Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.

Supporting Information

Organophotoredox-catalyzed redox-neutral cascade involving *N*-(acyloxy)phthalimides and maleimides

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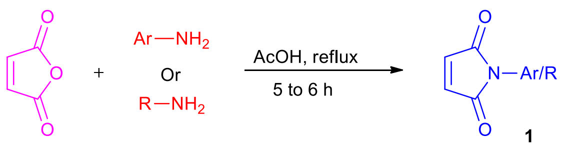
General Information: Photoredox reactions were performed under an argon atmosphere for all the reaction set, using pre-dried glassware and standard glass tubes. All the solvents were dried with calcium hydride and freshly distilled under argon. The following starting materials and the reaction components *N*-phenyl, methyl and ethyl maleimides, *N*-hydroxyphthalimide, maleic anhydride, aniline and alkyl amine derivatives, α-bromoacetic acid, phenol derivatives, *N*,*N*´-diisopropylcarbodiimide (DIC), 4-*N*,*N*-dimethylamino-pyridine (DMAP), NaH, DIPEA, Bu_3N, lutidine, all the photocatalysts and TEMPO were obtained from commercial sources and were used without further purification. Other maleimides and phthalimide ester derivatives were synthesized by the synthetic procedures mentioned below. Yields refer to isolated compounds, estimated to be >95% pure as determined by ^{1}H NMR and ^{13}C NMR. All optimized photoredox reactions were conducted under the photo irradiation using 36 W Kessil blue LED (440 nm) lamp. Thin layer chromatography (TLC) was performed on Merck pre-coated silica gel 60 F254 aluminum sheets with detection under UV light at 254 nm. Chromatographic separations were carried out on Chempure silica gel (60-120 mesh or 100−200 mesh). Nuclear magnetic resonance (NMR) spectroscopy was performed using JEOL 400 MHz and Bruker 500 MHz spectrometers. If not otherwise specified, chemical shifts (δ) are provided in ppm. HRMS spectra were recorded using Bruker Maxis Impact mass spectrometer (TOF). Fluorescence experiment was recorded with a **"HITACHI f-7000"** Scientific Spectrofluorometer.

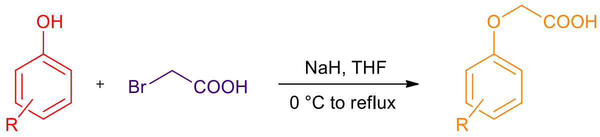
Synthetic procedure of starting materials:

(A) General Procedure to the Direct Synthesis of Maleimides:[1]



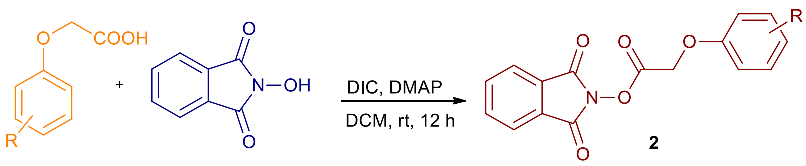
To a stirred solution of maleic anhydride (2.45 gm, 25 mmol, 2.5 equiv) in acetic acid (15 mL) was added the amine (10 mmol, 1 equiv). The reaction mixture was stirred at reflux for 6 h, and then the acetic acid was removed in vacuo. The residue was dissolved in CH_2Cl_2 (20 mL) and washed with aqueous $NaHCO_3$ (2 × 30 mL), HCl (1 M, 2 × 30 mL), and saturated aqueous NaCl (30 mL). The organic layer was separated, dried over Na_2SO_4, and the solvent was removed in vacuo. Maleimides **1** were further purified by 60-120 mesh silica gel column chromatography using 20% ethylacetate in hexane as the eluent to obtain **1b-l**.

(B) General Procedure for the Synthesis of *α*-alkoxy Carboxylic Acids:[2]



An oven dried 250 mL three-necked flask was equipped with a magnetic stir bar and a reflux condenser. Sodium hydride (1.20 g, 60% dispersion in mineral oil, 30 mmol, 3 equiv) was then suspended in dry THF (20 mL) at 0 ˚C under argon. Phenol derivative (10 mmol), dissolved in dry THF (30 mL), was then added slowly. After 30 min, bromoacetic acid (1.39 gm, 10 mmol, 1 equiv), dissolved in dry THF (30 mL), was added drop wise. The mixture was heated to reflux, and the progress of the reaction was monitored by TLC. Upon completion of the reaction, as shown by TLC, the mixture was cooled down to room temperature and diluted with water (60 mL). The mixture was extracted with hexane (2 x 30 mL), the aqueous layer was acidified with HCl (2 M) until pH 2 was reached and extracted with DCM (3 x 30 mL). The combined organic layers were dried over Na_2SO_4, the solvent was removed under reduced pressure and the crude mixture was purified by column chromatography on silica gel (petroleum ether / ethyl acetate) to give the pure *α*-alkoxy carboxylic acids.

(C) General procedure for the synthesis of *N*-(acyloxy)phthalimides:[3]

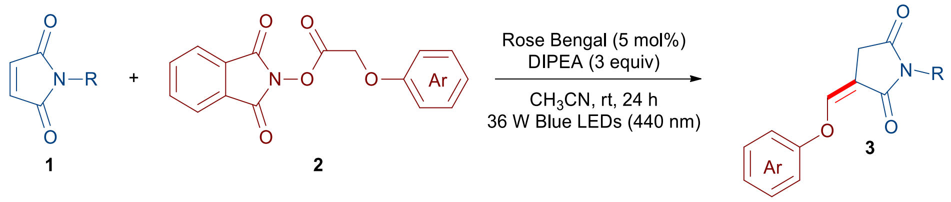


The *N*-hydroxyphthalimide (1.63 g, 10 mmol, 1.1 equiv), corresponding carboxylic acid (12 mmol, 1.2 equiv), *N,N´*-dicyclohexylcarbodiimide (2.47 g, 12 mmol, 1.2 equiv) and 4-dimethylaminopyridine (0.61 g, 0.50 mmol, 5 mol%) were added in a pre-dried reaction flask. DCM (15 mL) was then added and the orange reaction mixture was stirred for 12 h at room temperature. The white precipitate was filtered off and the solution was concentrated by evaporation. Purification by silica gel column chromatography using 20% ethyl acetate in hexane delivered the *N*-(acyloxy)phthalimides **2**.

Optimization study for the organophotoredox catalyzed cascade radical annulation:

1-phenyl-1H-pyrrole-2,5-dione (**1a**, 43 mg, 0.25 mmol, 1.0 equiv), *N*-(acyloxy)phthalimide (**2a**, 0.275 mmol, 90 mg, 1.1 equiv), photocatalyst (2-5 mol%), and organic base (0.90 mmol, 3.0 equiv) were placed in a pre-dried 15 mL reaction tube. The tube was degassed and purged with argon three times. Solvent (3.0 mL) was added, and the mixture was irradiated under 36 W 440 nm Kessil blue LED lamp and stirred for 24 h under argon atmosphere using a balloon filled with argon gas. The reaction mixture was then concentrated under vacuum, and purified by silica gel column chromatography using 7-10% ethyl acetate in hexane to deliver the annulated product **3aa**.

General procedure for the organophotoredox catalyzed addition/oxidation cascade involving *N*-(acyloxy)phthalimides and Maleimides (GP):



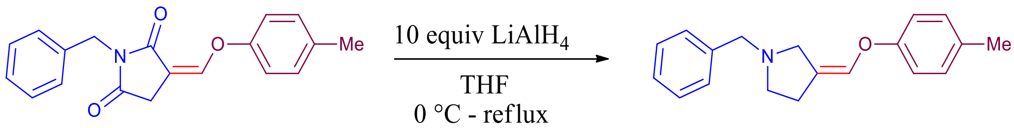
N-aryl/alkyl maleimide derivative **1** (0.25 mmol, 1.0 equiv), *N*-(acyloxy)phthalimide **2** (0.275 mmol, 1.1 equiv), Rose Bengal (13 mg, 15 µmol, 5 mol%), and DIPEA (116 mg, 0.90 mmol, 3.0 equiv) were placed in a pre-dried 15 mL reaction tube. The tube was degassed and purged with argon three times. Acetonitrile (3.0 mL) was added, and the mixture was irradiated using 36 W Kessil blue LED (440 nm) lamp and stirred for 24 h under argon atmosphere using a balloon filled with argon gas. The reaction mixture was then concentrated under vacuum, and purified by silica gel column chromatography using 8-10% ethyl acetate in hexane to deliver the annulated product **3.**

Gram Scale Synthesis of 3aa:

1-phenyl-1H-pyrrole-2,5-dione **1a** (8.0 g, 4.0 mmol, 1.0 equiv), 1,3-dioxoisoindolin-2-yl 2-(*p*-tolyloxy)acetate (**2a**, 1.37 g, 4.4 mmol, 1.1 equiv), photocatalyst (240 µmol, 5 mol%), and DIPEA (12.0 mmol, 3.0 equiv) were placed in a pre-dried 100 mL two neck round bottom flask. The flask was degassed and purged with argon three times. Acetonitrile (48.0 mL) was added, and the mixture was irradiated under 36 W 440 nm Kessil blue LED lamp and stirred for 24 h under argon atmosphere using a balloon filled with argon gas. The reaction mixture was then concentrated under vacuum, and purified by silica gel column chromatography using 8% ethyl acetate in hexane to deliver the annulated product **3aa** (750 mg, 64%) as an isolated product.

Product Derivation:

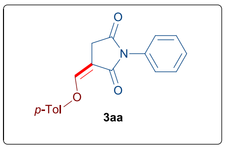
1) Synthesis of (*Z*)-1-benzyl-3-((*p*-tolyloxy)methylene)pyrrolidine



$LiAlH_4$ (10 equiv) was slowly added to a solution of pyrrolidinedione (0.2 mmol) in dry THF (3 ml) at 0 °C and the resulting reaction mixture was refluxed for 5h. Following which, the solution was cooled to 0 °C, EtOAc (10 ml) was added and product was extracted. The reaction mixture was concentrated and purified by column chromatography using silica gel. The product was isolated in 55% yield (31 mg).

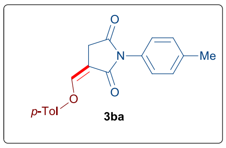
Report of NMR spectra:

(*Z*)-1-phenyl-3-((*p*-tolyloxy)methylene)pyrrolidine-2,5-dione (3aa): **GP** was

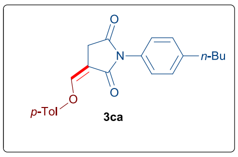


followed using Rose Bengal (13 mg, 5.0 mol %), *N*-phenyl maleimide **1a** (43 mg, 0.25 mmol), and 1,3-dioxoisoindolin-2-yl 2-(*p*-tolyloxy)acetate **2a** (86 mg, 0.275 mmol). After 24 h, purification by column chromatography using 8% ethyl acetate in hexanes yielded **3aa** (61 mg, 83%). **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.83 (s, 1H), 7.49 (t, J = 7.7 Hz, 2H), 7.39 (t, J = 7.4 Hz, 1H), 7.35 (d, J = 7.5 Hz, 2H), 7.19 (d, J = 8.2 Hz, 2H), 7.02 (d, J = 8.4 Hz, 2H), 3.56 (d, J = 1.8 Hz, 2H), 2.36 (s, 3H). **^{13}CNMR** (126 MHz, $CDCl_3$) δ 173.2, 169.9, 154.6, 150.0, 135.1, 132.2, 130.7, 129.3, 128.6, 126.7, 117.3, 106.9, 31.3, 20.9. HRMS-ESI (m/z): calcd for $C_{18}H_{15}NO_3$ [M + Na]$^+$ 316.0944; found 316.0944.

(*Z*)-1-(p-tolyl)-3-((*p*-tolyloxy)methylene)pyrrolidine-2,5-dione (3ba): **GP** was followed using Rose Bengal (13 mg, 5.0 mol %), 1-(*p*-tolyl)-1H-pyrrole-2,5-dione **1b** (47 mg, 0.25 mmol), and 1,3-dioxoisoindolin-2-yl 2-(*p*-tolyloxy)acetate **2a** (86 mg, 0.275 mmol). After 24 h, purification by column chromatography using 8% ethyl acetate in hexanes yielded **3ba** (56 mg, 73%). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.82 (t, J = 2.0 Hz, 1H), 7.29 (d, J = 8.4 Hz, 2H), 7.23 – 7.16 (m, 4H), 7.01 (d, J = 8.5 Hz, 2H), 3.54 (d, J = 1.8 Hz, 2H), 2.39 (s, 3H), 2.35 (s, 3H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 173.3, 170.0, 154.5, 149.8, 138.6, 135.0, 130.6, 129.9, 129.5, 126.5, 117.2, 106.9, 31.3, 21.3, 20.8. HRMS-ESI (m/z): calcd for $C_{19}H_{17}NO_3$ [M + Na]$^+$ 330.1101; found 330.1157.

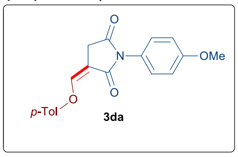


(*Z*)-1-(4-(*tert*-butyl)phenyl)-3-((*p*-tolyloxy)methylene)pyrrolidine-2,5-dione (3ca): **GP** was followed using Rose bengal (13 mg, 5.0 mol %), 1-(4-(*tert*-butyl)phenyl)-1H-pyrrole-2,5-dione **1c** (57 mg, 0.25 mmol), and 1,3-dioxoisoindolin-2-yl 2-(*p*-tolyloxy)acetate **2a** (86 mg, 0.275 mmol). After 24 h, purification by column chromatography using 8% ethyl acetate in hexanes yielded **3ca** (69 mg, 79%). **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.82 (s, 1H), 7.29 (d, J = 7.6 Hz, 2H), 7.23 (d, J = 8.0 Hz, 2H), 7.19 (d, J = 7.9 Hz, 2H), 7.02 (d, J = 7.8 Hz, 2H), 3.54 (s, 2H), 2.64 (t, J = 7.6 Hz, 2H), 2.35 (s, 3H), 1.63 (s, 2H), 1.37 (dd, J = 14.6, 7.3 Hz, 2H), 0.93 (t, J = 7.2 Hz, 3H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 173.3, 170.1, 154.5, 149.9, 143.5, 135.0, 130.6, 129.6, 129.3, 126.4, 117.2, 106.9, 35.5, 33.5, 31.3, 22.5, 20.8, 14.0. HRMS-ESI (m/z): calcd for $C_{22}H_{23}NO_3$ [M + H]$^+$ 350.1751; found 350.1749.

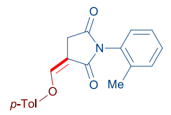


(*Z*)-1-(4-methoxyphenyl)-3-((*p*-tolyloxy)methylene)pyrrolidine-2,5-dione (3da):

GP was followed using Rose Bengal (13 mg, 5.0 mol %), 1-(4-methoxyphenyl)-1H-pyrrole-2,5-dione **1d** (51 mg, 0.25 mmol), and 1,3-dioxoisoindolin-2-yl 2-(*p*-tolyloxy)acetate **2a** (86 mg, 0.275 mmol). After 24 h, purification by column chromatography using 10% ethyl acetate in hexanes yielded **3da** (53 mg, 66%). **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.81 (s, 1H), 7.25 (d, J = 8.6 Hz, 2H), 7.18 (d, J = 8.3 Hz, 2H), 7.02 – 6.97 (m, 4H), 3.82 (s, 3H), 3.53 (d, J = 1.5 Hz, 2H), 2.35 (s, 3H). **^{13}CNMR** (126 MHz, $CDCl_3$) δ 173.4, 170.1, 159.6, 154.5, 149.8, 135.0, 130.6, 127.9, 124.8, 117.2, 114.6, 106.9, 55.6, 31.2, 20.8. HRMS-ESI (m/z): calcd for $C_{19}H_{17}NO_4$ [M + Na]$^+$ 346.1050; found 346.1058.

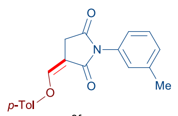


(*Z*)-1-(o-tolyl)-3-((*p*-tolyloxy)methylene)pyrrolidine-2,5-dione (3ea):


3ea

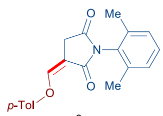
GP was followed using Rose Bengal (13 mg, 5.0 mol %), 1-(*o*-tolyl)-1H-pyrrole-2,5-dione **1e** (47 mg, 0.25 mmol), and 1,3-dioxoisoindolin-2-yl 2-(*p*-tolyloxy)acetate **2a** (86 mg, 0.275 mmol). After 24 h, purification by column chromatography using 10% ethyl acetate in hexanes yielded **3ea** (57 mg, 74%). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.83 (t, *J* = 2.1 Hz, 1H), 7.39 – 7.28 (m, 3H), 7.19 (d, *J* = 8.5 Hz, 2H), 7.12 (d, *J* = 7.4 Hz, 1H), 7.02 (d, *J* = 8.5 Hz, 2H), 3.59 (d, *J* = 2.2 Hz, 2H), 2.36 (s, 3H), 2.19 (s, 3H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 173.2, 169.9, 154.5, 149.9, 136.0, 135.1, 131.3, 130.6, 129.6, 128.3, 127.1, 117.2, 107.0, 31.4, 20.9, 18.0. HRMS-ESI (m/z): calcd for $C_{19}H_{17}NO_3$ [M + Na]$^+$ 330.1101; found 330.1092.

(*Z*)-1-(*m*-tolyl)-3-((*p*-tolyloxy)methylene)pyrrolidine-2,5-dione (3fa): **GP** was


3fa

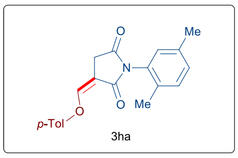
followed using Rose Bengal (13 mg, 5.0 mol %), 1-(*m*-tolyl)-1H-pyrrole-2,5-dione **1f** (47 mg, 0.25 mmol), and 1,3-dioxoisoindolin-2-yl 2-(*p*-tolyloxy)acetate **2a** (86 mg, 0.275 mmol). After 24 h, purification by column chromatography using 10% ethyl acetate in hexanes yielded **3fa** (66 mg, 86%). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.82 (t, *J* = 2.1 Hz, 1H), 7.37 (t, *J* = 7.7 Hz, 1H), 7.23 – 7.16 (m, 3H), 7.13 (d, *J* = 8.1 Hz, 2H), 7.02 (d, *J* = 8.6 Hz, 2H), 3.55 (d, *J* = 2.3 Hz, 2H), 2.40 (s, 3H), 2.36 (s, 3H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 173.3, 170.0, 154.5, 149.9, 139.3, 135.0, 132.0, 130.6, 129.5, 129.1, 127.4, 123.9, 117.2, 106.9, 31.3, 21.5, 20.8. HRMS-ESI (m/z): calcd for $C_{19}H_{17}NO_3$ [M + Na]$^+$ 330.1101; found 330.1101.

(*Z*)-1-(2,6-dimethylphenyl)-3-((*p*-tolyloxy)methylene)pyrrolidine-2,5-dione


3ga

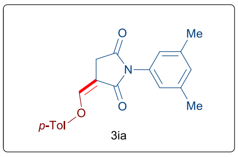
(3ga): **GP** was followed using Rose Bengal (13 mg, 5.0 mol %), 1-(2,6-dimethylphenyl)-1H-pyrrole-2,5-dione **1g** (50 mg, 0.25 mmol), and 1,3-dioxoisoindolin-2-yl 2-(*p*-tolyloxy)acetate **2a** (86 mg, 0.275 mmol). After 24 h, purification by column chromatography using 9% ethyl acetate in hexanes yielded **3ga** (41 mg, 51%). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.87 (t, *J* = 2.1 Hz, 1H), 7.29 (dd, *J* = 6.3, 2.0 Hz, 1H), 7.23 (d, *J* = 8.6 Hz, 2H), 7.19 (d, *J* = 7.6 Hz, 2H), 7.09 – 7.05 (m, 2H), 3.65 (d, *J* = 2.2 Hz, 2H), 2.39 (s, 3H), 2.18 (s, 6H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 173.0, 169.7, 154.5, 149.9, 136.2, 135.1, 130.6, 129.6, 128.6, 117.3, 115.2, 107.0, 31.4, 20.8, 18.0. HRMS-ESI (m/z): calcd for $C_{20}H_{19}NO_3$ [M + H]$^+$ 322.1438; found 322.1446.

(*Z*)-1-(2,5-dimethylphenyl)-3-((*p*-tolyloxy)methylene)pyrrolidine-2,5-dione (3ha):



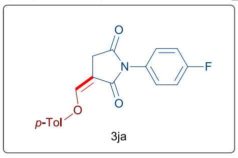
GP was followed using Rose Bengal (13 mg, 5.0 mol %), 1-(2,5-dimethylphenyl)-1H-pyrrole-2,5-dione **1h** (50 mg, 0.25 mmol), and 1,3-dioxoisoindolin-2-yl 2-(*p*-tolyloxy)acetate **2a** (86 mg, 0.275 mmol). After 24 h, purification by column chromatography using 10% ethyl acetate in hexanes yielded **3ha** (60 mg, 75%). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.82 (t, *J* = 2.1 Hz, 1H), 7.19 (d, *J* = 8.4 Hz, 2H), 7.16 – 7.09 (m, 2H), 7.04 – 6.98 (m, 3H), 3.57 (d, *J* = 1.1 Hz, 2H), 2.35 (s, 6H), 2.14 (s, 3H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 173.3, 170.1, 154.5, 149.8, 139.6, 135.6, 135.0, 132.0, 130.6, 128.6, 128.0, 127.8, 117.2, 107.1, 31.4, 21.3, 20.8, 17.9. HRMS-ESI (m/z): calcd for $C_{20}H_{19}NO_3$ $[M + H]^+$ 322.1438; found 322.1446.

(*Z*)-1-(3,5-dimethylphenyl)-3-((*p*-tolyloxy)methylene)pyrrolidine-2,5-dione (3ia):



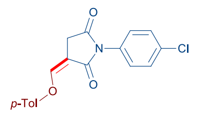
GP was followed using Rose Bengal (13 mg, 5.0 mol %), 1-(3,5-dimethylphenyl)-1H-pyrrole-2,5-dione **1i** (50 mg, 0.25 mmol), and 1,3-dioxoisoindolin-2-yl 2-(*p*-tolyloxy)acetate **2a** (86 mg, 0.275 mmol). After 24 h, purification by column chromatography using 10% ethyl acetate in hexanes yielded **3ia** (56 mg, 70%). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.81 (t, *J* = 2.1 Hz, 1H), 7.19 (d, *J* = 8.4 Hz, 2H), 7.02 (t, *J* = 5.7 Hz, 3H), 6.92 (s, 2H), 3.54 (d, *J* = 2.0 Hz, 2H), 2.35 (s, 9H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 173.4, 170.0, 154.5, 149.8, 139.1, 135.0, 131.9, 130.6, 124.6, 117.2, 107.0, 31.3, 21.4, 20.8. HRMS-ESI (m/z): calcd for $C_{20}H_{19}NO_3$ $[M + Na]^+$ 344.1257; found 344.1252.

(*Z*)-1-(4-fluorophenyl)-3-((*p*-tolyloxy)methylene)pyrrolidine-2,5-dione (3ja):



GP was followed using Rose Bengal (13 mg, 5.0 mol %), 1-(4-fluorophenyl)-1H-pyrrole-2,5-dione **1j** (48 mg, 0.25 mmol), and 1,3-dioxoisoindolin-2-yl 2-(*p*-tolyloxy)acetate **2a** (86 mg, 0.275 mmol). After 24 h, purification by column chromatography using 10% ethyl acetate in hexanes yielded **3ja** (56 mg, 72%). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.83 (t, *J* = 2.2 Hz, 1H), 7.36 – 7.30 (m, 2H), 7.21 – 7.13 (m, 4H), 7.01 (d, *J* = 8.5 Hz, 2H), 3.56 (d, *J* = 2.0 Hz, 2H), 2.36 (s, 3H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 173.1, 169.8, 162.3 (d, *J* = 248.7 Hz), 154.5, 150.2, 135.2, 130.7, 128.5 (d, J = 8.7 Hz), 128.1 (d, J = 3.1 Hz), 117.2, 116.3 (d, J = 22.9 Hz), 106.6, 31.3, 20.9. ^{19}**F NMR** (376 MHz, $CDCl_3$) δ -112.5. HRMS-ESI (m/z): calcd for $C_{18}H_{14}NFO_3$ [M + H]$^+$ 312.1030; found 312.1023.

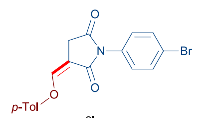
(*Z*)-1-(4-chlorophenyl)-3-((*p*-tolyloxy)methylene)pyrrolidine-2,5-dione (3ka):



3ka

GP was followed using Rose Bengal (13 mg, 5.0 mol %), 1-(4-chlorophenyl)-1H-pyrrole-2,5-dione **1k** (52 mg, 0.25 mmol), and 1,3-dioxoisoindolin-2-yl 2-(*p*-tolyloxy)acetate **2a** (86 mg, 0.275 mmol). After 24 h, purification by column chromatography using 10% ethyl acetate in hexanes yielded **3ka** (66 mg, 81%). ^{1}**H NMR** (400 MHz, $CDCl_3$) δ 7.83 (t, J = 2.1 Hz, 1H), 7.45 (d, J = 8.9 Hz, 2H), 7.35 – 7.28 (m, 2H), 7.19 (d, J = 8.6 Hz, 2H), 7.01 (d, J = 8.5 Hz, 2H), 3.55 (d, J = 2.0 Hz, 2H), 2.36 (s, 3H). ^{13}**C NMR** (126 MHz,) δ 172.9, 169.6, 154.5, 150.3, 135.2, 134.3, 130.7, 129.4, 127.9, 117.2, 106.5, 31.3, 20.9. HRMS-ESI (m/z): calcd for $C_{18}H_{14}NClO_3$ [M + Na]$^+$ 350.0554; found 350.0394.

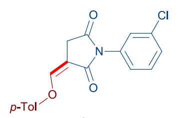
(*Z*)-1-(4-bromophenyl)-3-((*p*-tolyloxy)methylene)pyrrolidine-2,5-dione (3la):



3la

GP was followed using Rose Bengal (13 mg, 5.0 mol %), 1-(4-bromophenyl)-1H-pyrrole-2,5-dione **1l** (63 mg, 0.25 mmol), and 1,3-dioxoisoindolin-2-yl 2-(*p*-tolyloxy)acetate **2a** (86 mg, 0.275 mmol). After 24 h, purification by column chromatography using 10% ethyl acetate in hexanes yielded **3la** (72 mg, 78%). ^{1}**H NMR** (500 MHz, $CDCl_3$) δ 7.82 (t, J = 2.1 Hz, 1H), 7.60 (d, J = 8.7 Hz, 2H), 7.25 (d, J = 6.3 Hz, 2H), 7.18 (d, J = 8.2 Hz, 2H), 7.00 (d, J = 8.5 Hz, 2H), 3.54 (d, J = 2.1 Hz, 2H), 2.34 (s, 3H). ^{13}**C NMR** (126 MHz, $CDCl_3$) δ 172.8, 169.5, 154.5, 150.4, 135.2, 132.4, 131.2, 130.7, 128.2, 122.4, 117.2, 106.5, 31.3, 20.9. HRMS-ESI (m/z): calcd for $C_{18}H_{14}NBrO_3$ [M + Na]$^+$ 394.0049; found 394.0034.

(*Z*)-1-(3-chlorophenyl)-3-((*p*-tolyloxy)methylene)pyrrolidine-2,5-dione (3ma):

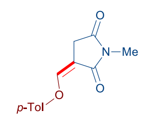


3ma

GP was followed using Rose Bengal (13 mg, 5.0 mol %), 1-(3-chlorophenyl)-1H-pyrrole-2,5-dione **1m** (52 mg, 0.25 mmol), and 1,3-

dioxoisoindolin-2-yl 2-(*p*-tolyloxy)acetate **2a** (86 mg, 0.275 mmol). After 24 h, purification by column chromatography using 10% ethyl acetate in hexanes yielded **3ma** (44 mg, 54%). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.84 (t, *J* = 2.1 Hz, 1H), 7.45 – 7.33 (m, 3H), 7.31 – 7.26 (m, 1H), 7.20 (d, *J* = 8.5 Hz, 2H), 7.02 (d, *J* = 8.5 Hz, 2H), 3.56 (d, *J* = 2.2 Hz, 2H), 2.36 (s, 3H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 172.7, 169.4, 154.5, 150.4, 135.2, 134.8, 133.2, 130.7, 130.1, 128.7, 127.0, 124.9, 117.2, 106.5, 31.3, 20.9. HRMS-ESI (m/z): calcd for $C_{18}H_{14}NClO_3$ [M + Na]$^+$ 350.0554; found 350.0551.

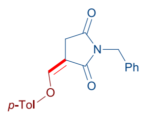
(*Z*)-1-methyl-3-((*p*-tolyloxy)methylene)pyrrolidine-2,5-dione (3na): **GP** was



3na

followed using Rose Bengal (13 mg, 5.0 mol %), 1-methyl-1H-pyrrole-2,5-dione **1n** (28 mg, 0.25 mmol), and 1,3-dioxoisoindolin-2-yl 2-(*p*-tolyloxy)acetate **2a** (86 mg, 0.275 mmol). After 24 h, purification by column chromatography using 10% ethyl acetate in hexanes yielded **3na** (48 mg, 84%). **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.72 (t, *J* = 2.0 Hz, 1H), 7.17 (d, *J* = 8.4 Hz, 2H), 7.04 – 6.95 (m, 2H), 3.37 (d, *J* = 1.9 Hz, 2H), 3.06 (s, 3H), 2.34 (s, 3H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 174.3, 171.0, 154.5, 148.9, 134.9, 130.6, 117.2, 107.3, 31.1, 24.8, 20.8. HRMS-ESI (m/z): calcd for $C_{13}H_{13}NO_3$ [M + Na]$^+$ 254.0788; found 254.0783.

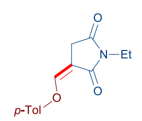
(*Z*)-1-benzyl-3-((*p*-tolyloxy)methylene)pyrrolidine-2,5-dione (3oa): **GP** was



3oa

followed using Rose Bengal (13 mg, 5.0 mol %), 1-benzyl-1H-pyrrole-2,5-dione **1o** (47 mg, 0.25 mmol), and 1,3-dioxoisoindolin-2-yl 2-(*p*-tolyloxy)acetate **2a** (86 mg, 0.275 mmol). After 24 h, purification by column chromatography using 10% ethyl acetate in hexanes yielded **3oa** (44 mg, 58%). **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.69 (s, 1H), 7.39 (d, *J* = 7.3 Hz, 2H), 7.27 (dt, *J* = 12.0, 6.3 Hz, 3H), 7.14 (d, *J* = 8.0 Hz, 2H), 6.94 (d, *J* = 8.0 Hz, 2H), 4.71 (s, 2H), 3.35 (s, 2H), 2.31 (s, 3H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 173.8, 170.6, 154.5, 149.2, 136.2, 134.9, 130.6, 128.9, 128.8, 128.0, 117.2, 107.1, 42.3, 31.2, 20.8. HRMS-ESI (m/z): calcd for $C_{19}H_{17}NO_3$ [M + Na]$^+$ 330.1101; found 330.1108.

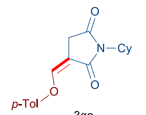
(*Z*)-1-ethyl-3-((*p*-tolyloxy)methylene)pyrrolidine-2,5-dione (3pa): **GP** was



3pa

followed using Rose Bengal (13 mg, 5.0 mol %), 1-ethyl-1H-pyrrole-2,5-dione **1p** (31 mg, 0.25 mmol), and 1,3-dioxoisoindolin-2-yl 2-(*p*-tolyloxy)acetate **2a** (86 mg, 0.275 mmol). After 24 h, purification by column chromatography using 10% ethyl acetate in hexanes yielded **3pa** (40 mg, 66%). **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.70 (d, *J* = 2.0 Hz, 1H), 7.16 (d, *J* = 8.2 Hz, 2H), 6.97 (d, *J* = 8.5 Hz, 2H), 3.62 (q, *J* = 7.2 Hz, 2H), 3.35 (d, *J* = 2.0 Hz, 2H), 2.33 (s, 3H), 1.20 (t, *J* = 7.2 Hz, 3H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 174.0, 170.7, 154.5, 148.8, 134.9, 130.6, 117.1, 107.3, 3.6, 31.1, 20.8, 13.3. HRMS-ESI (m/z): calcd for $C_{14}H_{15}NO_3$ [M + Na]$^+$ 268.0944; found 268.0941.

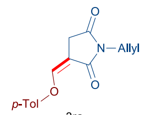
(*Z*)-1-cyclohexyl-3-((*p*-tolyloxy)methylene)pyrrolidine-2,5-dione (3qa): **GP**



3qa

was followed using Rose Bengal (13 mg, 5.0 mol %), 1-cyclohexyl-1H-pyrrole-2,5-dione **1q** (45 mg, 0.25 mmol), and 1,3-dioxoisoindolin-2-yl 2-(*p*-tolyloxy)acetate **2a** (86 mg, 0.275 mmol). After 24 h, purification by column chromatography using 10% ethyl acetate in hexanes yielded **3qa** (60 mg, 80%). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.65 (t, *J* = 2.1 Hz, 1H), 7.16 (d, *J* = 8.4 Hz, 2H), 6.97 (d, *J* = 8.5 Hz, 2H), 4.04 (tt, *J* = 12.3, 3.8 Hz, 1H), 3.30 (d, *J* = 2.3 Hz, 2H), 2.33 (s, 3H), 2.26 – 2.12 (m, 2H), 1.89 – 1.77 (m, 2H), 1.70 – 1.54 (m, 2H), 1.44 – 1.11 (m, 4H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 174.2, 171.0, 154.6, 148.6, 134.8, 130.5, 117.2, 107.3, 51.6, 31.0, 29.1, 26.0, 25.2, 20.8. HRMS-ESI (m/z): calcd for $C_{18}H_{21}NO_3$ [M + Na]$^+$ 322.1414; found 322.1410.

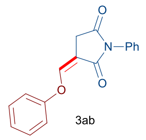
(*Z*)-1-allyl-3-((*p*-tolyloxy)methylene)pyrrolidine-2,5-dione (3ra):



3ra

GP was followed using Rose Bengal (13 mg, 5.0 mol %), 1-allyl-1H-pyrrole-2,5-dione **1r** (34 mg, 0.25 mmol), and 1,3-dioxoisoindolin-2-yl 2-(*p*-tolyloxy)acetate **2a** (86 mg, 0.275 mmol). After 24 h, purification by column chromatography using 10% ethyl acetate in hexanes yielded **3ra** (54 mg, 84%). **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.71 (t, *J* = 2.1 Hz, 1H), 7.16 (d, *J* = 8.5 Hz, 2H), 6.97 (d, *J* = 8.5 Hz, 2H), 5.82 (ddt, *J* = 16.0, 10.3, 5.8 Hz, 1H), 5.20 (ddd, *J* = 13.7, 11.2, 1.1 Hz, 2H), 4.17 (d, *J* = 5.8 Hz, 2H), 3.37 (d, *J* = 2.1 Hz, 2H), 2.33 (s, 3H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 173.6, 170.3, 154.5, 149.0, 134.9, 131.1, 130.5, 118.1, 117.1, 107.1, 40.7, 31.1, 20.8. HRMS-ESI (m/z): calcd for $C_{15}H_{15}NO_3$ [M + H]$^+$ 258.1125; found 258.1125.

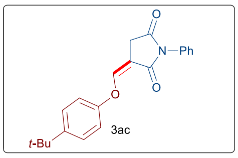
(*Z*)-3-(phenoxymethylene)-1-phenylpyrrolidine-2,5-dione (3ab):



3ab

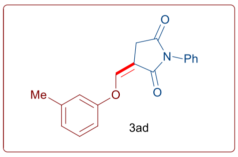
GP was followed using Rose Bengal (13 mg, 5.0 mol %), 1-phenyl-1H-pyrrole-2,5-dione **1a** (43 mg, 0.25 mmol), and 1,3-dioxoisoindolin-2-yl 2-phenoxyacetate **2b** (82 mg, 0.275 mmol). After 24 h, purification by column chromatography using 10% ethyl acetate in hexanes yielded **3ab** (47 mg, 68%). **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.90 (s, 1H), 7.52 (t, *J* = 7.7 Hz, 2H), 7.47 – 7.41 (m, 3H), 7.39 (d, *J* = 7.7 Hz, 2H), 7.26 (t, *J* = 7.4 Hz, 1H), 7.17 (d, *J* = 8.0 Hz, 2H), 3.61 (d, *J* = 1.9 Hz, 2H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 173.1, 169.8, 156.5, 149.5, 132.2, 130.3, 129.3, 128.6, 126.7, 125.4, 117.4, 107.4, 31.3. HRMS-ESI (m/z): calcd for $C_{17}H_{13}NO_3$ [M + Na]$^+$ 302.0788; found 302.0799.

(*Z*)-3-((4-(*tert*-butyl)phenoxy)methylene)-1-phenylpyrrolidine-2,5-dione (3ac):



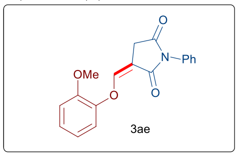
GP was followed using Rose Bengal (13 mg, 5.0 mol %), 1-phenyl-1H-pyrrole-2,5-dione **1a** (43 mg, 0.25 mmol), and 1,3-dioxoisoindolin-2-yl 2-(4-(*tert*-butyl)phenoxy)acetate **2c** (97 mg, 0.275 mmol). After 24 h, purification by column chromatography using 10% ethyl acetate in hexanes yielded **3ac** (71 mg, 85%). **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.85 (t, *J* = 2.0 Hz, 1H), 7.49 (t, *J* = 7.7 Hz, 2H), 7.45 – 7.38 (m, 3H), 7.35 (d, *J* = 7.4 Hz, 2H), 7.06 (d, *J* = 8.8 Hz, 2H), 3.57 (d, *J* = 2.0 Hz, 2H), 1.33 (s, 9H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 173.2, 169.9, 154.4, 149.9, 148.5, 132.2, 129.2, 128.6, 127.1, 126.7, 116.9, 106.9, 34.6, 31.5, 31.3. HRMS-ESI (m/z): calcd for $C_{21}H_{21}NO_3$ [M + Na]$^+$ 358.1414; found 358.1406.

(*Z*)-1-phenyl-3-((*m*-tolyloxy)methylene)pyrrolidine-2,5-dione (3ad):



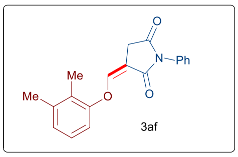
GP was followed using Rose Bengal (13 mg, 5.0 mol %), 1-phenyl-1H-pyrrole-2,5-dione **1a** (43 mg, 0.25 mmol), and 1,3-dioxoisoindolin-2-yl 2-(*m*-tolyloxy)acetate **2d** (85 mg, 0.275 mmol). After 24 h, purification by column chromatography using 10% ethyl acetate in hexanes yielded **3ad** (49 mg, 67%). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.86 (t, *J* = 2.2 Hz, 1H), 7.49 (t, *J* = 7.7 Hz, 2H), 7.43 – 7.37 (m, 3H), 7.29 (d, *J* = 7.8 Hz, 1H), 7.03 (d, *J* = 7.3 Hz, 1H), 6.94 (dd, *J* = 11.1, 2.9 Hz, 2H), 3.56 (d, *J* = 2.0 Hz, 2H), 2.39 (s, 3H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 173.1, 169.9, 156.5, 149.6, 140.6, 132.2, 129.9, 129.2, 128.6, 126.7, 126.1, 118.1, 114.3, 107.1, 31.3, 21.5. HRMS-ESI (m/z): calcd for $C_{18}H_{15}NO_3$ [M + Na]$^+$ 316.0944; found 316.0933.

(*Z*)-3-((2-methoxyphenoxy)methylene)-1-phenylpyrrolidine-2,5-dione (3ae):



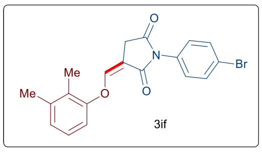
GP was followed using Rose Bengal (13 mg, 5.0 mol %), 1-phenyl-1H-pyrrole-2,5-dione **1a** (43 mg, 0.25 mmol), and 1,3-dioxoisoindolin-2-yl 2-(2-methoxyphenoxy)acetate **2e** (90 mg, 0.275 mmol). After 24 h, purification by column chromatography using 10% ethyl acetate in hexanes yielded **3ae** (42 mg, 54%). **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.70 (t, *J* = 2.1 Hz, 1H), 7.48 (t, *J* = 7.7 Hz, 2H), 7.39 (t, *J* = 7.5 Hz, 1H), 7.36 – 7.33 (m, 2H), 7.20 (td, *J* = 8.2, 1.5 Hz, 1H), 7.12 (dd, *J* = 8.0, 1.5 Hz, 1H), 7.00 (dd, *J* = 8.2, 1.1 Hz, 1H), 6.96 (td, *J* = 7.9, 1.3 Hz, 1H), 3.88 (s, 3H), 3.57 (d, *J* = 2.1 Hz, 2H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ ^{13}C NMR (126 MHz, $CDCl_3$) δ 173.3, 170.0, 152.4, 150.4, 145.7, 134.4, 132.3, 129.2, 128.5, 126.8, 121.2, 120.1, 113.1, 105.9, 56.1, 31.3. HRMS-ESI (m/z): calcd for $C_{18}H_{15}NO_4$ [M + Na]$^+$ 332.0893; found 332.0884.

(*Z*)-3-((2,3-dimethylphenoxy)methylene)-1-phenylpyrrolidine-2,5-dione (3af):



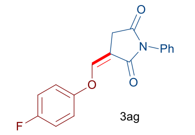
GP was followed using Rose Bengal (13 mg, 5.0 mol %), 1-phenyl-1H-pyrrole-2,5-dione **1a** (43 mg, 0.25 mmol), and 1,3-dioxoisoindolin-2-yl 2-(2,3-dimethylphenoxy)acetate **2f** (89 mg, 0.275 mmol). After 24 h, purification by column chromatography using 10% ethyl acetate in hexanes yielded **3af** (45 mg, 59%). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.76 (t, *J* = 2.1 Hz, 1H), 7.53 – 7.44 (m, 2H), 7.44 – 7.37 (m, 1H), 7.37 – 7.32 (m, 2H), 7.03 (d, *J* = 11.0 Hz, 2H), 6.93 (d, *J* = 8.1 Hz, 1H), 3.54 (d, *J* = 2.3 Hz, 2H), 2.32 (s, 3H), 2.26 (s, 3H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 173.2, 169.9, 153.0, 150.9, 135.2, 132.3, 132.2, 129.2, 128.6, 128.0, 128.0, 126.7, 116.9, 106.4, 31.3, 20.8, 15.9. HRMS-ESI (m/z): calcd for $C_{19}H_{17}NO_3$ [M + Na]$^+$ 330.1101; found 330.1105.

(*Z*)-1-(4-bromophenyl)-3-((2,3-dimethylphenoxy)methylene)pyrrolidine-2,5-dione (3lf):



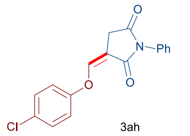
GP was followed using Rose Bengal (13 mg, 5.0 mol %), 1-(4-bromophenyl)-1H-pyrrole-2,5-dione **1l** (63 mg, 0.25 mmol), and 2-(2-(2,3-dimethylphenoxy)acetyl)isoindoline-1,3-dione **2f** (89 mg, 0.275 mmol). After 24 h, purification by column chromatography using 10% ethyl acetate in hexanes yielded **3lf** (61 mg, 63%). **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.75 (s, 1H), 7.61 (d, *J* = 8.6 Hz, 2H), 7.26 (s, 2H), 7.08 – 6.99 (m, 2H), 6.92 (d, *J* = 8.1 Hz, 1H), 3.53 (d, *J* = 2.0 Hz, 2H), 2.32 (s, 3H), 2.26 (s, 3H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 172.8, 169.6, 153.0, 151.2, 135.3, 132.4, 132.4, 131.3, 128.2, 128.0, 122.3, 117.0, 106.1, 31.3, 20.8, 15.9. HRMS-ESI (m/z): calcd for $C_{19}H_{16}NBrO_3$ [M + Na]$^+$ 408.0206; found 408.0213.

(*Z*)-3-((4-fluorophenoxy)methylene)-1-phenylpyrrolidine-2,5-dione (3ag):


3ag

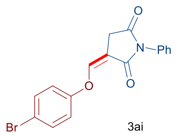
GP was followed using Rose Bengal (13 mg, 5.0 mol %), 1-phenyl-1H-pyrrole-2,5-dione **1a** (43 mg, 0.25 mmol), and 1,3-dioxoisoindolin-2-yl 2-(4-fluorophenoxy)acetate **2g** (87 mg, 0.275 mmol). After 24 h, purification by column chromatography using 10% ethyl acetate in hexanes yielded **3ag** (53 mg, 71%). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.78 (t, *J* = 2.3 Hz, 1H), 7.53 – 7.45 (m, 2H), 7.41 (dd, *J* = 4.9, 3.7 Hz, 1H), 7.35 (dd, *J* = 8.3, 1.3 Hz, 2H), 7.10 (d, *J* = 6.5 Hz, 4H), 3.56 (d, *J* = 2.0 Hz, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 173.0, 169.7, 159.9 (d, *J* = 243.9 Hz), 152.6, 149.6, 132.1, 129.3, 128.7, 126.7, 119.0 (d, *J* = 8.2 Hz), 116.9 (d, *J* = 23.6 Hz), 107.5, 31.2. **^{19}F NMR** (376 MHz, $CDCl_3$) δ -117.2. HRMS-ESI (m/z): calcd for $C_{17}H_{12}NFO_3$ [M + H]$^+$ 298.0874; found 298.0884.

(*Z*)-3-((4-chlorophenoxy)methylene)-1-phenylpyrrolidine-2,5-dione (3ah):


3ah

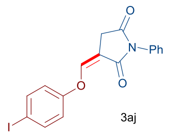
GP was followed using Rose Bengal (13 mg, 5.0 mol %), 1-phenyl-1H-pyrrole-2,5-dione **1a** (43 mg, 0.25 mmol), and 1,3-dioxoisoindolin-2-yl 2-(4-chlorophenoxy)acetate **2h** (91 mg, 0.275 mmol). After 24 h, purification by column chromatography using 10% ethyl acetate in hexanes yielded **3ah** (55 mg, 70%). **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.80 (t, *J* = 2.2 Hz, 1H), 7.49 (t, *J* = 7.7 Hz, 2H), 7.42 – 7.32 (m, 5H), 7.08 (d, *J* = 8.9 Hz, 2H), 3.57 (d, *J* = 2.2 Hz, 2H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 172.9, 169.6, 155.0, 148.9, 134.5, 130.7, 130.3, 129.3, 128.7, 126.7, 118.7, 108.1, 31.3. HRMS-ESI (m/z): calcd for $C_{17}H_{12}NClO_3$ [M + H]$^+$ 314.0578; found 314.0575.

(*Z*)-3-((4-bromophenoxy)methylene)-1-phenylpyrrolidine-2,5-dione (3ai):


3ai

GP was followed using Rose Bengal (13 mg, 5.0 mol %), 1-phenyl-1H-pyrrole-2,5-dione **1a** (43 mg, 0.25 mmol), and 1,3-dioxoisoindolin-2-yl 2-(4-bromophenoxy)acetate **2i** (103 mg, 0.275 mmol). After 24 h, purification by column chromatography using 10% ethyl acetate in hexanes yielded **3ai** (58 mg, 65%). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.80 (t, *J* = 2.2 Hz, 1H), 7.56 – 7.45 (m, 4H), 7.43 – 7.38 (m, 1H), 7.37 – 7.32 (m, 2H), 7.03 (d, *J* = 8.9 Hz, 2H), 3.57 (d, *J* = 2.3 Hz, 2H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 173.1, 169.6, 155.4, 148.8, 133.3, 132.2, 129.3, 128.9, 126.7, 119.1, 118.2, 108.2, 31.3. HRMS-ESI (m/z): calcd for $C_{17}H_{12}NBrO_3$ [M + Na]$^+$ 379.9893; found 379.9893.

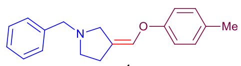
(*Z*)-3-((4-iodophenoxy)methylene)-1-phenylpyrrolidine-2,5-dione (3aj):



3aj

GP was followed using Rose Bengal (13 mg, 5.0 mol %), 1-phenyl-1H-pyrrole-2,5-dione **1a** (43 mg, 0.25 mmol), and 1,3-dioxoisoindolin-2-yl 2-(4-iodophenoxy)acetate **2j** (116 mg, 0.275 mmol). After 24 h, purification by column chromatography using 10% ethyl acetate in hexanes yielded **3aj** (63 mg, 62%). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.80 (t, *J* = 2.2 Hz, 1H), 7.76 – 7.65 (m, 2H), 7.54 – 7.44 (m, 2H), 7.44 – 7.38 (m, 1H), 7.34 (dd, *J* = 8.4, 1.2 Hz, 2H), 6.91 (d, *J* = 8.9 Hz, 2H), 3.56 (d, *J* = 2.2 Hz, 2H). **^{13}C NMR** (126 MHz,) δ NMR (126 MHz,) δ 172.9, 169.4, 156.3, 148.6, 139.5, 132.4, 129.9, 128.7, 127.0, 119.7, 108.2, 88.2, 31.3. HRMS-ESI (m/z): calcd for $C_{17}H_{12}NIO_3$ [M + H]$^+$ 427.9754; found 427.9768.

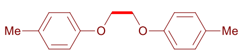
(*Z*)-1-benzyl-3-((*p*-tolyloxy)methylene)pyrrolidine (4):



4

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.40 – 7.27 (m, 5H), 7.08 (d, *J* = 8.5 Hz, 2H), 6.85 (d, *J* = 8.5 Hz, 2H), 6.37 (t, *J* = 1.9 Hz, 1H), 3.69 (s, 2H), 3.23 (s, 2H), 2.74 (t, *J* = 6.2 Hz, 2H), 2.61 (t, *J* = 6.2 Hz, 2H), 2.29 (s, 3H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 155.7, 133.8, 131.9, 130.3, 129.4, 128.3, 127.6, 122.4, 116.0, 60.7, 55.9, 53.9, 26.6, 20.6. HRMS-ESI (m/z): calcd for $C_{19}H_{21}NO$ [M + H]$^+$ 280.1696; found 280.1696.

1,2-bis(*p*-tolyloxy)ethane (6)[4]:

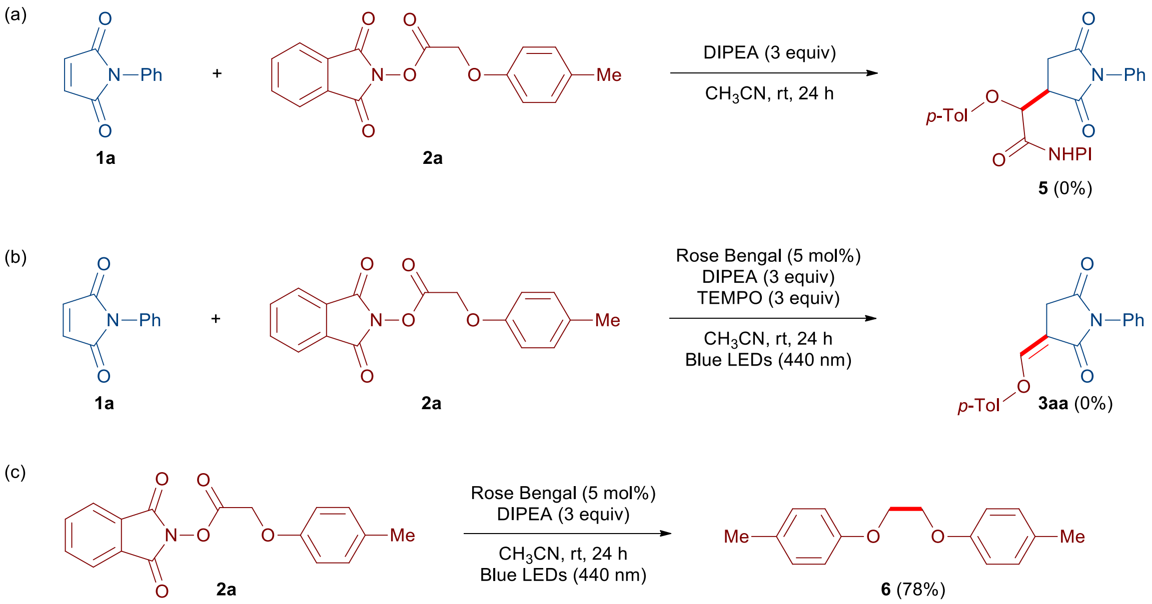


6

GP was followed using Rose Bengal (13 mg, 5.0 mol %), 1,3-dioxoisoindolin-2-yl 2-(*p*-tolyloxy)acetate **2a** (86 mg, 0.275 mmol). After 24 h, purification by column chromatography using 10% ethyl acetate in hexanes yielded **6** (42 mg, 78%). **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.09 (d, *J* = 8.2 Hz, 4H), 6.85 (d, *J* = 8.5 Hz, 4H), 4.28 (s, 4H), 2.29 (s, 6H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 156.7, 130.1, 114.8, 66.9, 20.6.

Procedure of Control Experiments (Scheme 2):

(A) To check the probability of ionic nucleophilic conjugate addition followed by radical decarboxylation and oxidation cascade, we performed the performed the reaction in absence of light and photocatalyst. *N*-phenyl maleimide derivative **1a** (0.25 mmol, 50 mg, 1.0 equiv), *N*-(acyloxy)phthalimide **2a** (0.275 mmol, 90 mg, 1.1 equiv), and DIPEA (116 mg, 0.90 mmol, 3.0 equiv) were placed in a pre-dried 15 mL reaction tube. The tube was degassed and purged with argon three times. Acetonitrile (3.0 mL) was added, and the mixture was placed in dark and stirred for 24 h under argon atmosphere using a balloon filled with argon gas. No indication of formation of **5** was observed.



(B) To confirm the radical assisted mechanism, the reaction was performed under standard condition along with 3 equiv of free radical scavenger TEMPO. *N*-phenyl maleimide **1a** (0.25 mmol, 50 mg, 1.0 equiv), *N*-(acyloxy)phthalimide **2a** (0.275 mmol, 90 mg, 1.1 equiv), Rose Bengal (13 mg, 15 µmol, 5 mol%), DIPEA (116 mg, 0.90 mmol, 3.0 equiv) and TEMPO (0.75 mmol, 117 mg, 3.0 equiv) were placed in a pre-dried 15 mL reaction tube. The tube was degassed and purged with argon three times. Acetonitrile (3.0 mL) was added, and the mixture was irradiated using 36 W Kessil blue LED (440 nm) lamp and stirred for 24 h under argon atmosphere using a balloon filled with argon gas. Product **3aa** was not formed.

(C) Furthermore, the transformation was carried out in absence of the coupling partner maleimide. *N*-(acyloxy)phthalimide **2a** (0.275 mmol, 90 mg, 1.1 equiv), Rose Bengal (13 mg, 15 µmol, 5 mol%) and DIPEA (116 mg, 0.90 mmol, 3.0 equiv) were placed in a pre-dried 15 mL reaction tube. The tube was degassed and purged with argon three times. Acetonitrile (3.0 mL) was added, and the mixture was irradiated using 36 W Kessil blue LED (440 nm) lamp and stirred for 24 h under argon atmosphere using a balloon filled with argon gas. Homocoupled product **6** was formed with 78% isolated yield. The characterization data of the compound matched with the literature reported data.[4]

Photophysical studies:

(A) Preparation of the Stock Solution:

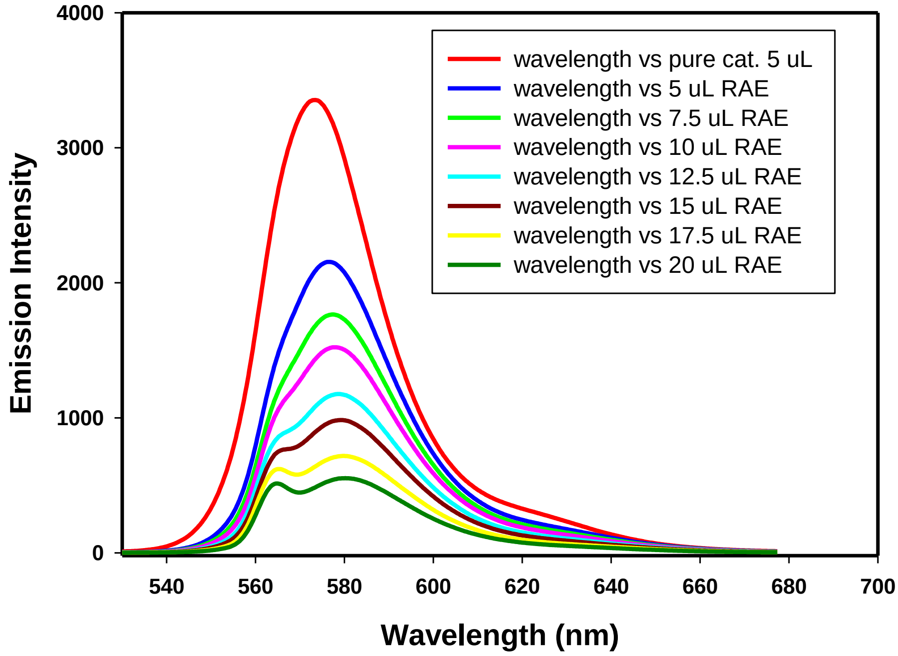
1 mM solution of the Rose bengal catalyst was prepared in a sample vial by dissolving 2.59 mg of the catalyst in 4 mL of MeCN (spectroscopic grade, purchased from Spectrochem). The freshly prepared solution was used for the spectroscopic measurement. The required amount was taken using micro pipette from the mother solution as an aliquot and it was diluted further by dissolving in 1 mL of MeCN in the cuvette. Similarly, 4 mL 0.3 M solution of diisopropyl ethyl amine (DIPEA), phthalimido ester (**2a**) and *N*-phenyl maleimide (**1a**) were prepared by dissolving the requisite amount of each substrate in MeCN. Freshly prepared of those solutions were used for the quenching experiment.

(B) Luminescence quenching Experiment methods:

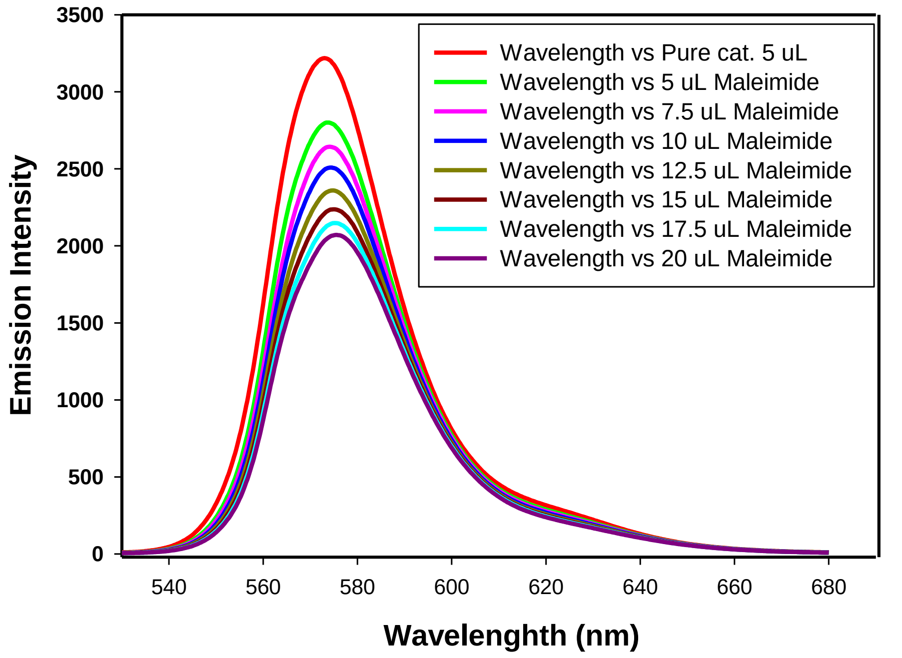
Fluorescence emission spectra of the photocatalyst in presence of different reactions components (**1a**, **2a** and DIPEA) were recorded and analysed in detail to estimate the light emission properties of the pure catalyst system and their distractions by external interference from the substrates. Emission intensities of Eosin Y were recorded with a **"HITACHI f-7000"** Scientific Spectrofluorometer using a 10.0 mm quartz cuvette. The catalyst exhibits an absorption maxima at 538 nm (confirmed from literature).4 Hence, the sample solution of Rose bengal with a proper concentration of 1 mM in MeCN was excited (degassed for 15 mins before recording the spectra) with a wavelength of 500 nm and the emission maxima was found to be observed at 573 nm. The individual substrate **1a** and **2a** were silent to show any emission feature in that region. To study the quenching behaviour of rose bengal, different concentration of **2a** was added to the catalyst solution and the emission spectra was measured following the aforementioned procedure. The quenching effect of the redox active phthalimide ester was quite significant on the photocatalyst; the intensity of the emission maxima decreased gradually upon increasing the concentration of **2a**. Few set of solutions with different concentration of the ester were used; the experiment was repeated and finally the Stern-Volmer plot was depicted. DIPEA was hardly to impose any quenching effect on the emission intensities of the catalyst even with high concentration of that. On the other hand, no significant change in the emission maxima [almost similar to DIPEA, slightly higher] of Eosin Y was observed when *N*-phenyl maleimide (**1a**) was used as the quencher. The corresponding Stern-Volmer plots were drawn for all the cases.

(C) Luminescence Spectra:

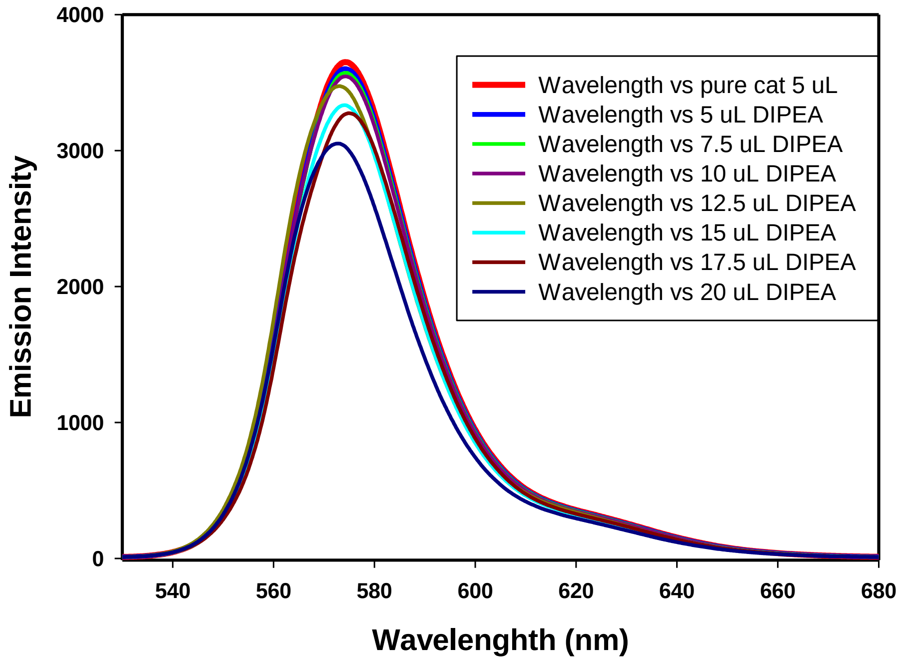
Luminescence spectra of Rose Bengal (1 mM) as a function of concentration of Phthalimido ester (0.3 M) in degassed MeCN with excitation at 480 nm

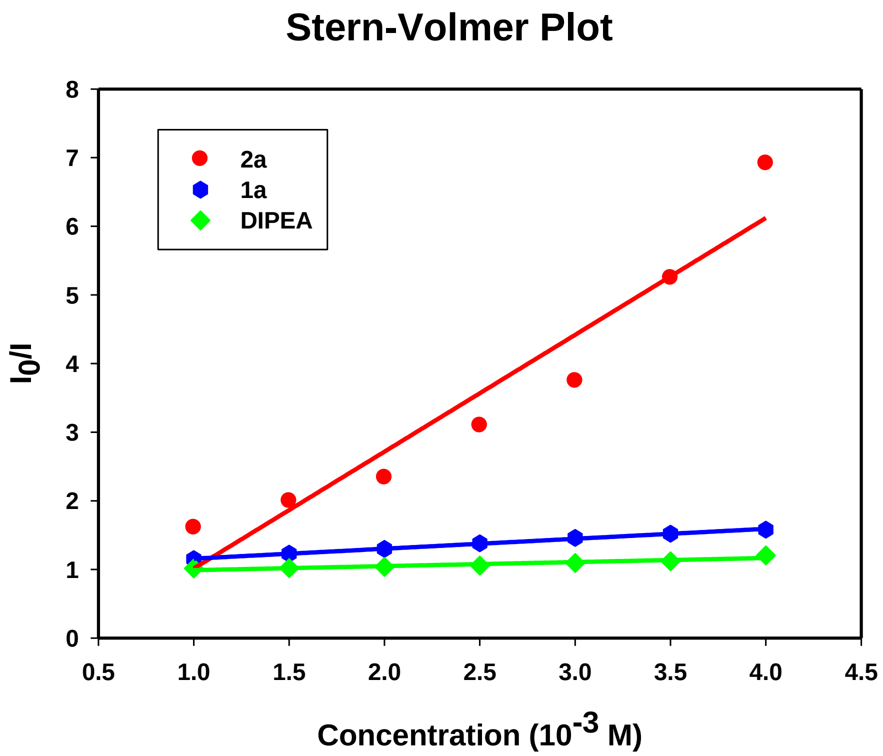


Luminescence spectra of Rose Bengal (1 mM) as a function of concentration of Maleimide (0.3 M) in degassed MeCN with excitation at 480 nm



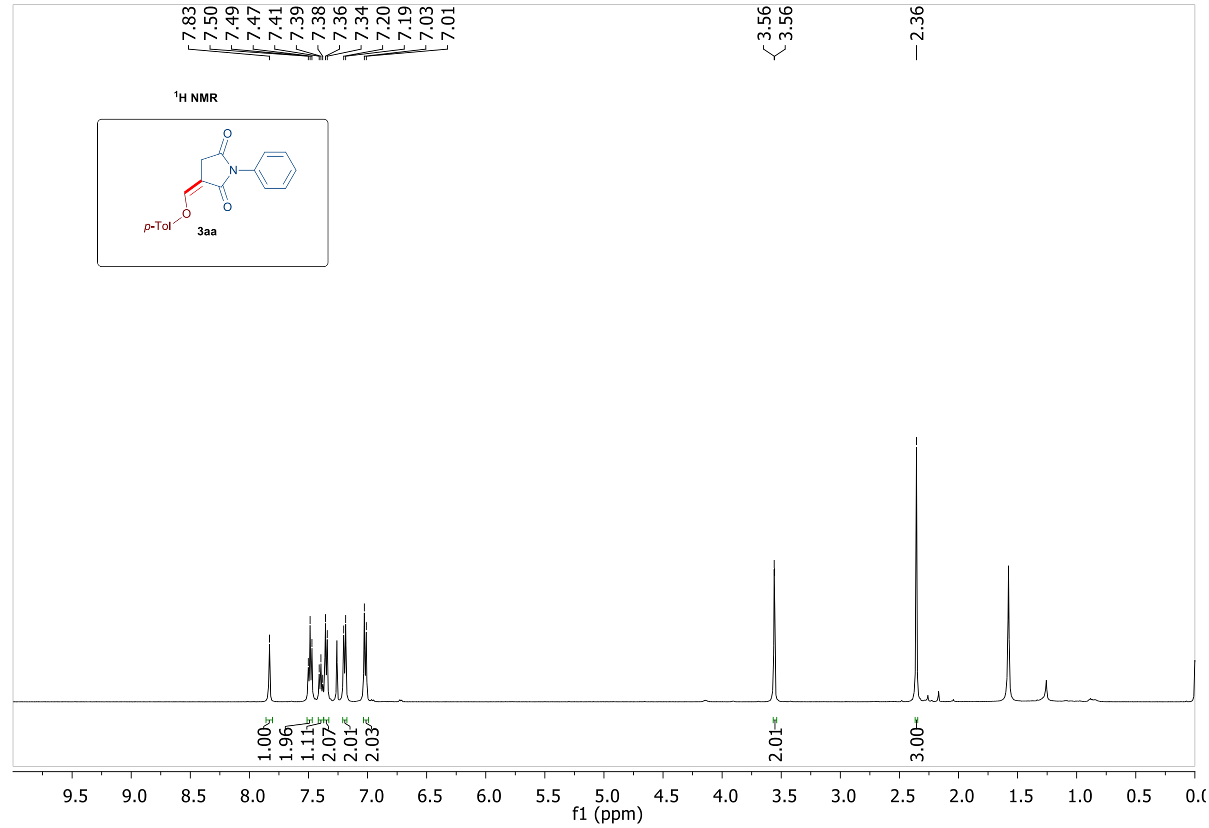
Luminescence spectra of Rose Bengal (1 mM) as a function of concentration of DIPEA (0.3 M) in degassed MeCN with excitation at 480 nm





Stern-Volmer Plot
2a
1a
DIPEA
I_0/I
0
1
2
3
4
5
6
7
8
0.5
1.0
1.5
2.0
2.5
3.0
3.5
4.0
4.5
Concentration (10^{-3} M)

NMR SPECTRA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7.38
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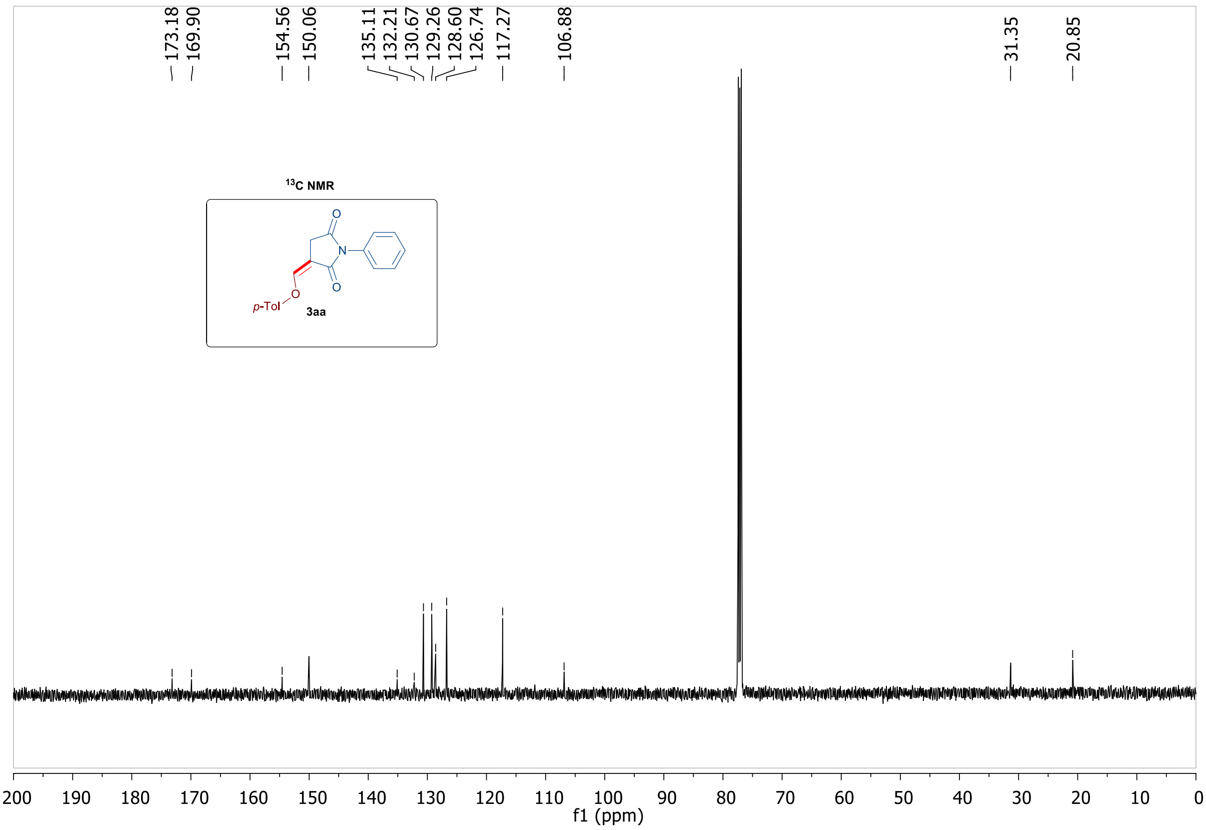
7.34
7.20
7.19
7.03
7.01
3.56
3.56
2.36
^{1}H NMR
p-Tol
3aa
1.00
1.96
1.11
2.07
2.01
2.03
2.01
3.00
f1 (ppm)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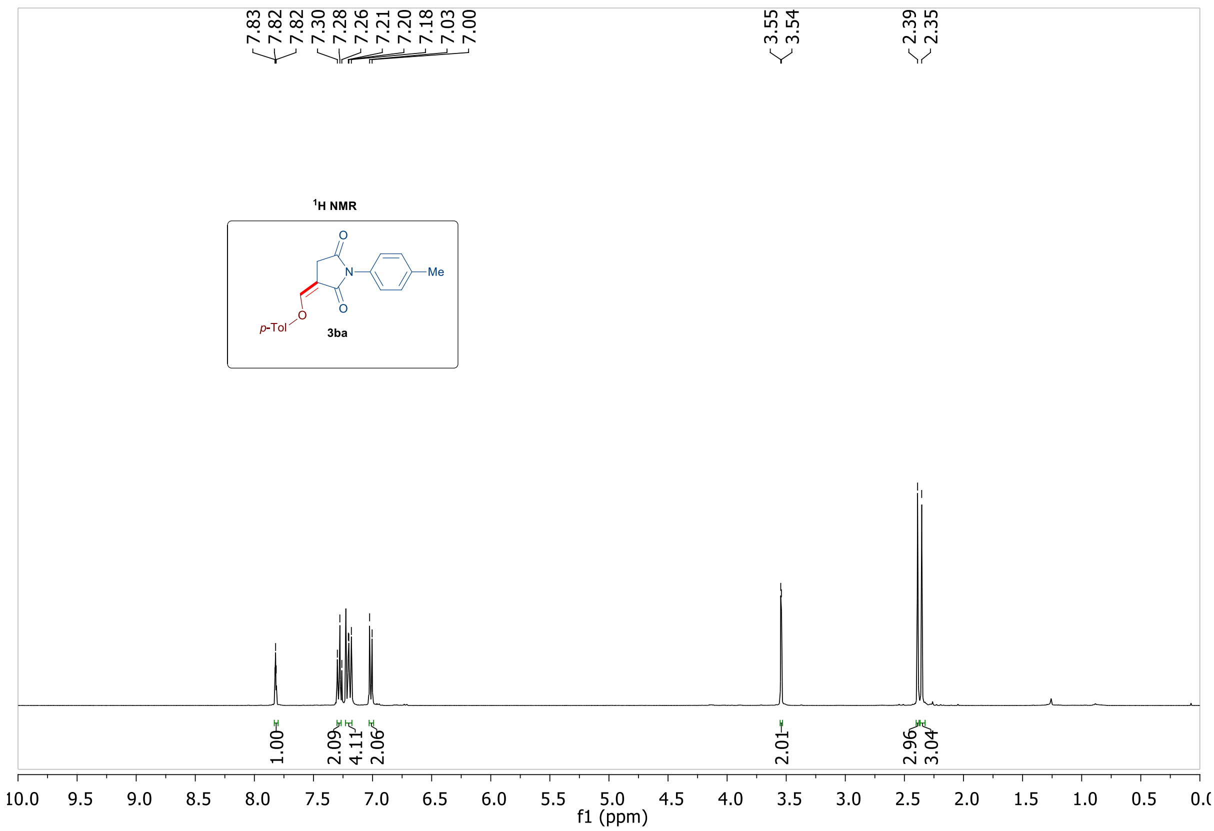
20.85
^{13}C NMR
p-Tol
3aa
f1 (ppm)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2.39
2.35
1H NMR
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N
Me
O
O
p-Tol
3ba
1.00
2.09
4.11
2.06
2.01
2.96
3.04
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
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2.0
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1.0
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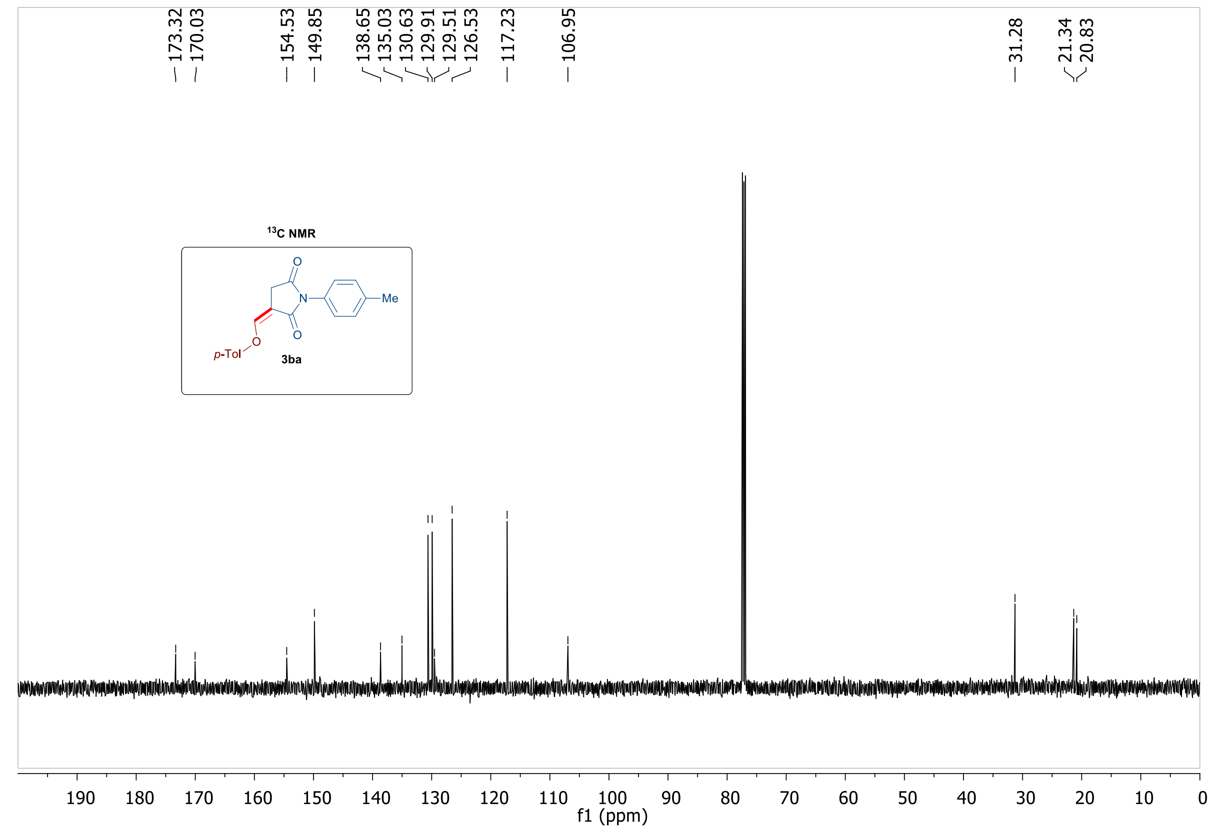
0.0
f1 (ppm)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21.34
20.83
13C NMR
O
N
Me
O
O
p-Tol
3ba
190
180
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120
110
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50
40
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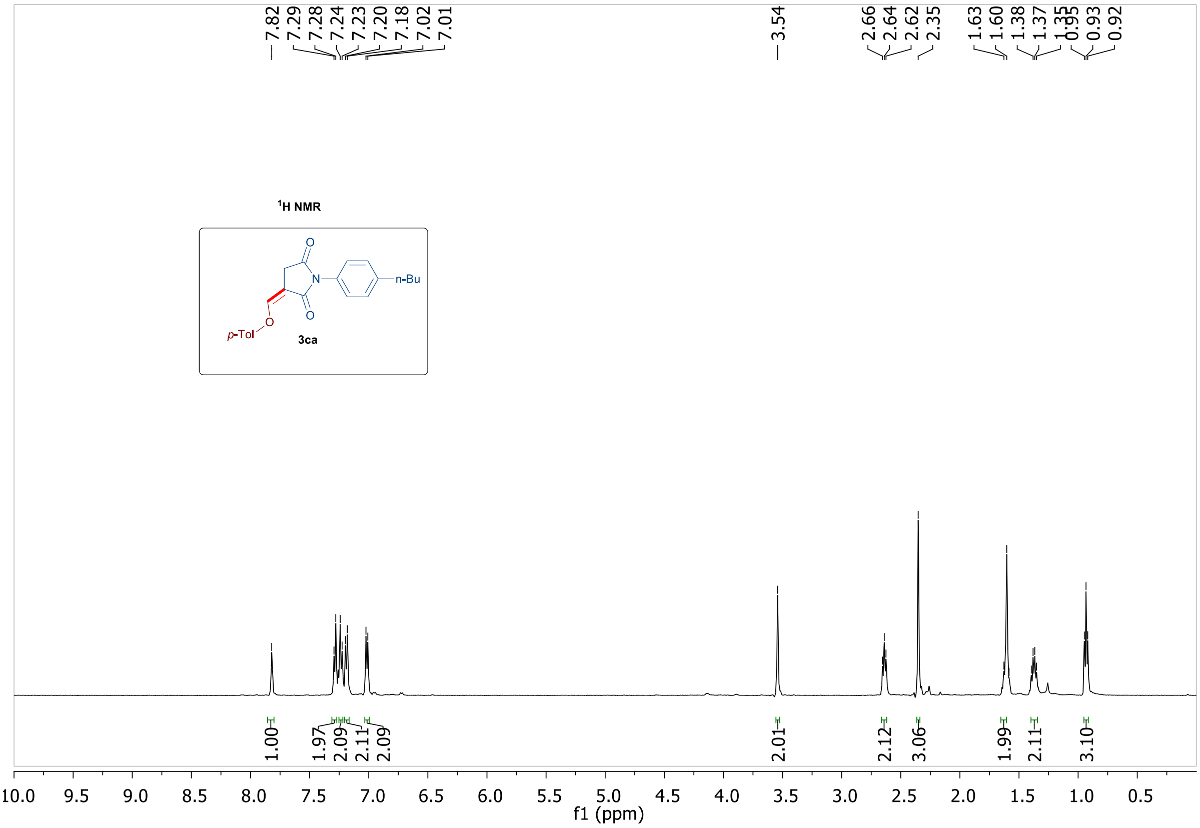
20
10
0
f1 (ppm)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1.60
1.38
1.37
1.35
0.95
0.93
0.92
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N
n-Bu
O
O
p-Tol
3ca
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1.97
2.09
2.11
2.09
2.01
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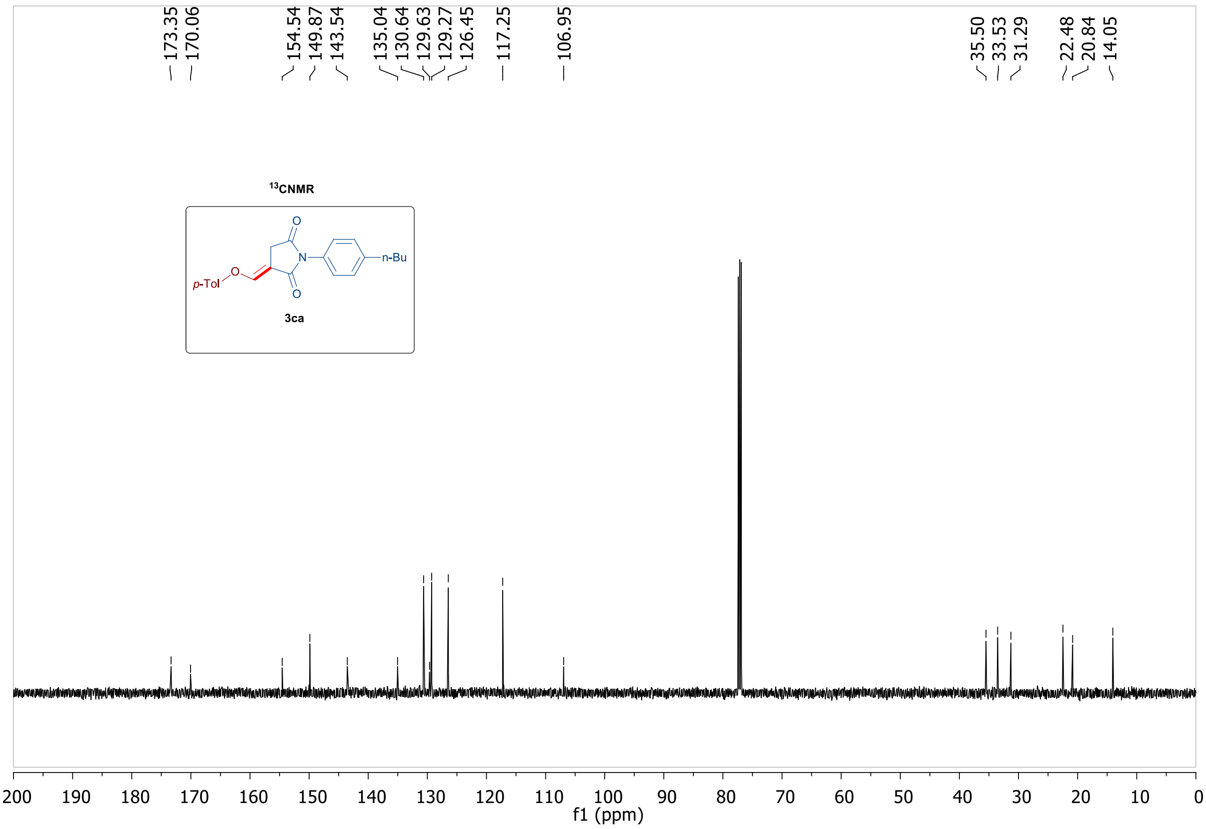
1.99
2.11
3.10
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
f1 (ppm)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31.29
22.48
20.84
14.05
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O
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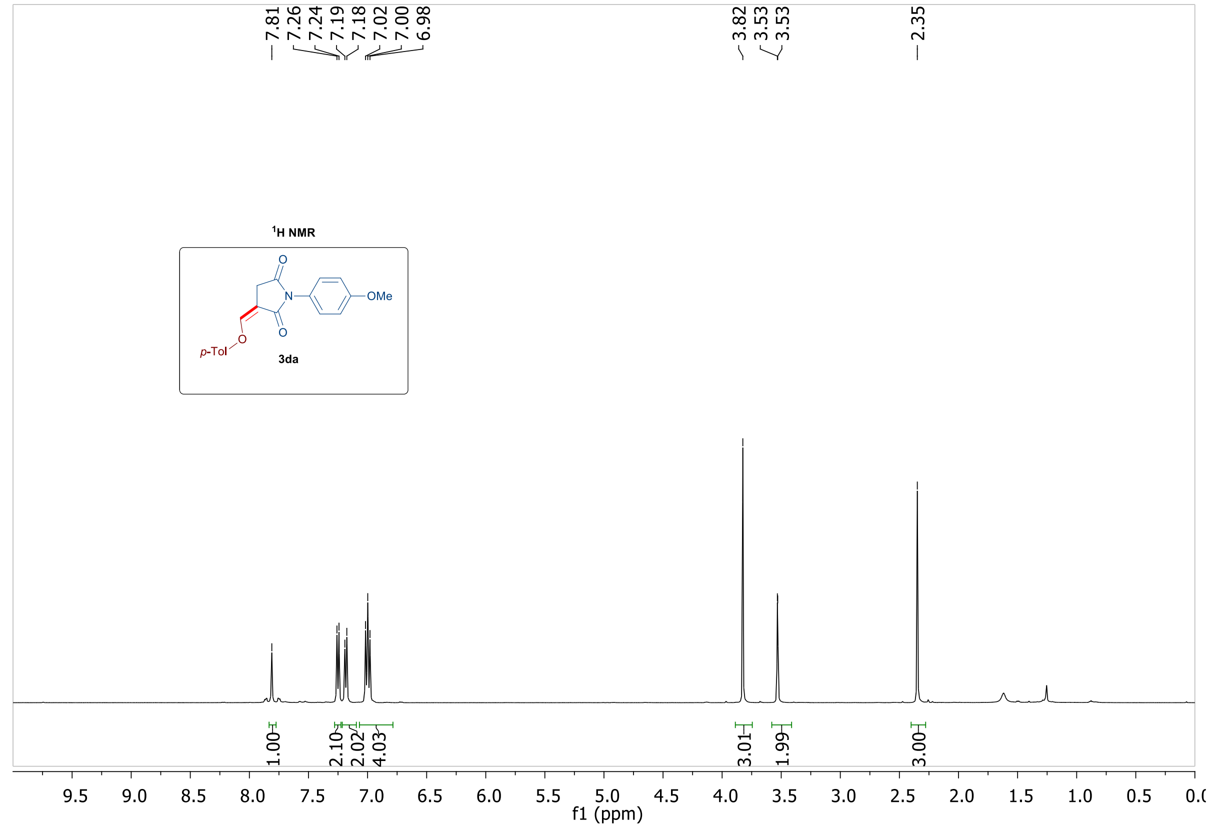
f1 (ppm)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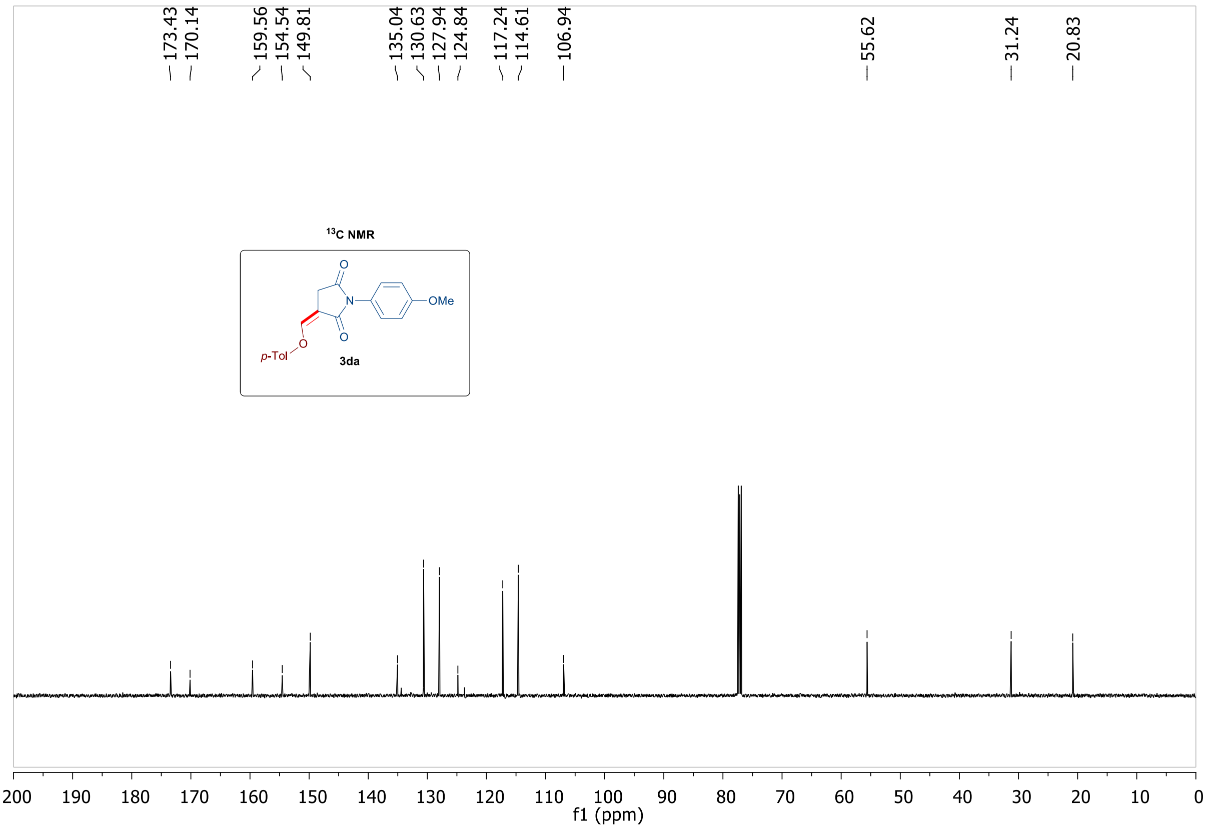
1.99
3.00
f1 (ppm)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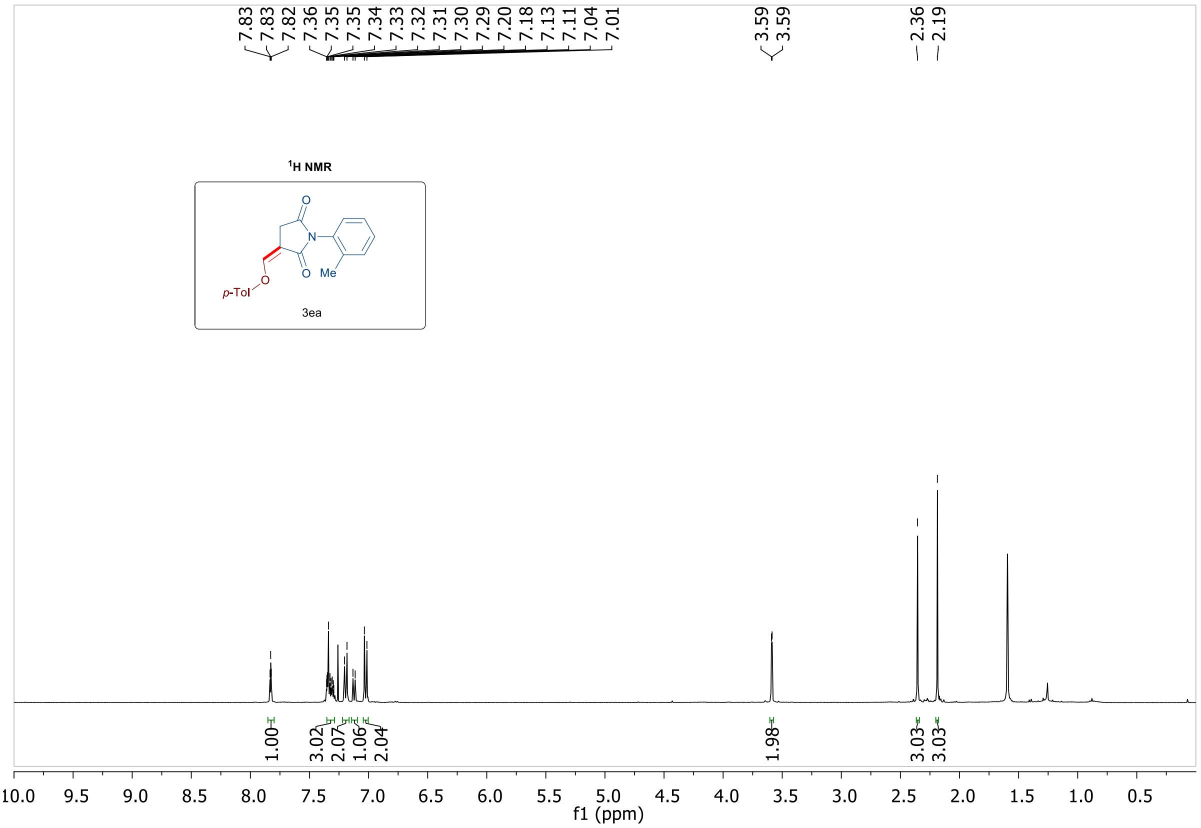
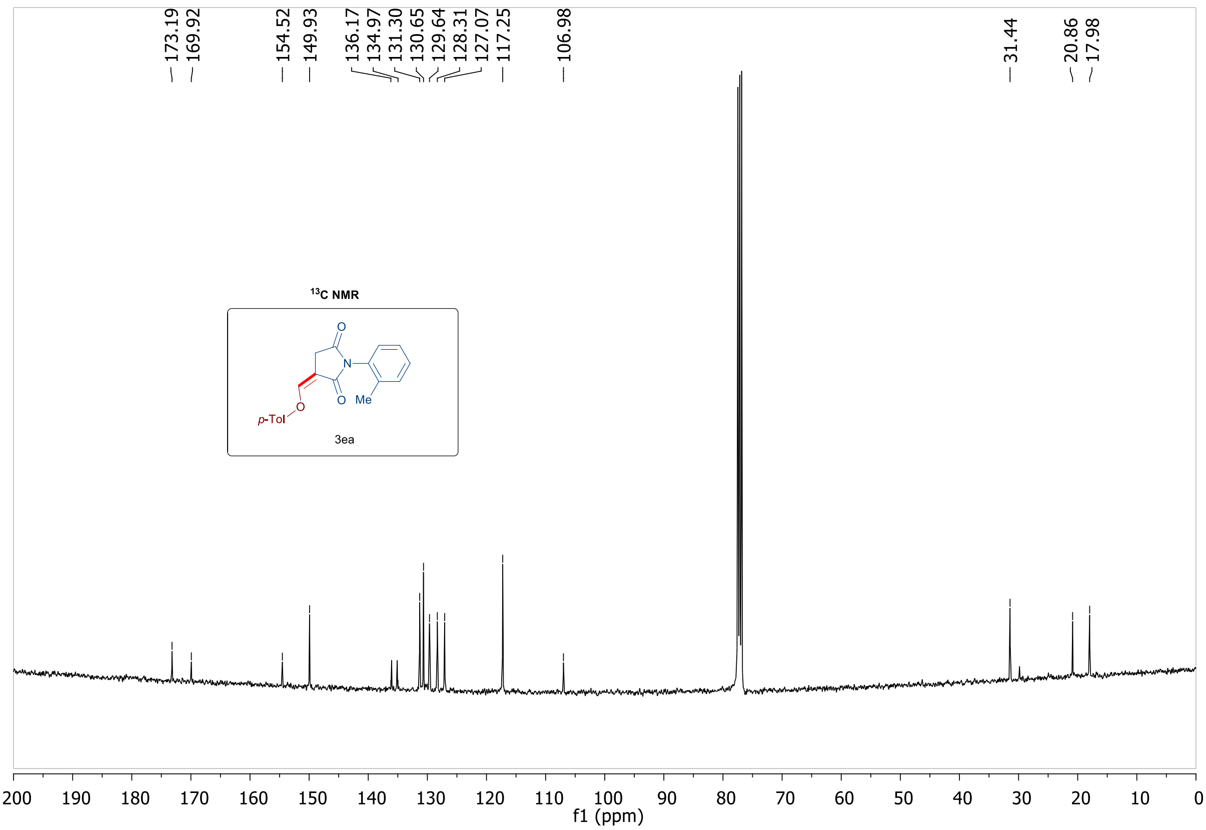
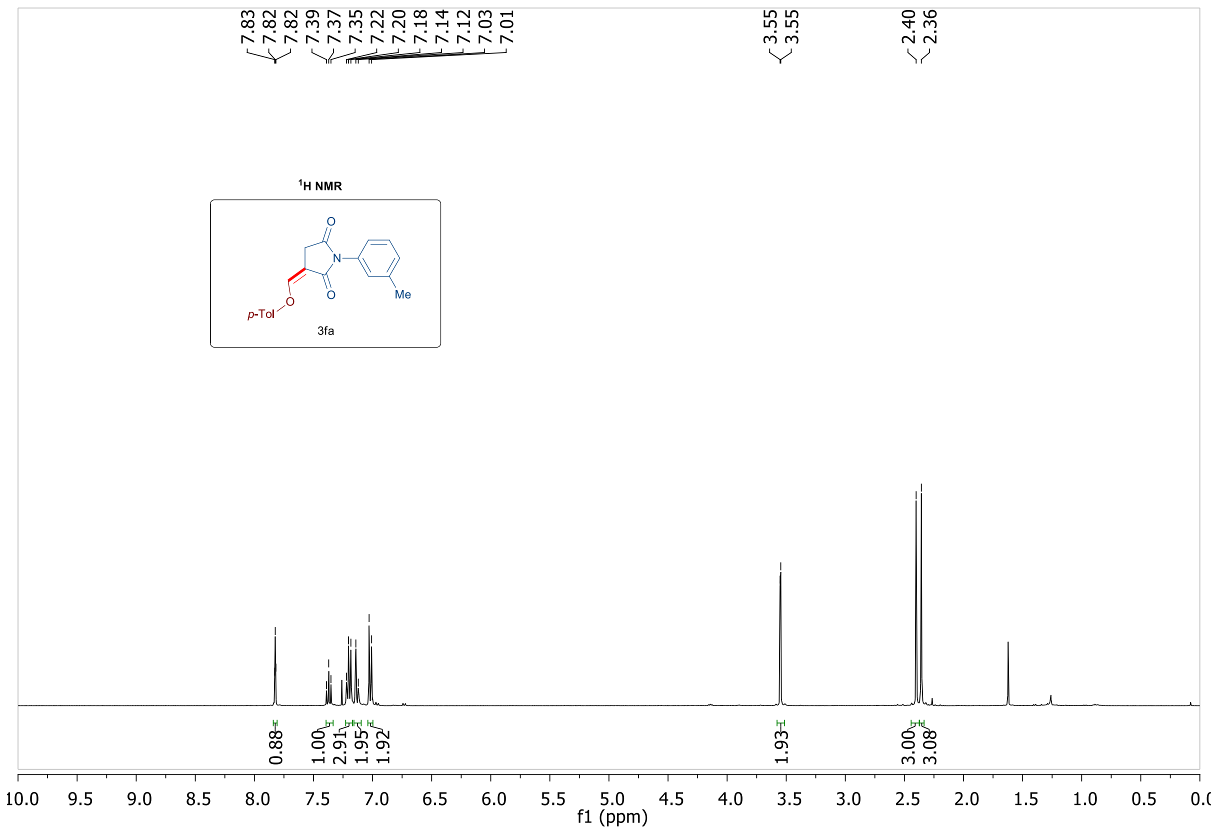
OMe
p-Tol
3da
f1 (ppm)



1H NMR
3ea



13C NMR
3ea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3.55
2.40
2.36
1H NMR
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N
O
O
p-Tol
Me
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1.00
2.91
1.95
1.92
1.93
3.00
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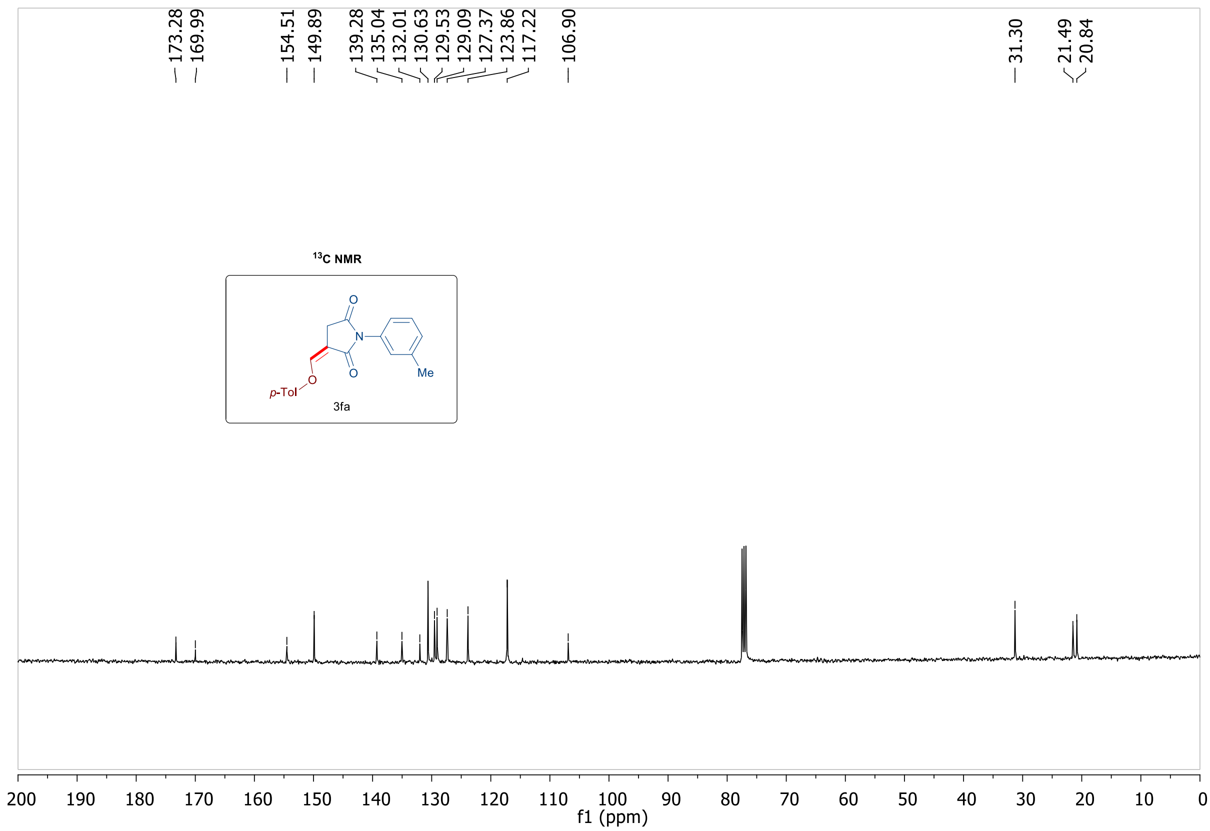
f1 (ppm)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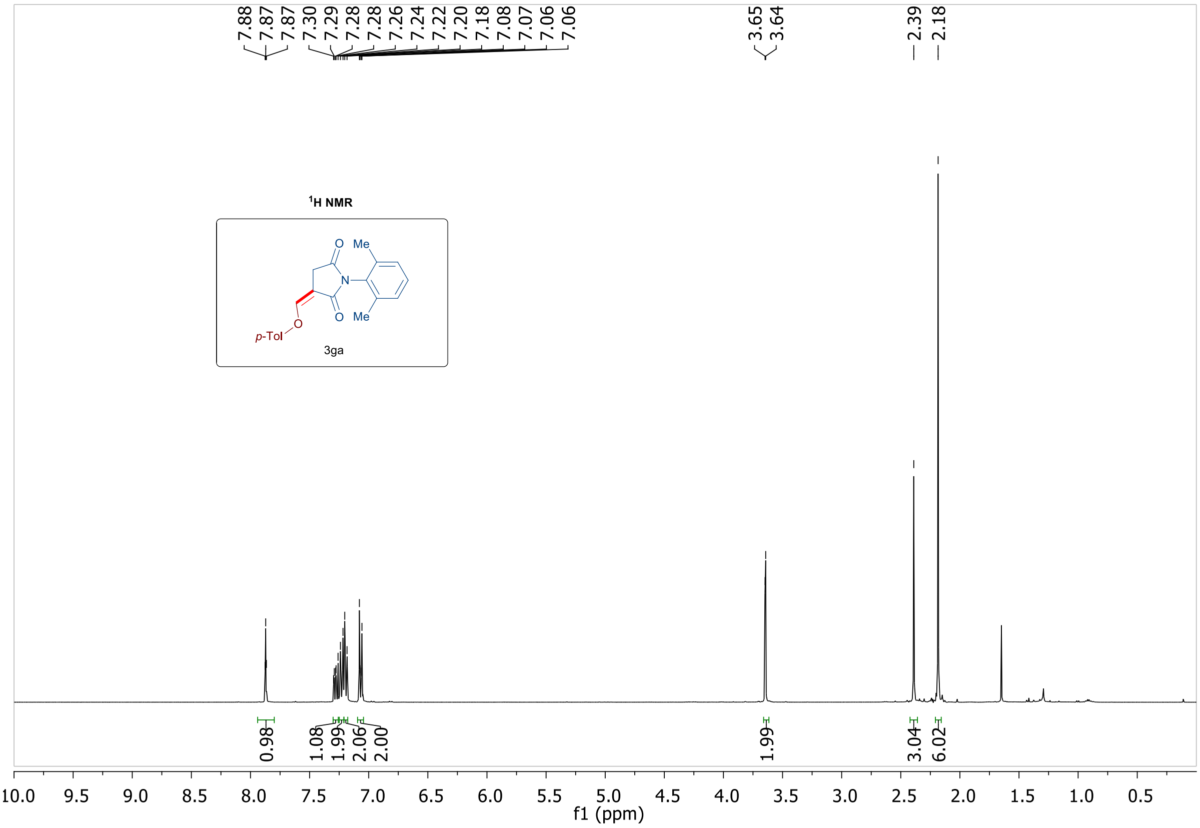
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7.07
7.06
7.06
3.65
3.64
2.39
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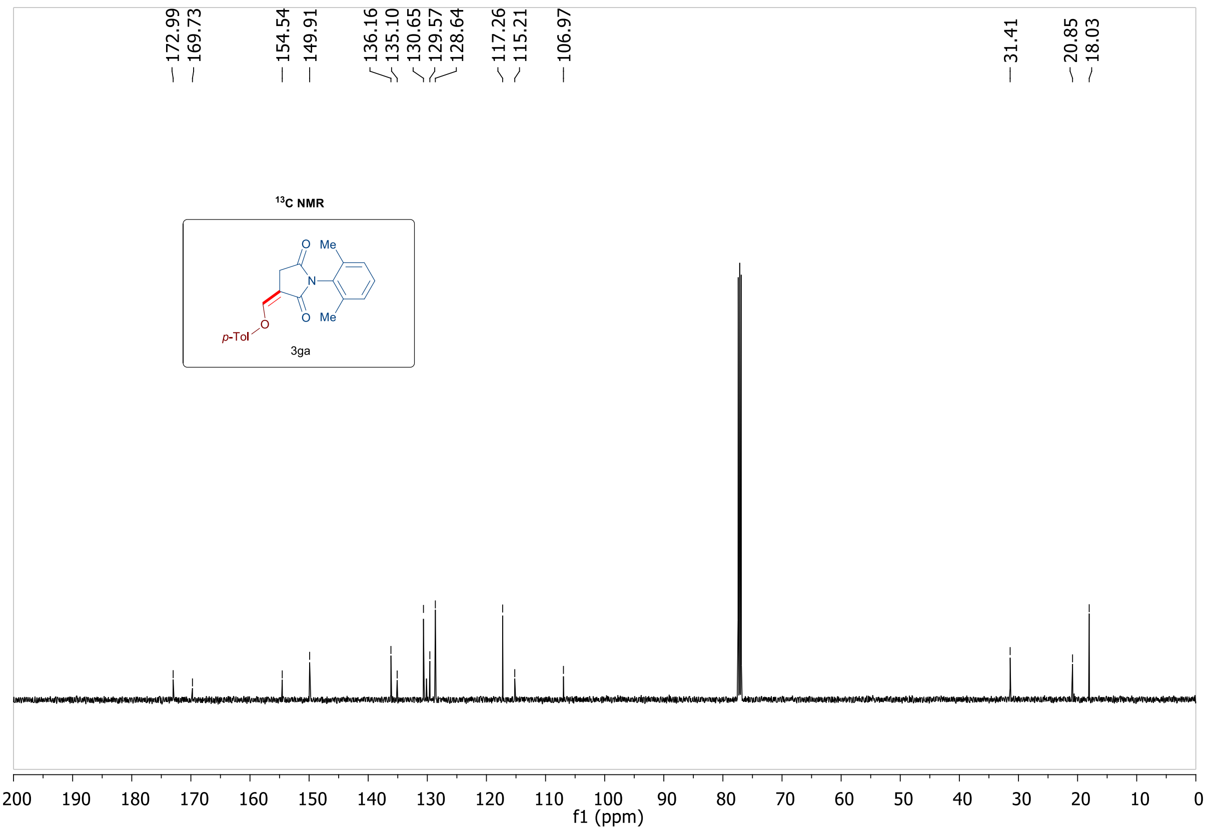
1.99
2.06
2.00
1.99
3.04
6.02
f1 (ppm)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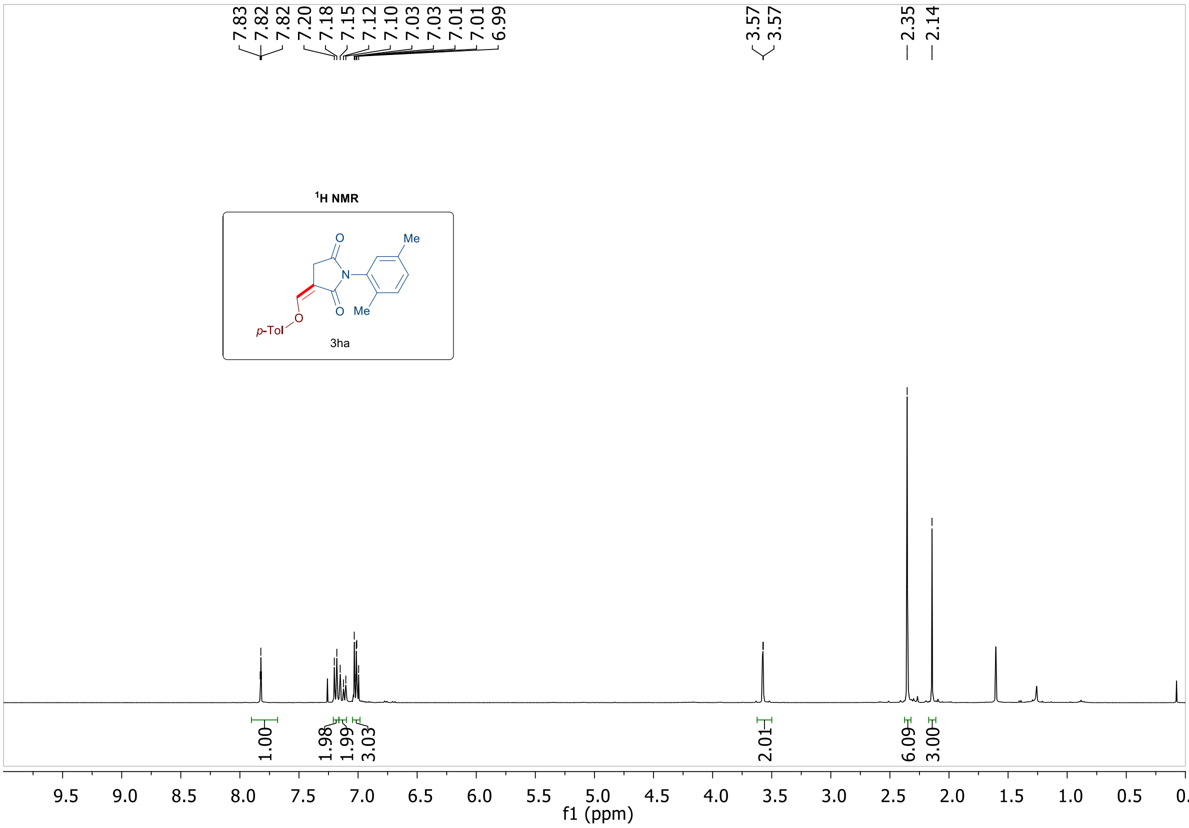
18.03
¹³C NMR
3ga
f1 (ppm)



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7.82
7.20
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7.15
7.12
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7.03
7.01
7.01
6.99
3.57
3.57
2.35
2.14
¹H NMR
O
Me
N
O
Me
p-Tol
O
3ha
1.00
1.98
1.99
3.03
2.01
6.09
3.00
9.5
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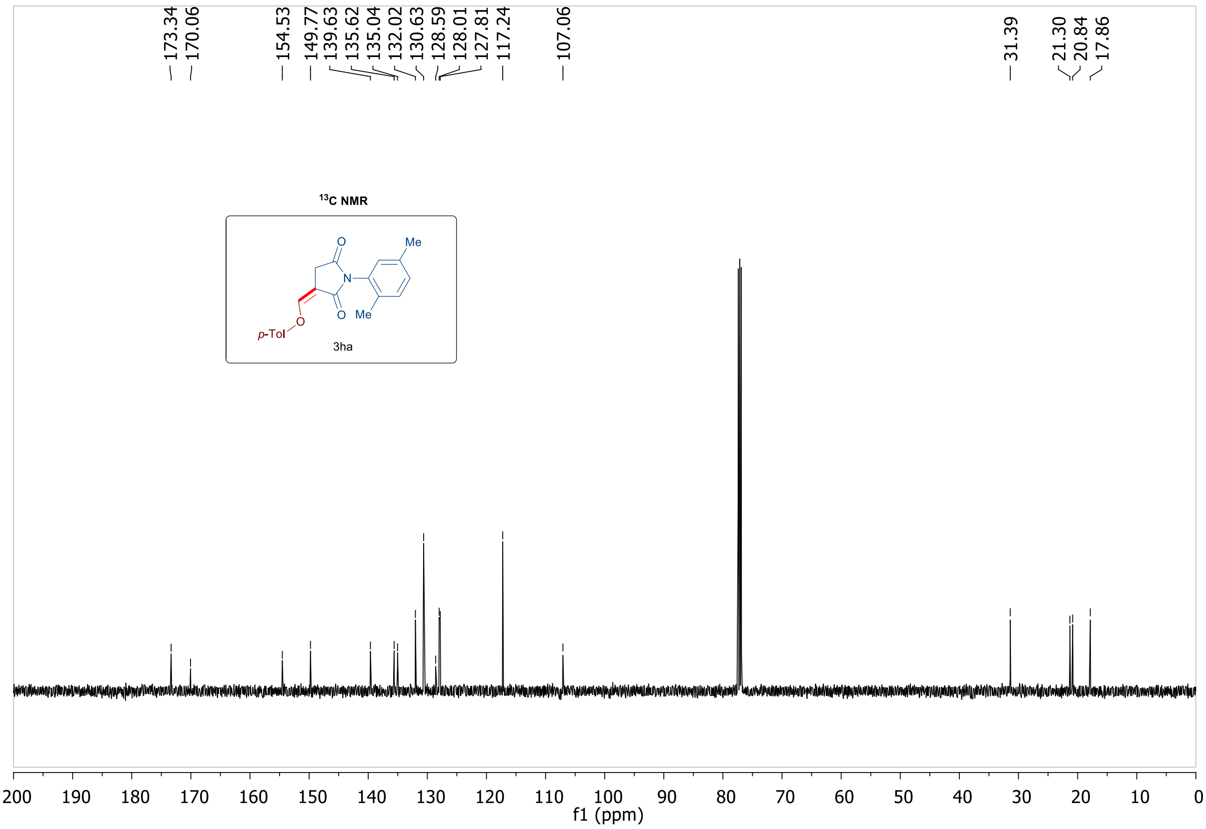
f1 (ppm)



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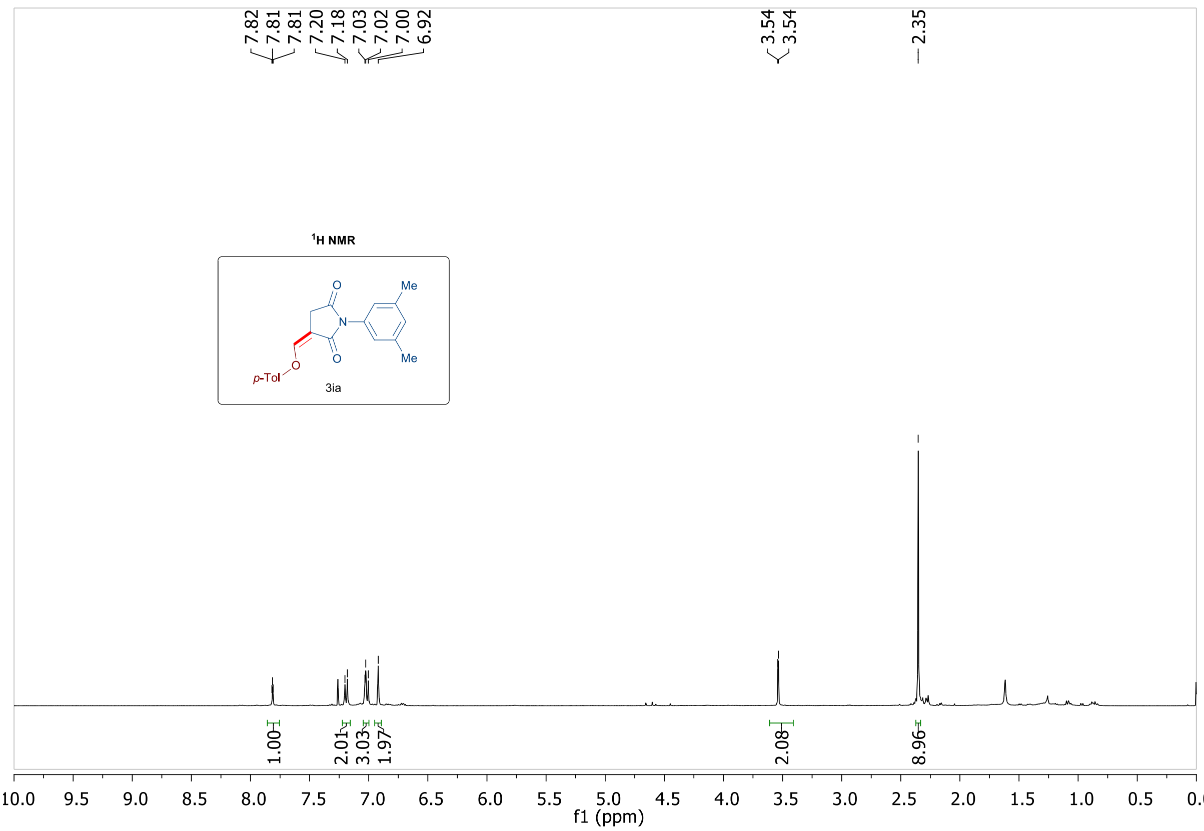
N
O
Me
p-Tol
O
3ha
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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7.81
7.20
7.18
7.03
7.02
7.00
6.92
3.54
3.54
2.35
1H NMR
O
N
Me
Me
O
O
p-Tol
3ia
1.00
2.01
3.03
1.97
2.08
8.96
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
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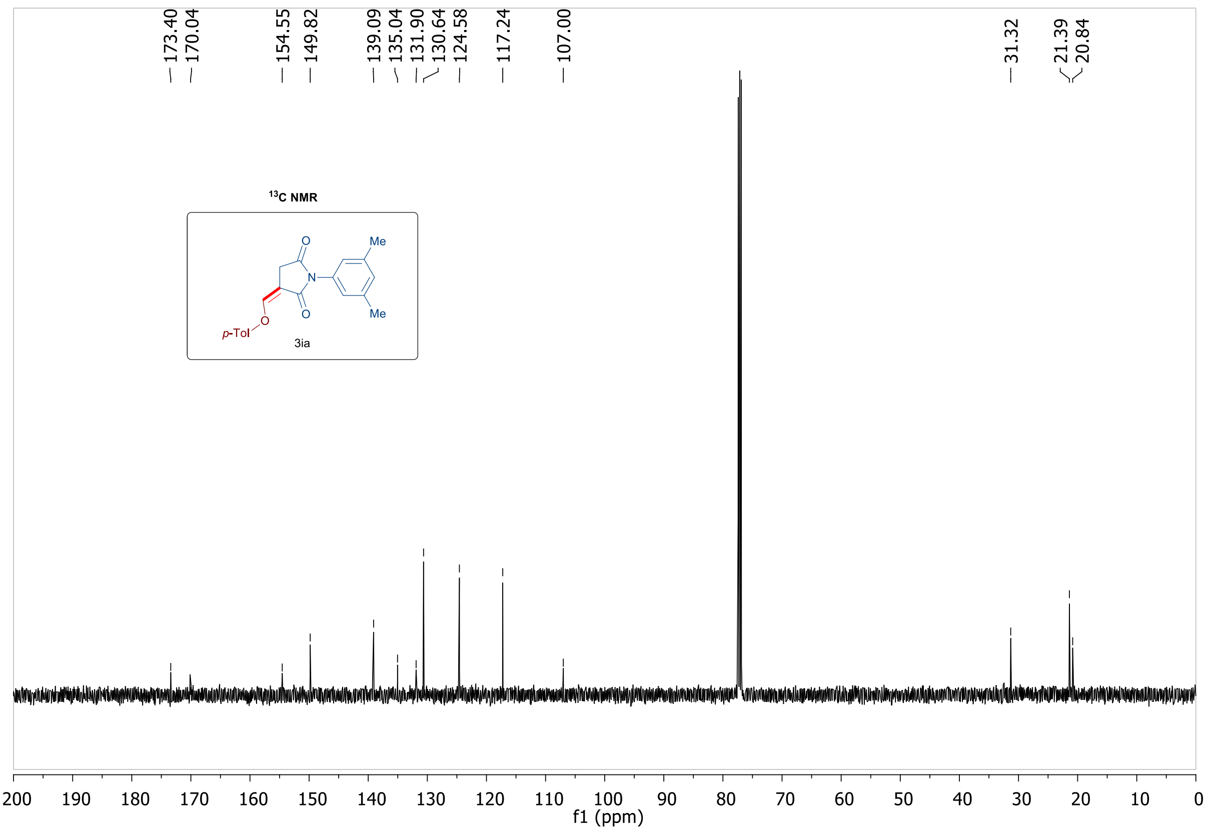
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107.00
31.32
21.39
20.84
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Me
Me
O
O
p-Tol
3ia
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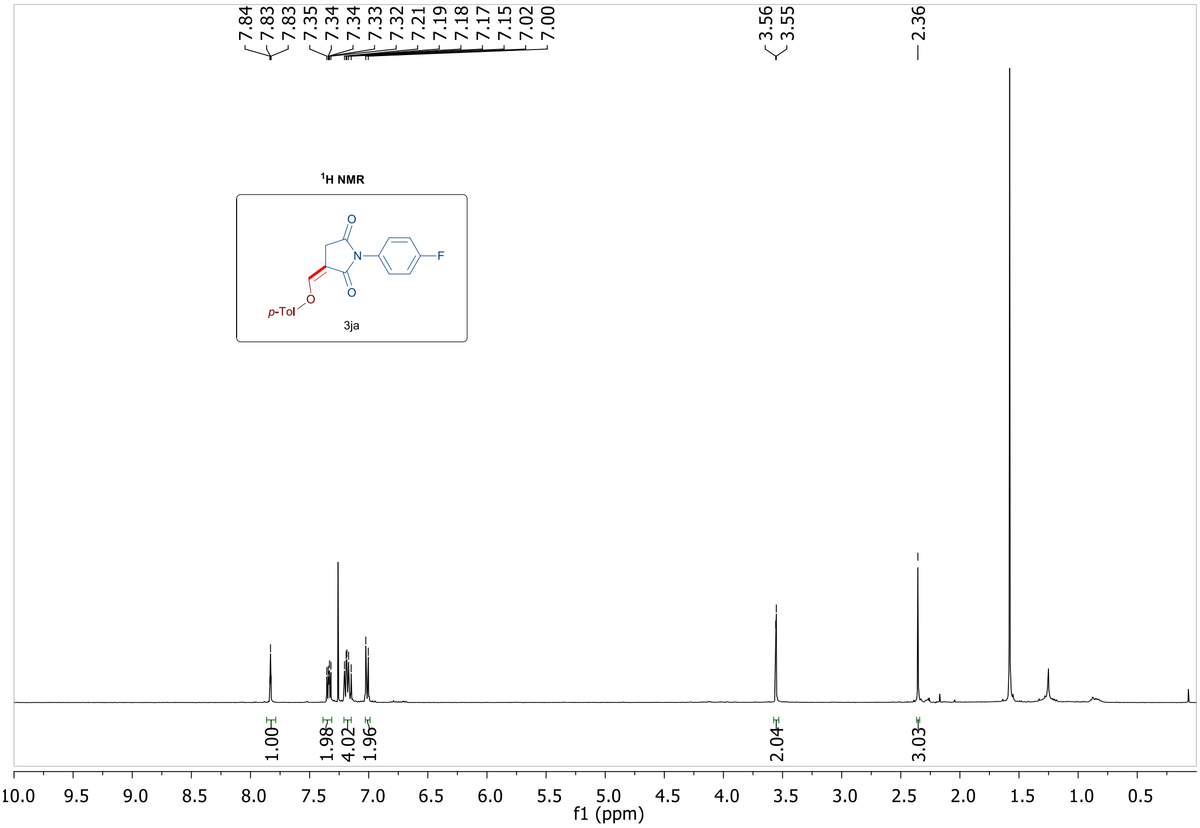
f1 (ppm)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7.32
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7.15
7.02
7.00
3.56
3.55
2.36
¹H NMR
O
N
F
O
O
p-Tol
3ja
1.00
1.98
4.02
1.96
2.04
3.03
10.0
9.5
9.0
8.5
8.0
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7.0
6.5
6.0
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3.0
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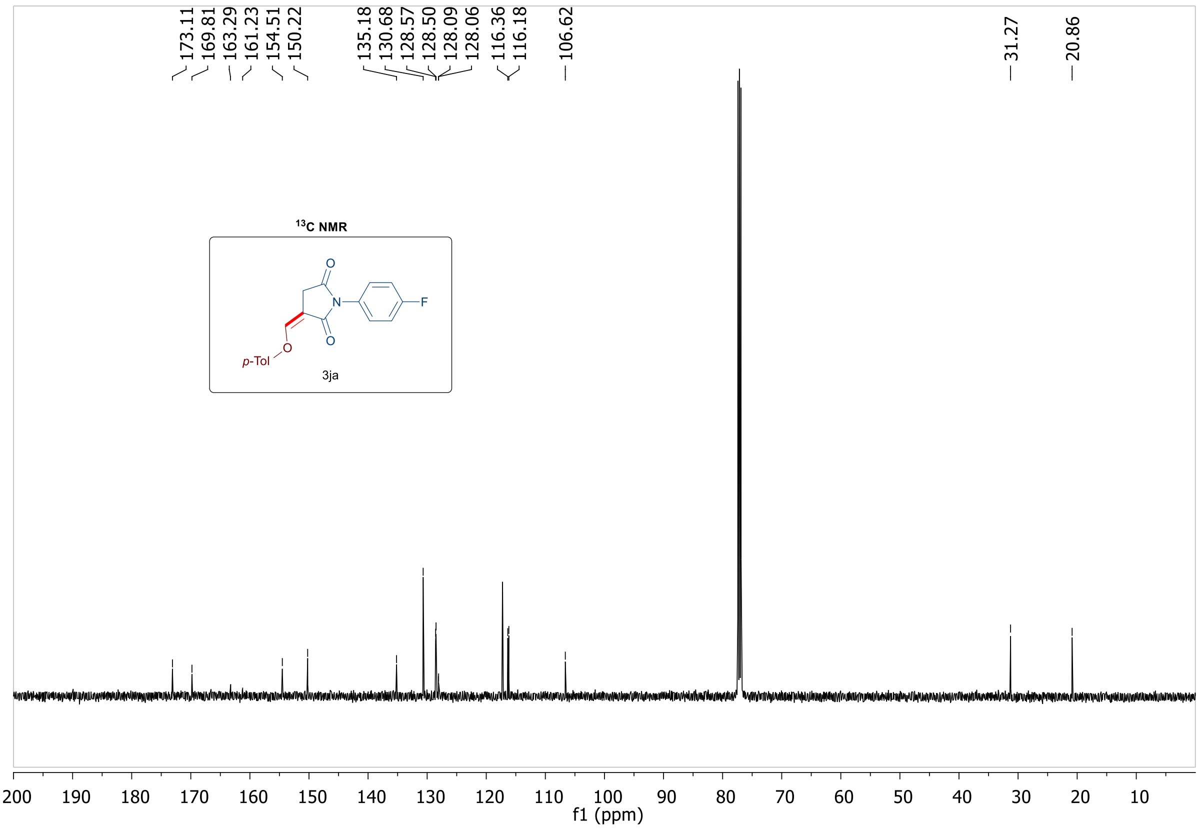
0.5
f1 (ppm)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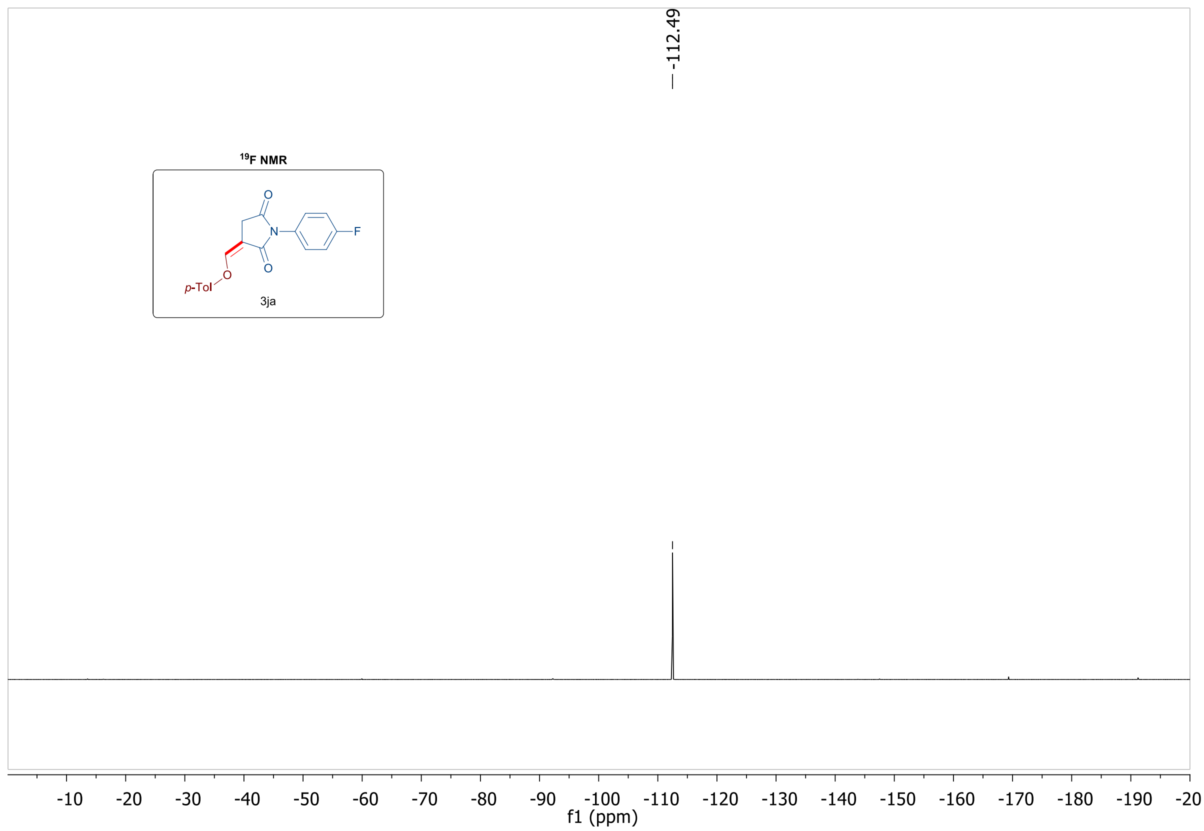
116.36
116.18
106.62
31.27
20.86
¹³C NMR
O
N
F
O
O
p-Tol
3ja
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)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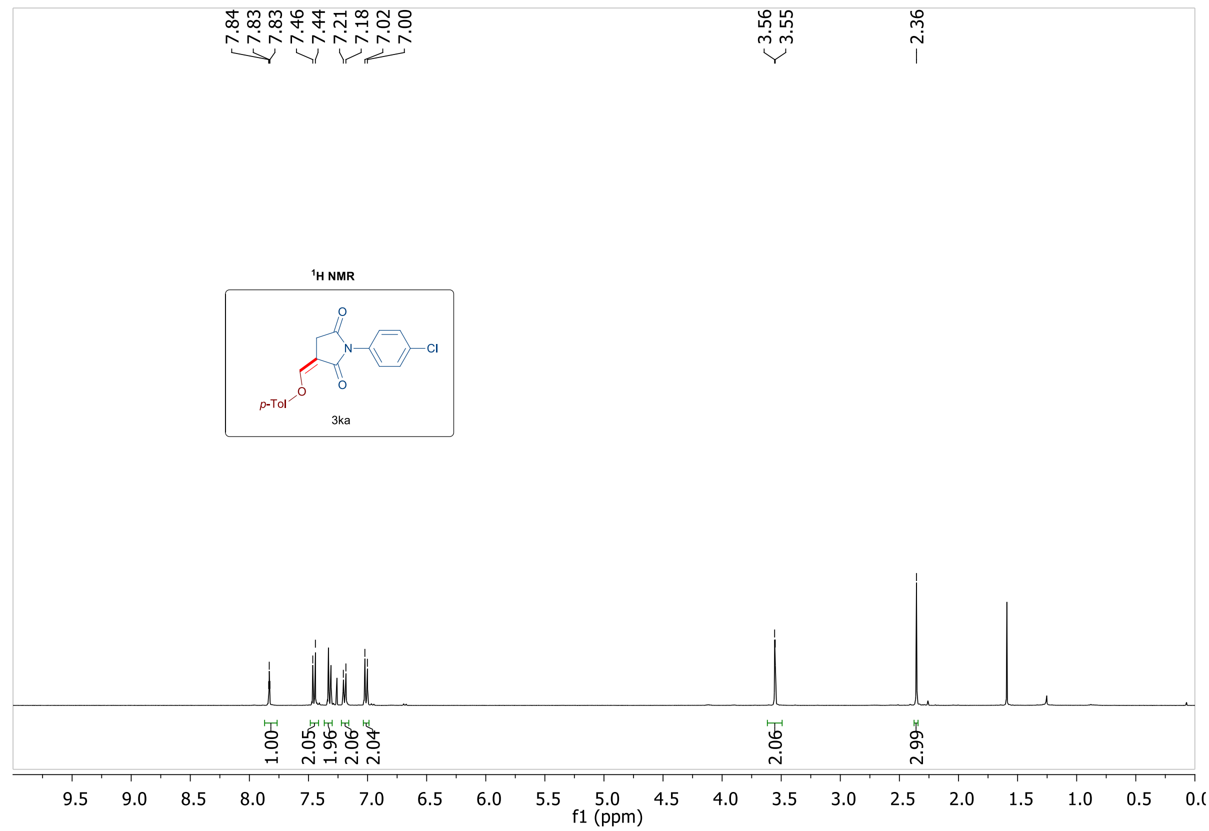
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3.55
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p-Tol
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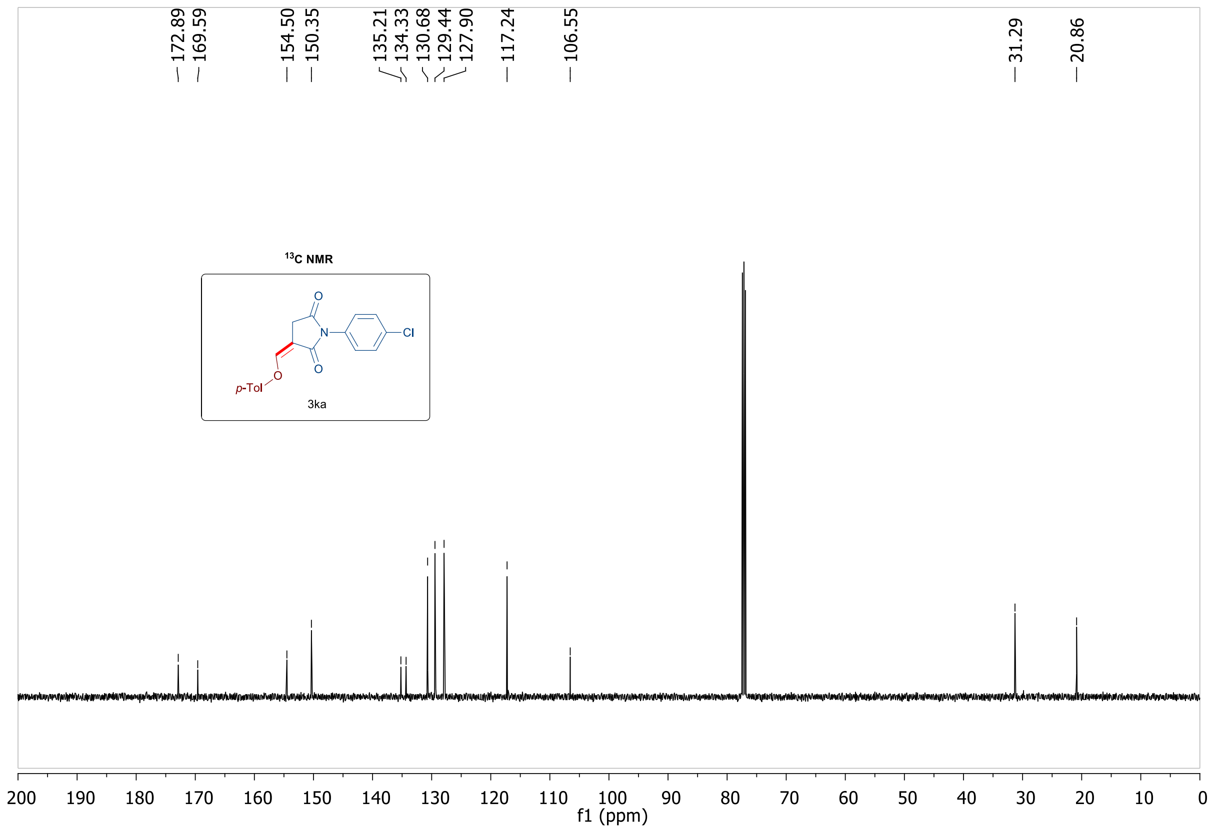
2.04
2.06
2.99
f1 (ppm)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¹³C NMR
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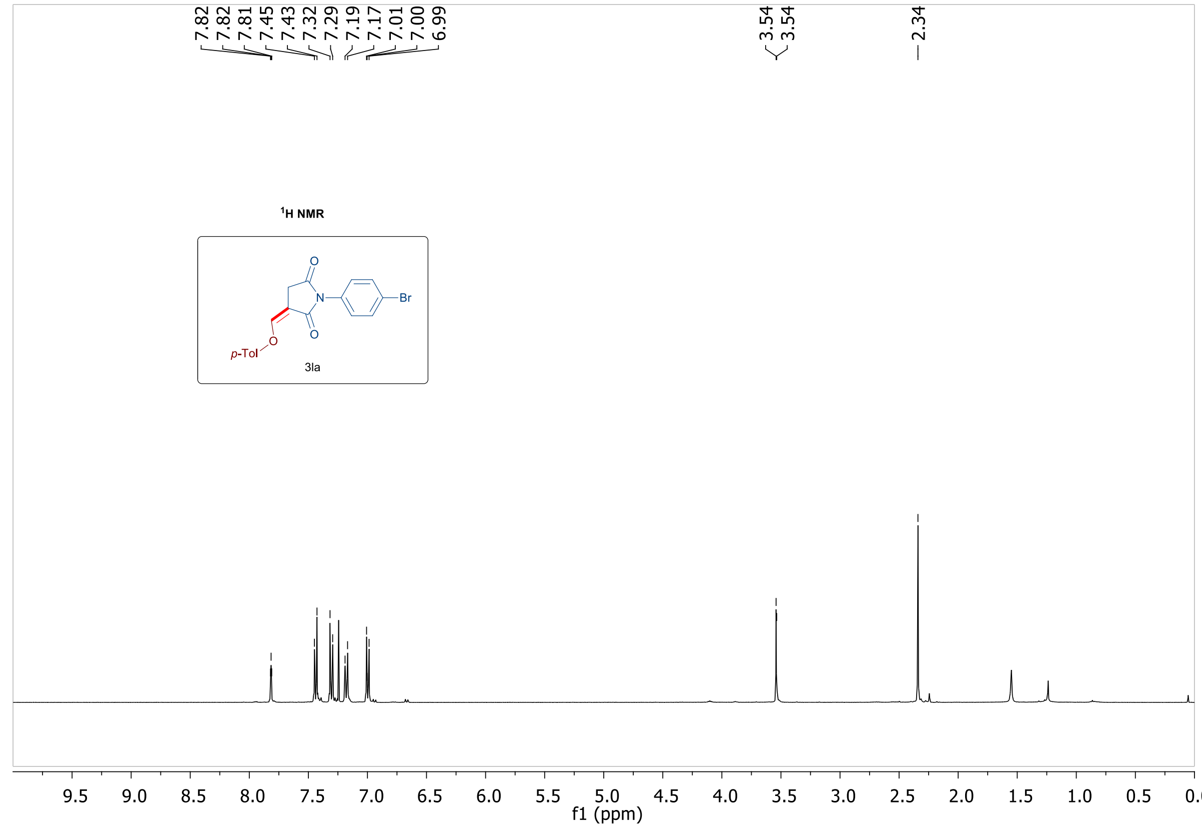
p-Tol
f1 (ppm)



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7.01
7.00
6.99
3.54
3.54
2.34
1H NMR
O
N
Br
O
O
p-Tol
3la
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9.0
8.5
8.0
7.5
7.0
6.5
6.0
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4.0
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3.0
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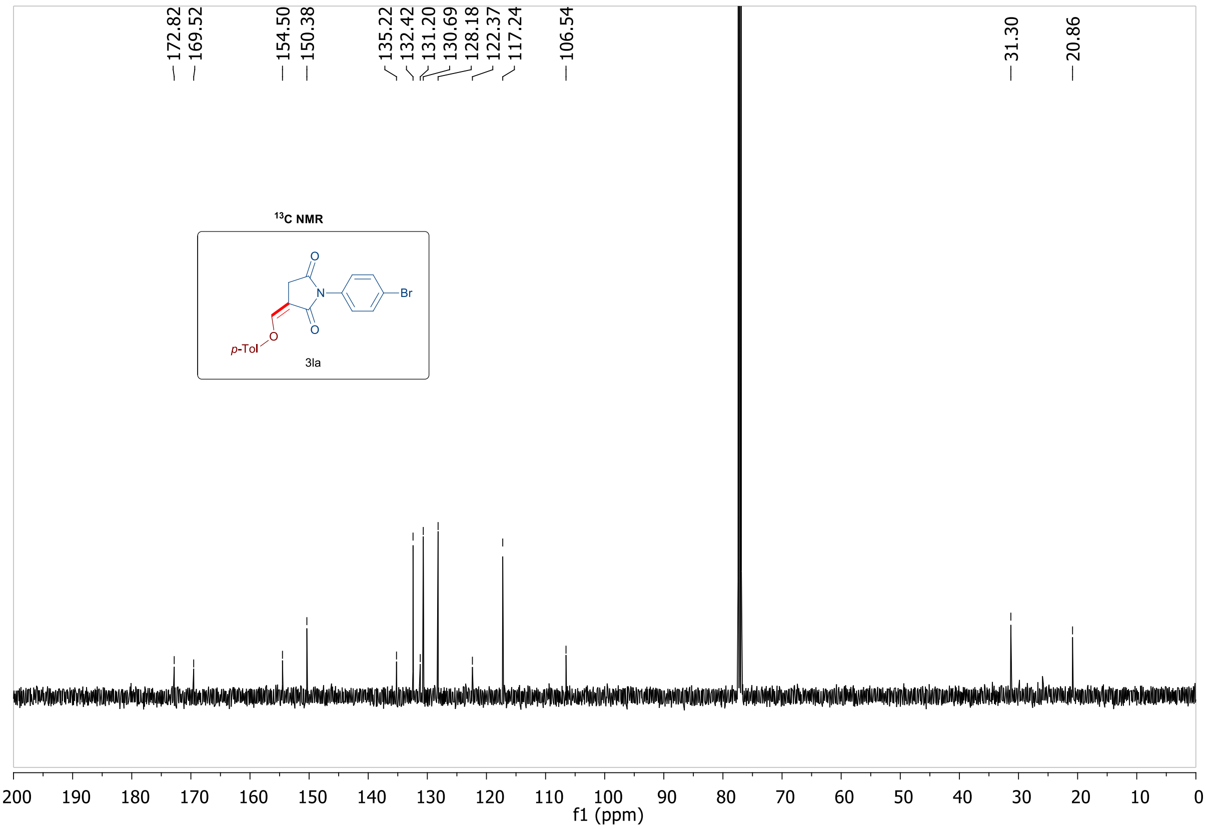
0.5
f1 (ppm)



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130.69
128.18
122.37
117.24
106.54
31.30
20.86
13C NMR
O
N
Br
O
O
p-Tol
3la
200
190
180
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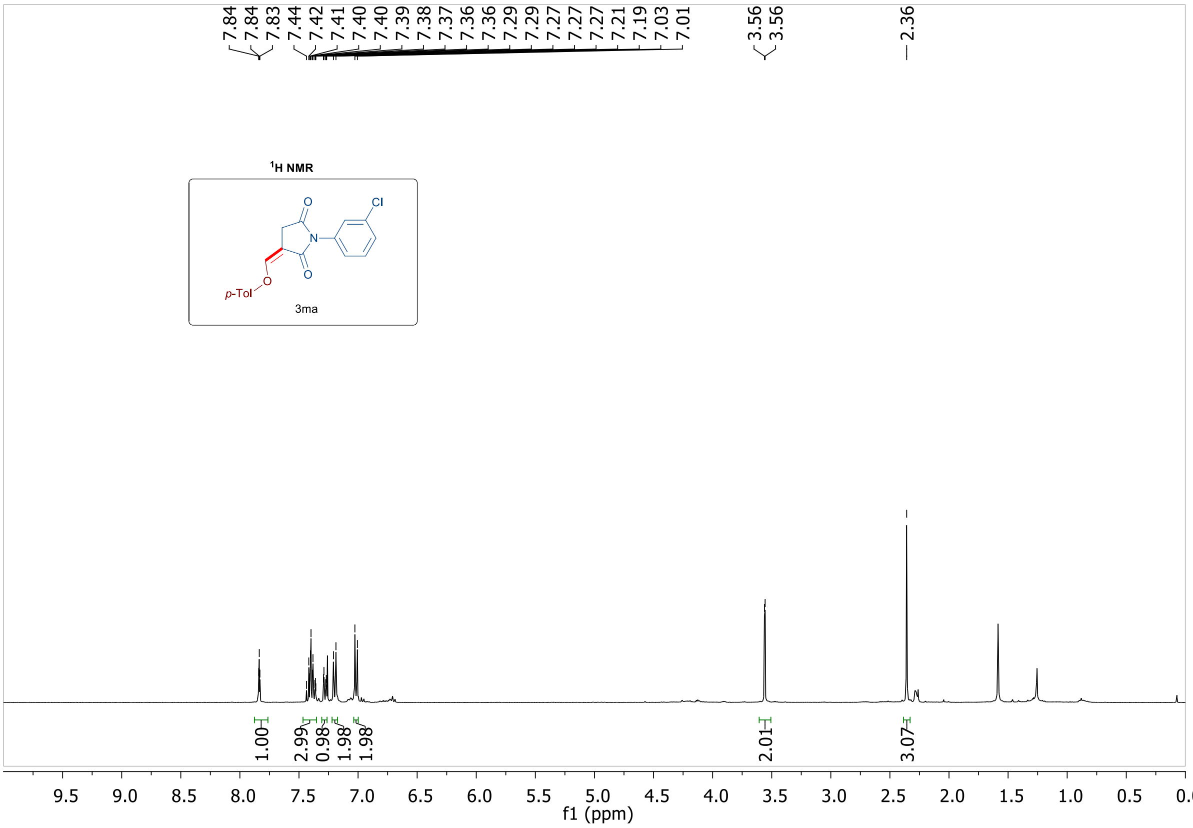
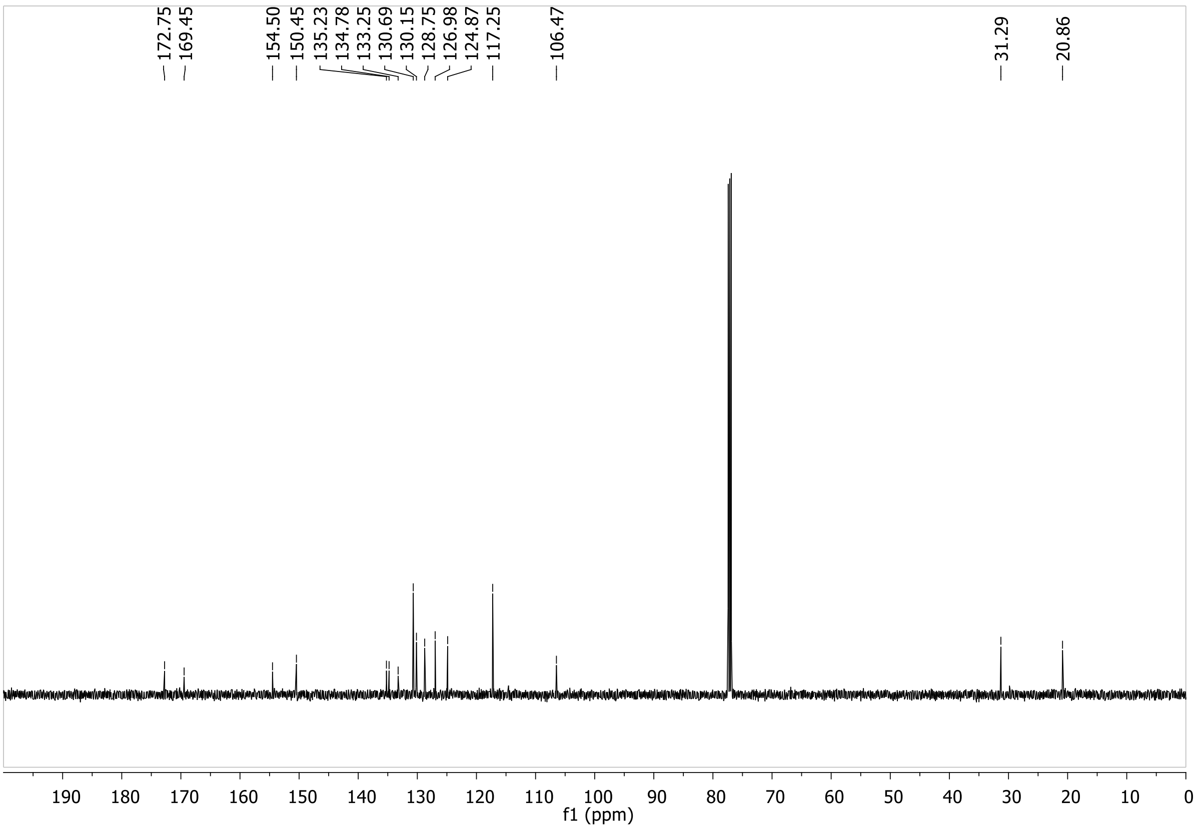
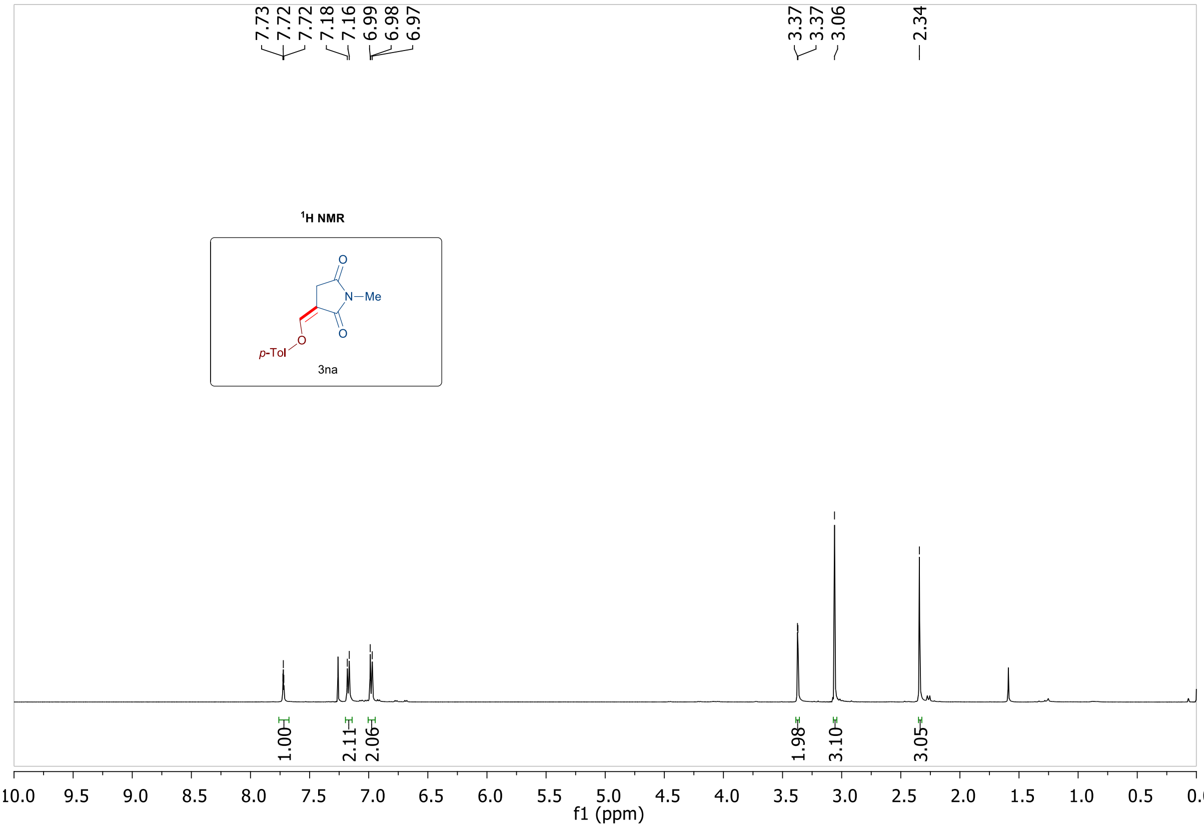
f1 (ppm)







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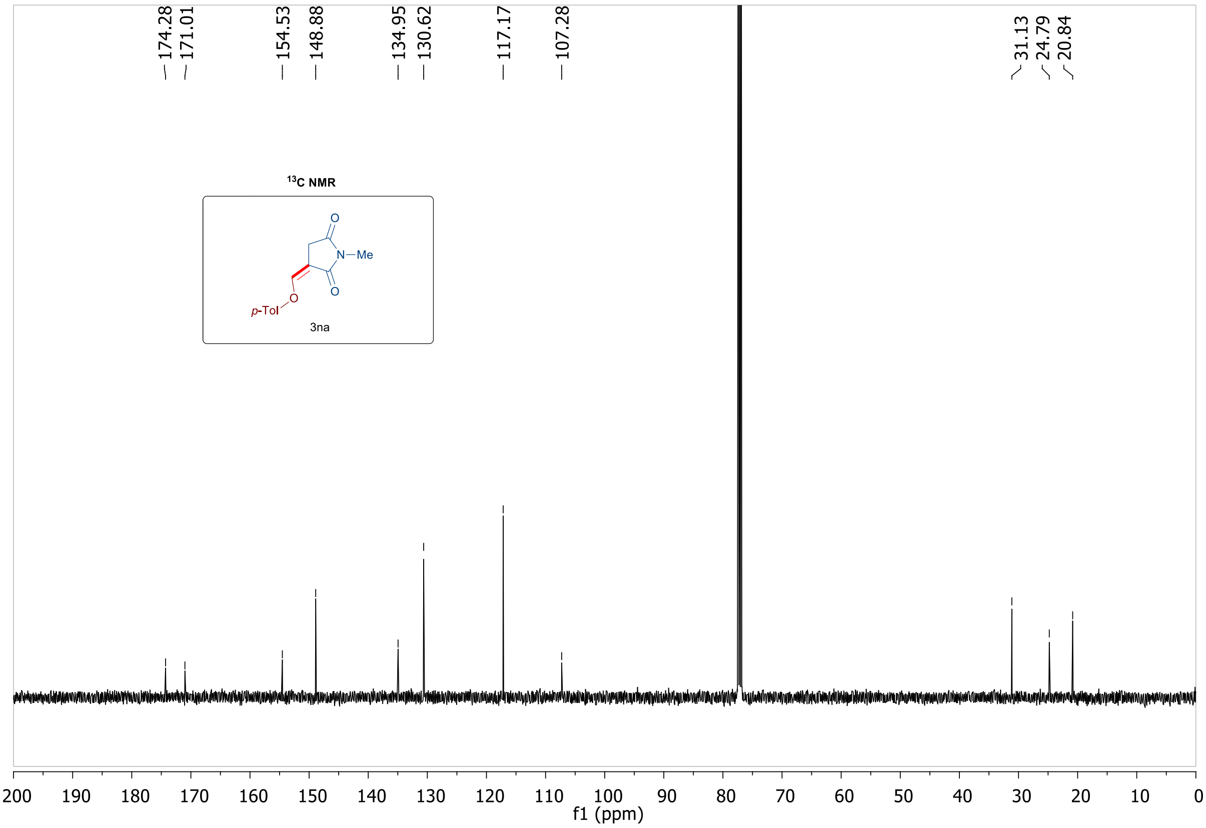
7.16
6.99
6.98
6.97
3.37
3.37
3.06
2.34
¹H NMR
O
N—Me
O
p-Tol
O
3na
1.00
2.11
2.06
1.98
3.10
3.05
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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130.62
117.17
107.28
31.13
24.79
20.84
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N–Me
O
p-Tol
O
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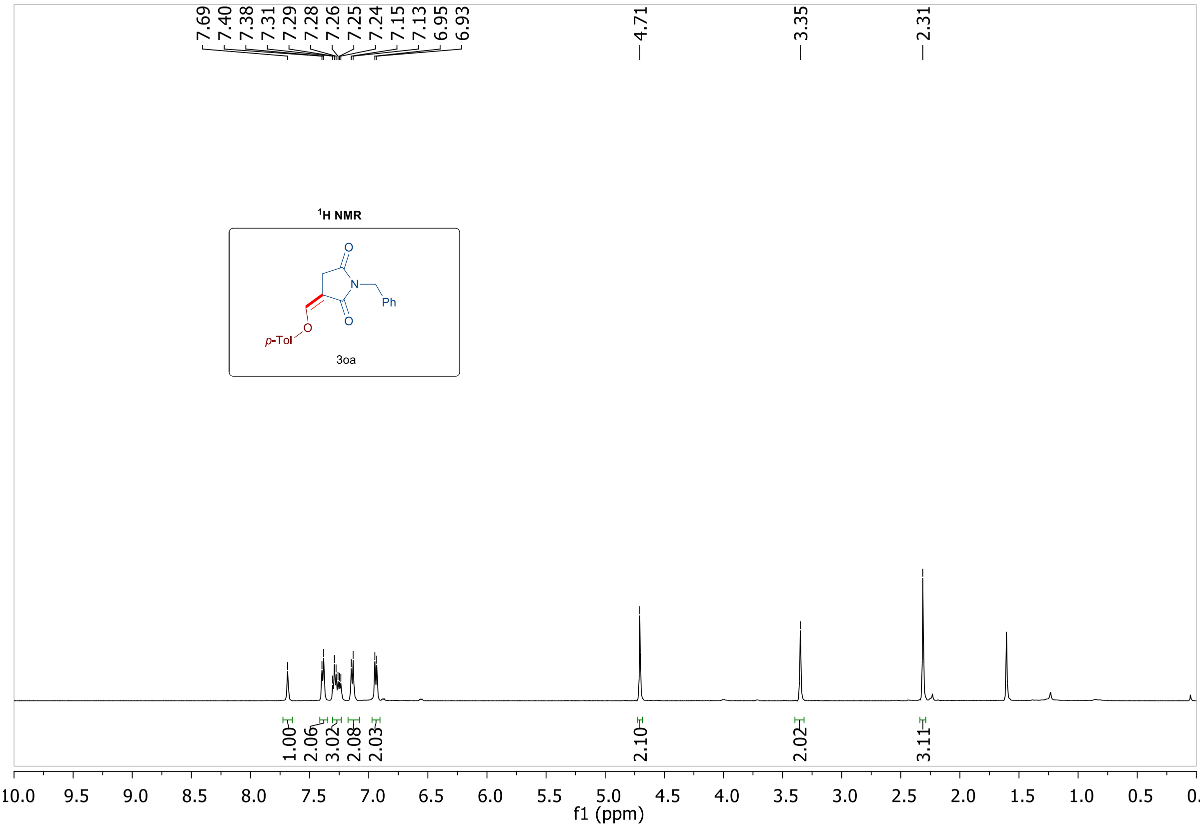
f1 (ppm)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7.26
7.25
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6.93
4.71
3.35
2.31
1H NMR
O
N
Ph
O
O
p-Tol
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2.06
3.02
2.08
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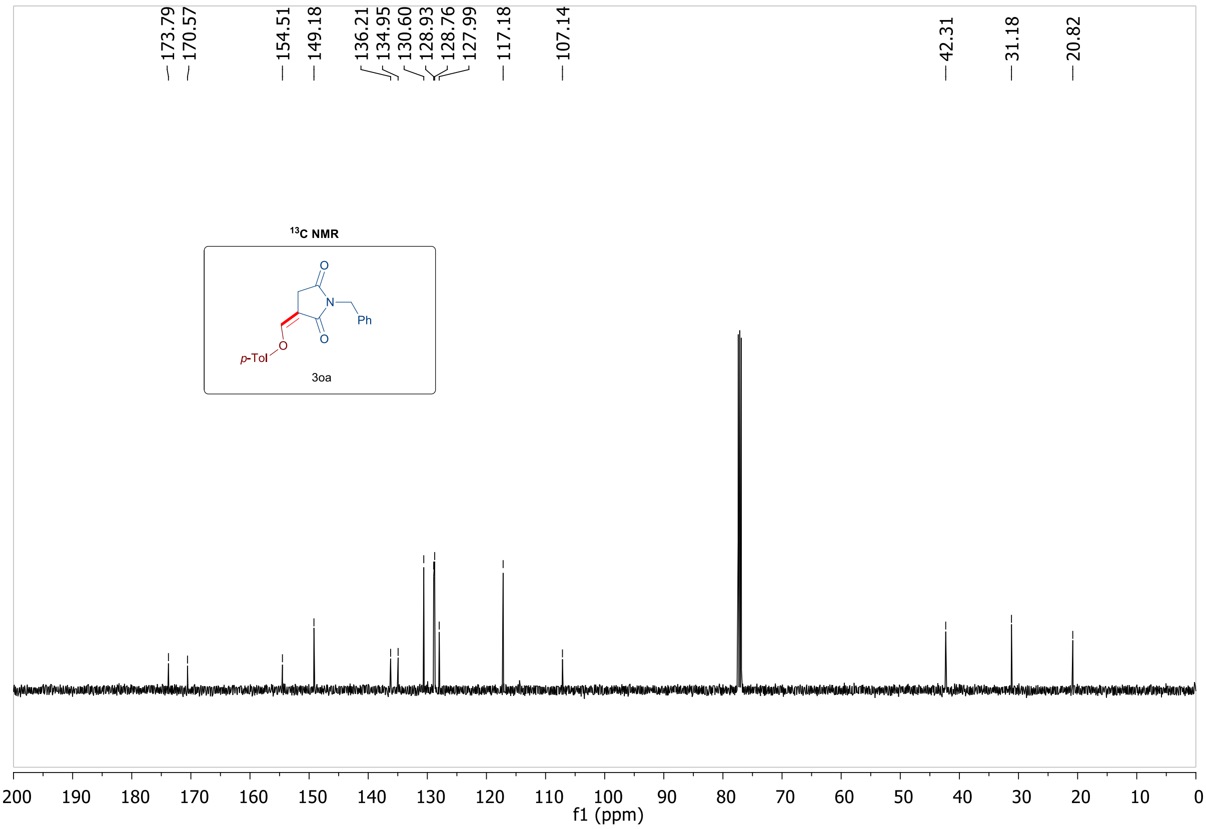
2.10
2.02
3.11
f1 (ppm)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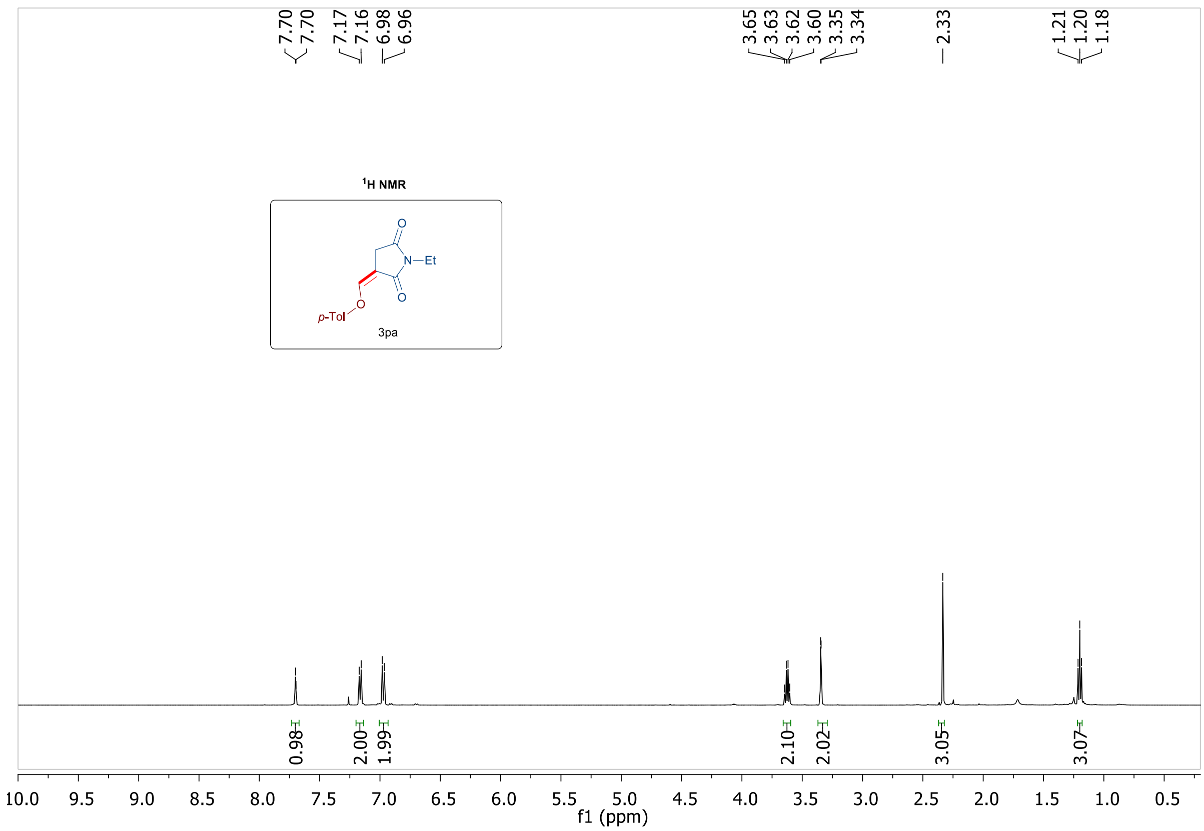
31.18
20.82
13C NMR
O
N
Ph
O
O
p-Tol
3oa
f1 (ppm)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3.35
3.34
2.33
1.21
1.20
1.18
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p-Tol
3pa
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2.02
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3.07
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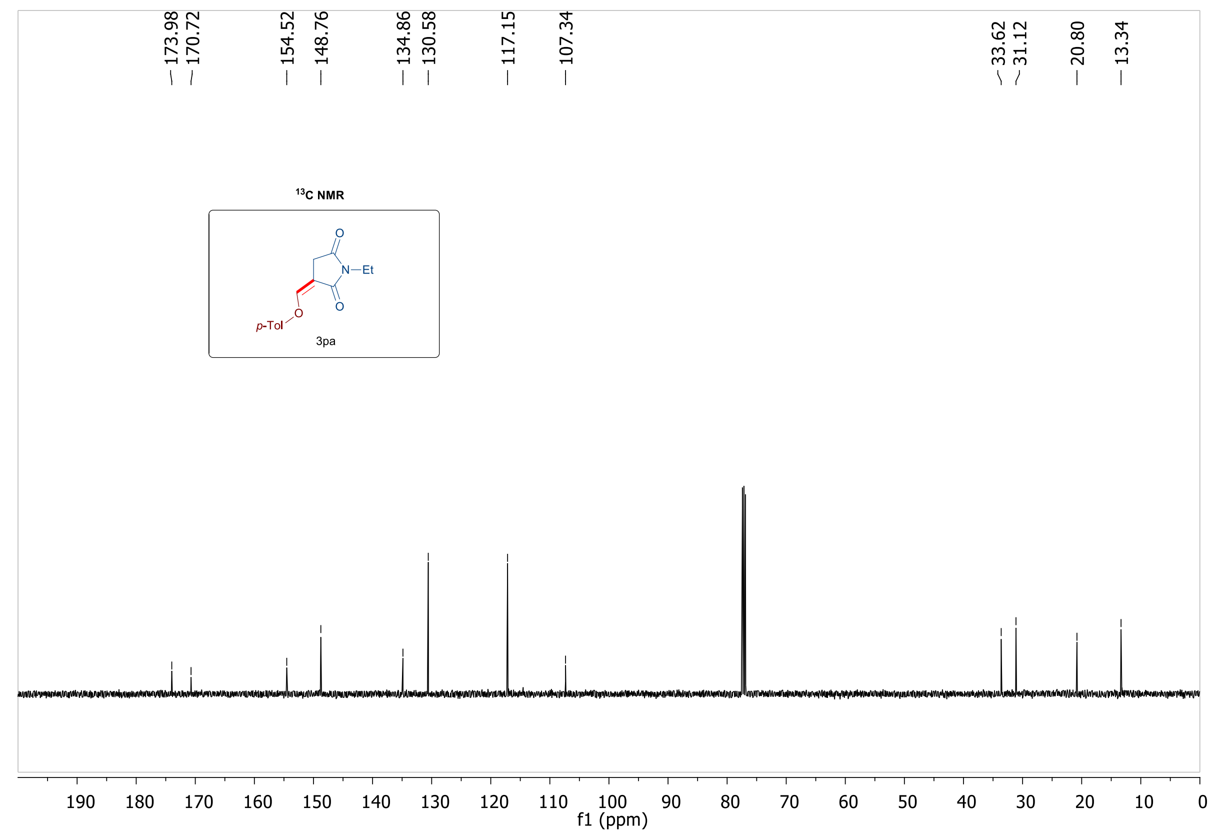
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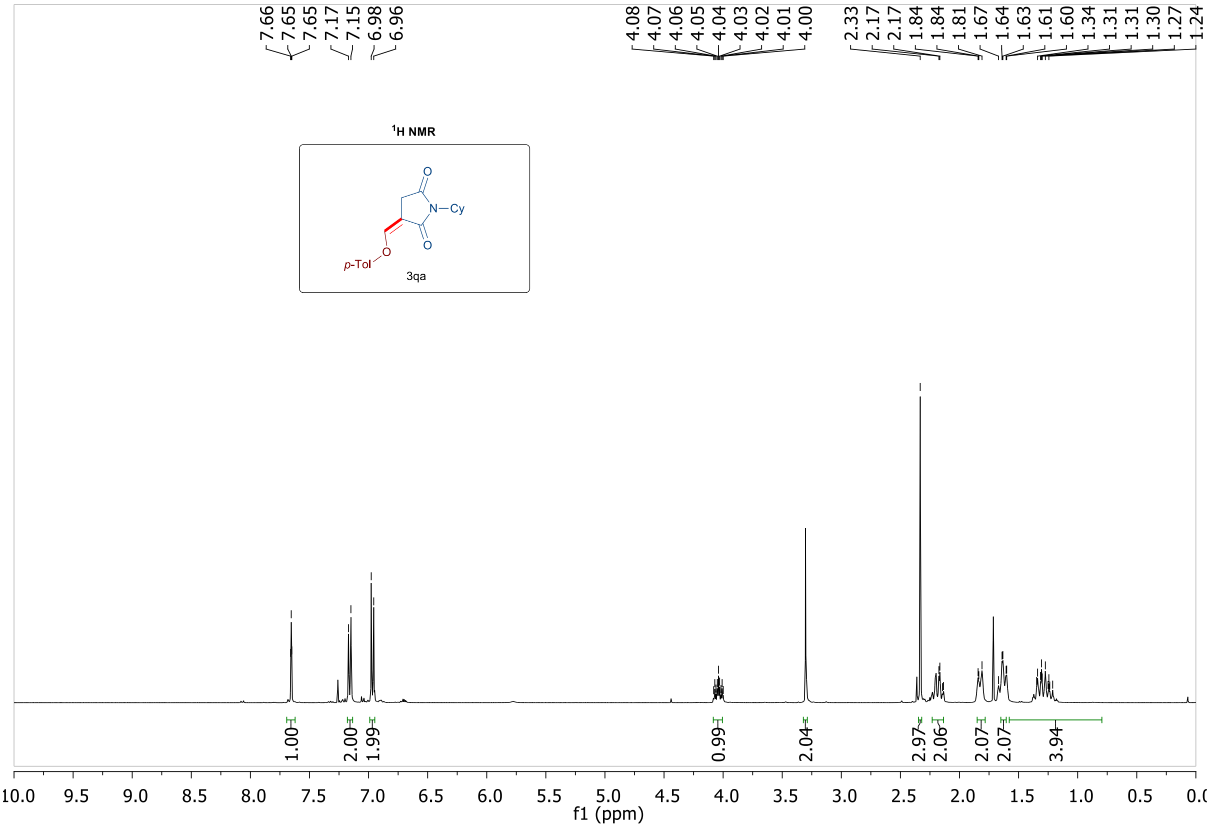
p-Tol
3pa
f1 (ppm)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4.03
4.02
4.01
4.00
2.33
2.17
2.17
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1.84
1.81
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1.63
1.61
1.60
1.34
1.31
1.31
1.30
1.27
1.24
1H NMR
N
Cy
O
O
O
p-Tol
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1.00
2.00
1.99
0.99
2.04
2.97
2.06
2.07
2.07
3.94
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9.5
9.0
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8.0
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6.0
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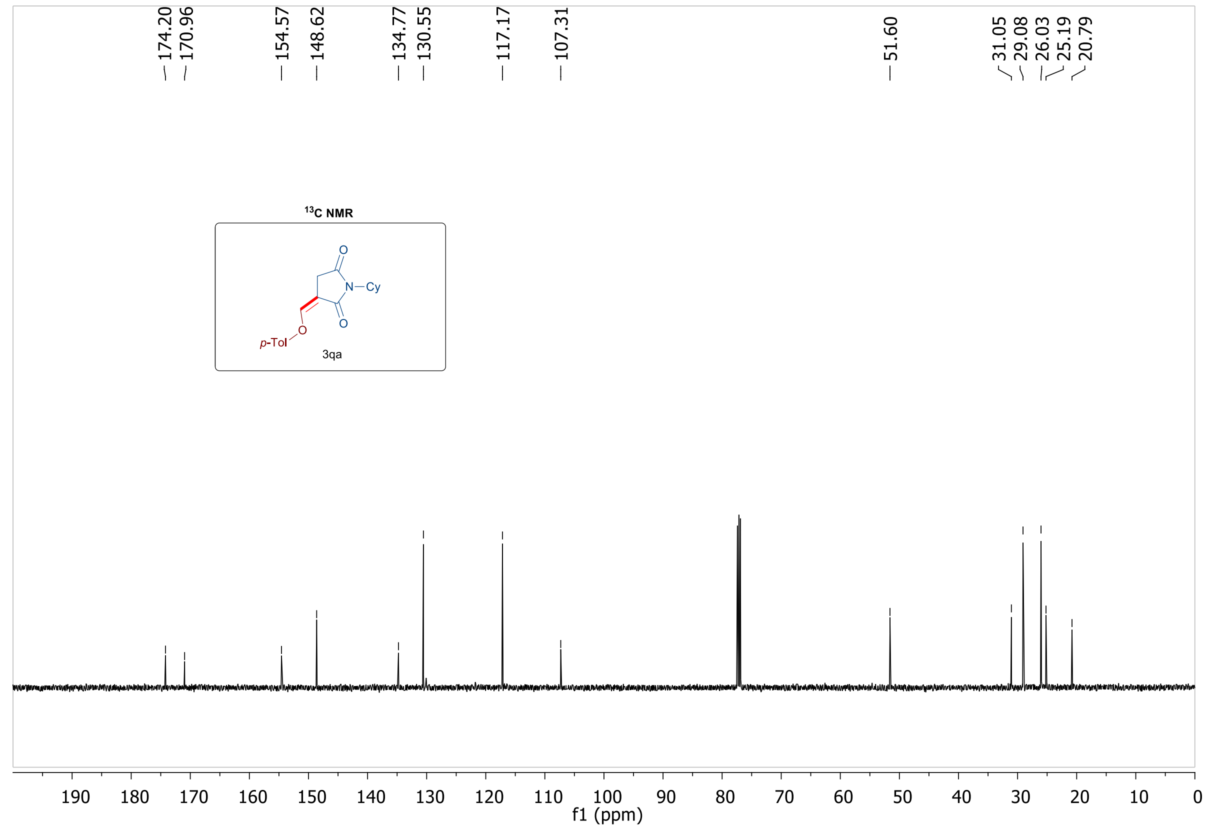
f1 (ppm)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107.31
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31.05
29.08
26.03
25.19
20.79
13C NMR
N
Cy
O
O
O
p-Tol
3qa
190
180
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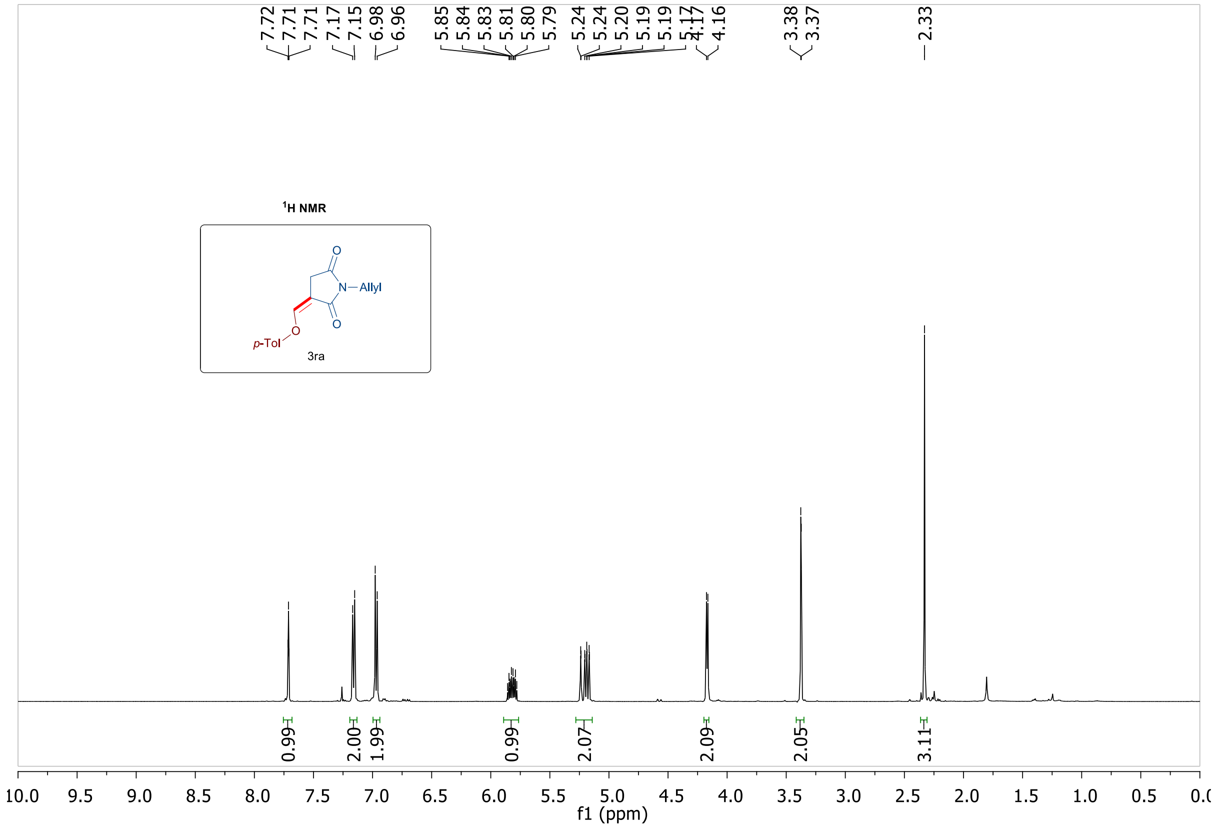
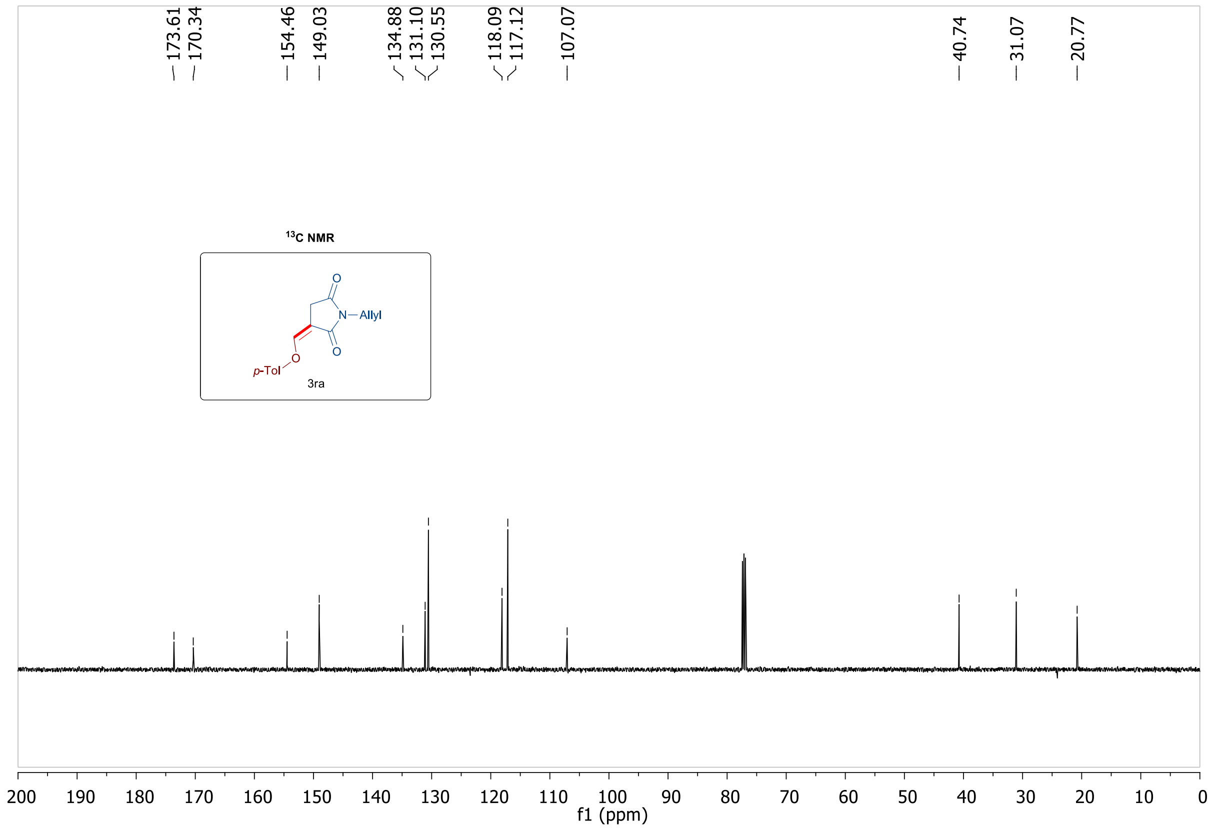
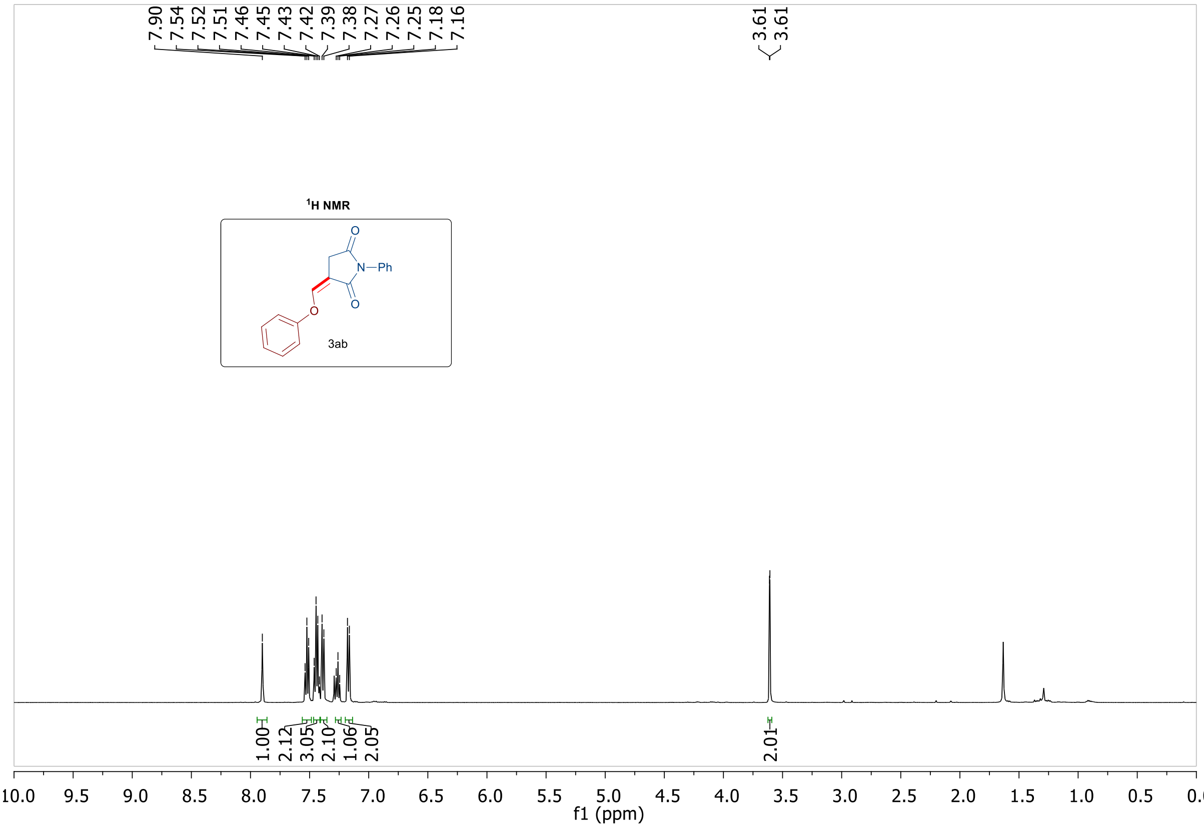
10
0
f1 (ppm)



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7.25
7.18
7.16
3.61
3.61
1H NMR
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N—Ph
O
O
3ab
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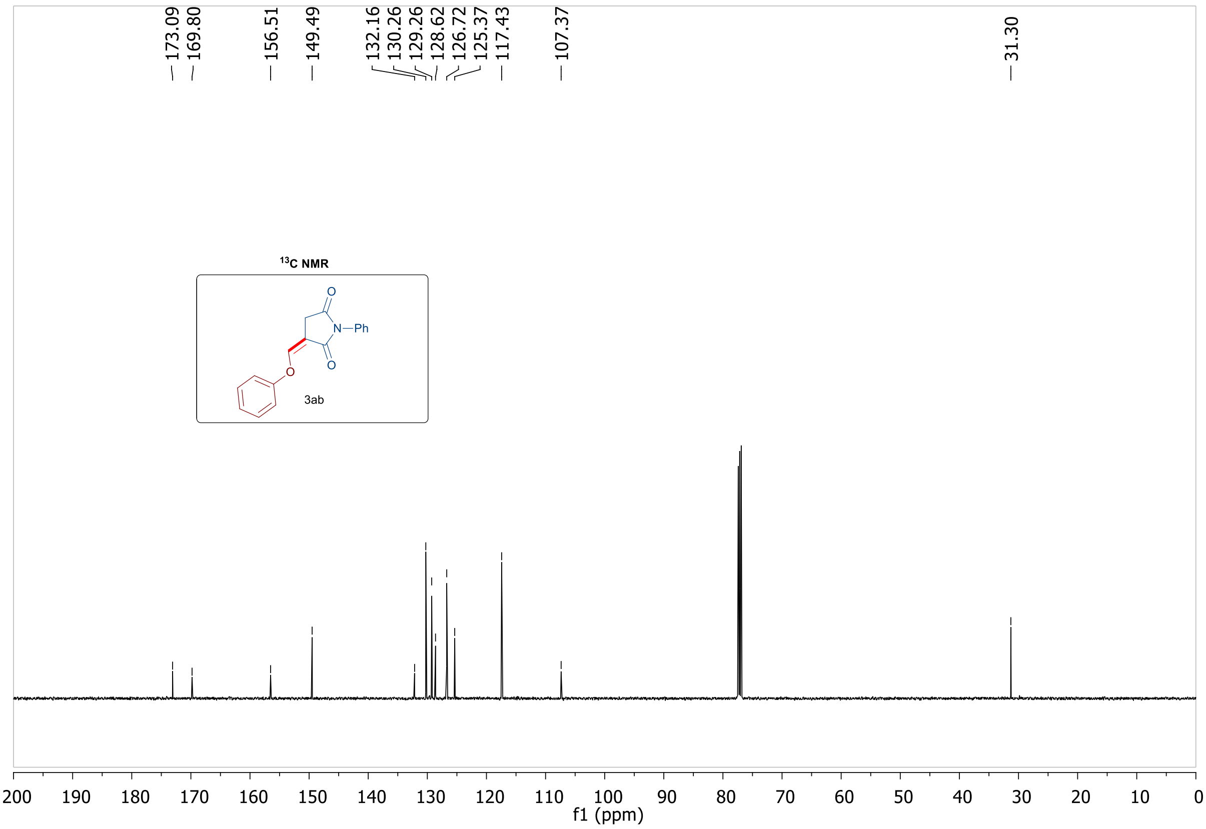
2.12
3.05
2.10
1.06
2.05
2.01
f1 (ppm)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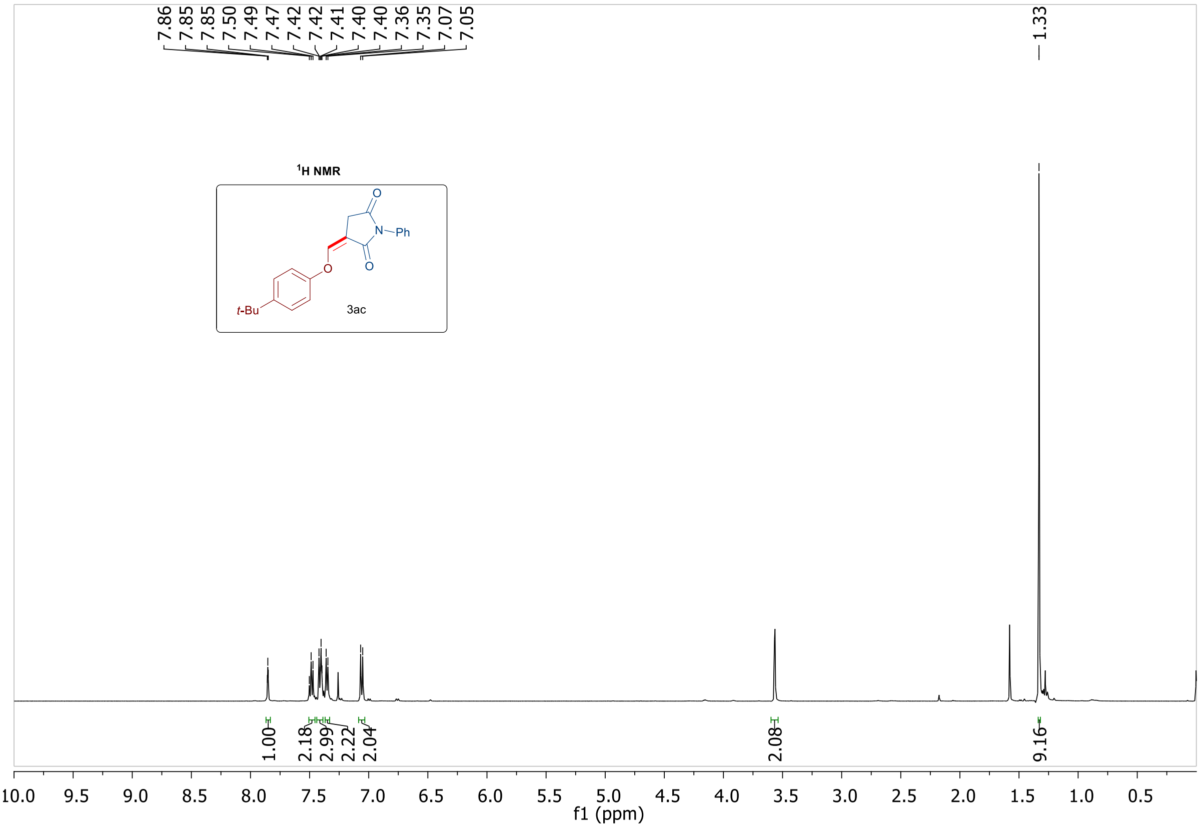
O
3ab
f1 (ppm)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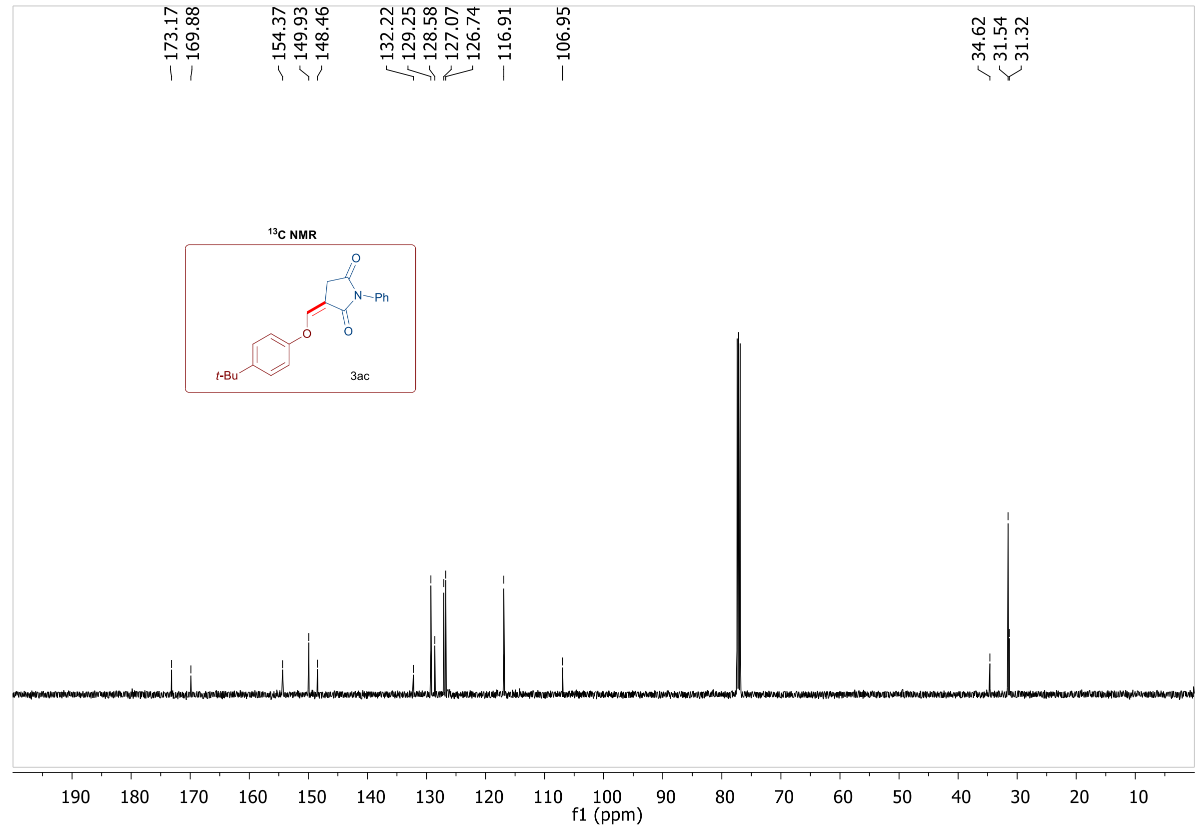
1H NMR
O
N
Ph
O
O
t-Bu
3ac
1.00
2.18
2.99
2.22
2.04
2.08
9.16
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
f1 (ppm)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106.95
34.62 31.54 31.32
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N
Ph
O
O
t-Bu
3ac
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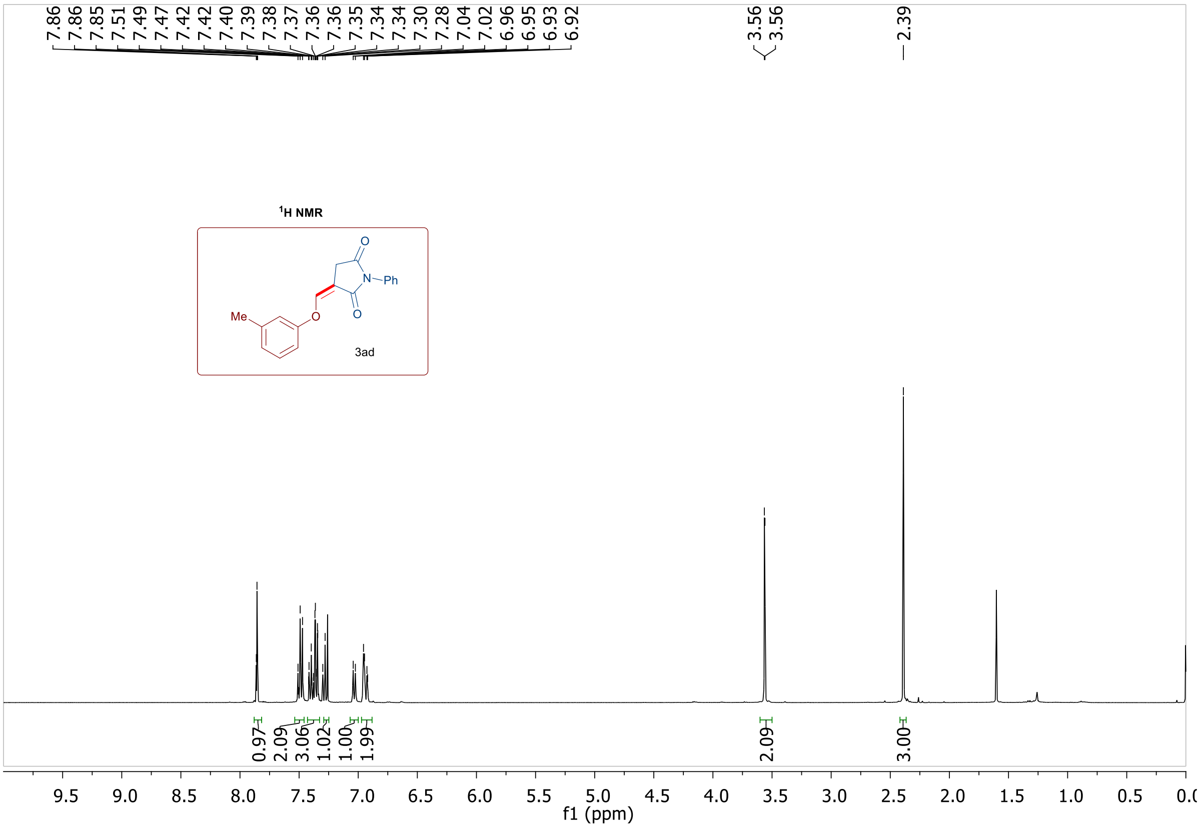
f1 (ppm)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7.34
7.34
7.30
7.28
7.04
7.02
6.96
6.95
6.93
6.92
3.56
3.56
2.39
1H NMR
Me
O
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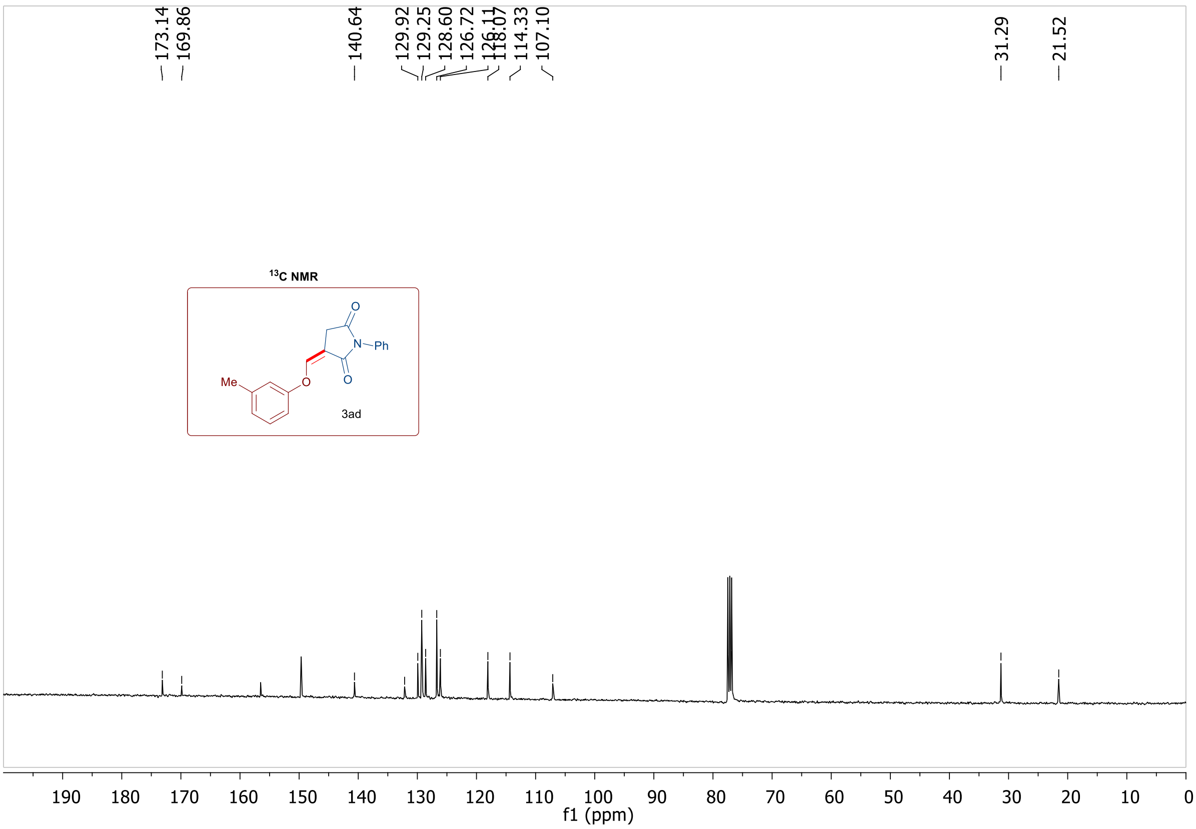
3.00
f1 (ppm)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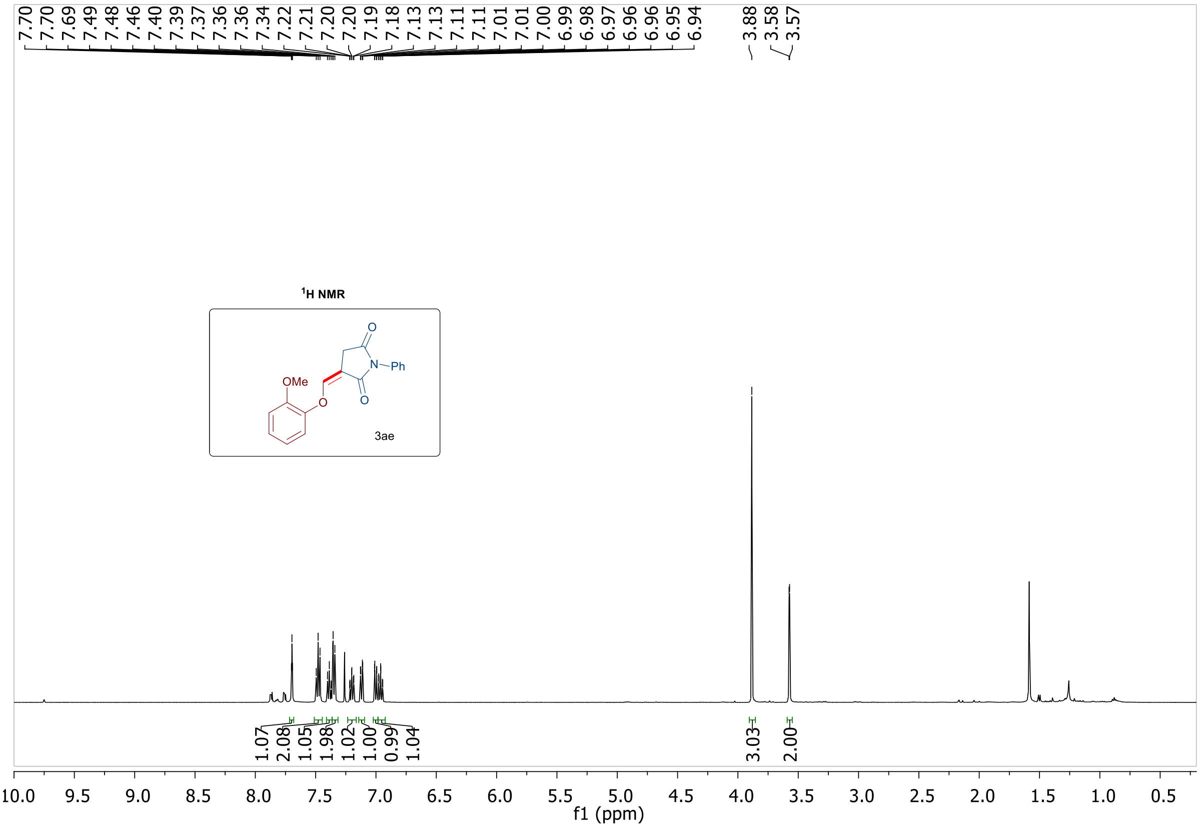
f1 (ppm)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7.19
7.18
7.13
7.13
7.11
7.11
7.01
7.01
7.00
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6.98
6.97
6.96
6.96
6.95
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3.58
3.57
¹H NMR
OMe
O
N
Ph
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1.00
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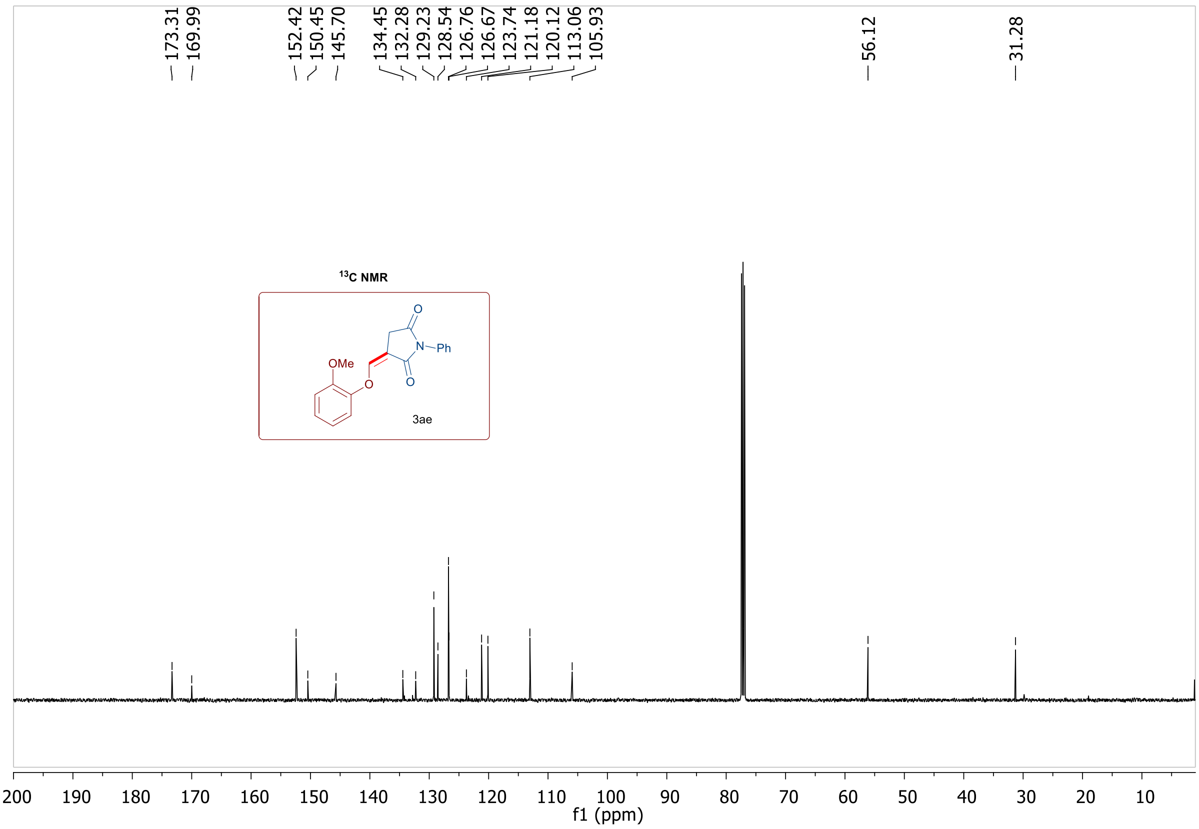
1.04
3.03
2.00
f1 (ppm)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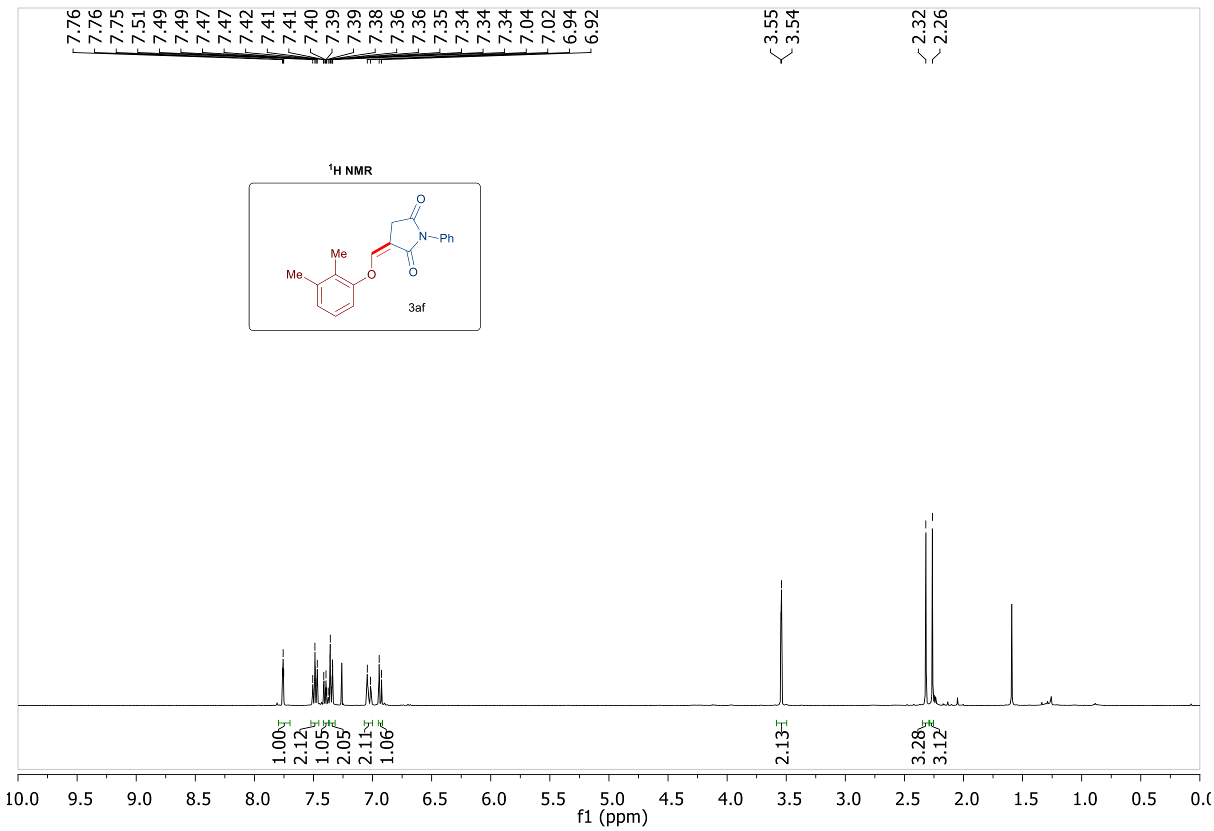
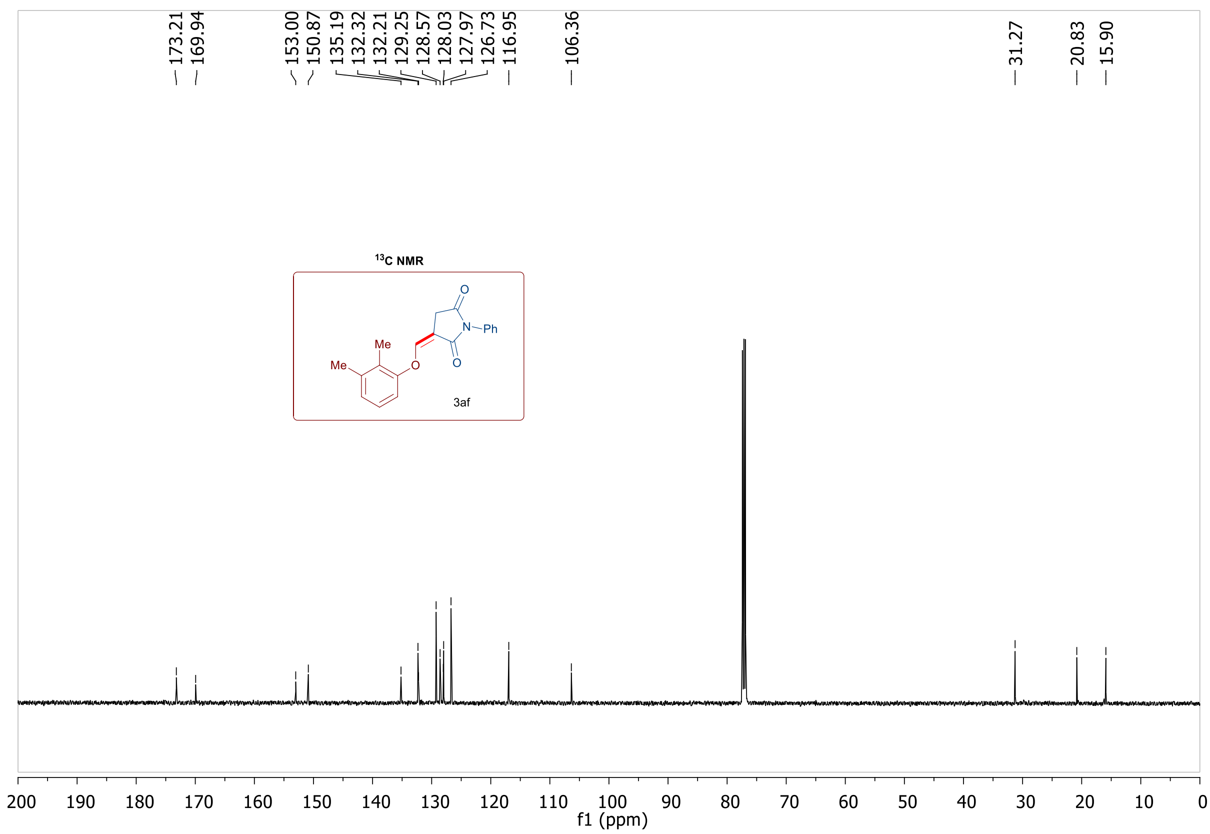
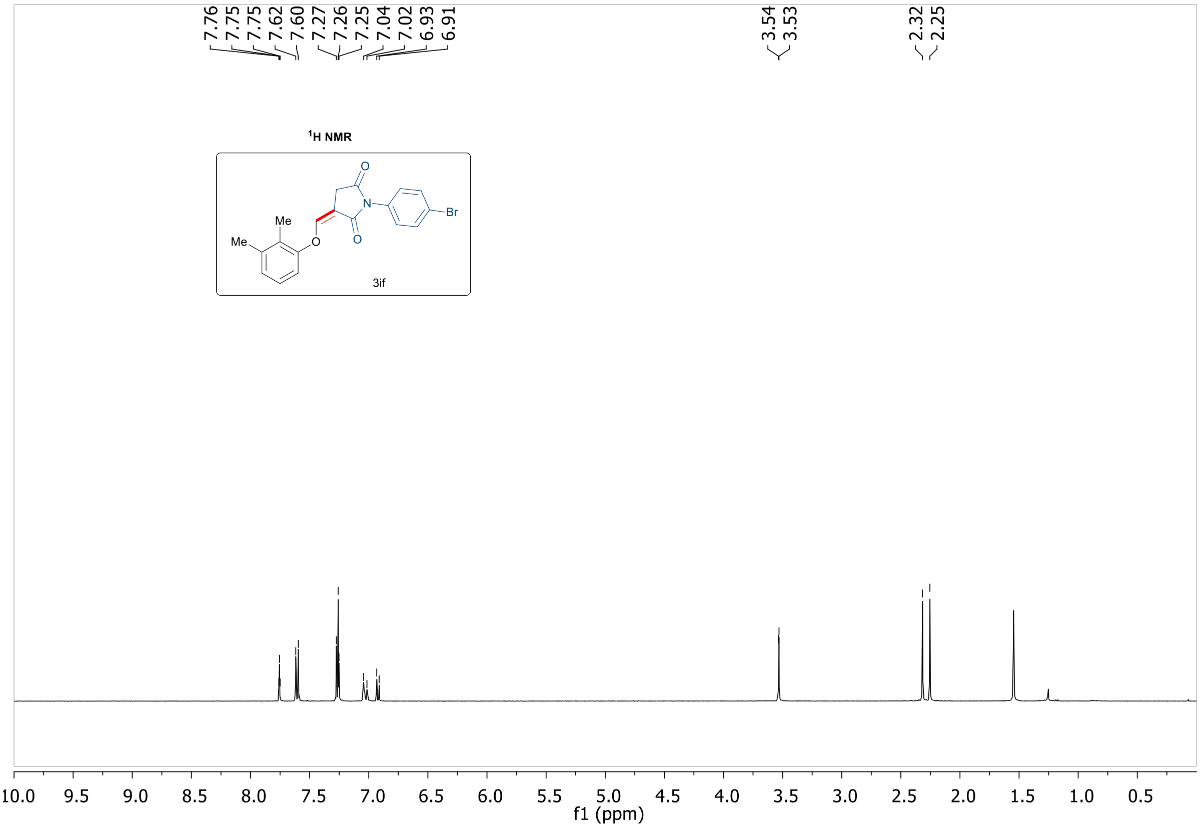
105.93
56.12
31.28
¹³C NMR
OMe
O
N
Ph
3ae
f1 (ppm)



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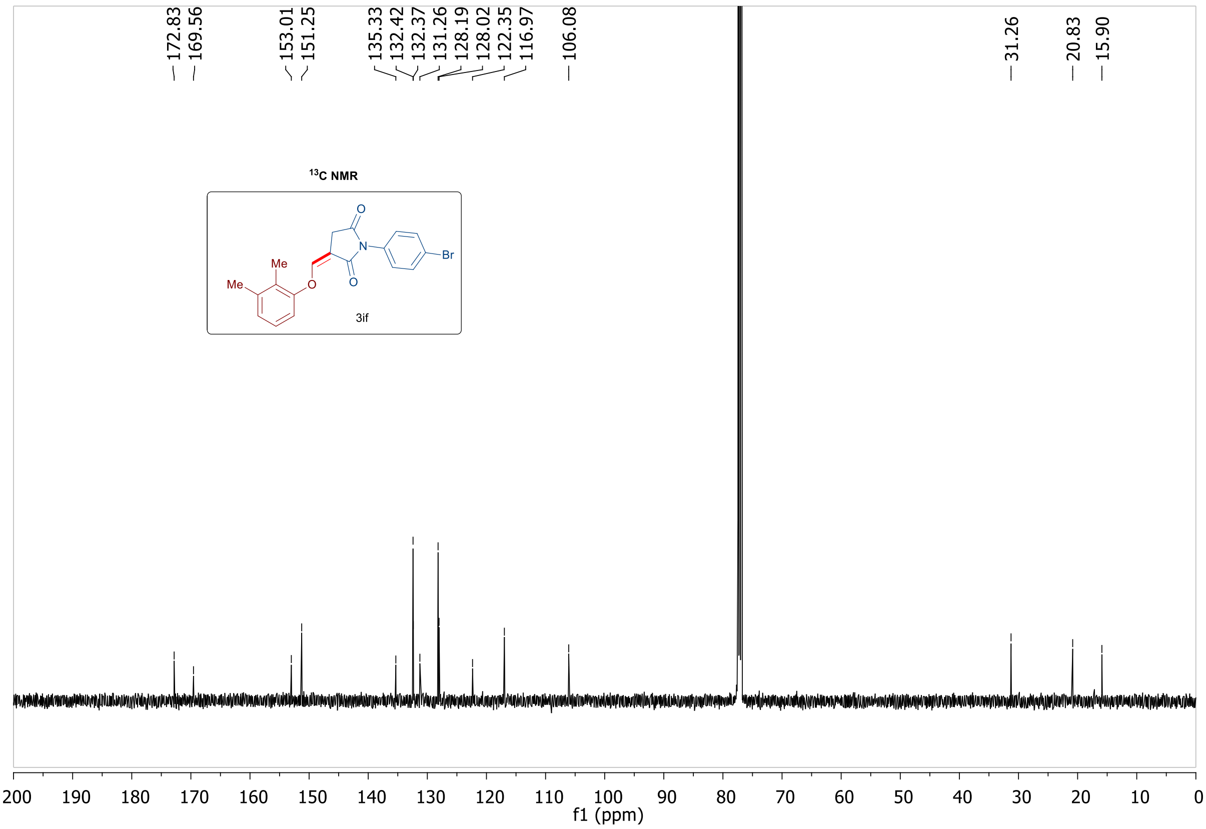
7.02
6.93
6.91
3.54
3.53
2.32
2.25
1H NMR
Me
Me
O
O
N
O
Br
3if
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
f1 (ppm)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106.08
31.26
20.83
15.90
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Me
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N
O
Br
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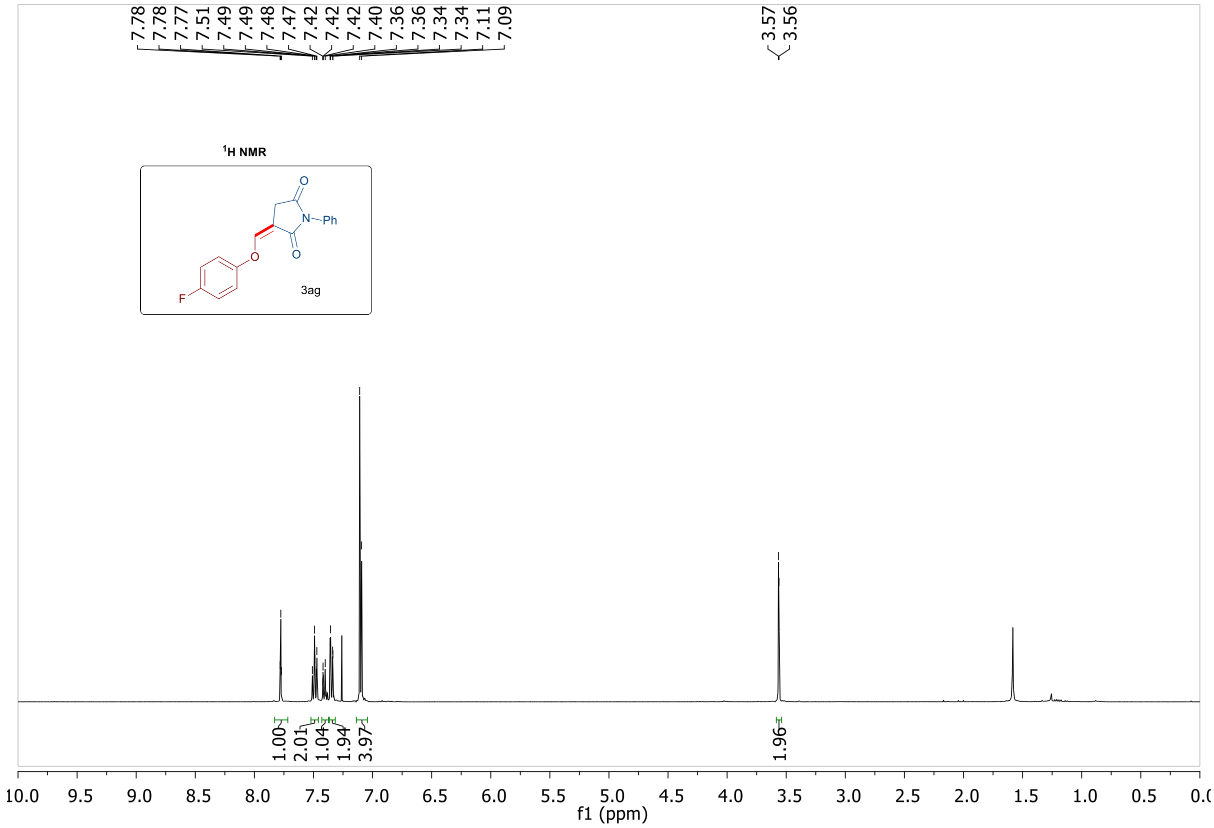
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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7.34
7.11
7.09
3.57
3.56
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Ph
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O
F
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2.01
1.04
1.94
3.97
1.96
10.0
9.5
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8.0
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6.0
5.5
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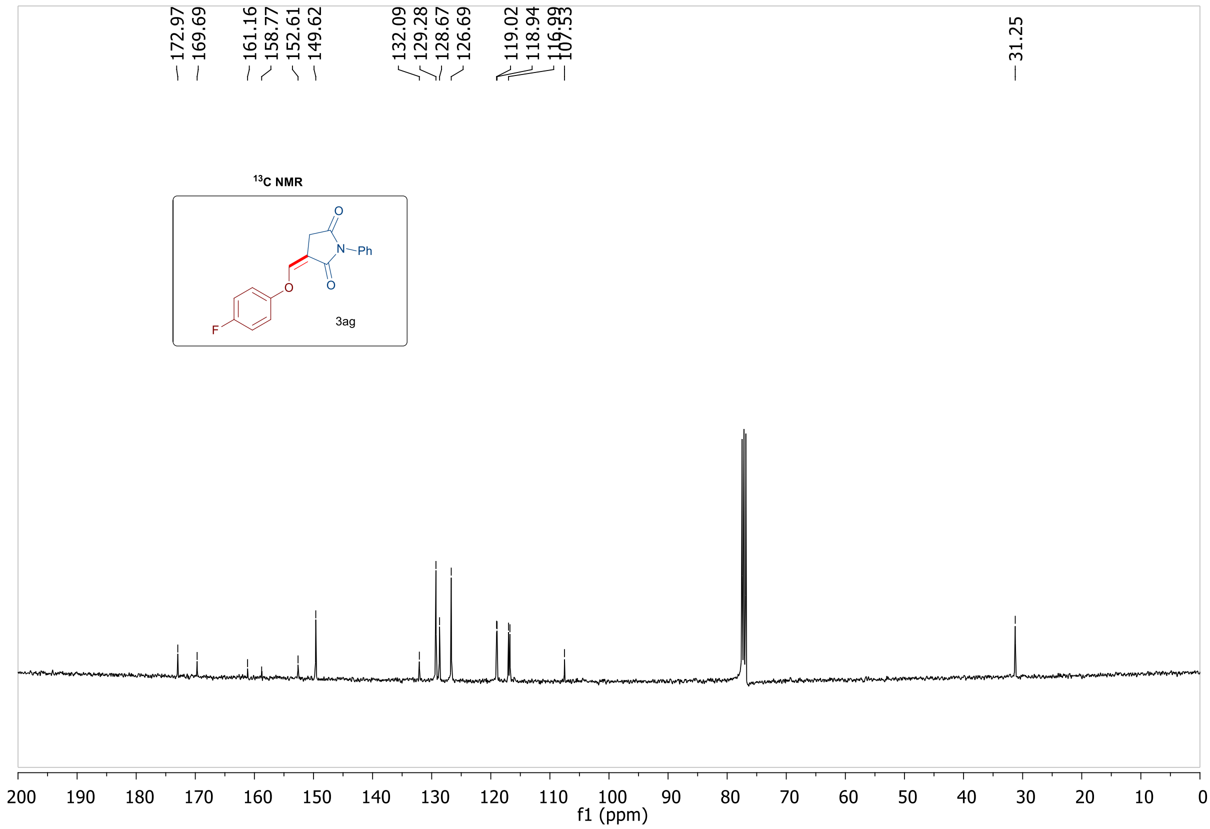
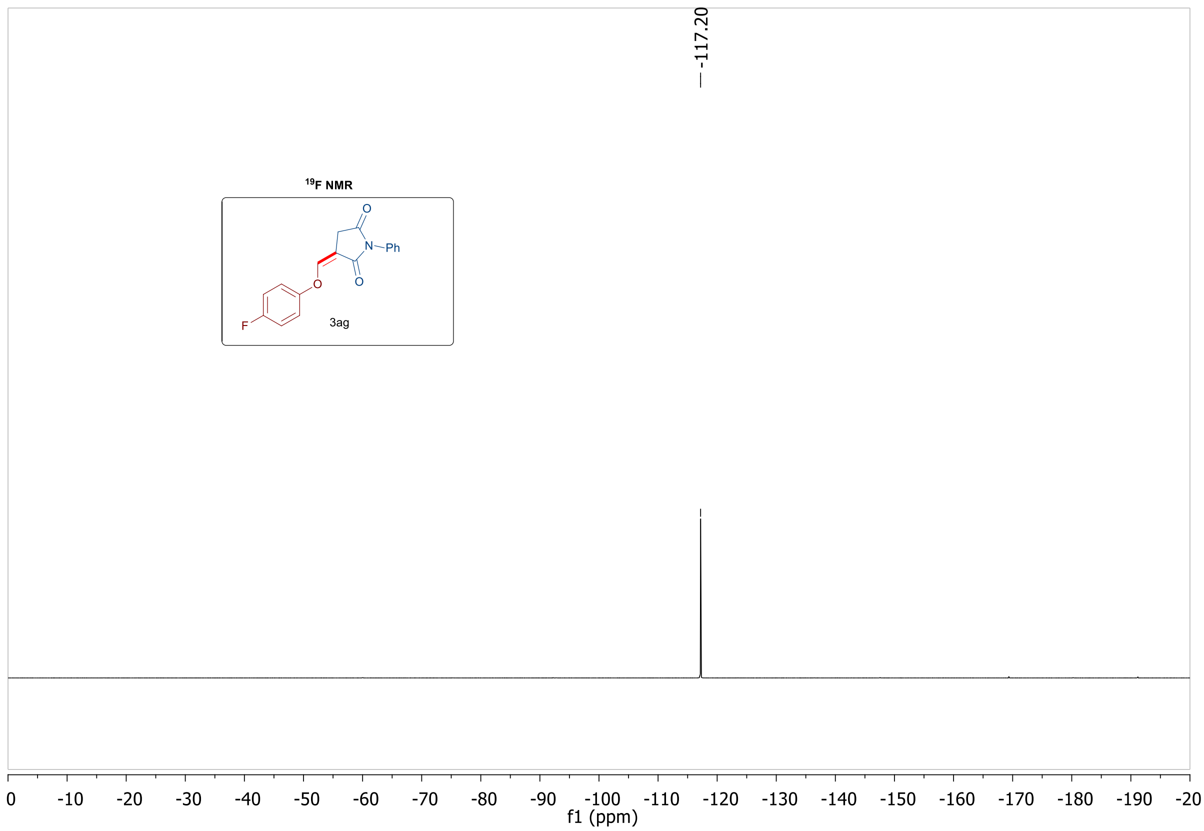
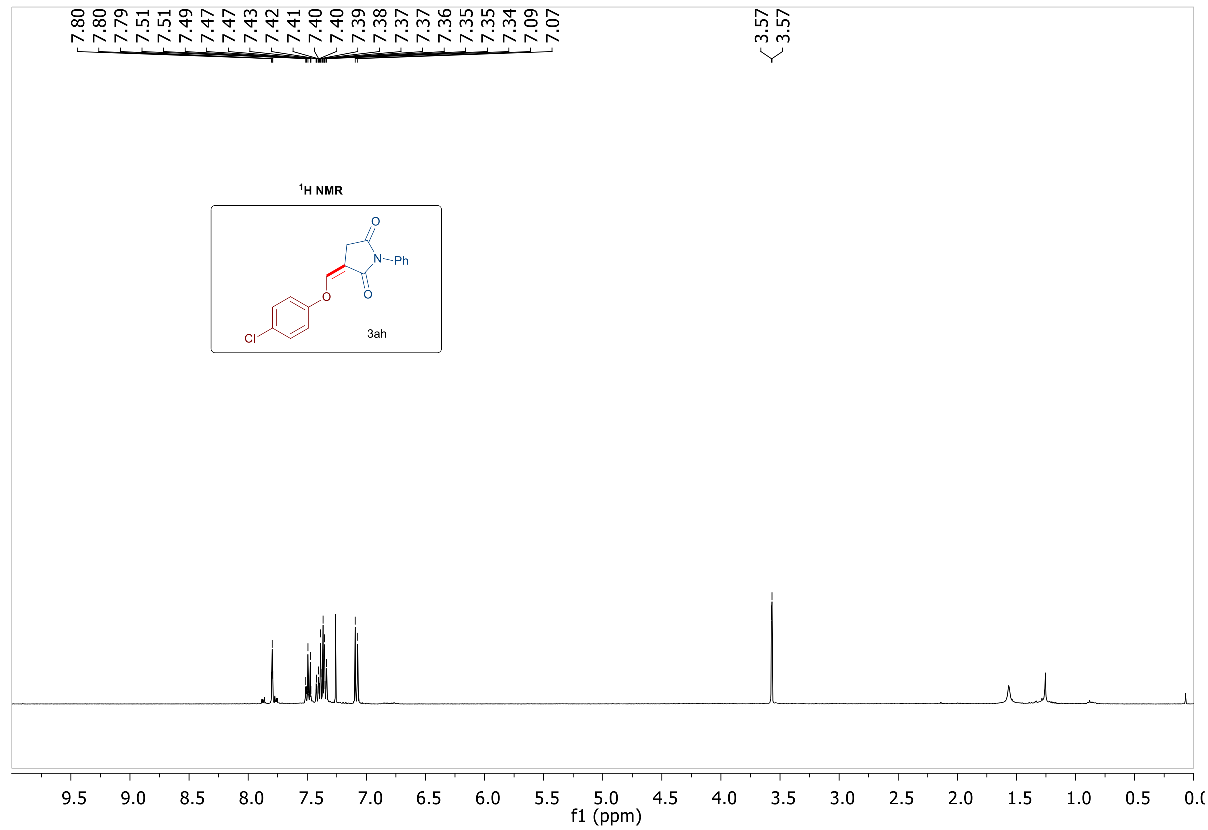
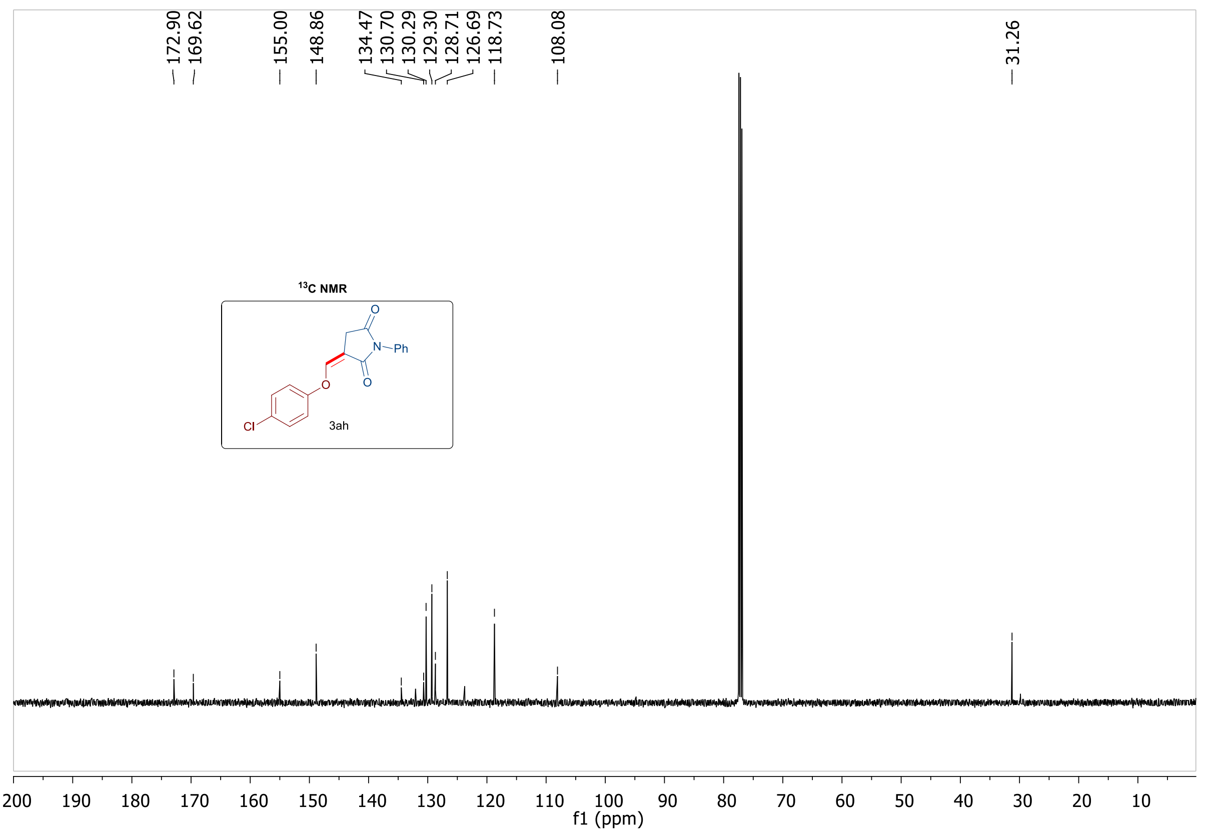
0.0
f1 (ppm)


172.97
169.69
161.16
158.77
152.61
149.62
132.09
129.28
128.67
126.69
119.02
118.94
116.99
107.53
31.25
13C NMR
O
N
Ph
O
O
F
3ag
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

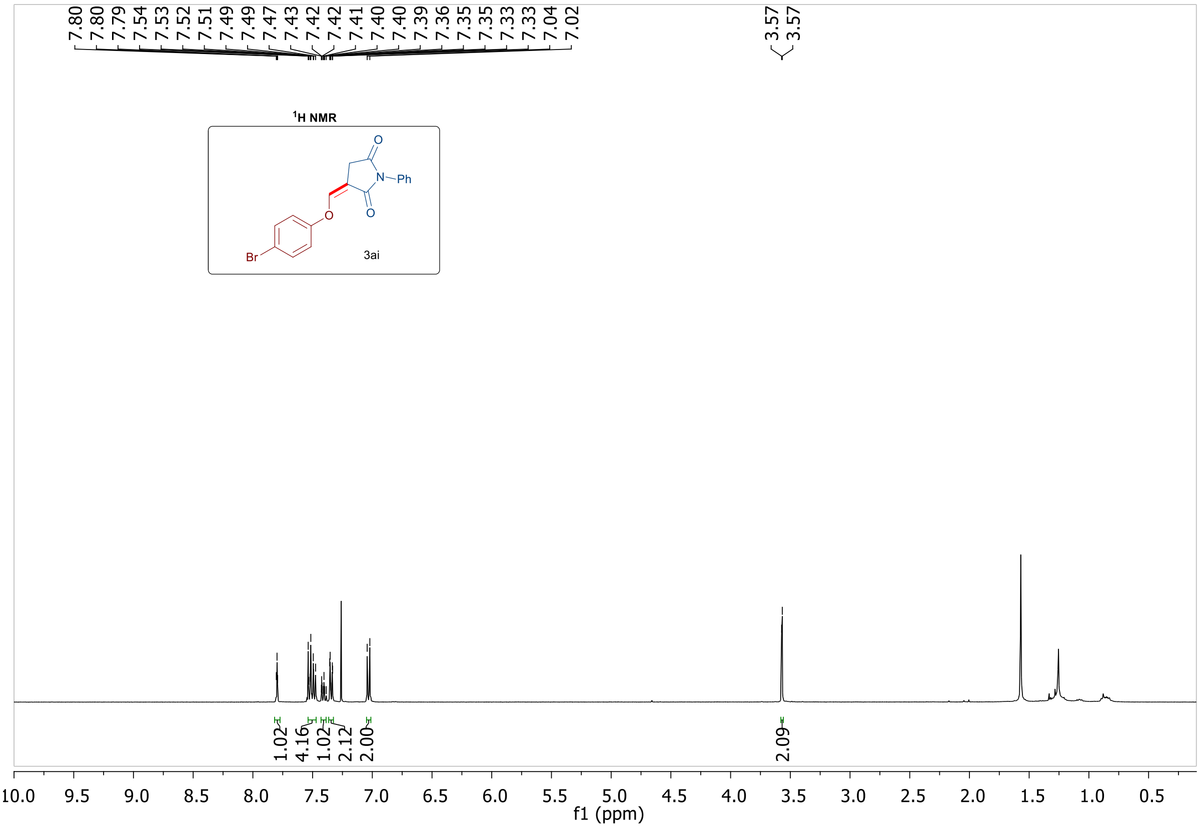

-117.20
19F NMR
O
N
Ph
O
O
F
3ag
0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -20
f1 (ppm)

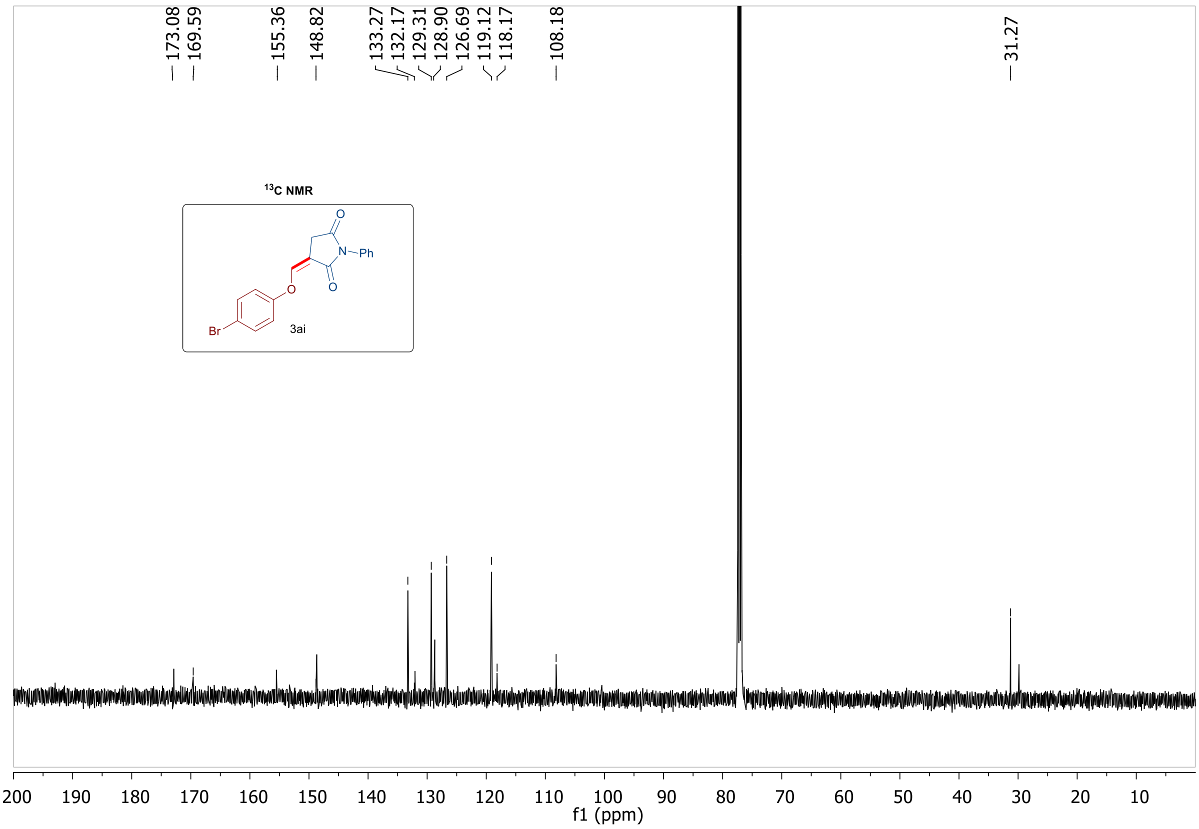


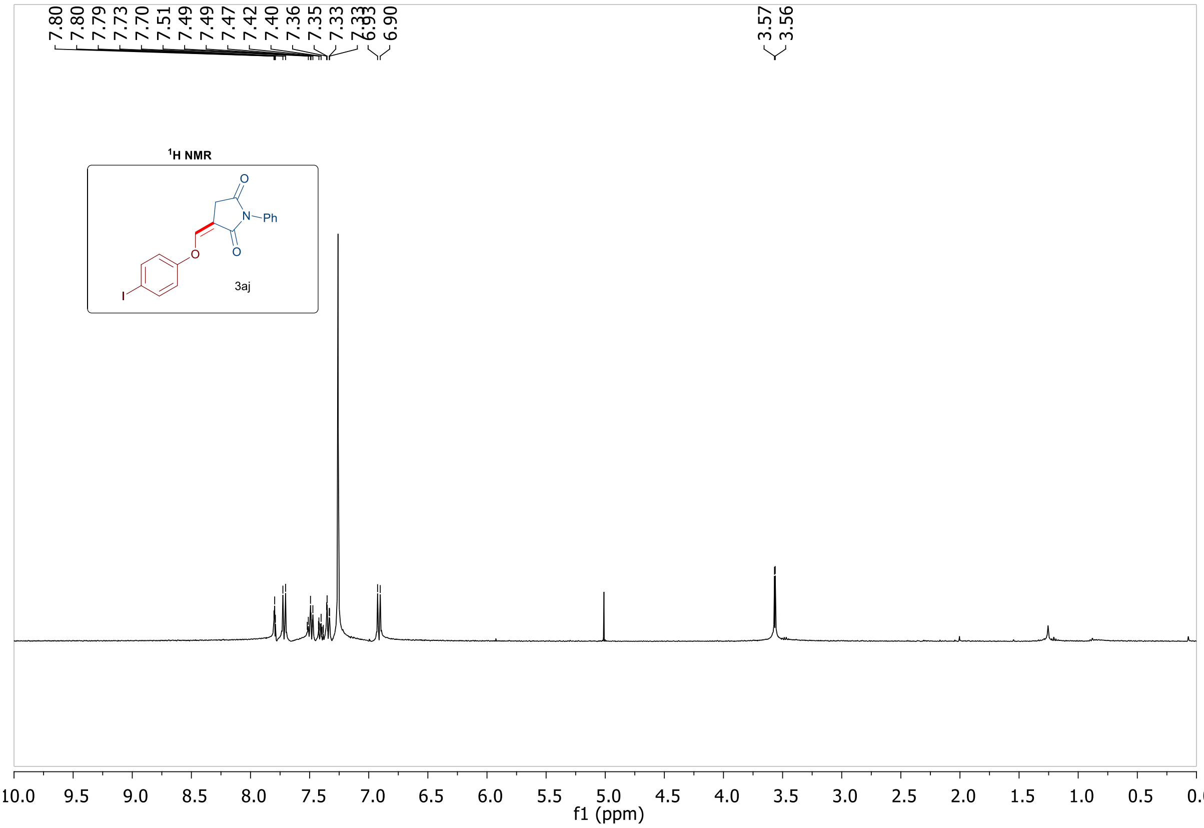
7.80
7.80
7.79
7.51
7.51
7.49
7.47
7.47
7.43
7.42
7.41
7.40
7.40
7.39
7.38
7.37
7.37
7.36
7.35
7.35
7.34
7.09
7.07
3.57
3.57
¹H NMR
O
N
Ph
O
O
Cl
3ah
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)

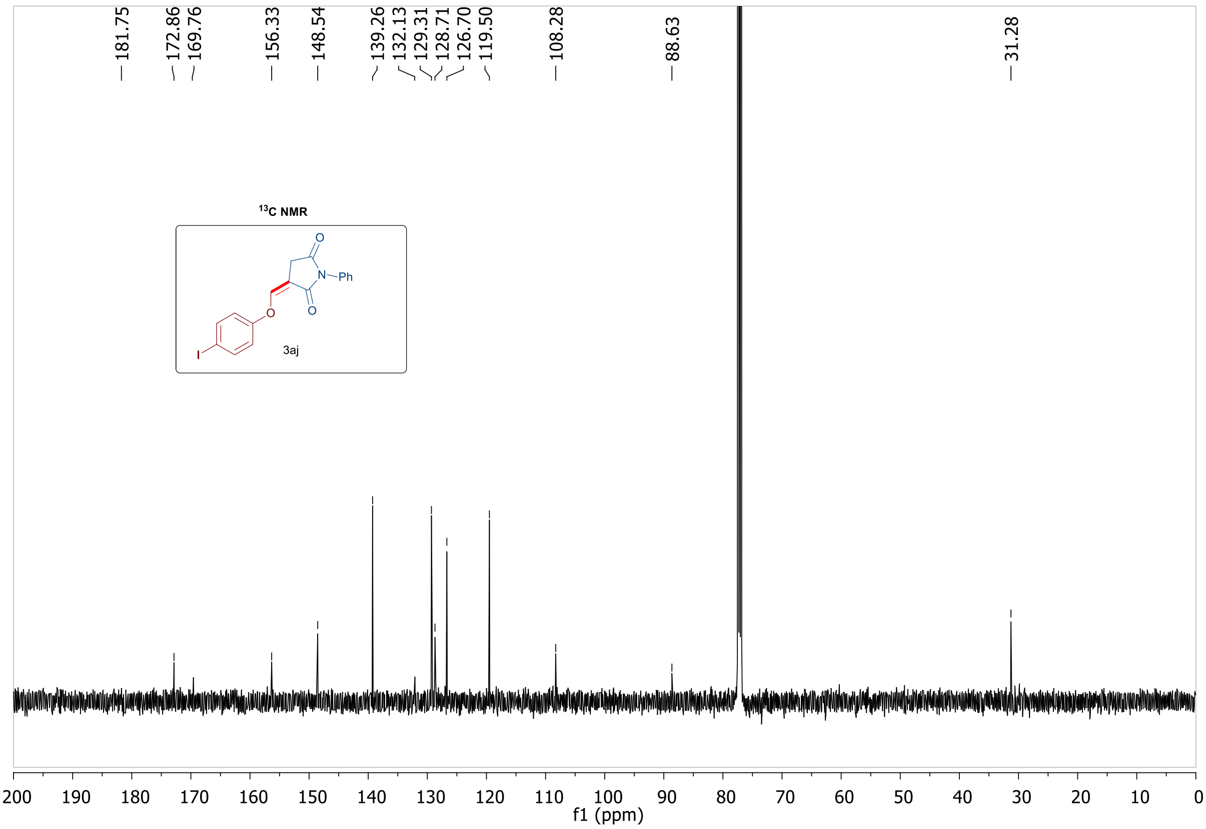


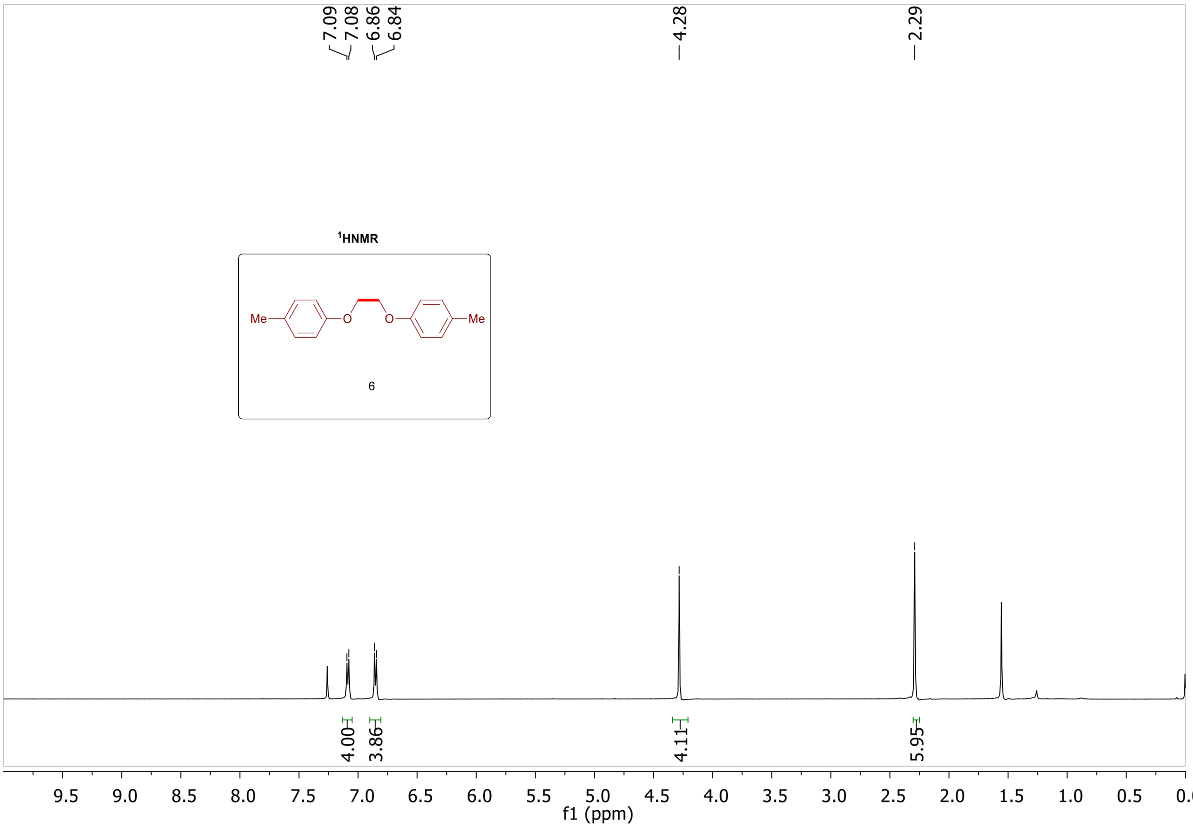
172.90
169.62
155.00
148.86
134.47
130.70
130.29
129.30
128.71
126.69
118.73
108.08
31.26
¹³C NMR
O
N
Ph
O
O
Cl
3ah
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

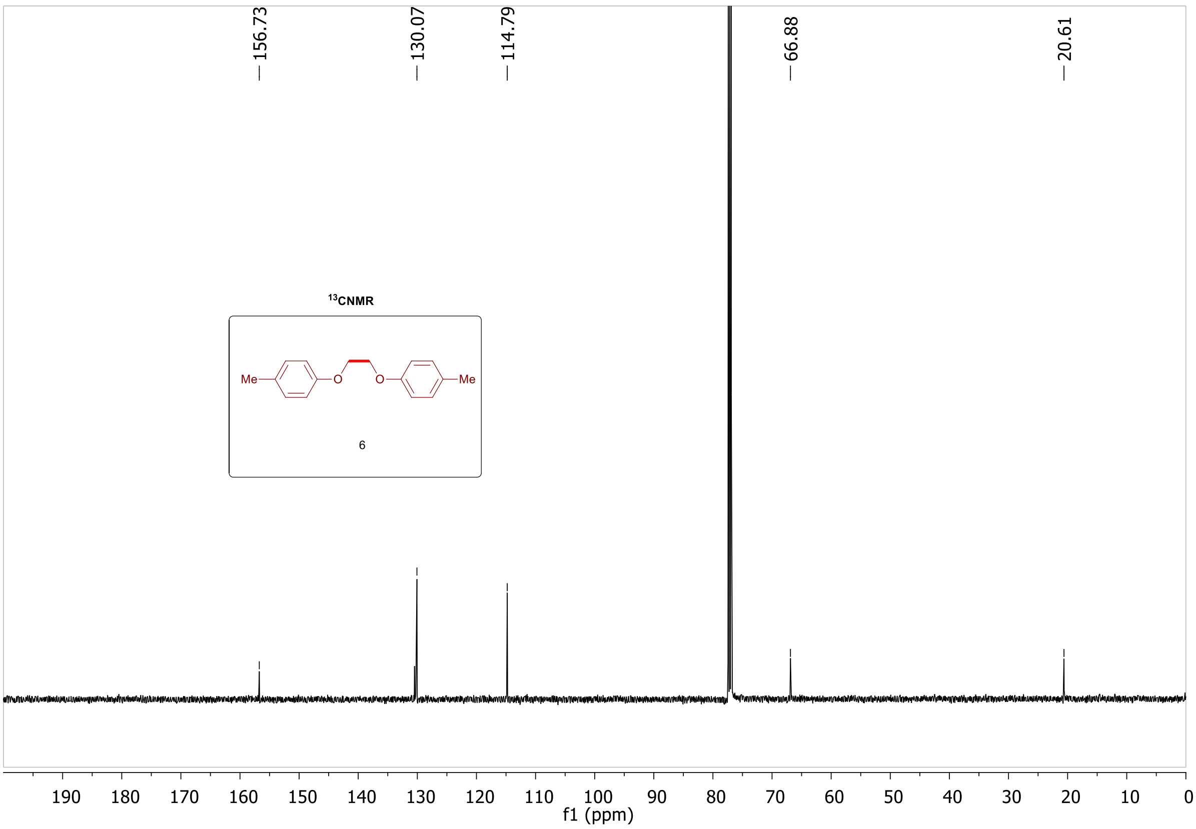

7.80
7.80
7.79
7.54
7.53
7.52
7.51
7.49
7.49
7.47
7.43
7.42
7.42
7.41
7.40
7.39
7.36
7.35
7.35
7.33
7.33
7.04
7.02
3.57
3.57
^{1}H NMR
O
N
Ph
O
O
Br
3ai
1.02
4.16
1.02
2.12
2.00
2.09
f1 (ppm)

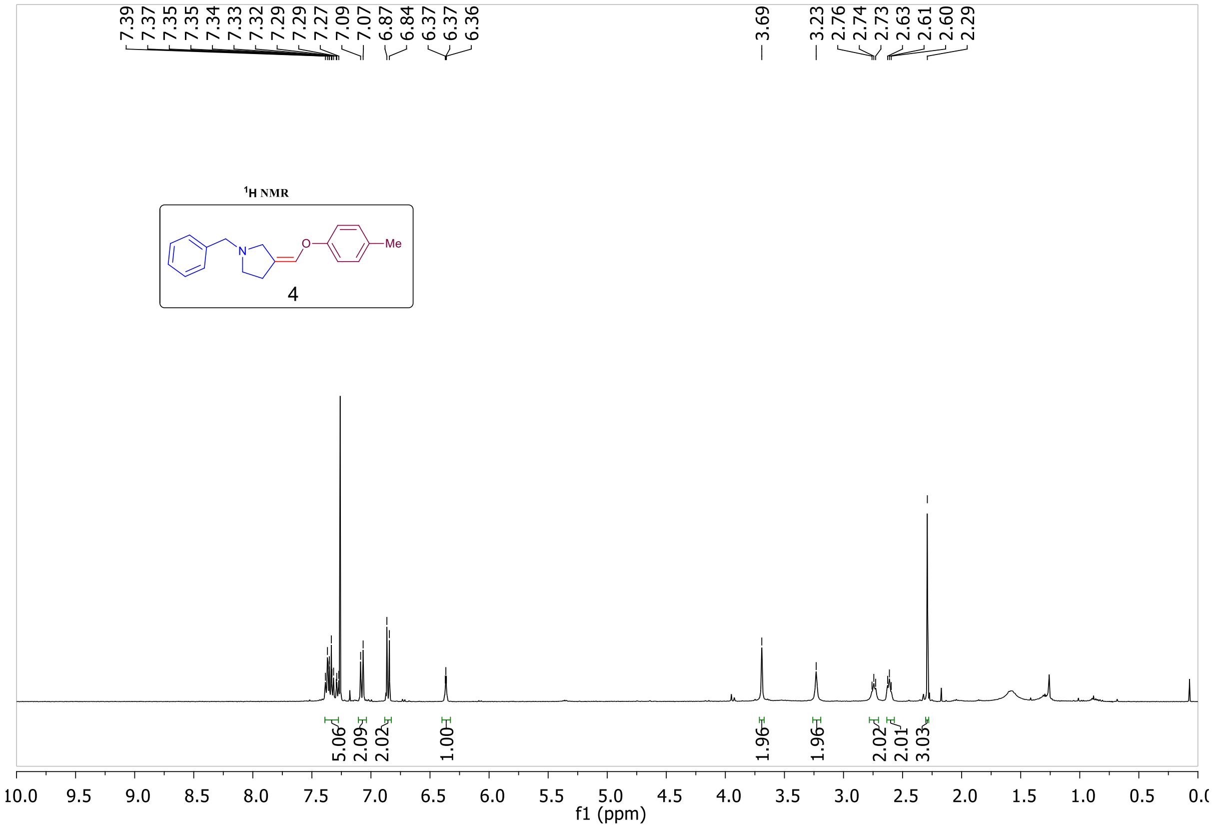

173.08
169.59
155.36
148.82
133.27
132.17
129.31
128.90
126.69
119.12
118.17
108.18
31.27
^{13}C NMR
O
N
Ph
O
O
Br
3ai
f1 (ppm)

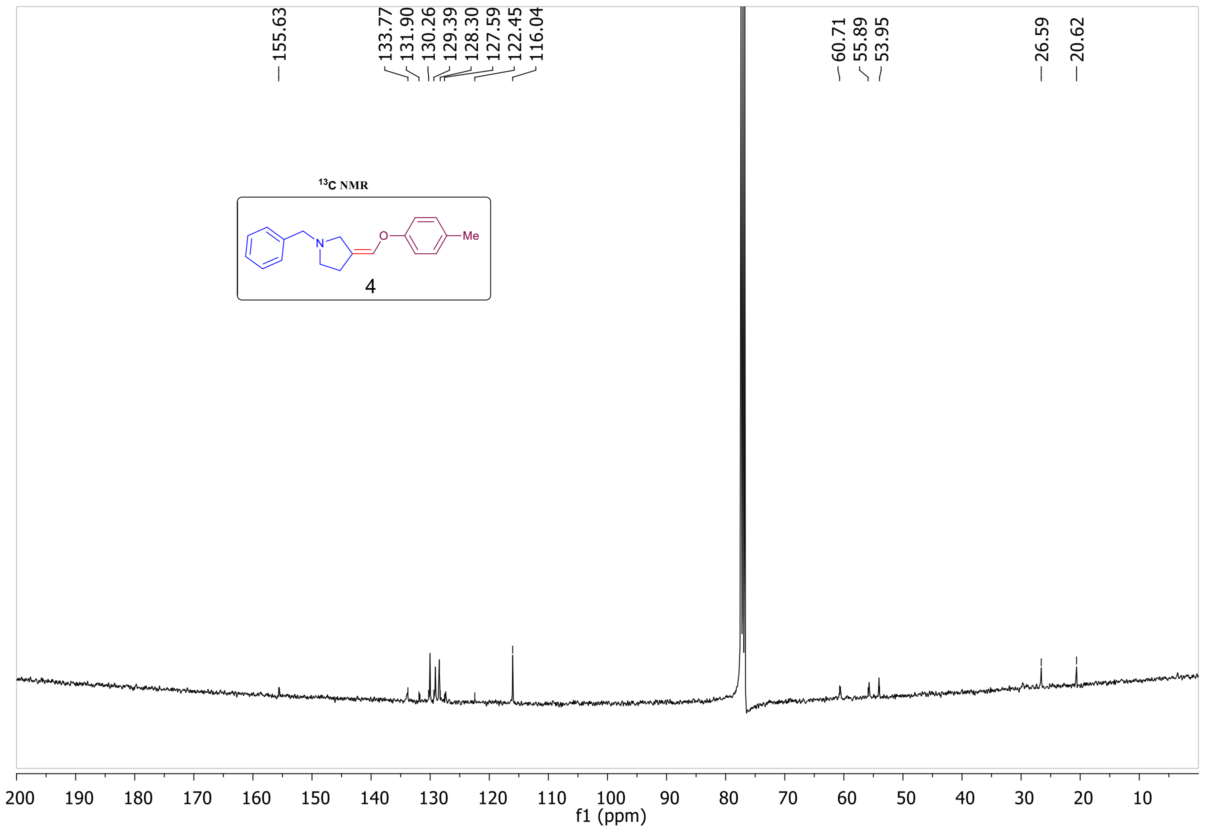

7.80
7.80
7.79
7.73
7.70
7.51
7.49
7.49
7.47
7.42
7.40
7.36
7.35
7.33
7.33
6.93
6.90
3.57
3.56
1H NMR
O
N
Ph
O
O
I
3aj
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)


181.75
172.86
169.76
156.33
148.54
139.26
132.13
129.31
128.71
126.70
119.50
108.28
88.63
31.28
13C NMR
O
N
Ph
O
O
I
3aj
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

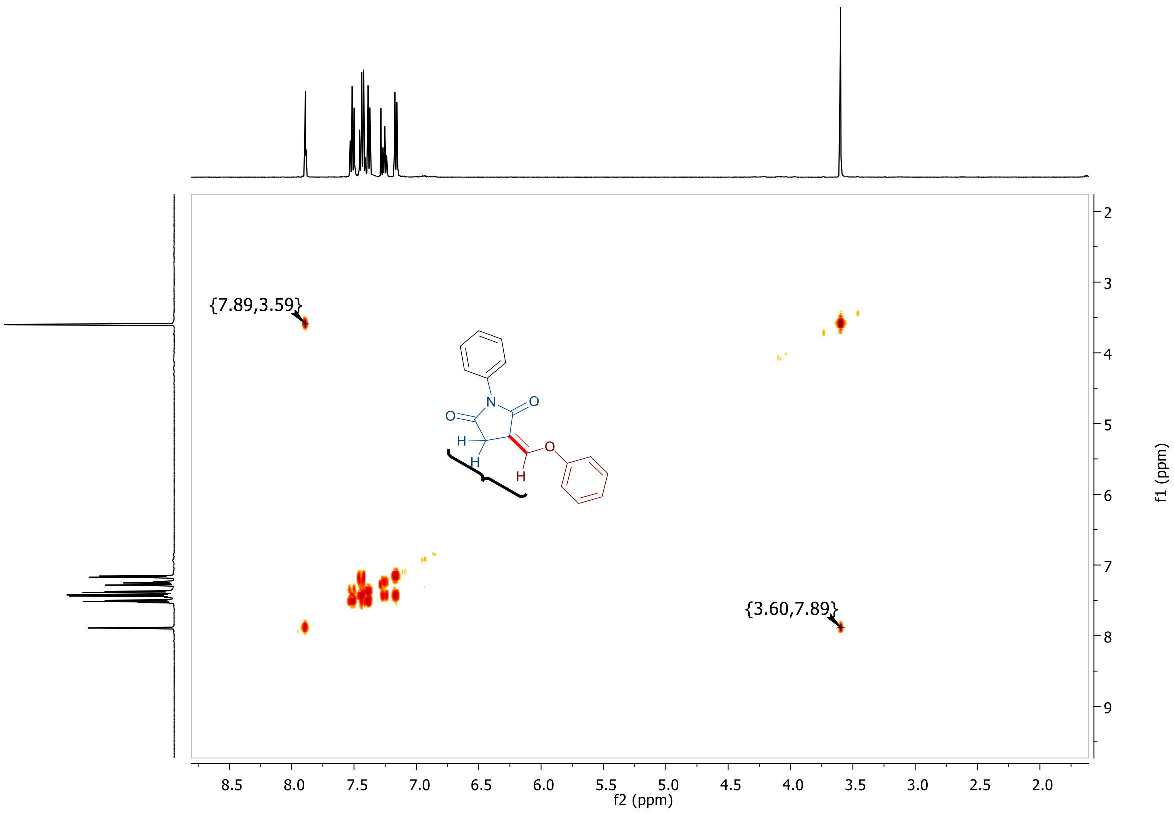

7.09
7.08
6.86
6.84
4.28
2.29
¹HNMR
Me
O
O
Me
6
4.00
3.86
4.11
5.95
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)


156.73
130.07
114.79
66.88
20.61
¹³CNMR
Me
O
O
Me
6
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

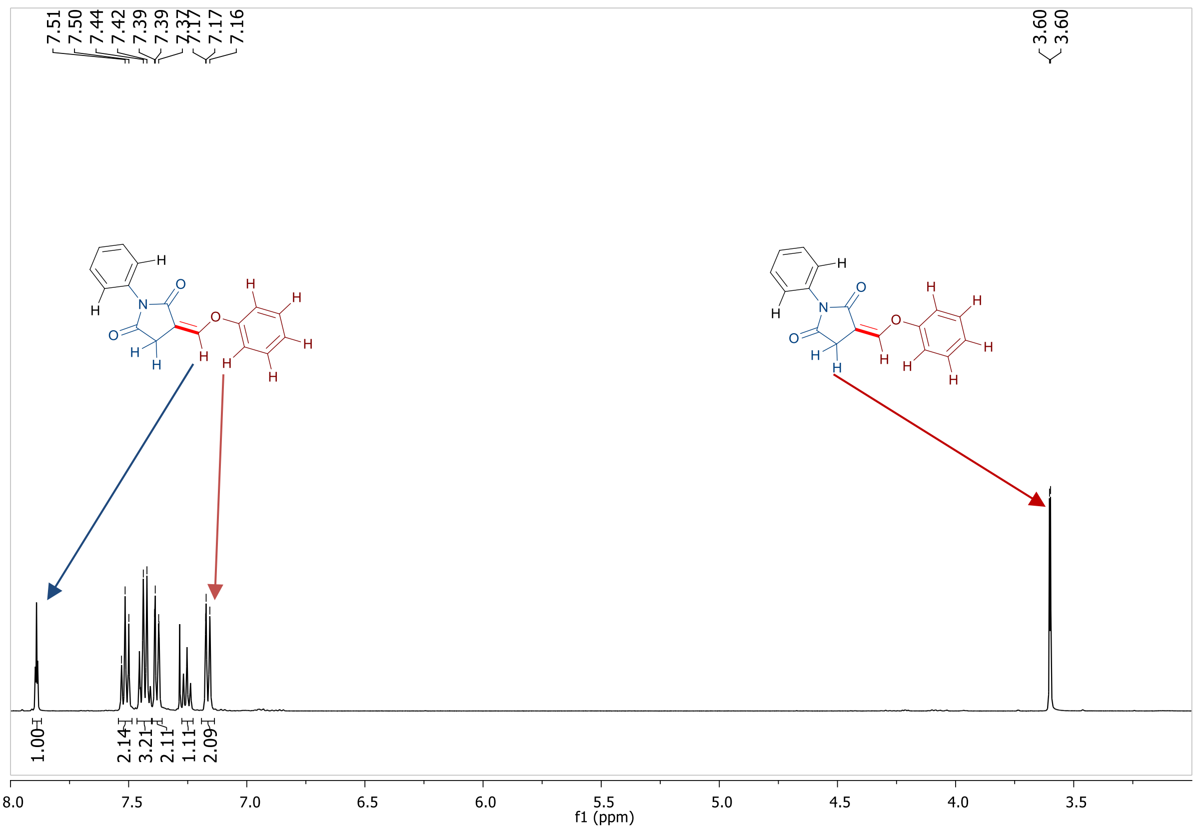

7.39
7.37
7.35
7.35
7.34
7.33
7.32
7.29
7.29
7.27
7.09
7.07
6.87
6.84
6.37
6.37
6.36
3.69
3.23
2.76
2.74
2.73
2.63
2.61
2.60
2.29
1H NMR
N
O
Me
4
5.06
2.09
2.02
1.00
1.96
1.96
2.02
2.01
3.03
f1 (ppm)

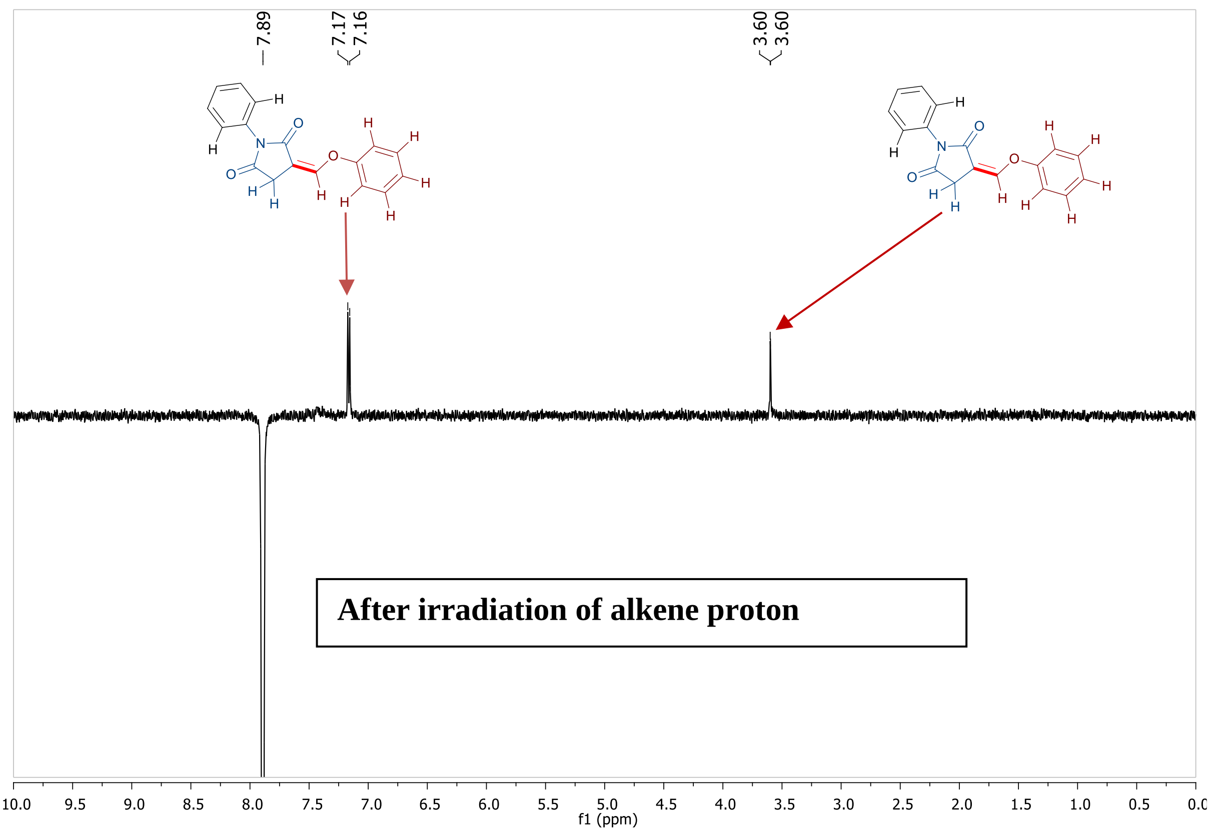

155.63
133.77
131.90
130.26
129.39
128.30
127.59
122.45
116.04
60.71
55.89
53.95
26.59
20.62
13C NMR
N
O
Me
4
f1 (ppm)

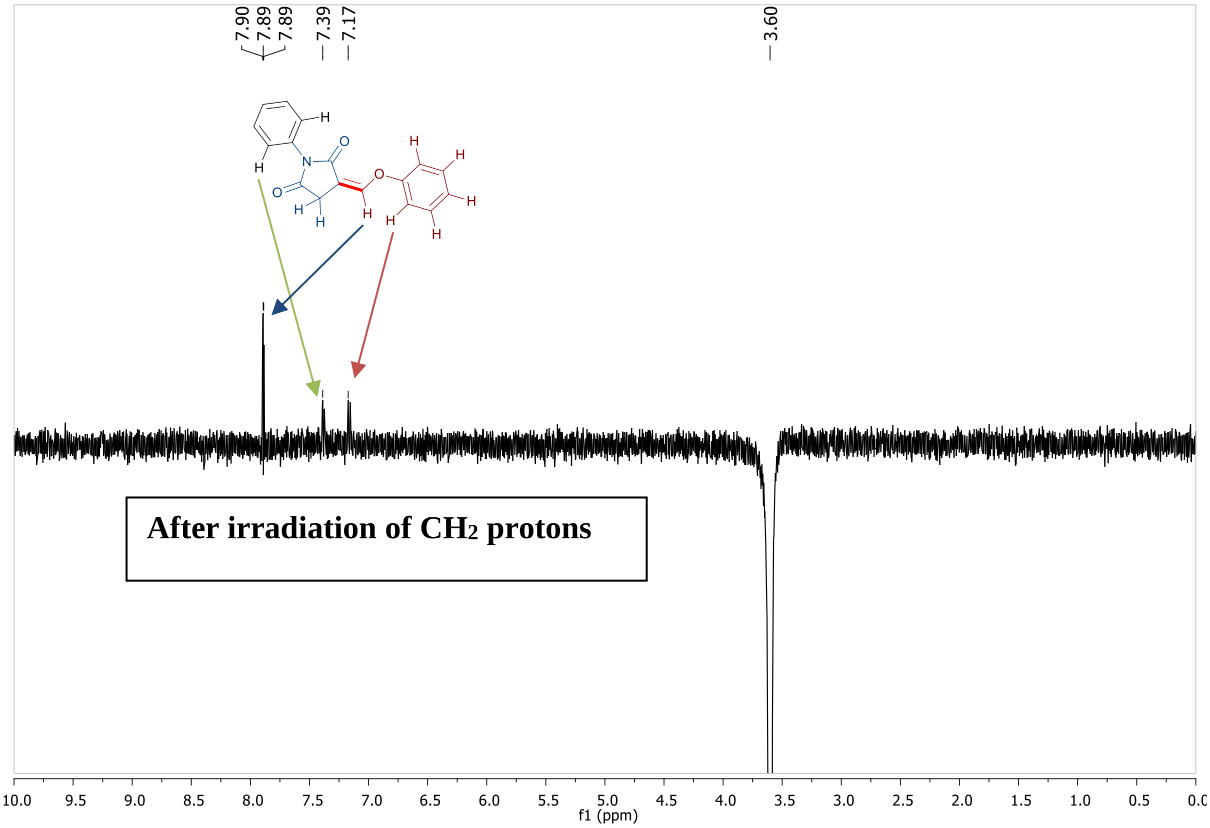
COSY Experiment of 3ab.



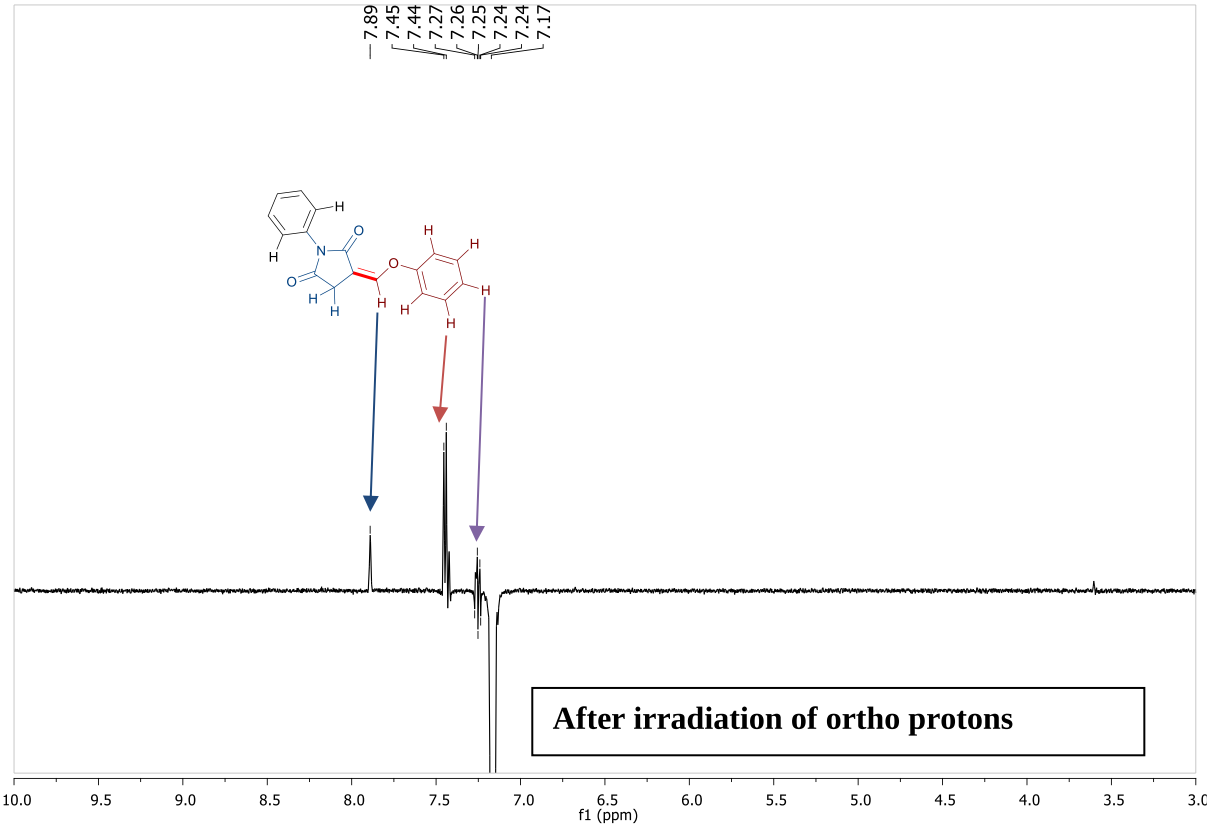
NOE Experiment of 3ab.


7.51
7.50
7.44
7.42
7.39
7.39
7.37
7.17
7.17
7.16
3.60
3.60
1.00
2.14
3.21
2.11
1.11
2.09
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
f1 (ppm)


7.89
7.17
7.16
3.60
3.60
After irradiation of alkene proton
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)



7.90
7.89
7.89
7.39
7.17
3.60
After irradiation of CH2 protons
f1 (ppm)



7.89
7.45
7.44
7.27
7.26
7.25
7.24
7.24
7.17
After irradiation of ortho protons
f1 (ppm)

Computational details

(a) Method: All calculations were carried out using the Gaussian09 program package.[5] Geometries of all the intermediates and transition states were optimized in vacuum without any constraints with Truhlar's meta-GGA M06-2X[6] functional in conjunction with Pople's 6-31G(d,p)[7] double-ζ split valence basis set for all the atoms. The M06-2X functional was chosen as it reliably accounts for the various non-covalent interactions like C•----HC, O---H and N---H hydrogen bonds, in addition to properly describing the kinetics and thermochemistry.[6, 8] Harmonic vibrational frequencies were computed considering the ideal-gas rigid rotor simple harmonic approximations, at the same level of theory, to distinguish transition states (with one imaginary mode) from minima (with all real modes). Furthermore, the electronic energies were refined by single point calculations at M06-2X employing a higher quality double-ζ split valence basis set, 6-31++G(d,p), consisting of diffuse functions and polarization functions on all atoms. Solvent effects for acetonitrile (ε = 35.688) were introduced with Truhlar's Solvation Model Density (SMD) approach to the single-point energies at M06-2X/6-31++G(d,p). Relative Gibbs free energies reported in the main text are evaluated by adding thermal corrections obtained from vibrational analyses to the solvent-phase electronic energies. In order to predict the kinetically controlled diastereo-selectivity within the framework of the transition state theory at a given temperature, the following principle was utilized:

$$\frac{[Z\text{−}alkene]}{[E\text{−}alkene]} = \frac{k_{Z-alkene}}{k_{E-alkene}} = e^{-\Delta\Delta G^{\ddagger}/RT} \quad (1)$$

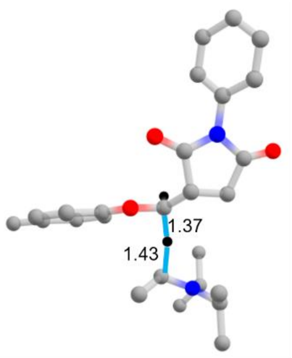
where, $\Delta\Delta G^{\ddagger} = \Delta G_{Z-alkene}{}^{\ddagger} - \Delta G_{E-alkene}{}^{\ddagger}$ (2)

Here, RT was taken as 0.593 kcal/mol, considering the experimental temperature is 298 K.

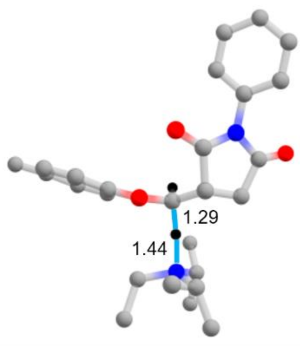
$\Delta\Delta G^{\ddagger}$ was evaluated to be -1.6 kcal/mol from the free energy barriers of **TS-*Z*** (19.5 kcal/mol) and **TS-*E*** (21.1 kcal/mol). Hence the selectivity for Z-alkene product (**3aa**) was calculated to be 14.85 as compared to E-alkene (**3aa'**).

(b) Optimized geometries of transition states.[a]

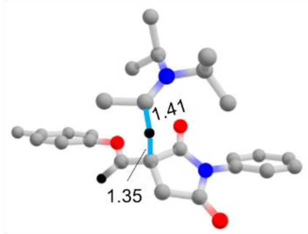
[a]Colour Code: carbon(grey), oxygen (red), nitrogen (blue), hydrogen (black). Unimportant hydrogen atoms are not shown for clarity. Bond distances shown are in units of Å.



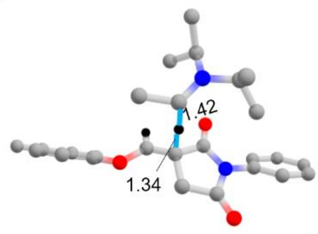
TS-*H abstraction*



TS-*deprotonation*



TS-*Z*



TS-*E*

(c) Absolute free energies of all species in a.u. evaluated at M06-2X/6-31++G(d,p).[a]

Species	E_{sol} (a.u.)	G_{corr} (a.u.)	G (a.u.)
F	-976.055059	0.268681	-975.786378
***i*-Pr$_2$EtN**	-370.871525	0.229509	-370.642016
TS-*deprotonation*	-1346.93935	0.518004	-1346.42135
H	-975.611119	0.253371	-975.357748
***i*-Pr$_2$EtNH$^+$**	-371.343965	0.245873	-371.098092
***i*-Pr$_2$NCHCH$_3$• (G)**	-370.219605	0.212388	-370.007217
TS-*H abstraction*	-1346.26006	0.497439	-1345.76263
I	-975.451428	0.256075	-975.195353
RC-*Z*	-1345.74973	0.493518	-1345.25621
TS-*Z*	-1345.71192	0.486845	-1345.22508
J	-974.822433	0.243347	-974.579086
I'	-975.451673	0.255483	-975.19619
RC-*E*	-1345.75089	0.493014	-1345.25787
TS-*E*	-1345.71529	0.491011	-1345.22428
J'	-974.813219	0.242635	-974.570584

(d) XYZ coordinates of computed species.

F

Charge = 1, Multiplicity = 2

C	-4.499536000	1.375224000	-0.053592000
C	-4.627325000	0.469727000	1.037203000
C	-3.502352000	1.127495000	-1.041321000
H	-5.384978000	0.653739000	1.791765000
H	-3.402312000	1.826753000	-1.865134000
C	-3.812996000	-0.619369000	1.133787000
C	-2.669651000	0.047470000	-0.967752000
H	-3.887305000	-1.332536000	1.947121000
H	-1.899280000	-0.099462000	-1.711679000
C	-2.816521000	-0.859162000	0.130251000
C	-5.364008000	2.581949000	-0.145004000
H	-5.536106000	2.877143000	-1.182020000
H	-6.320111000	2.434379000	0.359770000
H	-4.855804000	3.420489000	0.351699000
O	-2.135314000	-1.953705000	0.316917000
C	-1.049313000	-2.421765000	-0.512188000
H	-1.238295000	-3.490946000	-0.623123000
C	0.264175000	-2.174756000	0.213905000
C	0.648739000	-0.698006000	0.187490000
N	2.011659000	-0.608690000	0.014401000
C	2.600969000	-1.865746000	-0.264973000
C	1.477679000	-2.887599000	-0.381775000
H	1.349765000	-3.112506000	-1.446960000
C	2.759722000	0.613167000	0.065838000
C	3.946109000	0.647522000	0.794327000
C	2.296171000	1.735853000	-0.614925000
H	4.294903000	-0.240134000	1.308329000
H	1.369951000	1.687318000	-1.174760000
C	4.678085000	1.829106000	0.835429000
C	3.034120000	2.913348000	-0.556554000
H	5.605781000	1.861923000	1.395941000
H	2.680894000	3.793111000	-1.083558000
C	4.224209000	2.961343000	0.164284000
H	4.799462000	3.880091000	0.200119000
O	3.772641000	-2.059297000	-0.409389000
O	-0.137001000	0.221187000	0.291412000
H	1.756715000	-3.811218000	0.125239000
H	0.129767000	-2.458790000	1.264117000
H	-1.076911000	-1.948818000	-1.495783000

***i*-Pr$_2$EtN**

Charge = 0, Multiplicity = 1

N	-0.059024000	-0.190296000	-0.468707000
C	0.074423000	1.206236000	-0.841739000
C	0.613203000	2.197947000	0.202341000
H	0.545955000	3.217810000	-0.190127000
H	0.050781000	2.155668000	1.138049000
H	1.664446000	2.005972000	0.433008000
H	-1.126922000	0.354496000	2.057257000
C	-1.862861000	0.253126000	1.255470000
H	-2.119221000	1.256598000	0.898401000
H	-2.772350000	-0.186427000	1.676617000
C	-1.332990000	-0.616091000	0.106158000
H	-1.153093000	-1.620991000	0.510358000
C	-2.399914000	-0.753729000	-0.984578000
H	-2.641148000	0.219582000	-1.424668000
H	-3.326542000	-1.167070000	-0.574617000
H	-2.041022000	-1.407600000	-1.782195000
H	-0.915456000	1.545579000	-1.166397000
H	0.709802000	1.275918000	-1.734011000
C	1.118968000	-0.932848000	-0.033803000
H	0.878570000	-1.992638000	-0.206199000
C	2.329231000	-0.614892000	-0.909674000
H	2.699031000	0.401805000	-0.743547000
H	3.145262000	-1.303404000	-0.675162000
H	2.076643000	-0.723040000	-1.967730000
C	1.469475000	-0.801832000	1.458416000
H	0.626695000	-1.105284000	2.086620000
H	2.317872000	-1.447611000	1.708007000
H	1.736659000	0.225206000	1.721741000

TS-*deprotonation*

Charge = 1, Multiplicity = 2

Imaginary mode = -964.88 cm^{-1}

C	2.258573000	4.578113000	0.346906000
C	1.766078000	4.363941000	-0.948257000
C	2.245262000	3.506455000	1.244267000
H	1.765114000	5.185211000	-1.659059000
H	2.629235000	3.650366000	2.250160000
C	1.275153000	3.128472000	-1.335860000
C	1.752391000	2.257040000	0.877872000
H	0.873627000	2.956082000	-2.327685000
H	1.764548000	1.443436000	1.595733000
C	1.264959000	2.086168000	-0.413240000
C	2.773414000	5.932710000	0.754104000
H	3.230620000	5.904131000	1.745050000
H	3.518350000	6.299028000	0.042496000
H	1.957737000	6.662013000	0.778875000
O	0.765186000	0.890479000	-0.889076000
C	0.397777000	-0.111976000	-0.051790000
H	1.423660000	-0.883572000	0.091053000
C	-0.710835000	-0.947273000	-0.659620000
C	-1.977280000	-0.065466000	-0.729647000
N	-3.007581000	-0.730685000	-0.083123000
C	-2.609615000	-1.954864000	0.474971000
C	-1.127714000	-2.157125000	0.173165000
H	-0.600745000	-2.234753000	1.130097000
C	-4.341232000	-0.213226000	0.021048000
C	-5.422603000	-1.067167000	-0.186121000
C	-4.531786000	1.131618000	0.328819000
H	-5.255113000	-2.112824000	-0.414698000
H	-3.679210000	1.782765000	0.477736000
C	-6.713193000	-0.560052000	-0.076509000
C	-5.827619000	1.625252000	0.424158000
H	-7.559071000	-1.220788000	-0.232033000
H	-5.983675000	2.672571000	0.657609000
C	-6.917688000	0.783399000	0.225273000
H	-7.926262000	1.173782000	0.305199000
O	-3.312020000	-2.708086000	1.088501000
O	-2.026294000	1.022349000	-1.240489000
H	-1.010614000	-3.112328000	-0.342926000
H	-0.450466000	-1.205818000	-1.690549000
H	0.170700000	0.230562000	0.964775000
N	2.623403000	-1.672819000	0.077566000
C	2.631337000	-2.381723000	1.400998000
H	1.968979000	-3.243082000	1.255807000
C	4.017615000	-2.876895000	1.824668000
H	4.659957000	-2.037655000	2.106746000
H	4.519762000	-3.464877000	1.057003000
H	3.896602000	-3.508424000	2.707899000
C	2.052306000	-1.507900000	2.513862000
H	1.005789000	-1.248995000	2.345550000
H	2.629016000	-0.587266000	2.646397000
H	2.104420000	-2.058068000	3.455587000
C	3.634020000	-0.599232000	-0.109595000
H	3.717060000	-0.085887000	0.852017000
H	3.198181000	0.118015000	-0.811462000
C	5.022654000	-1.001567000	-0.607613000
H	5.003360000	-1.389518000	-1.625895000
H	5.636740000	-0.097796000	-0.618524000
H	5.514606000	-1.730015000	0.035162000
C	2.311977000	-2.550923000	-1.099762000
H	1.301291000	-2.920938000	-0.881060000
C	3.221891000	-3.774104000	-1.230317000
H	3.154137000	-4.437631000	-0.366364000
H	4.266600000	-3.497359000	-1.385888000
H	2.895116000	-4.343198000	-2.104258000
C	2.256929000	-1.752218000	-2.400684000
H	1.684733000	-0.826425000	-2.308992000
H	1.778785000	-2.371525000	-3.162933000
H	3.254084000	-1.501364000	-2.767772000

H

Charge = 0, Multiplicity = 2

C	5.852250000	-0.603695000	-0.342288000
C	5.178616000	-1.310407000	0.661880000
C	5.193196000	0.465843000	-0.943705000
H	5.673547000	-2.146605000	1.148812000

H	5.699803000	1.036764000	-1.717051000
C	3.890965000	-0.969109000	1.044035000
C	3.899921000	0.831127000	-0.571013000
H	3.357419000	-1.516144000	1.813326000
H	3.413661000	1.686306000	-1.026973000
C	3.252791000	0.101225000	0.419218000
C	7.247936000	-0.998162000	-0.751904000
H	7.657249000	-0.298630000	-1.483991000
H	7.921589000	-1.017338000	0.109854000
H	7.260487000	-1.997233000	-1.198743000
O	1.984614000	0.392071000	0.860823000
C	1.144685000	1.060257000	0.033864000
C	-0.201017000	1.302563000	0.617232000
C	-1.128804000	0.080671000	0.498563000
N	-2.385215000	0.529405000	0.067098000
C	-2.401487000	1.903098000	-0.213733000
C	-0.988133000	2.431254000	-0.050629000
H	-0.601986000	2.658877000	-1.049934000
C	-3.523061000	-0.321090000	-0.076799000
C	-4.776426000	0.128113000	0.338166000
C	-3.369033000	-1.592729000	-0.628798000
H	-4.882493000	1.121553000	0.755016000
H	-2.387627000	-1.931975000	-0.934911000
C	-5.880502000	-0.704142000	0.192001000
C	-4.481149000	-2.417141000	-0.759259000
H	-6.856373000	-0.353673000	0.511210000
H	-4.361114000	-3.408094000	-1.184478000
C	-5.737817000	-1.977157000	-0.353165000
H	-6.602331000	-2.624079000	-0.460120000
O	-3.371739000	2.533523000	-0.547689000
O	-0.838481000	-1.062226000	0.736048000
H	-1.005298000	3.363426000	0.514630000
H	-0.077528000	1.481122000	1.691933000
H	1.254752000	0.869836000	-1.033713000

***i*-Pr$_2$EtNH$^+$**

Charge = 1, Multiplicity = 1

N	-0.066796000	-0.245138000	-0.544801000
C	0.086336000	1.222381000	-0.908972000
C	0.660845000	2.161721000	0.139670000
H	0.595483000	3.170865000	-0.274558000
H	0.110039000	2.156756000	1.079000000
H	1.713740000	1.965568000	0.342036000
H	-1.022500000	0.508790000	2.021597000
C	-1.785819000	0.371211000	1.255653000
H	-2.061297000	1.344777000	0.841618000
H	-2.674550000	-0.035038000	1.743875000
C	-1.379399000	-0.609034000	0.165098000
H	-1.175769000	-1.588585000	0.609025000
C	-2.470931000	-0.757995000	-0.888884000
H	-2.696763000	0.193833000	-1.378596000
H	-3.387887000	-1.100095000	-0.405211000
H	-2.208708000	-1.498650000	-1.651027000
H	-0.911351000	1.545326000	-1.214812000
H	0.718213000	1.238304000	-1.799454000
C	1.161836000	-0.958425000	0.031428000
H	0.899891000	-2.014906000	-0.098265000
C	2.382560000	-0.660570000	-0.828588000
H	2.745180000	0.361572000	-0.701560000
H	3.187041000	-1.334381000	-0.527263000
H	2.190143000	-0.839834000	-1.891143000
C	1.382521000	-0.710643000	1.516278000
H	0.540616000	-1.049458000	2.122525000
H	2.251509000	-1.300302000	1.817742000
H	1.596257000	0.332482000	1.748293000
H	-0.169413000	-0.692931000	-1.460309000

***i*-Pr$_2$NCHCH$_3$• (G)**

Charge = 0, Multiplicity = 2

C	-0.068135000	1.393464000	0.276361000
C	-1.228057000	2.215578000	-0.199484000
H	-1.710141000	1.750242000	-1.067416000
H	-0.890944000	3.211391000	-0.507275000
H	-2.005778000	2.369725000	0.561414000
H	0.850858000	1.910401000	0.526820000
N	0.089626000	0.066700000	-0.103474000
C	-0.964152000	-0.942168000	0.105166000
H	-0.482346000	-1.795550000	0.606352000

C	-1.502130000	-1.434106000	-1.239584000
H	-2.209004000	-2.258714000	-1.103172000
H	-0.686168000	-1.780245000	-1.880842000
H	-2.015658000	-0.618704000	-1.758329000
C	2.373824000	0.286635000	-1.036567000
H	1.918005000	0.380014000	-2.025332000
H	3.328787000	-0.237333000	-1.134491000
H	2.581853000	1.291764000	-0.660096000
C	1.446928000	-0.484475000	-0.099561000
H	1.353733000	-1.500105000	-0.504791000
C	2.027834000	-0.587527000	1.315371000
H	1.361983000	-1.159301000	1.969055000
H	2.154355000	0.408240000	1.750319000
H	3.003897000	-1.081485000	1.302354000
C	-2.092698000	-0.484109000	1.024846000
H	-2.698322000	-1.349741000	1.306999000
H	-1.691289000	-0.021955000	1.930434000
H	-2.751698000	0.234709000	0.533033000

TS-*H abstraction*

Charge = 1, Multiplicity = 3

Imaginary mode = -1629.16 cm^{-1}

C	3.143472000	4.389545000	0.149365000
C	2.531560000	4.261028000	-1.112766000
C	2.900317000	3.398992000	1.119665000
H	2.711105000	5.017119000	-1.870553000
H	3.374170000	3.487776000	2.092316000
C	1.707490000	3.194977000	-1.395345000
C	2.072088000	2.322406000	0.865776000
H	1.218519000	3.079786000	-2.356335000
H	1.904032000	1.573640000	1.630779000
C	1.465691000	2.220555000	-0.402348000
C	4.011595000	5.570928000	0.458448000
H	4.688015000	5.366910000	1.290100000
H	4.600599000	5.867397000	-0.412398000
H	3.389070000	6.428746000	0.737835000
O	0.650655000	1.233753000	-0.775650000
C	0.307920000	0.168183000	0.045486000
H	1.472304000	-0.544050000	-0.042006000
C	-0.899665000	-0.528045000	-0.518697000
C	-2.149409000	0.363975000	-0.403831000
N	-3.214713000	-0.438006000	-0.011332000
C	-2.816581000	-1.748004000	0.304470000
C	-1.297869000	-1.813967000	0.199106000
H	-0.905994000	-1.849771000	1.221928000
C	-4.568123000	0.022236000	0.090140000
C	-5.598560000	-0.779198000	-0.396687000
C	-4.831664000	1.260039000	0.672503000
H	-5.376583000	-1.742857000	-0.838469000
H	-4.017192000	1.873946000	1.036675000
C	-6.910690000	-0.331369000	-0.290270000
C	-6.148380000	1.698598000	0.761697000
H	-7.717449000	-0.953599000	-0.662064000
H	-6.358879000	2.663467000	1.210241000
C	-7.188420000	0.905608000	0.284858000
H	-8.213695000	1.251239000	0.361268000
O	-3.546893000	-2.643409000	0.627346000
O	-2.174916000	1.548727000	-0.616901000
H	-1.005471000	-2.735715000	-0.305927000
H	-0.746429000	-0.698869000	-1.591472000
H	0.201467000	0.459303000	1.096132000
N	2.848749000	-2.300655000	0.128217000
C	3.215817000	-2.624466000	1.515767000
H	3.103486000	-3.708994000	1.606725000
C	4.675849000	-2.268788000	1.809592000
H	4.834210000	-1.187213000	1.815507000
H	5.345570000	-2.713394000	1.069887000
H	4.946844000	-2.651319000	2.796417000
C	2.252316000	-1.962587000	2.504275000
H	1.217722000	-2.238311000	2.282897000
H	2.343111000	-0.872270000	2.472850000
H	2.486586000	-2.288723000	3.519947000
C	2.825697000	-0.946275000	-0.252524000
H	3.338106000	-0.349510000	0.505068000
C	3.182245000	-0.527878000	-1.668273000
H	2.323871000	-0.534894000	-2.345315000
H	3.562547000	0.495772000	-1.637206000
H	3.966153000	-1.157798000	-2.102059000

C	2.478769000	-3.438472000	-0.723469000
H	1.884320000	-4.091071000	-0.069340000
C	3.736919000	-4.211053000	-1.144827000
H	4.313624000	-4.547050000	-0.279665000
H	4.377122000	-3.581634000	-1.768887000
H	3.447309000	-5.091761000	-1.723184000
C	1.612650000	-3.084056000	-1.928255000
H	0.849825000	-2.343697000	-1.672614000
H	1.105548000	-3.992378000	-2.261945000
H	2.201263000	-2.709631000	-2.766819000

I

Charge = 1, Multiplicity = 1

C	5.491523000	0.911578000	0.285494000
C	5.493594000	-0.183385000	-0.590664000
C	4.271667000	1.358699000	0.802620000
H	6.434196000	-0.534677000	-1.003239000
H	4.251933000	2.223752000	1.457359000
C	4.316947000	-0.827985000	-0.946378000
C	3.074671000	0.731058000	0.472216000
H	4.305340000	-1.674034000	-1.624032000
H	2.119648000	1.116553000	0.817306000
C	3.144667000	-0.357595000	-0.380188000
C	6.778214000	1.612727000	0.623981000
H	6.666532000	2.250088000	1.502361000
H	7.576507000	0.892704000	0.817439000
H	7.097297000	2.242763000	-0.211905000
O	1.943851000	-1.030058000	-0.752245000
C	1.077335000	-1.333438000	0.107287000
H	1.311608000	-1.160184000	1.163673000
C	-0.233147000	-1.765998000	-0.345927000
C	-1.031423000	-0.393624000	-0.517073000
N	-2.265163000	-0.585208000	0.038352000
C	-2.418896000	-1.836325000	0.683494000
C	-1.087970000	-2.576915000	0.619667000
H	-0.676211000	-2.614827000	1.633465000
C	-3.313030000	0.400108000	-0.028054000
C	-4.594859000	-0.003770000	-0.390401000
C	-3.020546000	1.727523000	0.270808000
H	-4.801049000	-1.044172000	-0.611866000
H	-2.012972000	2.019370000	0.543444000
C	-5.604583000	0.950553000	-0.445954000
C	-4.039317000	2.670870000	0.199997000
H	-6.608575000	0.648225000	-0.721901000
H	-3.823046000	3.709047000	0.426174000
C	-5.329124000	2.284277000	-0.155272000
H	-6.120828000	3.023709000	-0.207145000
O	-3.422168000	-2.220422000	1.203798000
O	-0.559697000	0.571251000	-1.048433000
H	-1.252176000	-3.603292000	0.290483000
H	-0.162297000	-2.174888000	-1.358952000

RC-*Z*

Charge = 1, Multiplicity = 2

C	6.116855000	0.118747000	0.783043000
C	5.869276000	-0.988482000	-0.031302000
C	5.049653000	0.972436000	1.076675000
H	6.686481000	-1.658798000	-0.281738000
H	5.220600000	1.839527000	1.708549000
C	4.600724000	-1.247243000	-0.540199000
C	3.773125000	0.728119000	0.583614000
H	4.419166000	-2.096662000	-1.190619000
H	2.938960000	1.377856000	0.828408000
C	3.559949000	-0.382170000	-0.223316000
C	7.489444000	0.371973000	1.349625000
H	7.606582000	-0.121807000	2.319507000
H	8.267593000	-0.012895000	0.687019000
H	7.665938000	1.439421000	1.499134000
O	2.281081000	-0.571045000	-0.730568000
C	1.834217000	-1.852230000	-0.790630000
H	2.117031000	-2.507435000	0.031883000
C	0.537368000	-2.029550000	-1.508664000
C	-0.572168000	-1.285254000	-0.759391000
N	-1.400871000	-2.211233000	-0.164635000
C	-1.118311000	-3.539329000	-0.561147000
C	0.070076000	-3.489860000	-1.507259000
H	0.833245000	-4.192920000	-1.166059000
C	-2.475374000	-1.846447000	0.700063000
C	-3.776231000	-2.235212000	0.395341000

C	-2.198446000	-1.075781000	1.827386000
H	-3.965400000	-2.857374000	-0.472581000
H	-1.169980000	-0.813521000	2.055591000
C	-4.815842000	-1.825700000	1.225973000
C	-3.245055000	-0.663729000	2.645285000
H	-5.832261000	-2.130085000	1.000878000
H	-3.035432000	-0.069095000	3.528690000
C	-4.554680000	-1.033723000	2.341916000
H	-5.369889000	-0.720261000	2.985331000
O	-1.748876000	-4.495144000	-0.209796000
O	-0.699882000	-0.078018000	-0.667567000
H	-0.263726000	-3.826015000	-2.491570000
H	0.613897000	-1.594281000	-2.511287000
N	-1.549031000	2.833941000	-0.743538000
C	-2.971476000	2.600810000	-1.167865000
H	-3.445751000	3.580836000	-1.040407000
C	-3.614409000	1.577899000	-0.230052000
C	-3.104746000	2.175303000	-2.620161000
H	-2.608878000	2.865777000	-3.307568000
H	-2.726439000	1.160521000	-2.776617000
H	-4.167560000	2.167972000	-2.868612000
H	-3.075472000	0.628350000	-0.287145000
H	-4.650327000	1.420013000	-0.538328000
H	-3.627378000	1.904173000	0.812244000
C	-1.418563000	3.507390000	0.589957000
H	-2.454236000	3.697855000	0.879772000
C	-0.739674000	4.869783000	0.474761000
C	-0.821943000	2.556570000	1.624525000
H	-1.340561000	1.594224000	1.599387000
H	0.241961000	2.373288000	1.465110000
H	-0.942751000	2.999177000	2.616112000
H	0.325727000	4.805645000	0.252453000
H	-0.847978000	5.387743000	1.430341000
H	-1.220001000	5.479202000	-0.294809000
C	-0.559736000	2.411902000	-1.443016000
H	-0.818305000	1.913987000	-2.371415000
C	0.890729000	2.492170000	-1.156136000
H	1.235632000	1.454032000	-1.056252000
H	1.158086000	3.056627000	-0.269931000
H	1.393590000	2.919271000	-2.028970000

TS-Z

Charge = 1, Multiplicity = 2

Imaginary mode = -1134.76 cm^{-1}

C	-6.077844000	-1.293626000	-0.291005000
C	-5.549407000	-0.546704000	0.761804000
C	-5.188955000	-1.881457000	-1.200751000
H	-6.221359000	-0.068791000	1.468021000
H	-5.581951000	-2.459496000	-2.032092000
C	-4.173835000	-0.388533000	0.922492000
C	-3.815953000	-1.741684000	-1.061935000
H	-3.784728000	0.220427000	1.732621000
H	-3.118810000	-2.192510000	-1.759366000
C	-3.330055000	-1.004421000	0.009576000
C	-7.563313000	-1.474431000	-0.454110000
H	-7.852491000	-2.506030000	-0.232073000
H	-8.121109000	-0.817540000	0.215473000
H	-7.873218000	-1.260337000	-1.480139000
O	-1.937932000	-0.874014000	0.078174000
C	-1.334308000	-0.788500000	1.240459000
H	-1.925736000	-0.973010000	2.136241000
C	0.022249000	-0.428634000	1.309485000
C	0.920105000	-0.762591000	0.129678000
N	2.080695000	-1.320725000	0.645200000
C	2.108731000	-1.346376000	2.052855000
C	0.810041000	-0.734936000	2.568434000
H	0.319846000	-1.447029000	3.236167000
C	3.175341000	-1.744022000	-0.177104000
C	4.476573000	-1.390838000	0.177189000
C	2.916946000	-2.491564000	-1.323489000
H	4.661111000	-0.823564000	1.082123000
H	1.897931000	-2.752617000	-1.583851000
C	5.530560000	-1.802088000	-0.631685000
C	3.980569000	-2.887075000	-2.127299000
H	6.546725000	-1.540313000	-0.357588000
H	3.785512000	-3.468350000	-3.021823000
C	5.285920000	-2.546256000	-1.782892000
H	6.112925000	-2.862927000	-2.409092000
O	3.016789000	-1.750815000	2.721652000

O	0.685077000	-0.534512000	-1.031938000
H	1.063240000	0.152817000	3.156828000
H	0.077225000	0.906545000	1.114857000
N	0.596491000	2.682541000	-0.208512000
C	2.042167000	3.031597000	-0.242330000
H	2.224937000	3.362732000	-1.267879000
C	2.911246000	1.805065000	0.021955000
C	2.362469000	4.195605000	0.693842000
H	1.669307000	5.026780000	0.541711000
H	2.331179000	3.900247000	1.746653000
H	3.375124000	4.549634000	0.488459000
H	2.729028000	1.405978000	1.027917000
H	3.966239000	2.083868000	-0.032803000
H	2.722599000	1.021121000	-0.715718000
C	-0.086713000	2.753484000	-1.522780000
H	0.645039000	2.327191000	-2.219283000
C	-0.326338000	4.223104000	-1.880931000
C	-1.358038000	1.926081000	-1.655748000
H	-1.217993000	0.915277000	-1.268981000
H	-2.220592000	2.404806000	-1.188048000
H	-1.577331000	1.840835000	-2.722733000
H	-1.038151000	4.673794000	-1.183272000
H	-0.746863000	4.288402000	-2.887046000
H	0.596077000	4.808763000	-1.860974000
C	0.054002000	2.311393000	0.971889000
H	0.732988000	2.515248000	1.801775000
C	-1.408254000	2.488776000	1.323406000
H	-2.056006000	1.751637000	0.842883000
H	-1.759899000	3.484562000	1.039609000
H	-1.516010000	2.385657000	2.405467000

J

Charge = 1, Multiplicity = 2

C	5.806106000	-0.665477000	0.146072000
C	5.409534000	0.698006000	0.127750000
C	4.810580000	-1.670346000	0.085133000
H	6.174548000	1.465754000	0.182338000
H	5.107481000	-2.714016000	0.102243000
C	4.088242000	1.064127000	0.049587000
C	3.484513000	-1.334796000	0.007598000
H	3.815933000	2.112342000	0.045613000
H	2.688674000	-2.071217000	-0.039044000
C	3.114478000	0.037634000	-0.012804000
C	7.248097000	-1.039332000	0.211829000
H	7.574840000	-1.413457000	-0.766780000
H	7.879511000	-0.191918000	0.479381000
H	7.407351000	-1.849358000	0.929060000
O	1.805653000	0.225565000	-0.087900000
C	1.160602000	1.410590000	-0.147591000
H	1.755434000	2.316496000	-0.173652000
C	-0.183687000	1.396469000	-0.175928000
C	-1.018108000	0.146139000	-0.116971000
N	-2.343348000	0.573350000	-0.074971000
C	-2.478809000	1.975351000	-0.135890000
C	-1.084755000	2.583735000	-0.236973000
H	-1.009570000	3.134034000	-1.180813000
C	-3.454369000	-0.321511000	0.011090000
C	-4.522365000	-0.008481000	0.852901000
C	-3.451223000	-1.492131000	-0.748288000
H	-4.513294000	0.907383000	1.430530000
H	-2.612948000	-1.721855000	-1.394068000
C	-5.598609000	-0.883828000	0.929073000
C	-4.533510000	-2.358345000	-0.656778000
H	-6.433168000	-0.646291000	1.579370000
H	-4.538289000	-3.269473000	-1.244668000
C	-5.606699000	-2.057791000	0.178880000
H	-6.449548000	-2.737220000	0.244545000
O	-3.512815000	2.578263000	-0.116258000
O	-0.623931000	-0.992811000	-0.103360000
H	-0.934890000	3.297133000	0.578746000

I'

Charge = 1, Multiplicity = 1

C	5.715819000	-0.733707000	-0.395734000
C	5.010492000	-0.141081000	-1.451871000
C	5.141281000	-0.735173000	0.879763000
H	5.447950000	-0.124814000	-2.445226000
H	5.686275000	-1.167944000	1.712349000
C	3.761418000	0.430917000	-1.253324000

C	3.889309000	-0.175274000	1.112462000
H	3.206083000	0.893341000	-2.061668000
H	3.479002000	-0.141379000	2.116902000
C	3.232408000	0.375198000	0.024883000
C	7.078251000	-1.324557000	-0.630964000
H	7.402750000	-1.928933000	0.217099000
H	7.080857000	-1.952721000	-1.524799000
H	7.816032000	-0.531170000	-0.783613000
O	1.939084000	0.965198000	0.170082000
C	1.074912000	0.526568000	0.967521000
H	1.290076000	-0.370543000	1.556730000
C	-0.231276000	1.173113000	1.086182000
C	-1.302508000	0.031556000	1.024776000
N	-2.301241000	0.467706000	0.195088000
C	-2.035499000	1.725075000	-0.400331000
C	-0.654424000	2.198525000	0.048306000
H	0.000837000	2.220363000	-0.826484000
C	-3.495168000	-0.292880000	-0.063617000
C	-4.728463000	0.351719000	-0.035194000
C	-3.388334000	-1.653849000	-0.335228000
H	-4.787643000	1.413762000	0.170652000
H	-2.418360000	-2.137077000	-0.347171000
C	-5.876739000	-0.389878000	-0.290923000
C	-4.547089000	-2.383058000	-0.577138000
H	-6.842690000	0.102614000	-0.276657000
H	-4.476202000	-3.445012000	-0.784475000
C	-5.788748000	-1.753612000	-0.558300000
H	-6.689141000	-2.325937000	-0.753123000
O	-2.772632000	2.302437000	-1.141591000
O	-1.190821000	-1.005727000	1.620644000
H	-0.727444000	3.214389000	0.437427000
H	-0.298603000	1.534234000	2.125736000

RC-*E*

Charge = 1, Multiplicity = 2

C	-5.628219000	-0.886554000	-0.559262000
C	-4.735601000	-1.526355000	-1.417334000
C	-5.214841000	-0.651891000	0.758319000
H	-5.041522000	-1.745272000	-2.436435000
H	-5.900777000	-0.180299000	1.456899000
C	-3.460473000	-1.912089000	-1.002388000
C	-3.951321000	-1.025436000	1.193669000
H	-2.810957000	-2.442084000	-1.688343000
H	-3.634611000	-0.863946000	2.219427000
C	-3.068613000	-1.636130000	0.302613000
C	-7.013359000	-0.503823000	-1.010763000
H	-7.293182000	0.485461000	-0.639673000
H	-7.087397000	-0.493655000	-2.099966000
H	-7.753848000	-1.215837000	-0.633701000
O	-1.816587000	-1.911424000	0.809861000
C	-0.816240000	-2.323026000	-0.009840000
H	-0.879743000	-2.049264000	-1.059733000
C	0.508452000	-2.419517000	0.661954000
C	1.394388000	-1.198887000	0.370620000
N	2.665584000	-1.635961000	0.087088000
C	2.777641000	-3.051785000	0.089997000
C	1.379347000	-3.614588000	0.247573000
H	1.070713000	-4.018979000	-0.721946000
C	3.769714000	-0.776835000	-0.206485000
C	4.921957000	-0.848628000	0.570065000
C	3.682822000	0.093918000	-1.288903000
H	4.976175000	-1.554551000	1.391278000
H	2.783318000	0.105088000	-1.896529000
C	5.997007000	-0.020937000	0.261635000
C	4.758779000	0.925835000	-1.581535000
H	6.902281000	-0.074876000	0.856357000
H	4.700962000	1.603708000	-2.426920000
C	5.915096000	0.869024000	-0.806784000
H	6.758190000	1.508943000	-1.043991000
O	3.811437000	-3.641242000	-0.037257000
O	1.031184000	-0.035078000	0.388665000
H	1.379943000	-4.437184000	0.962776000
H	0.334048000	-2.426043000	1.744407000
N	-0.434241000	2.763690000	0.378280000
C	0.717503000	3.636275000	-0.025048000
H	0.235183000	4.511391000	-0.474239000
C	1.550380000	2.890080000	-1.063113000
C	1.563576000	4.099073000	1.151077000
H	0.954949000	4.518108000	1.956771000

H	2.195071000	3.297526000	1.544479000
H	2.232975000	4.883874000	0.793276000
H	1.982620000	1.995901000	-0.607505000
H	2.356434000	3.539369000	-1.412676000
H	0.956739000	2.587407000	-1.930300000
C	-1.565739000	2.756704000	-0.606220000
H	-1.122757000	3.220779000	-1.490541000
C	-2.691643000	3.661478000	-0.113583000
C	-2.013105000	1.346686000	-0.994806000
H	-1.171415000	0.646099000	-0.967316000
H	-2.811324000	0.964635000	-0.355546000
H	-2.405293000	1.376235000	-2.013887000
H	-3.166619000	3.261856000	0.785276000
H	-3.453200000	3.733473000	-0.893215000
H	-2.328419000	4.669562000	0.102311000
C	-0.387805000	2.056057000	1.445959000
H	0.533581000	2.129326000	2.016373000
C	-1.437090000	1.155116000	1.976434000
H	-1.212663000	0.140084000	1.621827000
H	-2.444762000	1.418269000	1.663783000
H	-1.378052000	1.150156000	3.066377000

TS-*E*

Charge = 1, Multiplicity = 2

Imaginary mode = -1059.30 cm^{-1}

C	-6.426825000	-1.084727000	-0.407720000
C	-5.394682000	-1.799210000	-1.021529000
C	-6.106922000	-0.237070000	0.658215000
H	-5.625208000	-2.472658000	-1.841418000
H	-6.896655000	0.322230000	1.150629000
C	-4.075787000	-1.680398000	-0.593441000
C	-4.797511000	-0.097068000	1.101298000
H	-3.288768000	-2.270795000	-1.052363000
H	-4.540850000	0.555141000	1.928822000
C	-3.803012000	-0.816888000	0.457217000
C	-7.854108000	-1.252498000	-0.856303000
H	-8.430609000	-0.340564000	-0.687807000
H	-7.909205000	-1.503560000	-1.917484000
H	-8.339315000	-2.059511000	-0.298468000
O	-2.498727000	-0.655095000	0.950785000
C	-1.493305000	-0.578692000	0.109949000
H	-1.701097000	-0.550893000	-0.958945000
C	-0.192559000	-0.456547000	0.621636000
C	0.916002000	-0.814260000	-0.339421000
N	1.877497000	-1.504934000	0.376501000
C	1.545724000	-1.650071000	1.742636000
C	0.183136000	-1.007247000	1.980627000
H	-0.520898000	-1.762453000	2.339562000
C	3.117514000	-1.945282000	-0.191328000
C	4.302328000	-1.751541000	0.517952000
C	3.119275000	-2.544366000	-1.448712000
H	4.280970000	-1.301906000	1.503729000
H	2.188964000	-2.682635000	-1.986388000
C	5.502278000	-2.171284000	-0.045509000
C	4.328656000	-2.950669000	-2.002196000
H	6.426871000	-2.033158000	0.504318000
H	4.337007000	-3.417835000	-2.980947000
C	5.518848000	-2.767927000	-1.303434000
H	6.458039000	-3.094334000	-1.736835000
O	2.238213000	-2.173187000	2.568198000
O	0.952259000	-0.505256000	-1.508830000
H	0.281607000	-0.251483000	2.765034000
H	0.066463000	0.862901000	0.683483000
N	1.057707000	2.769524000	-0.065928000
C	2.491834000	2.893544000	0.303718000
H	2.951913000	3.416326000	-0.539081000
C	3.136660000	1.515170000	0.425659000
C	2.690881000	3.750809000	1.551404000
H	2.150964000	4.697658000	1.471239000
H	2.371374000	3.238317000	2.463345000
H	3.754876000	3.970706000	1.663373000
H	2.704057000	0.961607000	1.268144000
H	4.207232000	1.620205000	0.616231000
H	3.005480000	0.931314000	-0.490344000
C	0.743188000	3.147716000	-1.463617000
H	1.619906000	2.811752000	-2.029494000
C	0.642334000	4.671757000	-1.562355000
C	-0.467561000	2.453873000	-2.076494000

H	-0.465776000	1.384970000	-1.849970000
H	-1.410562000	2.913703000	-1.776592000
H	-0.389095000	2.555440000	-3.161430000
H	-0.218072000	5.035246000	-0.993267000
H	0.509239000	4.963355000	-2.606879000
H	1.541355000	5.165199000	-1.184000000
C	0.193133000	2.270276000	0.845069000
H	0.638067000	2.227297000	1.840278000
C	-1.290544000	2.568086000	0.841604000
H	-1.838199000	1.999652000	0.084919000
H	-1.475669000	3.631253000	0.665425000
H	-1.698631000	2.300776000	1.818387000

J'

Charge = 1, Multiplicity = 2

C	-6.094437000	-0.505401000	-0.053350000
C	-5.129046000	-1.214085000	0.663836000
C	-5.701611000	0.655086000	-0.732362000
H	-5.416757000	-2.106004000	1.211652000
H	-6.440715000	1.220199000	-1.292593000
C	-3.803417000	-0.789948000	0.708113000
C	-4.386194000	1.096226000	-0.707319000
H	-3.070749000	-1.327059000	1.302480000
H	-4.072574000	1.989805000	-1.235190000
C	-3.454882000	0.354189000	0.006047000
C	-7.531205000	-0.953439000	-0.081566000
H	-7.919072000	-0.960225000	-1.103372000
H	-7.643840000	-1.956296000	0.333744000
H	-8.158764000	-0.274424000	0.503559000
O	-2.141159000	0.842280000	0.018150000
C	-1.139672000	-0.003705000	-0.074451000
H	-1.361721000	-1.049859000	-0.283579000
C	0.136003000	0.431258000	0.066580000
C	1.229954000	-0.497980000	-0.081209000
N	2.460568000	0.304507000	0.076327000
C	2.111289000	1.692522000	0.360137000
C	0.608133000	1.820345000	0.340589000
H	0.277516000	2.224235000	1.303023000
C	3.730611000	-0.176277000	-0.030769000
C	4.828678000	0.715765000	-0.291205000
C	3.986368000	-1.584976000	0.113821000
H	4.644154000	1.770437000	-0.428044000
H	3.166276000	-2.256459000	0.318139000
C	6.099557000	0.213442000	-0.392792000
C	5.272034000	-2.052146000	0.020410000
H	6.925084000	0.881678000	-0.609399000
H	5.468748000	-3.109895000	0.152222000
C	6.338031000	-1.167369000	-0.234718000
H	7.349442000	-1.551789000	-0.314938000
O	2.918318000	2.539788000	0.598952000
O	1.235840000	-1.678412000	-0.312030000
H	0.323843000	2.543809000	-0.431336000

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