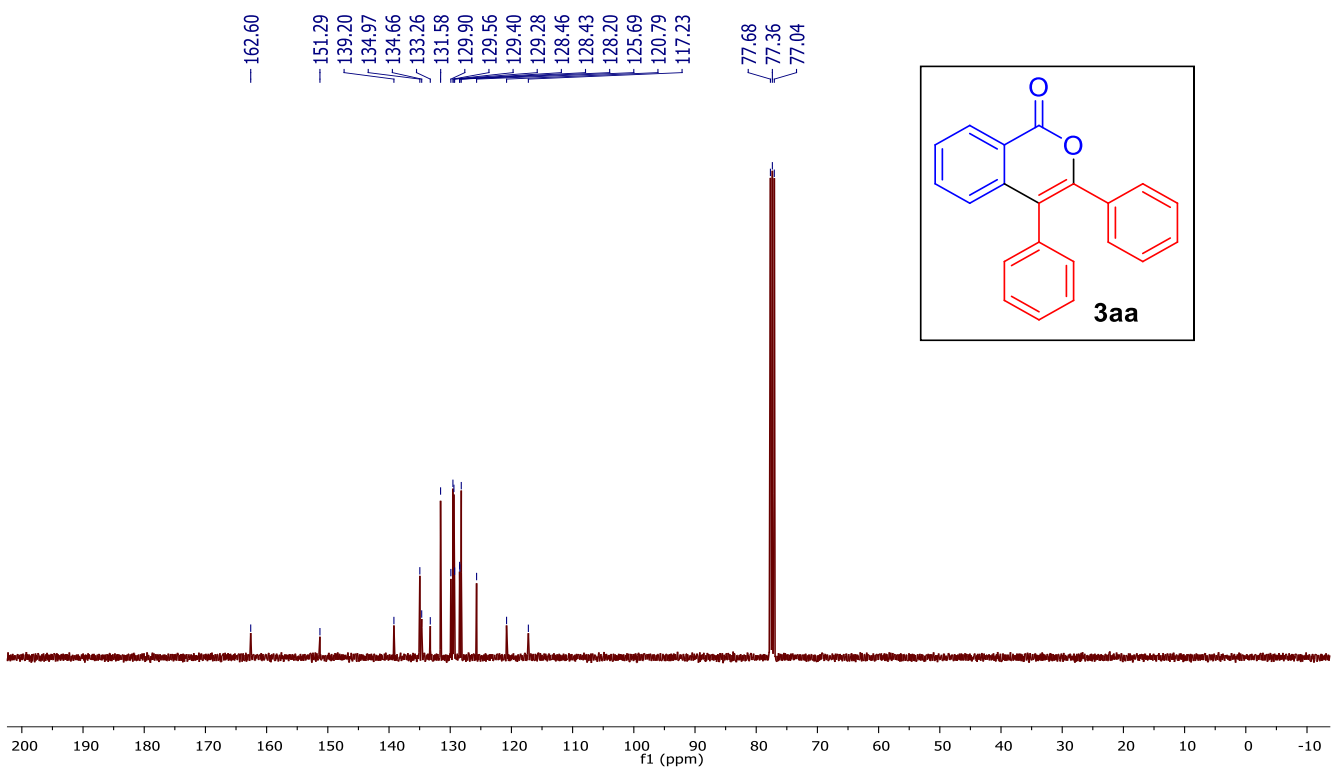


6.2 Copies of NMR spectra of the products

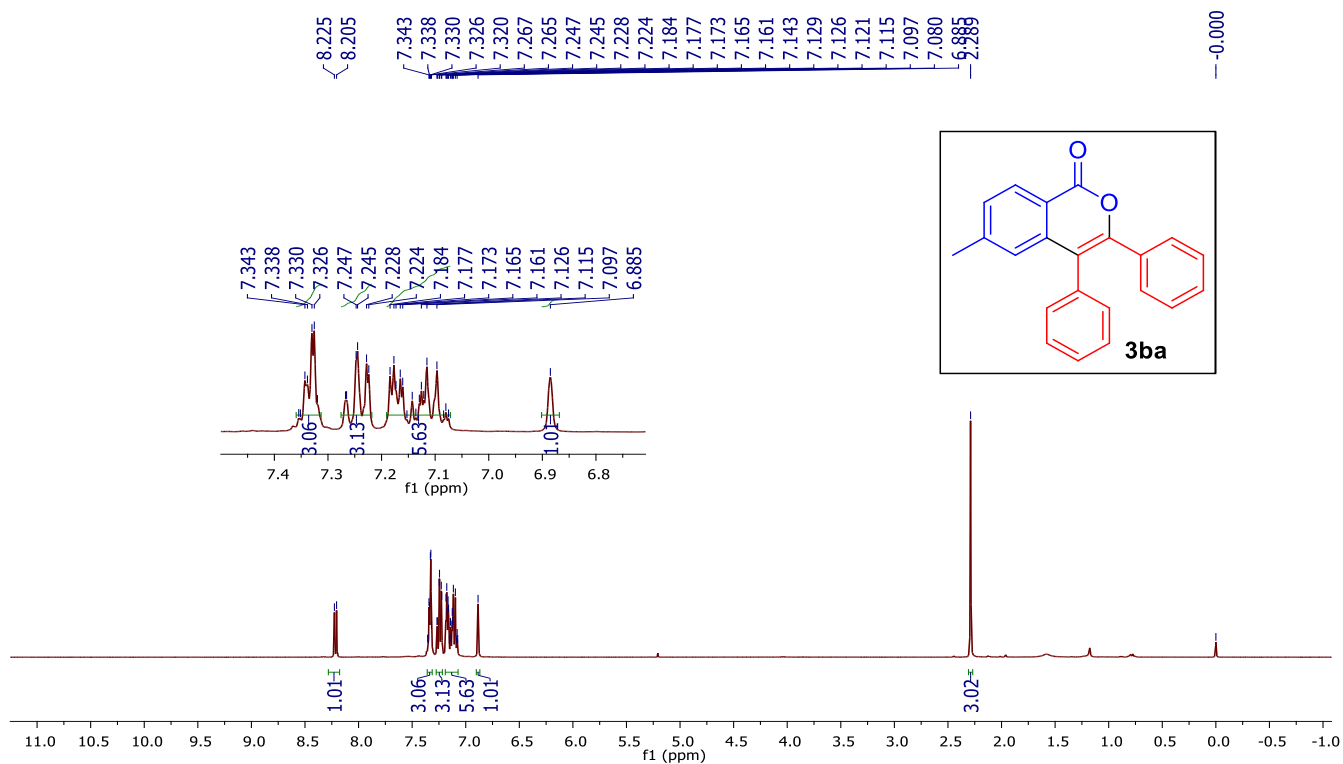
^1H NMR of 3aa (400 MHz, CDCl_3)



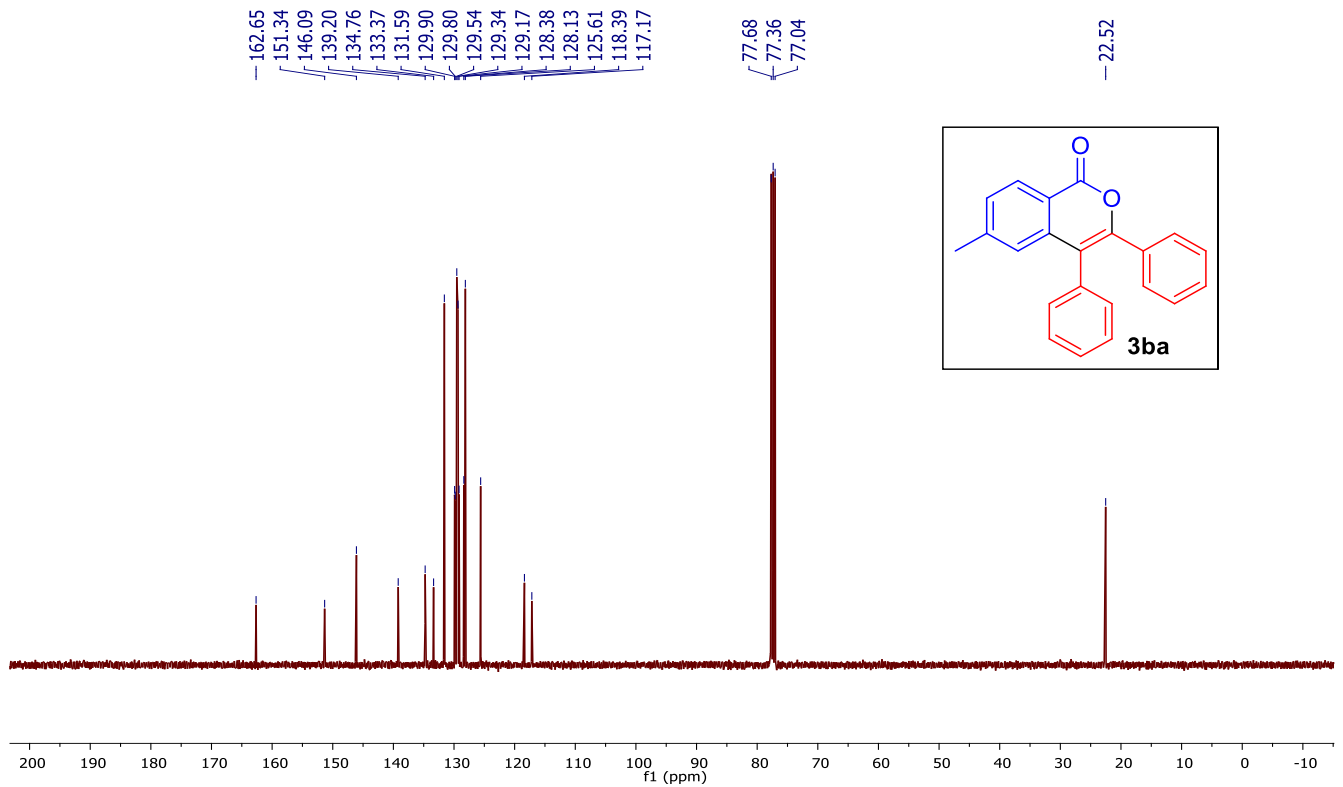
$^{13}\text{C}\{^1\text{H}\}$ NMR of 3aa (100 MHz, CDCl_3)



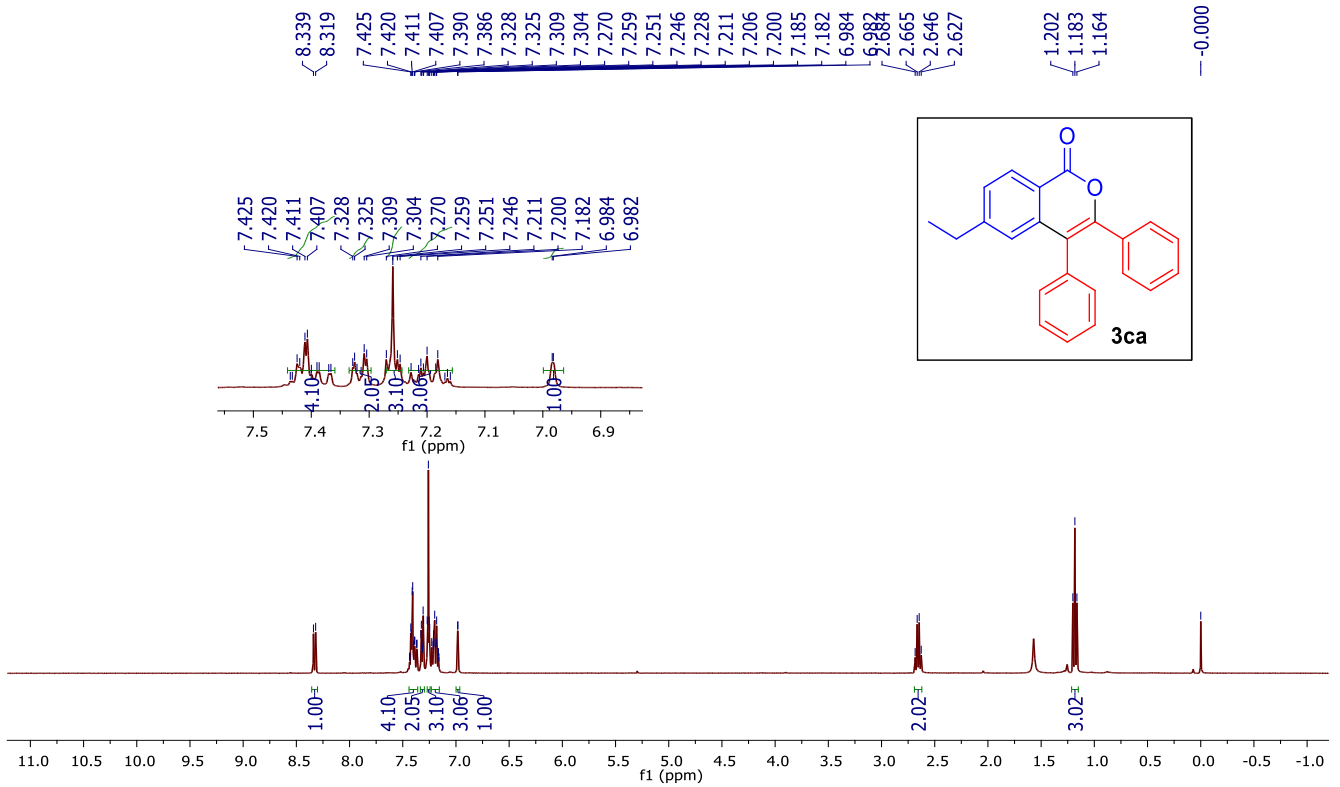
¹H NMR of 3ba (400 MHz, CDCl₃)



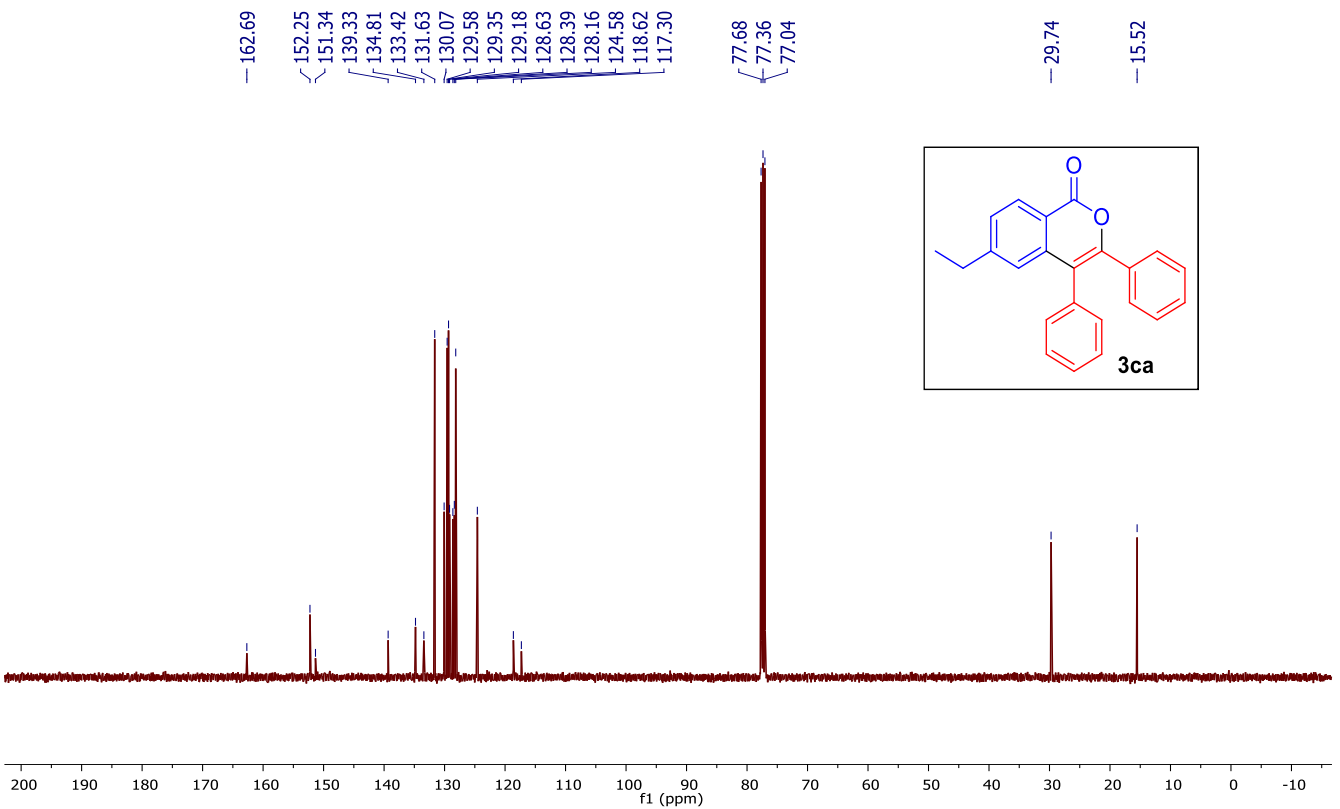
¹³C{¹H} NMR of 3ba (100 MHz, CDCl₃)



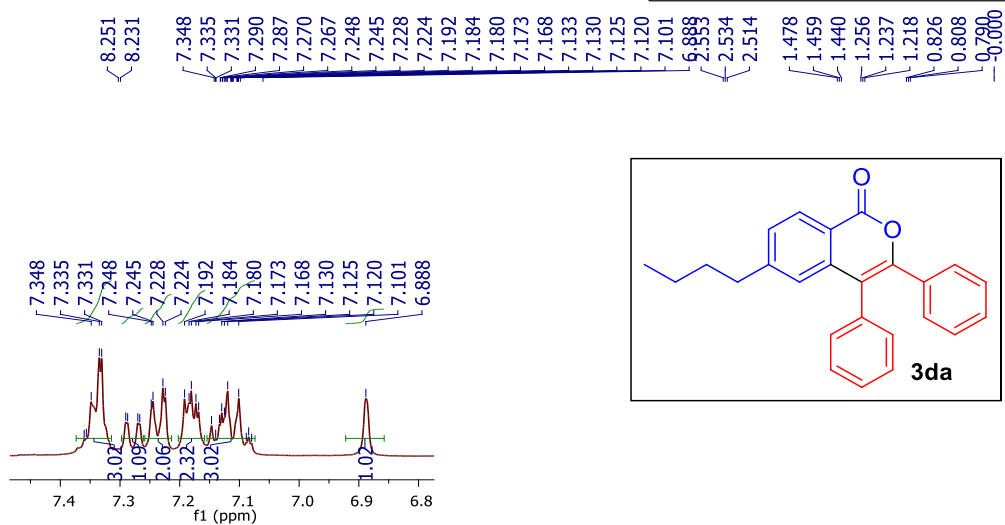
¹H NMR of 3ca (400 MHz, CDCl₃)



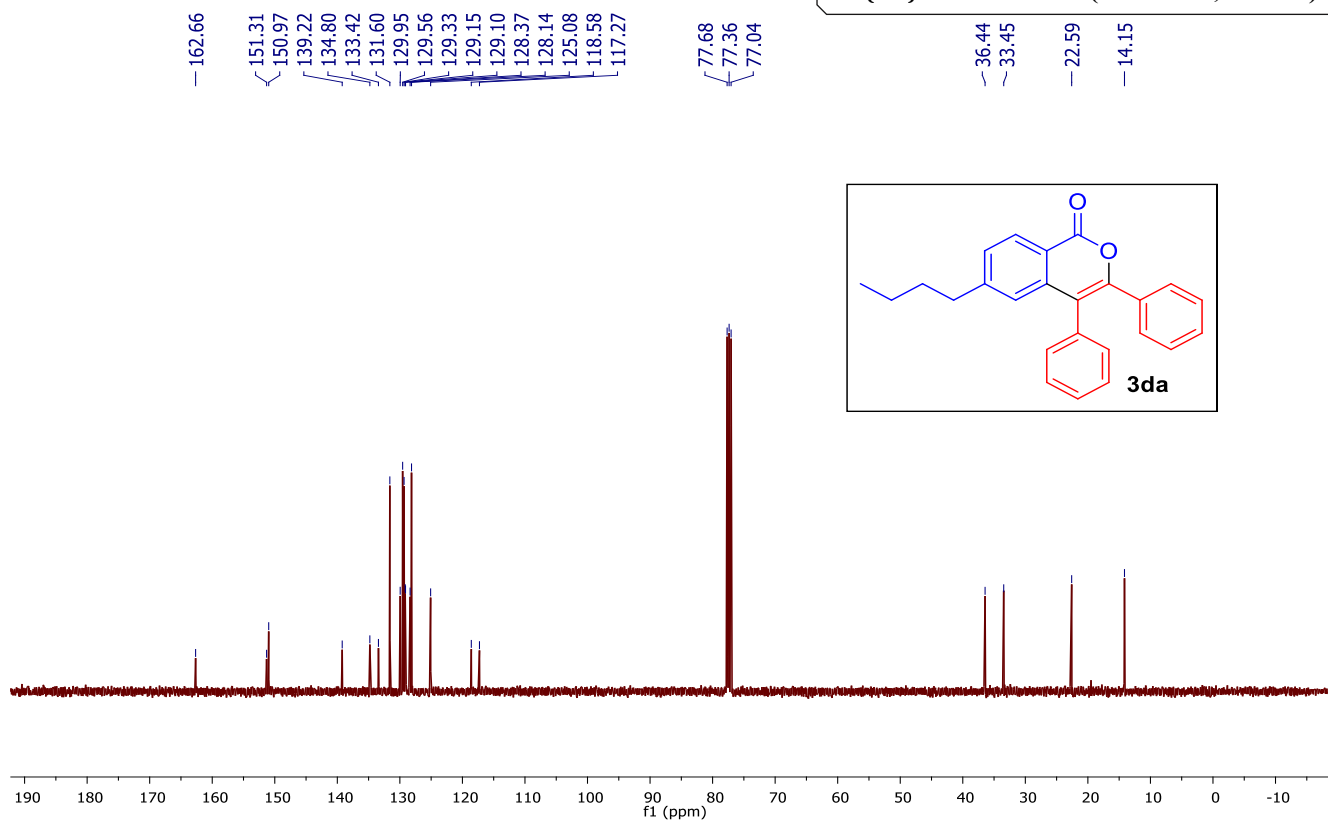
¹³C{¹H} NMR of 3ca (100 MHz, CDCl₃)



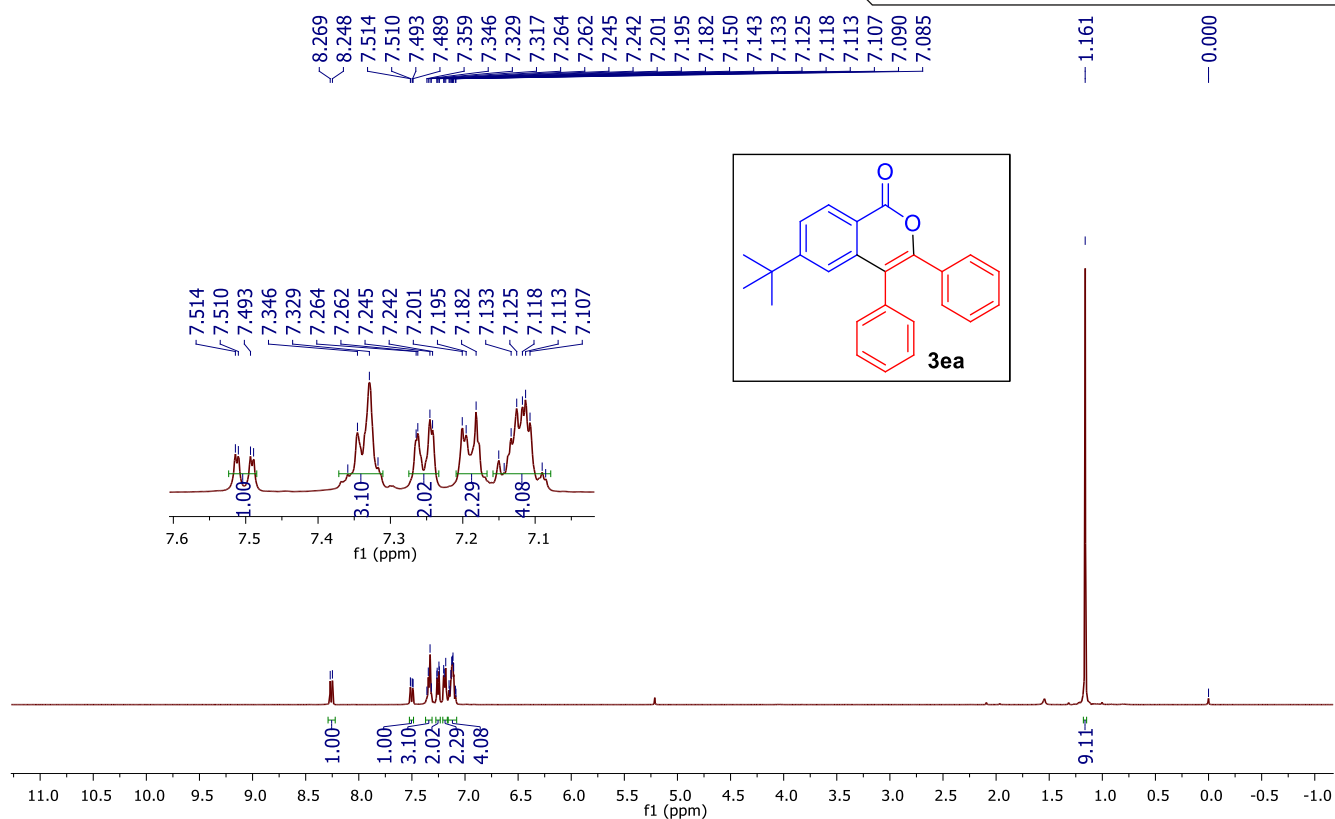
¹H NMR of 3da (400 MHz, CDCl₃)



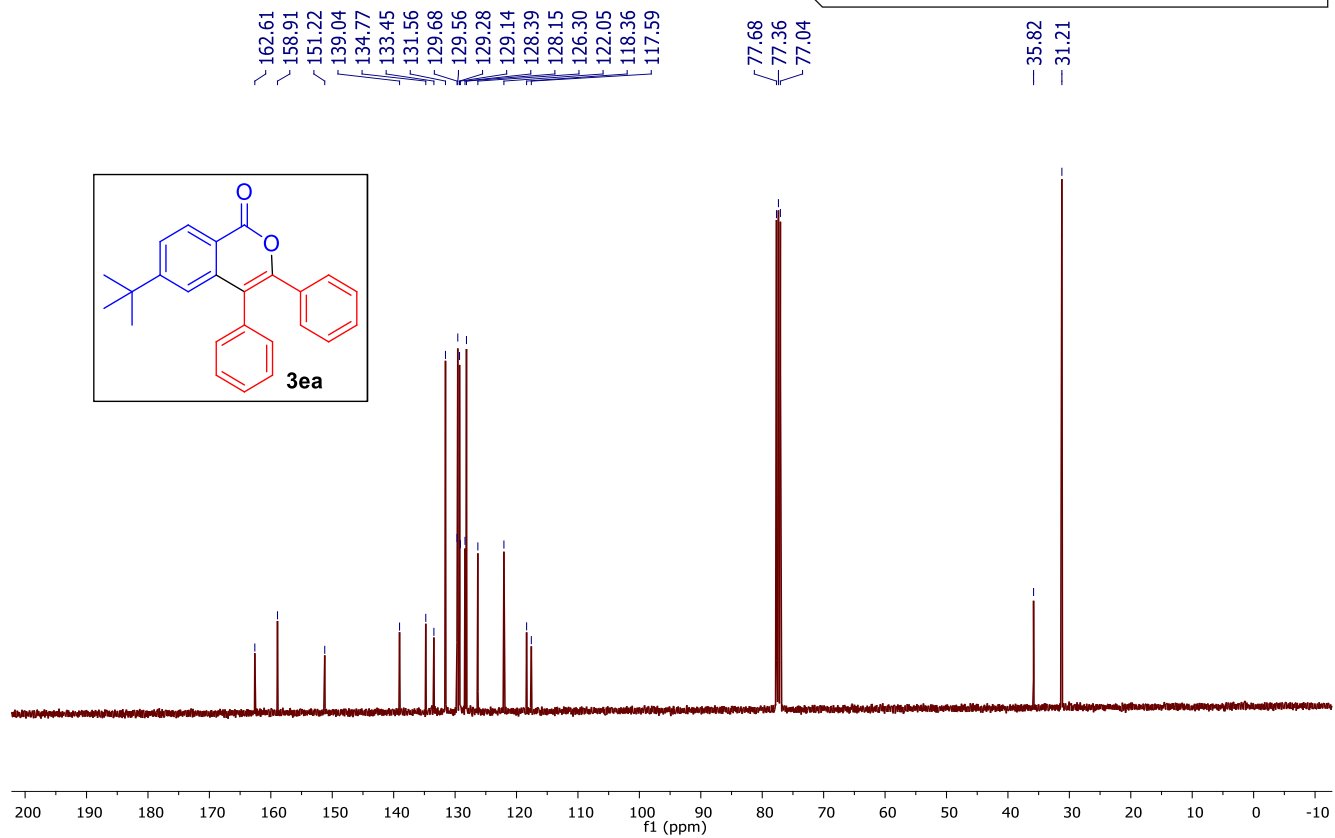
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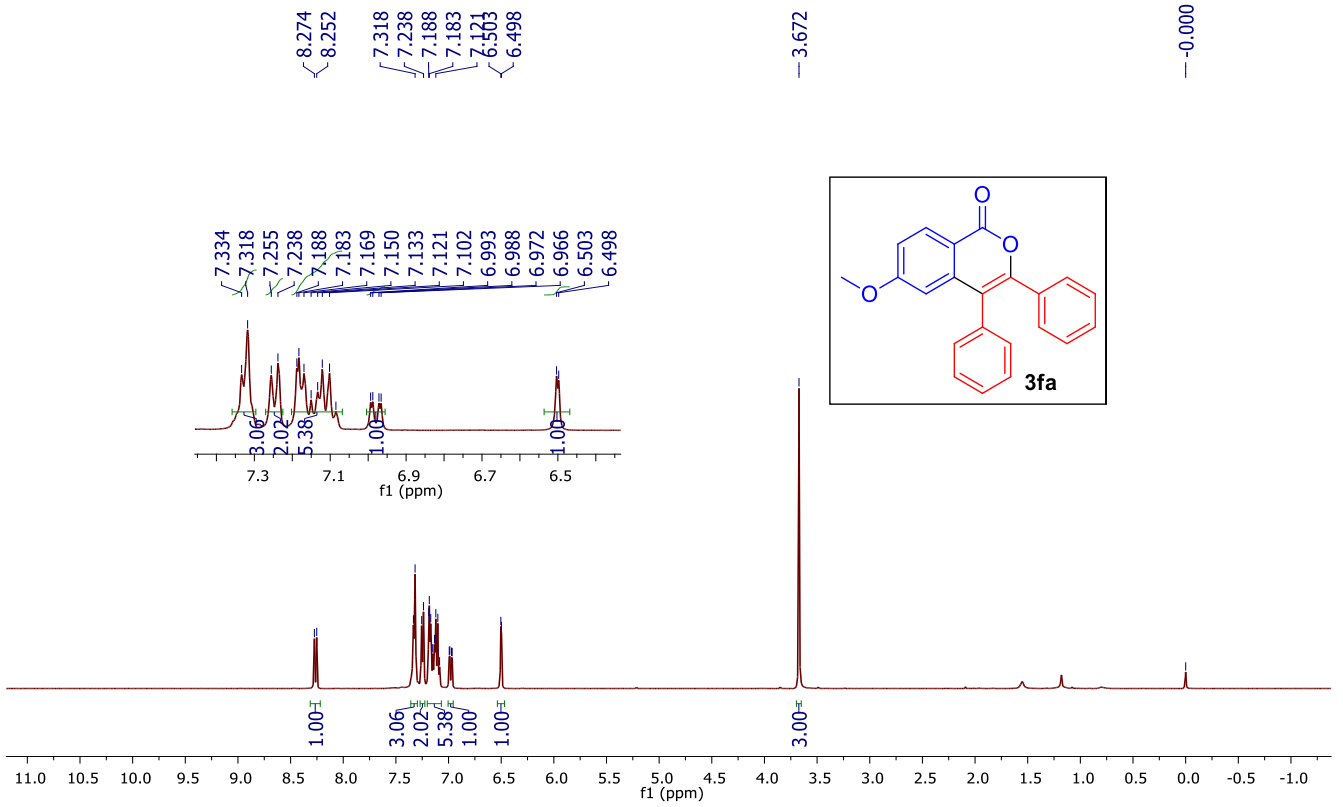
¹H NMR of 3ea (400 MHz, CDCl₃)



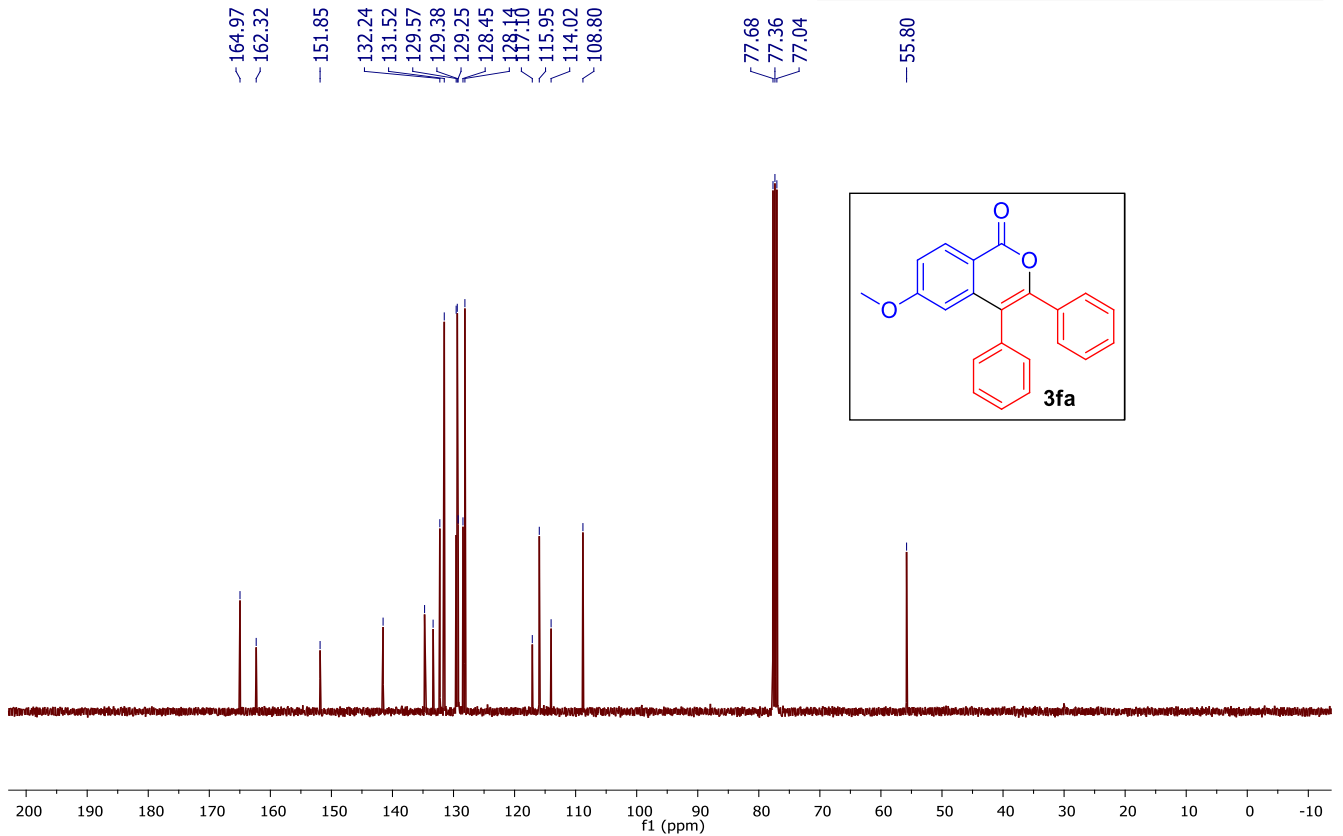
¹³C{¹H} NMR of 3ea (100 MHz, CDCl₃)



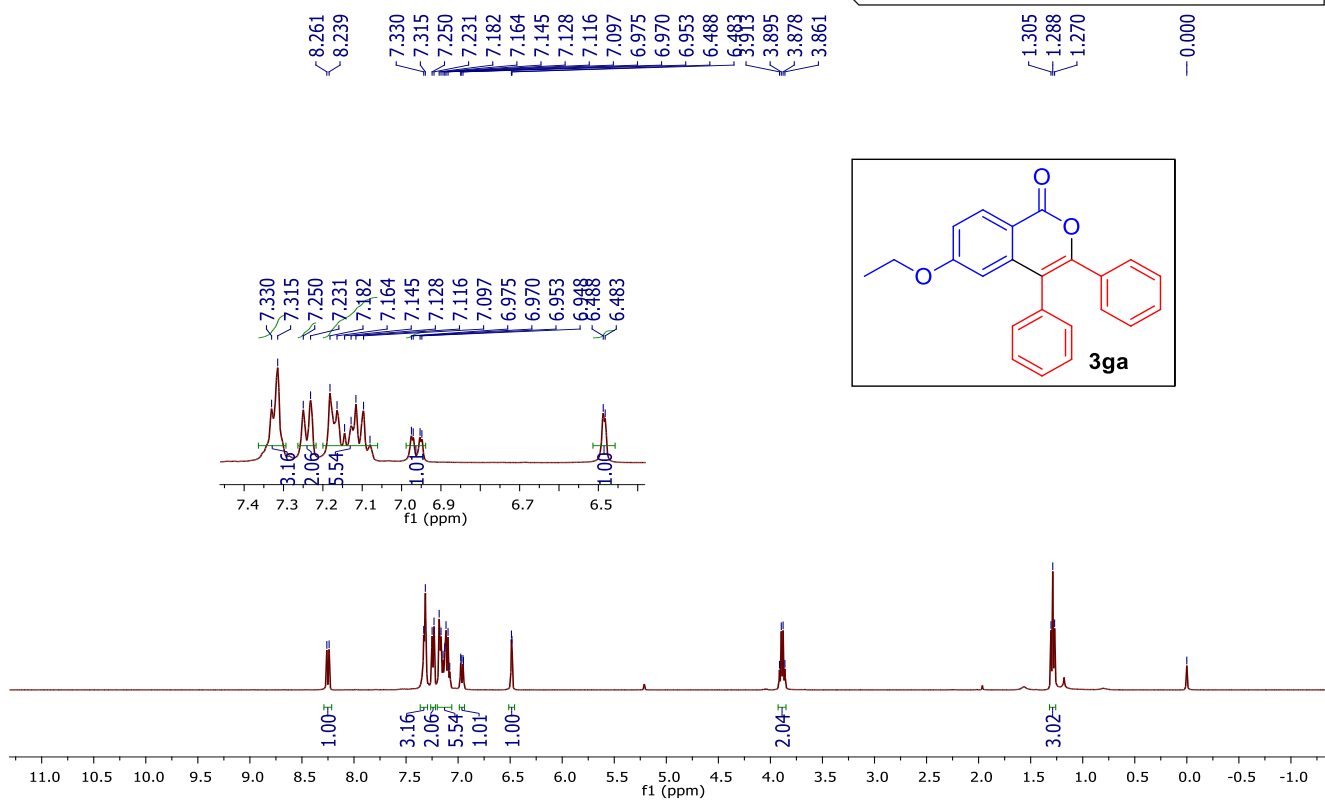
¹H NMR of 3fa (400 MHz, CDCl₃)



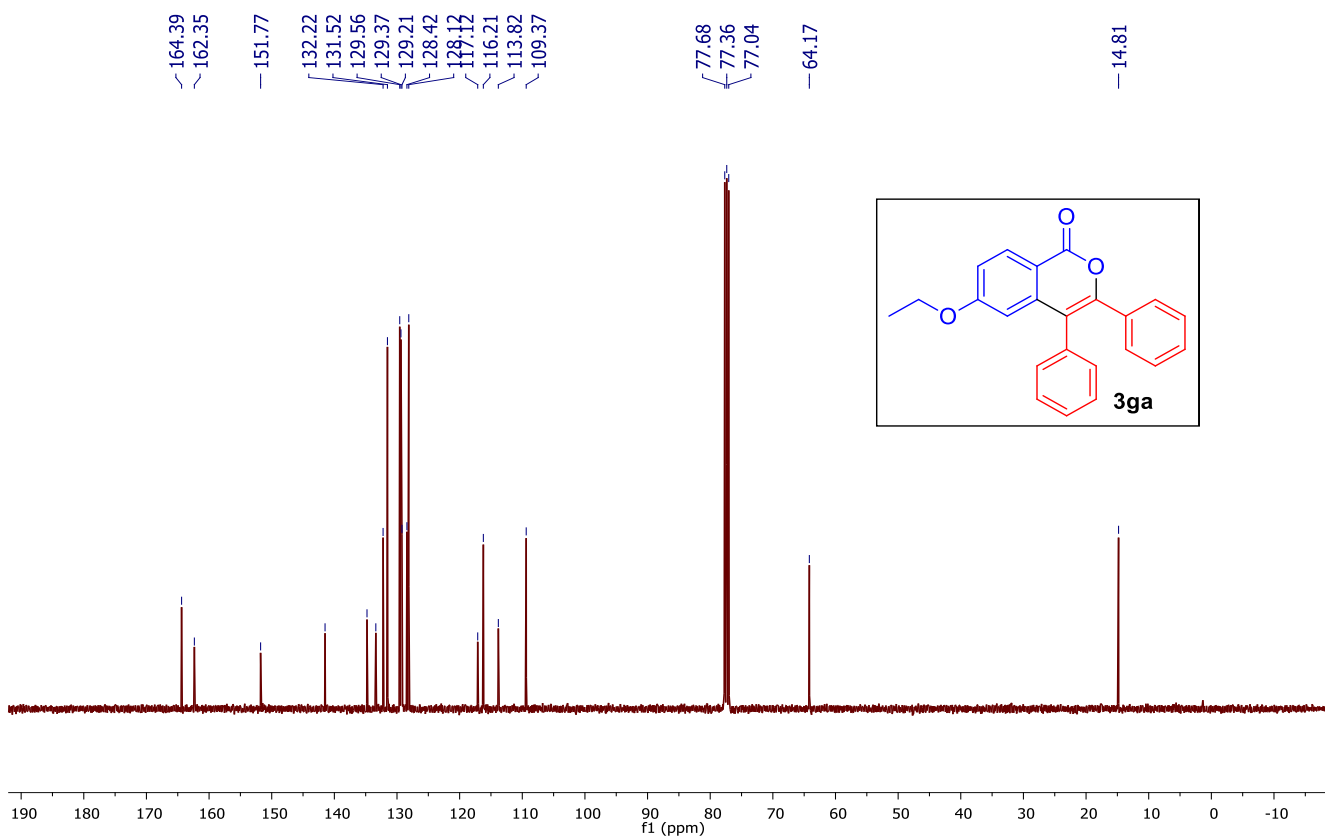
¹³C{¹H} NMR of 3fa (100 MHz, CDCl₃)



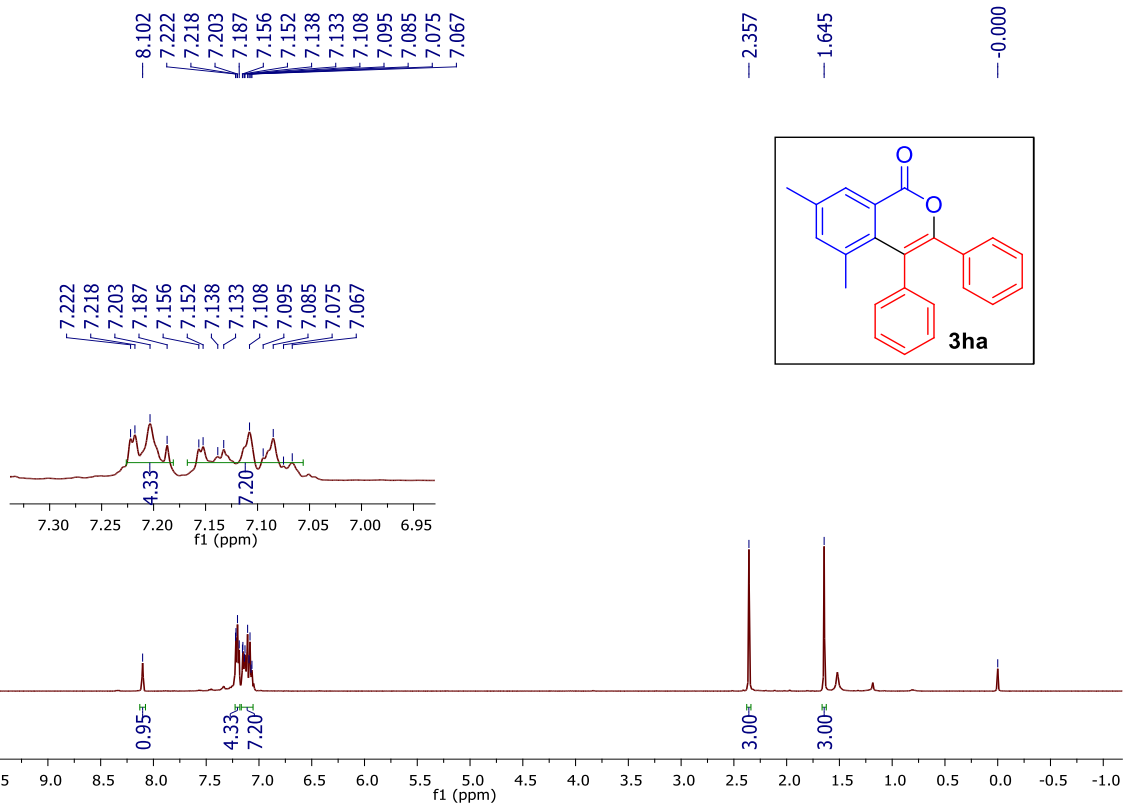
¹H NMR of 3ga (400 MHz, CDCl₃)



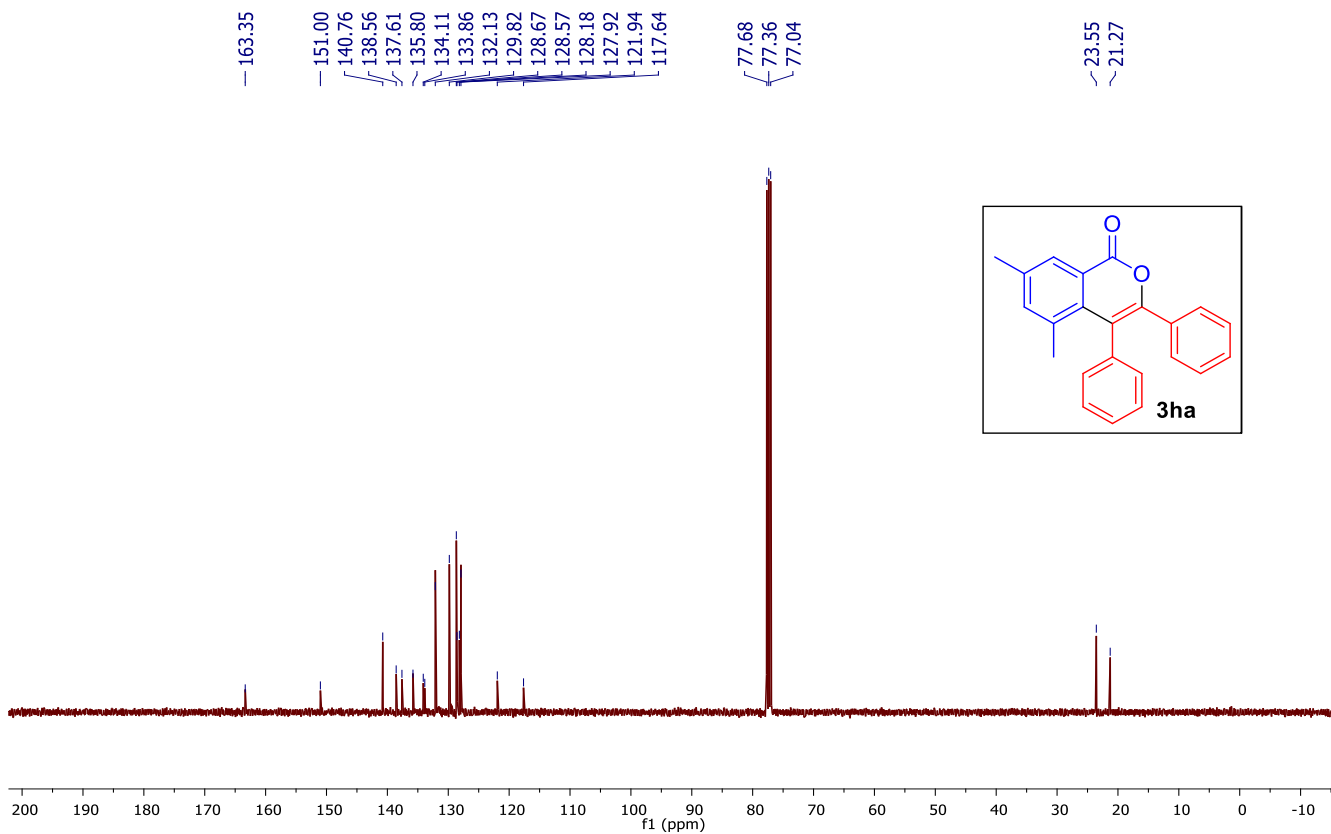
¹³C{¹H} NMR of 3ga (100 MHz, CDCl₃)



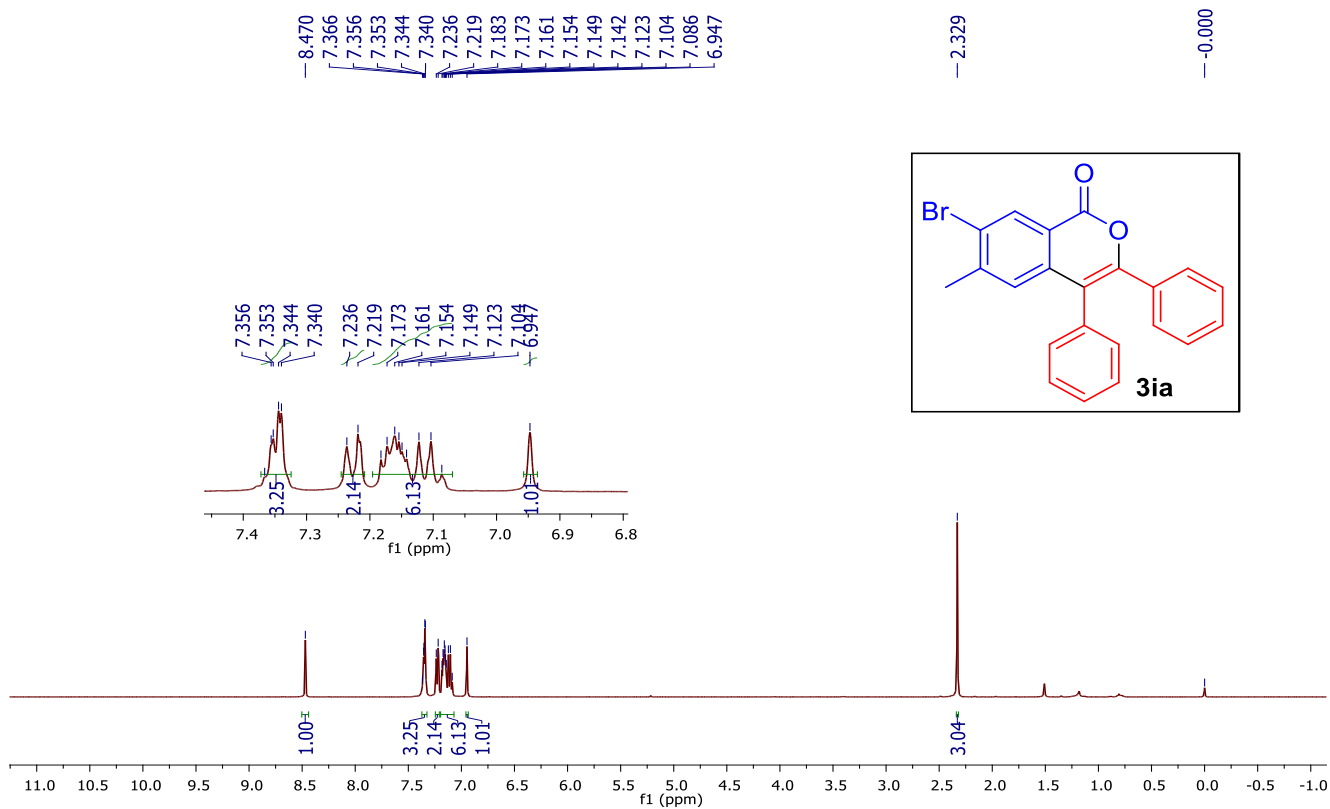
¹H NMR of 3ha (400 MHz, CDCl₃)



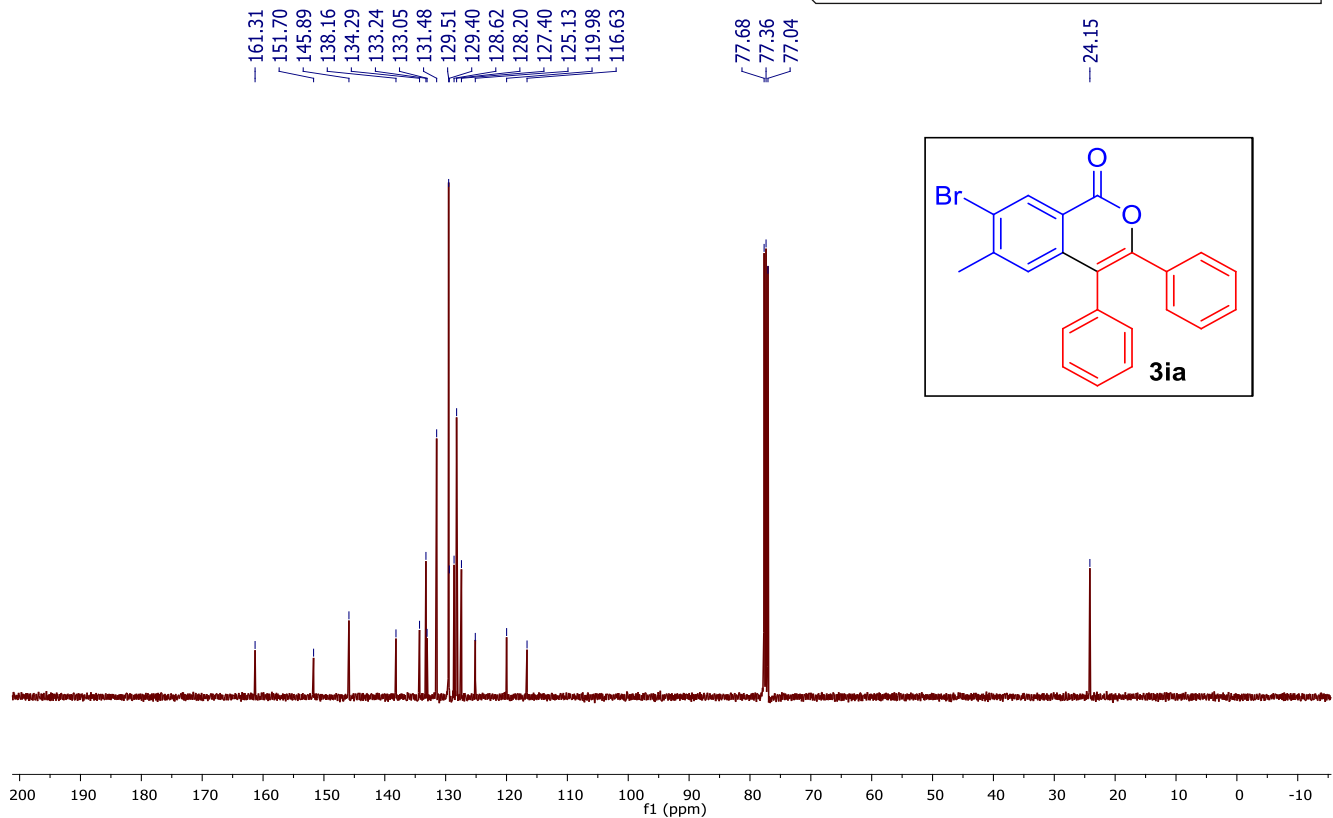
¹³C{¹H} NMR of 3ha (100 MHz, CDCl₃)



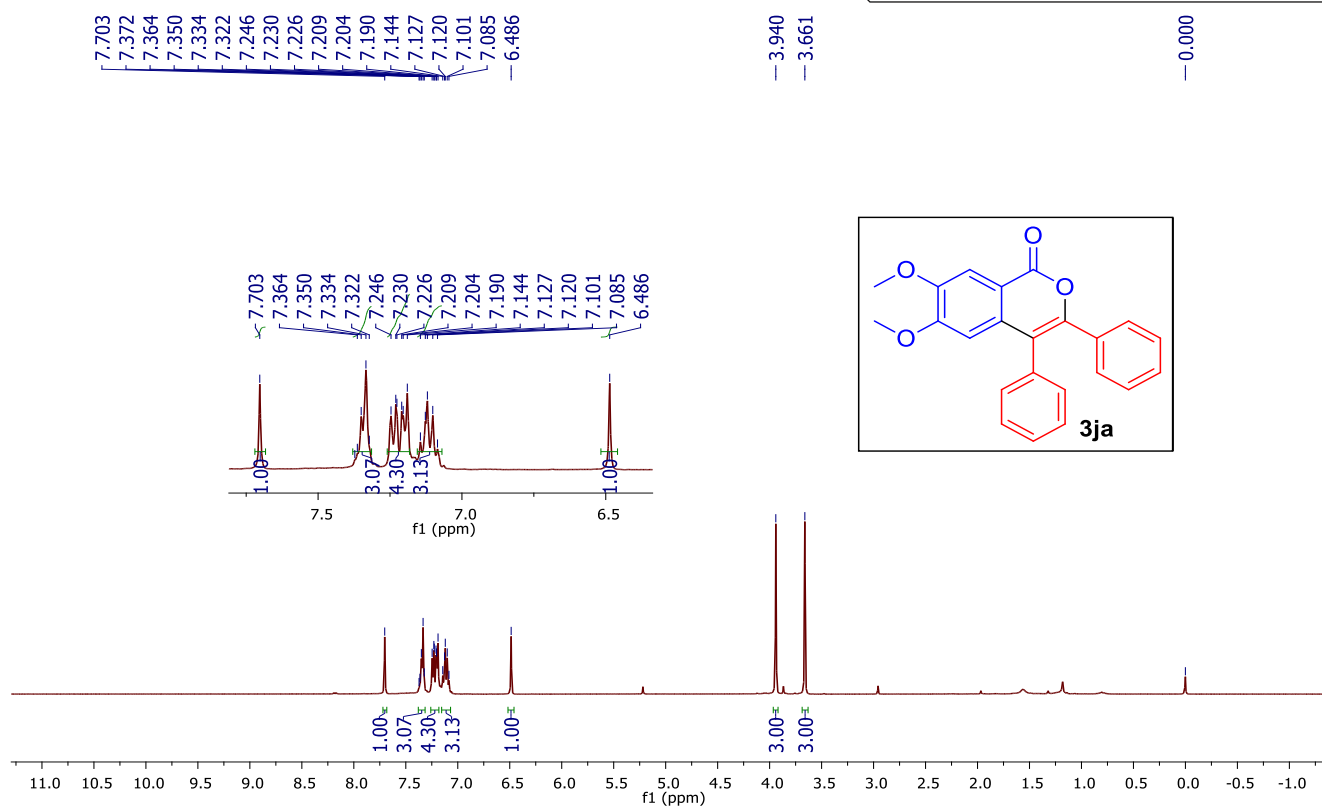
¹H NMR of 3ia (400 MHz, CDCl₃)



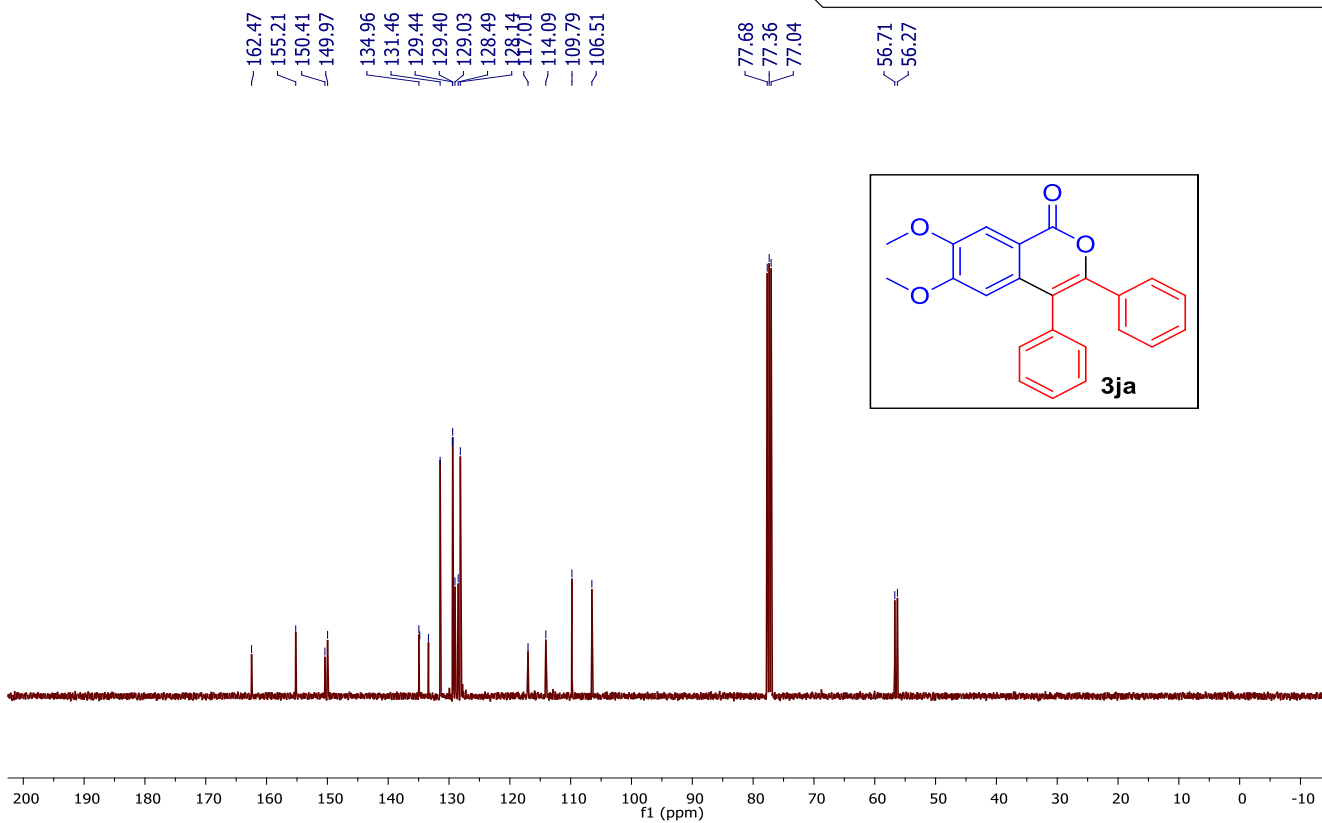
¹³C{¹H} NMR of 3ia (100 MHz, CDCl₃)



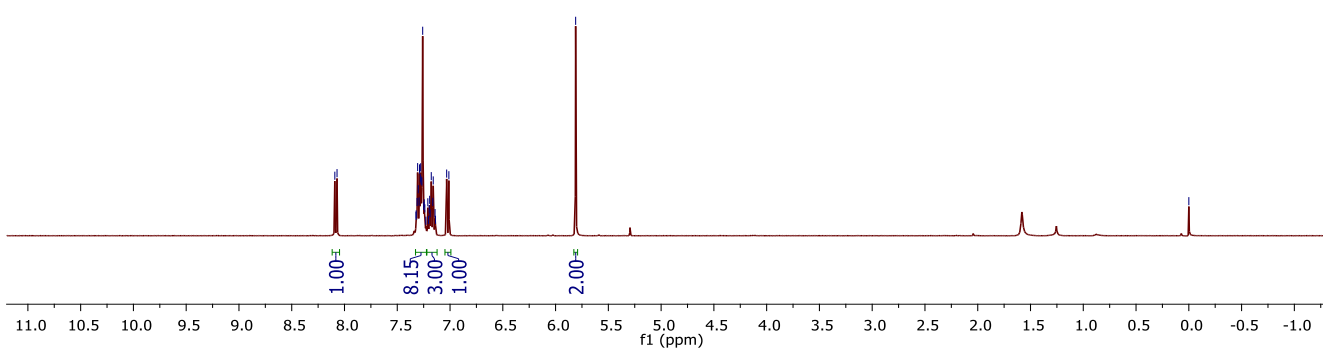
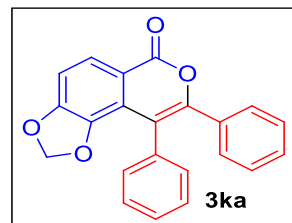
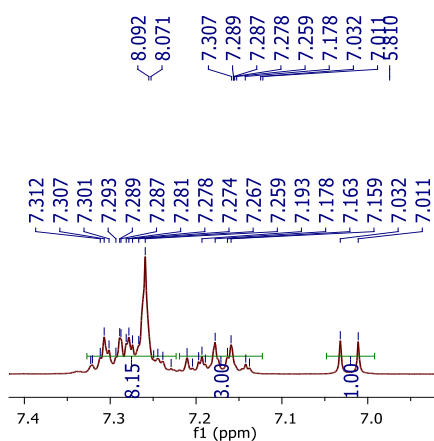
¹H NMR of 3ja (400 MHz, CDCl₃)



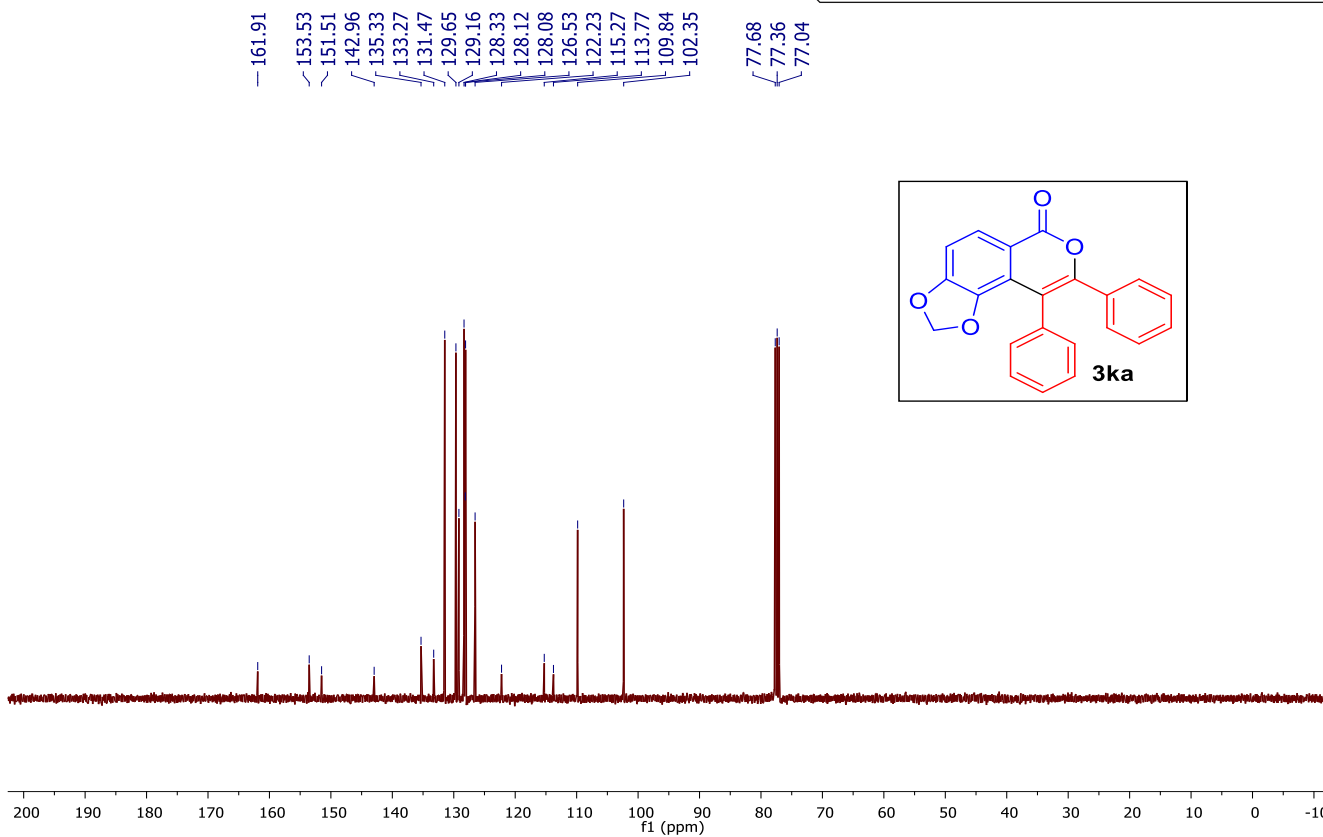
¹³C{¹H} NMR of 3ja (100 MHz, CDCl₃)



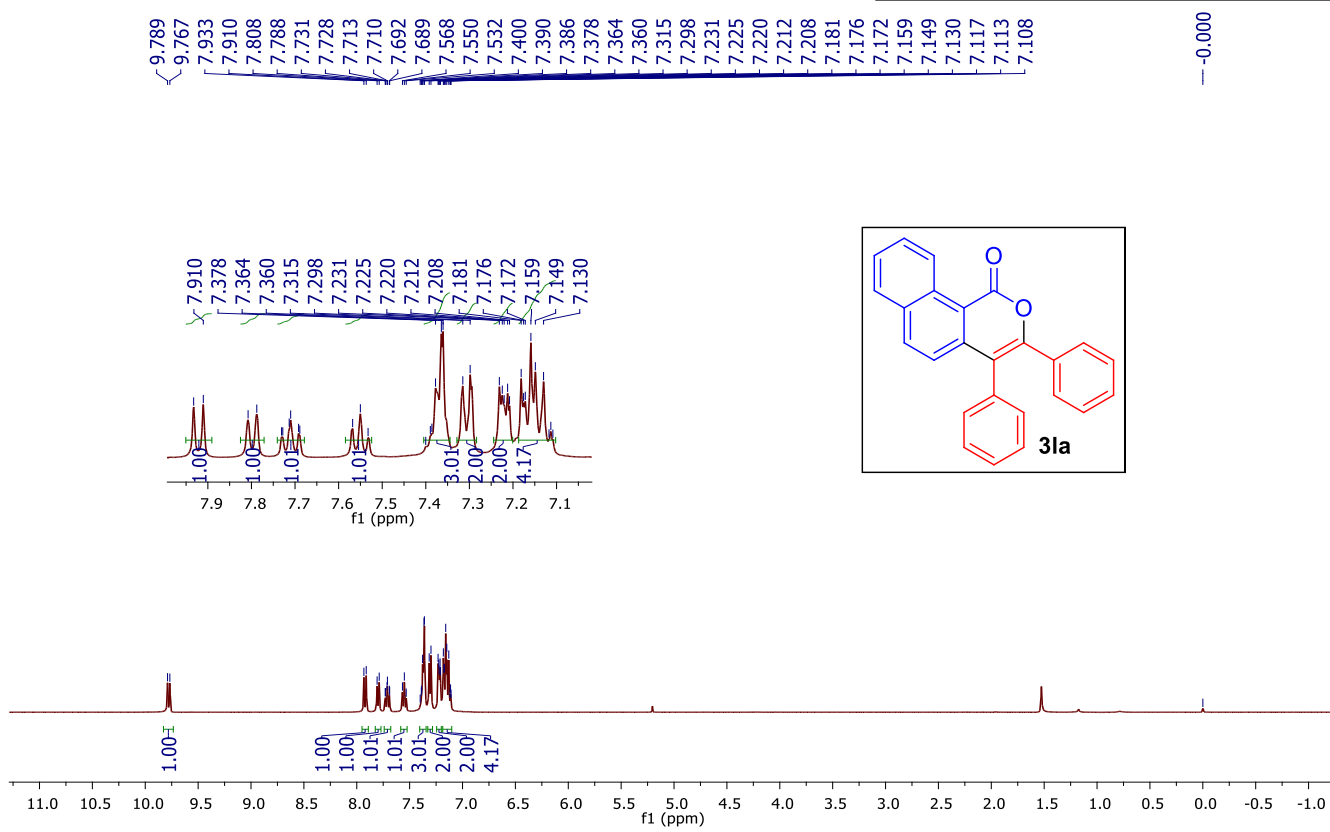
¹H NMR of 3ka (400 MHz, CDCl₃)



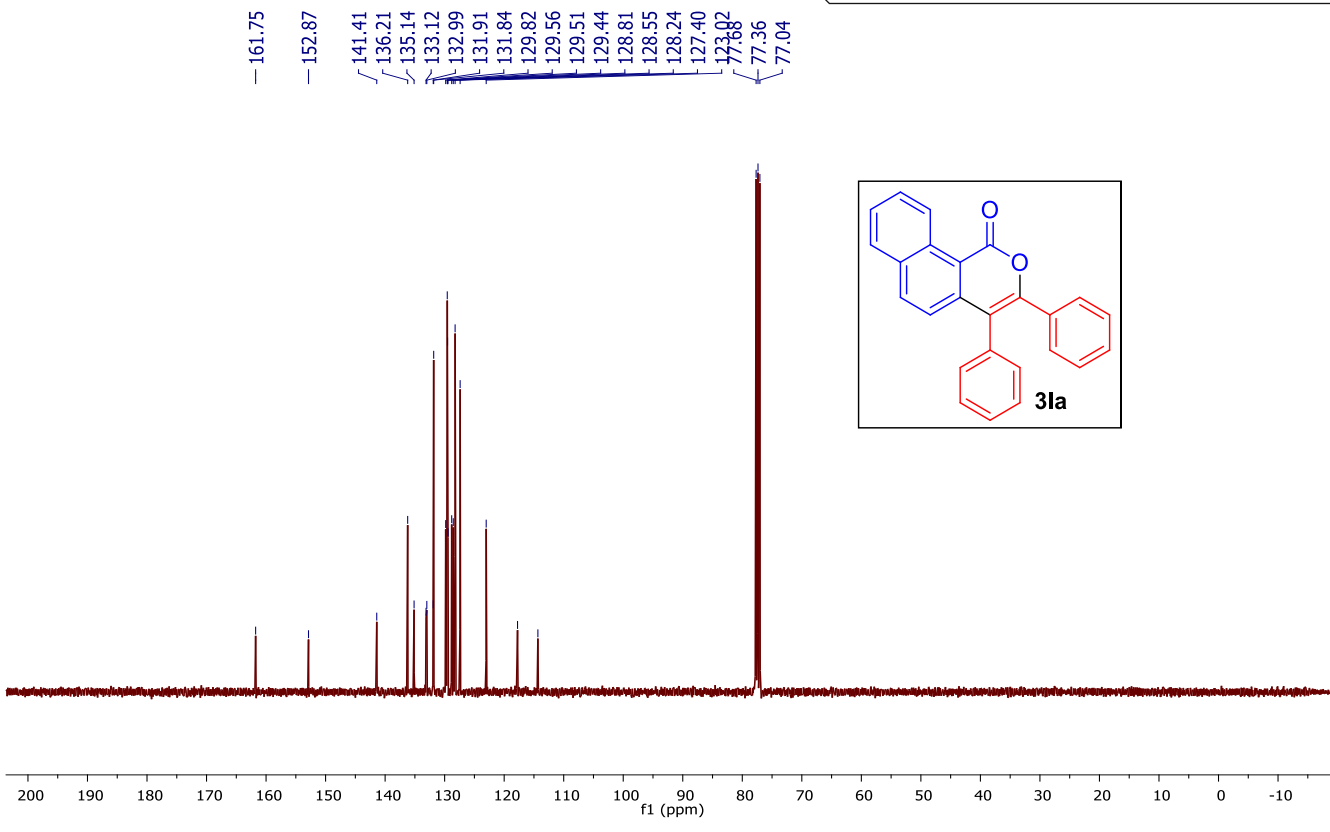
¹³C{¹H} NMR of 3ka (100 MHz, CDCl₃)



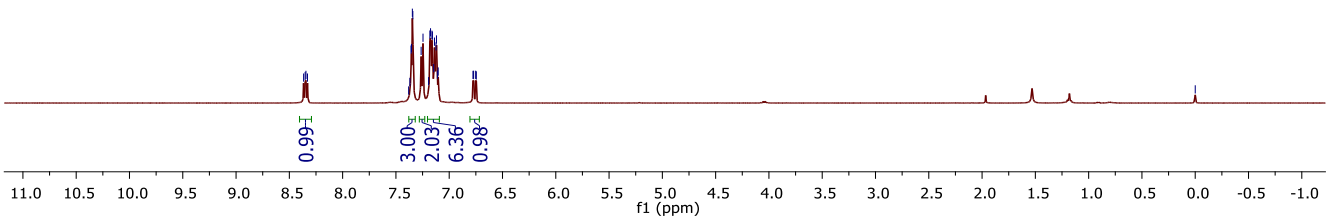
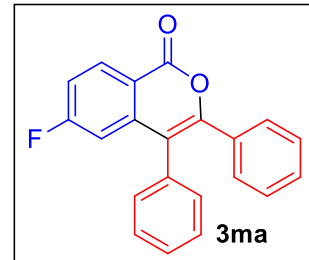
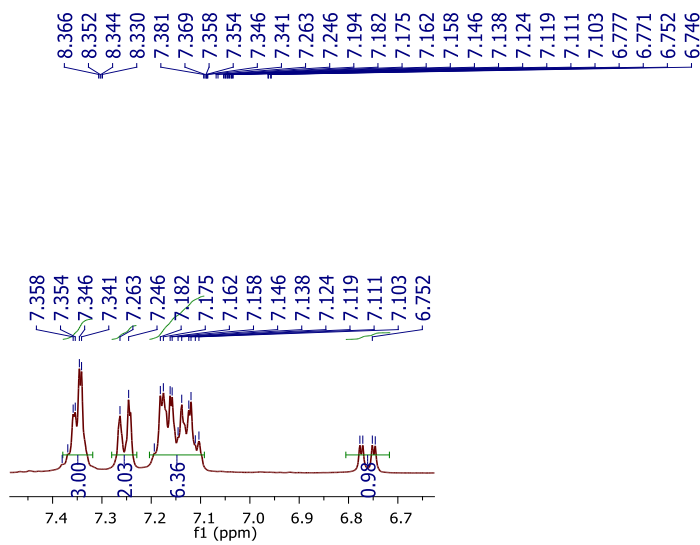
¹H NMR of 3la (400 MHz, CDCl₃)



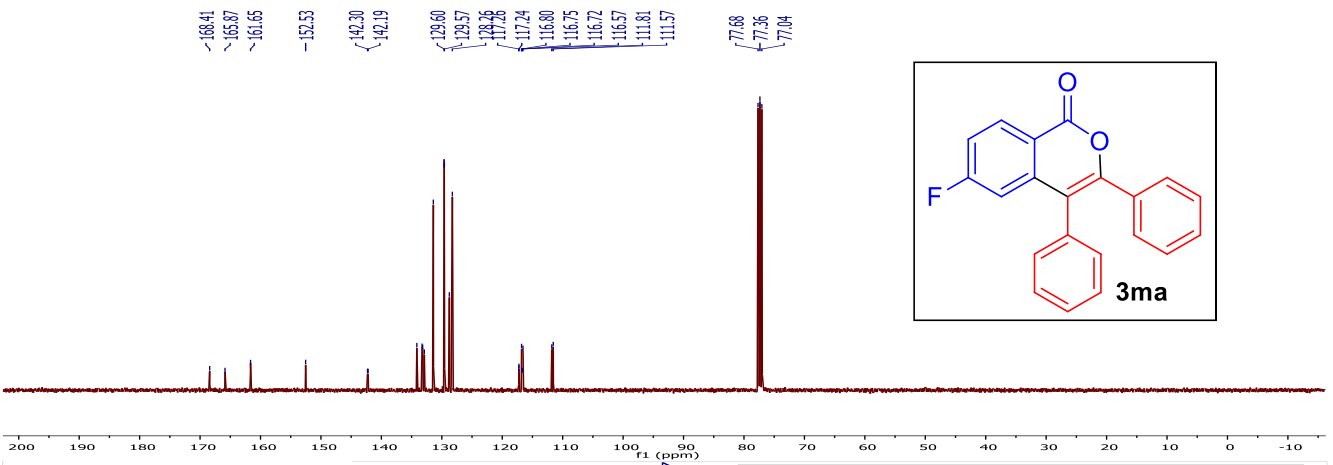
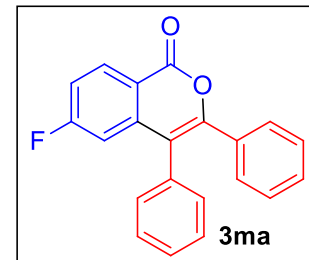
¹³C{¹H} NMR of 3la (100 MHz, CDCl₃)



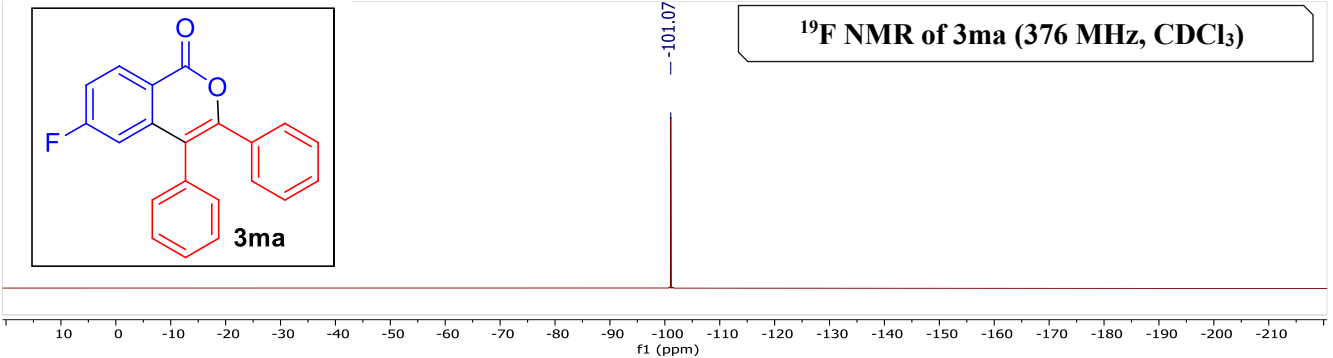
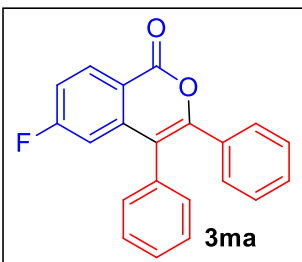
¹H NMR of 3ma (400 MHz, CDCl₃)



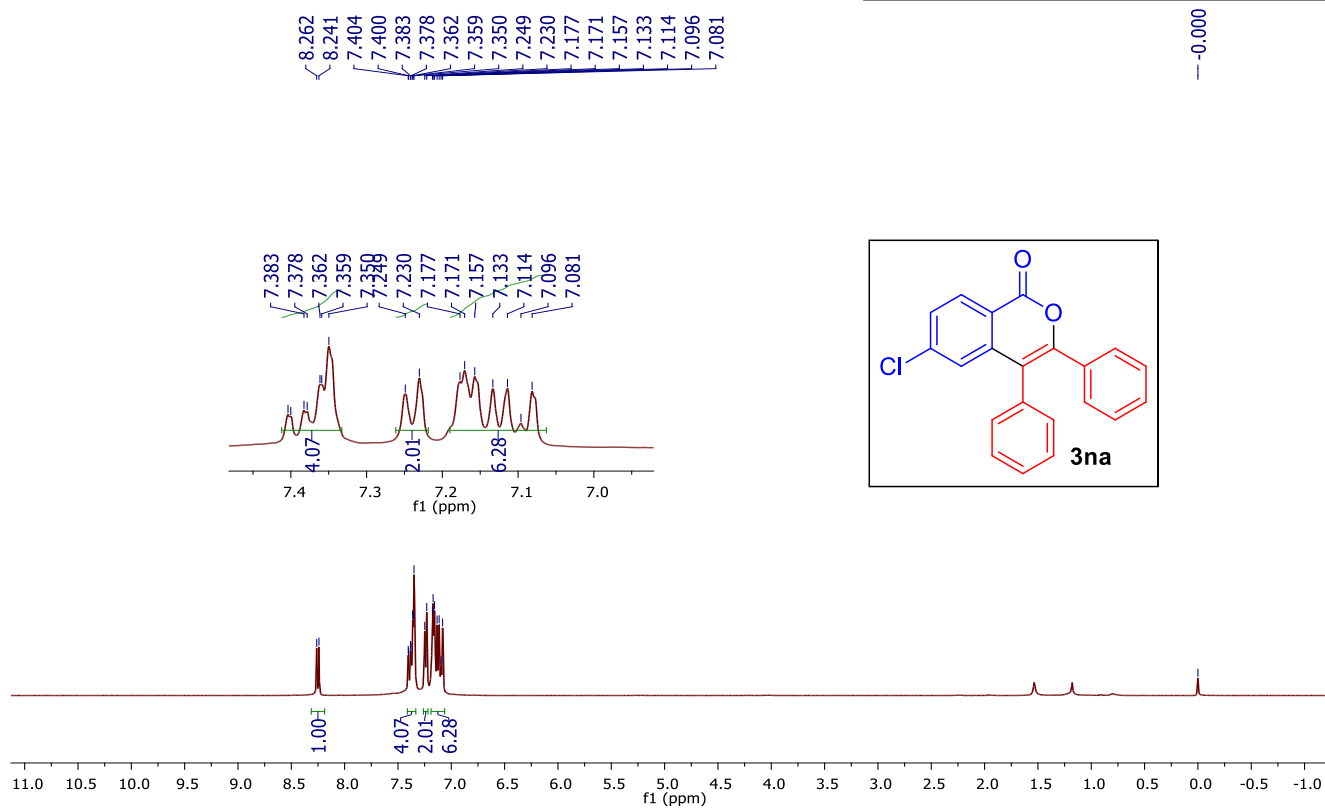
¹³C {¹H} NMR of 3ma (100 MHz, CDCl₃)



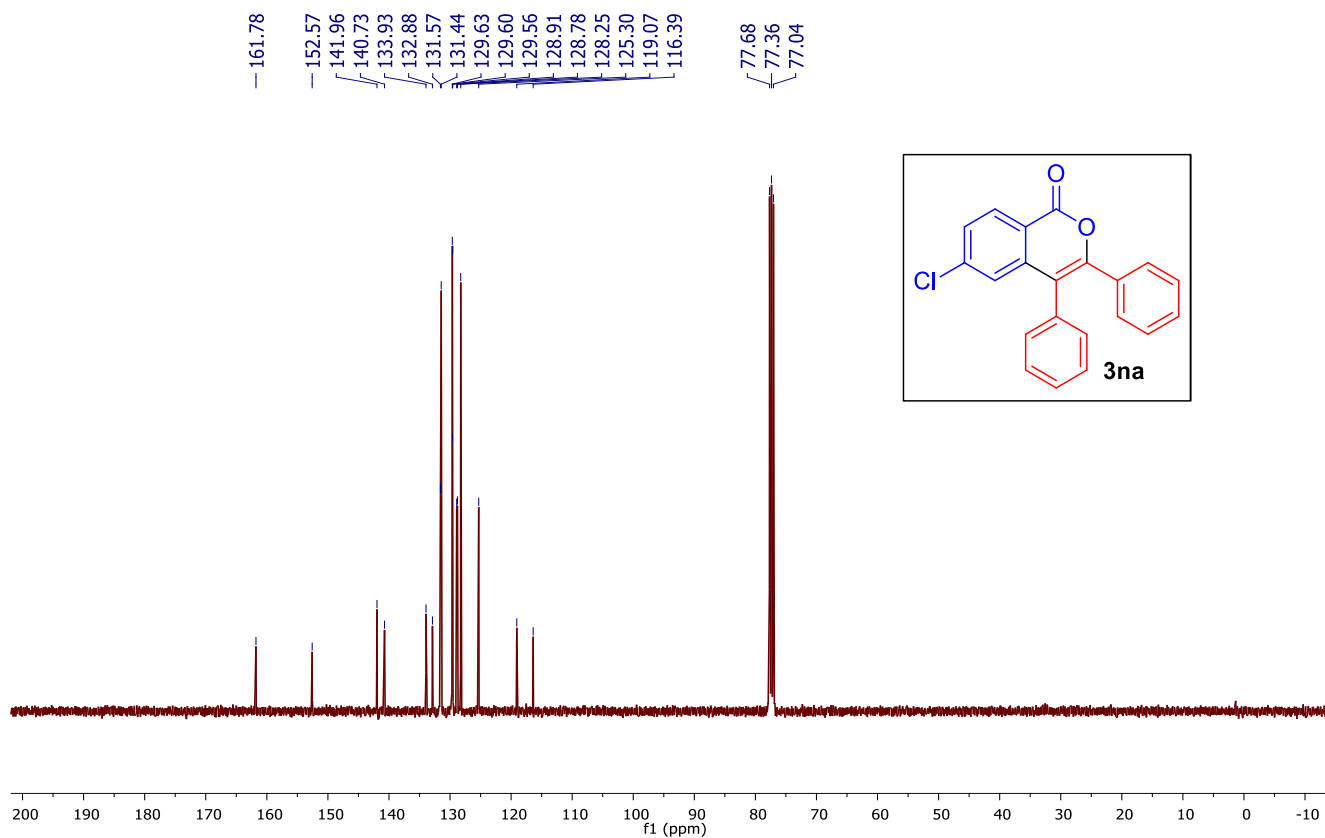
¹⁹F NMR of 3ma (376 MHz, CDCl₃)



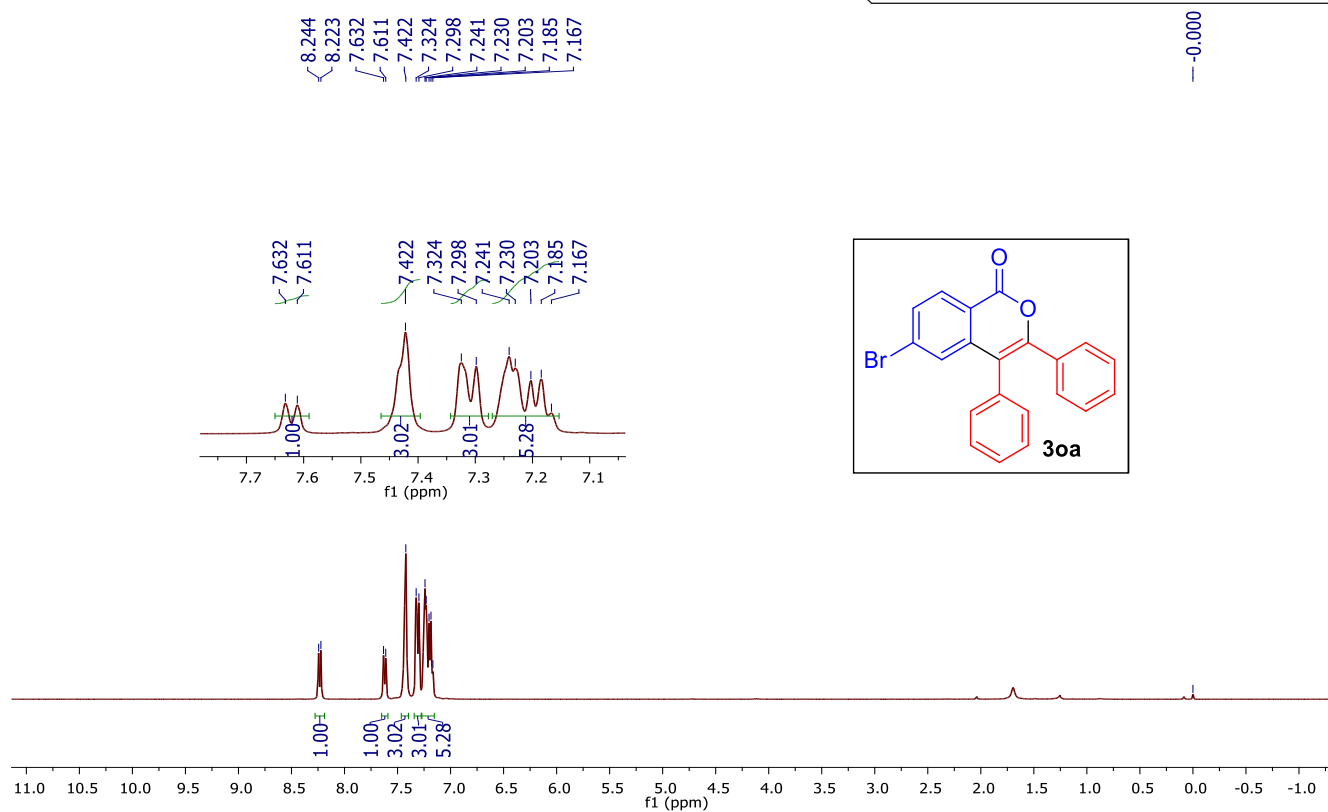
¹H NMR of 3na (400 MHz, CDCl₃)



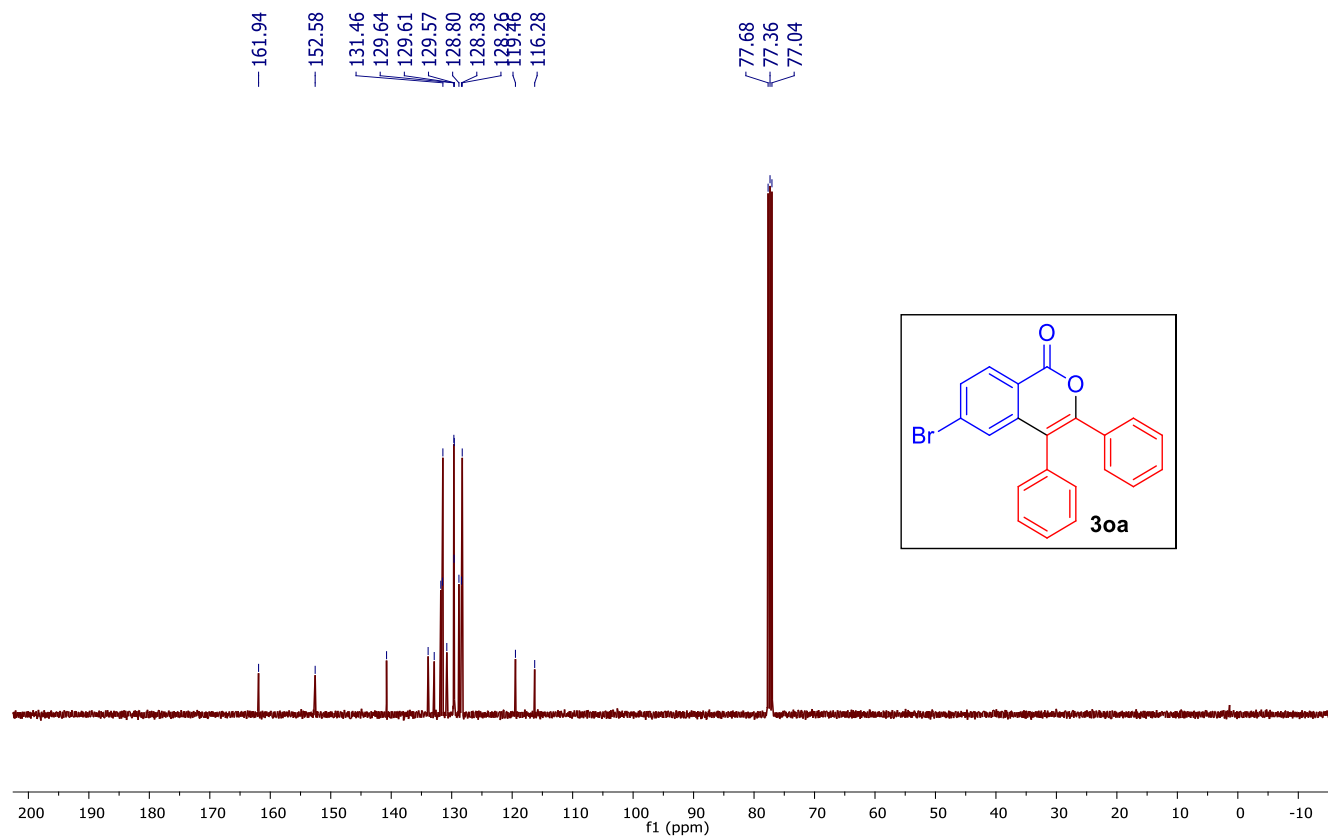
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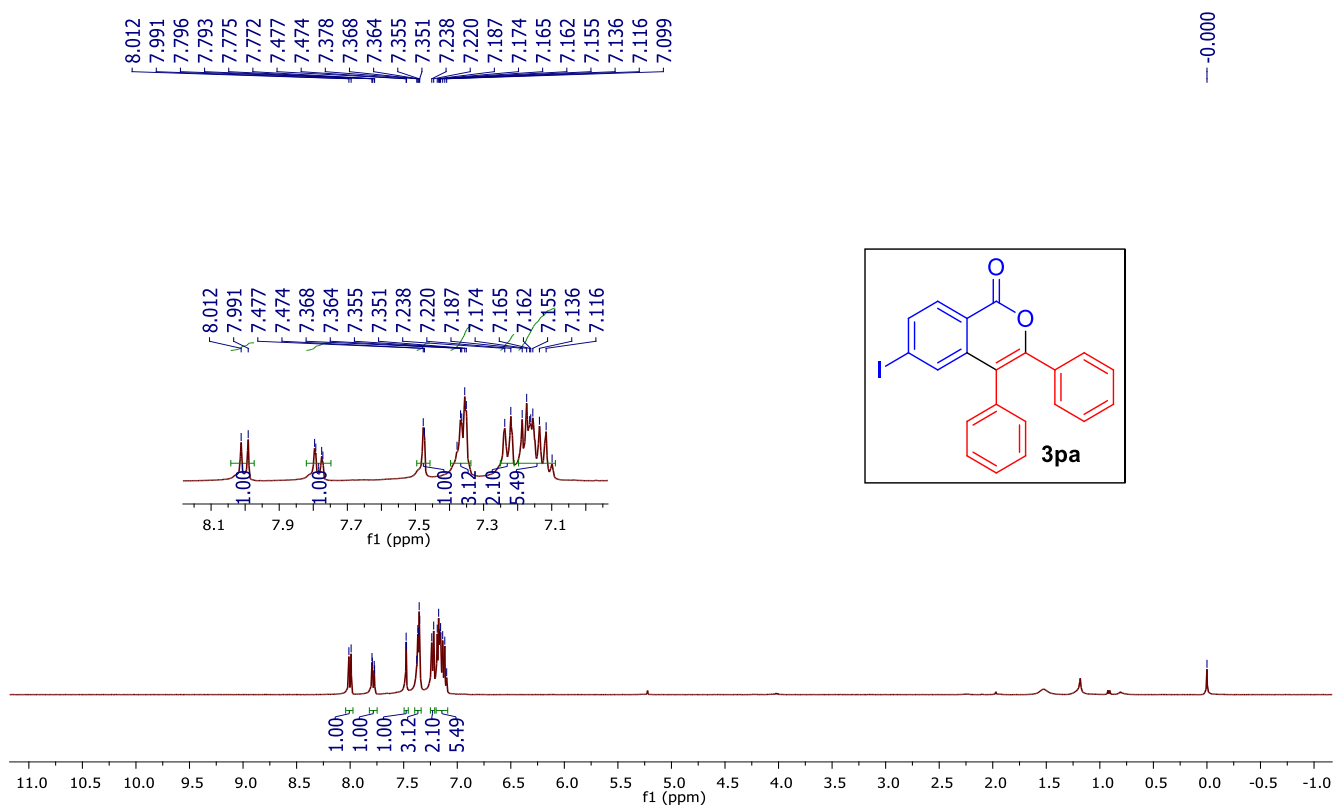
¹H NMR of 3oa (400 MHz, CDCl₃)



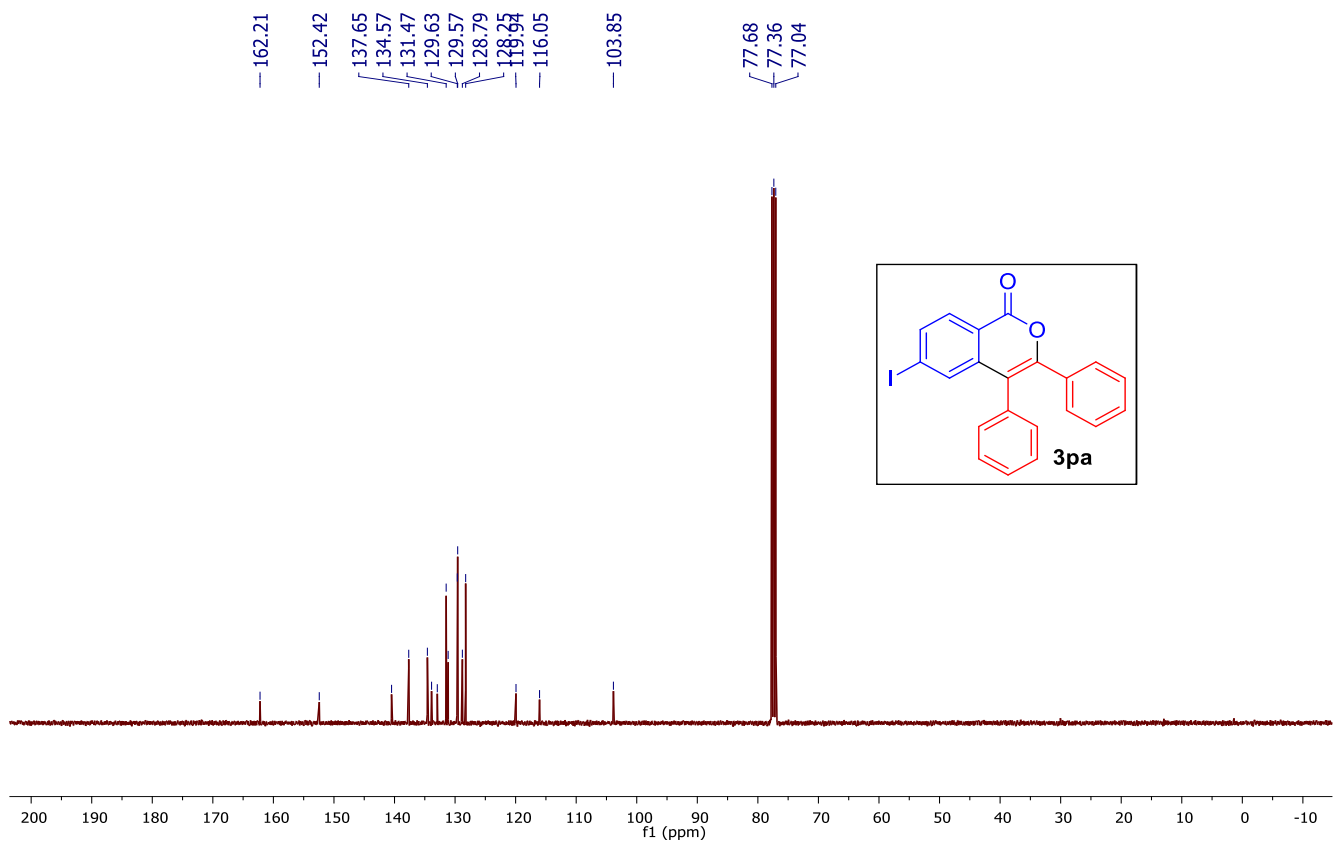
¹³C{¹H} NMR of 3oa (100 MHz, CDCl₃)



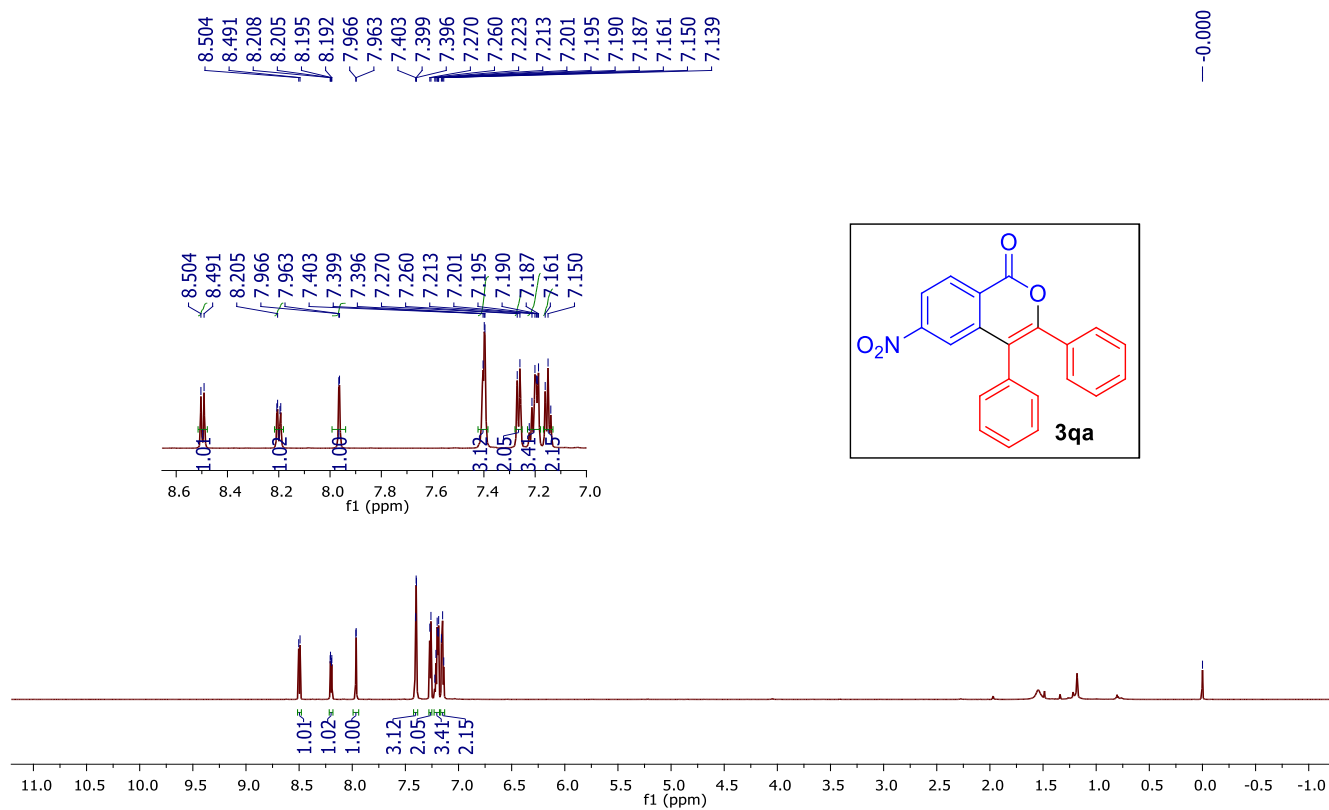
¹H NMR of 3pa (400 MHz, CDCl₃)



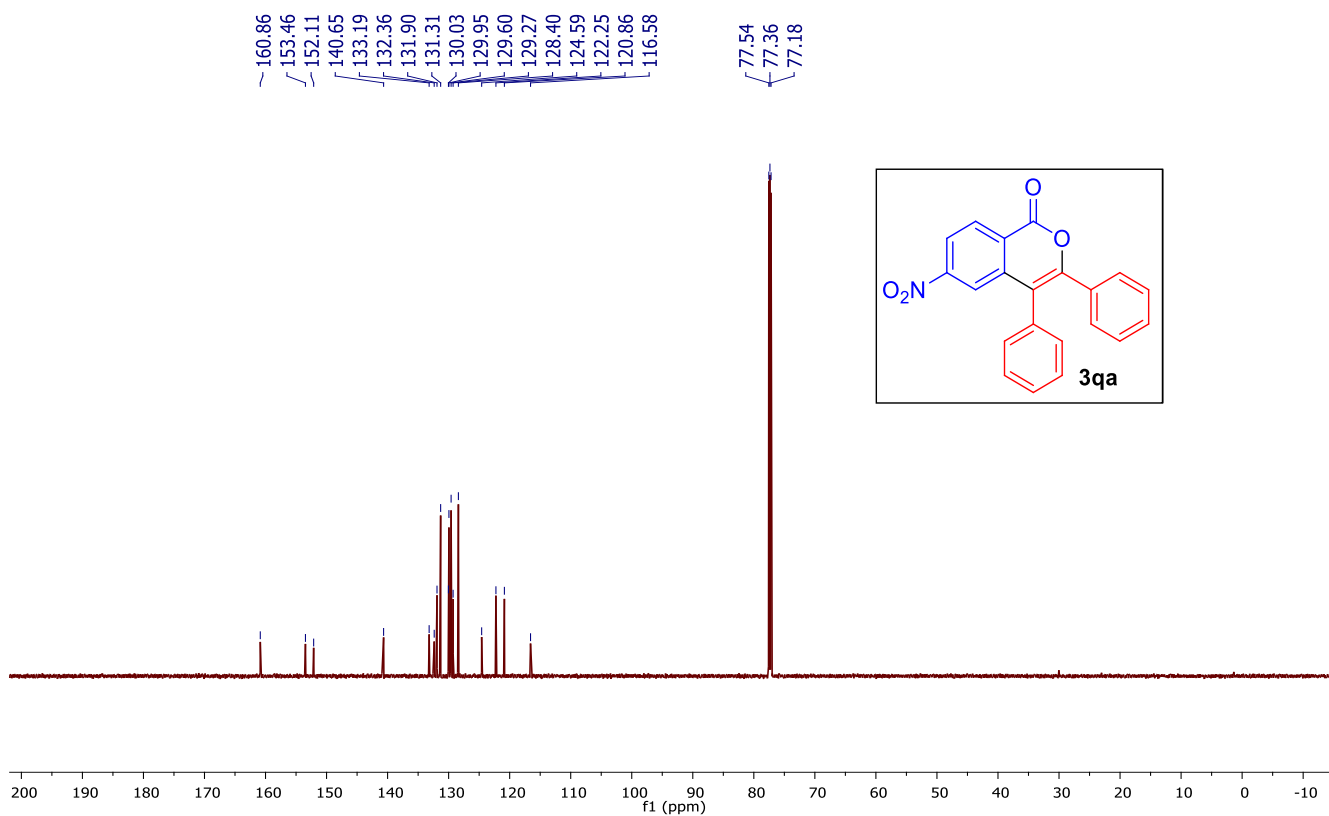
¹³C{¹H} NMR of 3pa (100 MHz, CDCl₃)



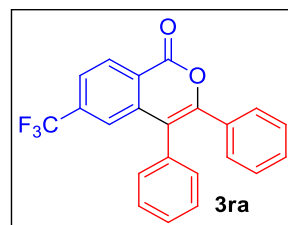
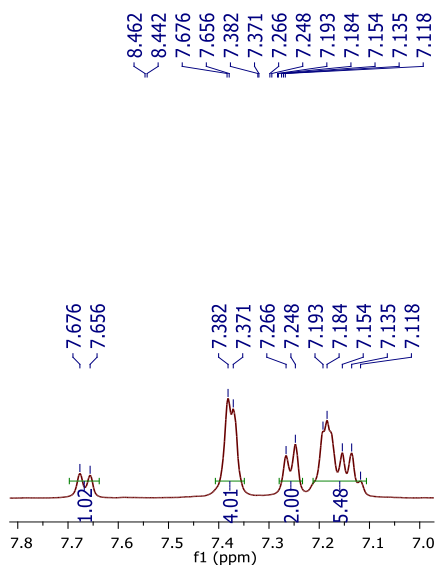
¹H NMR of 3qa (700 MHz, CDCl₃)



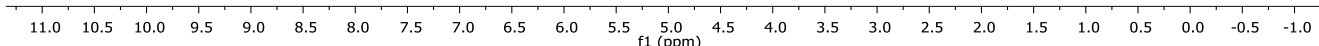
¹³C{¹H} NMR of 3qa (176 MHz, CDCl₃)



¹H NMR of 3ra (400 MHz, CDCl₃)

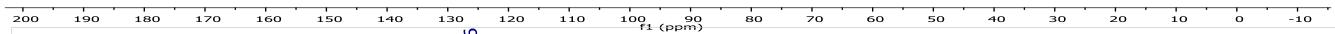
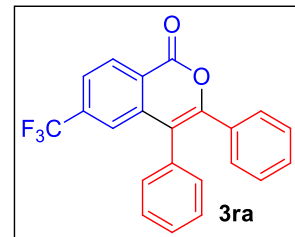


0.000



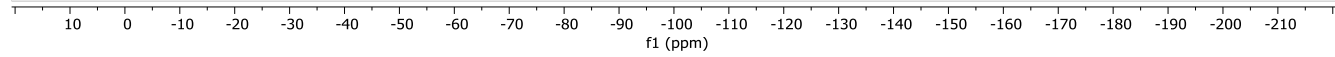
¹³C{¹H} NMR of 3ra (100 MHz, CDCl₃)

161.45, 152.75, 139.72, 133.62, 132.72, 131.41, 130.92, 129.75, 128.99, 128.33, 124.66, 124.63, 124.59, 123.13, 122.71, 122.67, 116.71, 116.81, 77.36, 77.04

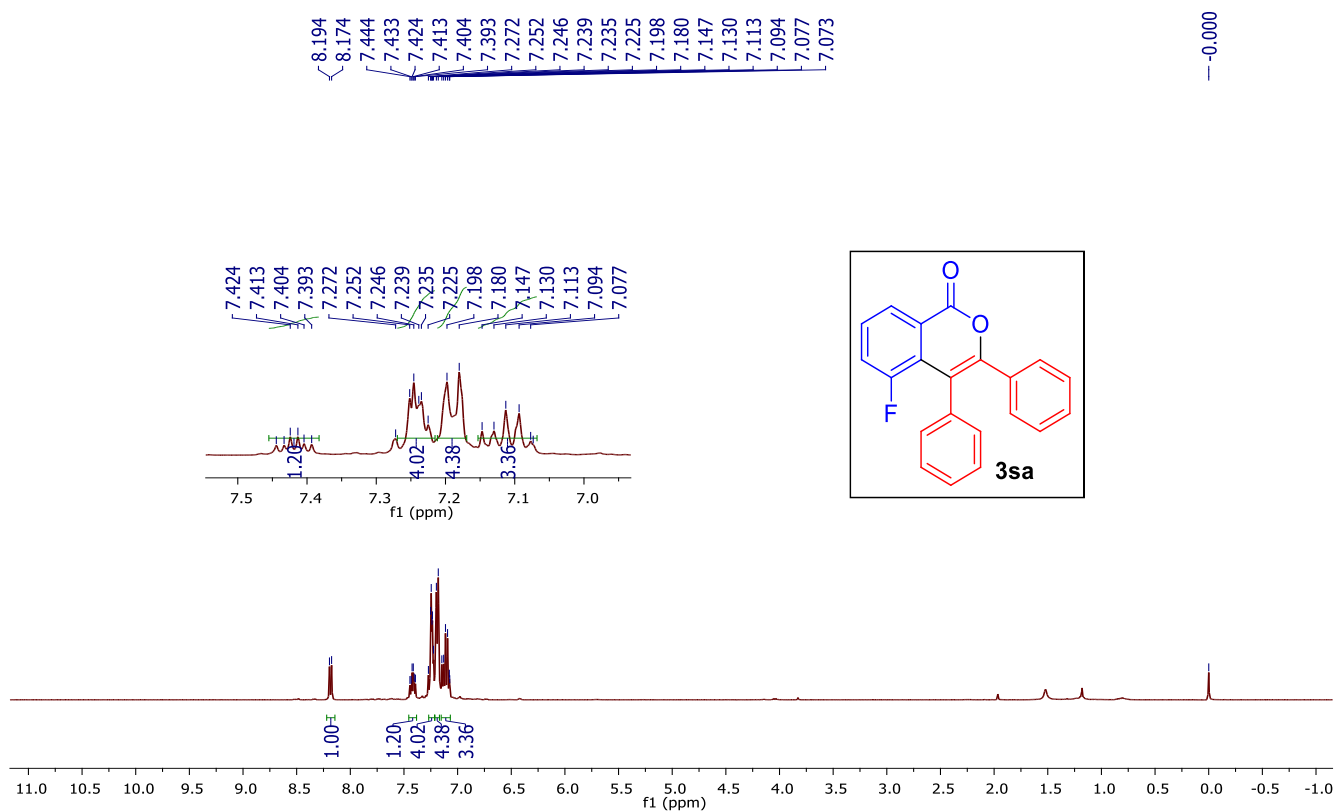


¹⁹F NMR of 3ra (376 MHz, CDCl₃)

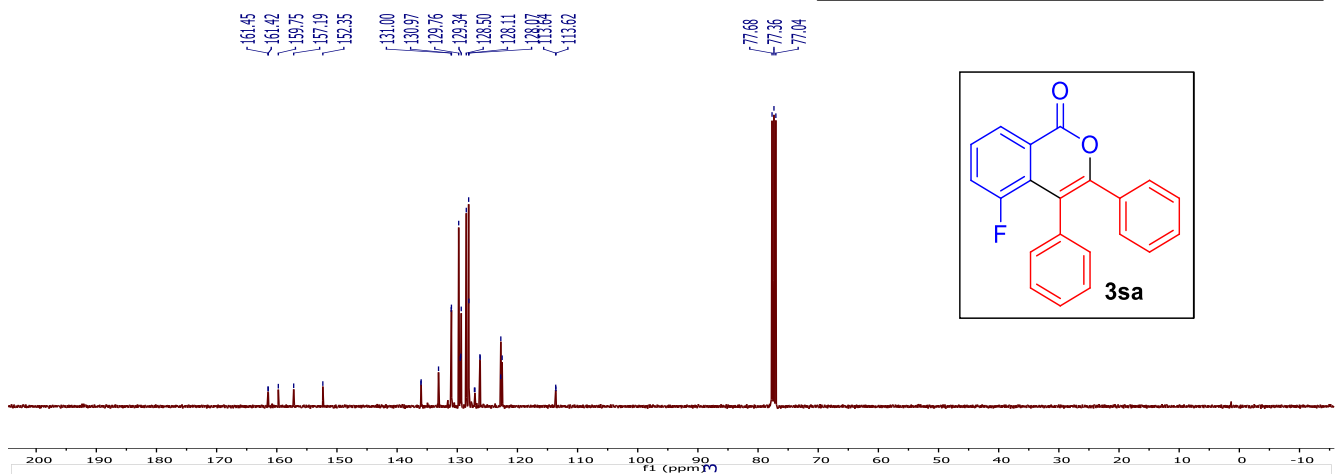
-63.36



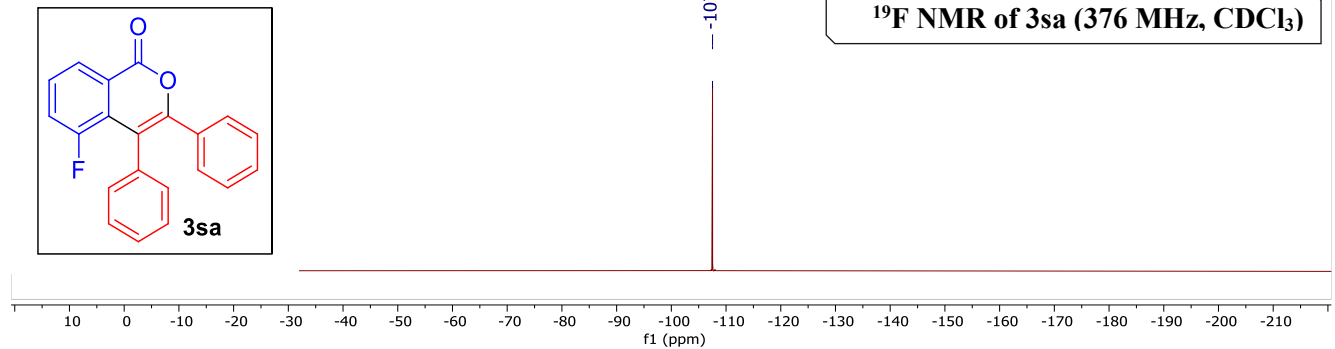
¹H NMR of 3sa (400 MHz, CDCl₃)



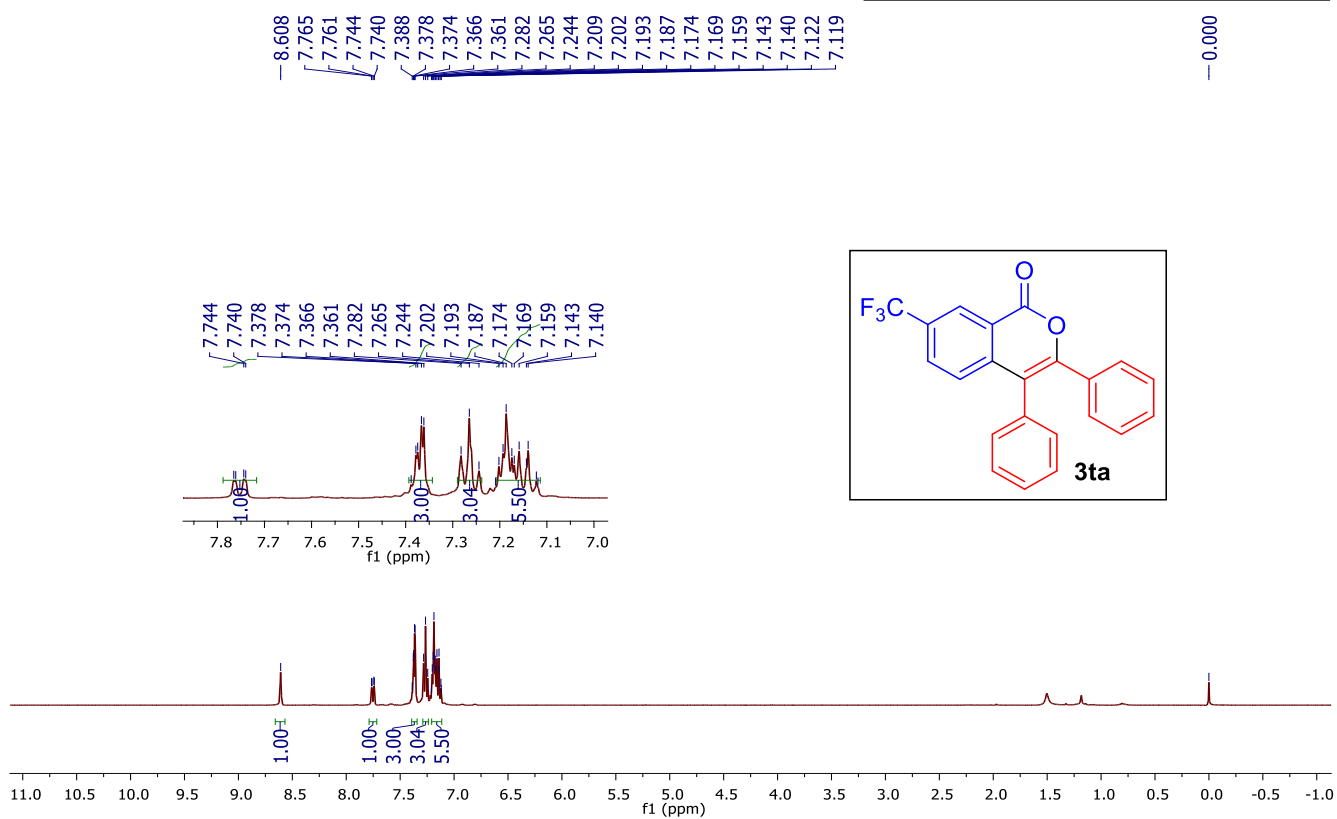
¹³C{¹H} NMR of 3sa (100 MHz, CDCl₃)



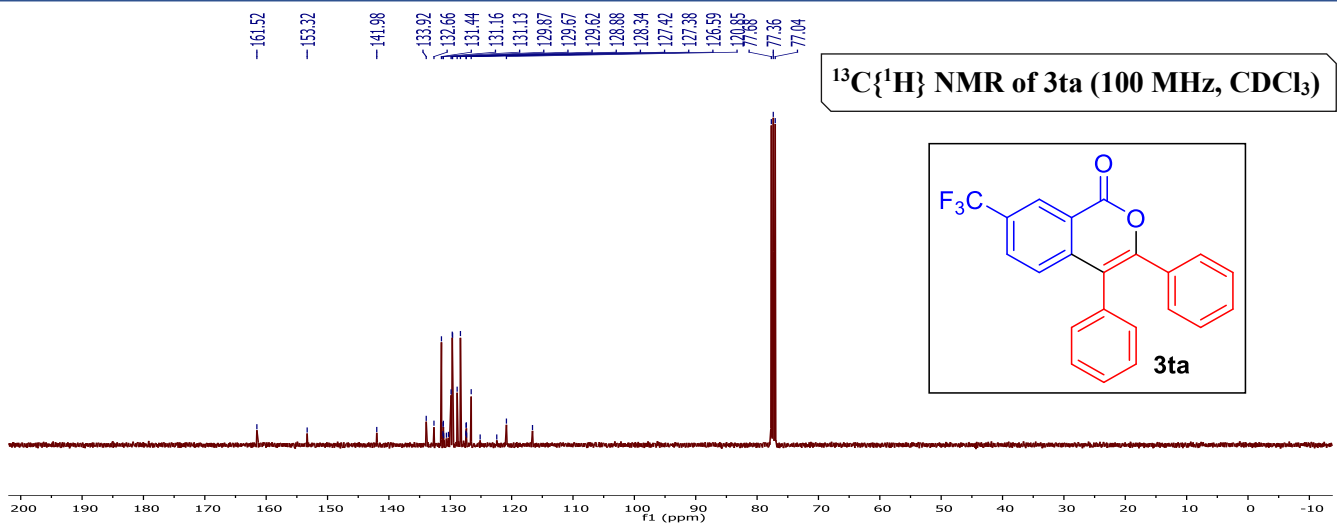
¹⁹F NMR of 3sa (376 MHz, CDCl₃)



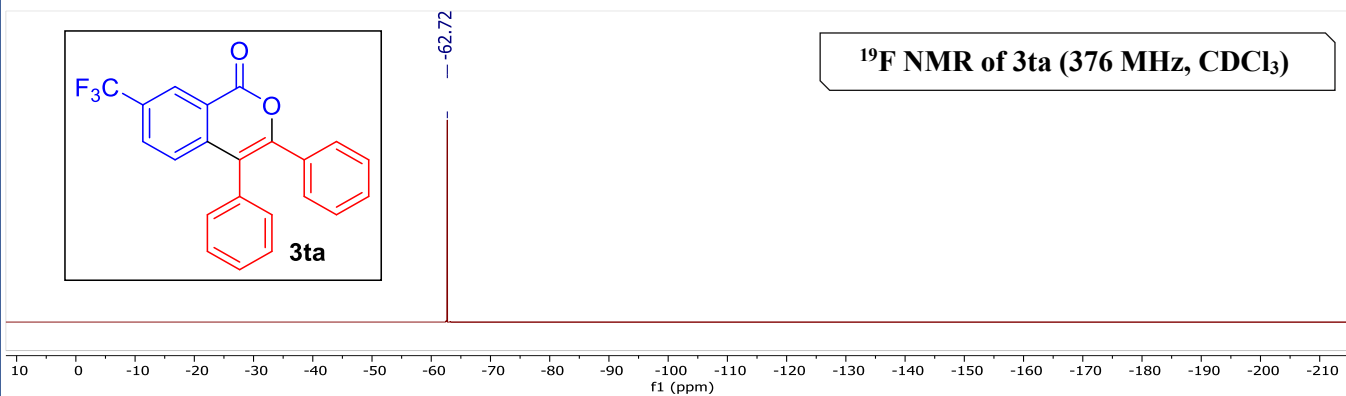
¹H NMR of 3ta (400 MHz, CDCl₃)



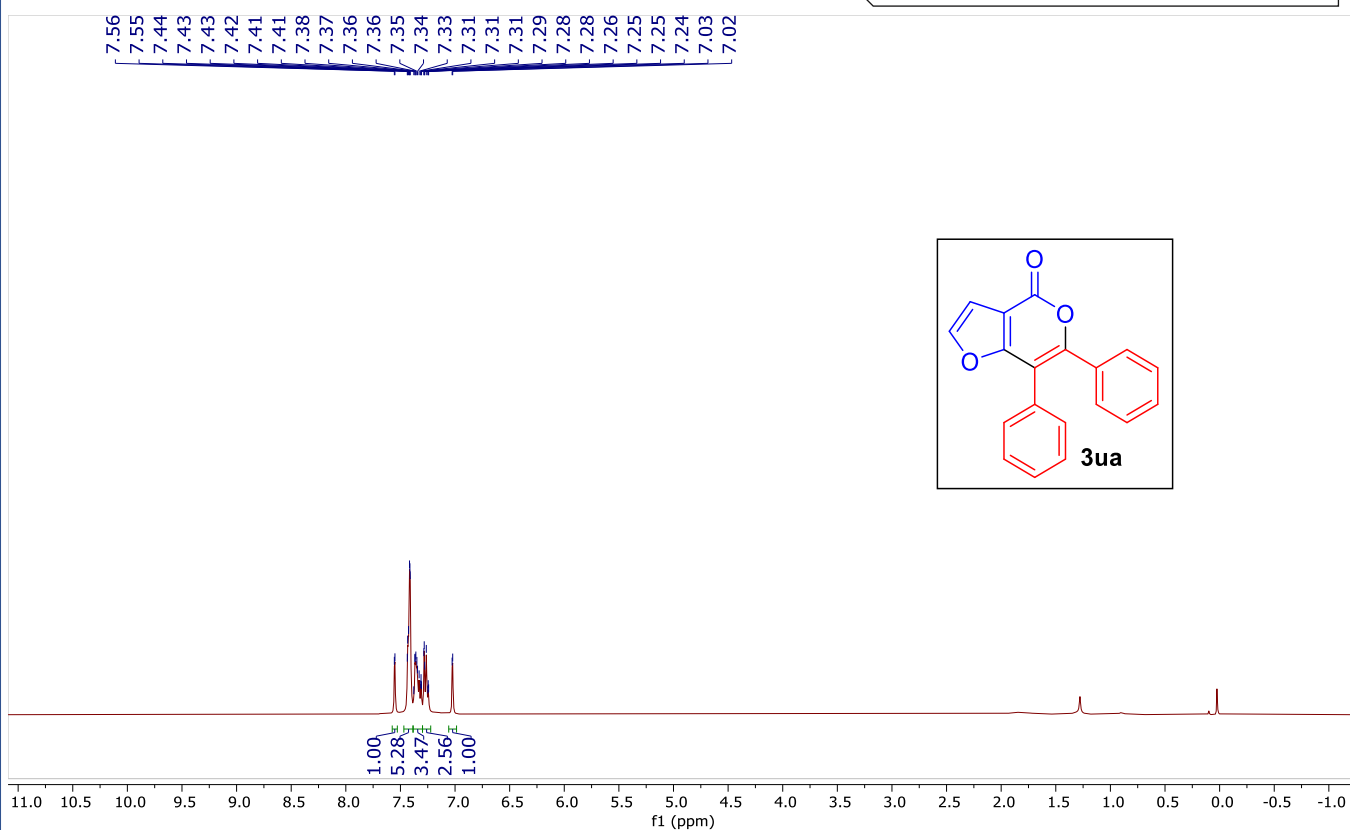
¹³C{¹H} NMR of 3ta (100 MHz, CDCl₃)



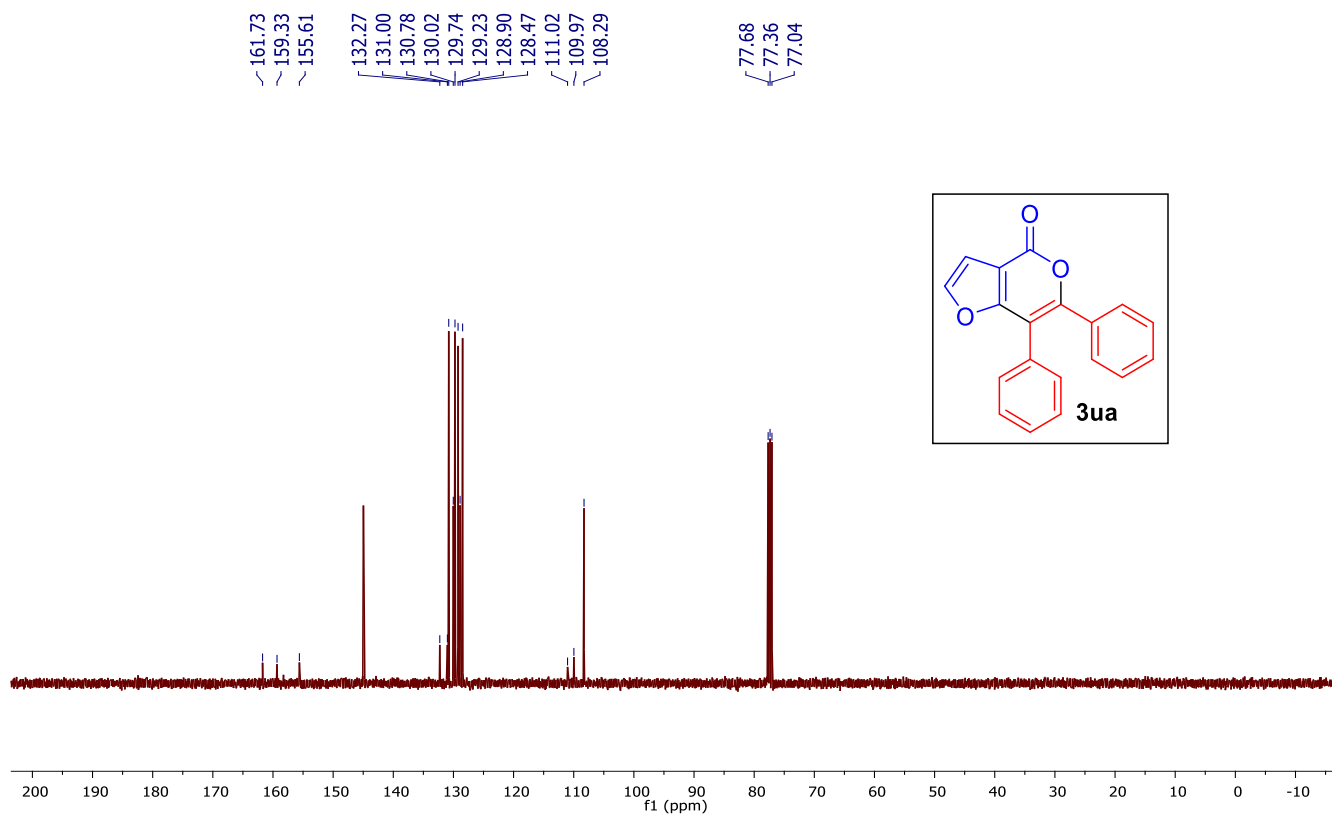
¹⁹F NMR of 3ta (376 MHz, CDCl₃)



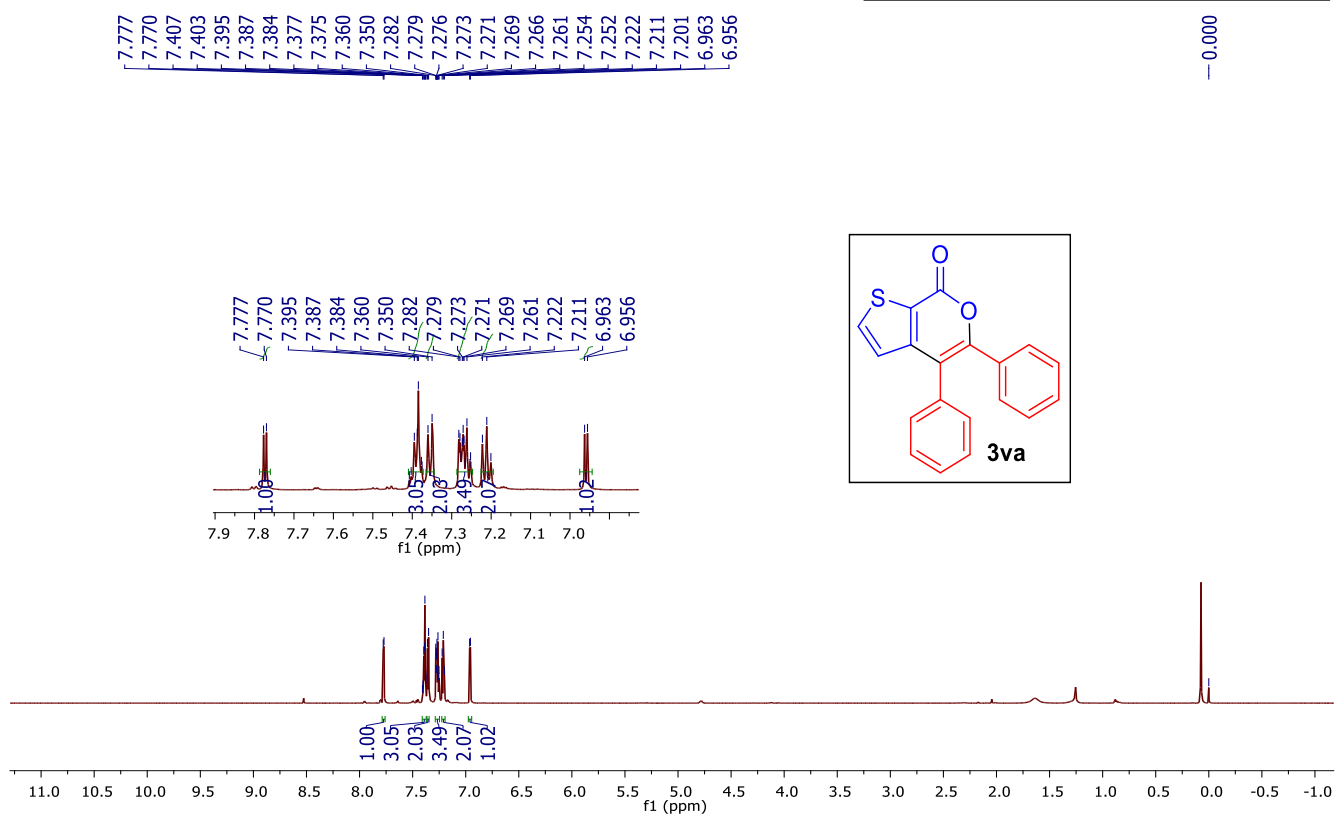
¹H NMR of 3ua (400 MHz, CDCl₃)



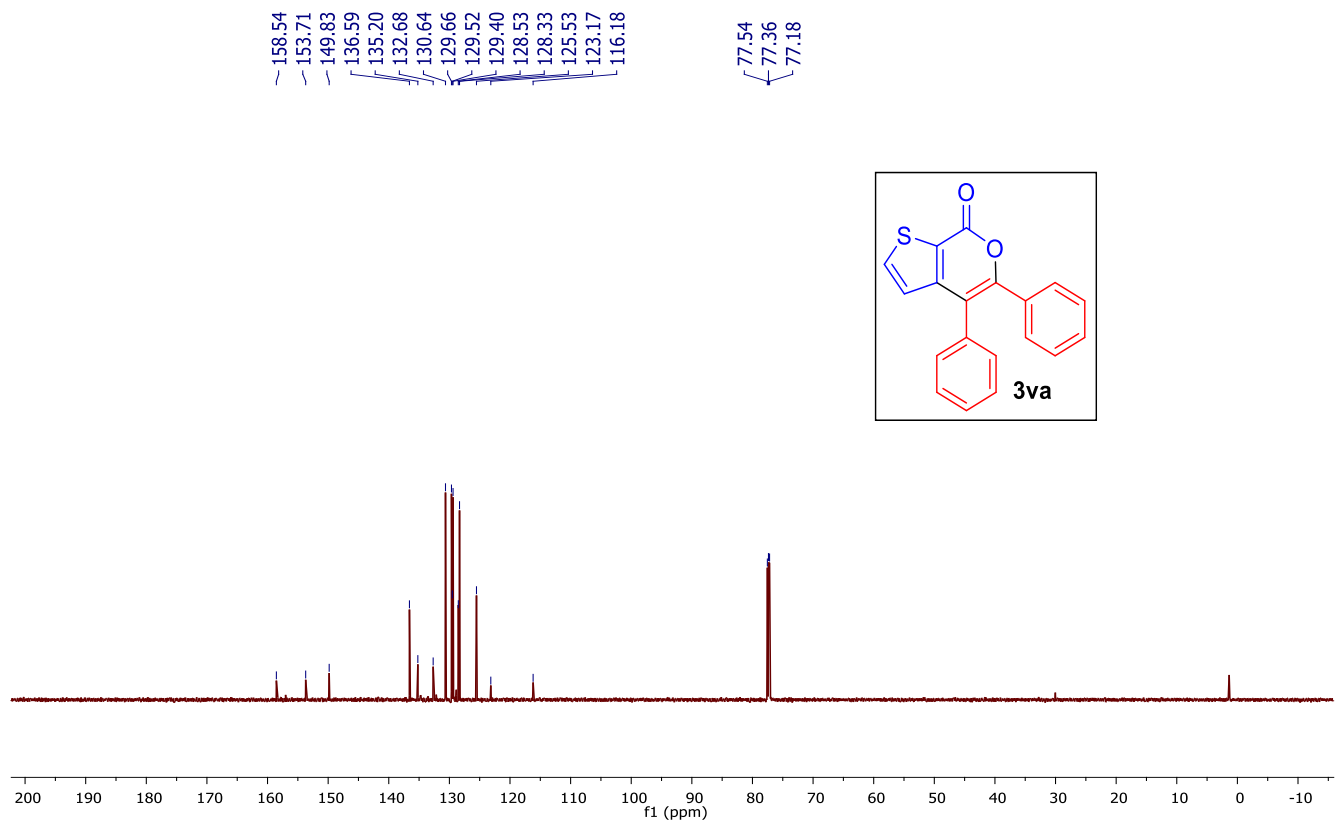
¹³C{¹H} NMR of 3ua (100 MHz, CDCl₃)



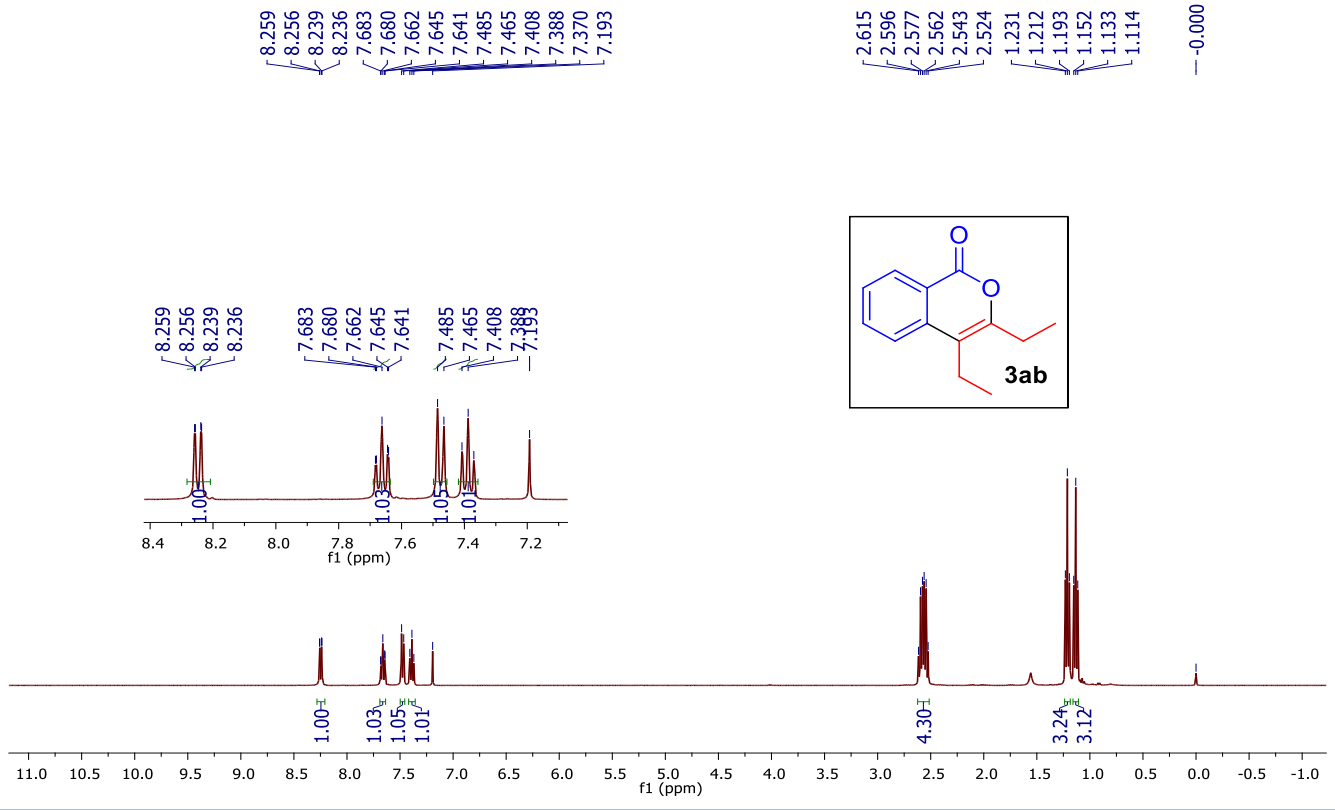
¹H NMR of 3va (700 MHz, CDCl₃)



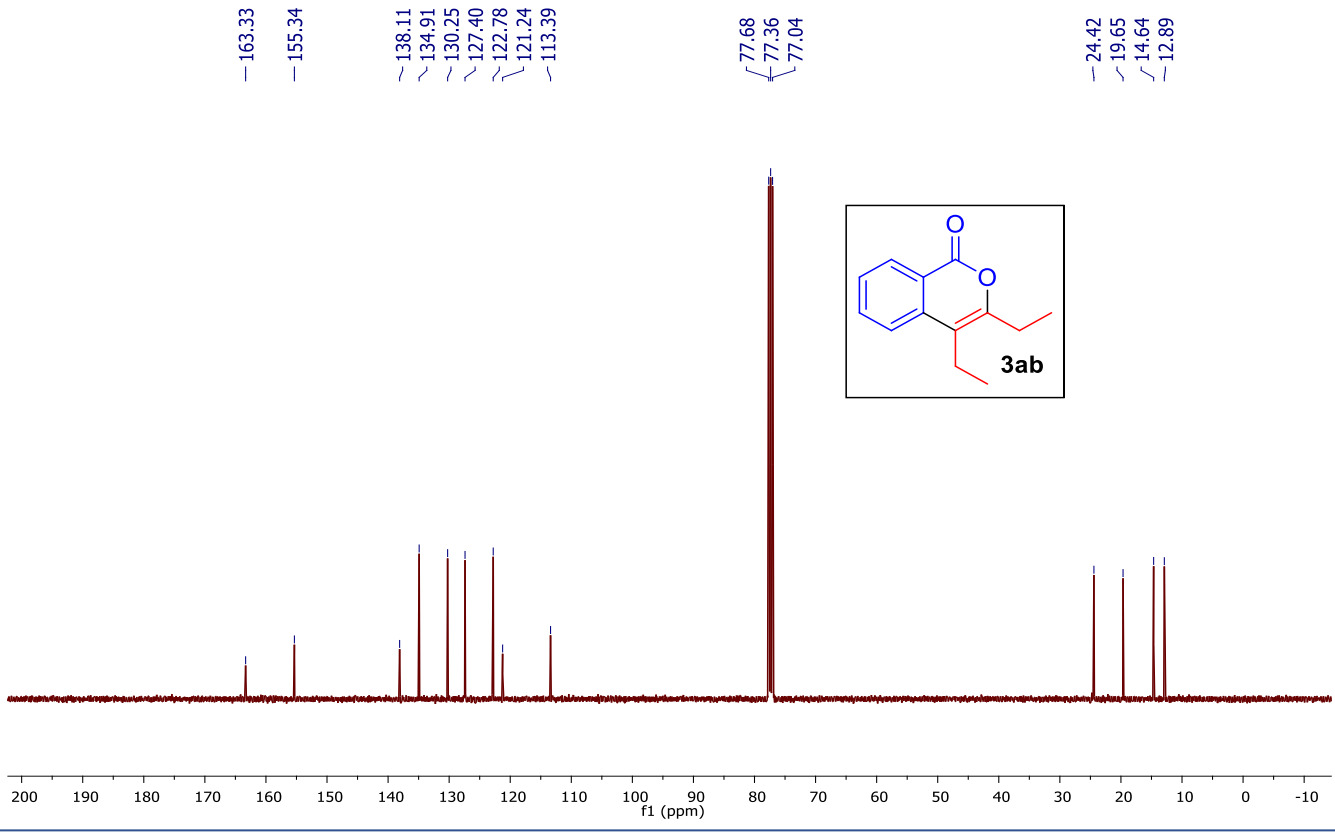
¹³C{¹H} NMR of 3va (176 MHz, CDCl₃)



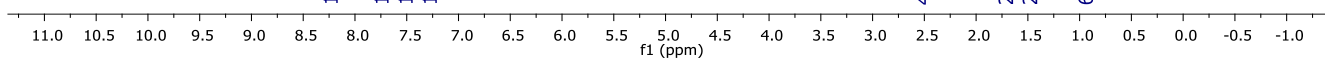
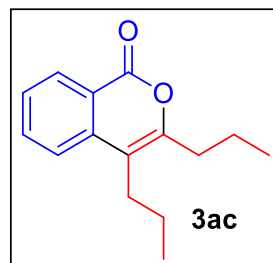
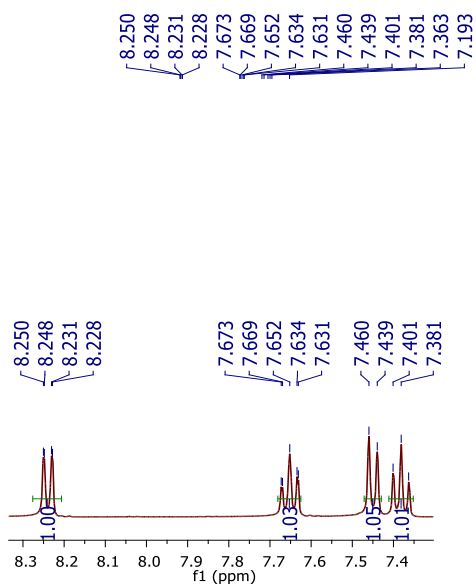
¹H NMR of 3ab (400 MHz, CDCl₃)



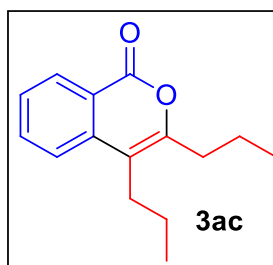
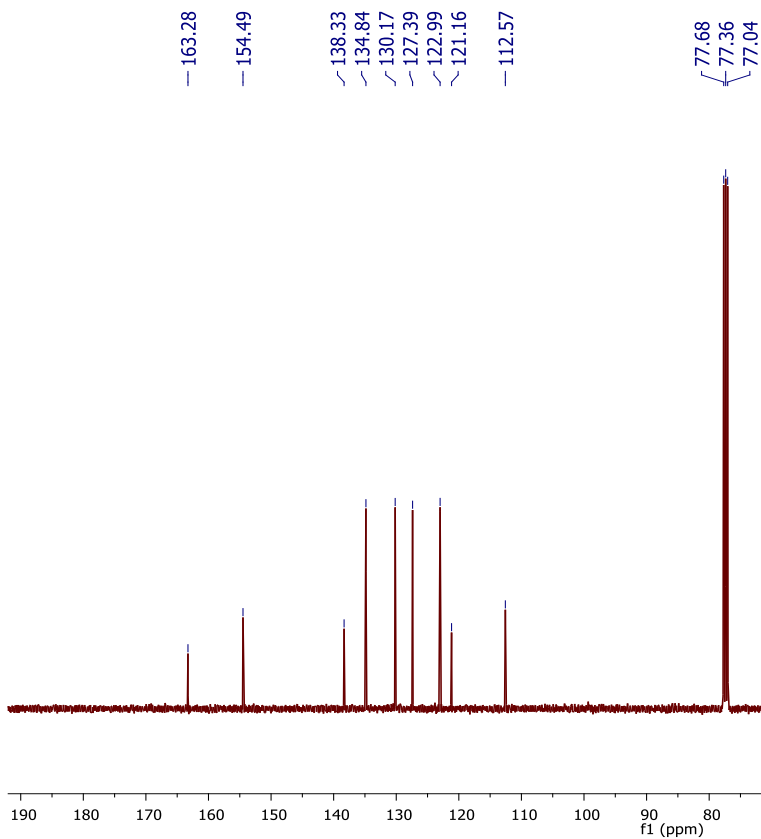
¹³C{¹H} NMR of 3ab (100 MHz, CDCl₃)



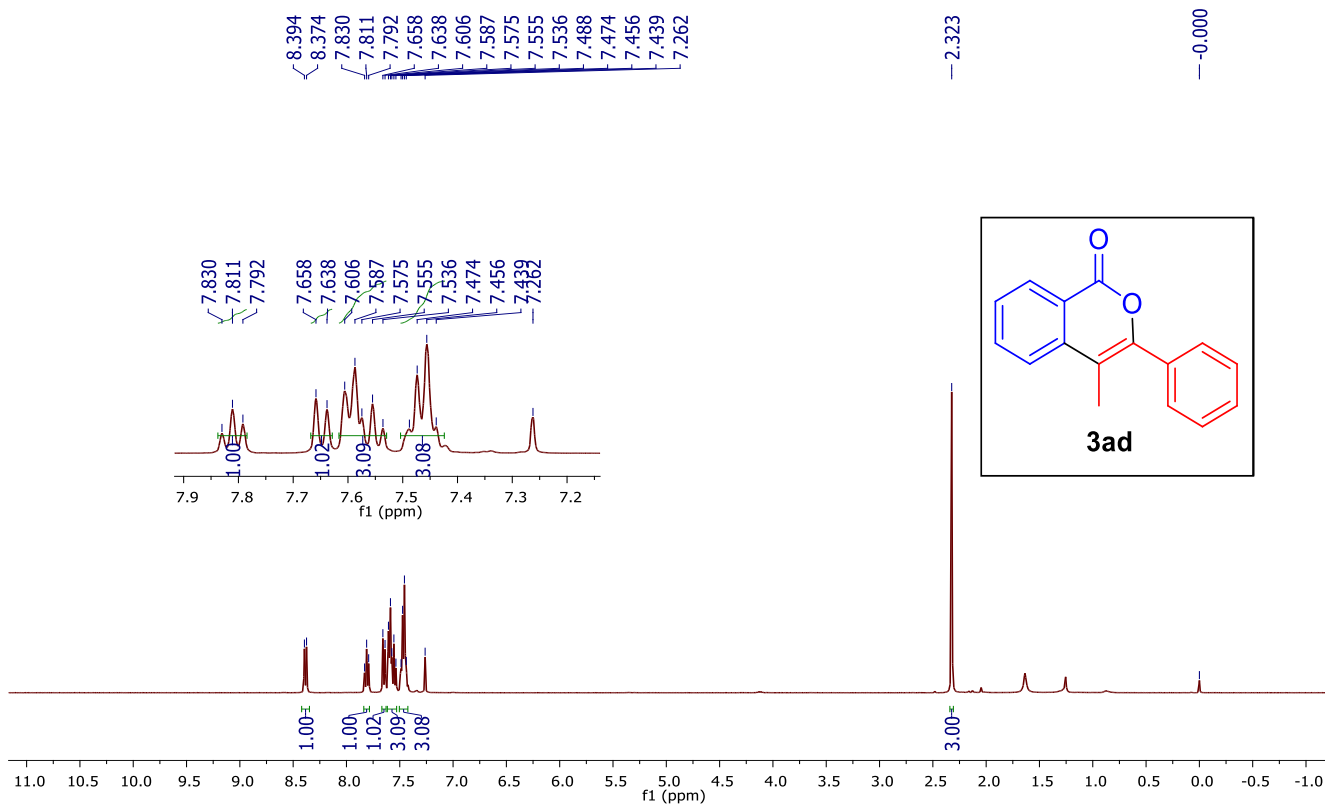
¹H NMR of 3ac (400 MHz, CDCl₃)



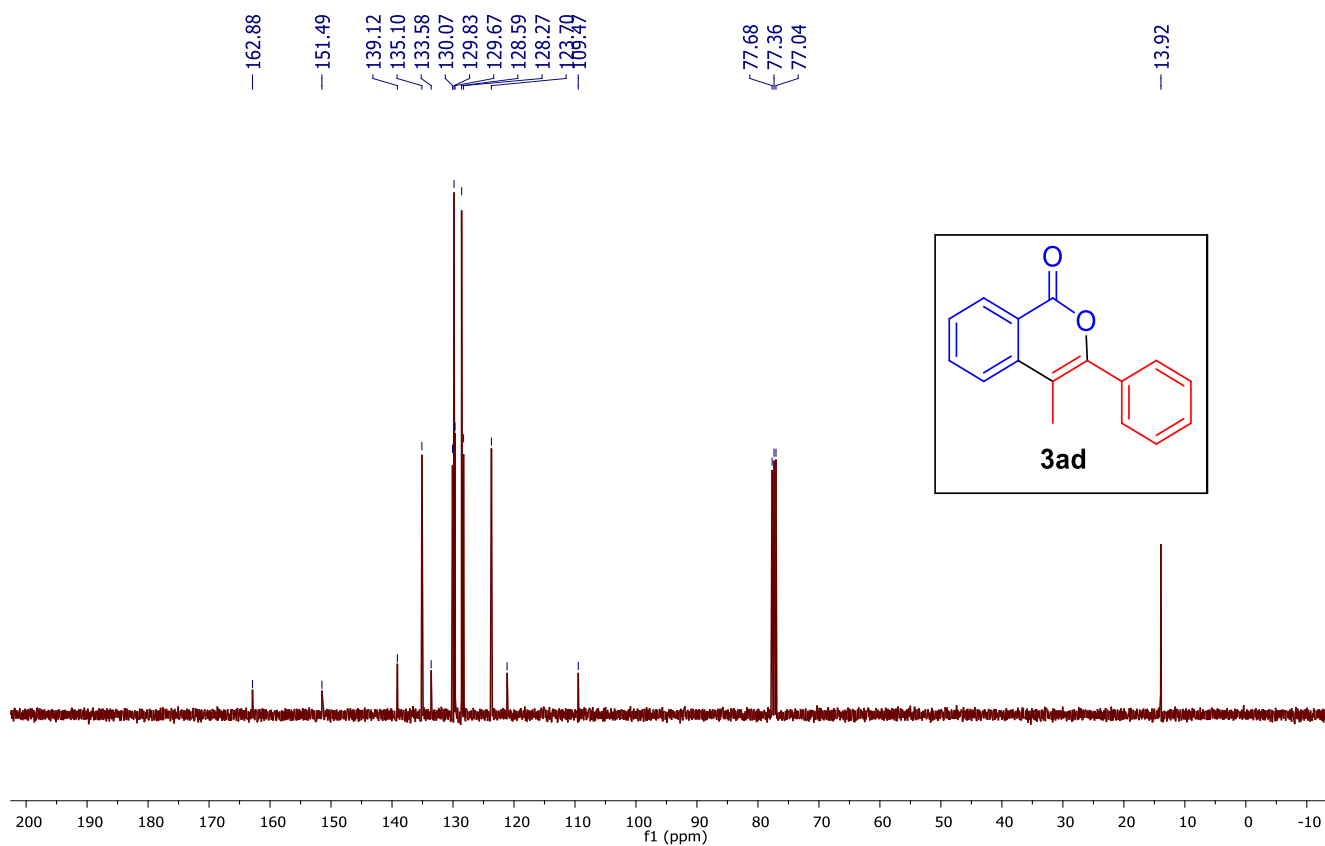
¹³C{¹H} NMR of 3ac (100 MHz, CDCl₃)



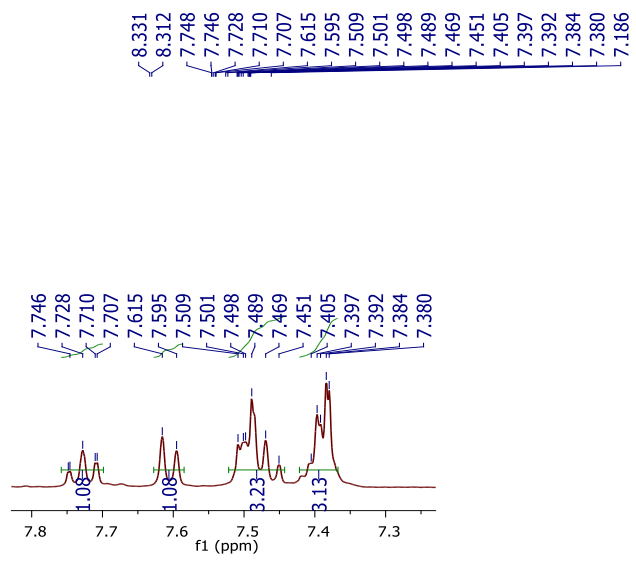
¹H NMR of 3ad (400 MHz, CDCl₃)



¹³C{¹H} NMR of 3ad (100 MHz, CDCl₃)



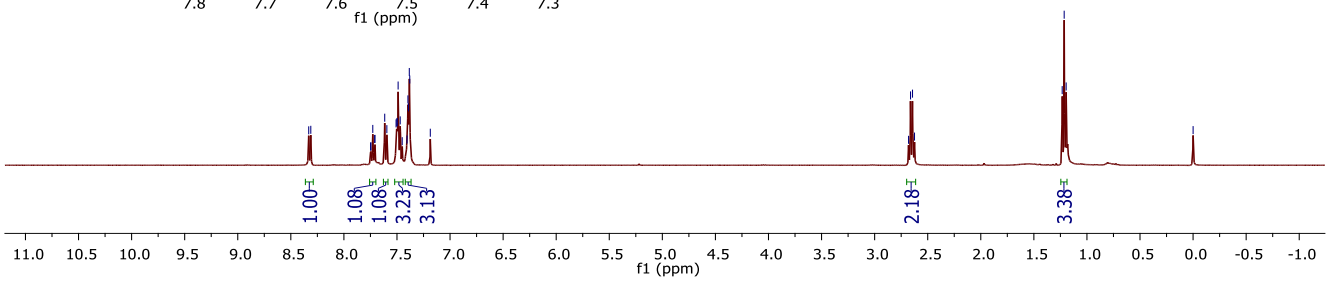
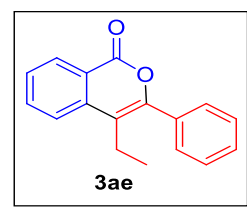
¹H NMR of 3ae (400 MHz, CDCl₃)



2.680
2.662
2.643
2.625

1.233
1.214
1.196

-0.000



¹³C{¹H} NMR of 3ae (100 MHz, CDCl₃)

162.80

151.67

138.02

135.03

133.79

130.37

129.73

129.29

128.68

128.18

123.75

121.68

115.57

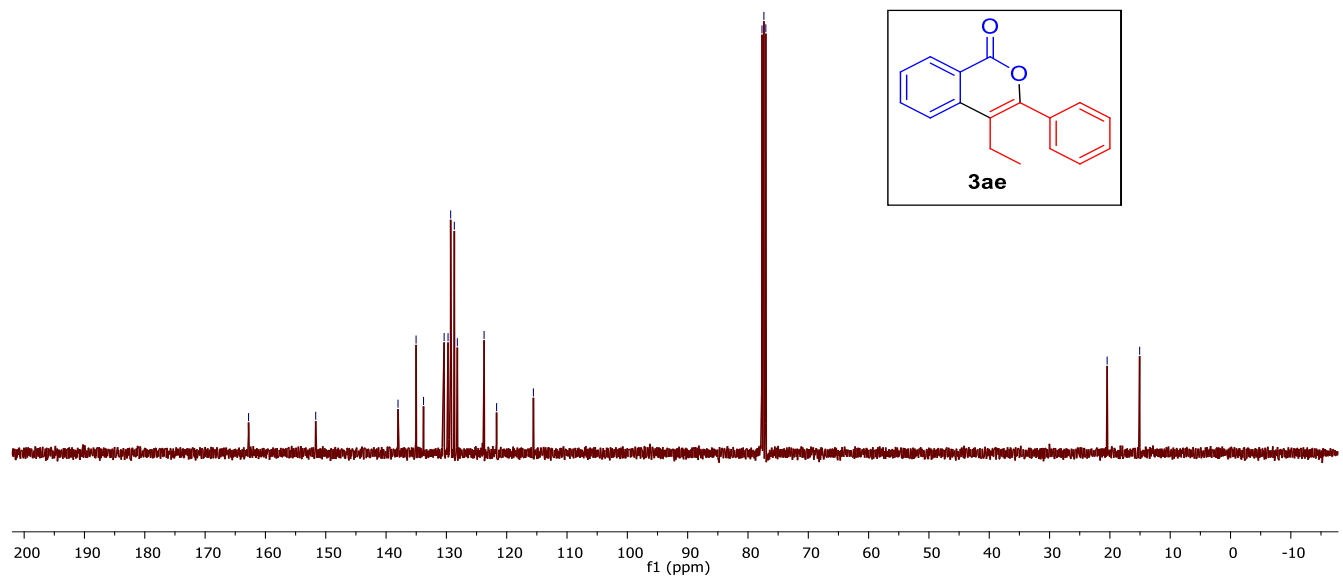
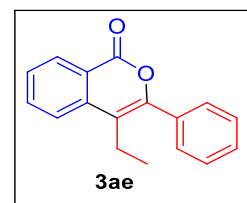
77.68

77.36

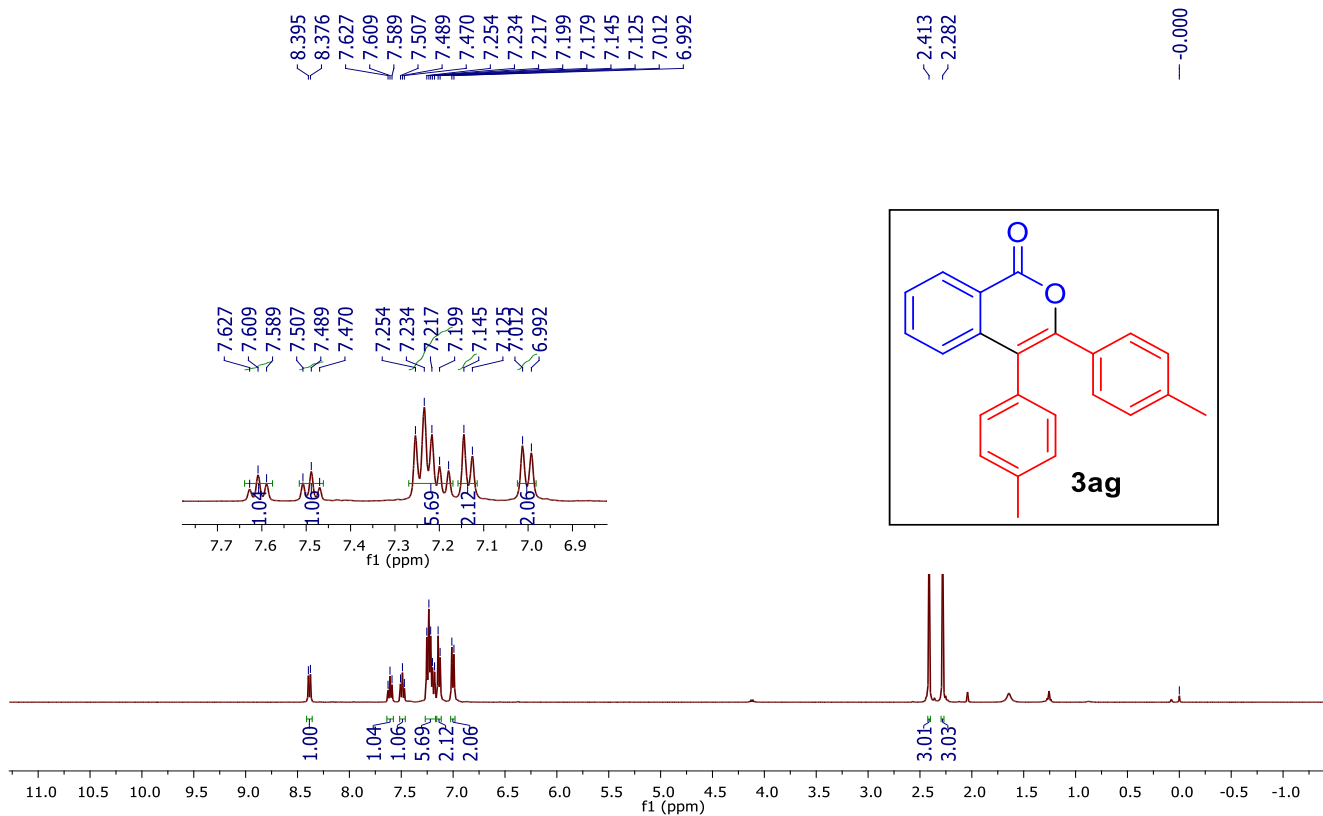
77.04

20.45

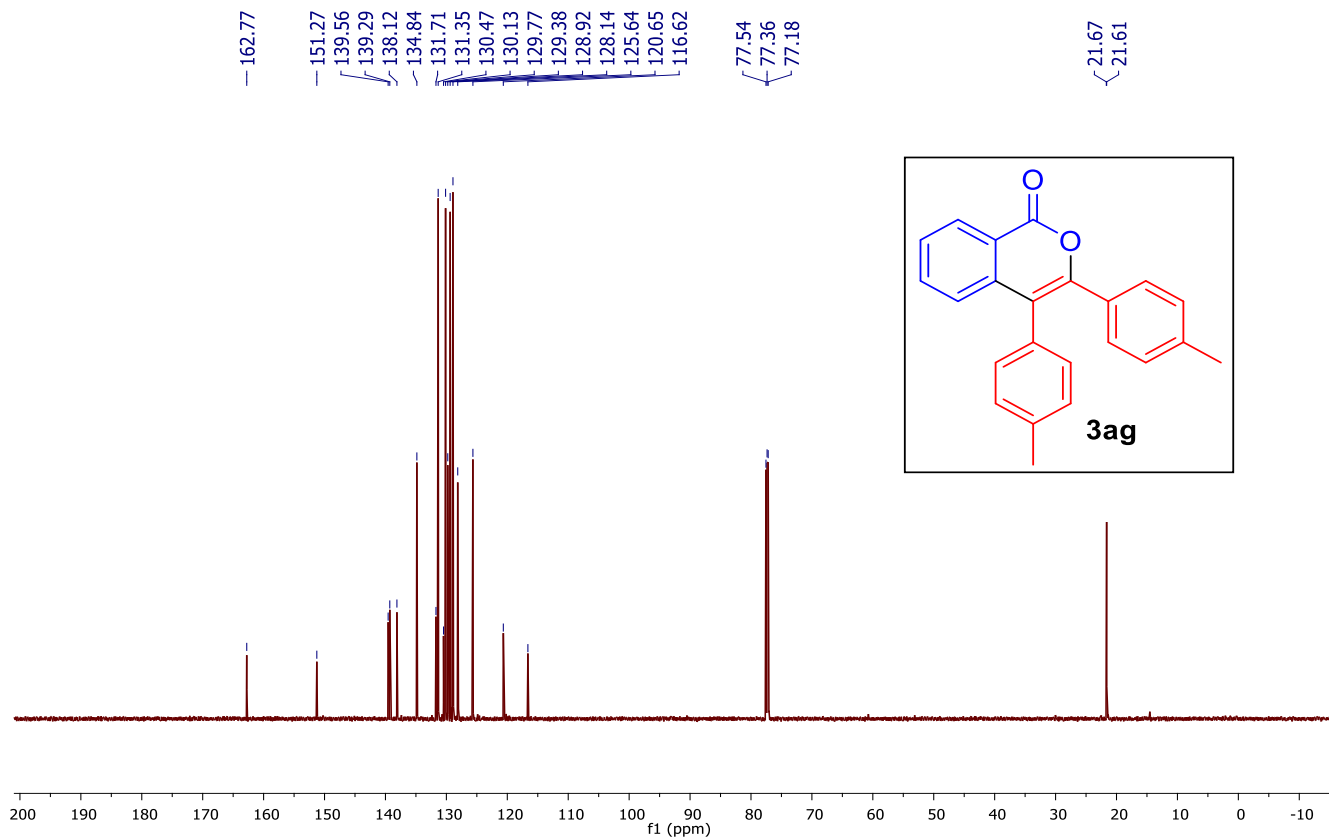
15.07



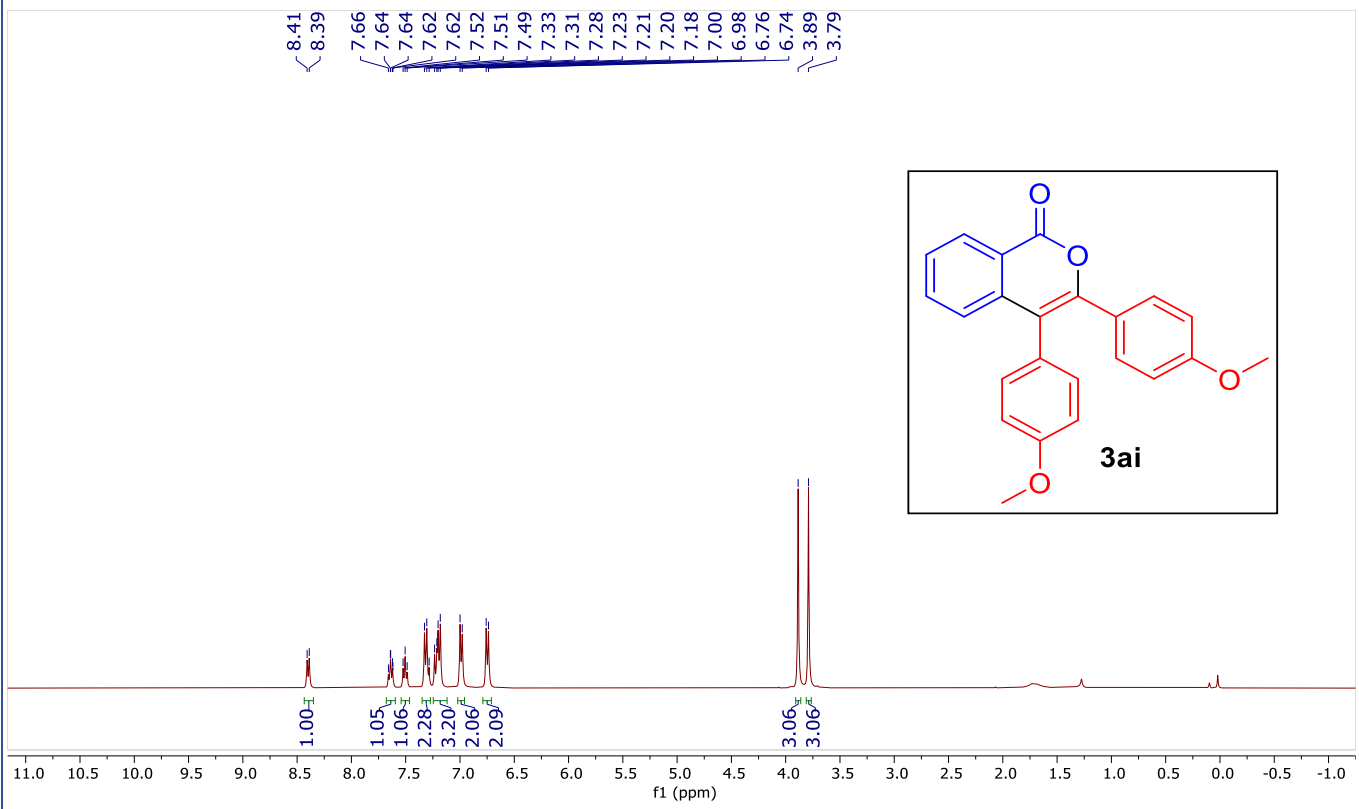
¹H NMR of 3ag (400 MHz, CDCl₃)



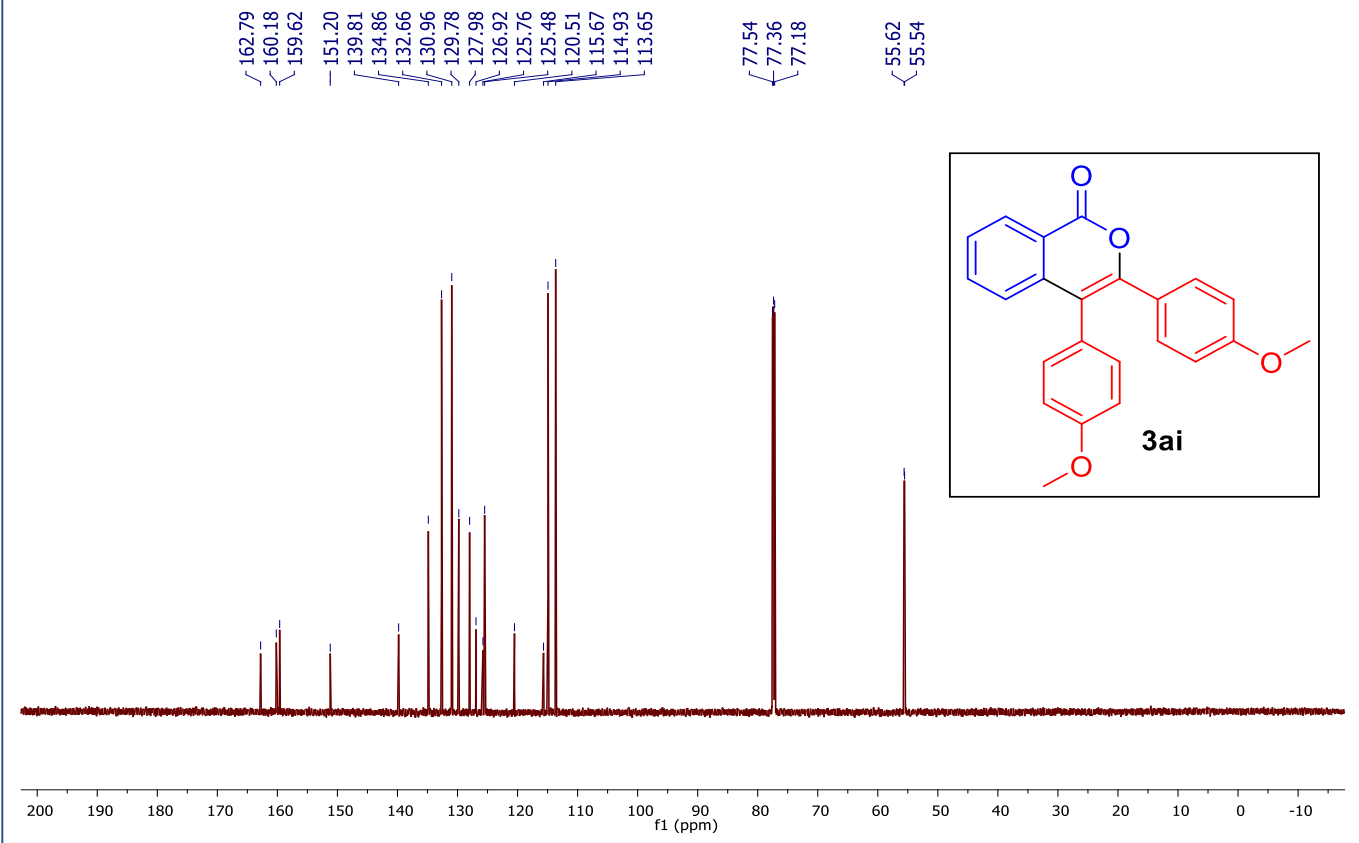
¹³C{¹H} NMR of 3ag (176 MHz, CDCl₃)



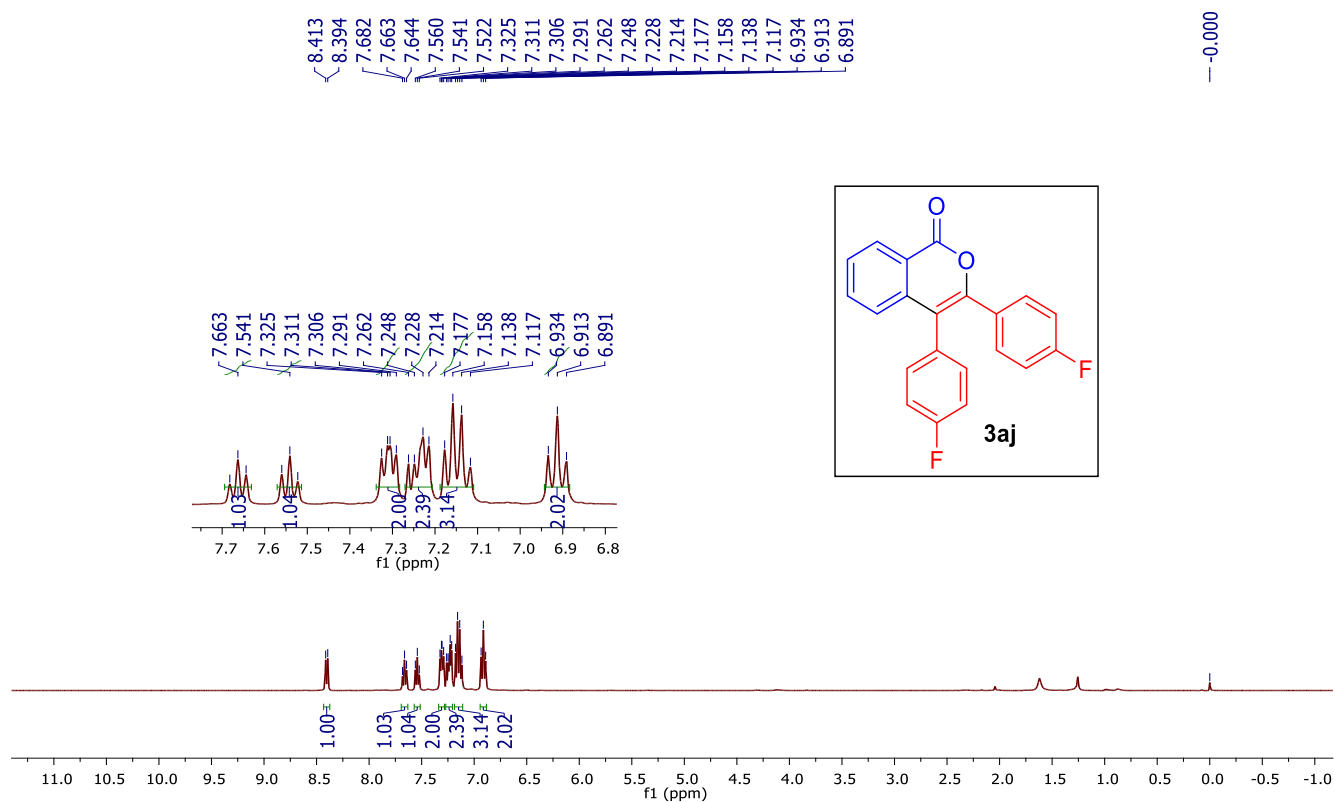
¹H NMR of 3ai (400 MHz, CDCl₃)



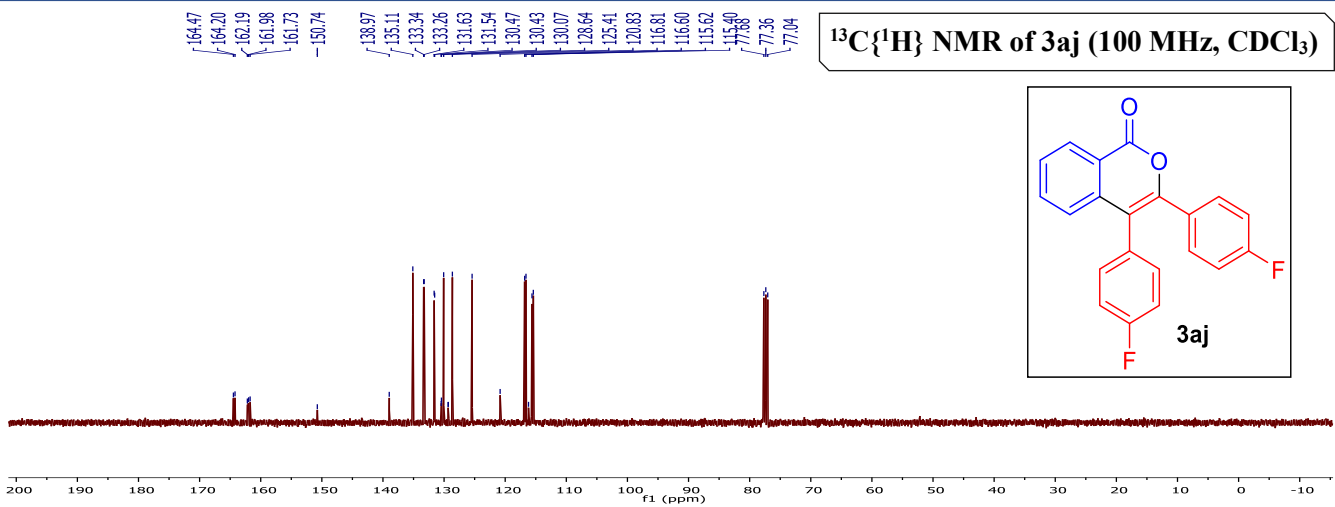
¹³C{¹H} NMR of 3ai (176 MHz, CDCl₃)



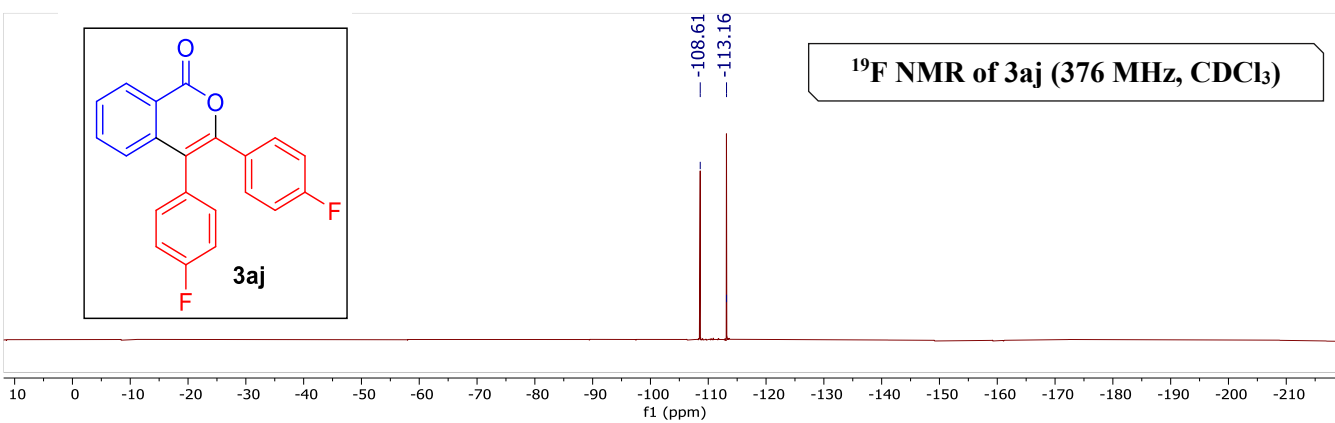
¹H NMR of 3aj (400 MHz, CDCl₃)



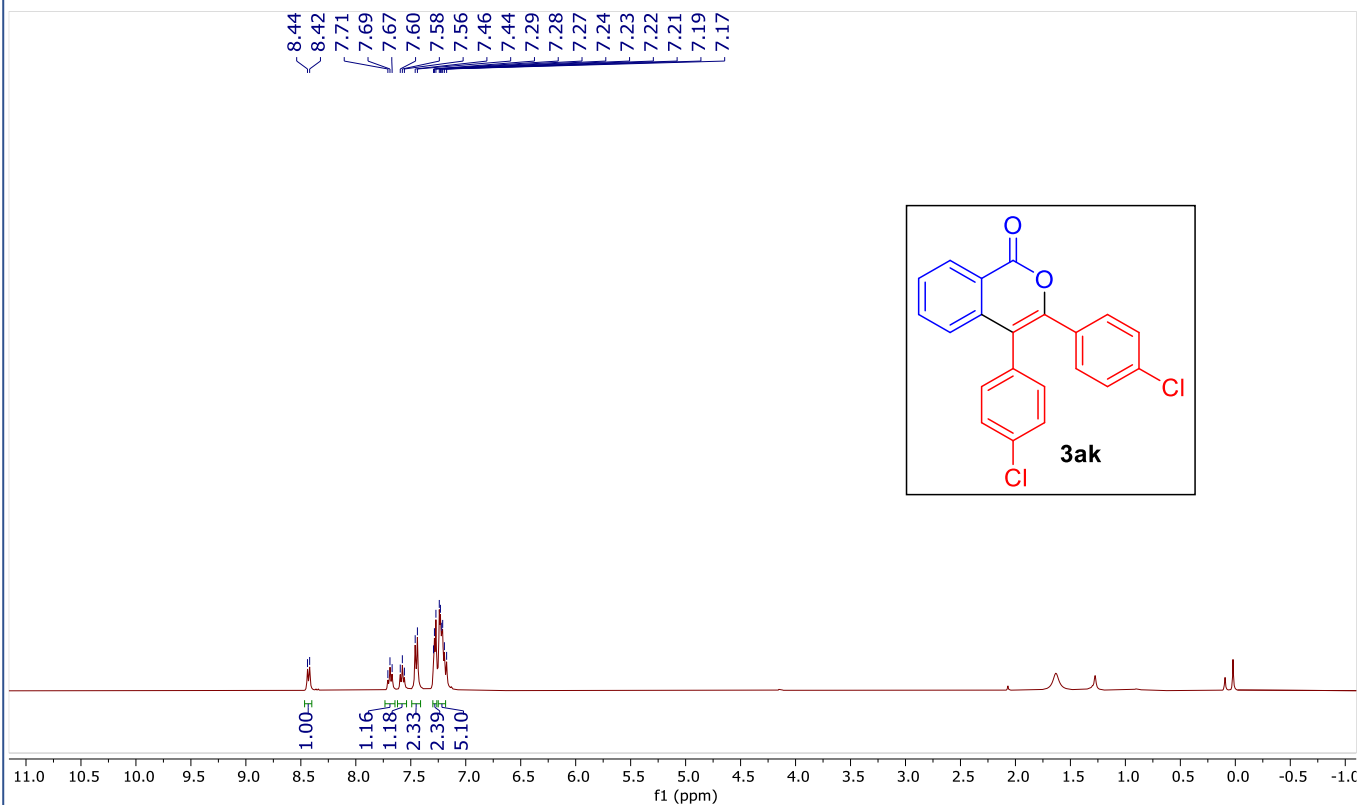
¹³C{¹H} NMR of 3aj (100 MHz, CDCl₃)



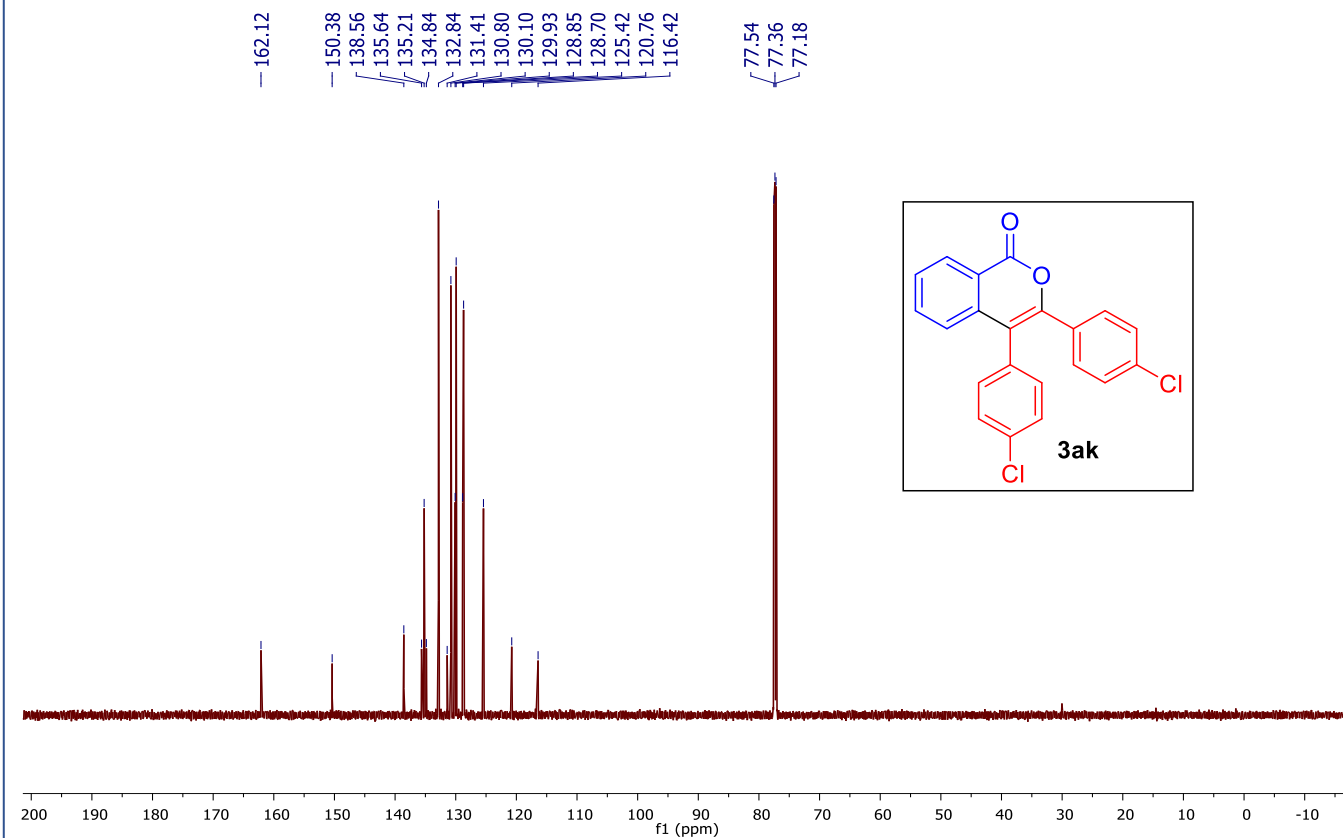
¹⁹F NMR of 3aj (376 MHz, CDCl₃)



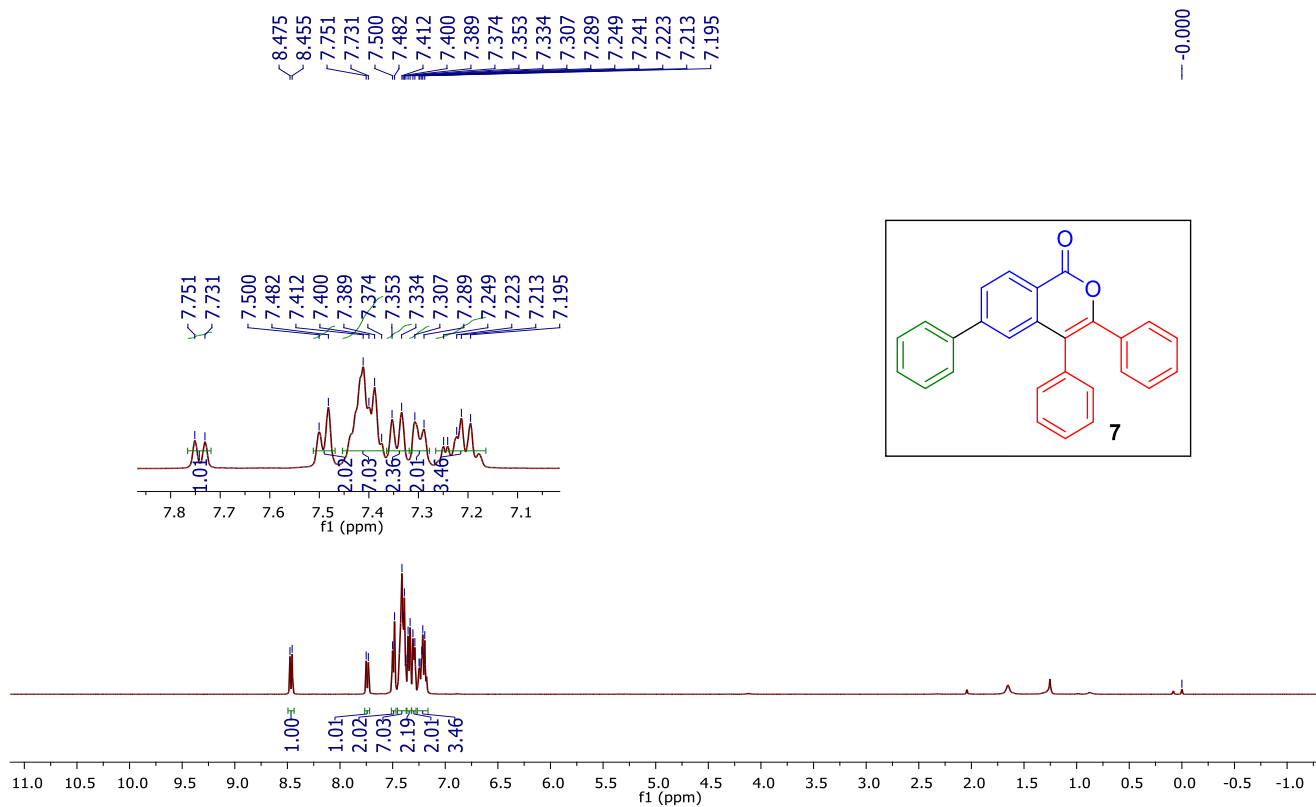
¹H NMR of 3ak (700 MHz, CDCl₃)



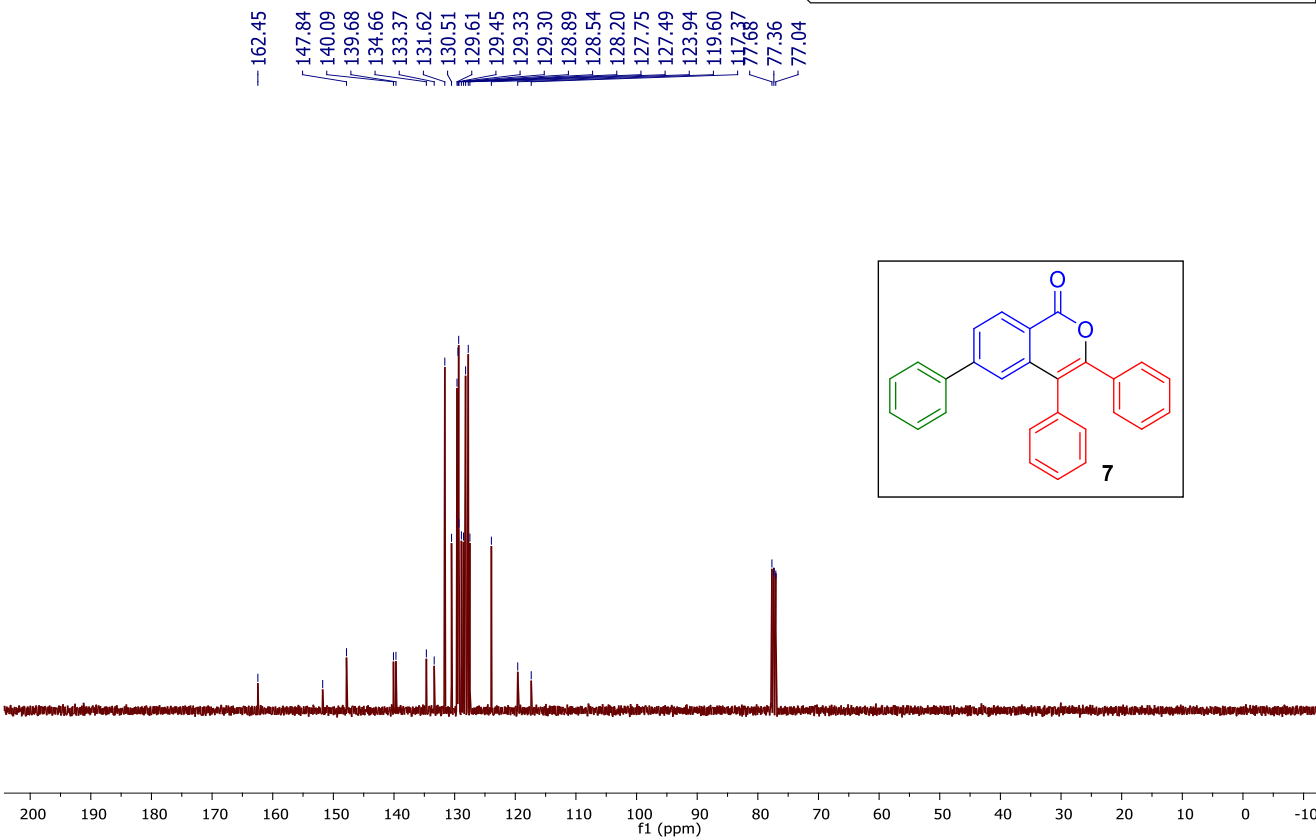
¹³C{¹H} NMR of 3ak (176 MHz, CDCl₃)



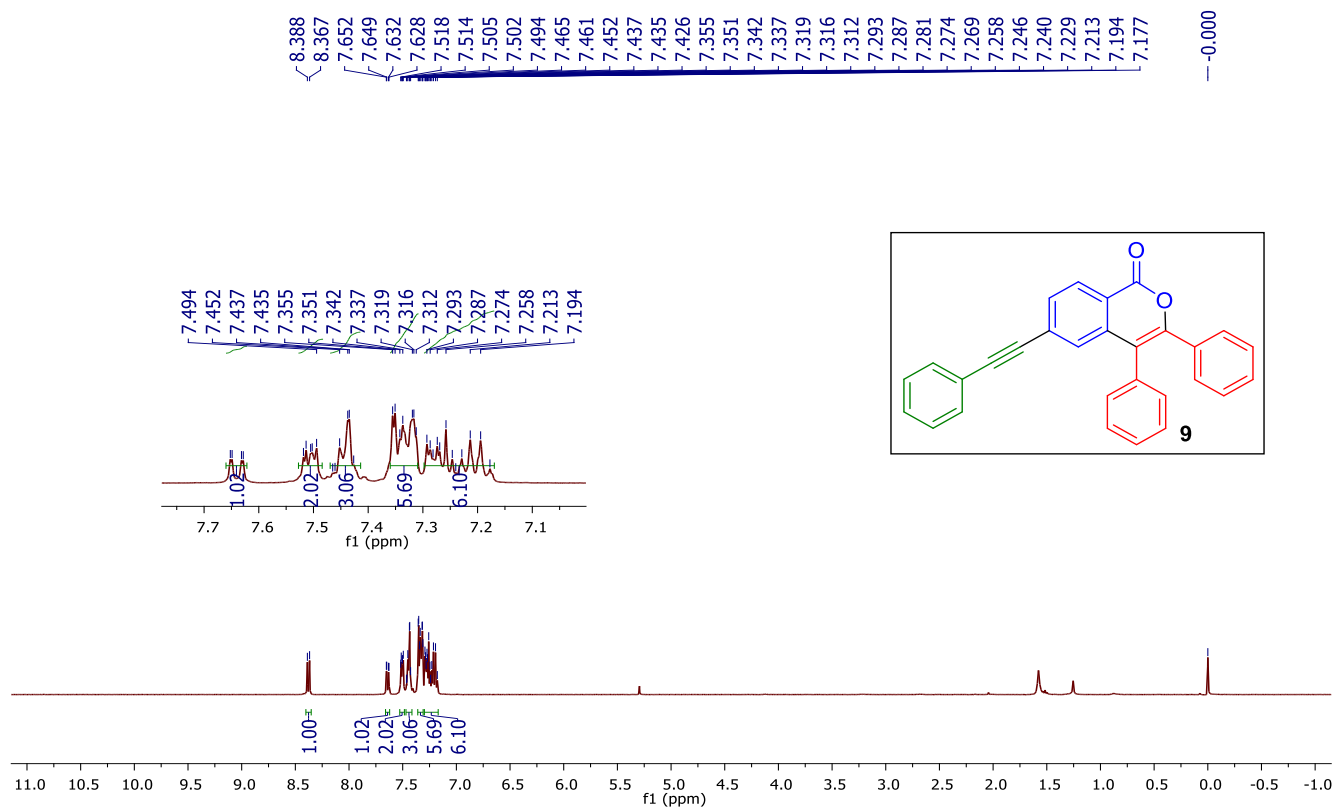
¹H NMR of 7 (400 MHz, CDCl₃)



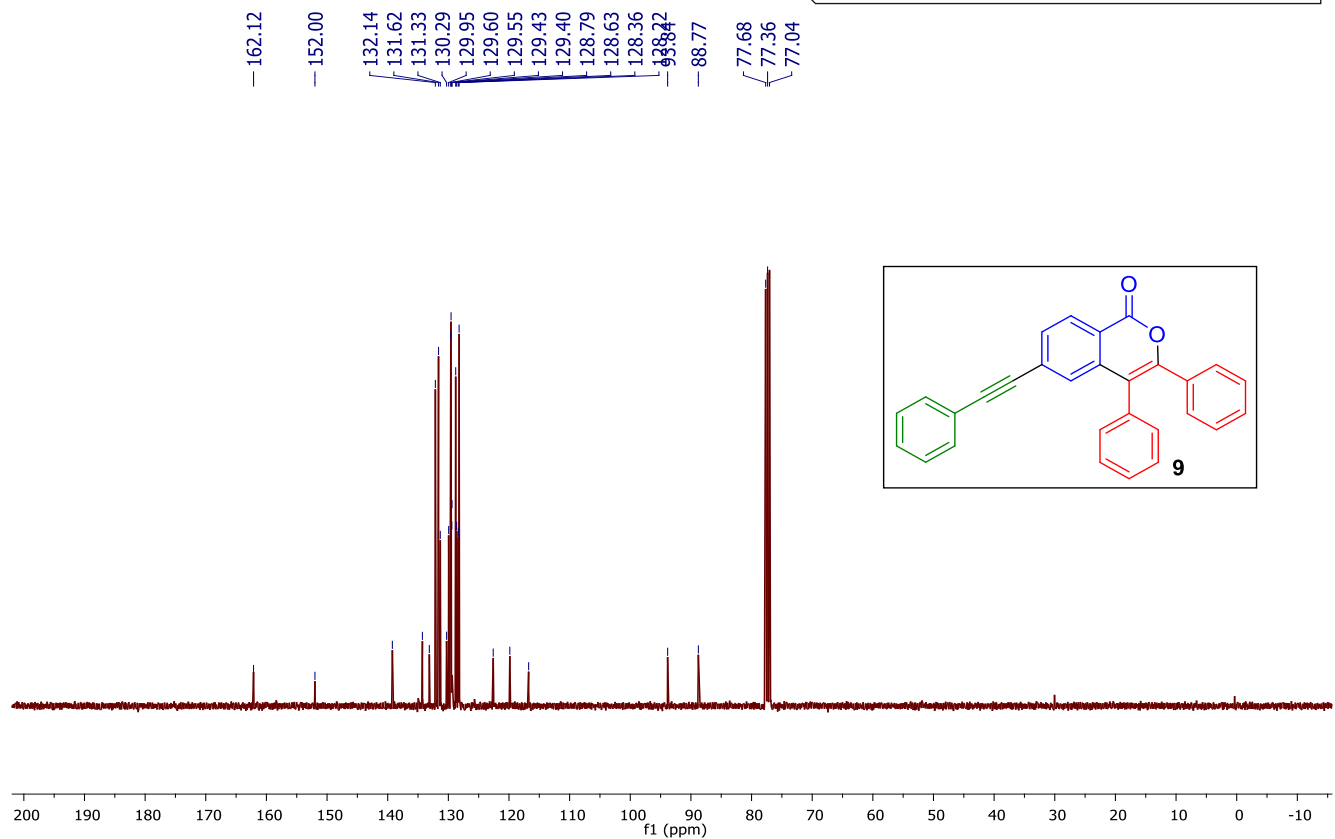
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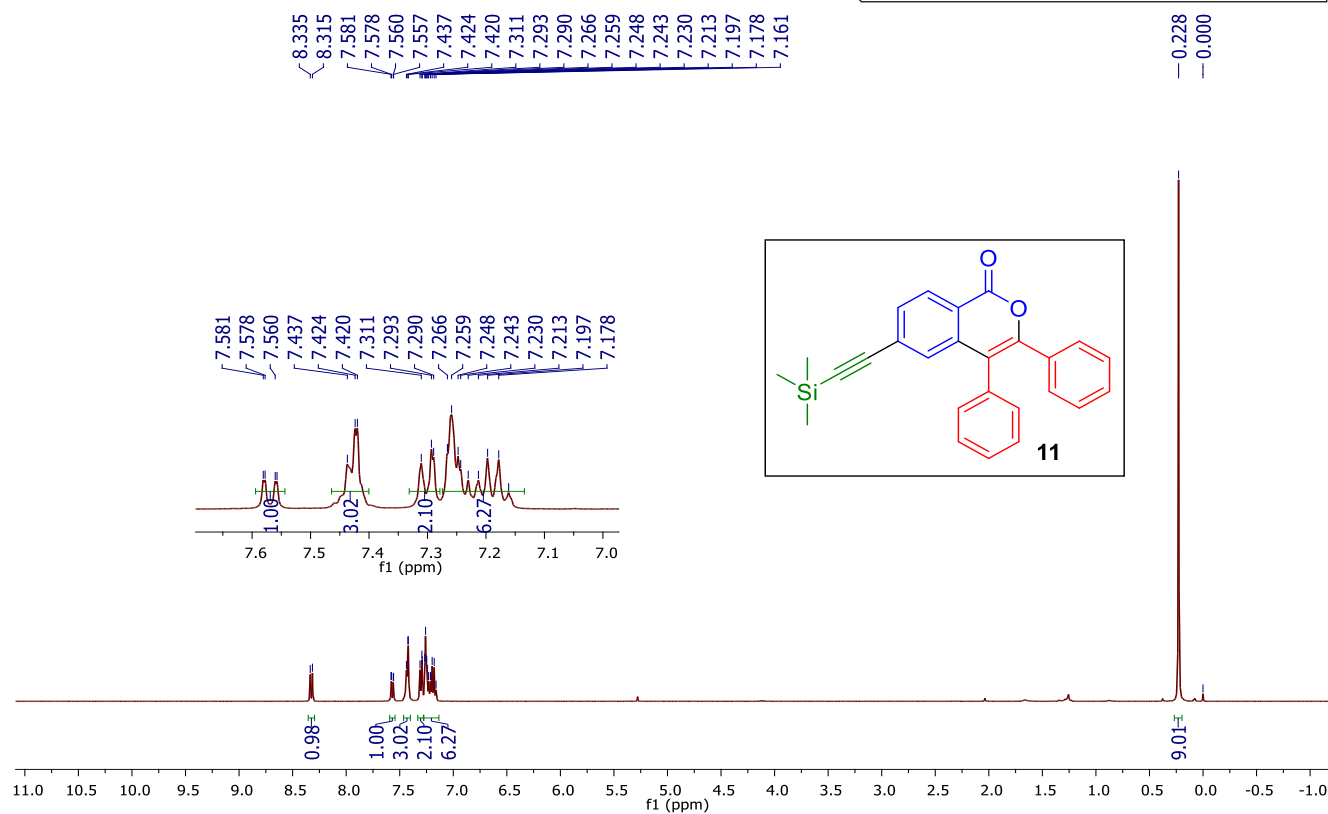
¹H NMR of 9 (400 MHz, CDCl₃)



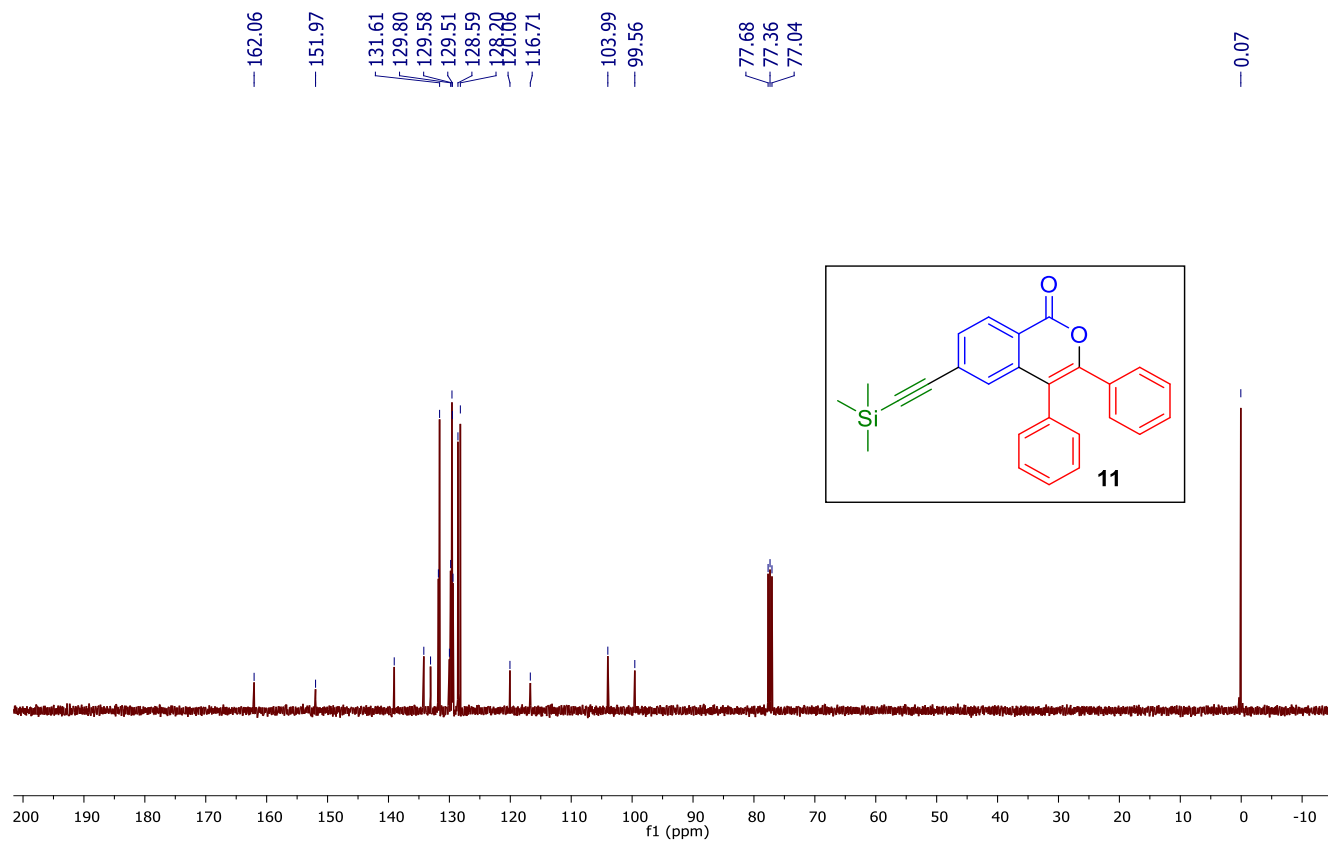
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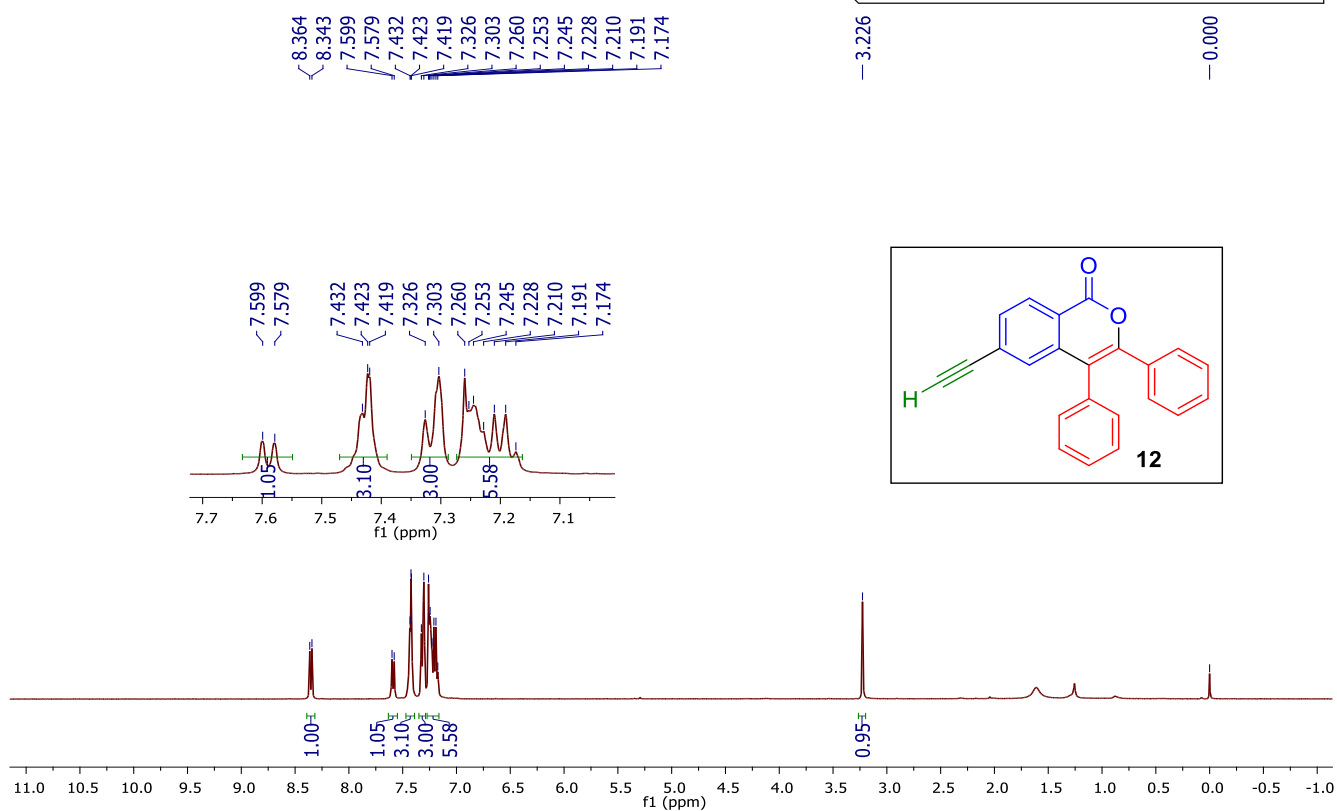
¹H NMR of 11 (400 MHz, CDCl₃)



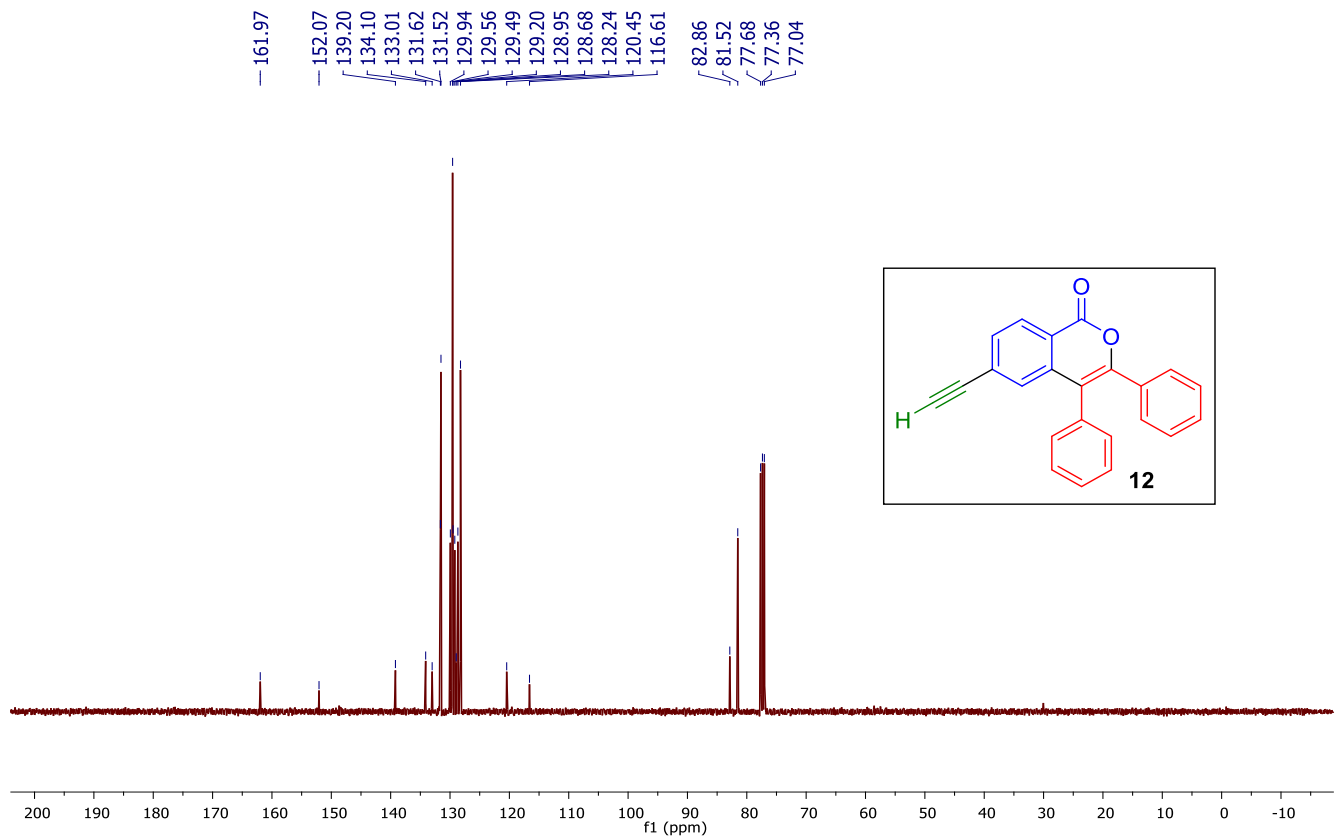
¹³C{¹H} NMR of 11 (100 MHz, CDCl₃)



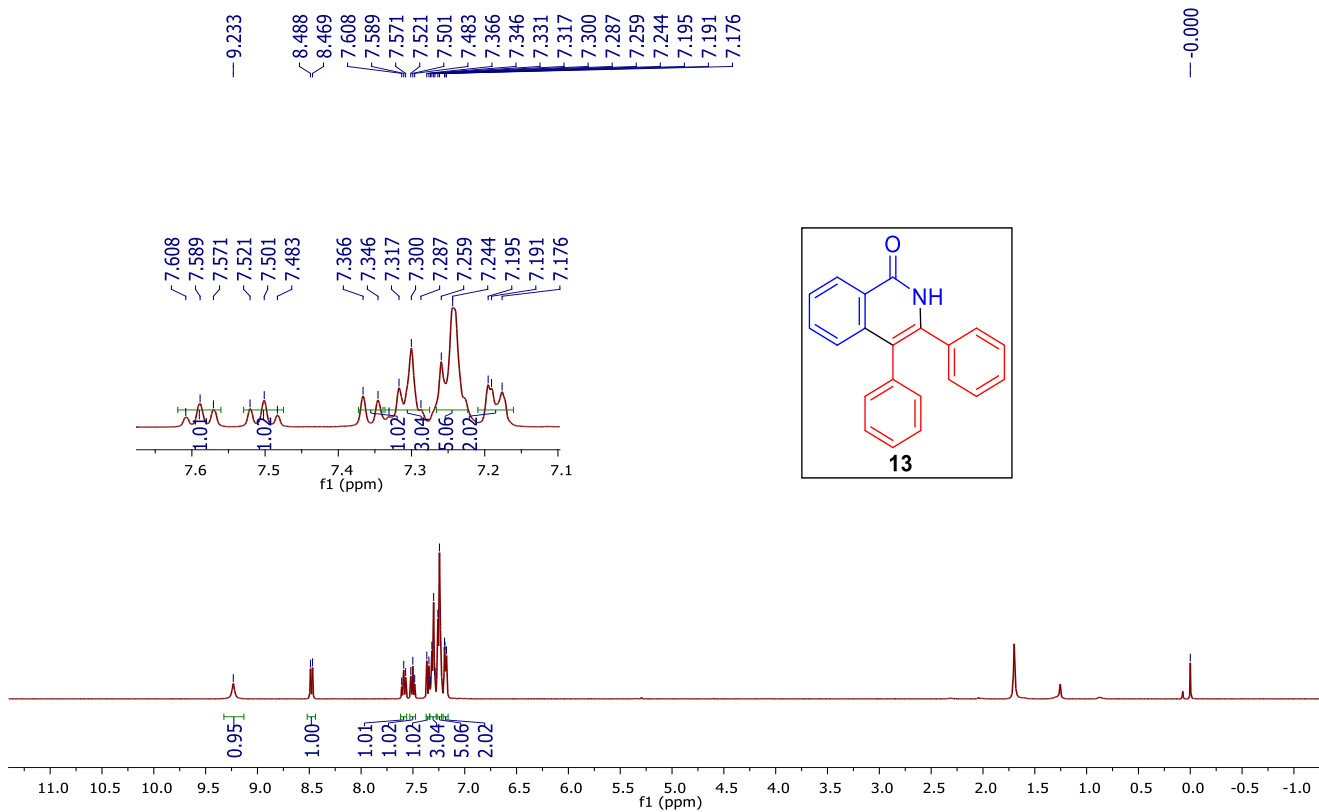
¹H NMR of 12 (400 MHz, CDCl₃)



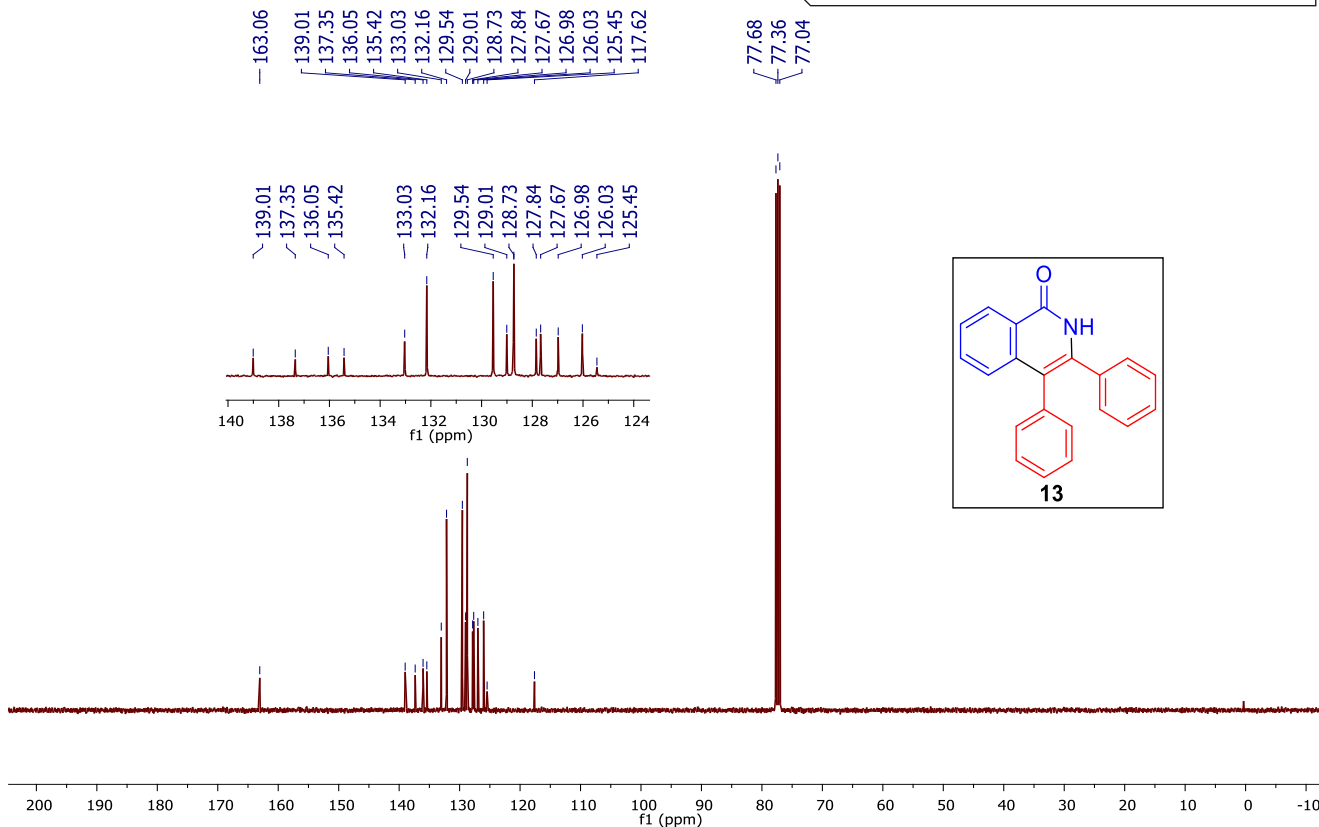
¹³C{¹H} NMR of 12 (100 MHz, CDCl₃)



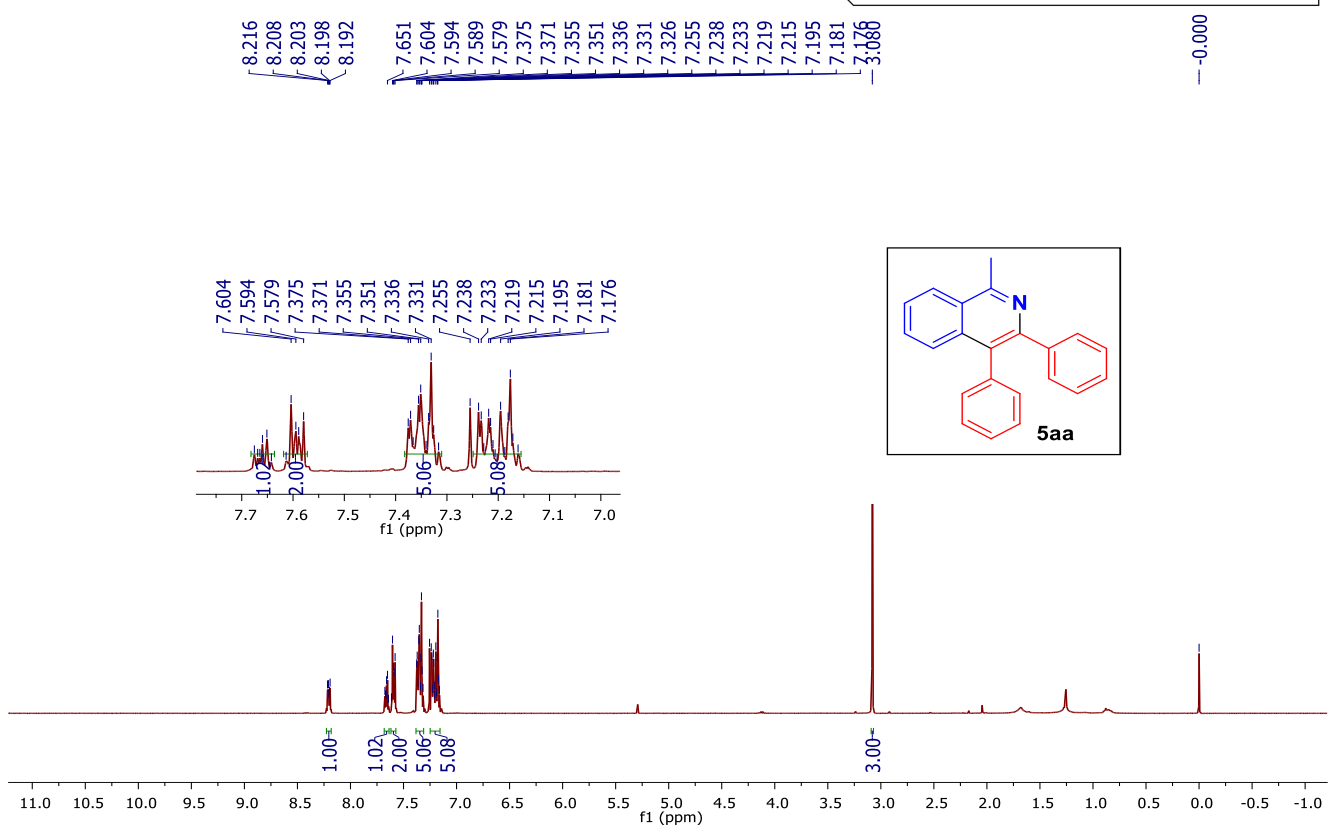
¹H NMR of 13 (400 MHz, CDCl₃)



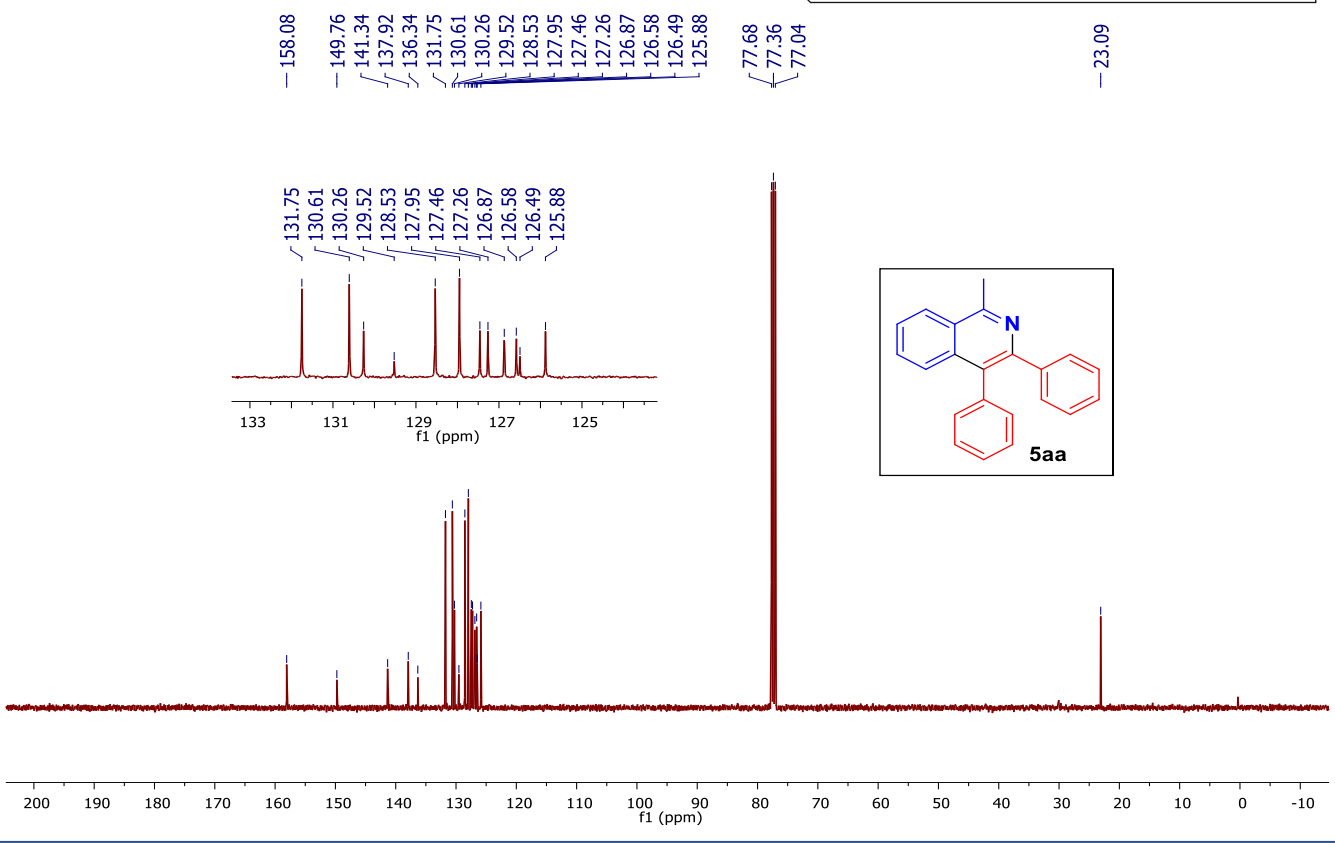
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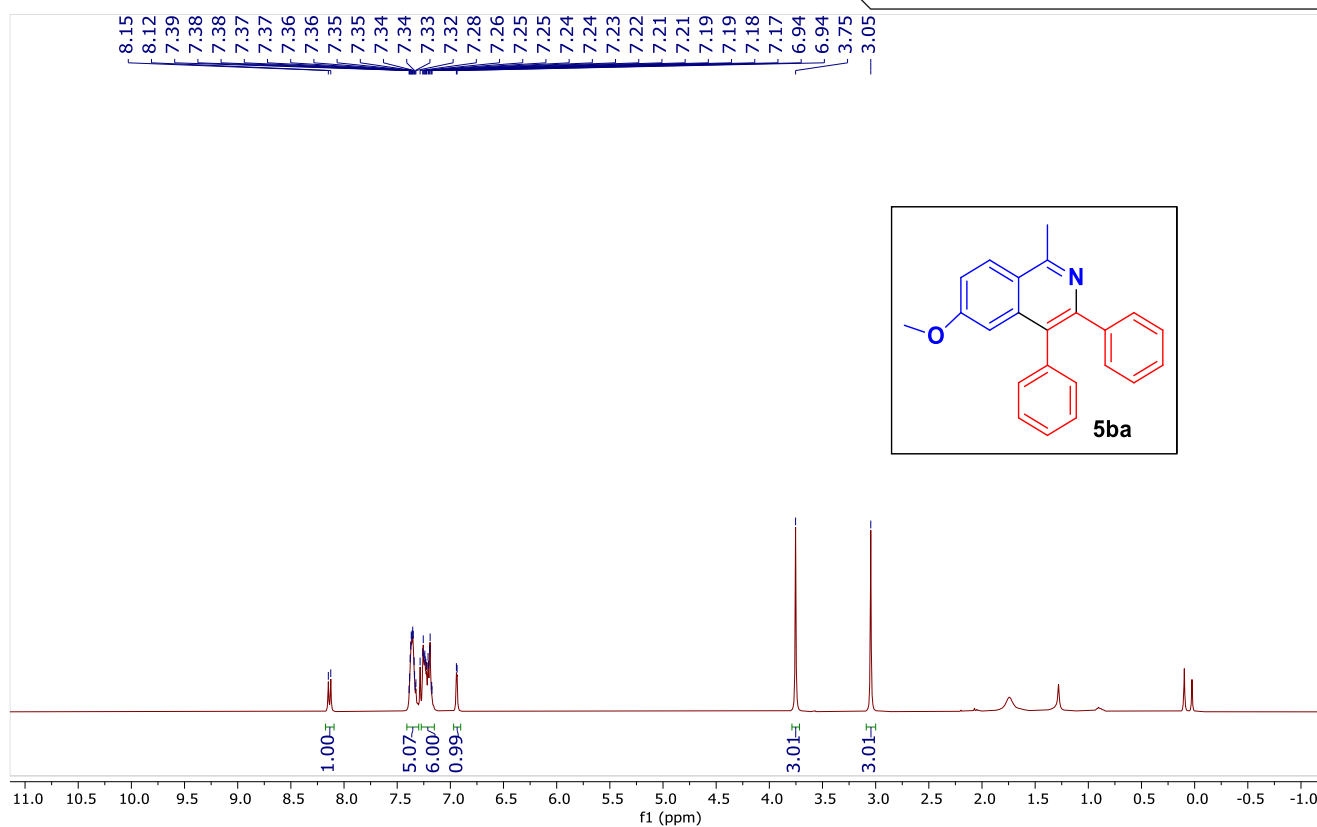
¹H NMR of 5aa (400 MHz, CDCl₃)



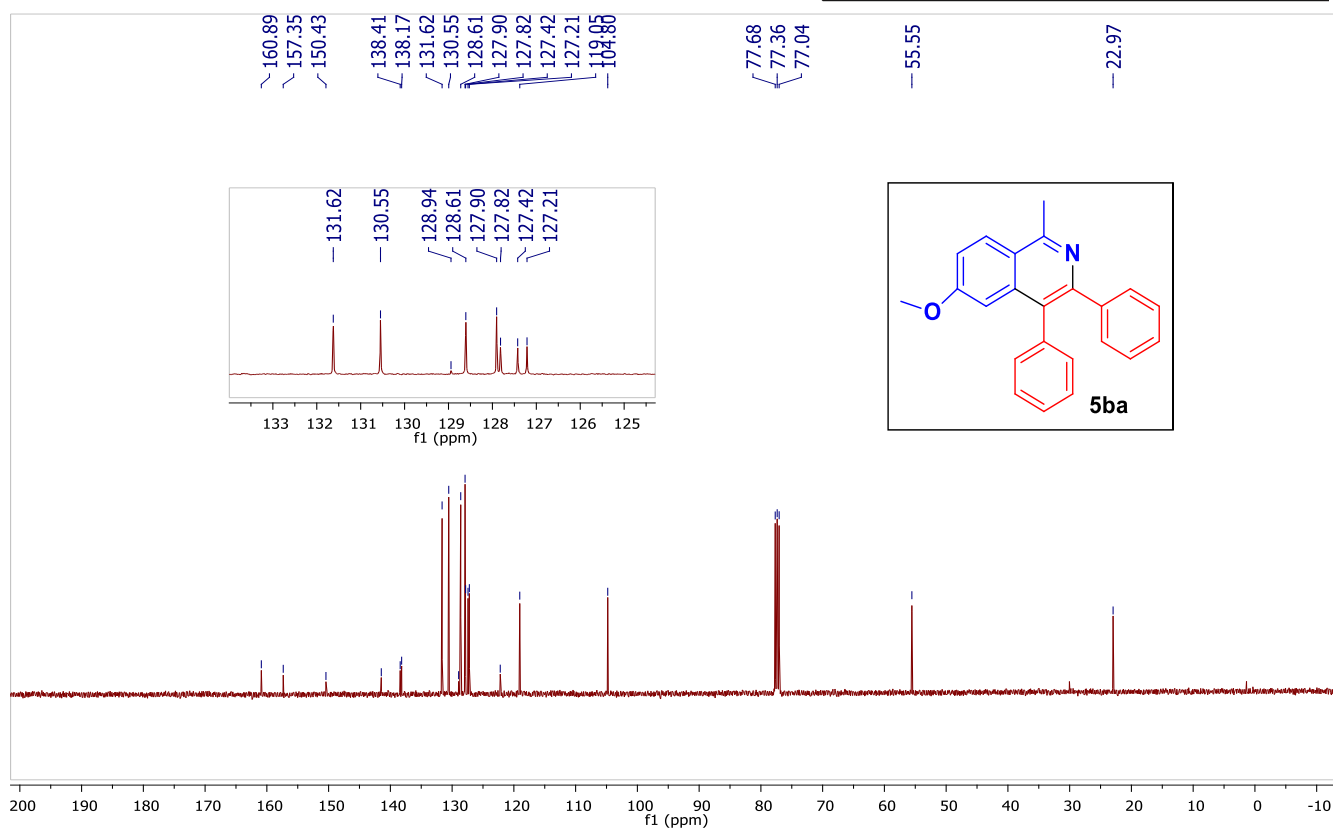
¹³C{¹H} NMR of 5aa (100 MHz, CDCl₃)



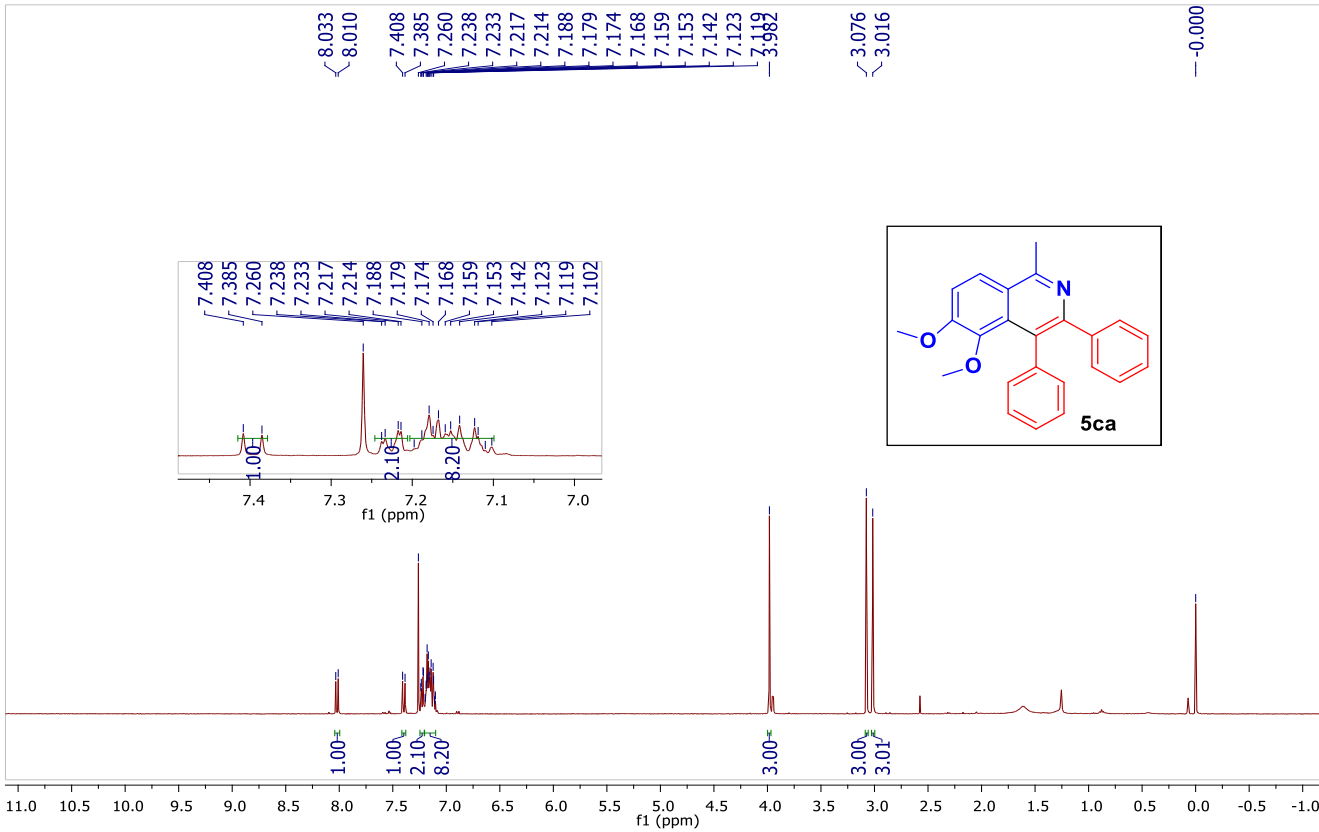
¹H NMR of 5ba (400 MHz, CDCl₃)



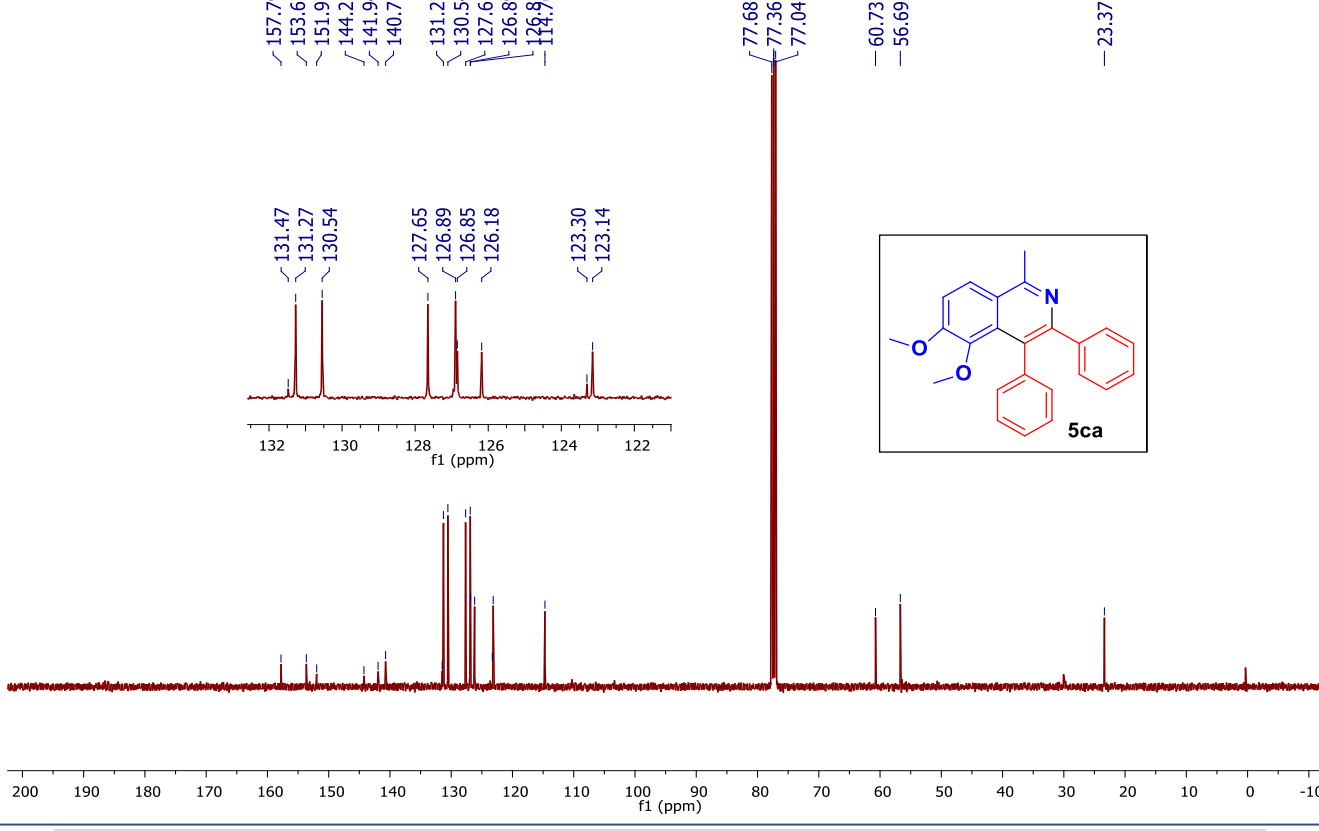
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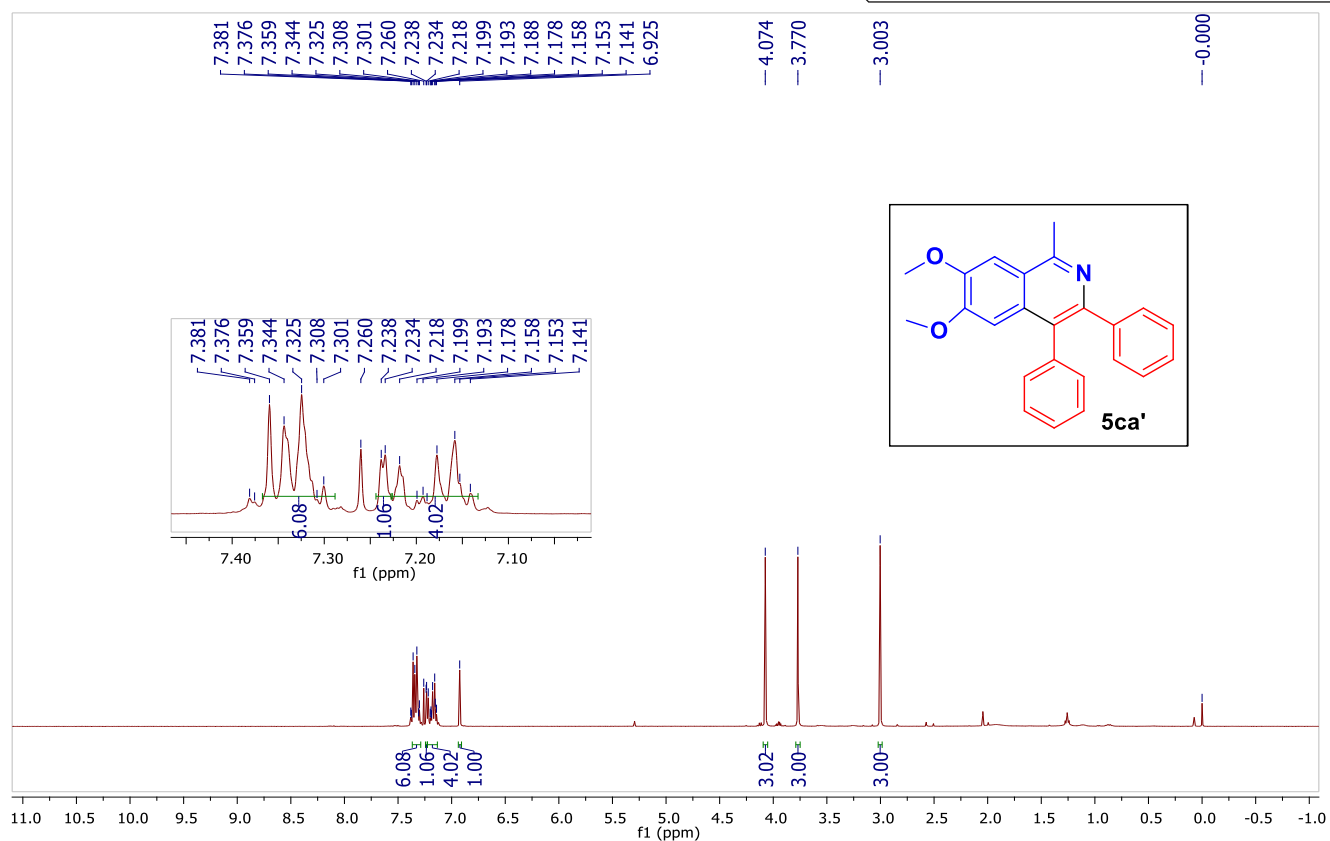
¹H NMR of 5ca (400 MHz, CDCl₃)



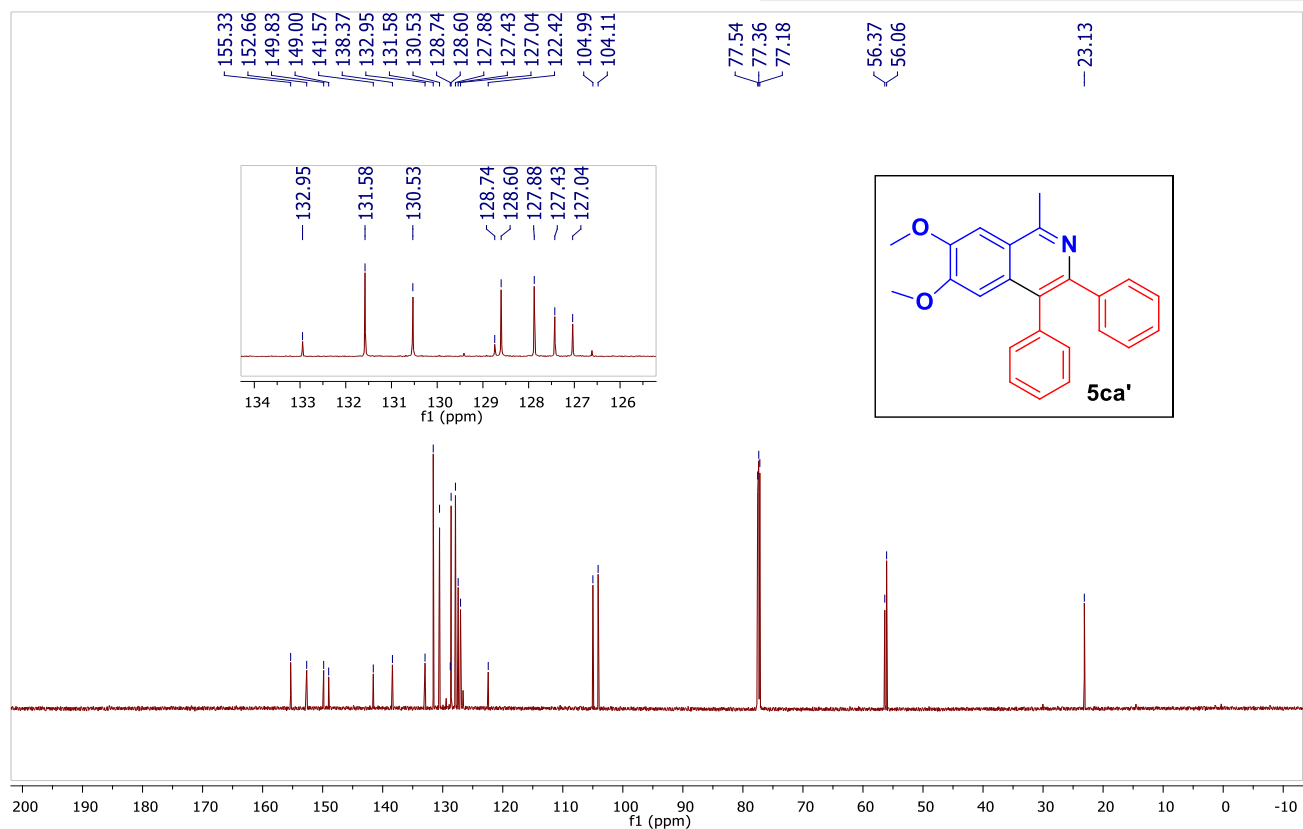
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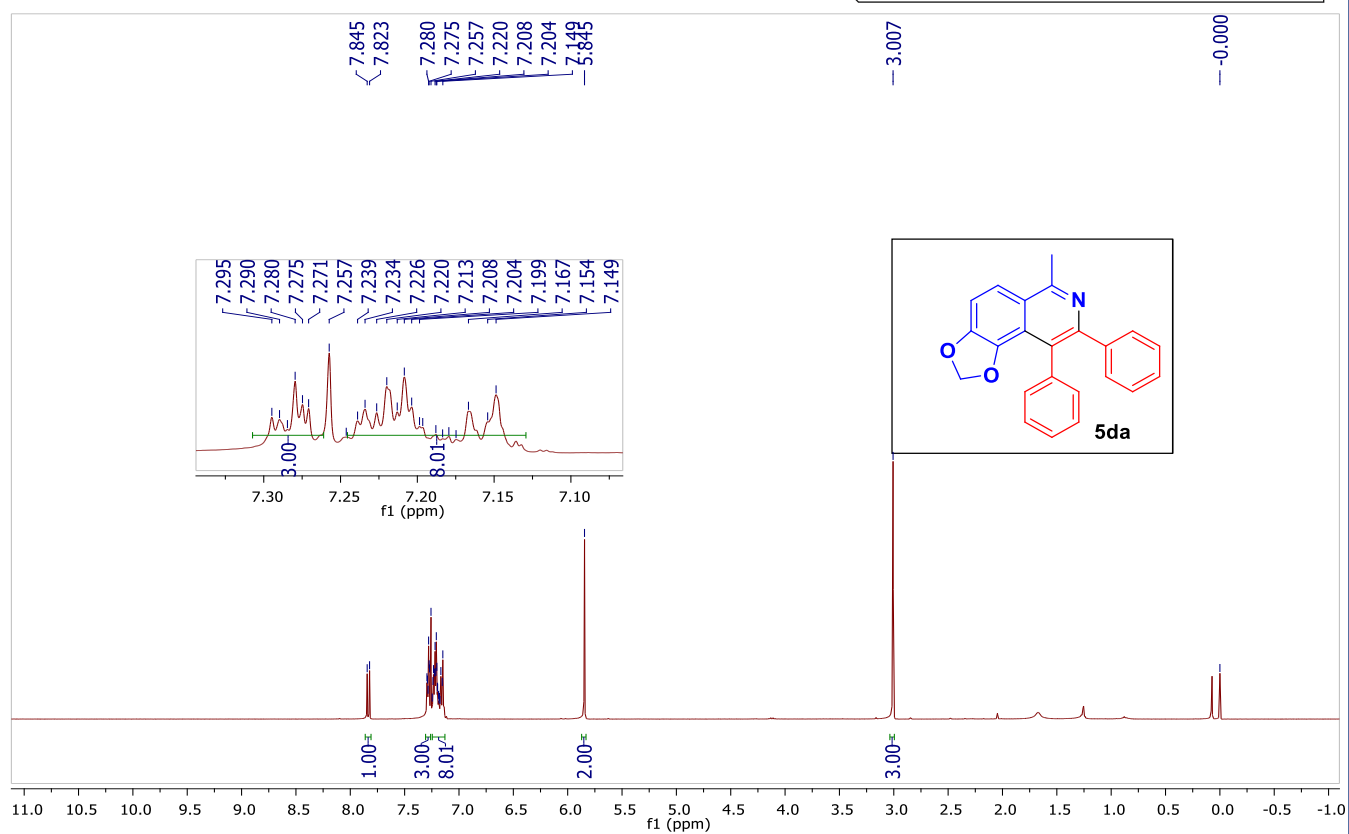
¹H NMR of 5ca' (400 MHz, CDCl₃)



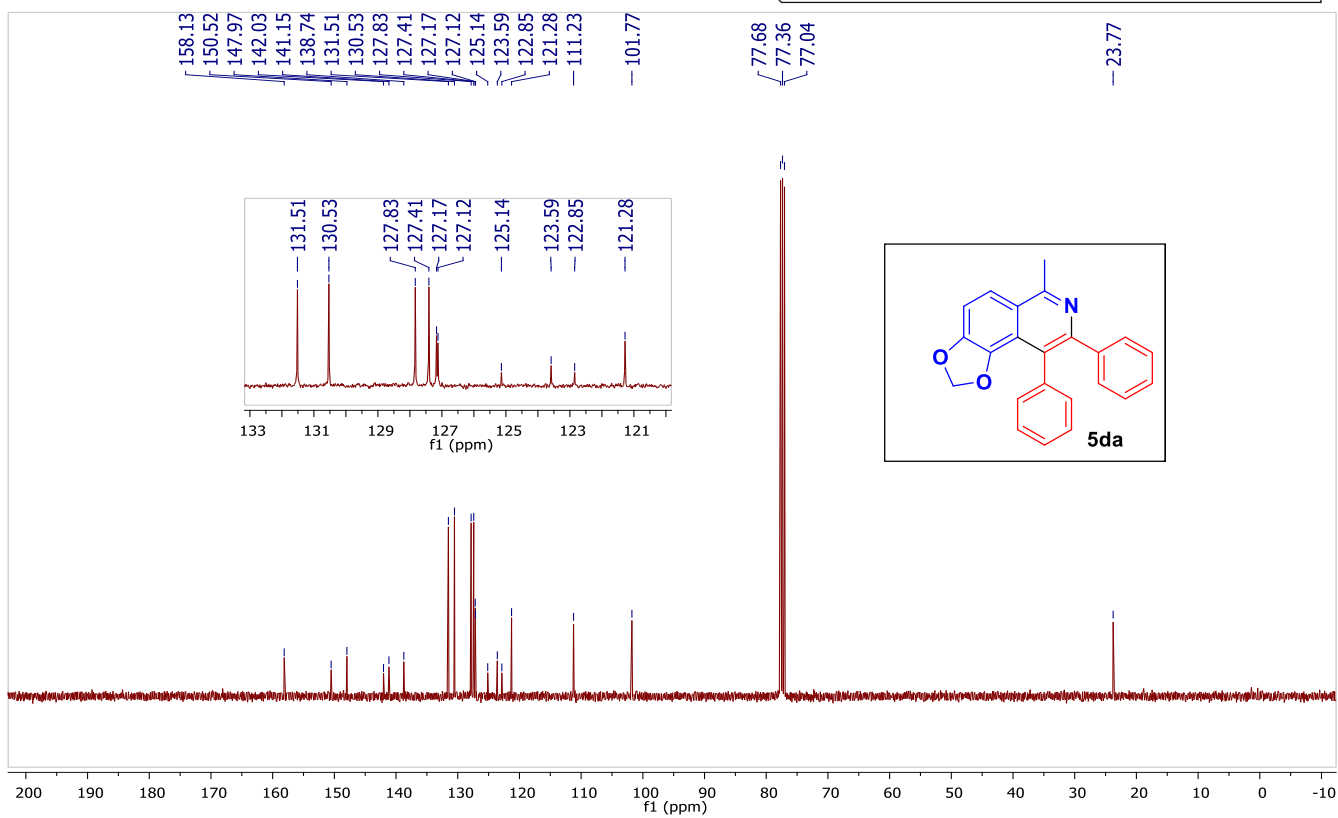
¹³C{¹H} NMR of 5ca' (176 MHz, CDCl₃)



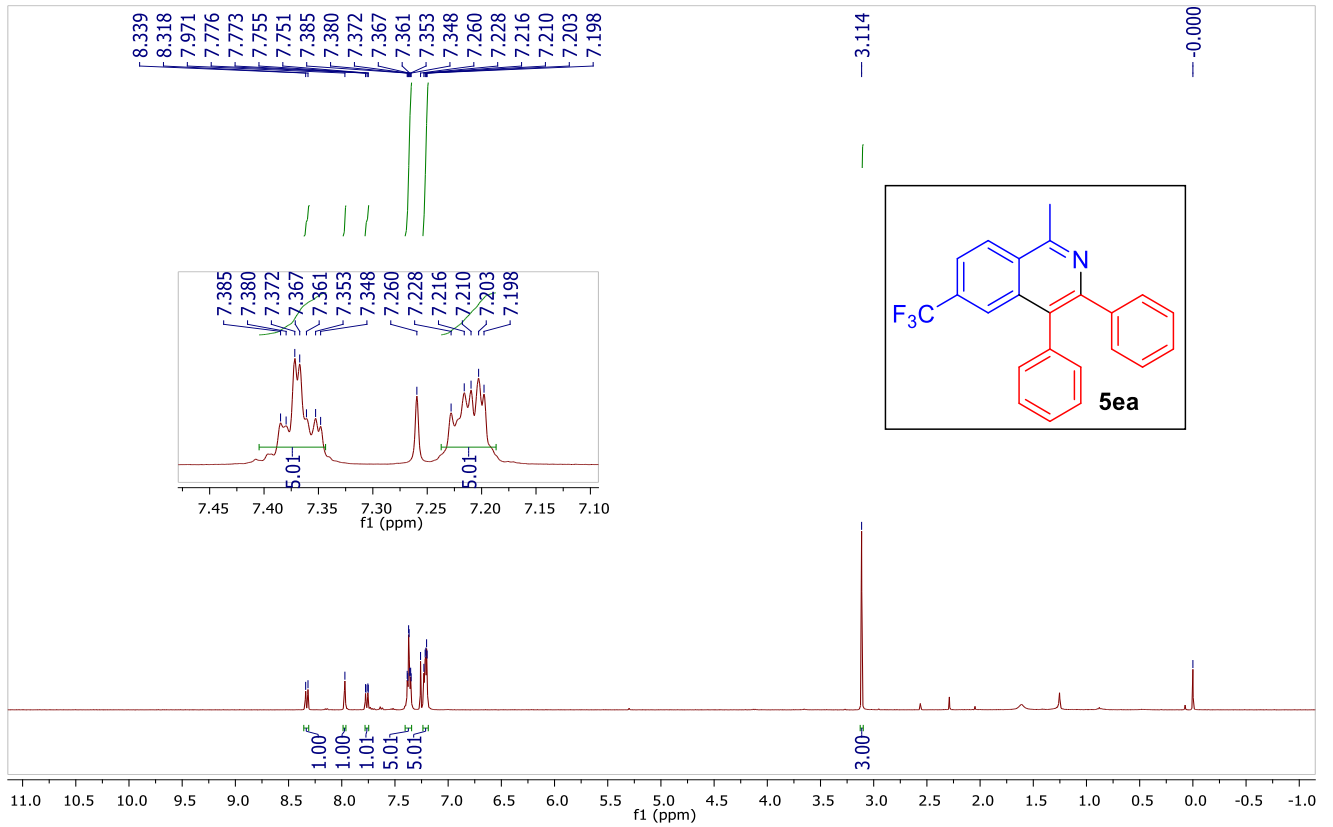
¹H NMR of 5da (400 MHz, CDCl₃)



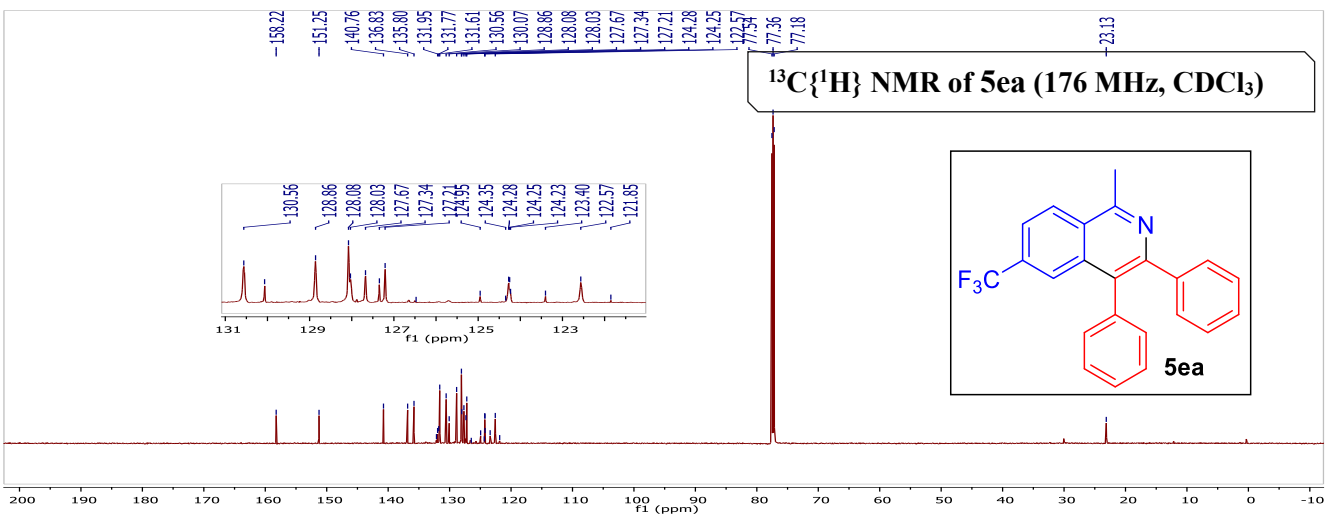
¹³C{¹H} NMR of 5da (100 MHz, CDCl₃)



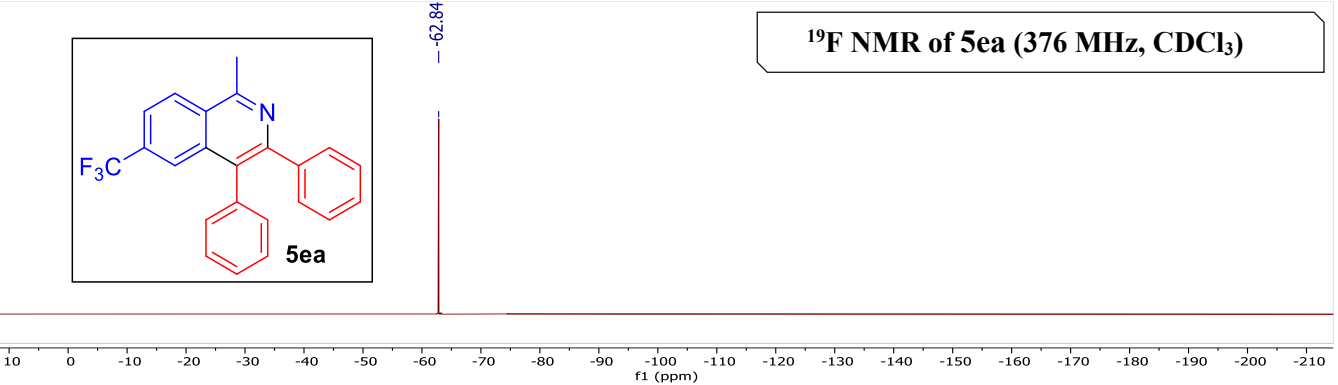
¹H NMR of 5ea (400 MHz, CDCl₃)



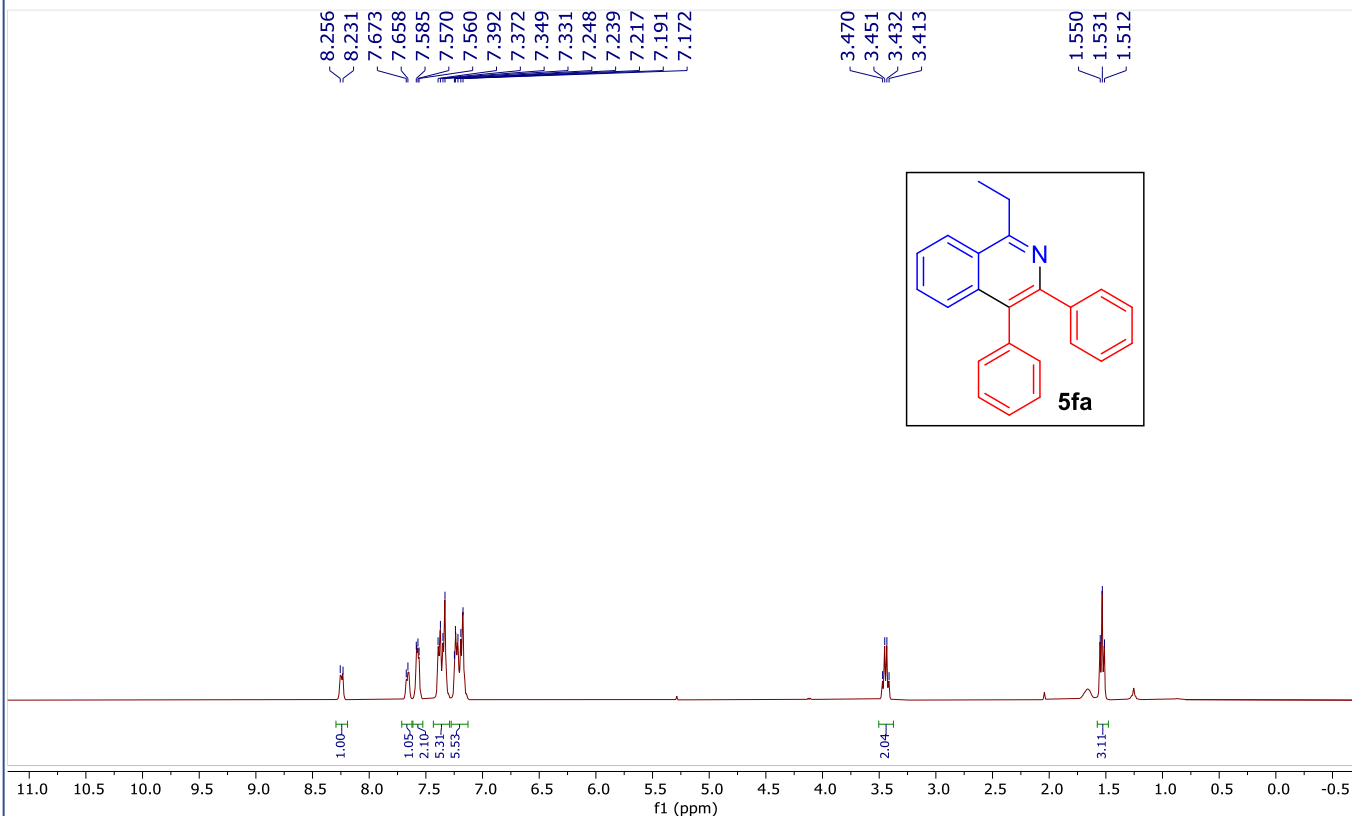
¹³C{¹H} NMR of 5ea (176 MHz, CDCl₃)



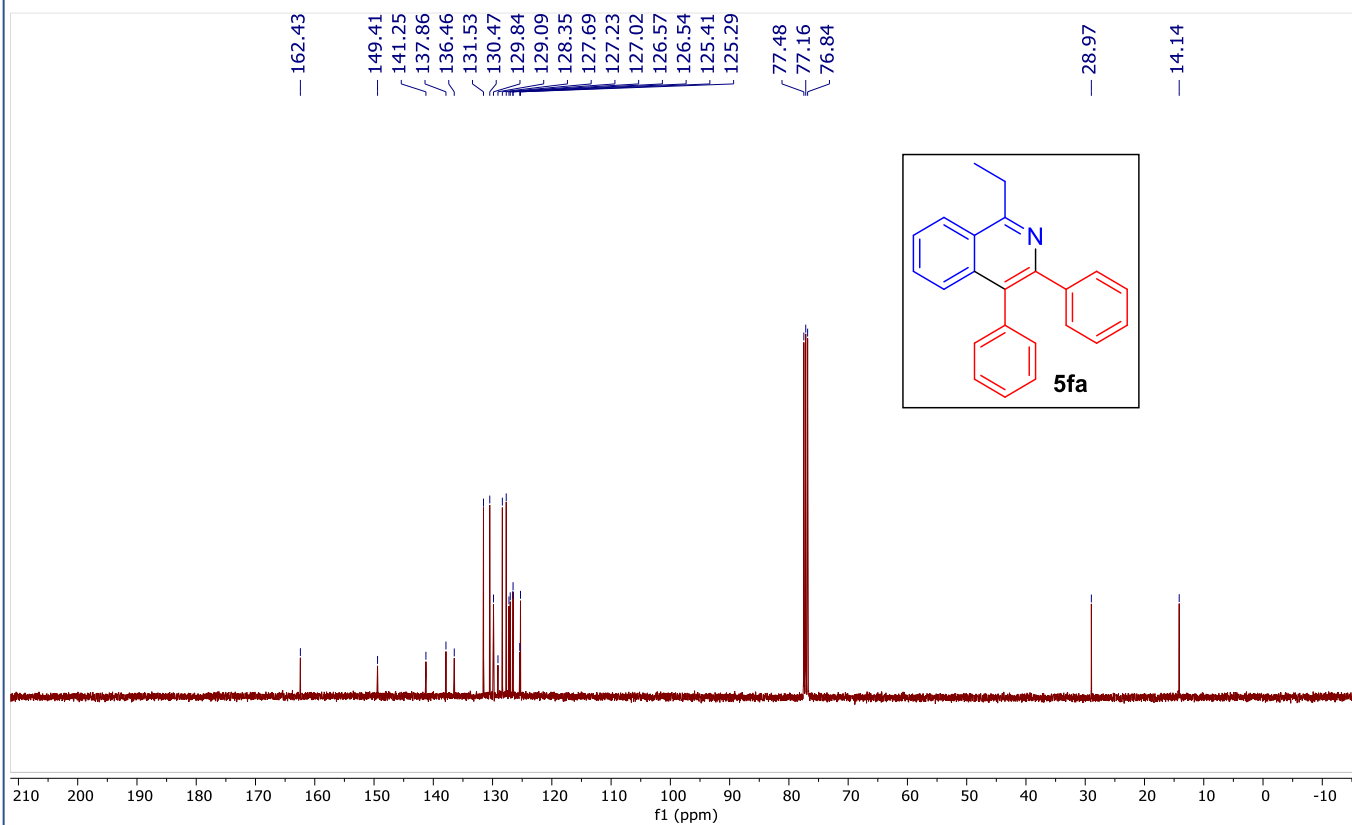
¹⁹F NMR of 5ea (376 MHz, CDCl₃)



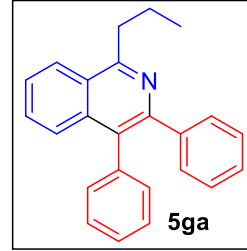
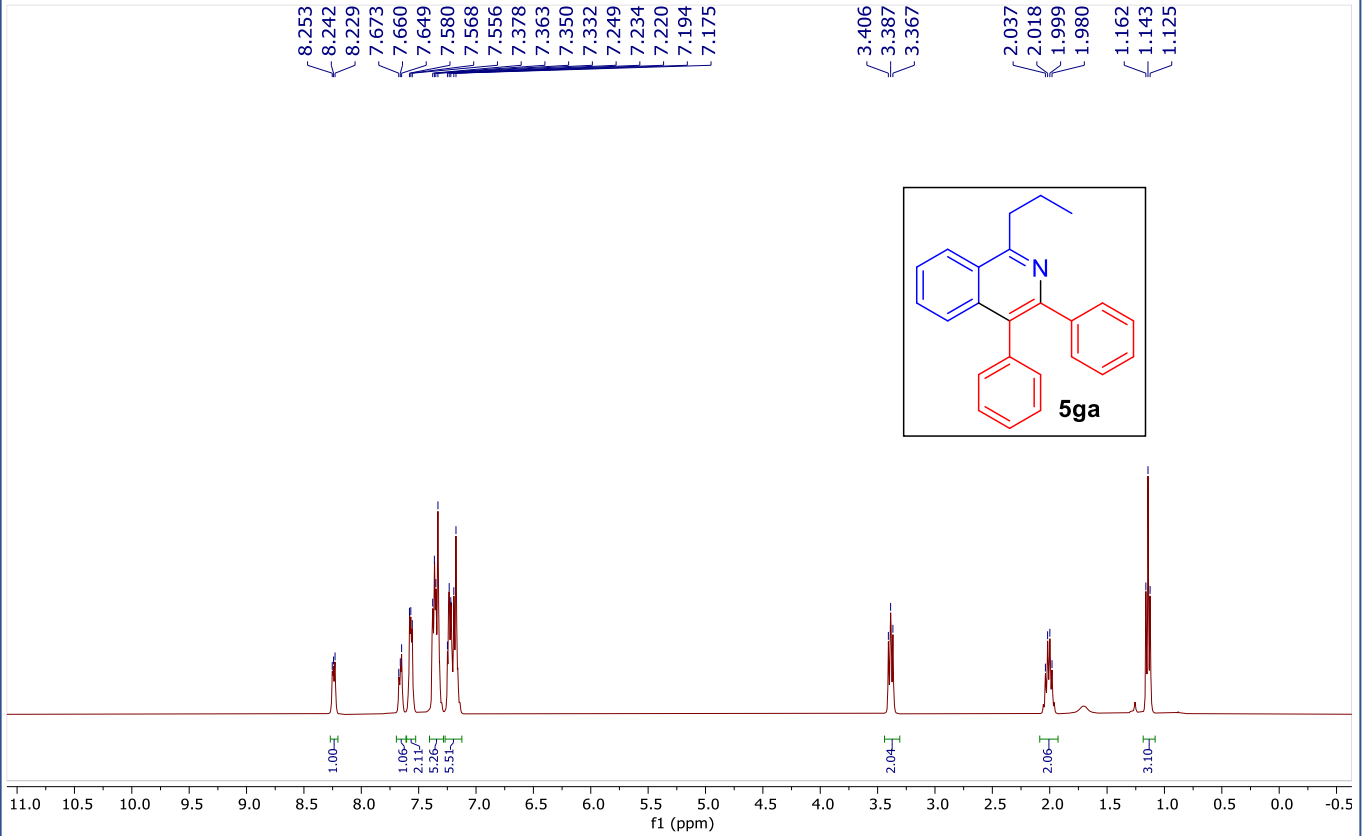
¹H NMR of 5fa (400 MHz, CDCl₃)



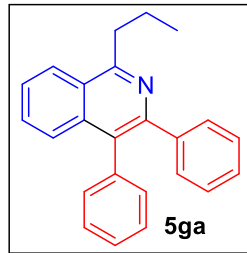
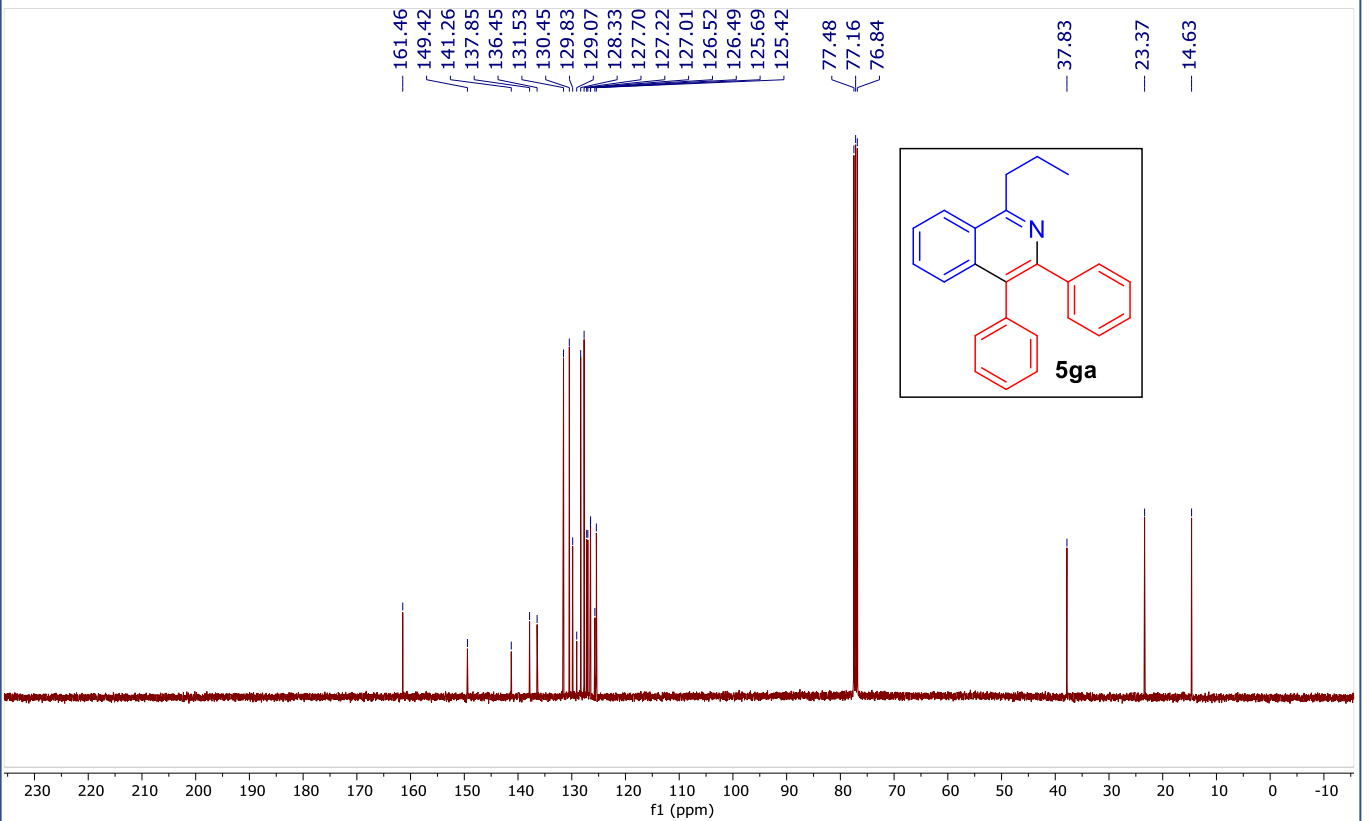
¹³C{¹H} NMR of 5fa (100 MHz, CDCl₃)



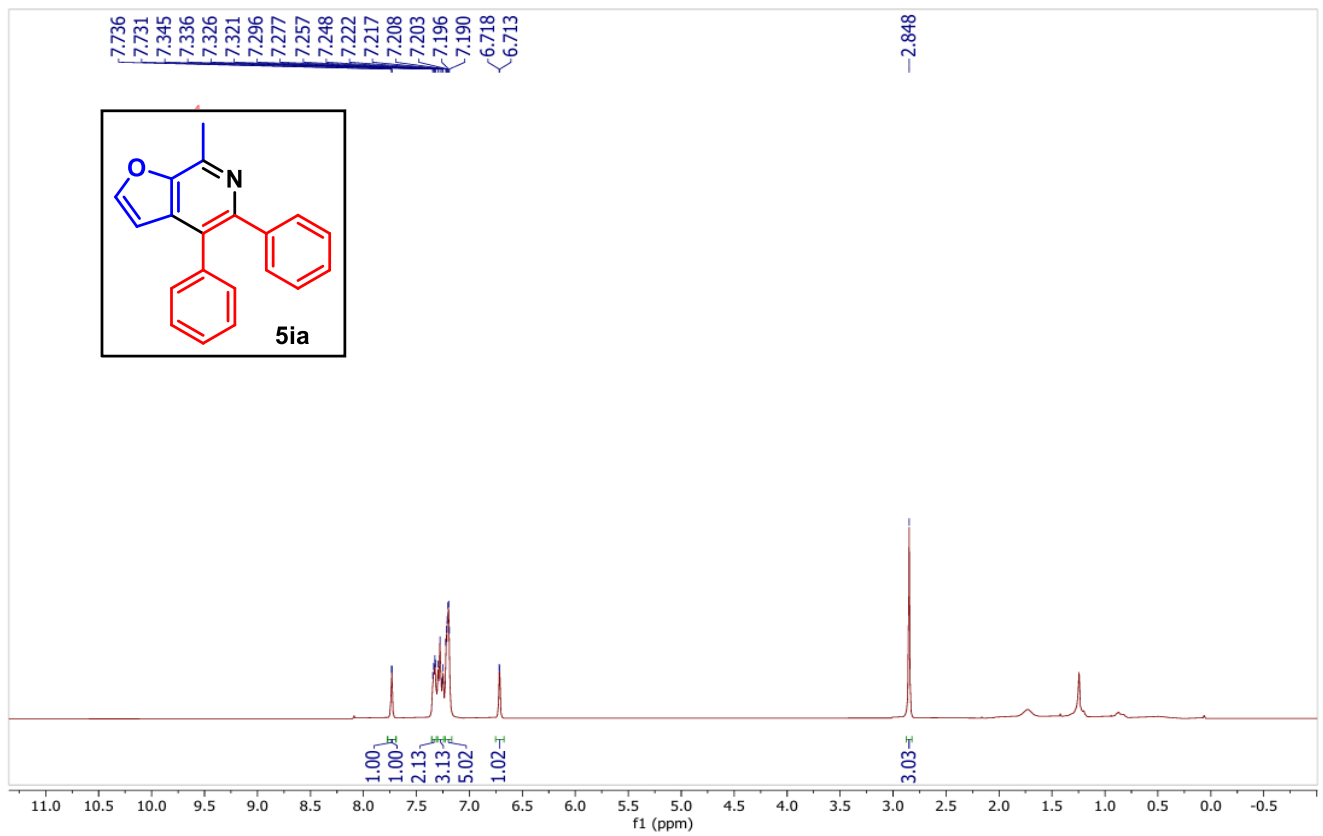
¹H NMR of 5ga (400 MHz, CDCl₃)



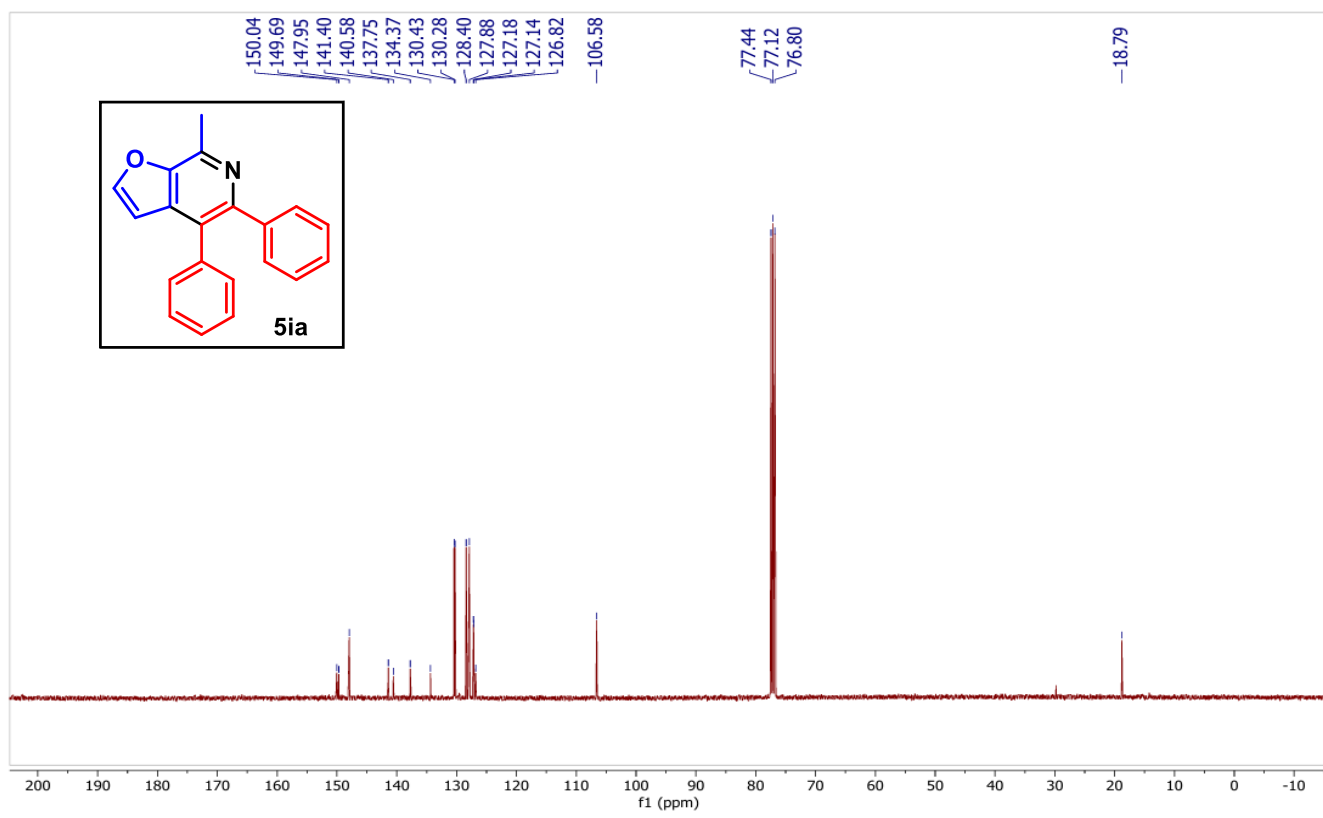
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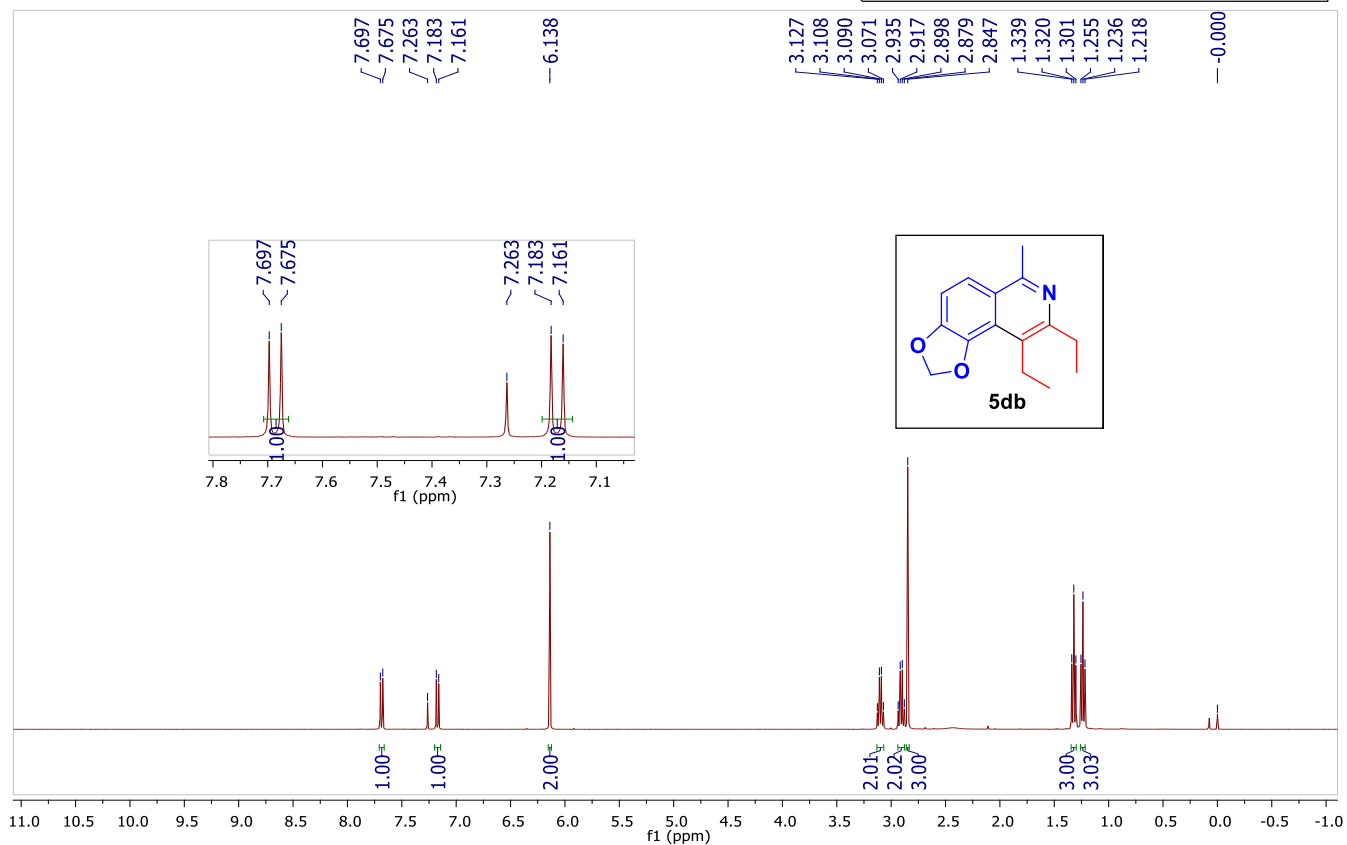
¹H NMR of 5ia (400 MHz, CDCl₃)



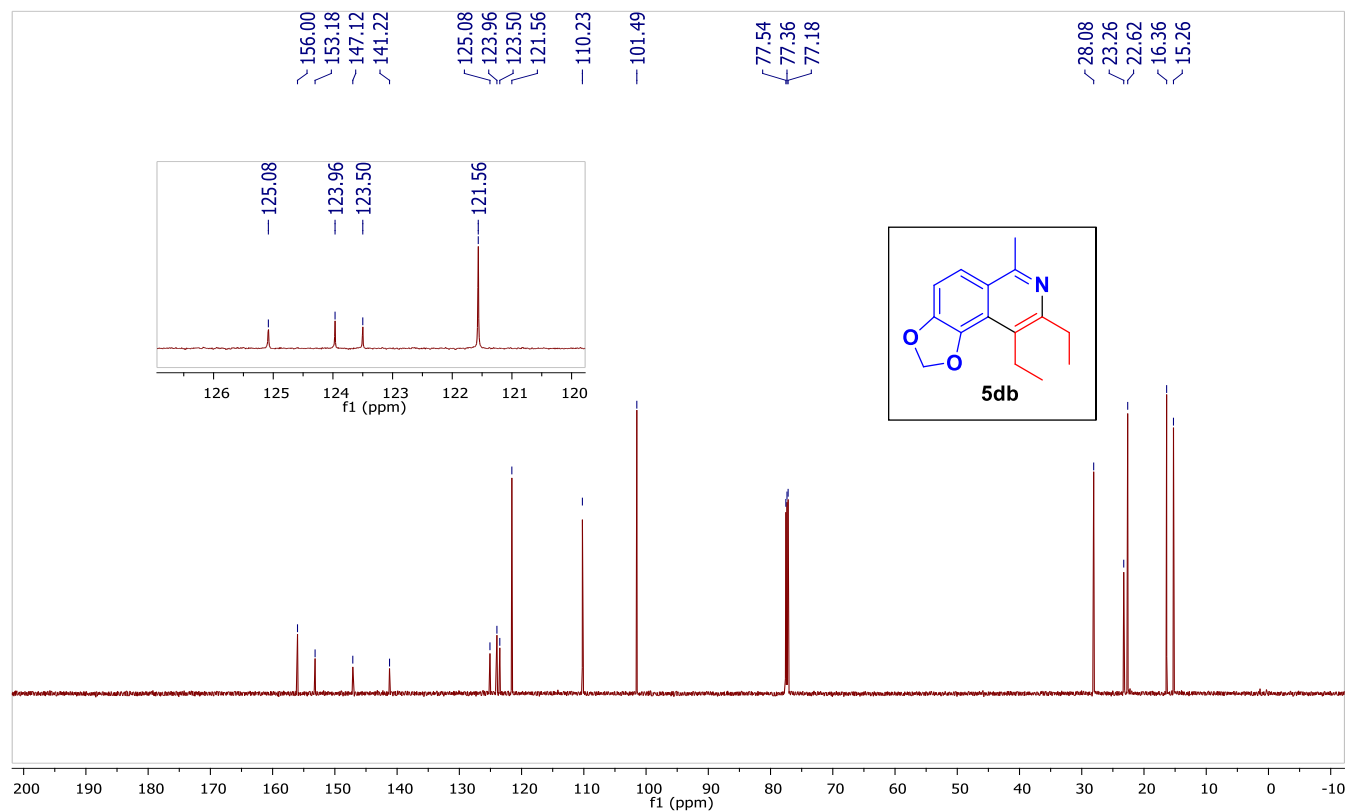
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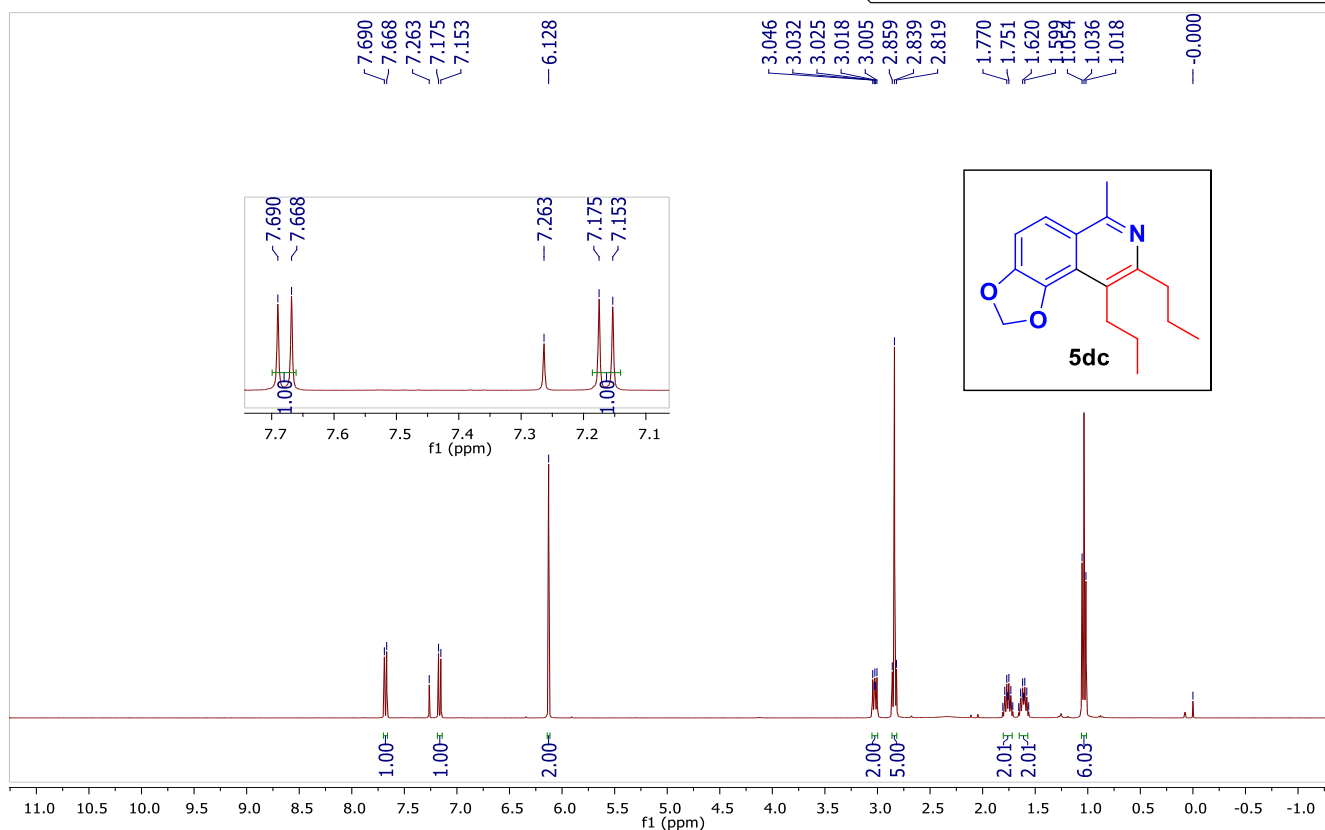
¹H NMR of 5db (400 MHz, CDCl₃)



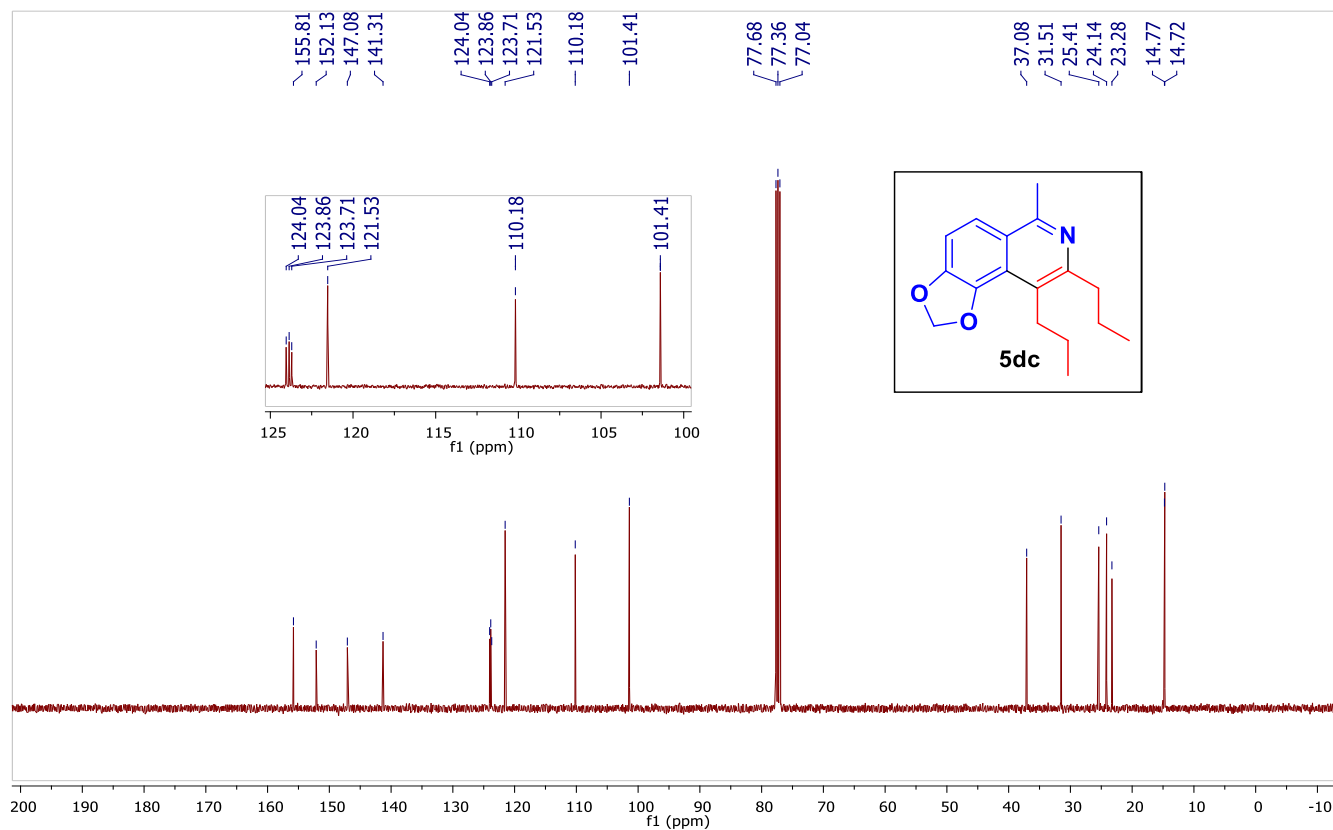
¹³C{¹H} NMR of 5db (176 MHz, CDCl₃)



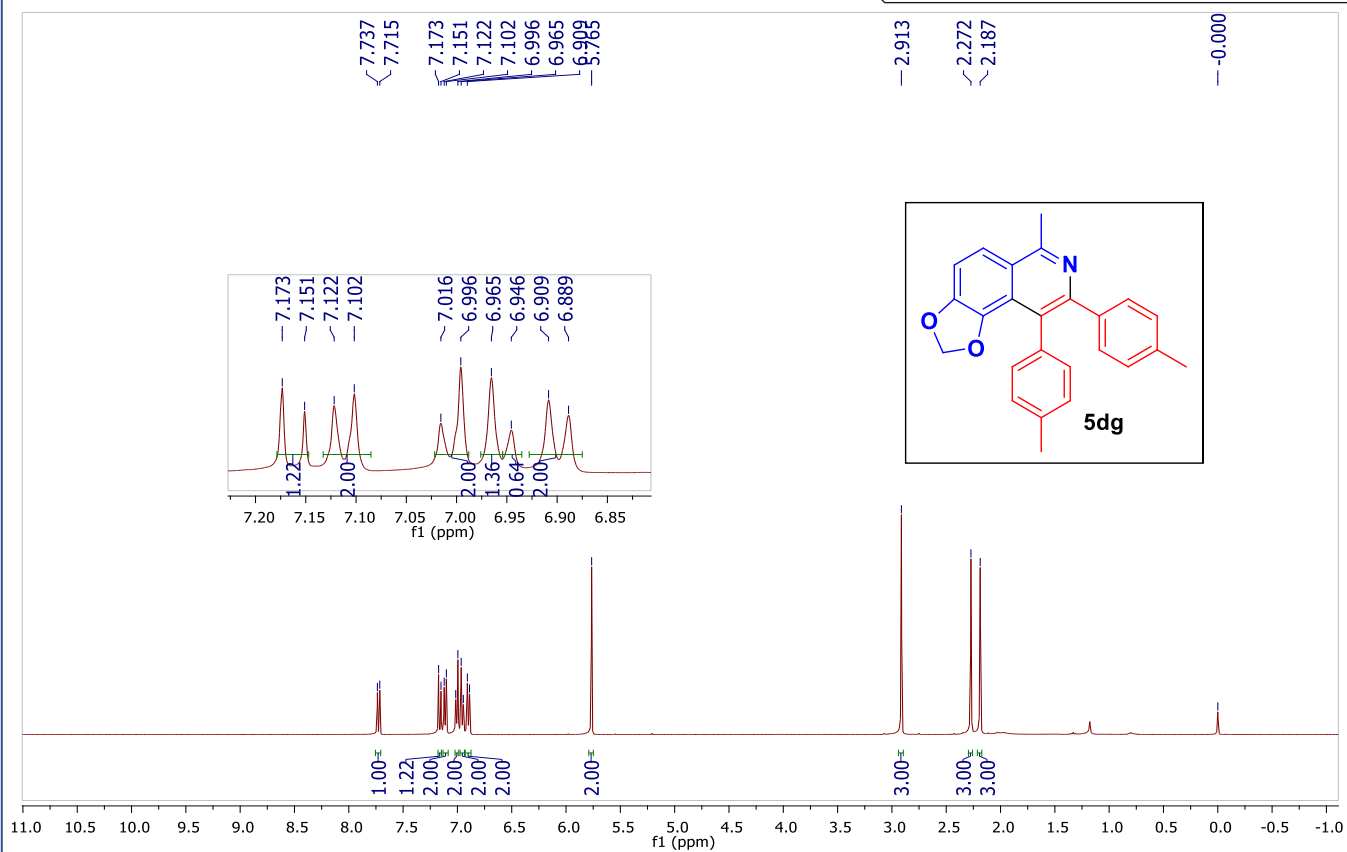
¹H NMR of 5dc (400 MHz, CDCl₃)



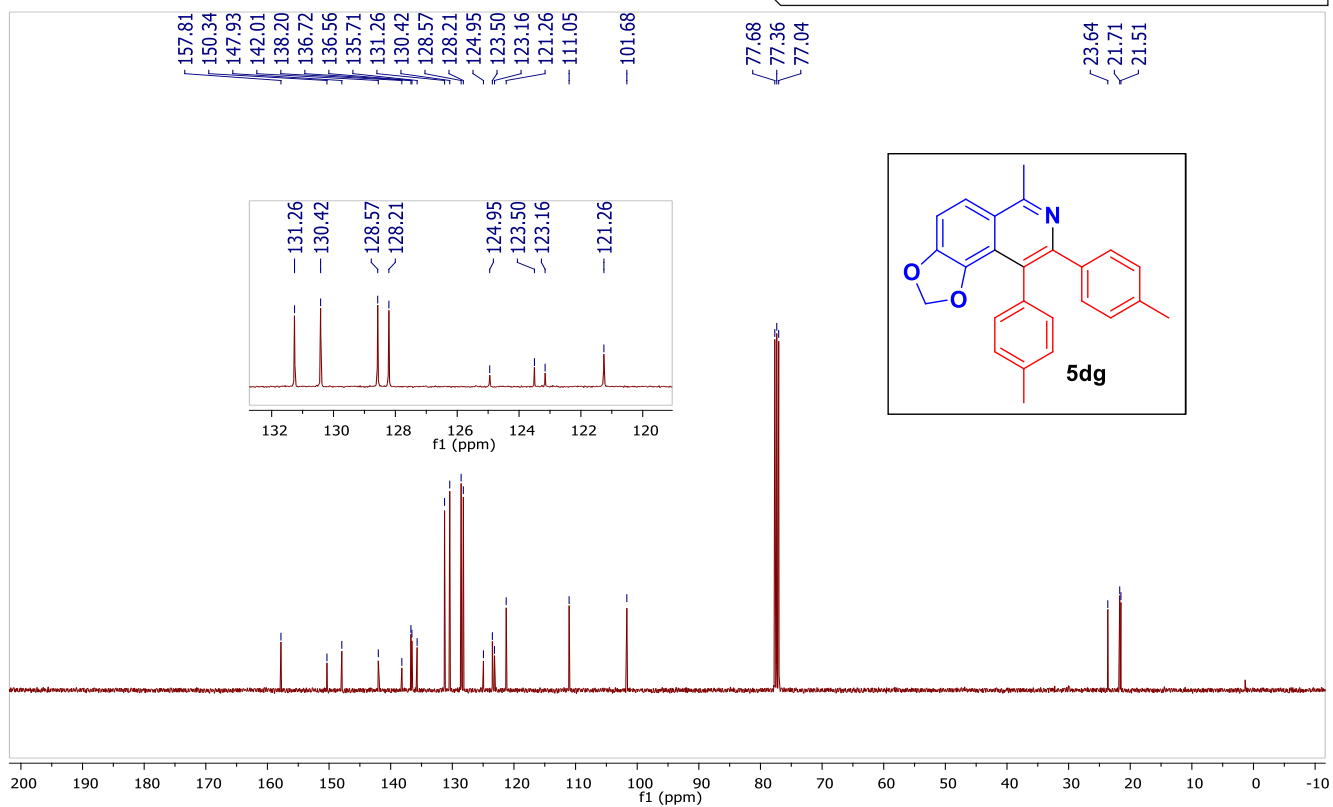
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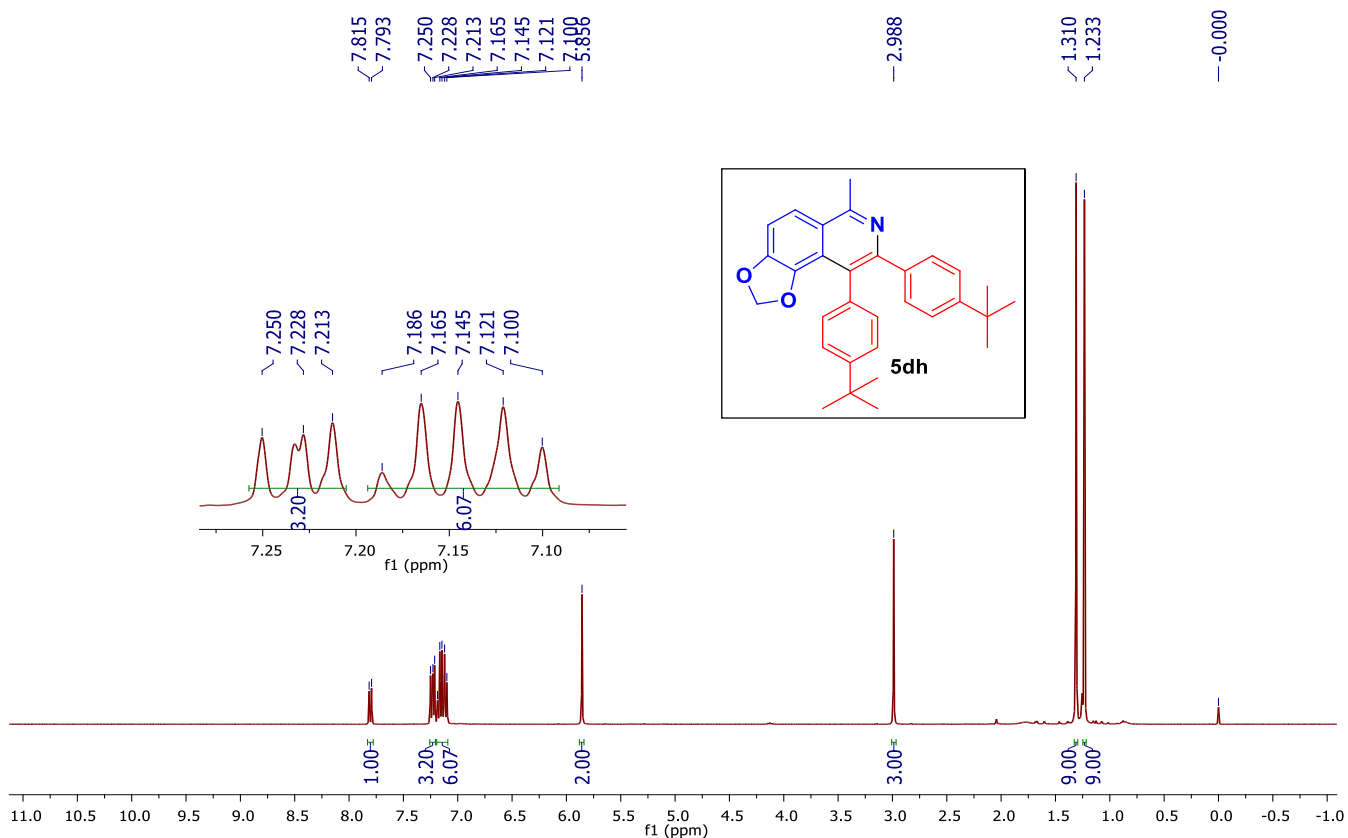
¹H NMR of 5dg (400 MHz, CDCl₃)



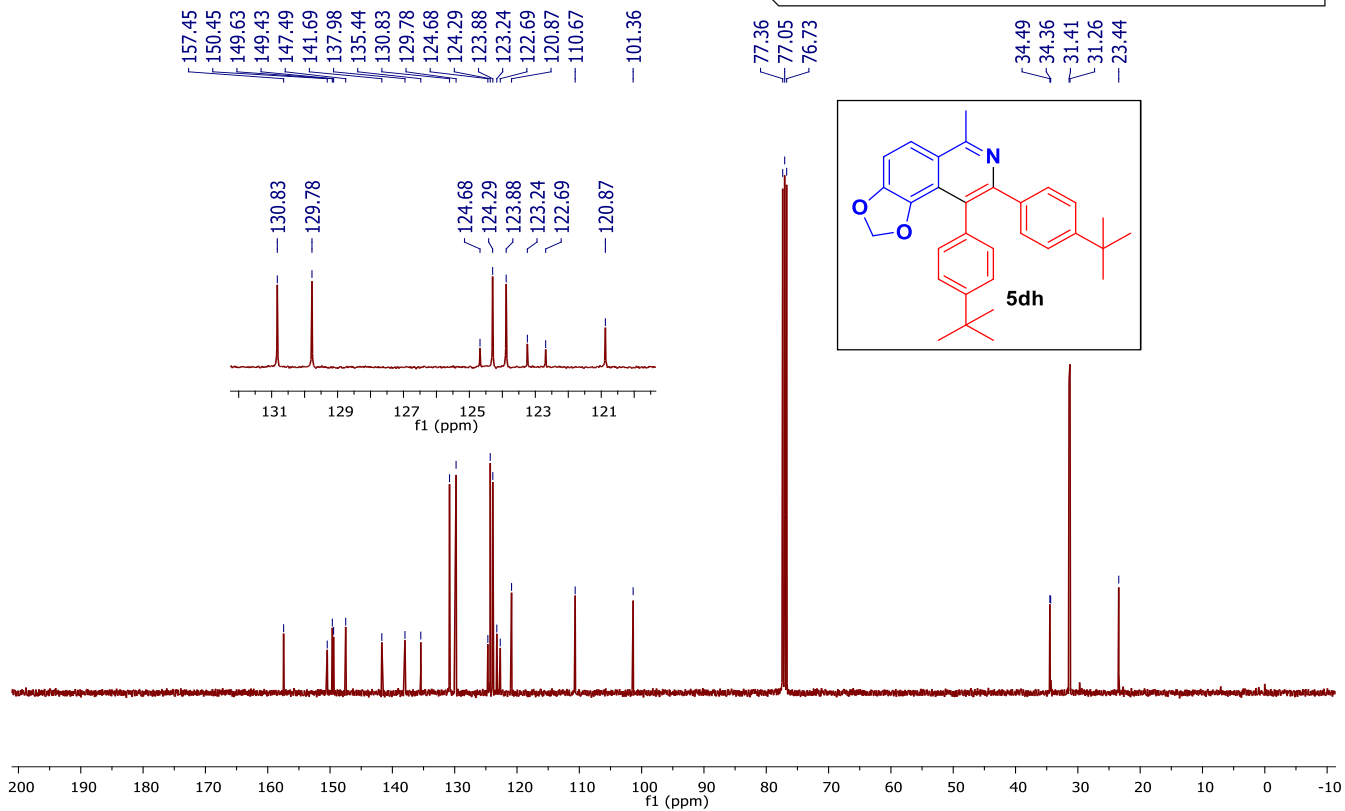
¹³C{¹H} NMR of 5dg (100 MHz, CDCl₃)



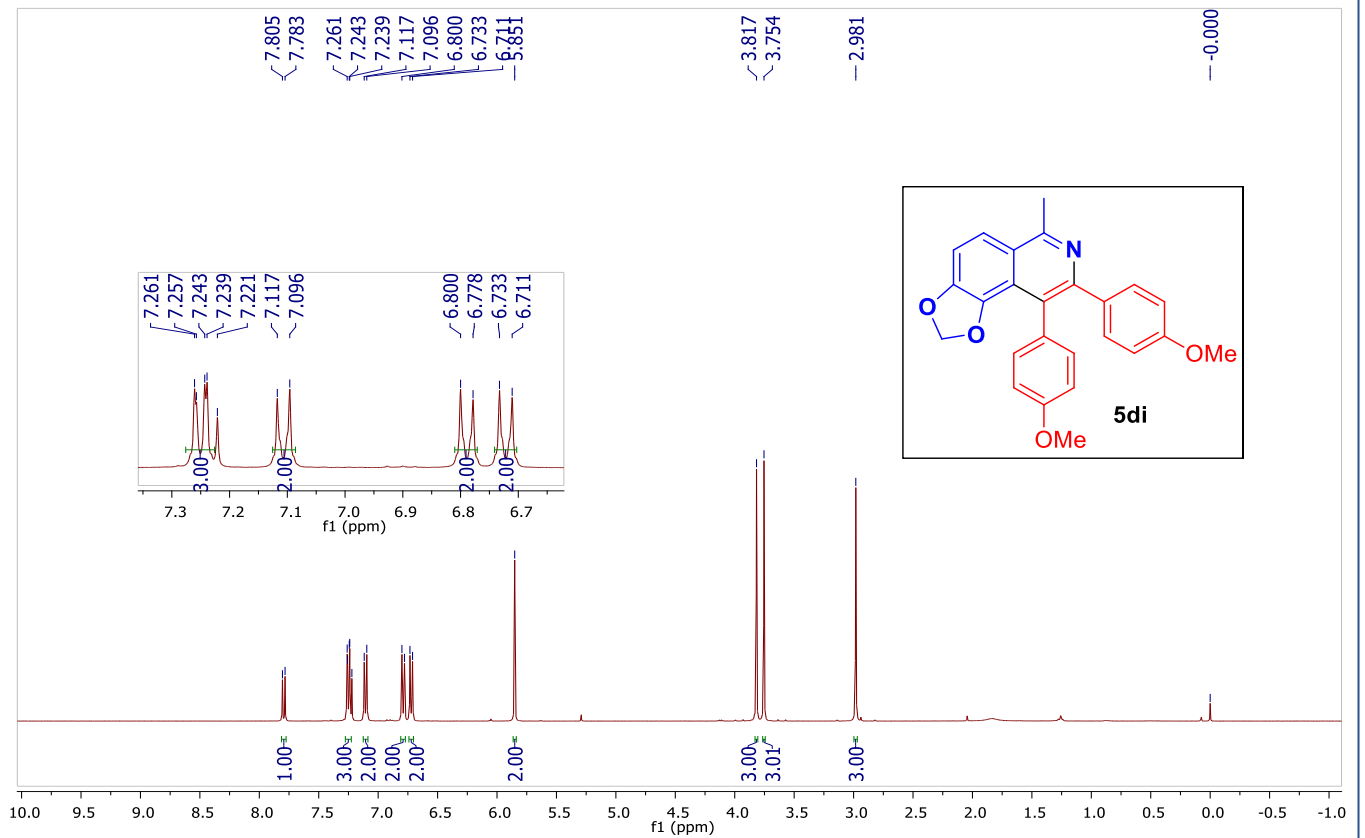
¹H NMR of 5dh (400 MHz, CDCl₃)



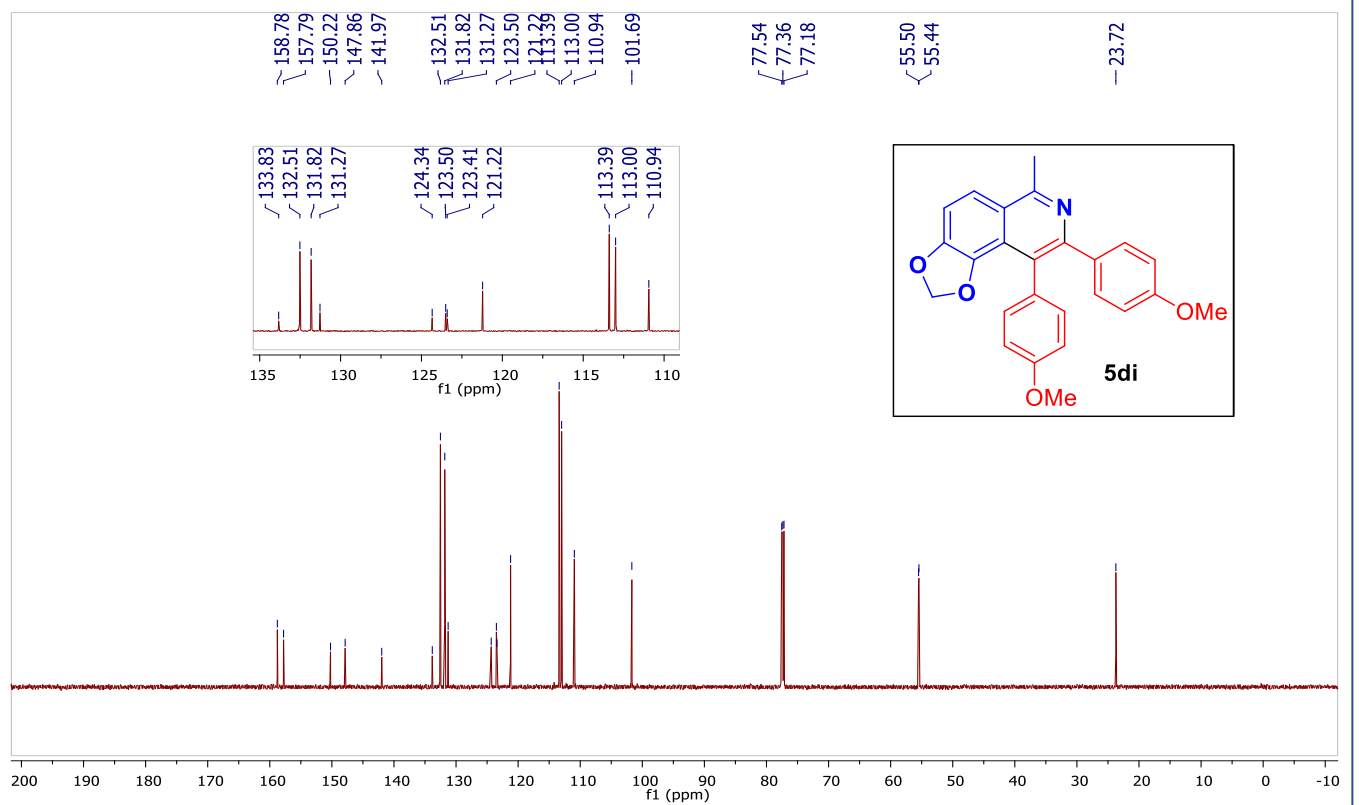
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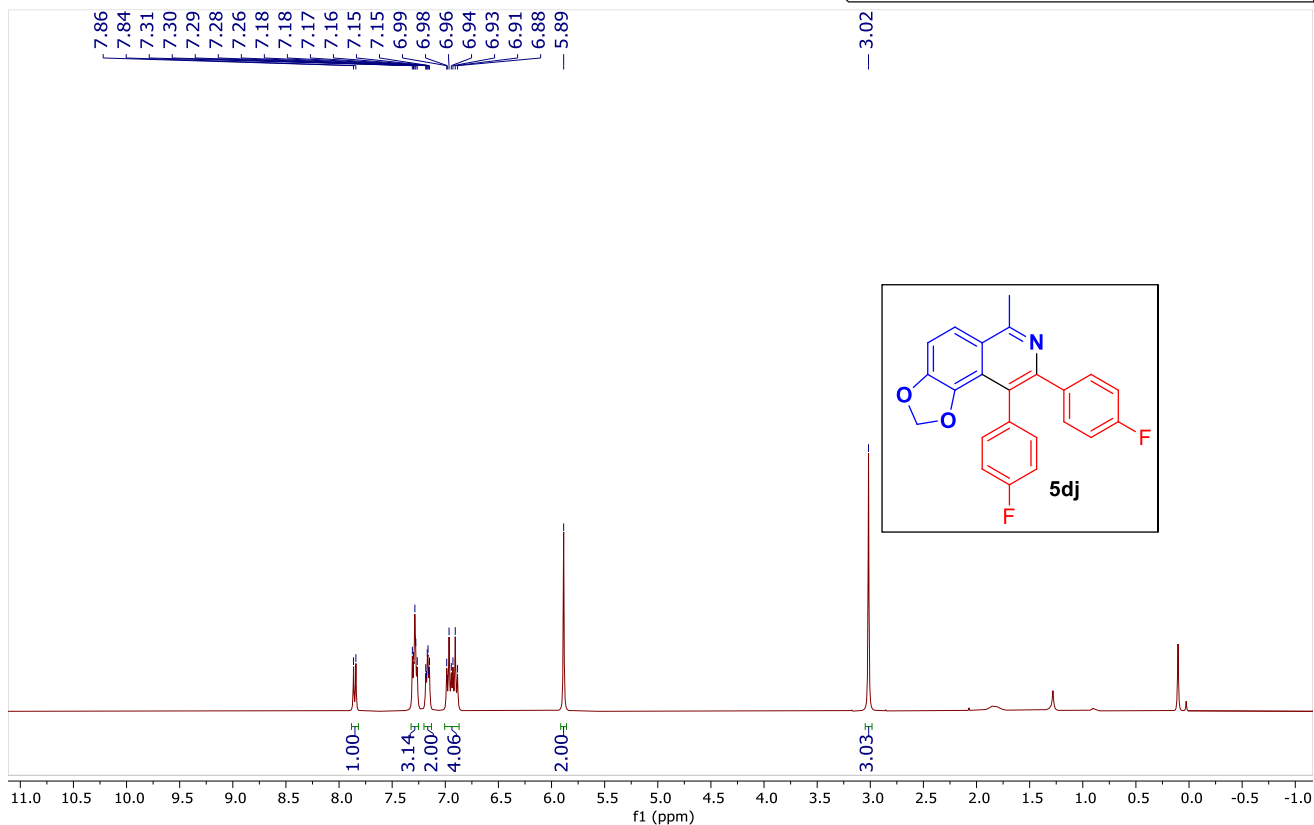
¹H NMR of 5di (400 MHz, CDCl₃)



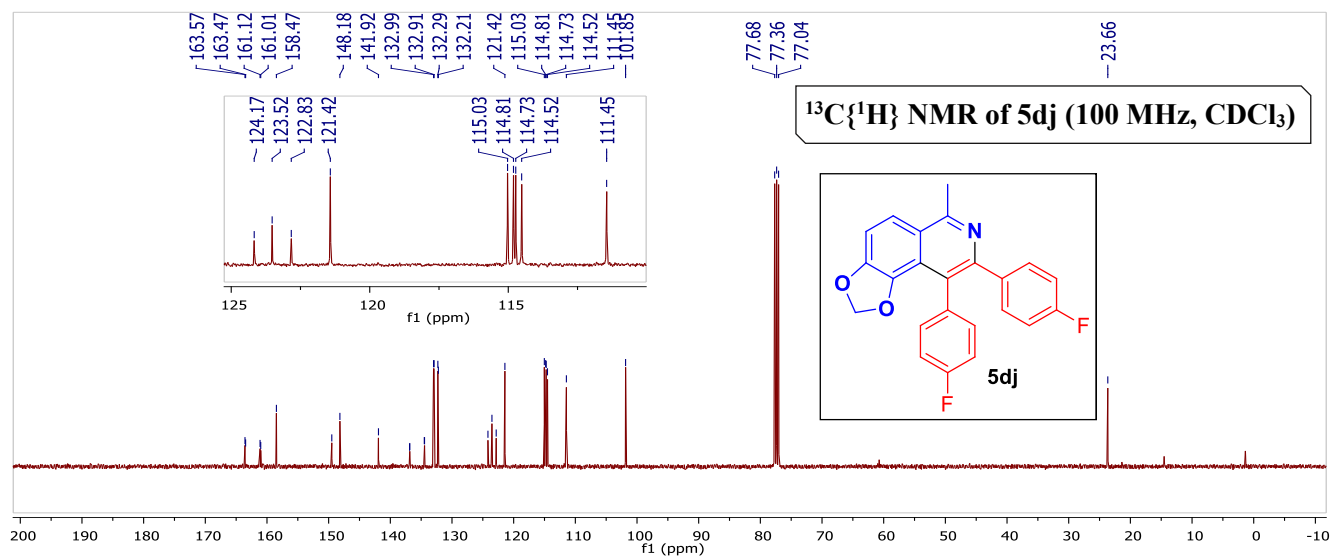
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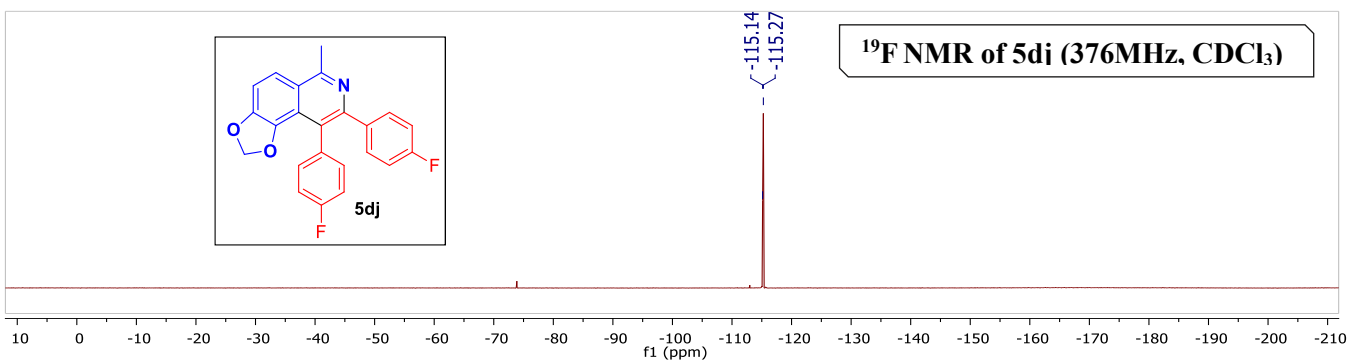
¹H NMR of 5dj (400 MHz, CDCl₃)



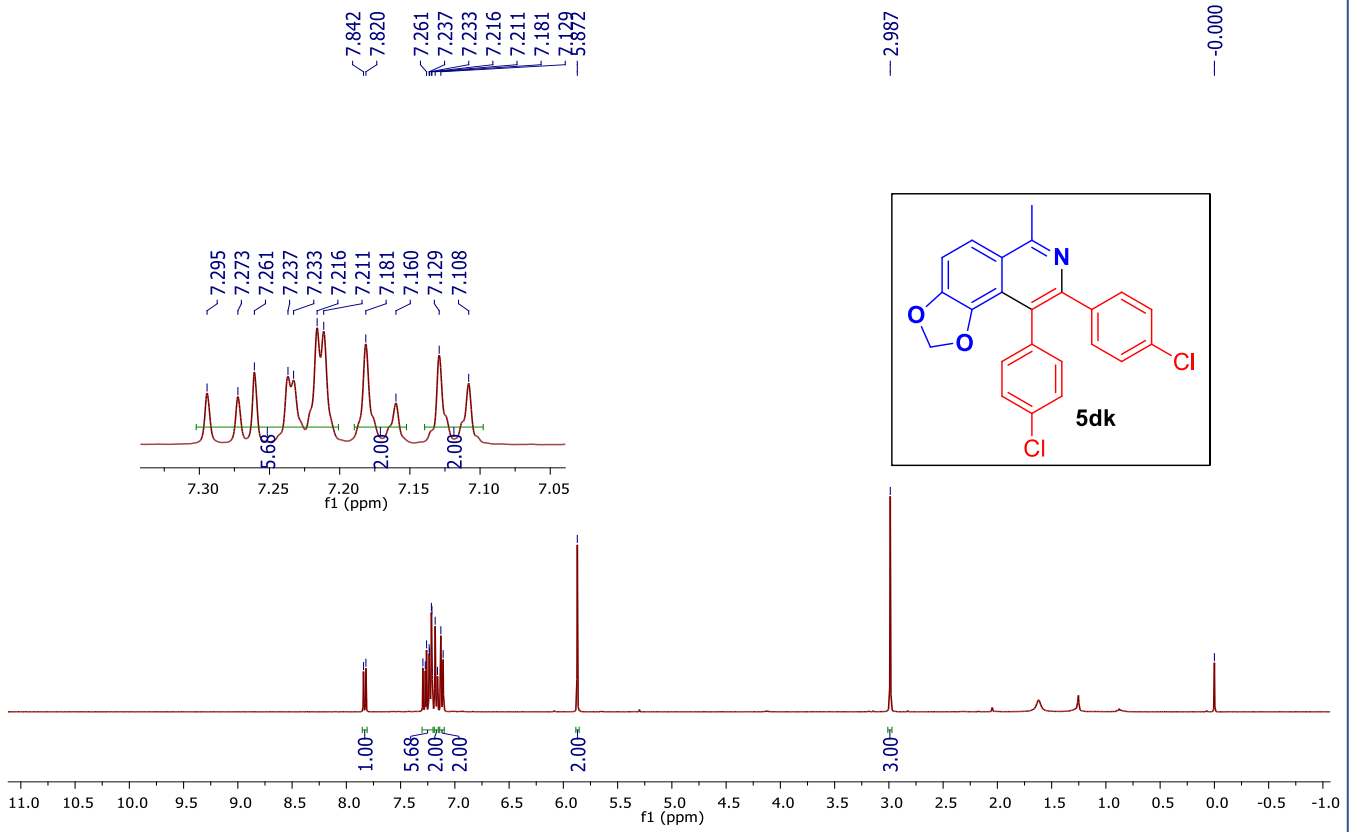
¹³C{¹H} NMR of 5dj (100 MHz, CDCl₃)



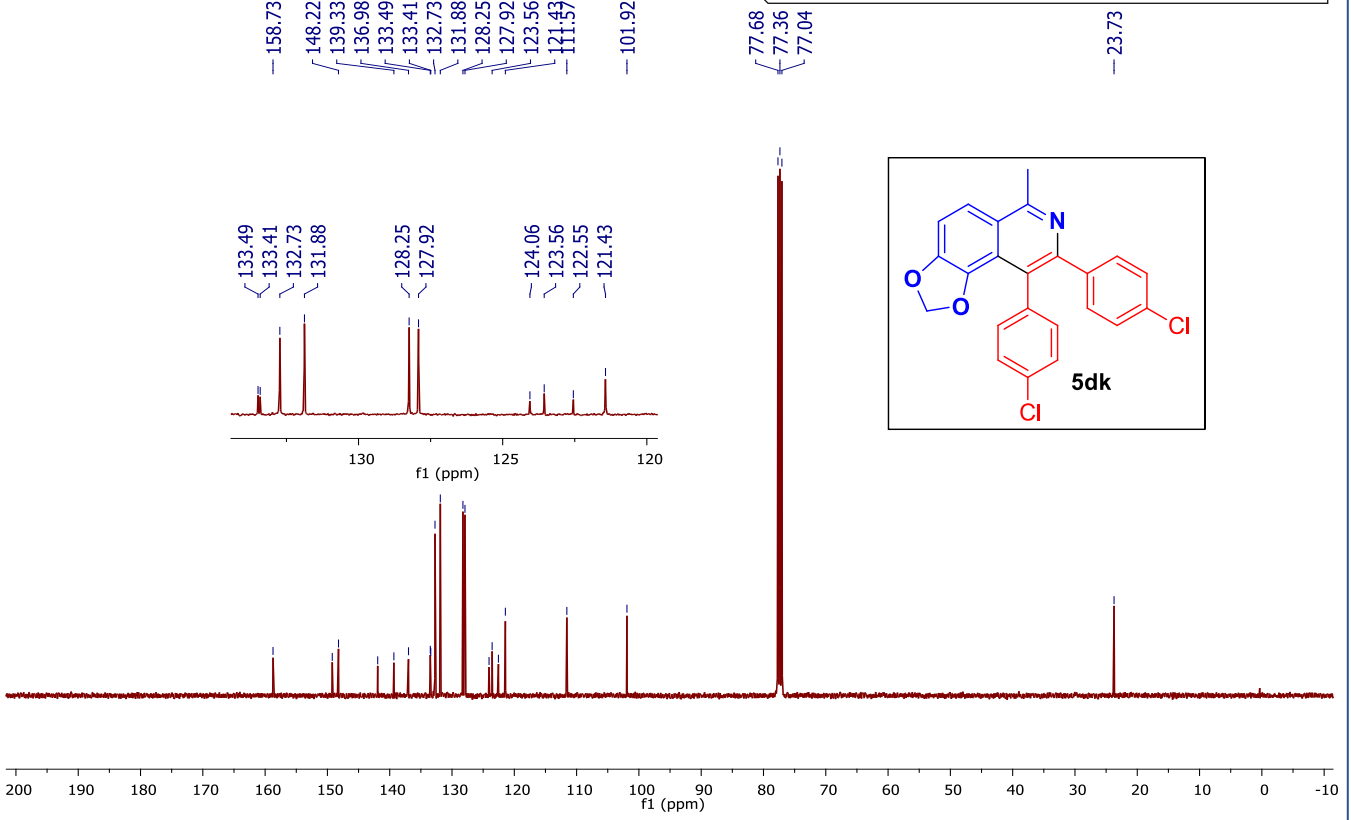
¹⁹F NMR of 5dj (376 MHz, CDCl₃)



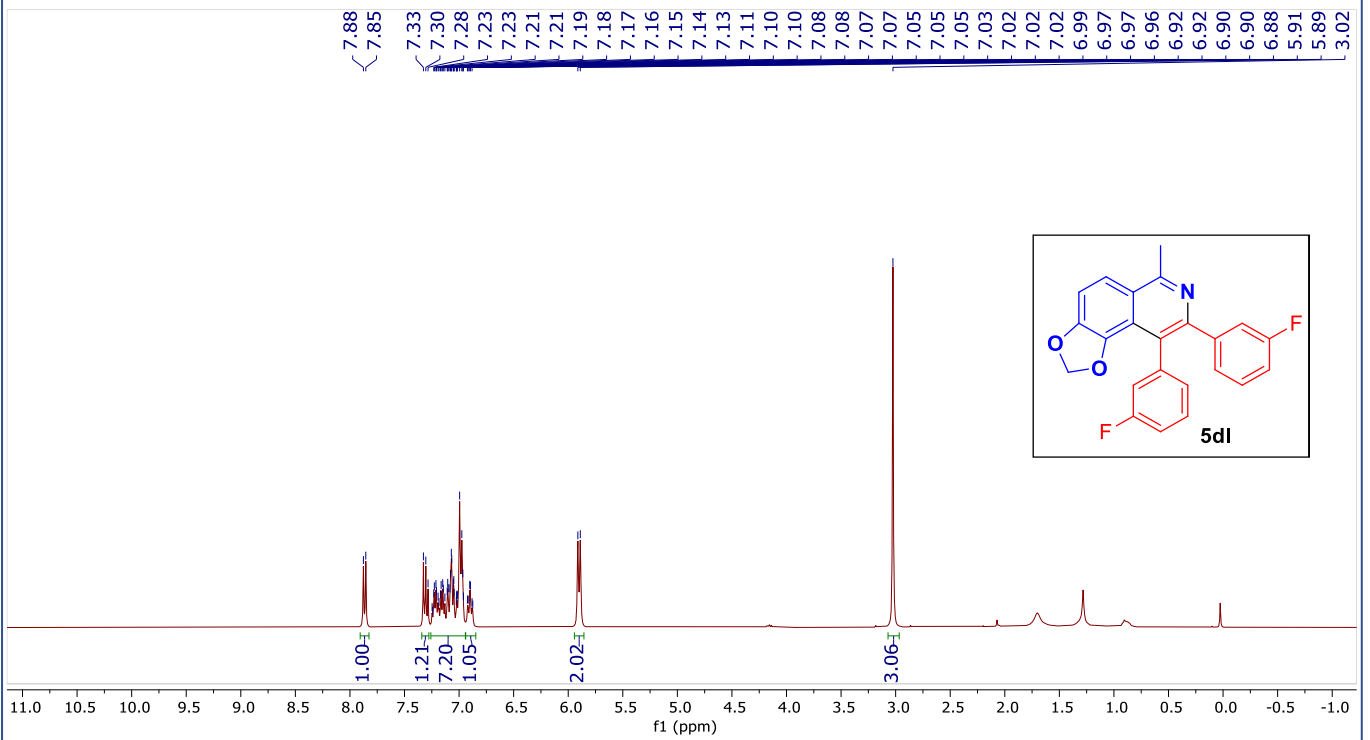
¹H NMR of 5dk (400 MHz, CDCl₃)



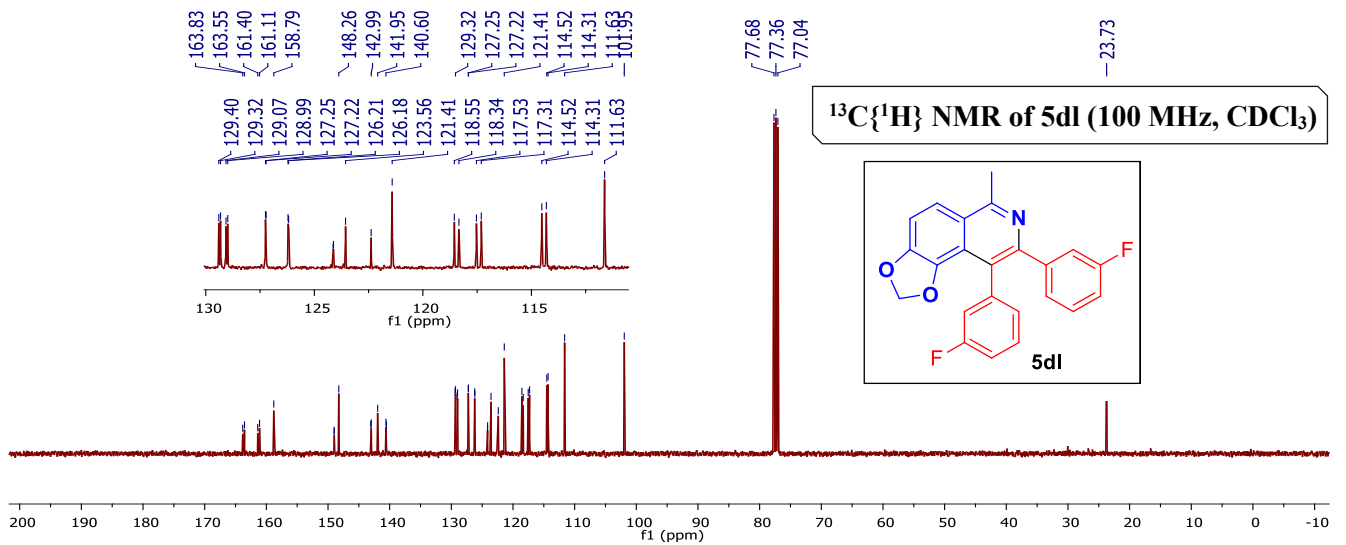
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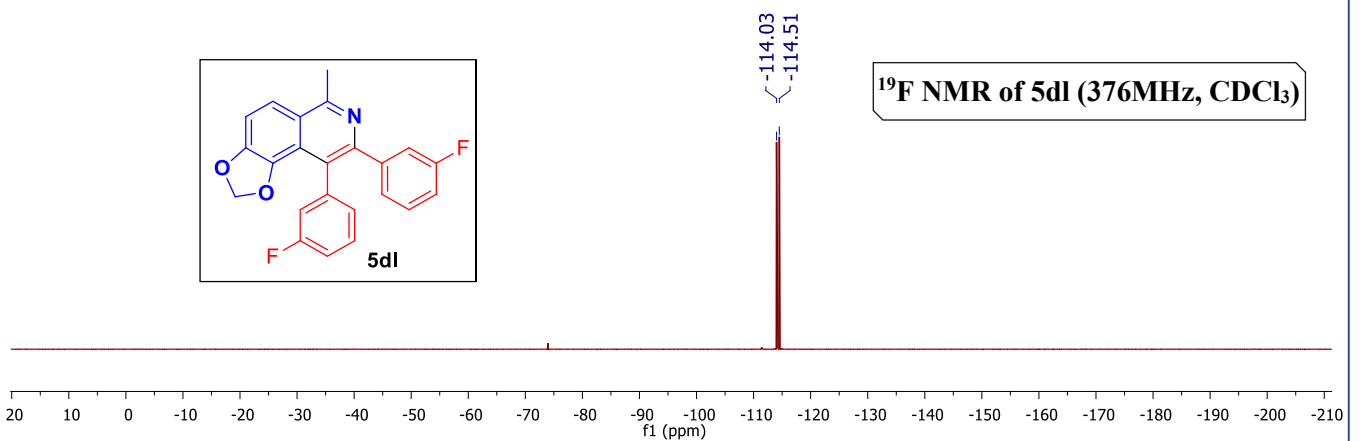
¹H NMR of 5dl (400 MHz, CDCl₃)



¹³C{¹H} NMR of 5dl (100 MHz, CDCl₃)



¹⁹F NMR of 5dl (376 MHz, CDCl₃)



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