

Supporting Information

Palladium Catalyzed Chemoselective Activation of sp^3 vs sp^2 C–Bonds: Oxidative Coupling to Form Quaternary Centers

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1. General Considerations

All non-aqueous reactions were carried out under an atmosphere of dry argon unless otherwise noted. Commercial reagents were used as received without additional purification unless otherwise noted. Dichloromethane was distilled from CaH_2 , and toluene was distilled from metallic sodium prior to use. Anhydrous 1,4-dioxane was purchased from Sigma Aldrich as 100 mL sure-seal bottles and stored in the glovebox. Activated carbon (Darco G-60) was dried overnight at 80 °C in vacuo. Reactions were monitored by thin layer chromatography (TLC) using Silicycle, glass-backed TLC plates with 250 μm silica and F254 indicator. Visualization was accomplished by UV light.

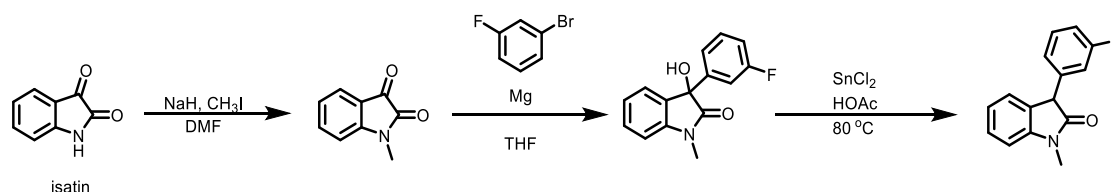
^1H NMR, ^{13}C NMR spectra were recorded on a AM-500 Fourier transform NMR spectrometer at 500 MHz, and 125 MHz respectively. Chemical shifts are reported relative to the solvent resonance peak δ 7.26 (CDCl_3) for ^1H NMR spectra and δ 77.16 (CDCl_3) for ^{13}C NMR spectra. Data are reported as follows: chemical shift, multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, b = broad singlet, m = multiplet), coupling constants, and number of protons. Accurate mass measurement analyses were conducted on either a GCMS with electron ionization (EI) or an LCMS with electrospray ionization (ESI). The signals were mass measured (TOF) against an internal lock mass reference of perfluorotributylamine (PFTBA) for EI-GCMS, and leucine enkephalin for ESI-LCMS. Waters software calibrates the instruments, and reports measurements, by use of neutral atomic masses; the mass of the electron is not subtracted (positive ions) or added (negative ions). Infrared spectra are reported in cm^{-1} . Melting points are uncorrected. Unless otherwise noted, yields refer to isolated material on the basis of product purity ($\geq 95\%$) by ^1H NMR following silica gel chromatography with Silica-P flash silica gel (50-63 μm mesh particle size).

Materials preparation: Cyanoarylacetates used in this study were prepared according to the literature.¹ 3-substituted oxindoles used in this study were prepared according to the literature.² Arylmalononitriles used in this study were prepared according to the literature.³ 3-Aryl benzofuran-2(3*H*)-one used in this study were prepared according to the literature.⁴ The dimer of 3-benzyl-1-methylindolin-2-one was synthesized according to the literature.⁵

2. Experimental Procedures and Characterization.

Synthesis and characterization of new starting materials

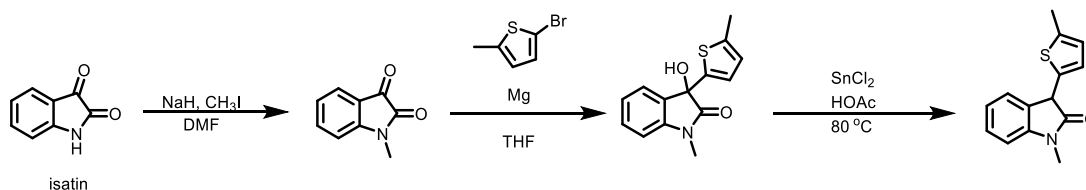
3-(3-fluorophenyl)-1-methylindolin-2-one:



This new compound was prepared according to the literature procedure.^{2c} The crude product was purified via column chromatography (eluent 12% EtOAc in hexanes) to give the title compound as white solid.

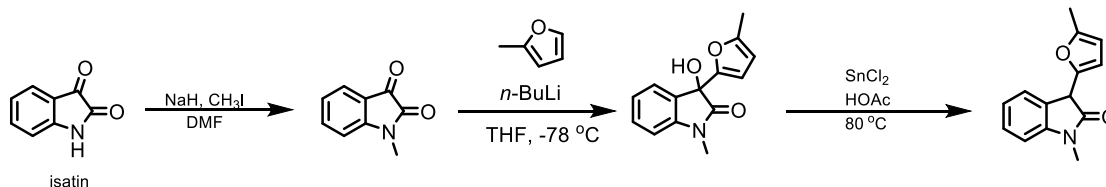
^1H NMR (500 MHz, CDCl_3) δ 7.36-7.27 (m, 2H), 7.17 (d, $J = 10.0$ Hz, 1H), 7.11-6.97 (m, 3H), 6.92-6.87 (m, 2H), 4.60 (s, 1H), 3.25 (s, 3H); ^{13}C NMR (125 MHz, CDCl_3) δ 175.2, 162.9 (d, $J_{\text{C-F}} = 245.0$ Hz), 144.4, 138.8 (d, $J_{\text{C-F}} = 7.5$ Hz), 130.2 (d, $J_{\text{C-F}} = 8.2$ Hz), 128.6, 128.0, 124.9, 124.2, 122.8, 115.2 (d, $J_{\text{C-F}} = 22.1$ Hz), 114.4 (d, $J_{\text{C-F}} = 21.0$ Hz), 108.2, 51.5 (d, $J_{\text{C-F}} = 1.6$ Hz), 26.4; IR (film) 2920, 1713, 1612, 1496, 1473, 1350, 1257, 752 cm^{-1} ; HRMS (EI) calcd for $\text{C}_{15}\text{H}_{13}\text{FNO}$ $[\text{M} + \text{H}]^+$ $m/z = 242.0981$; found 242.0979.

1-methyl-3-(5-methylthiophen-2-yl)indolin-2-one:



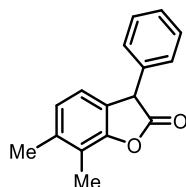
This new compound was prepared according to the literature procedure.^{2c} The crude product was purified via column chromatography (eluent 12% EtOAc in hexanes) to give the title compound as yellow solid. ¹H NMR (500 MHz, CDCl₃) δ 7.34 (t, *J* = 7.5 Hz, 2H), 7.09 (t, *J* = 7.5 Hz, 1H), 6.88 (d, *J* = 7.5 Hz, 1H), 6.78 (d, *J* = 3.5 Hz, 1H), 6.63-6.61 (m, 1H), 4.76 (s, 1H), 3.24 (s, 3H), 2.43 (s, 3H); ¹³C NMR (125 MHz, CDCl₃) δ 174.7, 144.1, 139.7, 135.3, 128.6, 128.0, 125.8, 125.0, 124.8, 122.6, 108.2, 47.1, 26.5, 15.2; IR (film) 2918, 1714, 1612, 1492, 1470, 1333, 1251, 1125, 751 cm⁻¹; HRMS (EI) calcd for C₁₄H₁₄NOS [M + H]⁺ *m/z* = 244.0796; found 244.0774.

1-methyl-3-(5-methylfuran-2-yl)indolin-2-one:



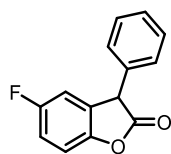
This new compound was prepared according to the literature procedure.^{2c, d} The crude product was purified via column chromatography (eluent 12% EtOAc in hexanes) to give the title compound as yellow solid. ¹H NMR (500 MHz, CDCl₃) δ 7.31 (q, *J* = 8.0 Hz, 2H), 7.07 (t, *J* = 7.5 Hz, 1H), 6.86 (d, *J* = 7.5 Hz, 1H), 6.11 (d, *J* = 3.0 Hz, 1H), 5.91 (d, *J* = 3.0 Hz, 1H), 4.69 (s, 1H), 3.26 (s, 3H), 2.25 (s, 3H); ¹³C NMR (125 MHz, CDCl₃) δ 173.7, 152.5, 146.7, 144.1, 128.5, 126.6, 124.7, 122.6, 108.6, 108.1, 106.2, 45.9, 26.4, 13.5; IR (film) 2918, 1718, 1612, 1495, 1470, 1346, 1253, 1085, 751 cm⁻¹; HRMS (EI) calcd for C₁₄H₁₃NO₂ [M]⁺ *m/z* = 227.0946; found 227.0943.

6,7-dimethyl-3-phenylbenzofuran-2(3*H*)-one:



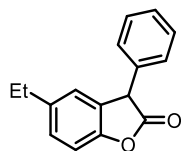
This new compound was prepared according to the literature procedure.⁴ The crude product was purified via column chromatography (eluent 6% EtOAc in hexanes) to give the title compound as white solid. ¹H NMR (500 MHz, CDCl₃) δ 7.37-7.30 (m, 3H), 7.23 (d, *J* = 7.4 Hz, 2H), 6.97 (d, *J* = 7.6 Hz, 1H), 6.92 (d, *J* = 7.6 Hz, 1H), 4.89 (s, 1H), 2.33 (s, 3H), 2.29 (s, 3H); ¹³C NMR (125 MHz, CDCl₃) δ 175.8, 152.7, 138.6, 135.6, 129.1, 128.3, 128.1, 125.5, 124.0, 122.0, 119.9, 50.5, 19.7, 12.1; IR (KBr, cm⁻¹) 2960, 1810, 1632, 1496, 1454, 1424, 1256, 1153, 1106, 1071, 1019, 974, 928, 911, 870, 822, 793, 747, 728, 701, 631; HRMS (EI-TOF) calcd for C₁₆H₁₄O₂ [M]⁺ *m/z* = 238.0994; found 238.1002.

5-fluoro-3-phenylbenzofuran-2(3H)-one:



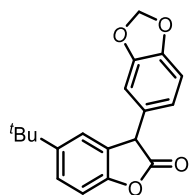
This new compound was prepared according to the literature procedure.⁴ The crude product was purified via column chromatography (eluent 6% EtOAc in hexanes) to give the title compound as white solid. ¹H NMR (500 MHz, CDCl₃) δ 7.40-7.35 (m, 3H), 7.22 (d, *J* = 6.5 Hz, 2H), 7.15 (dd, *J* = 8.8, 4.1 Hz, 1H), 7.07 (m, 1H), 6.94 (dd, *J* = 7.4, 2.6 Hz, 1H), 4.90 (s, 1H); ¹³C NMR (125 MHz, CDCl₃) δ 174.8, 159.7 (d, *J* = 243.0 Hz), 149.9, 134.6, 129.4, 128.7, 128.6, 128.3, 116.2 (d, *J* = 24.4 Hz), 112.8 (d, *J* = 25.5 Hz), 111.9 (d, *J* = 8.4 Hz), 50.3; IR (KBr, cm⁻¹) 2960, 1812, 1496, 1477, 1455, 1446, 1274, 1258, 1237, 1211, 1112, 1059, 922, 892, 843, 814, 740, 710, 696, 658, 504; HRMS (EI-TOF) calcd for C₁₄H₉O₂ [M]⁺ *m/z* = 228.0587; found 228.0575.

5-ethyl-3-phenylbenzofuran-2(3H)-one:



This new compound was prepared according to the literature procedure.⁴ The crude product was purified via column chromatography (eluent 6% EtOAc in hexanes) to give the title compound as white solid. ¹H NMR (500 MHz, CDCl₃) δ 7.40-7.34 (m, 3H), 7.24 (d, *J* = 6.8 Hz, 2H), 7.19 (d, *J* = 8.2 Hz, 1H), 7.10 (d, *J* = 8.2 Hz, 1H), 7.04 (s, 1H), 4.87 (s, 1H), 2.63 (q, *J* = 7.6 Hz, 2H), 1.22 (t, *J* = 7.6 Hz, 3H); ¹³C NMR (125 MHz, CDCl₃) δ 175.6, 152.1, 140.8, 135.4, 129.2, 128.7, 128.4, 128.2, 127.1, 124.7, 110.6, 50.0, 28.6, 15.9; IR (KBr, cm⁻¹) 2966, 2932, 1813, 1619, 1485, 1454, 1288, 1230, 1140, 1066, 1051, 1003, 919, 891, 822, 737, 709, 696, 659, 510; HRMS (EI-TOF) calcd for C₁₆H₁₄O₂ [M]⁺ *m/z* = 238.0994; found 238.0993.

3-(benzo[d][1,3]dioxol-5-yl)-5-(tert-butyl)benzofuran-2(3H)-one:

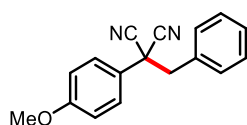


This new compound was prepared according to the literature procedure.⁴ The crude product was purified via column chromatography (eluent 7% EtOAc in hexanes) to give the title compound as white solid. ¹H NMR (500 MHz, CDCl₃) δ 7.38 (d, *J* = 8.5 Hz, 1H), 7.22 (s, 1H), 7.09 (d, *J* = 8.5 Hz, 1H), 6.80 (d, *J* = 8.0 Hz, 1H), 6.72 (d, *J* = 7.5 Hz, 1H), 6.66 (s, 1H), 5.96 (d, 2H), 4.77 (s, 1H), 1.30 (d, 9H); ¹³C NMR (125 MHz, CDCl₃) δ 175.7, 151.9, 148.4, 148.0, 147.7, 129.0, 126.6, 122.3, 122.0, 114.8, 110.3, 108.8, 108.7, 101.4, 49.9, 34.8, 31.7; IR (film) cm⁻¹ 2962, 2905, 1811, 1618, 1504, 1488, 1445, 1364, 1308, 1249, 1231, 1181, 1144, 1090, 1058, 1039, 930, 900, 820, 807; HRMS (EI-TOF) calcd C₁₉H₁₈O₄ [M]⁺ *m/z* = 310.1198; found 310.1205.

General Procedure and Characterization of the Products.

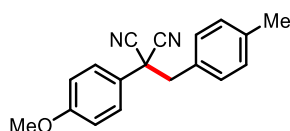
General Procedure A: Benzylation of Arylmalononitriles Under Stoichiometric Conditions. **1** (0.173 mmol) was added to a flame dried 8 mL microwave vial equipped with stir bar and brought into the glovebox. Pd(OAc)₂ (38.9 mg, 0.173 mmol) and the indicated tolyl analog (1.73 mL, 0.1 M) were added to the microwave vial, which was then sealed with a Teflon cap, removed from the glovebox, and placed in a 95 °C oil bath. After 24 h, the mixture was allowed to cool to ambient temperature, diluted with CH₂Cl₂ (3 mL), passed through celite with CH₂Cl₂, and concentrated. The resulting residue was purified by column chromatography to afford the alkylated arylmalononitrile **3**.

General Procedure B: Alkylation of Arylmalononitriles Under Catalytic Conditions. **1** (0.120 mmol), 2,6-dimethylbenzoquinone (16.4 mg, 0.120 mmol), and charcoal (54.0 mg, 10x weight of Pd(OAc)₂) were added to a flame dried 8 mL microwave vial equipped with stir bar and brought into the glovebox. PivOH (12.3 mg, 0.120 mmol), Pd(OAc)₂ (5.4 mg, 24.0 μmol), and indicated tolyl analog (1.20 mL, 0.1 M) were added to the microwave vial, which was then sealed with a Teflon cap, removed from the glovebox, and placed in a 115 °C oil bath. After 48 h, the mixture was allowed to cool to ambient temperature, diluted with CH₂Cl₂ (3 mL), passed through celite with CH₂Cl₂, and concentrated *in vacuo*. The crude mixture was then dissolved in CH₂Cl₂ and washed with 0.5 M NaOH/Na₂S₂O₄ twice. The organic layer was dried over Na₂SO₄, filtered, and concentrated. The resulting residue was purified by column chromatography to afford the alkylated arylmalononitrile **3**.



2-Benzyl-2-(4-methoxyphenyl)malononitrile. General Procedure **A** was followed using 2-(4-methoxyphenyl)malononitrile (29.8 mg, 0.173 mmol) and Pd(OAc)₂ (38.9 mg, 0.173 mmol) in toluene (1.73 mL, 0.1 M). Chromatography (5% EtOAc/Hexanes) provided product **3aa** as a white solid (43.4 mg) was isolated in 96% yield: ¹H NMR (500 MHz, CDCl₃) δ 7.33 (m, 5H), 7.14 (d, *J* = 6.5 Hz, 2H), 6.95 (dt, *J*₁ = 8.9 Hz, *J*₂ = 2.2 Hz, 2H), 3.84 (s, 3H), 3.43 (s, 2H); ¹³C NMR (125 MHz, CDCl₃) δ 160.8, 131.8, 130.7, 129.0, 128.9, 127.7, 123.4, 115.1, 115.0, 55.7, 48.7, 43.6; IR (film) 3032, 2935, 2849, 2323, 2247, 1608, 1586, 1511, 1494, 1456, 1438, 1301, 1255, 1187, 1178, 1088, 1029, 826, 814, 766, 702, 668, 537, 477; HRMS (EI-TOF) calcd for C₁₇H₁₄N₂O, [M]⁺ *m/z* = 262.1106; found 262.1122.

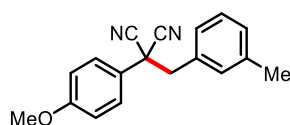
General Procedure **B** was followed using 2-(4-methoxyphenyl)malononitrile (26.0 mg, 0.151 mmol), Pd(OAc)₂ (6.8 mg, 30.2 μmol), 2,6-dimethylbenzoquinone (20.6 mg, 0.151 mmol), AcOH (8.6 μL, 0.151 mmol), charcoal (67.8 mg, 10 x weight of Pd), toluene (0.32 mL, 3.02 mmol), and 1,4-dioxane (1.16 mL, 0.13 M). Chromatography (5% EtOAc/Hexanes) provided product **3aa** as a white solid (38.2 mg) in 96% yield. See above for characterization.



2-(4-Methoxyphenyl)-2-(4-methylbenzyl)malononitrile. General Procedure **A** was followed using 2-(4-methoxyphenyl)malononitrile (25.6 mg, 0.149 mmol) and Pd(OAc)₂ (33.4 mg, 0.149 mmol) in *p*-

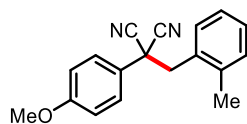
xylene (1.49 mL, 0.1 M) at 105 °C. Chromatography (5% EtOAc/Hexanes) provided product **3ab** as a white solid (15.1 mg) was isolated in 36% yield: ¹H NMR (500 MHz, CDCl₃) δ 7.36 (dt, *J*₁ = 8.8 Hz, *J*₂ = 2.1 Hz, 2H), 7.12 (d, *J* = 7.9 Hz, 2H), 7.03 (d, *J* = 8.0 Hz, 2H), 6.95 (dt, *J*₁ = 8.8 Hz, *J*₂ = 2.1 Hz, 2H), 3.85 (s, 3H), 3.40 (s, 2H), 2.34 (s, 3H); ¹³C NMR (125 MHz, CDCl₃) δ 160.8, 138.9, 130.6, 129.6, 128.8, 127.8, 123.6, 115.2, 115.0, 55.7, 48.5, 43.8, 21.4; IR (film) 3026, 2932, 2841, 2249, 1608, 1586, 1513, 1458, 1303, 1257, 1185, 1115, 1033, 821, 796, 720, 709, 667, 585, 539, 519, 495, 466; HRMS (EI-TOF) calcd for C₁₈H₁₆N₂O, [M]⁺ *m/z* = 276.1263; found 276.1245.

General Procedure **B** was followed using 2-(4-methoxyphenyl)malononitrile (21.5 mg, 0.125 mmol), Pd(OAc)₂ (5.6 mg, 25.0 μmol), 2,6-dimethylbenzoquinone (17.0 mg, 0.125 mmol), PivOH (12.8 mg, 0.125 mmol), charcoal (56.1 mg, 10 x weight of Pd), and *p*-xylene (1.25 mL, 0.1 M). Chromatography (5% EtOAc/Hexanes) provided product **3ab** as a white solid (9.3 mg) in 27% yield. See above for characterization.



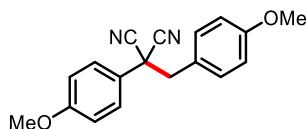
2-(4-Methoxyphenyl)-2-(3-methylbenzyl)malononitrile. General Procedure **A** was followed using 2-(4-methoxyphenyl)malononitrile (29.5 mg, 0.171 mmol) and Pd(OAc)₂ (38.5 mg, 0.171 mmol) in *m*-xylene (1.71 mL, 0.1 M) at 105 °C. Chromatography (5% EtOAc/Hexanes) provided product **3ac** as a white solid (27.9 mg) was isolated in 59% yield: ¹H NMR (500 MHz, CDCl₃) δ 7.37 (dt, *J*₁ = 8.9 Hz, *J*₂ = 2.1 Hz, 2H), 7.20 (t, *J* = 7.5 Hz, 1H), 7.16 (d, *J* = 7.7 Hz, 1H), 6.95 (m, 4H), 3.85 (s, 3H), 3.38 (s, 2H), 2.32 (s, 3H); ¹³C NMR (125 MHz, CDCl₃) δ 160.9, 138.6, 131.7, 131.4, 129.7, 128.7, 127.8, 127.7, 123.7, 115.2, 115.0, 55.7, 48.7, 43.6, 21.5; IR (film) 3014, 2935, 2850, 2249, 1609, 1585, 1510, 1464, 1442, 1421, 1305, 1258, 1184, 1032, 828, 788, 743, 721, 705, 611, 599, 585, 535; HRMS (EI-TOF) calcd for C₁₈H₁₆N₂O, [M]⁺ *m/z* = 276.1263; found 276.1254.

General Procedure **B** was followed using 2-(4-methoxyphenyl)malononitrile (20.7 mg, 0.120 mmol), Pd(OAc)₂ (5.4 mg, 24.0 μmol), 2,6-dimethylbenzoquinone (16.4 mg, 0.120 mmol), PivOH (12.3 mg, 0.120 mmol), charcoal (54.0 mg, 10 x weight of Pd), and *m*-xylene (1.20 mL, 0.1 M). Chromatography (5% EtOAc/Hexanes) provided product **3ac** as a white solid (21.7 mg) in 65% yield. See above for characterization.



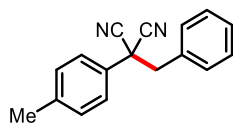
2-(4-Methoxyphenyl)-2-(2-methylbenzyl)malononitrile. General Procedure **A** was followed using 2-(4-methoxyphenyl)malononitrile (35.4 mg, 0.206 mmol) and Pd(OAc)₂ (46.2 mg, 0.206 mmol) in *o*-xylene (2.06 mL, 0.1 M) at 105 °C. Chromatography (5% EtOAc/Hexanes) provided product **3ad** as a white solid (34.7 mg) was isolated in 61% yield: ¹H NMR (500 MHz, CDCl₃) δ 7.34 (dt, *J*₁ = 8.9 Hz, *J*₂ = 2.2 Hz, 2H), 7.24 (dd, *J*₁ = 7.3 Hz, *J*₂ = 2.2 Hz, 1H), 7.18 (m, 3H), 6.93 (dt, *J*₁ = 8.9 Hz, *J*₂ = 2.2 Hz, 2H), 3.83 (s, 3H), 3.51 (s, 2H), 2.10 (s, 3H); ¹³C NMR (125 MHz, CDCl₃) δ 160.9, 138.1, 131.4, 131.1, 130.2, 129.0, 127.8, 126.4, 123.6, 115.4, 115.0, 55.7, 44.9, 43.0, 19.7; IR (film) 3022, 2917, 2849, 2324, 2248, 1609, 1512, 1463, 1303, 1260, 1185, 1032, 828, 772, 747, 729; HRMS (EI-TOF) calcd for C₁₈H₁₆N₂O, [M]⁺ *m/z* = 276.1263; found 276.1269.

General Procedure **B** was followed using 2-(4-methoxyphenyl)malononitrile (22.6 mg, 0.131 mmol), Pd(OAc)₂ (5.9 mg, 26.3 μmol), 2,6-dimethylbenzoquinone (17.9 mg, 0.131 mmol), PivOH (13.4 mg, 0.131 mmol), charcoal (58.9 mg, 10 x weight of Pd), and *o*-xylene (1.31 mL, 0.1 M). Chromatography (5% EtOAc/Hexanes) provided product **3ad** as a white solid (11.6 mg) in 32% yield. See above for characterization.

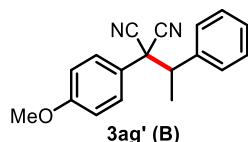
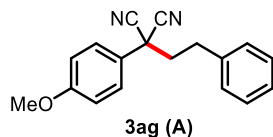


2-(4-Methoxybenzyl)-2-(4-methoxyphenyl)malononitrile. General Procedure **A** was followed using 2-(4-methoxyphenyl)malononitrile (26.2 mg, 0.152 mmol) and Pd(OAc)₂ (34.2 mg, 0.152 mmol) in *p*-methylanisole (1.52 mL, 0.1 M) at 95 °C. Chromatography (5% EtOAc/Hexanes) provided product **3ae** as a white solid (24.4 mg) was isolated in 55% yield: ¹H NMR (500 MHz, CDCl₃) δ 7.35 (d, *J* = 6.8 Hz, 2H), 7.04 (d, *J* = 6.7 Hz, 2H), 6.94 (d, *J* = 6.8 Hz, 2H), 6.83 (d, *J* = 6.7 Hz, 2H), 3.84 (s, 3H), 3.80 (s, 3H), 3.38 (s, 2H). Spectral data were in agreement with reported literature values.^{3a}

General Procedure **B** was followed using 2-(4-methoxyphenyl)malononitrile (19.6 mg, 0.114 mmol), Pd(OAc)₂ (5.1 mg, 22.8 μmol), 2,6-dimethylbenzoquinone (15.5 mg, 0.114 mmol), PivOH (11.6 mg, 0.114 mmol), charcoal (51.1 mg, 10 x weight of Pd), and *p*-methylanisole (1.14 mL, 0.1 M). Chromatography (5% EtOAc/Hexanes) provided product **3ae** as a white solid (32.4 mg) in 97 % yield. See above for characterization.



2-Benzyl-2-(*p*-tolyl)malononitrile. General Procedure **A** was followed using 2-(*p*-tolyl)malononitrile (32.0 mg, 0.204 mmol) and Pd(OAc)₂ (45.9 mg, 0.204 mmol) in toluene (2.04 mL, 0.1 M) at 95 °C. Chromatography (5% EtOAc/Hexanes) provided product **3ba** (43.0 mg) was isolated in 85% yield: ¹H NMR (500 MHz, CDCl₃) δ 7.33 (m, 5H), 7.25 (d, *J* = 8.4 Hz, 2H), 7.15 (d, *J* = 7.9 Hz, 2H), 3.43 (s, 2H), 2.40 (s, 3H); ¹³C NMR (125 MHz, CDCl₃) δ 140.3, 131.8, 130.6, 130.3, 128.9, 128.8, 128.7, 126.2, 114.9, 48.6, 43.9, 21.3; IR (film) 3032, 2928, 2855, 2252, 1509, 1496, 1456, 1236, 1089, 1017, 825, 809, 799, 764, 699, 572, 499, 477; HRMS (EI-TOF) calcd for C₁₇H₁₄N₂, [M]⁺ *m/z* = 246.1157; found 246.1154

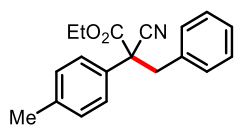


2-(4-Methoxyphenyl)-2-phenethylmalononitrile & 2-(4-methoxyphenyl)-2-(1-phenylethyl)malononitrile. General Procedure **A** was followed using 2-(4-methoxyphenyl)malononitrile (29.1 mg, 0.169 mmol) and Pd(OAc)₂ (37.9 mg, 0.169 mmol) in ethyl benzene (1.69 mL, 0.1 M) at 105 °C. Chromatography (5% EtOAc/Hexanes) provided products **3ag** and **3ag'** (34.9 mg combined, 1:3) were isolated in 75% yield: ¹H NMR (500 MHz, CDCl₃) δ 7.51 (dt, *J*₁ =

8.9 Hz, $J_2 = 2.2$ Hz, 2H_A), 7.27 (m, 3H_A, 3H_B), 7.22 (dt, $J_1 = 8.8$ Hz, $J_2 = 2.1$ Hz, 2H_B), 7.17 (d, $J = 6.9$ Hz, 2H_A), 7.11 (d, $J = 7.3$ Hz, 2H_B), 6.99 (dt, $J_1 = 8.8$ Hz, $J_2 = 2.2$ Hz, 2H_A), 6.87 (dt, $J_1 = 8.8$ Hz, $J_2 = 2.1$ Hz, 2H_B), 3.83 (s, 3H_A), 3.81 (s, 3H_B), 3.42 (q, $J = 7.1$ Hz, 1H_B), 2.91 (m, 2H_A), 2.47 (m, 2H_A), 1.63 (d, $J = 7.1$ Hz, 3H_B); ¹³C NMR (125 MHz, CDCl₃) δ A: 160.9, 138.5, 129.0, 128.9, 128.6, 127.1, 123.8, 115.3, 114.7, 55.7, 44.4, 41.7, 32.0 B: 160.7, 136.9, 128.9, 128.6, 128.5, 128.2, 127.3, 123.0, 114.6, 55.7, 51.2, 48.9, 16.9; IR (film) 3032, 2926, 2849, 2323, 2247, 1609, 1585, 1512, 1456, 1299, 1258, 1185, 1031, 829, 769, 701, 541; HRMS (EI-TOF) calcd for C₁₈H₁₆N₂O, [M]⁺ $m/z = 276.1263$; found 276.1248. General Procedure **B** was followed using 2-(4-methoxyphenyl)malononitrile (22.1 mg, 0.128 mmol), Pd(OAc)₂ (5.8 mg, 25.7 μmol), 2,6-dimethylbenzoquinone (17.4 mg, 0.128 mmol), PivOH (13.1 mg, 0.128 mmol), charcoal (57.6 mg, 10 x weight of Pd), and ethylbenzene (1.28 mL, 0.1 M). Chromatography (5% EtOAc/Hexanes) provided product as a white solid (18.8 mg 3:1) in 53% yield. See above for characterization.

General Procedure C – Alkylation of Cyanoacetate with Stoichiometric Pd in 1,4-Dioxane. The cyanoacetate **4** (0.098 mmol) and Pd(OAc)₂ (22.1 mg, 0.098 mmol) were added to a flame dried 8 mL microwave vial equipped with a stirbar and were brought into the glovebox. The indicated tolyl analog (1.96 mmol) and 1,4-dioxane (328 μL, 0.3 M) were added to the mixture. The microwave vial was sealed with a Teflon cap, removed from the glovebox and placed in a 95 °C oil bath. After 24 h, the mixture was allowed to cool to ambient temperature, diluted with CH₂Cl₂ (5 mL), passed through SiO₂ with 30% EtOAc/hexanes, and concentrated. The residue was chromatographed to afford the alkylated cyanoarylacacetate derivative.

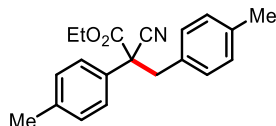
General Procedure D – Alkylation with Catalytic Pd in 1,4-Dioxane. The cyanoacetate **4** (0.098 mmol), Pd(OAc)₂ (4.4 mg, 0.0196 mmol), AcOH (5.9 mg, 0.098 mmol), K₂S₂O₈ (25.6 mg, 0.098 mmol), and activated carbon (44.0 mg, 10 x weight of Pd) were added to a flame dried 8 mL microwave vial equipped with a stirbar and were brought into the glovebox. The indicated tolyl analog (1.96 mmol) was added to the mixture followed by 1,4-dioxane (328 μL, 0.3 M). The microwave vial was sealed with a Teflon cap, removed from the glovebox, and placed in a 120 °C oil bath. After 45 h, the mixture was allowed to cool to ambient temperature, diluted with CH₂Cl₂ (5 mL), passed through SiO₂ with 30% EtOAc/hexanes, and concentrated. Chromatography afforded the alkylated cyanoarylacacetate derivative.



Ethyl 2-cyano-3-phenyl-2-(p-tolyl)propanoate. General procedure **C** was followed with **4a** (20 mg, 0.098 mmol), and Pd(OAc)₂ (22.1 mg, 0.098 mmol), toluene (210 μL, 1.96 mmol), and 1,4-dioxane (380 μL, 0.3 M). Chromatography (5% EtOAc/hexanes) afforded **5aa** (23.3 mg) in 81% yield. ¹H NMR (500 MHz, Chloroform-*d*) δ 7.43 (d, $J = 8.3$ Hz, 2H), 7.26 (m, 3H), 7.23-7.15 (m, 4H), 4.27-4.14 (m, 2H), 3.69 (d, $J = 13.7$ Hz, 1H), 3.31 (d, $J = 13.5$ Hz, 1H), 2.37 (s, 3H), 1.20 (t, $J = 7.1$ Hz, 3H); ¹³C NMR (125 MHz, Chloroform-*d*) δ 167.6, 139.0, 134.4, 131.6, 130.5, 129.9, 128.4, 127.8, 126.3, 118.3, 63.4, 55.6, 44.2, 21.2, 13.9; IR (film) 2981, 2923, 2249, 1739, 1512, 1497, 1455, 1297, 1248, 1222, 1090, 1037,

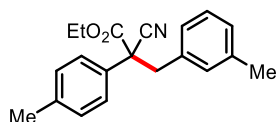
1022, 857, 834, 804, 765, 749, 730, 699, 649, 512, 483 cm^{-1} ; HRMS (ESI-TOF) calcd for $\text{C}_{19}\text{H}_{19}\text{NO}_2\text{Na}$ $[\text{M}+\text{Na}]^+$ $m/z = 316.1313$; found = 316.1312.

General procedure **D** was followed with **4a** and toluene. Chromatography (5% EtOAc/hexanes) provided **5aa** (22.8 mg) in 79% yield. See above for characterization.



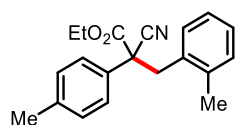
Ethyl 2-cyano-2,3-di-*p*-tolylpropanoate. General procedure **C** was followed with **4a** and *para*-xylene. Chromatography (eluent 5% EtOAc/hexanes) provided **5ab** (11.5 mg) in 38% yield: ¹H NMR (500 MHz, Chloroform-*d*) δ 7.45-7.41 (m, 2H), 7.22-7.18 (m, 2H), 7.06 (s, 4H), 4.26-4.13 (m, 2H), 3.65 (d, $J = 13.6$ Hz, 1H), 3.25 (d, $J = 13.7$ Hz, 1H), 2.36 (s, 3H), 2.30 (s, 3H), 1.19 (t, $J = 7.1$ Hz, 3H); ¹³C NMR (125 MHz, Chloroform-*d*) δ 167.7, 139.0, 137.5, 131.7, 131.3, 130.4, 129.8, 129.1, 126.3, 118.3, 63.3, 55.8, 43.9, 21.3, 21.2, 13.9; IR (film) 2981, 2925, 2249, 1740, 1513, 1445, 1367, 1296, 1246, 1223, 1214, 1194, 1114, 1094.98, 1039, 1022, 858, 818, 734, 714, 648, 632, 508 cm^{-1} ; HRMS (ESI-TOF) calcd for $\text{C}_{20}\text{H}_{21}\text{NO}_2\text{Na}$, $[\text{M}+\text{Na}]^+$ $m/z = 330.1470$; found = 330.1469.

General procedure **D** was followed with ethyl 2-cyano-2-(*p*-tolyl)acetate and *para*-xylene. Chromatography (5% EtOAc/hexanes) provided **5ab** (14.5 mg) in 48% yield. See above for characterization.



Ethyl 2-cyano-3-(*m*-tolyl)-2-(*p*-tolyl)propanoate. General procedure **C** was followed with ethyl 2-cyano-2-(*p*-tolyl)acetate **4a** and *meta*-xylene. Chromatography (5% EtOAc/hexanes) to provided **5ac** (51.0 mg) in 69% yield: ¹H NMR (500 MHz, Chloroform-*d*) δ 7.47-7.41 (m, 2H), 7.23-7.18 (m, 2H), 7.14 (t, $J = 7.6$ Hz, 1H), 7.10-7.05 (m, 1H), 7.01-6.94 (m, 2H), 4.27-4.13 (m, 2H), 3.66 (d, $J = 13.5$ Hz, 1H), 3.25 (d, $J = 13.5$ Hz, 1H), 2.37 (s, 3H), 2.29 (s, 3H), 1.20 (t, $J = 7.1$ Hz, 3H); ¹³C NMR (125 MHz, Chloroform-*d*) δ 167.7, 139.0, 138.0, 134.3, 131.7, 131.3, 129.8, 128.6, 128.3, 127.5, 126.3, 118.3, 63.3, 55.6, 44.2, 21.5, 21.2, 13.9; IR (film) 2981, 2924, 2249, 1740, 1511, 1488, 1445, 1367, 1298, 1214, 1195, 1129, 1096, 1040, 1022, 855, 809, 787, 737, 702, 510 cm^{-1} ; HRMS(ESI) calcd for $\text{C}_{20}\text{H}_{21}\text{NO}_2\text{Na}$, $[\text{M}+\text{Na}]^+$ $m/z = 330.1470$; found = 330.1475.

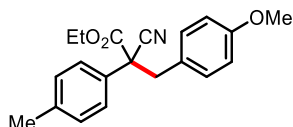
General procedure **D** was followed with ethyl 2-cyano-2-(*p*-tolyl)acetate and *meta*-xylene. Chromatography (5% EtOAc/hexanes) provided **5ac** (20.5 mg) in 68% yield. See above for characterization.



Ethyl 2-cyano-3-(*o*-tolyl)-2-(*p*-tolyl)propanoate. General procedure **C** was followed with ethyl 2-cyano-2-(*p*-tolyl)acetate **4a** and *ortho*-xylene. Chromatography (5% EtOAc/hexanes) provided **5ad** (18.5 mg) in 61% yield: ¹H NMR (500 MHz, Chloroform-*d*) δ 7.42-7.36 (m, 2H), 7.22-7.18 (m, 2H), 7.18-

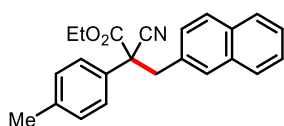
7.11 (m, 2H), 7.11-7.03 (m, 2H), 4.32-4.19 (m, 2H), 3.73 (d, $J = 14.2$ Hz, 1H), 3.40 (d, $J = 14.2$ Hz, 1H), 2.37 (s, 3H), 2.21 (s, 3H), 1.23 (t, $J = 7.1$ Hz, 3H); ^{13}C NMR (125 MHz, Chloroform- d) δ 168.0, 139.0, 137.9, 132.9, 132.0, 130.8, 130.3, 129.8, 127.8, 126.4, 125.9, 118.4, 63.5, 54.8, 40.4, 21.2, 20.0, 14.0; IR (film) 2925, 2249, 1740, 1511, 1496, 1446, 1382, 1367, 1295, 1223, 1116, 1094, 1055, 1033, 857, 809, 763, 737, 649, 533, 515 cm^{-1} ; HRMS (ESI-TOF) calcd for $\text{C}_{20}\text{H}_{21}\text{NO}_2\text{Na}$, $[\text{M}+\text{Na}]^+ m/z = 330.1470$; found = 330.1467.

General procedure **D** was followed with ethyl 2-cyano-2-(*p*-tolyl)acetate and *ortho*-xylene. Chromatography (5% EtOAc/hexanes) provided **5ad** (18.7 mg) in 62% yield. See above for characterization.



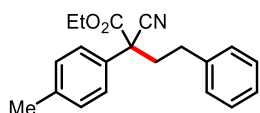
Ethyl 2-cyano-3-(4-methoxyphenyl)-2-(*p*-tolyl)propanoate. General procedure **C** was followed using ethyl 2-cyano-2-(*p*-tolyl)acetate **4a** and 1-methylanisole. Chromatography (8% EtOAc/hexanes) provided **5ae** (13.3 mg) in 42% yield as a solid: ^1H NMR (500 MHz, Chloroform- d) δ 7.42 (d, $J = 8.3$ Hz, 2H), 7.20 (d, $J = 8.1$ Hz, 2H), 7.13-7.04 (m, 2H), 6.78 (d, $J = 8.6$ Hz, 2H), 4.20 (m, 2H), 3.78 (s, 3H), 3.63 (d, $J = 13.7$ Hz, 1H), 3.24 (d, $J = 13.7$ Hz, 1H), 2.36 (s, 3H), 1.20 (t, $J = 7.1$ Hz, 3H); ^{13}C NMR (125 MHz, Chloroform- d) δ 167.7, 159.2, 139.0, 131.6, 129.8, 126.4, 126.3, 118.4, 113.8, 77.4, 63.3, 55.9, 55.3, 43.5, 21.2, 14.0; IR (film) 2925, 2249, 1736, 1512, 1464, 1453, 1445, 1303, 1249, 1214, 1198, 1177, 1116, 1047, 1030, 1005, 847, 826, 813, 750, 523, 513 cm^{-1} ; HRMS(ESI-TOF) calcd for $\text{C}_{20}\text{H}_{22}\text{NO}_3$, $[\text{M}+\text{H}]^+ m/z = 324.1600$; found = 324.1600; Melting point 72-75 $^\circ\text{C}$.

General procedure **D** was followed with ethyl 2-cyano-2-(*p*-tolyl)acetate (20 mg, 0.078 mmol), $\text{Pd}(\text{OAc})_2$ (3.5 mg, 0.015 mmol), AcOH (4.7 mg, 0.078 mmol), $\text{K}_2\text{S}_2\text{O}_8$ (21.1 mg, 0.078 mmol), activated carbon (35 mg, 10x weight of Pd), 1-methylanisole (250 μL , 1.56 mmol), and 1,4-dioxane (380 μL , 0.3 M). Chromatography (5% EtOAc/hexanes) provided **5ae** (2.8 mg) in 9% yield. See above for characterization.



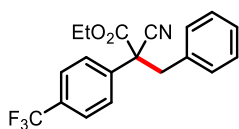
Ethyl 2-cyano-3-(naphthalen-2-yl)-2-(*p*-tolyl)propanoate. General procedure **C** was followed with ethyl 2-cyano-2-(*p*-tolyl)acetate **4a** and 2-methylnaphthalene. Chromatography (5% EtOAc/hexanes) provided **5af** (22.7 mg) in 67% yield: ^1H NMR (500 MHz, Chloroform- d) δ 7.78 (m, 2H), 7.73 (d, $J = 8.4$ Hz, 1H), 7.69 (d, $J = 1.7$ Hz, 1H), 7.50-7.42 (m, 3H), 7.29-7.25 (m, 2H), 7.21 (d, $J = 8.0$ Hz, 2H), 4.29-4.13 (m, 2H), 3.86 (d, $J = 13.6$ Hz, 1H), 3.47 (d, $J = 13.6$ Hz, 1H), 2.38 (s, 3H), 1.18 (t, $J = 7.1$ Hz, 3H); ^{13}C NMR (125 MHz, Chloroform- d) δ 167.6, 139.1, 133.3, 132.9, 131.9, 131.6, 129.9, 129.7, 128.3, 128.1, 128.0, 127.7, 126.4, 126.2, 126.1, 118.3, 63.4, 55.7, 44.4, 21.2, 13.9; IR (film) 2981, 2249, 1739, 1510, 1444, 1367, 1289, 1221, 1195, 1157, 1127, 1094, 1040, 1021, 896, 856, 818, 749, 667, 512, 476 cm^{-1} ; HRMS (ESI-TOF) calcd $\text{C}_{23}\text{H}_{21}\text{NO}_2\text{Na}$, $[\text{M}+\text{Na}]^+ m/z = 366.1470$; found = 366.1473.

General procedure **D** was followed with ethyl 2-cyano-2-(*p*-tolyl)acetate and 2-methylnaphthalene. Chromatography (5% EtOAc/hexanes) provided **5af** (22.3 mg) in 66% yield. See above for characterization.

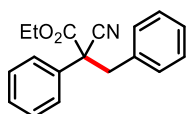


Ethyl 2-cyano-4-phenyl-2-(*p*-tolyl)butanoate. General procedure **C** was followed with ethyl 2-cyano-2-(*p*-tolyl)acetate **4a** and ethylbenzene. Chromatography (8% EtOAc/hexanes) provided **5ag** (9.98 mg) in 33% yield as a colorless liquid: $^1\text{H NMR}$ (500 MHz, Chloroform-*d*) δ 7.48-7.43 (m, 2H), 7.28 (dd, $J = 8.2, 6.8$ Hz, 2H), 7.25-7.17 (m, 5H), 4.27-4.18 (m, 2H), 2.84-2.60 (m, 4H), 2.36 (s, 3H), 1.28-1.23 (m, 3H); $^{13}\text{C NMR}$ (125 MHz, Chloroform-*d*) δ 167.7, 140.2, 139.0, 131.6, 130.0, 128.7, 128.6, 126.5, 126.1, 118.6, 63.4, 53.9, 40.1, 32.0, 21.2, 14.0; IR (film) 2926, 2249, 1741, 1511, 1497, 1454, 1367, 1294, 1231, 1194, 1129, 1095, 1020, 968, 857, 813, 750, 736, 699, 557, 516 cm^{-1} ; HRMS (ESI-TOF) calcd $\text{C}_{20}\text{H}_{22}\text{NO}_2$ $[\text{M}+\text{H}]^+$ $m/z = 308.1651$ found = 308.1653.

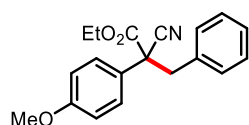
General procedure **D** was followed with ethyl 2-cyano-2-(*p*-tolyl)acetate and ethyl benzene. Chromatography (8% EtOAc/hexanes) provided **5ag** (4.23 mg) in 14% yield as a colorless liquid. See above for characterization.



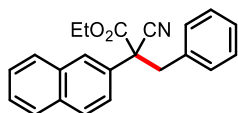
Ethyl 2-cyano-3-phenyl-2-(4-(trifluoromethyl)phenyl)propanoate. General procedure **D** was followed with **4b** (20 mg, 0.078 mmol), $\text{Pd}(\text{OAc})_2$ (3.5 mg, 0.015 mmol), AcOH (4.7 mg, 0.078 mmol), $\text{K}_2\text{S}_2\text{O}_8$ (21.1 mg, 0.078 mmol), activated carbon (35 mg, 10 x weight of Pd), toluene (166 μL , 1.56 mmol), and 1,4-dioxane (260 μL , 0.3 M). Chromatography (5% EtOAc/hexanes) provided **5ba** (46.5 mg) in 69% yield. $^1\text{H NMR}$ (500 MHz, Chloroform-*d*) δ 7.72-7.64 (m, 4H), 7.30-7.23 (m, 3H), 7.18-7.11 (m, 2H), 4.30-4.17 (m, 2H), 3.72 (d, $J = 13.7$ Hz, 1H), 3.33 (d, $J = 13.7$ Hz, 1H), 1.21 (t, $J = 7.1$ Hz, 3H); $^{13}\text{C NMR}$ (125 MHz, Chloroform-*d*) δ 166.9, 138.2, 133.5, 131.2, 130.4, 128.6, 128.1, 127.1, 124.0 (q, $J_{\text{C-F}} = 270.1$ Hz), 117.5, 77.4, 63.9, 55.8, 44.4, 13.9; IR (film) 2983, 2249, 1743, 1414, 1325, 1301, 1249, 1223, 1168, 1121, 1090, 1070, 1037, 1018, 846, 818, 743, 723, 700, 683, 628, 600 cm^{-1} ; HRMS (ESI-TOF) calcd for $\text{C}_{19}\text{H}_{16}\text{F}_3\text{NO}_2\text{Na}$, $[\text{M}+\text{Na}]^+$ $m/z = 370.1031$; found = 370.1034.



Ethyl 2-cyano-2,3-diphenylpropanoate. General procedure **D** was followed with **4c** (20 mg, 0.105 mmol), $\text{Pd}(\text{OAc})_2$ (4.75 mg, 0.0211 mmol), AcOH (6.34 mg, 0.105 mmol), $\text{K}_2\text{S}_2\text{O}_8$ (28.6 mg, 0.105 mmol), activated carbon (48 mg, 10 x weight of Pd), toluene (225 μL , 2.11 mmol), and 1,4-dioxane (352 μL , 0.3 M). Chromatography (5% EtOAc/hexanes) provided **5ca** (17.1 mg) in 58% yield. $^1\text{H NMR}$ (500 MHz, Chloroform-*d*) δ 7.58-7.51 (m, 2H), 7.44-7.35 (m, 3H), 7.26 (m, 3H), 7.20-7.13 (m, 2H), 4.28-4.16 (m, 2H), 3.70 (d, $J = 13.6$ Hz, 1H), 3.33 (d, $J = 13.6$ Hz, 1H), 1.21 (d, $J = 7.1$ Hz, 3H); $^{13}\text{C NMR}$ (125 MHz, Chloroform-*d*) δ 167.5, 134.5, 134.2, 130.5, 129.2, 129.1, 128.4, 127.9, 126.5, 118.1, 63.4, 55.9, 44.3, 13.9; IR (film) 2925, 2250, 1739, 1497, 1497, 1297, 1297, 1219, 1094, 1082, 1034, 1004, 856, 771, 747, 729, 695, 635, 611, 569, 507, 486 cm^{-1} ; HRMS (ESI-TOF) calcd for $\text{C}_{18}\text{H}_{18}\text{NO}_2$, $[\text{M}+\text{H}]^+$ $m/z = 280.1338$; found = 280.1344.



Ethyl 2-cyano-2-(4-methoxyphenyl)-3-phenylpropanoate. General procedure **D** was followed with **4d** (20 mg, 0.091 mmol), Pd(OAc)₂ (4.1 mg, 0.0182 mmol), AcOH (5.46 mg, 0.091 mmol), K₂S₂O₈ (24.5 mg, 0.091 mmol), activated carbon (41 mg, 10 x weight of Pd), toluene (194 μ L, 1.82 mmol), and 1,4-dioxane (304 μ L, 0.3 M). Chromatography (5% EtOAc/hexanes) provided **5da** (17.5 mg) in 62% yield. ¹H NMR (500 MHz, Chloroform-*d*) δ 7.49-7.43 (m, 2H), 7.26 (m, 3H), 7.17 (m, 2H), 6.94-6.88 (m, 2H), 4.20 (m, 2H), 3.82 (s, 3H), 3.67 (d, *J* = 13.6, 1H), 3.30 (d, *J* = 13.6 Hz, 1H), 1.20 (t, *J* = 7.1, 1.9 Hz, 3H); ¹³C NMR (125 MHz, Chloroform-*d*) δ 167.7, 160.0, 134.3, 130.5, 128.4, 127.8, 127.8, 126.4, 118.1, 114.5, 63.3, 55.5, 55.2, 44.3, 13.9; IR (film) 2930, 2249, 1738, 1608, 1510, 1455, 1443, 1297, 1251, 1220, 1184, 1090, 1030, 856, 835, 807, 751, 734, 700, 635, 530, 485 cm⁻¹; HRMS(ESI) calcd for C₁₉H₁₉NO₃Na [M+Na]⁺ *m/z* = 332.1263; found = 332.1260.

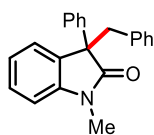


Ethyl 2-cyano-2-(naphthalen-2-yl)-3-phenylpropanoate. General procedure **D** was followed with **4e** (20 mg, 0.083 mmol), Pd(OAc)₂ (3.75 mg, 0.0167 mmol), AcOH (5.0 mg, 0.083 mmol), K₂S₂O₈ (22.5 mg, 0.083 mmol), activated carbon (38 mg, 10x weight of Pd), toluene (190 μ L, 1.67 mmol), and 1,4-dioxane (280 μ L, 0.3 M). Chromatography (5% EtOAc/hexanes) provided **5ea** (17.3 mg) in 63% yield. ¹H NMR (500 MHz, Chloroform-*d*) δ 8.02 (d, *J* = 2.0 Hz, 1H), 7.93-7.83 (m, 3H), 7.66 (dd, *J* = 8.7, 2.1 Hz, 1H), 7.58-7.51 (m, 2H), 7.29-7.16 (m, 5H), 4.30-4.17 (m, 2H), 3.81 (d, *J* = 13.7 Hz, 1H), 3.45 (d, *J* = 13.7 Hz, 1H), 1.20 (t, *J* = 7.1 Hz, 3H); ¹³C NMR (125 MHz, Chloroform-*d*) δ 167.5, 134.2, 133.2, 133.1, 131.6, 130.5, 129.2, 128.5, 128.5, 127.9, 127.8, 127.2, 127.0, 126.4, 123.3, 118.2, 63.5, 56.1, 44.1, 14.0; IR (film) 2982, 2249, 1739, 1497, 1454, 1366, 1296, 1218, 1126, 1091, 1036, 1004, 895, 860, 814, 773, 744, 719, 699, 654, 632, 476 cm⁻¹; HRMS (ESI-TOF) calcd for C₂₂H₁₉NO₂Na [M+Na]⁺ *m/z* = 352.1313 found; 352.1308.

General Procedure E – Alkylation of Oxindoles with Stoichiometric Pd in Neat Tolylyl Substrate. Oxindole (0.15 mmol) and Pd(OAc)₂ (50.5 mg, 0.225 mmol) were added to a flame-dried 8 mL microwave vial equipped with a stir bar and brought into the glovebox. The indicated tolylyl analog (0.1 M, 1.5 mL) was added to the mixture. The microwave vial was sealed with a Teflon cap, removed from the glovebox, and placed in a 120 °C oil bath. After 24 h, the mixture was allowed to cool to ambient temperature, diluted with CH₂Cl₂ (1 mL), passed through celite with CH₂Cl₂, and concentrated. The residue was chromatographed (EtOAc/hexanes) to afford the desired product.

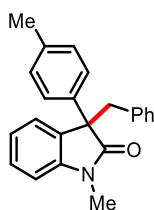
General Procedure F - Alkylation of Oxindoles with Catalytic Pd in Neat Tolylyl Substrate. Oxindole (0.15 mmol), Pd(OAc)₂ (6.7 mg, 0.03 mmol), K₂S₂O₈ (81.0 mg, 0.3 mmol), PivOH (15.3 mg, 0.15 mmol) and activated charcoal (67 mg, 10x weight of Pd) were added to a flame-dried 8 mL microwave vial equipped with a stir bar and brought into the glovebox. The indicated tolylyl analog (0.1 M, 1.5 mL) was added to the mixture. The microwave vial was sealed with a Teflon cap, removed from the glovebox, and

placed in a 120 °C oil bath. After 24 h, the mixture was allowed to cool to ambient temperature, diluted with CH₂Cl₂ (1 mL), passed through celite with CH₂Cl₂, and concentrated. The residue was chromatographed (EtOAc/hexanes) to afford the desired product.



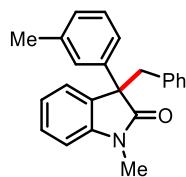
3-Benzyl-1-methyl-3-phenylindolin-2-one. General procedure **E** was followed using **6a** (33.4 mg, 0.15 mmol) and Pd(OAc)₂ (50.5 mg, 0.225 mmol) in toluene (1.5 mL, 0.1 M) at 120 °C for 24 h. Chromatography (6% EtOAc/hexanes) provided **7aa** (46.1 mg) in 98% yield as a white solid: ¹H NMR (500 MHz, CDCl₃) δ 7.51 (d, *J* = 9.5 Hz, 2H), 7.38-7.27 (m, 3H), 7.24-7.19 (m, 2H), 7.10-6.98 (m, 4H), 6.84 (d, *J* = 8.5 Hz, 2H), 6.61 (d, *J* = 12.0 Hz, 1H), 3.72 (d, *J* = 15.0 Hz, 1H), 3.46 (d, *J* = 15.0 Hz, 1H), 2.95 (s, 3H); HRMS (EI-TOF) calcd for C₂₂H₁₉NO [M]⁺ *m/z* = 313.1467; found 313.1469. Spectral data match those previously reported.⁶

General procedure **F** was followed using **6a** (33.4 mg, 0.15 mmol), Pd(OAc)₂ (6.7 mg, 0.03 mmol), K₂S₂O₈ (81.0 mg, 0.3 mmol), PivOH (15.3 mg, 0.15 mmol) and activated charcoal (67 mg, 10x weight of Pd) in toluene (1.5 mL, 0.1 M) at 120 °C for 24 h. Chromatography (6% EtOAc/hexanes) provided **7aa** (44.7 mg) in 96% yield. See above for characterization.



3-Benzyl-1-methyl-3-(p-tolyl)indolin-2-one. General procedure **E** was followed using **6b** (35.6 mg, 0.15 mmol) and Pd(OAc)₂ (50.5 mg, 0.225 mmol) in toluene (1.5 mL, 0.1 M) at 120 °C for 24 h. Chromatography (6% EtOAc/hexanes) provided **7ba** (45.7 mg) in 93% yield as a white solid: ¹H NMR (500 MHz, CDCl₃) δ 7.39 (d, *J* = 11.5 Hz, 2H), 7.24-7.15 (m, 4H), 7.10-6.99 (m, 4H), 6.85 (d, *J* = 8.5 Hz, 2H), 6.60 (d, *J* = 10.5 Hz, 1H), 3.71 (d, *J* = 18.0 Hz, 1H), 3.44 (d, *J* = 18.0 Hz, 1H), 2.95 (s, 3H), 2.34 (s, 3H); HRMS (EI-TOF) calcd for C₂₃H₂₁NO [M]⁺ *m/z* = 327.1623; found 327.1645. Spectral data match those previously reported.⁶

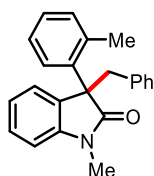
General procedure **F** was followed using **6b** (35.6 mg, 0.15 mmol), Pd(OAc)₂ (6.7 mg, 0.03 mmol), K₂S₂O₈ (81.0 mg, 0.3 mmol), PivOH (15.3 mg, 0.15 mmol) and activated charcoal (15.9 mg, 10x weight of Pd) in toluene (1.5 mL, 0.1 M) at 120 °C for 24 h. Chromatography (6% EtOAc/hexanes) provided **7ba** (45.7 mg) in 93% yield. See above for characterization.



3-Benzyl-1-methyl-3-(m-tolyl)indolin-2-one. General procedure **E** was followed using **6c** (35.6 mg, 0.15 mmol) and Pd(OAc)₂ (50.5 mg, 0.225 mmol) in toluene (1.5 mL, 0.1 M) at 120 °C for 24 h. Chromatography (6% EtOAc/hexanes) provided **7ca** (43.2 mg) in 88% yield as a white solid: ¹H NMR

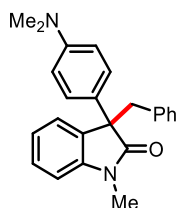
(500 MHz, CDCl₃) δ 7.30 (s, 1H), 7.25-7.19 (m, 4H), 7.10-6.97 (m, 5H), 6.82 (d, J = 6.5 Hz, 2H), 6.58 (d, J = 7.5 Hz, 1H), 3.70 (d, J = 12.5 Hz, 1H), 3.43 (d, J = 12.5 Hz, 1H), 2.93 (s, 3H), 2.33 (s, 3H); ¹³C NMR (125 MHz, CDCl₃) δ 177.9, 143.9, 139.9, 138.3, 135.9, 131.7, 130.1, 128.7, 128.4, 128.2, 128.0, 127.5, 126.7, 125.5, 124.4, 122.3, 108.1, 58.4, 44.0, 26.2, 21.8; IR (film) 3030, 2922, 1710, 1611, 1493, 1470, 1373, 1349, 1256, 1127, 1088, 1022, 754, 699 cm⁻¹; HRMS (EI-TOF) calcd for C₂₃H₂₁NO [M]⁺ m/z = 327.1623; found 327.1638.

General procedure **F** was followed using **6c** (35.6 mg, 0.15 mmol), Pd(OAc)₂ (6.7 mg, 0.03 mmol), K₂S₂O₈ (81.0 mg, 0.3 mmol), PivOH (15.3 mg, 0.15 mmol) and activated charcoal (67 mg, 10x weight of Pd) in toluene (1.5 mL, 0.1 M) at 120 °C for 24 h. Chromatography (6% EtOAc/hexanes) provided **7ca** (32.9 mg) in 67% yield. See above for characterization.



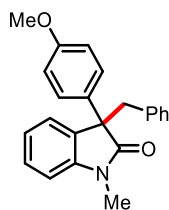
3-Benzyl-1-methyl-3-(o-tolyl)indolin-2-one. General procedure **E** was followed using **6d** (35.6 mg, 0.15 mmol) and Pd(OAc)₂ (50.5 mg, 0.225 mmol) in toluene (1.5 mL, 0.1 M) at 120 °C for 24 h. Chromatography (6% EtOAc/hexanes) provided **7da** (22.1 mg) in 45% yield as a pale yellow solid: ¹H NMR (500 MHz, CDCl₃) δ 7.81 (d, J = 10.5 Hz, 1H), 7.35 (td, J = 10.5, 1.5 Hz, 1H), 7.27-7.15 (m, 2H), 7.10-6.97 (m, 6H), 6.67 (d, J = 10.0 Hz, 2H), 6.45 (d, J = 10.5 Hz, 1H), 3.70 (d, J = 16.0 Hz, 1H), 3.54 (d, J = 16.0 Hz, 1H), 2.78 (s, 3H), 1.66 (s, 3H); ¹³C NMR (125 MHz, CDCl₃) δ 177.5, 143.8, 137.9, 137.1, 134.6, 132.0, 131.9, 129.9, 127.9, 127.5, 127.1, 126.9, 126.5, 125.9, 123.3, 122.5, 107.3, 57.8, 44.1, 25.5, 19.4; IR (film) 2928, 1713, 1611, 1493, 1469, 1347, 1252, 1089, 750, 700 cm⁻¹; HRMS (EI-TOF) calcd for C₂₃H₂₁NO [M]⁺ m/z = 327.1623; found 327.1615.

General procedure **F** was followed using **6d** (35.6 mg, 0.15 mmol), Pd(OAc)₂ (6.7 mg, 0.03 mmol), K₂S₂O₈ (81.0 mg, 0.3 mmol), PivOH (15.3 mg, 0.15 mmol) and activated charcoal (67 mg, 10x weight of Pd) in toluene (1.5 mL, 0.1 M) at 120 °C for 24 h. Chromatography (6% EtOAc/hexanes) provided **7da** (15.7 mg) in 32% yield. See above for characterization.



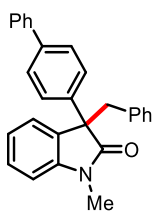
3-Benzyl-3-(4-(dimethylamino)phenyl)-1-methylindolin-2-one. General procedure **E** was followed using **6e** (39.9 mg, 0.15 mmol) and Pd(OAc)₂ (50.5 mg, 0.225 mmol) in toluene (1.5 mL, 0.1 M) at 120 °C for 24 h. Chromatography (8% EtOAc/hexanes) provided **7ea** (26.7 mg) in 50% yield as a white solid: ¹H NMR (500 MHz, CDCl₃) δ 7.36 (d, J = 9.0 Hz, 2H), 7.22-7.18 (m, 2H), 7.08- 7.00 (m, 4H), 6.85 (d, J = 6.5 Hz, 2H), 6.70 (d, J = 9.0 Hz, 2H), 6.59 (d, J = 7.5 Hz, 1H), 3.68 (d, J = 12.5 Hz, 1H), 3.41 (d, J = 12.5 Hz, 1H), 2.94 (s, 3H), 2.93 (s, 6H); ¹³C NMR (125 MHz, CDCl₃) δ 178.4, 149.9, 143.9, 136.2, 131.8, 130.2, 128.1, 128.0, 127.5, 126.5, 125.6, 122.1, 112.7, 107.9, 100.1, 57.6, 44.2, 40.7, 26.1; IR (film) 2922, 1710, 1610, 1520, 1493, 1470, 1372, 1349, 1126, 1088, 753, 700 cm⁻¹; HRMS (EI-TOF) calcd for C₂₄H₂₄N₂O [M]⁺ m/z = 356.1889; found 356.1891.

General procedure **F** was followed using **6e** (39.9 mg, 0.15 mmol), Pd(OAc)₂ (6.7 mg, 0.03 mmol), K₂S₂O₈ (81.0 mg, 0.3 mmol), PivOH (15.3 mg, 0.15 mmol) and activated charcoal (67 mg, 10x weight of Pd) in toluene (1.5 mL, 0.1 M) at 120 °C for 24 h. Chromatography (8% EtOAc/hexanes) provided **7ea** (3.2 mg) in 6% yield. See above for characterization.



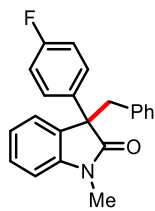
3-Benzyl-3-(4-methoxyphenyl)-1-methylindolin-2-one. General procedure **E** was followed using **6f** (38.0 mg, 0.15 mmol) and Pd(OAc)₂ (50.5 mg, 0.225 mmol) in toluene (1.5 mL, 0.1 M) at 120 °C for 24 h. Chromatography (9% EtOAc/hexanes) provided **7fa** (49.9 mg) in 97% yield as a pale yellow solid: ¹H NMR (500 MHz, CDCl₃) δ 7.43 (d, *J* = 12.5 Hz, 2H), 7.24-7.18 (m, 2H), 7.08-7.01 (m, 4H), 6.90-6.82 (m, 4H), 6.61 (d, *J* = 11.0 Hz, 1H), 3.79 (s, 3H), 3.67 (d, *J* = 17.5 Hz, 1H), 3.42 (d, *J* = 17.5 Hz, 1H), 2.95 (s, 3H); HRMS (EI-TOF) calcd for C₂₃H₂₁NO₂ [M]⁺ *m/z* = 343.1572; found 343.1570. Spectral data match those previously reported.⁷

General procedure **F** was followed using **6f** (38.0 mg, 0.15 mmol), Pd(OAc)₂ (6.7 mg, 0.03 mmol), K₂S₂O₈ (81.0 mg, 0.3 mmol), PivOH (15.3 mg, 0.15 mmol) and activated charcoal (67 mg, 10x weight of Pd) in toluene (1.5 mL, 0.1 M) at 120 °C for 24 h. Chromatography (9% EtOAc/hexanes) provided **7fa** (37.6 mg) in 73% yield. See above for characterization.



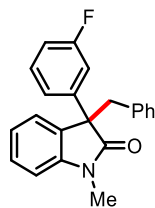
3-((1,1'-Biphenyl)-4-yl)-3-benzyl-1-methylindolin-2-one. General procedure **E** was followed using **6g** (44.9 mg, 0.15 mmol) and Pd(OAc)₂ (50.5 mg, 0.225 mmol) in toluene (1.5 mL, 0.1 M) at 120 °C for 24 h. Chromatography (7% EtOAc/hexanes) provided **7ga** (57.3 mg) in 98% yield as a white solid: ¹H NMR (500 MHz, CDCl₃) δ 7.62-7.60 (m, 6H), 7.47 (t, *J* = 7.5 Hz, 2H), 7.40-7.35 (m, 1H), 7.31-7.25 (m, 2H), 7.16-7.04 (m, 4H), 6.89 (d, *J* = 6.5 Hz, 2H), 6.67 (d, *J* = 8.0 Hz, 1H), 3.79 (d, *J* = 13.0 Hz, 1H), 3.52 (d, *J* = 13.0 Hz, 1H), 3.00 (s, 3H); ¹³C NMR (125 MHz, CDCl₃) δ 177.9, 143.9, 140.9, 140.5, 138.9, 135.8, 131.4, 130.2, 128.9, 128.4, 127.9, 127.6, 127.5, 127.2, 126.7, 125.7, 122.4, 108.2, 58.3, 44.2, 26.2; IR (film) 2922, 1711, 1611, 1491, 1371, 1098, 754, 699 cm⁻¹; HRMS (EI-TOF) calcd for C₂₈H₂₃NO [M]⁺ *m/z* = 389.1780; found 389.1785.

General procedure **F** was followed using **6g** (44.9 mg, 0.15 mmol), Pd(OAc)₂ (6.7 mg, 0.03 mmol), K₂S₂O₈ (81.0 mg, 0.3 mmol), PivOH (15.3 mg, 0.15 mmol) and activated charcoal (67 mg, 10x weight of Pd) in toluene (1.5 mL, 0.1 M) at 120 °C for 24 h. Chromatography (7% EtOAc/hexanes) provided **7ga** (46.7 mg) in 80% yield. See above for characterization.



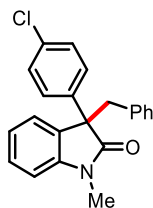
3-Benzyl-3-(4-fluorophenyl)-1-methylindolin-2-one. General procedure **E** was followed using **6h** (36.2 mg, 0.15 mmol) and Pd(OAc)₂ (50.5 mg, 0.225 mmol) in toluene (1.5 mL, 0.1 M) at 120 °C for 24 h. Chromatography (6% EtOAc/hexanes) provided **7ha** (48.7 mg) in 98% yield as a white solid: ¹H NMR (500 MHz, CDCl₃) δ 7.51-7.47 (m, 2H), 7.22 (td, *J* = 8.0, 1.5 Hz, 1H), 7.18 (d, *J* = 7.5 Hz, 1H), 7.11-6.99 (m, 6H), 6.82 (d, *J* = 7.0 Hz, 2H), 6.62 (d, *J* = 8.0 Hz, 1H), 3.65 (d, *J* = 13.0 Hz, 1H), 3.41 (d, *J* = 13.0 Hz, 1H), 2.95 (s, 3H); ¹³C NMR (125 MHz, CDCl₃) δ 178.0, 162.5 (d, *J*_{C-F} = 228.5 Hz), 144.1, 135.8 (d, *J*_{C-F} = 4.4 Hz), 131.3, 130.4, 129.4 (d, *J*_{C-F} = 8.0 Hz), 128.7, 127.8, 126.9, 125.9, 122.6, 115.7 (d, *J*_{C-F} = 21.1 Hz), 108.5, 100.4, 58.0, 44.8, 26.5; IR (film) 2924, 1711, 1611, 1508, 1373, 1234, 1162, 1088, 755, 700 cm⁻¹; HRMS (EI-TOF) calcd for C₂₂H₁₈FNO [M]⁺ *m/z* = 331.1372; found 331.1379.

General procedure **F** was followed using **6h** (36.2 mg, 0.15 mmol), Pd(OAc)₂ (6.7 mg, 0.03 mmol), K₂S₂O₈ (81.0 mg, 0.3 mmol), PivOH (15.3 mg, 0.15 mmol) and activated charcoal (67 mg, 10x weight of Pd) in toluene (1.5 mL, 0.1 M) at 120 °C for 24 h. Chromatography (6% EtOAc/hexanes) provided **7ha** (32.3 mg) in 65% yield. See above for characterization.



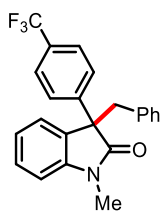
3-Benzyl-3-(3-fluorophenyl)-1-methylindolin-2-one. General procedure **E** was followed using **6i** (36.2 mg, 0.15 mmol) and Pd(OAc)₂ (50.5 mg, 0.225 mmol) in toluene (1.5 mL, 0.1 M) at 120 °C for 24 h. Chromatography (6% EtOAc/hexanes) provided **7ia** (47.2 mg) in 95% yield as a white solid: ¹H NMR (500 MHz, CDCl₃) δ 7.34-7.28 (m, 2H), 7.25-7.19 (m, 3H), 7.11-6.97 (m, 5H), 6.83 (d, *J* = 6.5 Hz, 2H), 6.62 (d, *J* = 8.0 Hz, 1H), 3.67 (d, *J* = 12.5 Hz, 1H), 3.44 (d, *J* = 12.5 Hz, 1H), 2.96 (s, 3H); ¹³C NMR (125 MHz, CDCl₃) δ 177.1, 162.8 (d, *J*_{C-F} = 244.4 Hz), 143.6, 142.1 (d, *J*_{C-F} = 7.1 Hz), 135.2, 130.6, 129.9 (d, *J*_{C-F} = 8.6 Hz), 128.4, 127.4, 126.6, 125.4, 122.9 (d, *J*_{C-F} = 2.7 Hz), 122.2, 114.7, 114.4 (d, *J*_{C-F} = 13.1 Hz), 114.2, 108.1, 57.9 (d, *J*_{C-F} = 1.6 Hz), 44.0, 26.0; IR (film) 2925, 1710, 1612, 1586, 1493, 1470, 1373, 1351, 1128, 1090, 755, 700 cm⁻¹; HRMS (EI-TOF) calcd for C₂₂H₁₈FNO [M]⁺ *m/z* = 331.1372; found 331.1364.

General procedure **F** was followed using **6i** (36.2 mg, 0.15 mmol), Pd(OAc)₂ (6.7 mg, 0.03 mmol), K₂S₂O₈ (81.0 mg, 0.3 mmol), PivOH (15.3 mg, 0.15 mmol) and activated charcoal (67 mg, 10x weight of Pd) in toluene (1.5 mL, 0.1 M) at 120 °C for 24 h. Chromatography (6% EtOAc/hexanes) provided **7ia** (48.7 mg) in 98% yield. See above for characterization.



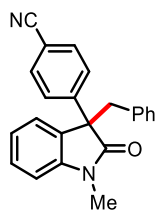
3-Benzyl-3-(4-chlorophenyl)-1-methylindolin-2-one. General procedure E was followed using **6j** (38.6 mg, 0.15 mmol) and Pd(OAc)₂ (50.5 mg, 0.225 mmol) in toluene (1.5 mL, 0.1 M) at 120 °C for 24 h. Chromatography (6% EtOAc/hexanes) provided **7ja** (45.4 mg) in 87% yield as a white solid: ¹H NMR (500 MHz, CDCl₃) δ 7.46 (d, *J* = 12.0 Hz, 2H), 7.32 (d, *J* = 12.0 Hz, 2H), 7.27-7.17 (m, 2H), 7.12-7.00 (m, 4H), 6.82 (d, *J* = 9.0 Hz, 2H), 6.63 (d, *J* = 10.5 Hz, 1H), 3.65 (d, *J* = 18.0 Hz, 1H), 3.42 (d, *J* = 18.0 Hz, 1H), 2.96 (s, 3H); HRMS (EI-TOF) calcd for C₂₂H₁₈ClNO [M]⁺ *m/z* = 347.1077; found 347.1076. Spectral data match those previously reported.⁶

General procedure F was followed using **6j** (38.6 mg, 0.15 mmol), Pd(OAc)₂ (6.7 mg, 0.03 mmol), K₂S₂O₈ (81.0 mg, 0.3 mmol), PivOH (15.3 mg, 0.15 mmol) and activated charcoal (67 mg, 10x weight of Pd) in toluene (1.5 mL, 0.1 M) at 120 °C for 24 h. Chromatography (6% EtOAc/hexanes) provided **7ja** (45.9 mg) in 88% yield. See above for characterization.



3-Benzyl-1-methyl-3-(4-(trifluoromethyl)phenyl)indolin-2-one. General procedure E was followed using **6k** (43.7 mg, 0.15 mmol) and Pd(OAc)₂ (50.5 mg, 0.225 mmol) in toluene (1.5 mL, 0.1 M) at 120 °C for 24 h. Chromatography (6% EtOAc/hexanes) provided **7ka** (52.1 mg) in 91% yield as a white solid: ¹H NMR (500 MHz, CDCl₃) δ 7.63 (d, *J* = 8.5 Hz, 2H), 7.58 (d, *J* = 8.5 Hz, 2H), 7.25-7.18 (m, 2H), 7.11-6.99 (m, 4H), 6.82 (d, *J* = 7.0 Hz, 2H), 6.62 (d, *J* = 7.5 Hz, 1H), 3.70 (d, *J* = 13.0 Hz, 1H), 3.43 (d, *J* = 13.0 Hz, 1H), 2.94 (s, 3H); ¹³C NMR (125 MHz, CDCl₃) δ 176.9, 143.7, 135.0, 130.3, 129.9, 128.5, 127.7, 127.4, 126.7, 125.4 (q, *J*_{C-F} = 3.6 Hz), 125.1 (q, *J*_{C-F} = 270.6 Hz), 122.3, 108.2, 58.1, 44.0, 26.1; IR (film) 2965, 1713, 1615, 1496, 1327, 1234, 1124, 756, 700 cm⁻¹; HRMS (EI-TOF) calcd for C₂₃H₁₈F₃NO [M]⁺ *m/z* = 381.1340; found 381.1340.

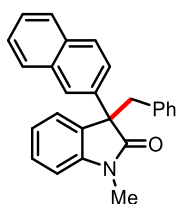
General procedure F was followed using **6k** (43.7 mg, 0.15 mmol), Pd(OAc)₂ (6.7 mg, 0.03 mmol), K₂S₂O₈ (81.0 mg, 0.3 mmol), PivOH (15.3 mg, 0.15 mmol) and activated charcoal (67 mg, 10x weight of Pd) in toluene (1.5 mL, 0.1 M) at 120 °C for 24 h. Chromatography (6% EtOAc/hexanes) provided **7ka** (36.0 mg) in 63% yield. See above for characterization.



4-(3-Benzyl-1-methyl-2-oxoindolin-3-yl)benzonitrile. General procedure E was followed using **6l**

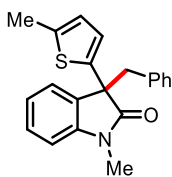
(37.2 mg, 0.15 mmol) and Pd(OAc)₂ (50.5 mg, 0.225 mmol) in toluene (1.5 mL, 0.1 M) at 120 °C for 24 h. Chromatography (8% EtOAc/hexanes) provided **7la** (38.1 mg) in 75% yield as a white solid: ¹H NMR (500 MHz, CDCl₃) δ 7.67-7.62 (m, 4H), 7.26 (t, *J* = 6.5 Hz, 1H), 7.18 (d, *J* = 7.0 Hz, 1H), 7.13-7.00 (m, 4H), 6.80 (d, *J* = 7.0 Hz, 2H), 6.65 (d, *J* = 7.5 Hz, 1H), 3.65 (d, *J* = 13.0 Hz, 1H), 3.43 (d, *J* = 13.0 Hz, 1H), 2.96 (s, 3H); ¹³C NMR (125 MHz, CDCl₃) δ 176.8, 145.1, 143.8, 134.9, 132.4, 130.1, 129.9, 128.9, 128.4, 127.7, 126.9, 125.6, 122.6, 118.8, 111.5, 108.6, 58.4, 44.3, 26.4; IR (film) 2928, 1710, 1611, 1494, 1470, 1372, 1259, 1127, 756, 700 cm⁻¹; HRMS (EI-TOF) calcd for C₂₃H₁₈N₂O [M]⁺ *m/z* = 338.1419; found 338.1418.

General procedure **F** was followed using **6l** (37.2 mg, 0.15 mmol), Pd(OAc)₂ (6.7 mg, 0.03 mmol), K₂S₂O₈ (81.0 mg, 0.3 mmol), PivOH (15.3 mg, 0.15 mmol) and activated charcoal (67 mg, 10x weight of Pd) in toluene (1.5 mL, 0.1 M) at 120 °C for 24 h. Chromatography (8% EtOAc/hexanes) provided **7la** (45.1 mg) in 89% yield. See above for characterization.

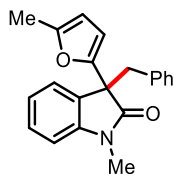


3-Benzyl-1-methyl-3-(naphthalen-2-yl)indolin-2-one. General procedure **E** was followed using **6m** (40.9 mg, 0.15 mmol) and Pd(OAc)₂ (50.5 mg, 0.225 mmol) in toluene (1.5 mL, 0.1 M) at 120 °C for 24 h. Chromatography (7% EtOAc/hexanes) provided **7ma** (53.9 mg) in 99% yield as a yellow solid: ¹H NMR (500 MHz, CDCl₃) δ 7.93 (s, 1H), 7.84-7.80 (m, 3H), 7.62 (dd, *J* = 9.0, 2.0 Hz, 1H), 7.48-7.46 (m, 2H), 7.27-7.23 (m, 2H), 7.13-7.01 (m, 4H), 6.88 (d, *J* = 7.0 Hz, 2H), 6.65 (d, *J* = 8.0 Hz, 1H), 3.83 (d, *J* = 12.5 Hz, 1H), 3.59 (d, *J* = 12.5 Hz, 1H), 2.99 (s, 3H); HRMS (EI-TOF) calcd for C₂₆H₂₁NO [M]⁺ *m/z* = 363.1623; found 363.1641. Spectral data match those previously reported.⁶

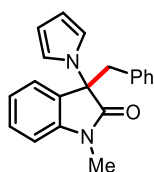
General procedure **F** was followed using **6m** (40.9 mg, 0.15 mmol), Pd(OAc)₂ (6.7 mg, 0.03 mmol), K₂S₂O₈ (81.0 mg, 0.3 mmol), PivOH (15.3 mg, 0.15 mmol) and activated charcoal (67 mg, 10x weight of Pd) in toluene (1.5 mL, 0.1 M) at 120 °C for 24 h. Chromatography (7% EtOAc/hexanes) provided **7ma** (45.2 mg) in 83% yield. See above for characterization.



3-Benzyl-1-methyl-3-(5-methylthiophen-2-yl)indolin-2-one. General procedure **E** was followed using **6n** (36.5 mg, 0.15 mmol) and Pd(OAc)₂ (50.5 mg, 0.225 mmol) in toluene (1.5 mL, 0.1 M) at 120 °C for 24 h. Chromatography (6% EtOAc/hexanes) provided **7na** (4.5 mg) in 9% yield as a red oil: ¹H NMR (500 MHz, CDCl₃) δ 7.29 (d, *J* = 7.5 Hz, 1H), 7.23 (t, *J* = 7.5 Hz, 1H), 7.10-7.00 (m, 4H), 6.85 (d, *J* = 7.0 Hz, 2H), 6.80 (d, *J* = 3.5 Hz, 1H), 6.61 (d, *J* = 7.5 Hz, 2H), 3.59 (d, *J* = 12.5 Hz, 1H), 3.42 (d, *J* = 12.5 Hz, 1H), 2.96 (s, 3H), 2.44 (s, 3H); ¹³C NMR (125 MHz, CDCl₃) δ 176.8, 143.7, 140.8, 139.8, 135.5, 130.8, 130.2, 128.7, 127.6, 126.8, 125.4, 125.3, 124.9, 122.3, 108.2, 56.2, 46.1, 26.3, 15.5; IR (film) 2921, 1715, 1611, 1492, 1470, 1368, 1098, 754, 700 cm⁻¹; HRMS (EI-TOF) calcd for C₂₁H₁₉NOS [M]⁺ *m/z* = 333.1187; found 333.1170.

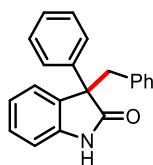


3-Benzyl-1-methyl-3-(5-methylfuran-2-yl)indolin-2-one. General procedure E was followed using **6o** (34.1 mg, 0.15 mmol) and Pd(OAc)₂ (50.5 mg, 0.225 mmol) in toluene (1.5 mL, 0.1 M) at 120 °C for 24 h. Chromatography (6% EtOAc/hexanes) provided **7oa** (19.5 mg) in 41% yield as a yellow oil: ¹H NMR (500 MHz, CDCl₃) δ 7.25-7.19 (m, 2H), 7.07-7.01 (m, 4H), 6.82 (d, *J* = 6.5 Hz, 2H), 6.60 (d, *J* = 8.0 Hz, 1H), 6.07 (d, *J* = 3.0 Hz, 1H), 5.89 (d, *J* = 2.0 Hz, 1H), 3.52 (d, *J* = 13.0 Hz, 1H), 3.49 (d, *J* = 13.0 Hz, 1H), 2.97 (s, 3H), 2.30 (s, 3H); ¹³C NMR (125 MHz, CDCl₃) δ 175.7, 152.5, 150.4, 143.6, 135.3, 130.2, 129.8, 128.5, 127.6, 126.7, 125.1, 122.3, 108.2, 107.9, 106.4, 54.9, 42.6, 26.2, 13.9; IR (film) 2924, 1714, 1611, 1494, 1470, 1374, 1090, 753, 700 cm⁻¹; HRMS (EI-TOF) calcd for C₂₁H₁₉NO₂ [M]⁺ *m/z* = 317.1416; found 317.1421.



3-benzyl-1-methyl-3-(1H-pyrrol-1-yl)indolin-2-one. General procedure E was followed using **6p** (31.8 mg, 0.15 mmol) and Pd(OAc)₂ (50.5 mg, 0.225 mmol) in toluene (1.5 mL, 0.1 M) at 120 °C for 24 h. Chromatography (6% EtOAc/hexanes) provided **7pa** (26.3 mg) in 58% yield as a white solid: ¹H NMR (500 MHz, CDCl₃) δ 7.29 (td, *J* = 8.0, 1.5 Hz, 1H), 7.17 (d, *J* = 7.5 Hz, 1H), 7.14-7.04 (m, 4H), 6.97 (t, *J* = 2.5 Hz, 2H), 6.78 (d, *J* = 7.0 Hz, 2H), 6.65 (d, *J* = 8.0 Hz, 1H), 6.23 (t, *J* = 2.5 Hz, 2H), 3.64 (d, *J* = 13.0 Hz, 1H), 3.61 (d, *J* = 13.0 Hz, 1H), 2.97 (s, 3H); ¹³C NMR (125 MHz, CDCl₃) δ 174.3, 143.8, 133.6, 130.3, 130.1, 127.9, 127.2, 126.9, 126.0, 122.6, 119.4, 108.9, 108.6, 67.5, 43.8, 26.2; IR (film) 2933, 1720, 1612, 1494, 1471, 1342, 1266, 1096, 755, 700 cm⁻¹; HRMS (EI-TOF) calcd for C₂₀H₁₈N₂O [M]⁺ *m/z* = 302.1419; found 302.1435.

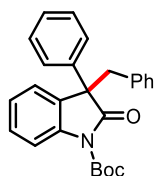
General procedure **F** was followed using **6p** (31.8 mg, 0.15 mmol), Pd(OAc)₂ (6.7 mg, 0.03 mmol), K₂S₂O₈ (81.0 mg, 0.3 mmol), PivOH (15.3 mg, 0.15 mmol) and activated charcoal (67 mg, 10x weight of Pd) in toluene (1.5 mL, 0.1 M) at 120 °C for 24 h. Chromatography (6% EtOAc/hexanes) provided **7pa** (15.4 mg) in 34% yield. See above for characterization.



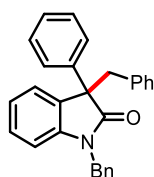
3-Benzyl-3-phenylindolin-2-one. General procedure E was followed using **6q** (31.3 mg, 0.15 mmol) and Pd(OAc)₂ (50.5 mg, 0.225 mmol) in toluene (1.5 mL, 0.1 M) at 120 °C for 24 h. Chromatography (7% EtOAc/hexanes) provided **7qa** (41.3 mg) in 92% yield as a white solid: ¹H NMR (500 MHz, CDCl₃) δ 8.43 (s, 1H), 7.49 (d, *J* = 7.5 Hz, 2H), 7.35 (t, *J* = 7.0 Hz, 2H), 7.30 (t, *J* = 7.5 Hz, 1H), 7.21-7.14 (m, 2H), 7.09-7.03 (m, 2H), 7.00 (t, *J* = 7.5 Hz, 2H), 6.90 (d, *J* = 7.0 Hz, 2H), 6.71 (d, *J* = 7.5 Hz, 1H), 3.72 (d, *J* = 13.0 Hz, 1H), 3.50 (d, *J* = 13.0 Hz, 1H); ¹³C NMR (125 MHz, CDCl₃) δ 180.5, 141.1, 139.9, 135.7, 132.1, 130.3, 128.8, 128.3, 127.8, 127.6, 127.3, 126.7, 125.9, 122.3, 110.1, 58.8, 43.6; IR (film)

3246, 1708, 1619, 1471, 751, 697 cm^{-1} ; HRMS (EI-TOF) calcd for $\text{C}_{21}\text{H}_{17}\text{NO}$ $[\text{M}]^+$ $m/z = 299.1310$; found 299.1298.

General procedure **F** was followed using **6q** (31.3 mg, 0.15 mmol), $\text{Pd}(\text{OAc})_2$ (6.7 mg, 0.03 mmol), $\text{K}_2\text{S}_2\text{O}_8$ (81.0 mg, 0.3 mmol), PivOH (15.3 mg, 0.15 mmol) and activated charcoal (67 mg, 10x weight of Pd) in toluene (1.5 mL, 0.1 M) at 120 °C for 24 h. Chromatography (7% EtOAc/hexanes) provided **7qa** (42.2 mg) in 94% yield. See above for characterization.

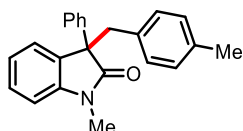


tert-Butyl 3-benzyl-2-oxo-3-phenylindoline-1-carboxylate. General procedure **E** was followed using **6r** (46.4 mg, 0.15 mmol) and $\text{Pd}(\text{OAc})_2$ (50.5 mg, 0.225 mmol) in toluene (1.5 mL, 0.1 M) at 95 °C for 24 h. Chromatography (9% EtOAc/hexanes) provided **7ra** (40.7 mg) in 68% yield as a white solid: ^1H NMR (500 MHz, CDCl_3) δ 7.62 (d, $J = 8.0$ Hz, 1H), 7.44 (d, $J = 7.5$ Hz, 2H), 7.34 (t, $J = 7.0$ Hz, 2H), 7.31-7.21 (m, 2H), 7.19-7.14 (m, 2H), 7.06 (t, $J = 7.5$ Hz, 1H), 7.02 (t, $J = 7.5$ Hz, 2H), 6.82 (d, $J = 7.0$ Hz, 2H), 3.78 (d, $J = 12.5$ Hz, 1H), 3.43 (d, $J = 12.5$ Hz, 1H), 1.54 (s, 9H); HRMS (EI-TOF) calcd for $\text{C}_{21}\text{H}_{17}\text{NO}$ $[\text{M}-\text{Boc}]^-$ $m/z = 299.1310$; found 299.1322. Spectral data match those previously reported.⁸ General procedure **F** was followed using **6r** (46.4 mg, 0.15 mmol), $\text{Pd}(\text{OAc})_2$ (6.7 mg, 0.03 mmol), $\text{K}_2\text{S}_2\text{O}_8$ (81.0 mg, 0.3 mmol), PivOH (15.3 mg, 0.15 mmol) and activated charcoal (67 mg, 10x weight of Pd) in toluene (1.5 mL, 0.1 M) at 95 °C for 24 h. Chromatography (9% EtOAc/hexanes) provided **7ra** (23.3 mg) in 39% yield. See above for characterization.

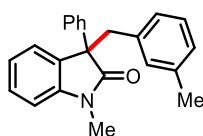


1,3-Dibenzyl-3-phenylindolin-2-one. General procedure **E** was followed using **6s** (44.9 mg, 0.15 mmol) and $\text{Pd}(\text{OAc})_2$ (50.5 mg, 0.225 mmol) in toluene (1.5 mL, 0.1 M) at 120 °C for 24 h. Chromatography (8% EtOAc/hexanes) provided **7sa** (57.8 mg) in 99% yield as a yellow solid: ^1H NMR (500 MHz, CDCl_3) δ 7.54 (d, $J = 8.0$ Hz, 2H), 7.40-7.29 (m, 4H), 7.18-7.05 (m, 8H), 6.94 (d, $J = 7.5$ Hz, 2H), 6.68 (d, $J = 6.5$ Hz, 2H), 6.45-6.43 (m, 1H), 4.90 (d, $J = 16.0$ Hz, 1H), 4.54 (d, $J = 16.0$ Hz, 1H), 3.84 (d, $J = 13.0$ Hz, 1H), 3.66 (d, $J = 13.0$ Hz, 1H); HRMS (EI-TOF) calcd for $\text{C}_{28}\text{H}_{23}\text{NO}$ $[\text{M}]^+$ $m/z = 389.1780$; found 389.1772. Spectral data match those previously reported.⁶

General procedure **F** was followed using **6s** (44.9 mg, 0.15 mmol), $\text{Pd}(\text{OAc})_2$ (6.7 mg, 0.03 mmol), $\text{K}_2\text{S}_2\text{O}_8$ (81.0 mg, 0.3 mmol), PivOH (15.3 mg, 0.15 mmol) and activated charcoal (67 mg, 10x weight of Pd) in toluene (1.5 mL, 0.1 M) at 120 °C for 24 h. Chromatography (8% EtOAc/hexanes) provided **7sa** (57.2 mg) in 98% yield. See above for characterization.

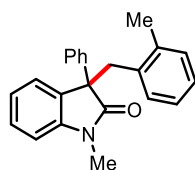


1-Methyl-3-(4-methylbenzyl)-3-phenylindolin-2-one. General procedure E was followed using **6a** (33.4 mg, 0.15 mmol) and Pd(OAc)₂ (50.5 mg, 0.225 mmol) in *p*-xylene (1.5 mL, 0.1 M) at 120 °C for 24 h. Chromatography (6% EtOAc/hexanes) provided **7ab** (18.2 mg) in 37% yield as a white solid: ¹H NMR (500 MHz, CDCl₃) δ 7.50 (d, *J* = 7.0 Hz, 2H), 7.34 (t, *J* = 7.5 Hz, 2H), 7.28 (t, *J* = 7.5 Hz, 1H), 7.25-7.20 (m, 2H), 7.07 (td, *J* = 7.5, 1.0 Hz, 1H), 6.82 (d, *J* = 8.0 Hz, 2H), 6.72 (d, *J* = 8.0 Hz, 2H), 6.64 (d, *J* = 8.0 Hz, 1H), 3.66 (d, *J* = 12.5 Hz, 1H), 3.43 (d, *J* = 12.5 Hz, 1H), 2.97 (s, 3H), 2.19 (s, 3H); HRMS (EI-TOF) calcd for C₂₃H₂₁NO [M]⁺ *m/z* = 327.1623; found 327.1624. Spectral data match those previously reported.⁶



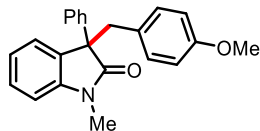
1-Methyl-3-(3-methylbenzyl)-3-phenylindolin-2-one. General procedure E was followed using **6a** (33.4 mg, 0.15 mmol) and Pd(OAc)₂ (50.5 mg, 0.225 mmol) in *m*-xylene (1.5 mL, 0.1 M) at 120 °C for 24 h. Chromatography (6% EtOAc/hexanes) provided **7ac** (29.9 mg) in 61% yield as a colorless oil: ¹H NMR (500 MHz, CDCl₃) δ 7.51 (d, *J* = 8.0 Hz, 2H), 7.35 (t, *J* = 7.0 Hz, 2H), 7.29 (t, *J* = 7.5 Hz, 1H), 7.24-7.19 (m, 2H), 7.07 (t, *J* = 7.0 Hz, 1H), 6.93-6.85 (m, 2H), 6.66-6.61 (m, 3H), 3.67 (d, *J* = 13.0 Hz, 1H), 3.42 (d, *J* = 13.0 Hz, 1H), 2.96 (s, 3H), 2.13 (s, 3H); ¹³C NMR (125 MHz, CDCl₃) δ 177.9, 143.9, 139.9, 137.0, 135.7, 131.5, 130.9, 128.7, 128.2, 127.5, 127.4, 127.3, 127.2, 127.1, 125.7, 122.2, 108.1, 58.4, 44.1, 26.2, 21.3; IR (film) 2922, 1711, 1611, 1492, 1470, 1373, 1348, 753, 696 cm⁻¹; HRMS (EI-TOF) calcd for C₂₃H₂₁NO [M]⁺ *m/z* = 327.1623; found 327.1612.

General procedure F was followed using **6a** (33.4 mg, 0.15 mmol), Pd(OAc)₂ (6.7 mg, 0.03 mmol), K₂S₂O₈ (81.0 mg, 0.3 mmol), PivOH (15.3 mg, 0.15 mmol) and activated charcoal (67 mg, 10x weight of Pd) in *m*-xylene (1.5 mL, 0.1 M) at 120 °C for 24 h. Chromatography (6% EtOAc/hexanes) provided **7ac** (23.6 mg) in 48% yield. See above for characterization.

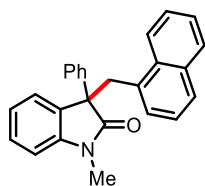


1-Methyl-3-(2-methylbenzyl)-3-phenylindolin-2-one. General procedure E was followed using **6a** (33.4 mg, 0.15 mmol) and Pd(OAc)₂ (50.5 mg, 0.225 mmol) in *o*-xylene (1.5 mL, 0.1 M) at 120 °C for 24 h. Chromatography (6% EtOAc/hexanes) provided **7ad** (30.4 mg) in 62% yield as a colorless oil: ¹H NMR (500 MHz, CDCl₃) δ 7.53 (d, *J* = 7.0 Hz, 2H), 7.34 (t, *J* = 7.5 Hz, 2H), 7.30-7.21 (m, 2H), 7.01-6.94 (m, 4H), 6.82 (td, *J* = 8.0, 2.0 Hz, 1H), 6.69 (d, *J* = 8.0 Hz, 1H), 6.66 (d, *J* = 8.0 Hz, 1H), 3.61 (s, 2H), 3.04 (s, 3H), 2.05 (s, 3H); ¹³C NMR (125 MHz, CDCl₃) δ 178.1, 143.7, 139.6, 137.2, 134.4, 130.8, 130.1, 129.5, 128.4, 128.2, 127.4, 127.3, 126.5, 125.9, 124.9, 121.9, 107.9, 57.6, 39.9, 26.1, 20.0; IR (film) 2930, 1712, 1611, 1493, 1470, 1372, 1348, 754, 696 cm⁻¹; HRMS (EI-TOF) calcd for C₂₃H₂₁NO [M]⁺ *m/z* = 327.1623; found 327.1630.

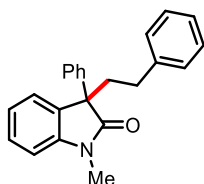
General procedure **F** was followed using **6a** (33.4 mg, 0.15 mmol), Pd(OAc)₂ (6.7 mg, 0.03 mmol), K₂S₂O₈ (81.0 mg, 0.3 mmol), PivOH (15.3 mg, 0.15 mmol) and activated charcoal (67 mg, 10x weight of Pd) in *o*-xylene (1.5 mL, 0.1 M) at 120 °C for 24 h. Chromatography (6% EtOAc/hexanes) provided **7ad** (17.7 mg) in 36% yield. See above for characterization.



3-(4-Ethoxybenzyl)-1-methyl-3-phenylindolin-2-one. General procedure **E** was followed using **6a** (33.4 mg, 0.15 mmol) and Pd(OAc)₂ (50.5 mg, 0.225 mmol) in 1-methoxy-4-methylbenzene (1.5 mL, 0.1 M) at 120 °C for 24 h. Chromatography (7% EtOAc/hexanes) provided **7ae** (21.1 mg) in 41% yield as a colorless oil: ¹H NMR (500 MHz, CDCl₃) δ 7.49 (d, *J* = 7.0 Hz, 2H), 7.34 (t, *J* = 7.5 Hz, 2H), 7.28 (d, *J* = 7.5 Hz, 1H), 7.24-7.20 (m, 2H), 7.07 (t, *J* = 6.5 Hz, 1H), 6.74 (d, *J* = 8.5 Hz, 2H), 6.63 (d, *J* = 7.5 Hz, 1H), 6.55 (d, *J* = 8.5 Hz, 2H), 3.69 (s, 3H), 3.64 (d, *J* = 13.0 Hz, 1H), 3.41 (d, *J* = 13.0 Hz, 1H), 2.97 (s, 3H); ¹³C NMR (125 MHz, CDCl₃) δ 178.0, 158.3, 143.9, 139.9, 131.5, 131.1, 128.7, 128.3, 127.9, 127.5, 127.4, 125.6, 122.3, 112.9, 108.2, 58.5, 55.2, 43.3, 26.2; IR (film) 2927, 1709, 1611, 1511, 1493, 1469, 1373, 1348, 1248, 1034, 751, 696 cm⁻¹; HRMS (EI-TOF) calcd for C₂₃H₂₁NO₂ [M]⁺ *m/z* = 343.1572; found 343.1569.



1-Methyl-3-(naphthalen-1-ylmethyl)-3-phenylindolin-2-one. General procedure **E** was followed using **6a** (33.4 mg, 0.15 mmol) and Pd(OAc)₂ (50.5 mg, 0.225 mmol) in 1-methylnaphthalene (1.5 mL, 0.1 M) at 120 °C for 24 h. Chromatography (7% EtOAc/hexanes) provided **7af** (5.9 mg) in 11% yield as a yellow solid: ¹H NMR (500 MHz, CDCl₃) δ 7.99-7.96 (m, 1H), 7.72-7.65 (m, 1H), 7.60-7.55 (m, 3H), 7.39-7.31 (m, 5H), 7.13 (t, *J* = 7.0 Hz, 1H), 7.09-7.01 (m, 3H), 6.82 (t, *J* = 7.5 Hz, 1H), 6.52 (d, *J* = 8.0 Hz, 1H), 4.22 (d, *J* = 13.5 Hz, 1H), 4.02 (d, *J* = 13.5 Hz, 1H), 2.92 (s, 3H); HRMS (EI-TOF) calcd for C₂₆H₂₁NO [M]⁺ *m/z* = 363.1623; found 363.1624. Spectral data match those previously reported.⁶



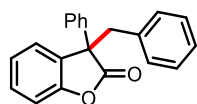
1-Methyl-3-phenethyl-3-phenylindolin-2-one. General procedure **E** was followed using **6a** (33.4 mg, 0.15 mmol) and Pd(OAc)₂ (50.5 mg, 0.225 mmol) in ethylbenzene (1.5 mL, 0.1 M) at 120 °C for 24 h. Chromatography (7% EtOAc/hexanes) provided **7ag** (33.4 mg) in 68% yield as a colorless oil: ¹H NMR (500 MHz, CDCl₃) δ 7.41-7.36 (m, 3H), 7.34-7.21 (m, 6H), 7.20-7.12 (m, 2H), 7.08 (d, *J* = 7.0 Hz, 2H), 6.94 (d, *J* = 7.5 Hz, 1H), 3.24 (s, 3H), 2.78-2.72 (m, 1H), 2.51-2.39 (m, 2H), 2.27-2.19 (m, 1H); HRMS (EI-TOF) calcd for C₂₃H₂₁NO [M]⁺ *m/z* = 327.1623; found 327.1640. Spectral data match those

previously reported.⁹

General procedure **F** was followed using **6a** (33.4 mg, 0.15 mmol), Pd(OAc)₂ (6.7 mg, 0.03 mmol), K₂S₂O₈ (81.0 mg, 0.3 mmol), PivOH (15.3 mg, 0.15 mmol) and activated charcoal (67 mg, 10x weight of Pd) in ethylbenzene (1.5 mL, 0.1 M) at 120 °C for 24 h. Chromatography (7% EtOAc/hexanes) provided **7ag** (22.6 mg) in 46% yield. See above for characterization.

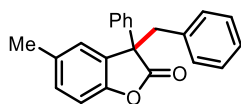
General Procedure G-Alkylation of Benzofuranones with Stoichiometric Pd Using neat Tolylyl Substrate. 3-Aryl benzofuran-2(3*H*)-one (0.178 mmol) and Pd(OAc)₂ (40.0 mg, 0.178 mmol, 100 mol%) were added to a flame-dried 8 mL microwave vial equipped with stirbar and were brought into the glovebox. The indicated tolylyl analog (0.1 M) was added to the mixture. The microwave vial was sealed with a Teflon cap, removed from the glovebox, and placed in a 120 °C oil bath. After 24 h, the mixture was allowed to cool to ambient temperature, diluted with CH₂Cl₂ (1 mL), passed through SiO₂ with 30% EtOAc/hexanes, and concentrated. The residue was chromatographed (EtOAc/hexanes) to afford the alkylated 3-aryl benzofuran-2(3*H*)-ones.

General procedure H – Alkylation of Benzofuranones with Catalytic Pd Using neat Tolylyl Substrate. 3-Aryl benzofuran-2(3*H*)-one (0.178 mmol), Pd(OAc)₂ (8 mg, 0.035 mmol, 20 mol%), PivOH (18.0 mg, 0.178 mmol, 1 equiv), K₂S₂O₈ (96.0 mg, 0.356 mmol, 2 equiv) and activated carbon (19.0 mg, 10x weight of Pd) were added to a flame-dried 8 mL microwave vial equipped with a stirbar and were brought into the glovebox. The indicated tolylyl analog (0.1M) was added to the mixture. The microwave vial was sealed with a Teflon cap, removed from the glovebox, and placed in a 120 °C oil bath. After 24 h, the mixture was allowed to cool to ambient temperature, diluted with CH₂Cl₂ (1 mL), passed through SiO₂ with 30% EtOAc/hexanes, and concentrated. The residue was chromatographed (EtOAc/hexanes) to afford the alkylated 3-aryl benzofuran-2(3*H*)-ones.

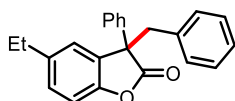


3-Benzyl-3-phenylbenzofuran-2(3*H*)-one. General procedure **G** was followed with 3-phenylbenzofuran-2(3*H*)-one and toluene. Chromatography (7% EtOAc/hexanes) afforded **9aa** (50 mg) in 94% yield as a white solid: ¹H NMR (500 MHz, CDCl₃) δ 7.53 (d, *J* = 7.6 Hz, 2H), 7.39 (t, *J* = 7.4 Hz, 2H), 7.34 (t, *J* = 6.7 Hz, 1H), 7.28 -7.23 (m, 2H), 7.19 (t, *J* = 7.4 Hz, 1H), 7.12 (d, *J* = 7.0 Hz, 1H), 7.08 (t, *J* = 7.1 Hz, 2H), 6.94 (d, *J* = 7.9 Hz, 1H), 6.87 (d, *J* = 6.7 Hz, 2H), 3.75 (d, *J* = 13.2 Hz, 1H), 3.54 (d, *J* = 13.2 Hz, 1H); ¹³C NMR (125 MHz, CDCl₃) δ 177.6, 153.2, 138.6, 134.9, 130.2, 129.3, 129.2, 129.0, 128.2, 128.1, 127.2, 127.2, 126.0, 124.0, 110.9, 57.9, 45.1; IR (film) 2960, 1799, 1619, 1497, 1478, 1463, 1289, 1230, 1125, 1061, 953, 879, 755, 724, 698, 655, 580, 519 cm⁻¹; HRMS (EI-TOF) calcd for C₂₁H₁₆O₂ [M]⁺ *m/z* = 300.1150; found 300.1153.

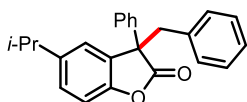
General procedure **H** was followed using 3-phenylbenzofuran-2(3*H*)-one and toluene (1.8 mL, 0.1 M) at 120 °C for 24 h. Chromatography (7% EtOAc/hexanes) provided **9aa** (48 mg) in 91% yield. See above for characterization.



3-Benzyl-5-methyl-3-phenylbenzofuran-2(3H)-one. General procedure **G** was followed using 5-methyl-3-phenylbenzofuran-2(3H)-one and toluene. Chromatography (5% EtOAc/hexanes) afforded **9ba** (55 mg) in 97% yield as a white solid: $^1\text{H NMR}$ (500 MHz, CDCl_3) δ 7.53 (d, $J = 7.9$ Hz, 2H), 7.39 (t, $J = 7.6$ Hz, 2H), 7.34 (t, $J = 7.3$ Hz, 1H), 7.12 (d, $J = 6.9$ Hz, 1H), 7.09 (t, $J = 7.1$ Hz, 2H), 7.05 (d, $J = 8.2$ Hz, 1H), 7.02 (s, 1H), 6.87 (d, $J = 7.0$ Hz, 2H), 6.82 (d, $J = 8.2$ Hz, 1H), 3.71 (d, $J = 13.1$ Hz, 1H), 3.53 (d, $J = 13.1$ Hz, 1H), 2.38 (s, 3H); $^{13}\text{C NMR}$ (125 MHz, CDCl_3) δ 177.9, 151.1, 138.8, 135.0, 133.6, 130.2, 129.6, 129.2, 128.9, 128.1, 128.1, 127.2, 127.1, 126.3, 110.5, 57.7, 44.9, 21.4; IR (film) 2960, 1795, 1486, 1455, 1448, 1230, 1148, 1131, 1087, 1062, 1034, 1001, 953, 868, 812, 767, 736, 725, 697, 644, 522; HRMS (EI-TOF) calcd for $\text{C}_{22}\text{H}_{18}\text{O}_2$ [M^+] $m/z = 314.1307$; found 314.1292. General procedure **H** was followed using 5-methyl-3-phenylbenzofuran-2(3H)-one and toluene. Chromatography (5% EtOAc/hexanes) provided **9ba** (53 mg) in 95% yield. See above for characterization.

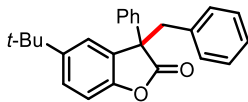


3-Benzyl-5-ethyl-3-phenylbenzofuran-2(3H)-one. General procedure **G** was followed with 5-ethyl-3-phenylbenzofuran-2(3H)-one and toluene. Chromatography (7% EtOAc/hexanes) afforded **9ca** (53 mg) in 94% yield as a faint yellow solid: $^1\text{H NMR}$ (500 MHz, CDCl_3) δ 7.55 (d, $J = 8.2$ Hz, 2H), 7.40 (t, $J = 7.6$ Hz, 2H), 7.34 (t, $J = 7.1$ Hz, 1H), 7.13 (d, $J = 7.1$ Hz, 1H), 7.09 (t, $J = 7.6$ Hz, 3H), 7.02 (s, 1H), 6.86 (t, $J = 8.2$ Hz, 3H), 3.72 (d, $J = 13.1$ Hz, 1H), 3.55 (d, $J = 13.1$ Hz, 1H), 2.67 (q, $J = 5.0$ Hz, 2H), 1.25 (t, $J = 10.0$ Hz, 3H); $^{13}\text{C NMR}$ (125 MHz, CDCl_3) δ 178.0, 151.2, 140.1, 138.7, 135.0, 130.2, 129.0, 128.9, 128.5, 128.1, 128.0, 127.2, 127.1, 125.4, 110.5, 57.6, 45.0, 28.7, 16.2; IR (film) 2960, 1797, 1496, 1484, 1455, 1228, 1147, 1131, 1087, 1066, 1054, 1034, 997, 953, 863, 821, 733, 696, 643, 529; HRMS (EI-TOF) calcd for $\text{C}_{21}\text{H}_{20}\text{O}_2$ [M^+] $m/z = 328.1463$; found 328.1467. General procedure **H** was followed using 5-ethyl-3-phenylbenzofuran-2(3H)-one and toluene. Chromatography (7% EtOAc/hexanes) provided **9ca** (52 mg) in 90% yield. See above for characterization.



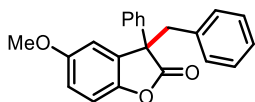
3-Benzyl-5-isopropyl-3-phenylbenzofuran-2(3H)-one. General procedure **G** was followed with 5-isopropyl-3-phenylbenzofuran-2(3H)-one and toluene. Chromatography (7% EtOAc/hexanes) afforded **9da** (58 mg) in 95% yield as a white solid: $^1\text{H NMR}$ (500 MHz, CDCl_3) δ 7.53 (d, $J = 8.0$ Hz, 2H), 7.39 (t, $J = 7.6$ Hz, 2H), 7.34 (t, $J = 7.6$ Hz, 1H), 7.13-7.05 (m, 4H), 7.01 (s, 1H), 6.86 (d, $J = 5.0$ Hz, 2H), 6.84 (d, $J = 5.0$ Hz, 1H), 3.70 (d, $J = 13.2$ Hz, 1H), 3.54 (d, $J = 13.1$ Hz, 1H), 2.96-2.88 (m, 1H), 1.26 (d, $J = 6.6$ Hz, 3H), 1.24 (d, $J = 6.5$ Hz, 3H); $^{13}\text{C NMR}$ (125 MHz, CDCl_3) δ 178.0, 151.2, 144.8, 138.6, 135.0, 130.2, 128.9, 128.7, 128.1, 128.0, 127.2, 127.1, 127.1, 124.1, 110.4, 57.6, 45.1, 34.0, 24.6, 24.0; IR (film) 2960, 1798, 1496, 1484, 1455, 1229, 1141, 1086, 1055, 1034, 993, 953, 881, 819,

778, 742, 729, 695, 642, 532; HRMS (EI-TOF) calcd for C₂₄H₂₂O₂ [M]⁺ *m/z* = 314.1620; found 314.1623. General procedure **H** was followed using 5-isopropyl-3-phenylbenzofuran-2(3*H*)-one and toluene. Chromatography (7% EtOAc/hexanes) provided **9da** (55 mg) in 90% yield. See above for characterization.



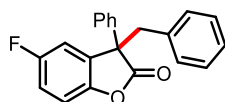
3-Benzyl-5-(tert-butyl)-3-phenylbenzofuran-2(3*H*)-one. General procedure **G** was followed with 5-(tert-butyl)-3-phenylbenzofuran-2(3*H*)-one and toluene. Chromatography (7% EtOAc/hexanes) afforded **9ea** (59 mg) in 93% yield as a white solid: ¹H NMR (500 MHz, CDCl₃) δ 7.53 (d, *J* = 7.7 Hz, 2H), 7.39 (t, *J* = 7.5 Hz, 2H), 7.34 (t, *J* = 7.3 Hz, 1H), 7.27 (d, *J* = 2.1 Hz, 1H), 7.15 (s, 1H), 7.11 (d, *J* = 7.2 Hz, 1H), 7.06 (t, *J* = 4.2 Hz, 2H), 6.87 (d, *J* = 8.5 Hz, 1H), 6.84 (d, *J* = 7.2 Hz, 2H), 3.69 (d, *J* = 13.2 Hz, 1H), 3.56 (d, *J* = 13.2 Hz, 1H), 1.32 (s, 9H); ¹³C NMR (125 MHz, CDCl₃) δ 178.1, 151.0, 147.0, 138.6, 135.1, 130.2, 128.9, 128.3, 128.1, 128.0, 127.3, 127.1, 125.8, 123.5, 110.1, 57.5, 45.2, 34.8, 31.6; IR (film) 2962, 1801, 1488, 1456, 1365, 1263, 1233, 1144, 1087, 1060, 1035, 993, 954, 867, 820, 776, 744, 728, 697, 533; HRMS (EI-TOF) calcd for C₂₅H₂₄O₂ [M]⁺ *m/z* = 356.1776; found 356.1781.

General procedure **H** was followed using 5-(tert-butyl)-3-phenylbenzofuran-2(3*H*)-one and toluene. Chromatography (7% EtOAc/hexanes) provided **9ea** (56 mg) in 89% yield. See above for characterization



3-Benzyl-5-methoxy-3-phenylbenzofuran-2(3*H*)-one. General procedure **G** was followed with 5-methoxy-3-phenylbenzofuran-2(3*H*)-one (43 mg, 0.178 mmol) and toluene. Chromatography (5% EtOAc/hexanes) afforded **9fa** (58 mg) in 98% yield as a white solid: ¹H NMR (500 MHz, CDCl₃) δ 7.53 (d, *J* = 7.8 Hz, 2H), 7.40 (t, *J* = 7.7 Hz, 2H), 7.34 (t, *J* = 7.2 Hz, 1H), 7.16-7.09 (m, 3H), 6.91 (d, *J* = 7.3 Hz, 2H), 6.87 (d, *J* = 8.7 Hz, 1H), 6.79 (dd, *J* = 8.7, 2.5 Hz, 1H), 6.75 (s, 1H), 3.78 (s, 3H), 3.73 (d, *J* = 13.2 Hz, 1H), 3.54 (d, *J* = 13.2 Hz, 1H); ¹³C NMR (125 MHz, CDCl₃) δ 178.0, 156.1, 147.1, 138.5, 134.9, 130.2, 130.1, 129.0, 128.1, 128.1, 127.2, 127.1, 114.2, 111.9, 111.3, 58.1, 56.0, 44.8. IR (film) 2960, 1794, 1483, 1456, 1446, 1435, 1276, 1226, 1207, 1150, 1125, 1087, 1065, 1031, 996, 952, 870, 809, 733, 697, 528; HRMS (EI-TOF) calcd for C₂₂H₁₈O₃ [M]⁺ *m/z* = 330.1256; found 330.1256.

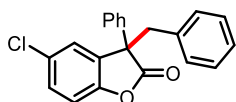
General procedure **H** was followed using 5-methoxy-3-phenylbenzofuran-2(3*H*)-one and toluene. Chromatography (7% EtOAc/hexanes) provided **9fa** (55 mg) in 93% yield. See above for characterization.



3-Benzyl-5-fluoro-3-phenylbenzofuran-2(3*H*)-one. General procedure **G** was followed with 5-fluoro-3-phenylbenzofuran-2(3*H*)-one and toluene. Chromatography (7% EtOAc/hexanes) afforded **9ga** (55 mg) in 96% yield as a white solid: ¹H NMR (500 MHz, CDCl₃) δ 7.50 (d, *J* = 7.1 Hz, 2H), 7.40 (t, *J* = 8.0 Hz, 2H), 7.35 (t, *J* = 6.6 Hz, 1H), 7.16-7.09 (m, 3H), 6.98-6.93 (m, 2H), 6.90 (d, *J* = 4.1 Hz, 2H),

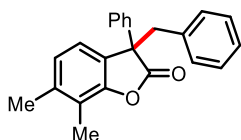
6.89 (s, 1H), 3.75 (d, $J = 13.2$ Hz, 1H), 3.52 (d, $J = 13.2$ Hz, 1H); ^{13}C NMR (125 MHz, CDCl_3) δ 177.4, 159.4 (d, $J = 242.7$ Hz), 149.0, 138.0, 134.5, 130.8 (d, $J = 8.5$ Hz), 130.1, 129.1, 128.4, 128.3, 127.4, 127.0, 115.9 (d, $J = 24.4$ Hz), 113.3 (d, $J = 25.3$ Hz), 111.9 (d, $J = 8.4$ Hz), 58.2, 44.8; IR (film) 3033, 1803, 1604, 1481, 1456, 1270, 1229, 1118, 1085, 1062, 996, 953, 871, 816, 768, 739, 697, 644, 526; HRMS (EI-TOF) calcd for $\text{C}_{21}\text{H}_{15}\text{FO}_2$ $[\text{M}]^+$ $m/z = 318.1056$; found 318.1056.

General procedure **H** was followed using 5-fluoro-3-phenylbenzofuran-2(3H)-one and toluene. Chromatography (7% EtOAc/hexanes) provided **9ga** (57 mg) in 98% yield. See above for characterization.



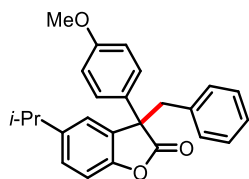
3-Benzyl-5-chloro-3-phenylbenzofuran-2(3H)-one. General procedure **G** was followed with 5-chloro-3-phenylbenzofuran-2(3H)-one and toluene. Chromatography (7% EtOAc/hexanes) afforded **9ha** (57 mg) in 97% yield as a white solid: ^1H NMR (500 MHz, CDCl_3) δ 7.49 (d, $J = 7.5$ Hz, 2H), 7.41 (t, $J = 7.4$ Hz, 2H), 7.36 (t, $J = 6.7$ Hz, 1H), 7.23 (dd, $J = 8.5, 2.2$ Hz, 1H), 7.20 (s, 1H), 7.15-7.11 (m, 3H), 6.88 (m, 3H), 3.74 (d, $J = 13.2$ Hz, 1H), 3.52 (d, $J = 13.2$ Hz, 1H); ^{13}C NMR (125 MHz, CDCl_3) δ 177.0, 151.5, 137.9, 134.4, 131.2, 130.1, 129.4, 129.3, 129.1, 128.4, 128.3, 127.4, 127.0, 126.0, 112.1, 57.9, 44.8; IR (film) 2960, 1805, 1497, 1468, 1456, 1422, 1263, 1231, 1132, 1086, 1060, 1034, 988, 952, 854, 816, 777, 727, 697, 641, 521; HRMS (EI-TOF) calcd for $\text{C}_{21}\text{H}_{15}\text{ClO}_2$ $[\text{M}]^+$ $m/z = 334.0761$; found 334.0778.

General procedure **H** was followed using 5-chloro-3-phenylbenzofuran-2(3H)-one and toluene. Chromatography (7% EtOAc/hexanes) provided **9ha** (57 mg) in 97% yield. See above for characterization.



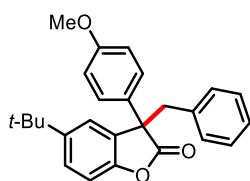
3-Benzyl-6,7-dimethyl-3-phenylbenzofuran-2(3H)-one. General procedure **G** was followed using 6,7-dimethyl-3-phenylbenzofuran-2(3H)-one and toluene. Chromatography (8% EtOAc/hexanes) afforded **9ia** (54 mg) in 93% yield as a faint yellow solid: ^1H NMR (500 MHz, CDCl_3) δ 7.54 (d, $J = 7.8$ Hz, 2H), 7.37 (t, $J = 7.4$ Hz, 2H), 7.32 (d, $J = 7.3$ Hz, 1H), 7.12 (d, $J = 6.9$ Hz, 1H), 7.09 (t, $J = 7.0$ Hz, 2H), 6.97 (d, $J = 7.7$ Hz, 1H), 6.90 (d, $J = 7.7$ Hz, 1H), 6.88 (d, $J = 8.1$ Hz, 2H), 3.67 (d, $J = 13.2$ Hz, 1H), 3.53 (d, $J = 13.2$ Hz, 1H), 2.27 (s, 3H), 2.08 (s, 3H); ^{13}C NMR (125 MHz, CDCl_3) δ 178.1, 151.9, 139.0, 138.3, 135.3, 130.3, 128.8, 128.0, 128.0, 127.2, 127.1, 125.8, 125.0, 122.8, 119.8, 58.0, 45.2, 19.7, 11.9; IR (film) 2960, 1800, 1455, 1260, 1048, 802, 698; HRMS (EI-TOF) calcd for $\text{C}_{23}\text{H}_{20}\text{O}_2$ $[\text{M}]^+$ $m/z = 328.1463$; found 328.1470.

General procedure **H** was followed using 6,7-dimethyl-3-phenylbenzofuran-2(3H)-one and toluene. Chromatography (8% EtOAc/hexanes) provided **9ia** (51 mg) in 89% yield. See above for characterization.



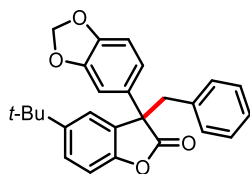
3-Benzyl-5-isopropyl-3-(4-methoxyphenyl)benzofuran-2(3H)-one. General procedure **G** was followed with 5-isopropyl-3-(4-methoxyphenyl)benzofuran-2(3H)-one and toluene. Chromatography (7% EtOAc/hexanes) afforded **9ja** (61 mg) in 92% yield as a white solid: ^1H NMR (500 MHz, CDCl_3) δ 7.44 (d, $J = 8.7$ Hz, 2H), 7.13-7.06 (m, 4 H), 6.97 (s, 1H), 6.92 (d, $J = 8.7$ Hz, 2H), 6.85 (d, $J = 8.5$ Hz, 3H), 3.82 (s, 3H), 3.66 (d, $J = 13.2$ Hz, 1H), 3.51 (d, $J = 13.1$ Hz, 1H), 2.92 (m, 1H), 1.26 (d, $J = 6.6$ Hz, 3H), 1.24 (d, $J = 6.5$ Hz, 3H); ^{13}C NMR (125 MHz, CDCl_3) δ 178.3, 159.3, 151.2, 144.7, 135.1, 130.6, 130.2, 128.9, 128.4, 128.0, 127.1, 127.0, 124.1, 114.2, 110.4, 56.9, 55.4, 45.2, 34.0, 24.6, 24.0; IR (film) 1798, 1609, 1510, 1484, 1456, 1295, 1252, 1230, 1184, 1141, 1084, 1056, 1033, 993, 956, 882, 822, 739, 700, 533; HRMS (EI-TOF) calcd for $\text{C}_{25}\text{H}_{24}\text{O}_3$ $[\text{M}]^+$ $m/z = 372.1725$; found 372.1725.

General procedure **H** was followed using 5-isopropyl-3-(4-methoxyphenyl)benzofuran-2(3H)-one and toluene. Chromatography (7% EtOAc/hexanes) provided **9ja** (57 mg) in 86% yield. See above for characterization.



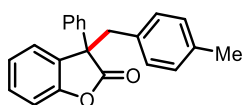
3-Benzyl-5-(tert-butyl)-3-(4-methoxyphenyl)benzofuran-2(3H)-one. General procedure **G** was followed with 5-(tert-butyl)-3-(4-methoxyphenyl)benzofuran-2(3H)-one and toluene. Chromatography (7% EtOAc/hexanes) afforded **9ka** (65 mg) in 94% yield as a white solid: ^1H NMR (500 MHz, CDCl_3) δ 7.43 (d, $J = 9.0$ Hz, 2H), 7.26 (dd, $J = 8.5, 2.1$ Hz, 1H), 7.11 (d, $J = 6.0$ Hz, 2H), 7.08 (s, 1H), 7.06 (d, $J = 7.0$ Hz, 1H), 6.91 (d, $J = 9.0$ Hz, 2H), 6.86 (d, $J = 8.5$ Hz, 1H), 6.83 (d, $J = 7.0$ Hz, 2H), 3.82 (s, 3H), 3.64 (d, $J = 13.2$ Hz, 1H), 3.52 (d, $J = 13.2$ Hz, 1H), 1.31 (s, 9H); ^{13}C NMR (125 MHz, CDCl_3) δ 178.4, 159.3, 151.0, 146.9, 135.2, 130.5, 130.2, 128.5, 128.4, 128.0, 127.1, 125.7, 123.4, 114.2, 110.0, 56.8, 55.4, 45.2, 34.7, 31.6; IR (film) 2960, 1798, 1510, 1487, 1463, 1291, 1252, 1234, 1183, 1144, 1083, 1059, 1033, 992, 955, 869, 836, 818, 735, 699, 533; HRMS (EI-TOF) calcd for $\text{C}_{26}\text{H}_{26}\text{O}_3$ $[\text{M}]^+$ $m/z = 386.1882$; found 386.1880.

General procedure **H** was followed using 5-(tert-butyl)-3-(4-methoxyphenyl)benzofuran-2(3H)-one and toluene (1.8 mL, 0.1 M). Chromatography (7% EtOAc/hexanes) provided **9ka** (62 mg) in 89 % yield. See above for characterization.



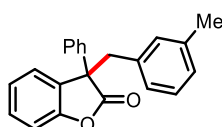
3-(Benzo[d][1,3]dioxol-5-yl)-3-benzyl-6-(tert-butyl)benzofuran-2(3H)-one. General procedure **G** was followed with 3-(benzo[d][1,3]dioxol-5-yl)-5-(tert-butyl)benzofuran-2(3H)-one and toluene

(1.8 mL, 0.1M). Chromatography (7% EtOAc/hexanes) afforded **9la** (66 mg) in 93% yield as a white solid: $^1\text{H NMR}$ (500 MHz, CDCl_3) δ 7.26 (dd, $J = 8.5, 2.1$ Hz, 1H), 7.11 (d, $J = 7.2$ Hz, 1H), 7.08 (s, 2H), 7.06 (d, $J = 7.0$ Hz, 2H), 6.91 (dd, $J = 8.2, 2.0$ Hz, 1H), 6.86 (d, $J = 8.5$ Hz, 1H), 6.83 (d, $J = 6.9$ Hz, 2H), 6.78 (d, $J = 8.2$ Hz, 1H), 5.98 (d, $J = 4.1$ Hz, 1H), 5.97 (d, $J = 4.1$ Hz, 1H), 3.60 (d, $J = 13.2$ Hz, 1H), 3.49 (d, $J = 13.2$ Hz, 1H), 1.31 (s, 9H); $^{13}\text{C NMR}$ (125 MHz, CDCl_3) δ 178.2, 150.9, 148.2, 147.4, 147.1, 135.0, 132.3, 130.2, 128.3, 128.0, 127.2, 125.9, 123.4, 120.9, 110.1, 108.3, 108.1, 101.4, 57.1, 45.2, 34.7, 31.6; IR (film) 2960, 1798, 1504, 1487, 1456, 1440, 1365, 1241, 1145, 1084, 1061, 1040, 993, 970, 935, 898, 875, 818, 734, 700; HRMS (EI-TOF) calcd for $\text{C}_{26}\text{H}_{24}\text{O}_4$ $[\text{M}]^+$ $m/z = 400.1675$; found 400.1688. General procedure **H** was followed using 3-(benzo[d][1,3]dioxol-5-yl)-5-(tert-butyl)benzofuran-2(3H)-one and toluene. Chromatography (7% EtOAc/hexanes) provided **9la** (64 mg) in 90 % yield. See above for characterization.



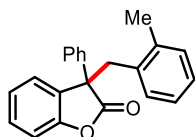
3-(4-Methylbenzyl)-3-phenylbenzofuran-2(3H)-one. General procedure **G** was followed with 3-phenylbenzofuran-2(3H)-one and *p*-xylene. Chromatography (7% EtOAc/hexanes) afforded **9ab** (38 mg) in 67% yield as a white solid: $^1\text{H NMR}$ (500 MHz, CDCl_3) δ 7.52 (d, $J = 8.0$ Hz, 2H), 7.38 (t, $J = 7.5$ Hz, 2H), 7.32 (t, $J = 7.8$ Hz, 1H), 7.29-7.23 (m, 2H), 7.19 (t, $J = 7.4$ Hz, 1H), 6.95 (d, $J = 7.9$ Hz, 1H), 6.88 (d, $J = 7.9$ Hz, 2H), 6.74 (d, $J = 8.0$ Hz, 2H), 3.69 (d, $J = 13.2$ Hz, 1H), 3.50 (d, $J = 13.2$ Hz, 1H), 2.22 (s, 3H); $^{13}\text{C NMR}$ (125 MHz, CDCl_3) δ 177.6, 153.2, 138.6, 136.8, 131.7, 130.0, 129.4, 129.2, 128.9, 128.8, 128.1, 127.1, 126.0, 124.0, 110.9, 57.6, 44.7, 21.1; IR (film) 2923, 1800, 1618, 1598, 1515, 1478, 1463, 1287, 1230, 1126, 1063, 1019, 954, 882, 815, 755, 730, 696, 652, 579; HRMS (EI-TOF) calcd for $\text{C}_{22}\text{H}_{18}\text{O}_2$ $[\text{M}]^+$ $m/z = 314.1307$; found 314.1305.

General procedure **H** was followed using 5-3-phenylbenzofuran-2(3H)-one and *p*-xylene. Chromatography (7% EtOAc/hexanes) provided **9ab** (23 mg) in 41% yield. See above for characterization.



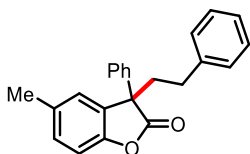
3-(3-Methylbenzyl)-3-phenylbenzofuran-2(3H)-one. General procedure **G** was followed with 3-phenylbenzofuran-2(3H)-one and *m*-xylene. Chromatography (7% EtOAc/hexanes) afforded **9ac** (43 mg) in 76% yield as a white solid: $^1\text{H NMR}$ (500 MHz, CDCl_3) δ 7.53 (d, $J = 7.1$ Hz, 2H), 7.38 (t, $J = 7.4$ Hz, 2H), 7.33 (t, $J = 7.3$ Hz, 1H), 7.28-7.23 (m, 2H), 7.19 (t, $J = 6.9$ Hz, 1H), 6.97-6.92 (m, 3H), 6.67 (s, 1H), 6.65 (d, $J = 7.3$ Hz, 1H), 3.70 (d, $J = 13.1$ Hz, 1H), 3.49 (d, $J = 13.1$ Hz, 1H), 2.15 (s, 3H); $^{13}\text{C NMR}$ (125 MHz, CDCl_3) δ 177.6, 153.2, 138.7, 137.6, 134.7, 131.0, 129.4, 129.2, 128.9, 128.1, 127.9, 127.2, 126.1, 126.1, 123.9, 110.9, 57.5, 45.0, 21.3; IR (film) 2960, 1798, 1478, 1462, 1447, 1228, 1125, 1096, 1062, 1036, 1019, 1002, 981, 955, 879, 789, 754, 728, 696, 655, 488; HRMS (EI-TOF) calcd for $\text{C}_{22}\text{H}_{18}\text{O}_2$ $[\text{M}]^+$ $m/z = 314.1307$; found 314.1317.

General procedure **H** was followed using 5-3-phenylbenzofuran-2(3H)-one and *m*-xylene. Chromatography (7% EtOAc/hexanes) provided **9ac** (30 mg) in 54% yield. See above for characterization.



3-(2-Methylbenzyl)-3-phenylbenzofuran-2(3H)-one. General procedure G was followed with 3-phenylbenzofuran-2(3H)-one and *o*-xylene. Chromatography (7% EtOAc/hexanes) afforded **9ad** (40 mg) in 72% yield a faint yellow solid: $^1\text{H NMR}$ (500 MHz, CDCl_3) δ 7.57 (d, $J = 7.2$ Hz, 2H), 7.40 (t, $J = 8.0$ Hz, 2H), 7.37-7.29 (m, 2H), 7.14 (td, $J = 7.6, 1.0$ Hz, 1H), 7.04-7.01 (m, 4H), 6.88 (t, $J = 6.4$ Hz, 1H), 6.62 (d, $J = 7.6$ Hz, 1H), 3.74 (d, $J = 13.8$ Hz, 1H), 3.64 (d, $J = 13.8$ Hz, 1H), 2.07 (s, 3H); $^{13}\text{C NMR}$ (125 MHz, CDCl_3) δ 177.8, 153.2, 138.4, 137.4, 133.5, 130.6, 129.8, 129.3, 128.9, 128.1, 127.4, 127.3, 126.4, 125.5, 123.8, 110.9, 56.6, 41.2, 20.0; IR (film) 2960, 1799, 1618, 1495, 1478, 1462, 1261, 1229, 1128, 1063, 1036, 1018, 980, 954, 881, 802, 755, 728, 695, 580, 487; HRMS (EI-TOF) calcd for $\text{C}_{22}\text{H}_{18}\text{O}_2$ $[\text{M}]^+$ $m/z = 314.1307$; found 314.1328.

General procedure H was followed using 5-3-phenylbenzofuran-2(3H)-one and *o*-xylene. Chromatography (7% EtOAc/hexanes) provided **9ad** (33 mg) in 58% yield. See above for characterization.



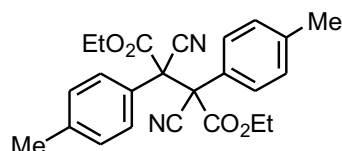
5-Methyl-3-phenethyl-3-phenylbenzofuran-2(3H)-one. General procedure G was followed with 5-methyl-3-phenylbenzofuran-2(3H)-one and ethylbenzene. Chromatography (7% EtOAc/hexanes) afforded **9be** (25 mg) in 43% yield as a faint yellow solid: $^1\text{H NMR}$ (500 MHz, CDCl_3) δ 7.41 (d, $J = 7.5$ Hz, 2H), 7.34 (t, $J = 7.6$ Hz, 2H), 7.29 (d, $J = 7.0$ Hz, 1H), 7.24 (d, $J = 7.7$ Hz, 2H), 7.18 (d, $J = 7.7$ Hz, 2H), 7.10 (m, 4H), 2.78-2.73 (m, 1H), 2.54-2.49 (m, 2H), 2.40 (s, 3H), 2.35- 2.30 (m, 1H); $^{13}\text{C NMR}$ (125 MHz, CDCl_3) δ 178.3, 151.4, 140.7, 138.9, 134.3, 129.9, 129.8, 128.9, 128.6, 128.4, 128.0, 126.8, 126.3, 125.5, 110.8, 56.0, 40.6, 31.4, 21.4; IR (film) 2962, 1798, 1601, 1484, 1448, 1260, 1228, 1131, 1091, 1063, 1018, 920, 888, 811, 734, 695, 648, 629, 507; HRMS (EI-TOF) calcd for fragments $\text{C}_{15}\text{H}_{12}\text{O}_2$ $[\text{M}-\text{PhCH}_2\text{CH}_2]^+$ $m/z = 224.0822$; found 224.0837 and C_8H_9 $[\text{PhCH}_2\text{CH}_2]^+$ $m/z = 105.0688$; found 105.0704.

General Procedure H was followed using 5-methyl-3-phenylbenzofuran-2(3H)-one and ethylbenzene. Chromatography (7% EtOAc/hexanes) provided **9be** (20 mg) in 34% yield. See above for characterization.

2. Mechanistic Studies

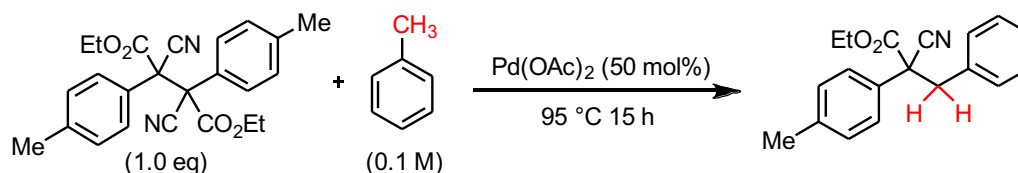
3-1. Cyanoarylacetate Dimer Studies

Preparation of Cu Complex. Cu(TMEDA)-Cl(OH) was prepared by sonicating CuCl with TMEDA in CH₃CN under aerobic conditions. Removal of the solvent yielded Cu(TMEDA)Cl(OH) as a blue-purple crystalline powder.¹⁰



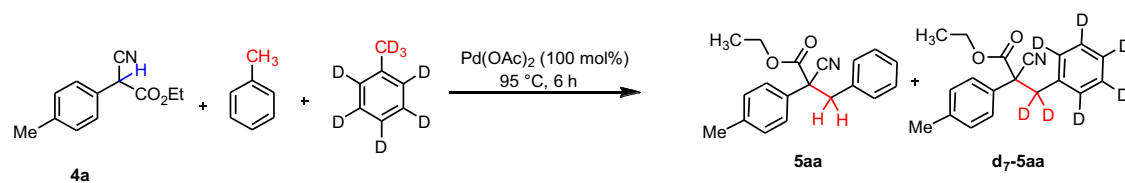
Diethyl 2,3-dicyano-2,3-di-*p*-tolylsuccinate 10. To a solution of ethyl 2-cyano-2-(*p*-tolyl)acetate (300 mg, 1.47 mmol) in MeOH (5 mL) was added Cu(TMEDA)Cl(OH) (60.6 mg, 10 mol%). After stirring for 5 min, the reaction mixture was quenched with 1 M HCl and extracted with EtOAc. Chromatography (10% EtOAc/hexanes) afforded a 1:1 mixture of the diastereomers of the title compound in 48% yield as a white oily solid: ¹H NMR (500 MHz, Chloroform-*d*) δ 7.13 (m, 5H), 6.98 (m, 3H), 4.47-4.34 (m, 2H), 4.33-4.21 (m, 2H), 2.36 (s, 6H), 1.33 (t, *J* = 7.1 Hz, 3H), 1.23 (t, *J* = 7.1 Hz, 3H); ¹³C NMR (126 MHz, Chloroform-*d*) δ 166.4, 144.7, 140.5, 140.4, 129.4, 129.3, 129.1, 128.7, 126.1, 116.4, 64.4, 64.2, 60.4, 21.3, 13.9, 13.7; IR (film) 2982, 2249, 1744, 1511, 1464, 1445, 1367, 1297, 1224, 1197, 1093, 1019, 850, 826, 789, 761, 726, 711, 695, 521, 510, 489 cm⁻¹; HRMS (ESI-TOF) (*m/z*): [M+H]⁺ calcd for C₂₄H₂₅N₂O₄, 405.1814; found, 405.1815.

Dimer with catalytic Pd



Cyanoarylacetate dimer **10** (20 mg, 0.049 mmol) and Pd(OAc)₂ (5.55 mg, 0.024 mmol) were added to a flame-dried 8 mL microwave vial equipped with a stirbar, and brought into the glovebox. Toluene (500 μL, 0.1 M) was added to the mixture. The microwave vial was sealed with a Teflon cap, removed from the glovebox and placed in a 95 °C oil bath. After 15 h, the mixture was allowed to cool to ambient temperature, diluted with CH₂Cl₂ (5 mL), passed through SiO₂ with 30% EtOAc/hexanes, and concentrated. The residue was analyzed using ¹H NMR in CDCl₃ solvent to determine the percentage of components using internal standard 4,4'-bis-*tert*-butyl-biphenyl (0.1 equiv) (NMR yield of **5aa** is 66%).

3-2. KIE Studies: d₈-toluene

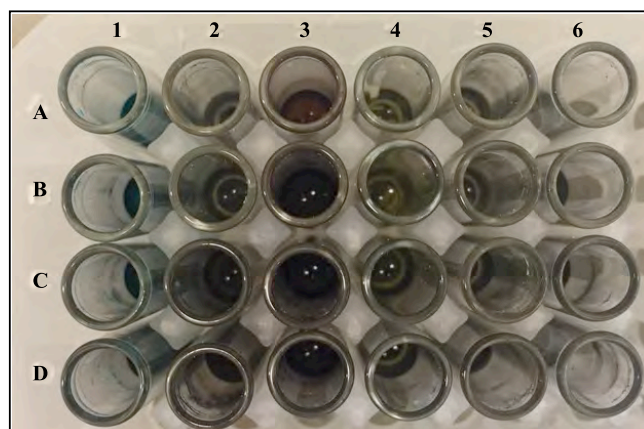
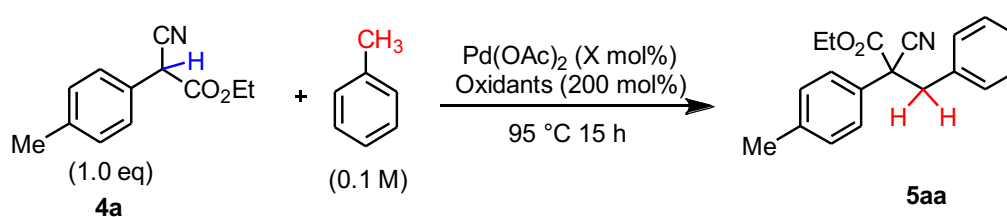


Ethyl 2-cyano-2-(*p*-tolyl)acetate **4a** (20 mg, 0.098 mmol) and Pd(OAc)₂ (22.06 mg, 0.098 mmol) were

added to a microwave vial followed by toluene (250 μ L, 2.35 mmol) and d_8 -toluene (250 μ L, 2.35 mmol). The vial was sealed with a Teflon cap, removed from the glovebox and placed in a 95 $^{\circ}$ C oil bath. After 7 h, the mixture was allowed to cool to ambient temperature, diluted with CH_2Cl_2 (1 mL), passed through SiO_2 with 30% EtOAc/hexanes, and concentrated. The resulting residue was chromatographed (7% EtOAc/hexanes) to afford a mixture of **5aa** and **d7-5aa** (22.4 mg) in 78% yield: $k_H/k_D = 2/1.028 = 1.945 \sim 2$. 1H NMR (500 MHz, Chloroform- d) δ 7.43 (d, $J = 8.3$ Hz, 2H), 7.26 (dt, $J = 4.7, 1.9$ Hz, 3H), 7.23-7.15 (m, 4H), 4.27-4.14 (m, 2H), 3.69 (d, $J = 13.7$ Hz, 1H), 3.31 (d, $J = 13.5$ Hz, 1H), 2.37 (s, 3H), 1.20 (t, $J = 7.1$ Hz, 3H).

4. Full Optimization Data

Table S1. HTE Study of Oxidants with Catalytic Pd.



HTE 24-well reactor

To a 24-well reactor equipped with 1 mL vials was added the indicated oxidant (Table S1, entries 1-6, 0.02 mmol, 200 μ L of a 0.1 M solution in THF), respectively. The solvent was evacuated on a Genevac. To A1:A6 vials was added $Pd(OAc)_2$ (0.0005 mmol) (25 μ L of a 0.02 M solution in THF), to B1:B6 vials was added $Pd(OAc)_2$ (0.001 mmol) (50 μ L of a 0.02 M solution in THF), to C1:C6 vials was added $Pd(OAc)_2$ (0.002 mmol) (75 μ L of a 0.02 M solution in THF) and to D1:D6 vials was added $Pd(OAc)_2$ (0.003 mmol) (100 μ L of a 0.02 M solution in THF). The solvent was evacuated on a Genevac. To each vial was added ethyl 2-cyano-2-(*p*-tolyl)acetate (0.01 mmol, 100 μ L of a 0.1 M solution in toluene). A parylene stir-bar was added to each vial. The reactor block was sealed, removed from the glovebox and stirred for 15 h on an Alligator tumble stirrer (1000 rpm) at 95 $^{\circ}$ C. The reactions were quenched via dilution with a solution of internal standard (4,4'-bis-*tert*-butyl-biphenyl) in MeCN (2.0 μ mol, 0.002 M, 500 μ L), and the contents were stirred for 15 minutes. Into a separate 24-well plate LC block was added 700 μ L of MeCN and 20 μ L of the diluted reaction mixtures. The 24-well plate LC block was sealed with a polypropylene 1 mL cap mat. The reaction mixtures were analyzed (P/IS and dimer/IS) using an Agilent

Technologies 1200 series HPLC with a 24 wellplate auto-sampler. Assay conditions: Acquity CORTECS BEH 1.6 μm C18; 50 mm x 2.1 mm; 1 mL/min; MeCN:H₂O:Ammonium Formate; gradient: 5% MeCN to 99% in 1.5 min, hold to 2.4 min to 5% MeCN at 2.41 min; ESC pos/neg; nebulizer: 700 L/hr; cone gas: 30 L/hr; source 150 °C; desolvation 450 °C; 210 nm: *t_R* of **5aa** = 5.36, IS = 7.24 and dimer = 5.48 min.

Catalyst quantity	Entry	1	2	3	4	5	6
5 mol% Pd(OAc) ₂	P/IS ^a	0.0	0.0	0.0	0.2	0.6	0.1
	Dimer/IS ^a	2.2	1.9	0.2	0.8	0.4	0.1
10 mol% Pd(OAc) ₂	P/IS ^a	0.4	0.0	0.0	0.3	0.7	0.1
	Dimer/IS ^a	2.0	2.2	0.0	0.8	0.4	0.1
20 mol% Pd(OAc) ₂	P/IS ^a	1.1	0.0	0.0	0.4	1.8	0.3
	Dimer/IS ^a	1.7	2.2	0.0	0.9	0.4	0.1
30 mol% Pd(OAc) ₂	P/IS ^a	1.3	0.0	0.0	0.5	2.4	0.6
	Dimer/IS ^a	1.5	2.1	0.0	1.2	0.0	0.2
oxidant		Cu(OAc)₂	Ag₂O	BQ	DMBQ	K₂S₂O₈	<i>t</i>BuootBu

^aDetermined by UPLC

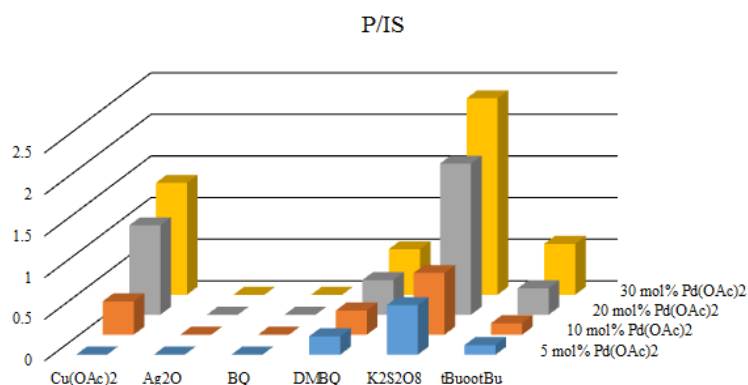
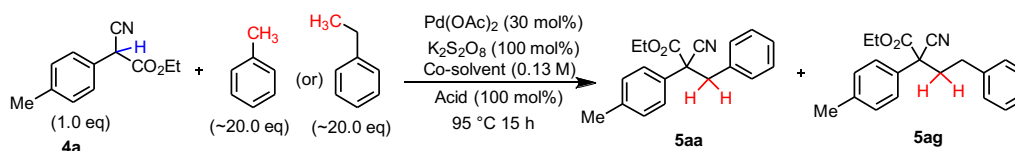


Table S2. HTE Screen of Co-solvents and Additives.

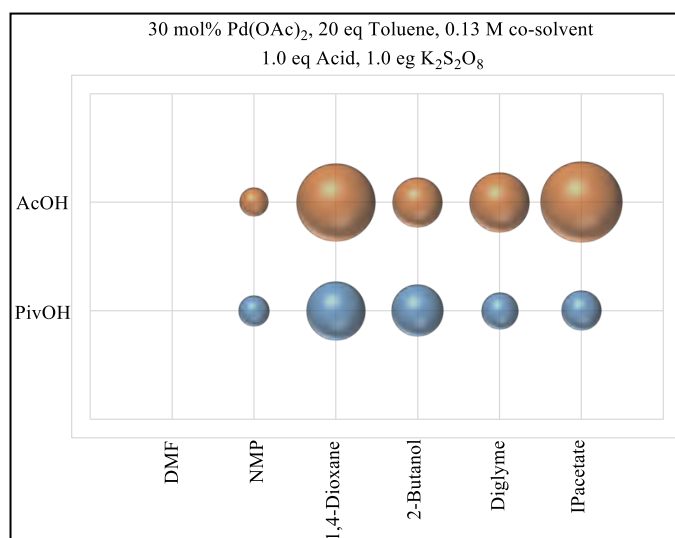


To a 24-well reactor equipped with 1 mL vials was added the was added Pd(OAc)₂ (0.003 mmol) (50 μL of a 0.078 M solution in THF). The solvent was evacuated on a Genevac. To each vial was added K₂S₂O₈ (0.01 mmol) (50 μL of a 0.26 M solution in THF). The solvent was evacuated on a Genevac. To A1:D1 vial was added ethyl 2-cyano-2-(*p*-tolyl)acetate (0.01 mmol, 100 μL of a 0.13 M solution in DMF). To A2:D2 vial was added ethyl 2-cyano-2-(*p*-tolyl)acetate (0.01 mmol, 100 μL of a 0.13 M solution in NMP). To A3:D3 vial was added ethyl 2-cyano-2-(*p*-tolyl)acetate (0.01 mmol, 100 μL of a 0.13 M solution in

1,4-dioxane). To A4:D4 vial was added ethyl 2-cyano-2-(*p*-tolyl)acetate (0.01 mmol, 100 μ L of a 0.13 M solution in 2-butanol). To A5:D5 vial was added ethyl 2-cyano-2-(*p*-tolyl)acetate (0.01 mmol, 100 μ L of a 0.13 M solution in diglyme). To A6:D6 vial was added ethyl 2-cyano-2-(*p*-tolyl)acetate (0.01 mmol, 100 μ L of a 0.13 M solution in isopropyl acetate). To A1:B6 vial was added toluene (28 μ L, 0.2 mmol). To C1:D6 vial was added ethylbenzene (32 μ L, 0.2 mmol). A parylene stir-bar was added to each vial. The reactor block was sealed, removed from the glovebox and stirred for 15 h on an Alligator tumble stirrer (1000 rpm) at 95 °C. The reactions were quenched via dilution with a solution of internal standard (4,4'-bis-*tert*-butyl-biphenyl) in MeCN (2.0 μ mol, 0.002 M, 500 μ L), and the contents were stirred for 15 minutes. Into a separate 24-well plate LC block was added 700 μ L of MeCN and 20 μ L of the diluted reaction mixtures. The 24-well plate LC block was sealed with a polypropylene 1 mL cap mat. The reaction mixtures were analyzed (P/IS and dimer/IS) using an Agilent Technologies 1200 series HPLC with a 24 wellplate auto-sampler. Assay conditions: Acquity CORTECS BEH 1.6 μ m C18; 50 mm x 2.1 mm; 1 mL/min; MeCN:H₂O:Ammonium Formate; gradient: 5% MeCN to 99% in 1.5 min, hold to 2.4 min to 5% MeCN at 2.41 min; ESC pos/neg; nebulizer: 700 L/hr; cone gas: 30 L/hr; source 150 °C; desolvation 450 °C; 210 nm: t_R of **5aa** = 5.36, IS = 7.24 and dimer = 5.48 min.

Acids		Entry	1	2	3	4	5	6
Toluene	PivOH	P/IS ^a	0.0	0.2	0.9	0.7	0.3	0.4
		Dimer/IS ^a	0.0	0.7	0.3	0.3	0.6	1.1
	AcOH	P/IS ^a	0.0	0.2	1.6	0.7	0.9	1.7
		Dimer/IS ^a	0.0	0.0	0.4	0.0	1.8	1.4
Ethyl benzene	PivOH	P/IS ^a	0.0	0.0	0.0	0.3	0.0	0.1
		Dimer/IS ^a	0.0	0.0	0.1	0.3	0.6	0.6
	AcOH	P/IS ^a	0.0	0.0	0.3	0.4	0.2	0.0
		Dimer/IS ^a	0.0	0.0	0.2	0.2	0.3	2.4
Solvents			DMF	NMP	Dioxane	butanol	Diglyme	Isoprpyl acetate

^aDetermined by UPLC



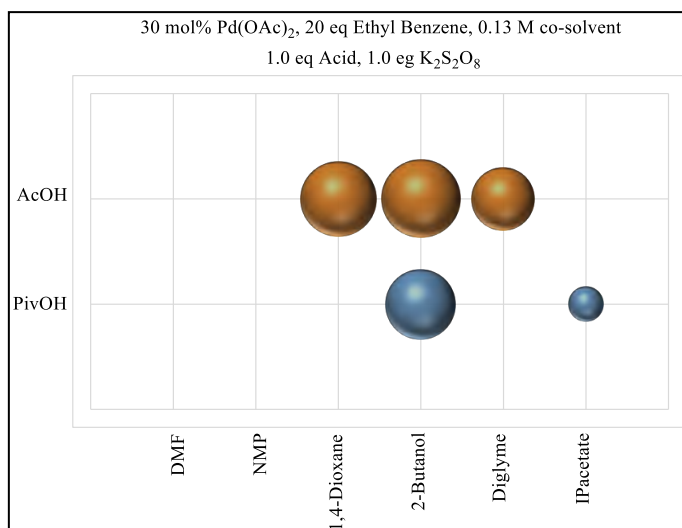
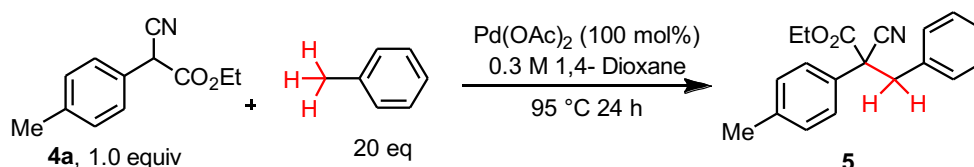


Table S3. Study of 1,4-Dioxane as Co-solvent with Stoichiometric Pd.



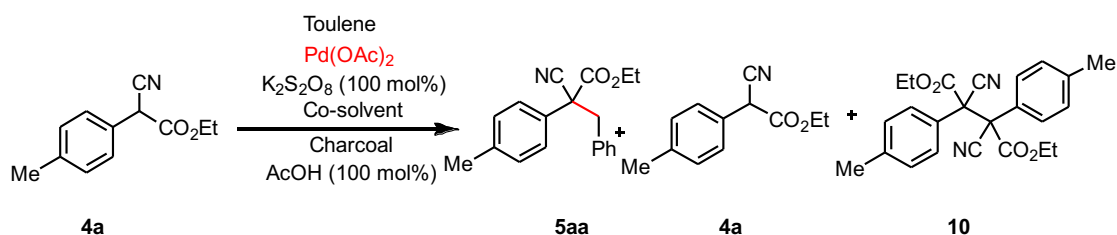
Ethyl 2-cyano-2-(*p*-tolyl)acetate (20 mg, 0.098 mmol) and Pd(OAc)₂ (22.1 mg, 0.098 mmol) and internal standard 4,4'-bis-*tert*-butyl-biphenyl (2.62 mg, 0.0098 mmol) were added to a flame-dried 8 mL microwave vial equipped with a stirbar and brought into the glovebox. The indicated tolyl analog (1.96 mmol) and 1,4-dioxane (320 μ L, 0.3 M) were added to the mixture. The microwave vial was sealed with a Teflon cap, removed from the glovebox, and placed in a 95 $^\circ$ C oil bath. After 24 h, the mixture was allowed to cool to ambient temperature, diluted with CH₂Cl₂ (5 mL), passed through SiO₂ with 30% EtOAc/hexanes, and concentrated. The residue was analyzed by ¹H NMR spectroscopy in CDCl₃ solvent to determine the percentage of components along with internal standard 4,4'-bis-*tert*-butyl-biphenyl (0.1 equiv).

Entry	Pd(OAc) ₂ equivalents (mol%)	Toluene (eq)	Co-Solvent 1,4-dioxane (quantity)	Temperature	Time (h)	% Components ^{a/b}		
						SM	Product	Dimer
1	100	~20	0.3 M	95 $^\circ$ C	24	9	68	2
2	100	~80	-	95 $^\circ$ C	24	10	62	-

^aConversion percentages were calculated using ¹H NMR with internal standard 4,4'- di-*ter*-butyl-biphenyl (0.1 equiv).

^bdata before normalization.

Table S4. Study of Catalytic Conditions at High Temperature.



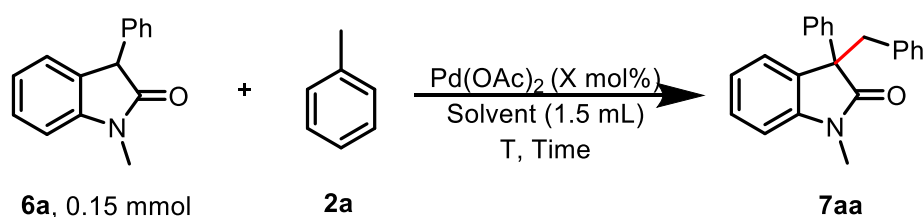
Entry	Pd(OAc) ₂ (mol%)	Toluene (eq)	Co-Solvent 1,4-dioxane (quantity)	Temperature	Time (h)	% Components ^a		
						SM	Product	Dimer
1	100	0.1 M	-	95 °C	15	14	86	-
2	30	20 eq	0.3 M	95 °C	45	38	59	3
3	30	20 eq	0.3 M	110 °C	72	18	82	-
4	10	20 eq	0.3 M	120 °C	45	33	67	-
5	20	20 eq	0.3 M	120 °C	45	18	82	-
6	30	20 eq	0.3 M	120 °C	45	12	88	-

^aConversion percentages were calculated using ¹H NMR with internal standard 4,4'-di-*tert*-butyl-biphenyl (0.1 equiv).

^bdata after normalization.

The study used general procedure to study the equivalents of Pd(OAc)₂ at different temperatures. After the respective times, the mixtures were allowed to cool to ambient temperature, diluted with CH₂Cl₂ (5 mL), passed through SiO₂ with 30% EtOAc/hexanes, and concentrated. The residue was analyzed by ¹H NMR spectroscopy in CDCl₃ solvent to determine the percentage of components along with internal standard 4,4'-bis-*tert*-butyl-biphenyl (0.1 equiv).

Table S5 Optimization Table for Oxindole 6a.



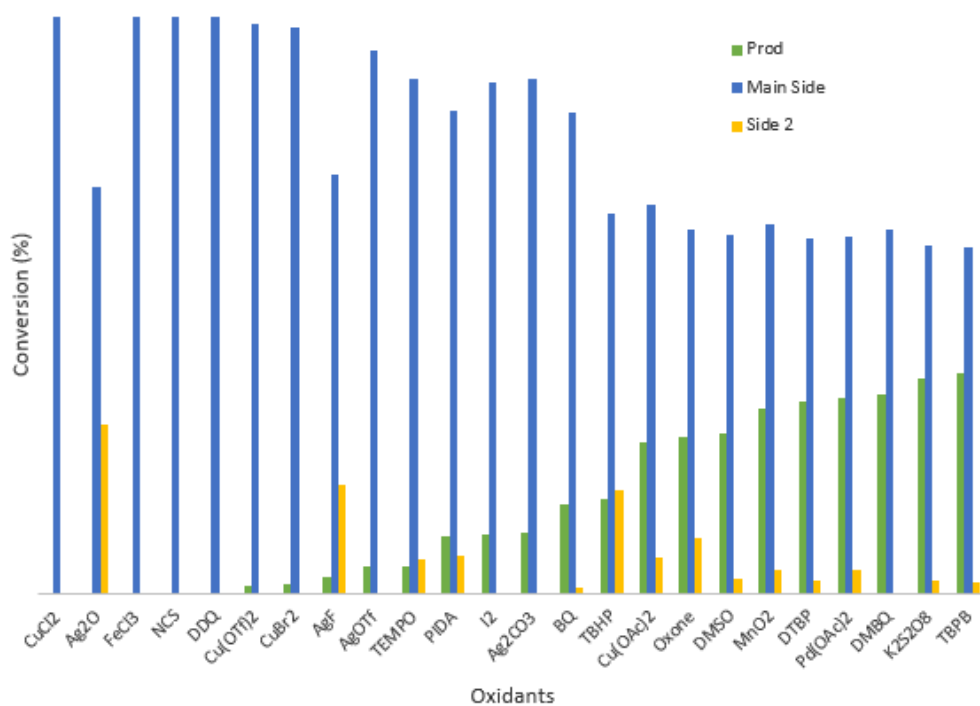
Entry	X	Solvent	T (°C)	Time (h)	Yield (%) ^b
1	100	Toluene	95	24	75
2	100	Dioxane	95	24	78 ^c
3	100	Dioxane	120	48	61 ^c
4	100	Toluene	120	48	80

5	100	Toluene	130	24	75
6	100	Toluene	120	24	81
7	120	Toluene	120	24	87
8	150	Toluene	120	24	96 (98) ^d

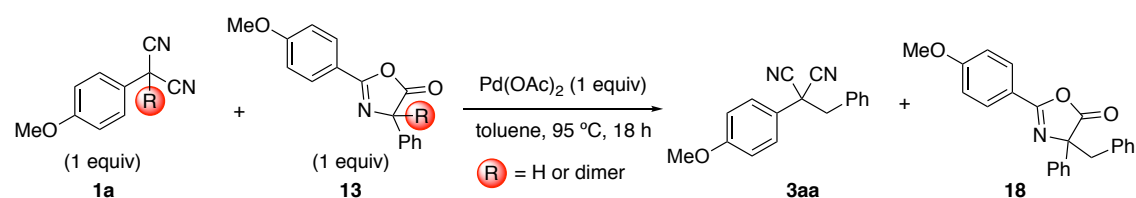
^a Reaction conditions: **6a** (0.15 mmol), **2a** (0.1 M), Pd(OAc)₂ (X mol%), solvent (1.5 mL) at T °C for indicated time under Argon unless otherwise specified. ^b Isolated yield. ^c **2a** (20 eq), dioxane (0.3 M) was employed. ^d run twice

Table S6 Oxidant Survey in the Oxindole Coupling

HTE oxidant screening was conducted in 10 μmol scale, using 24 different oxidants. The procedure was followed as described as Table S2.

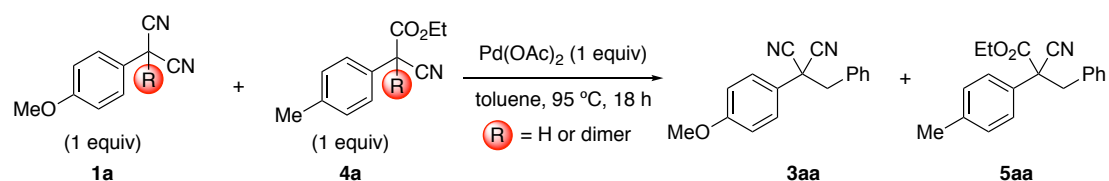


5. Competition Experiments.



To a dried microwave tube was added malononitrile **1a** (17.2 mg, 0.10 mmol, 1 equiv) or corresponding dimer (17.1 mg, 0.10 mmol, 1 equiv) followed by either azlactone **13** (26.7 mg, 0.10 mmol, 1 equiv) or corresponding dimer (26.6 mg, 0.10 mmol, 1 equiv) then 4,4'-di-*t*-Bu-biphenyl (10.5 mg, 0.08 mmol). The reaction vessel was brought into the glovebox before adding Pd(OAc)₂ (1 equiv) followed by toluene

(1 mL). The reaction was capped with a teflon-lined crimp cap, removed from the glovebox, then placed directly on 95 °C heat and stirred vigorously for 18 h. The reaction was cooled to room temperature, diluted with methylene chloride (approx. 4 mL), filtered through a plug of Celite (methylene chloride eluent), and concentrated by rotary evaporation. Reaction yields were determined by ¹H NMR analysis. **Monomers:** Mixture showed **3aa** (35%); **18** (54%). **Dimers:** Mixture showed **3aa** (19%), **18** (26%).



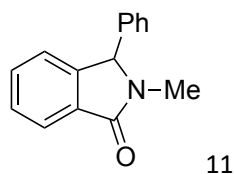
Monomers: To a dried pear flask was added malononitrile **1a** (17.2 mg, 0.10 mmol, 1 equiv) and 4,4'-di-*t*-Bu-biphenyl (10.5 mg, 0.08 mmol) before being brought into the glovebox, the mixture was dissolved in toluene (1 mL), sealed with a septa, removed from the glovebox, and placed under an argon atmosphere. To the pear flask was next added cyanoester **4a** (20.3 mg, 18.8 μL, 0.10 mmol, 1 equiv), before the substrate mixture was transferred to a separate microwave tube, under argon, containing Pd(OAc)₂ (22.4 mg, 0.10 mmol, 1 equiv) by syringe, and the reaction mixture placed directly on 95 °C heat and stirred vigorously for 18 h. The reaction was cooled to room temperature, diluted with methylene chloride (~ 4 mL), filtered through a plug of Celite (methylene chloride eluent), and concentrated by rotary evaporation. Reaction yields were determined by ¹H NMR. **Dimers:** Both dimers were solid and were prepared according to the **1a/13** procedure using **1a** dimer (17.1 mg, 0.10 mmol, 1 equiv) and **4a** dimer (20.2 mg, 0.10 mmol, 1 equiv). **Monomers:** Mixture showed **3aa** (84%). **Dimers:** Mixture showed **3aa** (43%).

6. BDE Calculations

Computational Methods

All structures were optimized using the uB3LYP¹¹⁻¹³ functional and 6-31g* basis set in Gaussian 09¹⁴. Frequency calculations were carried out at the same level of theory to confirm the local minima via the absence of imaginary frequencies. Global minima were found by performing dihedral scans using the PM3¹⁵ Hamiltonian.

Cartesian Coordinates

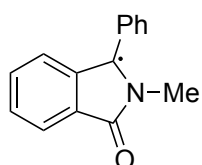


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G: -709.224795 Hartrees

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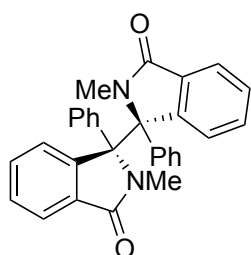


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C	2.48818200	0.72565600	-0.70942300
C	3.35637500	-1.52851700	0.68517000
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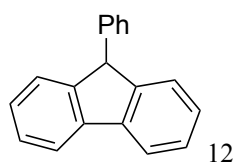
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C	1.44136200	-1.90467100	1.41692000
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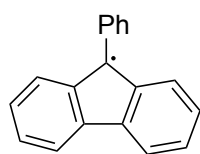
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C	2.51617400	3.01733800	0.34589000
C	1.29033500	3.46104500	-0.16270500
C	0.31891100	2.54340900	-0.57820300
C	0.59058600	1.18416000	-0.47754200
C	1.82175300	0.73486700	0.04061900
C	2.79115900	1.65221200	0.45214300
H	3.26084300	3.74229400	0.66394800
H	1.09045200	4.52684900	-0.23409000
H	-0.63568900	2.89009900	-0.96622700
H	3.74425800	1.31428800	0.85121100
C	-0.28225400	-0.00001200	-0.88390900
C	0.59062700	-1.18413300	-0.47757100
C	0.31903900	-2.54341800	-0.57824300
C	1.29049600	-3.46099100	-0.16275100
C	2.51632600	-3.01722900	0.34588000
C	2.79122300	-1.65210800	0.45216500
C	1.82176000	-0.73482000	0.04059900
H	-0.63555900	-2.89014000	-0.96625500
H	1.09068200	-4.52680400	-0.23417400
H	3.26100700	-3.74218100	0.66392000

H	3.74427500	-1.31406500	0.85124100
C	-1.68589700	-0.00005900	-0.29406500
C	-2.80882900	0.00000100	-1.12822800
C	-1.88158000	-0.00013900	1.09509600
C	-4.09996600	0.00000400	-0.59295900
H	-2.67316200	0.00004400	-2.20776600
C	-3.16694800	-0.00011900	1.63179200
H	-1.01824500	-0.00017100	1.75548800
C	-4.28256900	-0.00004100	0.78886600
H	-4.95948800	0.00010000	-1.25837900
H	-3.30001600	-0.00013500	2.71060100
H	-5.28494400	-0.00000100	1.20872600



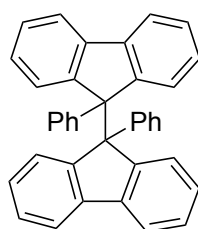
H: -731.577536 Hartrees

G: -731.632919 Hartrees

0 2

C	-2.67680800	3.01914600	-0.16069700
C	-1.34488800	3.45132400	-0.19599500
C	-0.29357900	2.53438000	-0.14320800
C	-0.58323000	1.16506400	-0.03813800
C	-1.94489000	0.73146800	-0.02792200
C	-2.98229700	1.65330100	-0.08451600
H	-3.48136300	3.74821100	-0.20400900
H	-1.12647400	4.51298200	-0.27305500
H	0.73343900	2.88145100	-0.19902400
H	-4.01909900	1.32589400	-0.07708600
C	0.27879500	0.00007500	0.00019200
C	-0.58312100	-1.16503400	0.03847400
C	-0.29338400	-2.53430100	0.14370200
C	-1.34462800	-3.45135100	0.19623900
C	-2.67657700	-3.01930900	0.16051700
C	-2.98216300	-1.65349600	0.08413900
C	-1.94480300	-0.73158600	0.02778400
H	0.73363400	-2.88132000	0.19980700
H	-1.12611000	-4.51297800	0.27341100
H	-3.48106400	-3.74846000	0.20363700
H	-4.01897800	-1.32614100	0.07638400
C	1.73714700	0.00012000	0.00004800

C	2.46671700	-0.94857200	-0.74961800
C	2.46687900	0.94871500	0.74957300
C	3.85888700	-0.94441800	-0.75128900
H	1.92979900	-1.66518700	-1.36295800
C	3.85909900	0.94447800	0.75099200
H	1.93018400	1.66537900	1.36305600
C	4.56318200	0.00002700	-0.00019700
H	4.39700000	-1.67669800	-1.34755900
H	4.39729400	1.67672900	1.34722200
H	5.64971500	-0.00004500	-0.00030800

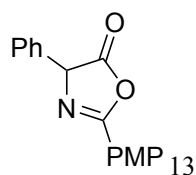


H: -1463.15725 Hartrees

G: -1463.24267 Hartrees

0 1			
C	-3.56632600	-1.43220400	-2.52492700
C	-2.92456600	-0.22240300	-2.80080800
C	-1.72686500	0.11797500	-2.16272200
C	-1.16429200	-0.75958100	-1.23517200
C	-1.83570300	-1.96264100	-0.94225900
C	-3.02502100	-2.30880100	-1.58568100
H	-4.49271500	-1.68493600	-3.03381000
H	-3.35915000	0.46908500	-3.51775500
H	-1.27289700	1.07629600	-2.38353500
H	-3.52742100	-3.24398700	-1.35187200
C	0.16024200	-0.67046700	-0.43231800
C	0.02686200	-1.91856600	0.46940400
C	0.83808400	-2.36861600	1.51287500
C	0.51319200	-3.55703100	2.17843600
C	-0.61004100	-4.30125200	1.80702600
C	-1.42965800	-3.85845400	0.76909500
C	-1.11058800	-2.66821000	0.11219300
H	1.71299300	-1.81028300	1.82376500
H	1.14540800	-3.90093400	2.99267100
H	-0.84819200	-5.22327500	2.33080300
H	-2.31185300	-4.42637500	0.48496900
C	1.34015600	-0.87164100	-1.43767500

C	2.34900000	-1.82736600	-1.22467600
C	1.40385200	-0.14934200	-2.64277000
C	3.37832600	-2.02920900	-2.14628900
H	2.33977900	-2.43599400	-0.33079800
C	2.43172700	-0.34456600	-3.56531800
H	0.64125800	0.57660700	-2.88277700
C	3.43117700	-1.28586800	-3.32303500
H	4.13634200	-2.77986500	-1.93744800
H	2.43876100	0.23847500	-4.48275200
H	4.22920700	-1.44413600	-4.04353500
C	0.20797600	0.69439600	0.47711600
C	-1.16001900	0.83143400	1.18465700
C	0.23030000	2.00589000	-0.34594200
C	-1.77290600	-0.00479100	2.11853400
C	-1.82067500	2.00525100	0.77706000
C	1.24546600	2.56027500	-1.12457200
C	-0.96077000	2.73516400	-0.15298700
C	-3.03896600	0.32667500	2.61425100
H	-1.28045200	-0.90072700	2.47639900
C	-3.08465600	2.33611000	1.26883500
C	1.04547400	3.79899600	-1.74504200
H	2.19254100	2.05268400	-1.25703100
C	-1.16163500	3.97146400	-0.76967600
C	-3.69517500	1.48523100	2.18957300
H	-3.51292300	-0.32683400	3.34180200
H	-3.58485300	3.24454800	0.94313800
C	-0.15308800	4.49762300	-1.57727300
H	1.83786400	4.22268800	-2.35619300
H	-2.08477700	4.52360900	-0.61314700
H	-4.67880300	1.72752200	2.58317000
H	-0.29326400	5.45992400	-2.06252600
C	1.39826700	0.74693600	1.46955200
C	1.20187300	1.01652200	2.83350000
C	2.72771100	0.61511500	1.02837200
C	2.27661700	1.12289500	3.71887000
H	0.19860900	1.14928100	3.21835600
C	3.80250100	0.71443300	1.91214600
H	2.93936700	0.41611000	-0.01312100
C	3.58506000	0.96642700	3.26683200
H	2.08120000	1.33041100	4.76794600
H	4.81451700	0.59761000	1.53265700
H	4.42198600	1.04566900	3.95552700

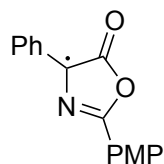


H: -897.679 Hartrees

G: -897.743 Hartrees

0 1

N	-0.72632000	-0.15875000	1.03634900
O	-2.22448200	2.78911500	-0.24865500
C	-1.96832300	0.59472000	0.91618100
H	-2.27559700	0.93973800	1.91527700
O	-0.22798900	1.70999700	-0.16490700
C	0.17414800	0.51133600	0.42309200
C	-1.58294000	1.84258200	0.10666100
C	-3.12603600	-0.18236800	0.29598600
C	-4.36253900	0.45042400	0.11289800
C	-2.97414700	-1.51914400	-0.08148900
C	-5.43191200	-0.24885200	-0.44484900
H	-4.48065100	1.49373600	0.39036700
C	-4.04906900	-2.21720400	-0.63635900
H	-2.01695200	-2.00647200	0.06906000
C	-5.27906700	-1.58561500	-0.82018700
H	-6.38587400	0.25221200	-0.58613300
H	-3.92142000	-3.25727500	-0.92505800
H	-6.11434600	-2.13008200	-1.25253200
C	1.58465200	0.16831000	0.27067600
C	2.46227500	0.98839100	-0.44812700
C	2.07713000	-1.01375500	0.85710900
C	3.80640500	0.64629800	-0.58808100
H	2.09233300	1.90120100	-0.90237500
C	3.40883900	-1.36019600	0.72368700
H	1.39524300	-1.64611200	1.41607300
C	4.28613600	-0.53248400	-0.00149200
H	4.46410300	1.29875100	-1.15012400
H	3.80418500	-2.26700600	1.16990800
O	5.57202000	-0.96327200	-0.07279000
C	6.51523400	-0.17488800	-0.78717400
H	7.46431400	-0.70793000	-0.71298400
H	6.23565000	-0.07432600	-1.84352300
H	6.62215300	0.82275900	-0.34278300

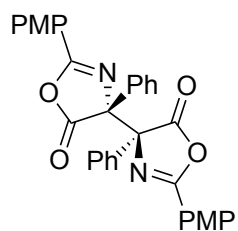


H: -897.085 Hartrees

G: -897.147 Hartrees

0 2

N	0.74411200	-0.39829900	0.00009300
O	2.11755000	2.81900000	-0.00011500
C	1.86897200	0.36089700	0.00003700
O	0.08368800	1.75941600	-0.00003100
C	-0.27272600	0.44486400	0.00010500
C	1.50009800	1.77763800	-0.00000300
C	3.20581500	-0.18497200	0.00000900
C	4.34356100	0.65315500	-0.00013200
C	3.38897300	-1.58623700	0.00011600
C	5.61894600	0.09830300	-0.00017100
H	4.20912900	1.72883500	-0.00019800
C	4.66767100	-2.12782100	0.00007800
H	2.51292700	-2.22595200	0.00022500
C	5.78882400	-1.28954100	-0.00006800
H	6.48709000	0.75180800	-0.00028400
H	4.79585500	-3.20695700	0.00016500
H	6.78812600	-1.71644400	-0.00010500
C	-1.67298800	0.10467100	0.00014700
C	-2.66613700	1.09950500	0.00028400
C	-2.06652300	-1.25256800	0.00006900
C	-4.01535000	0.76132200	0.00018100
H	-2.37319600	2.14403100	0.00036600
C	-3.40444600	-1.59395200	-0.00002200
H	-1.30014700	-2.02023700	0.00017700
C	-4.39279500	-0.59048100	-0.00009300
H	-4.76045600	1.54818900	0.00065600
H	-3.72270000	-2.63144000	-0.00010800
O	-5.67515700	-1.03295100	-0.00024400
C	-6.72771600	-0.07603000	-0.00018300
H	-6.69320400	0.55658200	-0.89591100
H	-7.65318300	-0.65367200	0.00020000
H	-6.69274100	0.55711000	0.89516900

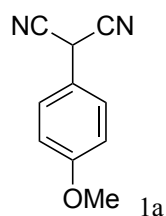


H: -1794.17 Hartrees

G: -1794.28 Hartrees

0 1			
N	-1.70524100	-0.69918300	0.39792200
O	-0.20405300	-0.05193300	-2.74862800
O	-2.22811000	-0.17350600	-1.74766100
C	-2.63106700	-0.45274300	-0.44832700
C	-0.84233500	-0.24331700	-1.75416300
C	0.32923600	-1.93432500	-0.24609700
C	1.29290900	-2.26584300	-1.20913400
C	0.07341700	-2.82788500	0.80382800
C	1.98497300	-3.47432200	-1.12059600
H	1.49214800	-1.58335300	-2.02684000
C	0.77276900	-4.03198300	0.88873100
H	-0.67473200	-2.57289900	1.54522800
C	1.72906100	-4.36021200	-0.07311800
H	2.72555800	-3.72203100	-1.87644500
H	0.56489600	-4.71484800	1.70826000
H	2.26992400	-5.30076900	-0.00807500
C	-4.06883400	-0.43696100	-0.20345400
C	-4.98033600	-0.16032200	-1.22907100
C	-4.55401100	-0.70693700	1.09099500
C	-6.35199200	-0.15060400	-0.98146300
H	-4.61481400	0.04944300	-2.22841900
C	-5.91292900	-0.69879000	1.34509400
H	-3.84479100	-0.92064700	1.88386200
C	-6.82460100	-0.42072200	0.30979400
H	-7.03645500	0.06633200	-1.79301800
H	-6.30355900	-0.90432700	2.33650300
C	0.43341600	0.60447200	0.30701300
C	2.63107600	0.45281100	0.44834600
C	-0.43341100	-0.60442600	-0.30700200
N	1.70524800	0.69923500	-0.39790800
C	0.84233900	0.24335500	1.75417100
O	0.20405800	0.05196300	2.74863600
O	2.22811800	0.17357100	1.74767700

C	4.06884300	0.43703500	0.20346900
C	4.98035400	0.16043000	1.22908800
C	4.55401000	0.70698900	-1.09098800
C	6.35200800	0.15070900	0.98147200
H	4.61484000	-0.04928500	2.22844900
C	5.91292500	0.69883000	-1.34509800
H	3.84478500	0.92067700	-1.88385600
C	6.82460300	0.42076400	-0.30980300
H	7.03648200	-0.06612300	1.79304600
H	6.30354800	0.90433300	-2.33651700
C	-0.32923800	1.93437000	0.24611500
C	-1.29296900	2.26584500	1.20910900
C	-0.07336000	2.82797400	-0.80375800
C	-1.98503400	3.47432300	1.12057900
H	-1.49225600	1.58331800	2.02677300
C	-0.77271400	4.03207200	-0.88865400
H	0.67483600	2.57302400	-1.54512300
C	-1.72906400	4.36025800	0.07315200
H	-2.72566500	3.72199700	1.87639400
H	-0.56479500	4.71497300	-1.70814100
H	-2.26992700	5.30081500	0.00811600
O	8.13593200	0.43840600	-0.66441400
O	-8.13593200	-0.43832100	0.66441100
C	-9.11337900	-0.16933200	-0.33201700
H	-10.07859800	-0.24088600	0.17172900
H	-8.99427800	0.83873300	-0.74910300
H	-9.07094000	-0.90594600	-1.14430800
C	9.11333300	0.16857100	0.33182600
H	8.99360000	-0.83947000	0.74878400
H	10.07852600	0.23954200	-0.17205200
H	9.07153000	0.90509800	1.14423300



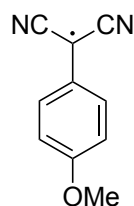
H: -570.37685 Hartrees

G: -570.43002 Hartrees

0 1

C	2.08685700	0.00184000	-0.28944600
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C	1.14670200	0.00806600	-1.33448700
C	-0.21003700	0.00672500	-1.05331600
C	-0.65930200	-0.00087200	0.27554100
C	0.27460100	-0.00700300	1.30870400
C	1.64557100	-0.00573800	1.03874400
H	1.50879200	0.01391800	-2.35730300
H	-0.92609700	0.01165600	-1.87081100
H	-0.05798900	-0.01293600	2.34404600
H	2.34842700	-0.01067200	1.86332600
C	4.39404700	-0.00237100	0.33340200
H	5.34709300	0.00045600	-0.19757300
H	4.32988400	0.88954900	0.96979000
H	4.32933400	-0.90165300	0.95928900
O	3.39038000	0.00379900	-0.67300600
C	-2.15761700	-0.00277600	0.59769800
H	-2.27861100	-0.00756000	1.68934100
C	-2.83505300	-1.21142000	0.08245100
C	-2.83595700	1.20976900	0.09292600
N	-3.34365700	-2.17355300	-0.31861300
N	-3.34530500	2.17491500	-0.29986600



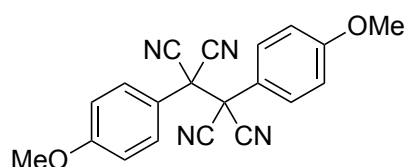
H: -569.775216 Hartrees

G: -569.82674 Hartrees

0 2

C	2.10734600	-0.29563800	-0.00018300
C	1.29059400	-1.44676000	-0.00005400
C	-0.08150500	-1.32785900	-0.00002800
C	-0.70294800	-0.04895900	-0.00001700
C	0.13212100	1.09510600	-0.00007400
C	1.51279700	0.97964100	-0.00014900
H	1.77109400	-2.41960200	-0.00002600
H	-0.69978000	-2.22018200	0.00004000
H	-0.31959200	2.08234200	-0.00006600
H	2.11973300	1.87724700	-0.00013200
C	4.33150300	0.58658500	0.00026600
H	5.33412100	0.15782900	0.00073500
H	4.19716100	1.20358700	-0.89610400

H	4.19644900	1.20369200	0.89648800
O	3.43832800	-0.52469800	-0.00010600
C	-2.13483900	0.08019800	-0.00000800
C	-2.97976400	-1.05579500	0.00012800
C	-2.76158500	1.35001300	-0.00001900
N	-3.65786000	-2.00700500	0.00006900
N	-3.25473000	2.40893100	0.00003700



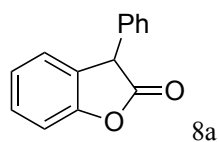
H: -1139.55881 Hartrees

G: -1139.63851 Hartrees

0 1

C	4.70936500	0.10843400	0.07160100
C	4.00887300	1.32016400	0.18417900
C	2.64121000	1.32079000	0.40671000
C	1.93678100	0.11047100	0.52124200
C	2.63969400	-1.09321700	0.41601400
C	4.01565000	-1.10248900	0.19152200
H	4.56003900	2.25038700	0.09593800
H	2.12205900	2.26928400	0.49566600
H	2.12154100	-2.04163300	0.51234800
H	4.52920700	-2.05332200	0.11651000
C	6.81192500	-0.97271100	-0.27715500
H	7.83783000	-0.64513600	-0.45120900
H	6.77358700	-1.57897400	0.63673500
H	6.47197100	-1.57468600	-1.12915200
O	6.04424200	0.21748000	-0.14356600
C	0.41282500	0.11020900	0.71817000
C	-0.02029700	1.30034300	1.47577200
C	-0.02113100	-1.08131400	1.47320600
N	-0.34157300	2.24896200	2.06052700
N	-0.34445400	-2.03177500	2.05388600
C	-0.41281300	0.10995600	-0.71815200
C	-1.93676600	0.11030600	-0.52121100
C	0.02031500	1.29981300	-1.47618300
C	0.02112300	-1.08184600	-1.47276200
C	-2.64115200	1.32066400	-0.40684200
C	-2.63971600	-1.09334400	-0.41579500

N	0.34158600	2.24821100	-2.06130000
N	0.34441800	-2.03251900	-2.05310800
C	-4.00881200	1.32011700	-0.18429200
H	-2.12196800	2.26912800	-0.49593500
C	-4.01567000	-1.10253700	-0.19128400
H	-2.12159500	-2.04179100	-0.51199900
C	-4.70934300	0.10842600	-0.07153100
H	-4.55994600	2.25037000	-0.09617600
H	-4.52925700	-2.05334300	-0.11612500
O	-6.04421400	0.21754700	0.14363200
C	-6.81202200	-0.97260400	0.27685300
H	-7.83785700	-0.64497500	0.45121700
H	-6.77391700	-1.57849300	-0.63729500
H	-6.47199500	-1.57497600	1.12854100

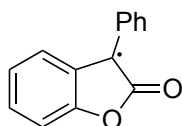


H: -689.754592 Hartrees

G: -689.80672 Hartrees

0 1			
C	-3.31099600	0.17226200	0.65586000
C	-2.04566000	0.58076000	0.26687900
C	-1.19021600	-0.20685600	-0.50308900
C	-1.60851400	-1.46879600	-0.91085100
C	-2.88262200	-1.91165700	-0.53385900
C	-3.71944000	-1.10011200	0.23863300
H	-3.94751700	0.81462300	1.25477900
H	-0.95647800	-2.10221000	-1.50599600
H	-3.22354300	-2.89483400	-0.84460700
H	-4.70461600	-1.45951000	0.52219700
C	0.07489700	0.57774500	-0.73770800
H	0.16502100	0.86762200	-1.79413900
C	-0.22619800	1.88875900	0.03032700
O	0.46256200	2.85942000	0.15648100
O	-1.49322100	1.80949300	0.59053300
C	1.39812900	-0.03732500	-0.29932400
C	2.58951700	0.42423400	-0.87277000
C	1.45949000	-1.02158600	0.69370800
C	3.81920800	-0.09192400	-0.46597200
H	2.55260100	1.19697400	-1.63621800

C	2.69051900	-1.53980200	1.09946500
H	0.54364200	-1.38848700	1.14752000
C	3.87326500	-1.07768500	0.52134700
H	4.73460000	0.27531800	-0.92204900
H	2.72251000	-2.30569900	1.86982600
H	4.83078500	-1.48319300	0.83670500

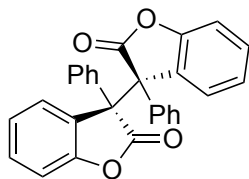


H: -689.148508 Hartrees

G: -689.199781 Hartrees

0 2

C	3.55022600	0.25359700	0.04601500
C	2.21346600	0.60657700	0.06261700
C	1.15391600	-0.33301600	-0.03627100
C	1.48720900	-1.69553800	-0.20312100
C	2.82682800	-2.06581100	-0.22217500
C	3.84726000	-1.10738700	-0.09072900
H	4.32542400	1.00770700	0.12837900
H	0.71567000	-2.44429300	-0.34066000
H	3.09074400	-3.11144600	-0.34990800
H	4.88575700	-1.42520500	-0.10845400
C	-0.05839200	0.41877700	0.01112600
C	0.34440700	1.83363400	0.10958400
O	-0.30238500	2.85503600	0.16296300
O	1.75034100	1.88632900	0.15724900
C	-1.43728900	-0.02158200	0.00903600
C	-2.48172800	0.85627000	-0.37186200
C	-1.78571200	-1.33776600	0.39475600
C	-3.80154000	0.42086600	-0.39077900
H	-2.23837600	1.87383300	-0.65075600
C	-3.10910400	-1.76196500	0.37856600
H	-1.01716900	-2.01242500	0.75406900
C	-4.12449400	-0.88843400	-0.02199700
H	-4.58582600	1.10843200	-0.69546700
H	-3.35189100	-2.77447700	0.68951200
H	-5.15830700	-1.22237800	-0.03701200



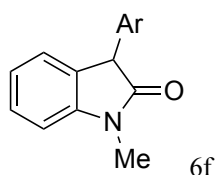
H: -1378.30879 Hartrees

G: -1378.3868 Hartrees

0 1

C	3.60444700	1.78435400	1.30297600
C	2.29426500	1.34627900	1.21870600
C	1.59577400	1.17546100	0.02578900
C	2.26804100	1.43877300	-1.16886400
C	3.59499500	1.88272700	-1.12166100
C	4.25487600	2.05996700	0.09678900
H	4.09176200	1.89778400	2.26533100
H	1.77420900	1.28414900	-2.11925700
H	4.11741600	2.08815300	-2.05146700
H	5.28414900	2.40705000	0.11191900
C	0.31254200	0.56527200	1.91737400
O	-0.49249100	0.16541700	2.71641600
O	1.54196300	1.00945100	2.33184700
C	-0.90225400	1.80764400	0.12699100
C	-2.14213300	1.74064600	0.78504800
C	-0.67754500	2.86771200	-0.76280700
C	-3.12662300	2.69989700	0.54689400
H	-2.33207300	0.95281000	1.50267900
C	-1.66502400	3.82430300	-0.99896600
H	0.27195300	2.95550600	-1.27560400
C	-2.89496100	3.74462700	-0.34729200
H	-4.07589900	2.62831400	1.07091800
H	-1.46532700	4.63453500	-1.69495700
H	-3.66262900	4.49169100	-0.53033700
C	-0.23482100	-0.67783000	-0.34155300
C	-1.50683600	-1.35234400	0.17952600
C	-2.46550100	-1.30580300	-0.83044100
C	0.17871600	0.71944700	0.37053200
C	0.94217300	-1.67522000	-0.37135800
C	1.46770300	-2.16225000	0.83681900
C	1.49146400	-2.15388300	-1.56839400
C	2.50811500	-3.08940700	0.84752700
H	1.06813800	-1.82619700	1.78704400
C	2.52852500	-3.08951500	-1.55659400

H	1.12641800	-1.79354800	-2.52240600
C	3.04328300	-3.56163500	-0.35146400
H	2.89615200	-3.44412500	1.79851300
H	2.93354000	-3.44410800	-2.50060300
H	3.85174700	-4.28743000	-0.34431000
C	-0.70490800	-0.30125000	-1.78339100
O	-0.08840800	0.23490400	-2.66632300
O	-2.00876500	-0.66788300	-1.97140400
C	-3.72968500	-1.86214000	-0.73702700
C	-4.04011800	-2.51996200	0.45603700
H	-5.02038200	-2.97183700	0.57810400
C	-3.09699000	-2.61075900	1.48348500
C	-1.82718200	-2.03859300	1.35124900
H	-1.12043300	-2.12171500	2.16523900
H	-3.34857200	-3.13439700	2.40093600
H	-4.43058500	-1.79086500	-1.56161800



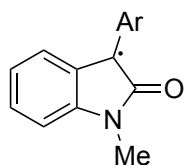
Ar = PMP

H: -823.655215 Hartrees

G: -823.717465 Hartrees

0 1			
C	2.64554100	-0.06000300	0.21894100
C	1.70890300	-1.93227000	-0.98495400
C	2.77260500	-2.72491000	-0.52648400
C	3.75574000	-2.17481300	0.29673800
C	3.70824500	-0.82852000	0.68288500
C	1.23759200	1.71874300	-0.19551800
H	0.93936700	-2.35972700	-1.62257600
H	2.82969400	-3.77042500	-0.81495100
H	4.57542500	-2.79650100	0.64678100
H	4.47729200	-0.40498600	1.32141300
C	0.65950800	0.49359300	-0.95414400
H	0.73270600	0.74569300	-2.02203400
C	1.64583100	-0.59899100	-0.60941500
C	3.19889400	2.17523800	1.27426100
H	3.25134300	1.81115300	2.30733400
H	4.21695200	2.25390400	0.87435500

H	2.72628500	3.15878200	1.25939000
O	0.78872300	2.84879200	-0.17227500
N	2.38795800	1.29746600	0.45724700
C	-0.80748900	0.26423000	-0.62076200
C	-1.22652300	-0.69125300	0.30583100
C	-1.78432500	1.07310400	-1.22458900
C	-2.57883400	-0.85630000	0.62280200
H	-0.49405800	-1.32881200	0.79178400
C	-3.12953400	0.92325700	-0.92000800
H	-1.48083200	1.83778200	-1.93413800
H	-2.86417100	-1.61355100	1.34435700
H	-3.88564300	1.54617500	-1.38766200
O	-4.88331000	-0.12005100	0.23585100
C	-5.35140300	-1.07474900	1.17353800
H	-6.43636700	-0.95803400	1.20457300
H	-5.10642900	-2.09989900	0.86443600
H	-4.93887200	-0.89383300	2.17515200
C	-3.53836700	-0.04634100	0.00795300



Ar = PMP

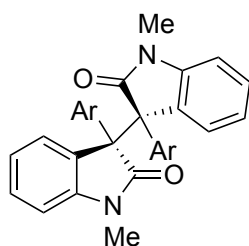
H: -823.048748 Hartrees

G: -823.109926 Hartrees

0 2

C	1.64680300	-0.67659600	-0.05076800
C	2.86604000	0.07120800	0.01634200
C	4.11330500	-0.54059700	-0.01622900
C	4.15759600	-1.93418500	-0.13795500
C	2.98018500	-2.69074400	-0.24190600
C	1.73222600	-2.07490300	-0.20630700
C	0.56390500	0.25772200	0.00046200
C	1.17694200	1.60964600	0.06131800
H	5.02695200	0.04291500	0.04193900
H	5.12180900	-2.43424100	-0.16615300
H	3.04313500	-3.76844400	-0.36094100
H	0.83597300	-2.67259200	-0.32729700
C	3.51726400	2.50759000	0.15368700

H	4.14128800	2.43619100	1.05262600
H	4.16782500	2.51552000	-0.72945100
H	2.94207700	3.43456300	0.18672900
N	2.56753600	1.41934800	0.09198800
O	0.64386300	2.71737100	0.09780500
C	-0.86001300	0.02791600	0.03681100
C	-1.40936400	-1.21398800	0.45091900
C	-1.77474300	1.04455700	-0.32790800
C	-2.77417500	-1.43123500	0.47248700
H	-0.75220600	-1.99875600	0.80655200
C	-3.14822500	0.83081100	-0.31455700
H	-1.38728500	2.01160800	-0.62255600
C	-3.66115000	-0.41334200	0.08003100
H	-3.18764000	-2.37853200	0.80431300
H	-3.80950200	1.63629800	-0.61315800
O	-4.98269400	-0.73021900	0.12847500
C	-5.93122500	0.26358200	-0.23506300
H	-5.80210500	0.57932500	-1.27820300
H	-6.91082300	-0.20253100	-0.11680800
H	-5.86382900	1.14136200	0.42007300



Ar = PMP

H: -1646.11137 Hartrees

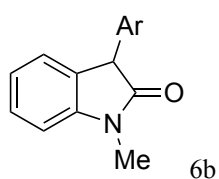
G: -1646.20861 Hartrees

0 1

C	-3.97016000	-0.75488800	-2.21215300
C	-2.64297600	-0.44681000	-1.92942300
C	-2.21225600	-0.07673500	-0.64258700
C	-3.14925200	-0.02021100	0.38485900
C	-4.49330500	-0.32606700	0.11976500
C	-4.89543900	-0.68929000	-1.16455600
H	-4.27926700	-1.04145400	-3.21233700
H	-2.85385500	0.26045900	1.38933400
H	-5.22117000	-0.27729200	0.92451800
H	-5.93812400	-0.92510900	-1.36033400
C	-0.38135400	-0.14145200	-2.17734200

O	0.69847100	-0.07624700	-2.73709000
C	-0.30023900	1.63975300	-0.42038200
C	1.00397600	2.08509500	-0.71981300
C	-1.20206100	2.58608400	0.07759900
C	1.38516100	3.40101800	-0.49780100
H	1.71604500	1.39929300	-1.15796500
C	-0.83143100	3.91545600	0.30483400
H	-2.22509100	2.30159000	0.29219100
C	0.47304400	4.32947800	0.02250100
H	2.39088700	3.73566600	-0.73270400
H	-1.57010600	4.60853500	0.69165500
C	0.05323400	-0.86423800	0.30837000
C	-0.38873100	-0.69988900	1.76148300
C	-0.93975600	-1.91394300	2.20867700
C	-0.70167700	0.17449800	-0.67579300
C	1.59794700	-0.92036600	0.18981400
C	2.43314500	-0.26953300	1.11533300
C	2.22519800	-1.65407900	-0.82743800
C	3.81742700	-0.33109300	1.02142500
H	2.00684900	0.29336900	1.93539600
C	3.61468100	-1.72895700	-0.93252100
H	1.62629300	-2.18188100	-1.55653600
C	4.42347200	-1.06130000	-0.00791400
H	4.44865200	0.17846900	1.74286200
H	4.04709400	-2.30900500	-1.73988100
C	-0.49097100	-2.29061100	-0.00777700
O	-0.50900300	-2.84877500	-1.09387600
C	-1.41714100	-2.08573600	3.50341900
C	-1.35001200	-0.99166600	4.37448700
H	-1.71751900	-1.09818700	5.39152800
C	-0.82496500	0.22780700	3.94852900
C	-0.34088100	0.37782600	2.63917500
H	0.04880500	1.33673600	2.31730400
H	-0.78717800	1.07090900	4.63220700
H	-1.83777700	-3.03233600	3.82795300
N	-0.95601000	-2.84650700	1.16629600
N	-1.56807700	-0.44739600	-2.81537000
C	-1.54245600	-4.16866400	1.23598900
H	-1.44254700	-4.62127600	0.24841300
H	-1.02075300	-4.78529600	1.97661200
H	-2.60440800	-4.11041400	1.50344900
C	-1.63054900	-0.83803600	-4.20712900
H	-2.32852700	-0.19840200	-4.75958700
H	-0.62739800	-0.72476500	-4.62023600

H	-1.94733300	-1.88347000	-4.30251100
O	5.78860800	-1.06565700	-0.01602300
O	0.94752900	5.59686800	0.20465100
C	0.05444600	6.58101200	0.69857600
H	-0.31833200	6.32442400	1.69942900
H	0.62990300	7.50692400	0.75587400
H	-0.80010200	6.72658800	0.02436000
C	6.44871300	-1.78535000	-1.04476100
H	6.19142600	-1.39692000	-2.03893300
H	7.51730300	-1.64725300	-0.86879200
H	6.21102100	-2.85677200	-1.00571500



Ar = *p*-tol

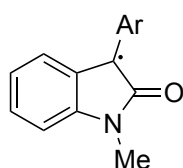
H: -748.456678 Hartrees

G: -748.517611 Hartrees

0 1

C	2.33627800	0.05923100	0.14455300
C	1.47149000	-1.96352800	-0.85188700
C	2.62165700	-2.63841100	-0.41442800
C	3.61105000	-1.95622100	0.29454400
C	3.48399600	-0.59131300	0.58573700
C	0.76920800	1.69377400	-0.29361300
H	0.69723300	-2.49421200	-1.39987000
H	2.74089300	-3.69625200	-0.62961900
H	4.49786200	-2.48781200	0.62897000
H	4.25750900	-0.06497800	1.13632700
C	0.24187500	0.37529100	-0.92260600
H	0.22598700	0.55184400	-2.00767900
C	1.32998600	-0.61323100	-0.57035000
C	2.78052900	2.40277600	0.99689000
H	2.92902700	2.12226100	2.04648100
H	3.76079000	2.52525600	0.52083500
H	2.23255100	3.34516500	0.94670200
O	0.23534800	2.78597600	-0.31927100
N	1.98891200	1.40848600	0.30369900
C	-1.17886000	0.06629500	-0.47365500
C	-2.25062500	0.72361200	-1.09149500

C	-1.45710000	-0.81519500	0.57584400
C	-3.56066200	0.49724100	-0.67710300
H	-2.05349200	1.42949300	-1.89382600
C	-2.77201400	-1.03981700	0.98585600
H	-0.64414100	-1.33261600	1.07663300
C	-3.84739800	-0.39299900	0.36673400
H	-4.37505900	1.02172400	-1.17238900
H	-2.96307800	-1.73044100	1.80455200
C	-5.27255000	-0.66212600	0.79066700
H	-5.73888000	-1.43122300	0.16010300
H	-5.32237400	-1.01631300	1.82572300
H	-5.89114800	0.23861800	0.71120600



Ar = *p*-tol

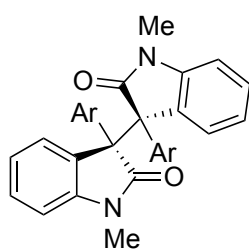
H: -747.848733 Hartrees

G: -747.909108 Hartrees

0 2

C	1.25359800	-0.68648400	0.05019700
C	2.49824000	0.01874500	-0.02844900
C	3.72279900	-0.63839100	-0.01028700
C	3.71675300	-2.03271000	0.10822900
C	2.51361300	-2.74788800	0.22293500
C	1.28900200	-2.08818100	0.20193000
C	0.20507900	0.28276800	0.01174600
C	0.86305900	1.61361600	-0.05578600
H	4.65677800	-0.08916100	-0.07742300
H	4.66238500	-2.56751600	0.12535500
H	2.54013100	-3.82737400	0.33886100
H	0.37123900	-2.65103700	0.32904400
C	3.23277600	2.43091700	-0.17338100
H	3.89343100	2.41614100	0.70199300
H	3.84279400	2.33821300	-1.07985200
H	2.68962100	3.37721300	-0.19973600
N	2.24669100	1.37580900	-0.09990800
O	0.36670100	2.73734900	-0.08781100
C	-1.22916600	0.09855300	-0.00596400
C	-1.81765400	-1.10988500	-0.44790500

C	-2.10442700	1.13371000	0.40555100
C	-3.19613600	-1.27996500	-0.45110300
H	-1.18857000	-1.90032700	-0.84124200
C	-3.47984700	0.94682900	0.40221700
H	-1.68363400	2.08013700	0.72092600
C	-4.05778200	-0.26226700	-0.01572200
H	-3.61561900	-2.21683700	-0.81115300
H	-4.12463400	1.75909100	0.73092900
C	-5.55287100	-0.46255800	0.01484700
H	-5.86899300	-1.23860100	-0.69007700
H	-5.89115100	-0.77171500	1.01344900
H	-6.08643500	0.46147600	-0.23354800



Ar = *p*-tol

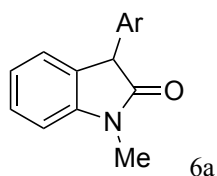
H: -1495.71336 Hartrees

G: -1495.81014 Hartrees

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C	-3.94652800	0.93395700	-1.77338000
C	-2.56954500	0.81672400	-1.61098100
C	-1.96471800	0.72507100	-0.34459600
C	-2.77562600	0.74650100	0.78627000
C	-4.16689500	0.86464900	0.64371000
C	-4.74217900	0.95738600	-0.62263700
H	-4.39159500	1.00077000	-2.76103400
H	-2.34506400	0.67570100	1.77859200
H	-4.79501900	0.88455800	1.52960200
H	-5.82044200	1.04854700	-0.72331300
C	-0.33515900	0.59659500	-2.08939100
O	0.67810800	0.52357500	-2.76086600
C	0.35365400	1.80491600	-0.00425000
C	1.69368500	1.98995900	-0.39083800
C	-0.21604900	2.77207300	0.83486000
C	2.42819800	3.07962000	0.07052200
H	2.15187500	1.29573300	-1.08203700
C	0.52752000	3.86133900	1.29285700
H	-1.25478600	2.69183300	1.13119200

C	1.86558200	4.03423600	0.92785000
H	3.46076400	3.19274700	-0.25347300
H	0.04885800	4.59288900	1.94055900
C	0.06402700	-0.80857600	0.09053100
C	-0.20971100	-0.91660700	1.59011700
C	-1.03417400	-2.03215200	1.82132000
C	-0.44922200	0.59526500	-0.52473400
C	1.52585400	-1.20502200	-0.24818400
C	2.56969000	-0.99770300	0.66357200
C	1.85245300	-1.81769100	-1.47099400
C	3.88129100	-1.36913200	0.36423000
H	2.37389600	-0.54870700	1.62842400
C	3.16141800	-2.19055200	-1.76103700
H	1.07855000	-2.00541100	-2.20232100
C	4.20569000	-1.97227200	-0.85316200
H	4.66212300	-1.18889300	1.10001300
H	3.37275000	-2.66168700	-2.71882500
C	-0.86898600	-1.92909600	-0.46303600
O	-1.11869100	-2.16774900	-1.63420900
C	-1.44282600	-2.40811100	3.09619900
C	-1.01787100	-1.62461000	4.17586900
H	-1.32436700	-1.89507700	5.18266300
C	-0.21579400	-0.50289800	3.97019400
C	0.19205300	-0.14514100	2.67532500
H	0.80071700	0.73998200	2.53089400
H	0.09867900	0.10217300	4.81553300
H	-2.07875500	-3.27401300	3.25144600
N	-1.37986100	-2.63412100	0.60679700
N	-1.60154300	0.77288700	-2.61187800
C	-2.29447800	-3.74649100	0.45453400
H	-2.39273700	-3.94239900	-0.61409700
H	-1.90535800	-4.63914100	0.95718100
H	-3.27894000	-3.50209400	0.87134100
C	-1.86825400	0.77307100	-4.03419500
H	-2.39806400	1.68587800	-4.33000800
H	-0.90514900	0.72932000	-4.54436500
H	-2.46918200	-0.09987300	-4.31541900
C	5.62231700	-2.37931800	-1.18294100
H	5.69173300	-3.45387800	-1.39375400
H	5.99143000	-1.85467900	-2.07324800
H	6.30585000	-2.15634500	-0.35740700
C	2.67847100	5.20104100	1.43742700
H	3.38034700	4.88755400	2.22184600
H	3.27495000	5.65383500	0.63694900

H	2.03810100	5.98051700	1.86304000
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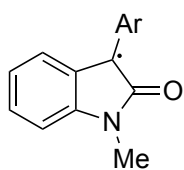


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H: -709.168029 Hartrees

G: -709.224027 Hartrees

0 1			
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C	1.96611100	0.14814000	-0.06208700
C	0.95859300	-0.61384600	0.55386900
C	1.15873800	-1.96672500	0.78066300
C	2.37234900	-2.55418200	0.39167400
C	3.36395800	-1.78361700	-0.21672300
H	3.95102800	0.17871300	-0.92900200
H	0.38170100	-2.56594300	1.24811000
H	2.53906300	-3.61327400	0.56503000
H	4.30025100	-2.24801700	-0.51429100
C	-0.20983500	0.29212300	0.87276600
H	-0.30853900	0.42024400	1.95974500
C	0.27238100	1.66521500	0.32978000
O	-0.33155700	2.71976500	0.35668500
C	-1.57064100	-0.09348400	0.31399500
C	-1.69697000	-0.77079700	-0.90553200
C	-2.73146600	0.28390600	0.99967200
C	-2.95770500	-1.07260500	-1.42128200
H	-0.80547200	-1.07201700	-1.44831000
C	-3.99260700	-0.01675700	0.48487500
H	-2.64499400	0.82205900	1.94013700
C	-4.10969600	-0.69786000	-0.72768700
H	-3.03866300	-1.60202200	-2.36712500
H	-4.88297200	0.28094900	1.03238700
H	-5.09126500	-0.93577000	-1.12884500
N	1.54693200	1.48049000	-0.18871100
C	2.31825700	2.54984600	-0.78632500
H	3.25705600	2.70707300	-0.24194900
H	2.54979900	2.32696500	-1.83474300
H	1.71147700	3.45532500	-0.73298900



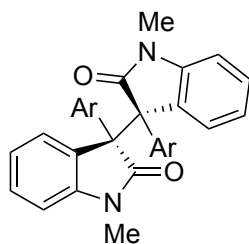
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H: -708.5594 Hartrees

G: -708.614617 Hartrees

0 2

C	-3.35660200	-0.50199800	-0.00932900
C	-2.10093700	0.09371800	-0.02995600
C	-0.89276700	-0.67318500	0.05156000
C	-0.99725600	-2.07135400	0.20864900
C	-2.25280700	-2.66868200	0.23228300
C	-3.41915500	-1.89429200	0.11467600
H	-4.26228400	0.09246100	-0.07825400
H	-0.10781900	-2.67771800	0.33736300
H	-2.33369900	-3.74494300	0.35248200
H	-4.39007200	-2.38156400	0.13402900
C	0.20183800	0.24079200	0.01068700
C	-0.38717000	1.60298000	-0.06192500
O	0.16664800	2.69910400	-0.09700600
C	1.62710400	-0.01723500	-0.00468700
C	2.54733200	0.96522000	0.43501500
C	2.14722600	-1.24906900	-0.46852100
C	3.91369900	0.70773900	0.43716000
H	2.16988900	1.92312600	0.76997700
C	3.51542000	-1.49543900	-0.46786800
H	1.47356500	-1.99454500	-0.87571000
C	4.40710400	-0.52237800	-0.00717100
H	4.60039400	1.47327500	0.78857800
H	3.88983800	-2.44573600	-0.83926500
H	5.47606100	-0.71756000	-0.00459500
N	-1.78139600	1.43566000	-0.10620900
C	-2.71264800	2.53950100	-0.18316200
H	-3.37263700	2.56139200	0.69250900
H	-2.12207900	3.45683700	-0.21289800
H	-3.32685800	2.47460500	-1.08916700



Ar = Ph

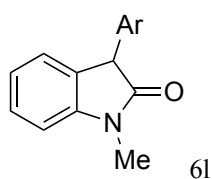
H: -1417.1356 Hartrees

G: -1417.22048 Hartrees

0 1

C	4.04581800	1.45497600	0.16526300
C	2.70769500	1.21864000	0.45400700
C	2.01360900	0.09070900	-0.01795600
C	2.69873500	-0.81955300	-0.81572100
C	4.04929000	-0.59806300	-1.12519200
C	4.71479100	0.52423100	-0.63756600
H	4.55564000	2.33575800	0.54262400
H	2.20274700	-1.69003600	-1.22657000
H	4.57441800	-1.31029200	-1.75500700
H	5.76111600	0.68536900	-0.88252900
C	0.57918800	1.51916300	1.24274500
O	-0.38859300	2.09044400	1.72395500
C	-0.59041400	0.11731000	-0.55206600
C	-2.01371400	0.09063900	0.01775500
C	-2.70773100	1.21801700	-0.45563000
C	0.59033900	0.11814500	0.55190100
C	-0.40853900	-0.97530400	-1.63572800
C	-0.87037000	-2.28391800	-1.42401600
C	0.21574700	-0.69399400	-2.86283400
C	-0.70684800	-3.27533200	-2.39222000
H	-1.37118100	-2.54151400	-0.50063900
C	0.36586500	-1.68228500	-3.83722600
H	0.60135800	0.29964000	-3.05443600
C	-0.09037900	-2.97951100	-3.60793900
H	-1.07483600	-4.27881500	-2.19447100
H	0.84732300	-1.43030500	-4.77860400
H	0.02788300	-3.74854000	-4.36676100
C	-0.57927900	1.51727600	-1.24504200
O	0.38839500	2.08758400	-1.72761900
C	-4.04583300	1.45481100	-0.16716200
C	-4.71486500	0.52511200	0.63683100
H	-5.76117900	0.68662500	0.88159400

C	-4.04944900	-0.59664200	1.12581400
C	-2.69891400	-0.81861400	0.81660600
H	-2.20299200	-1.68864200	1.22849400
H	-4.57463000	-1.30806300	1.75649600
H	-4.55560600	2.33514000	-0.54564300
N	-1.85635700	2.02325700	-1.22126900
N	1.85632800	2.02496100	1.21850900
C	-2.19256000	3.33322500	-1.73891900
H	-1.30217600	3.72836700	-2.22984800
H	-3.01150600	3.26436100	-2.46371000
H	-2.48950300	4.00599400	-0.92563400
C	2.19257300	3.33562100	1.73437000
H	2.48965900	4.00722100	0.92017200
H	1.30216300	3.73151500	2.22464300
H	3.01143000	3.26771300	2.45935200
C	0.40855700	-0.97289100	1.63719200
C	0.86998700	-2.28192200	1.42717200
C	-0.21517800	-0.68969600	2.86414800
C	0.70658100	-3.27192900	2.39683400
H	1.37037700	-2.54095800	0.50397600
C	-0.36516600	-1.67657200	3.83999500
H	-0.60043800	0.30430800	3.05451500
C	0.09065600	-2.97423800	3.61237000
H	1.07424200	-4.27578400	2.20036300
H	-0.84618000	-1.42313600	4.78121000
H	-0.02750200	-3.74216000	4.37232700



Ar = C₆H₄CN

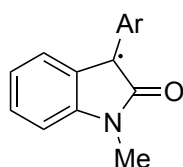
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G: -801.471894 Hartrees

0 1

C	-2.53031400	0.02440400	-0.19197800
C	-1.67352700	-1.96887400	0.87042400
C	-2.79780200	-2.66721900	0.40429100
C	-3.77030500	-2.01129900	-0.35144200
C	-3.65281300	-0.64972600	-0.66084400
C	-1.01122300	1.69379200	0.27658500

H	-0.91569700	-2.47923100	1.45926400
H	-2.91083000	-3.72225500	0.63506000
H	-4.63721900	-2.56115500	-0.70724600
H	-4.41484700	-0.14357700	-1.24505600
C	-0.48257100	0.39068000	0.94203700
H	-0.50229800	0.58176800	2.02441800
C	-1.53940500	-0.62205800	0.56679300
C	-2.98810500	2.35010200	-1.08929900
H	-3.09490000	2.05419900	-2.13937300
H	-3.98530500	2.45675700	-0.64655800
H	-2.46167600	3.30411200	-1.03233800
O	-0.49182600	2.79264200	0.30928900
N	-2.20036200	1.37809300	-0.35842600
C	0.95813800	0.11717500	0.53893600
C	1.29792200	-0.85718400	-0.40751700
C	1.97797500	0.89822700	1.10336300
C	2.62512900	-1.05992200	-0.77583900
H	0.52080700	-1.46677700	-0.85662700
C	3.30607700	0.70720500	0.74205100
H	1.72323000	1.67162000	1.82116000
C	3.64011900	-0.27942700	-0.20122600
H	2.88104600	-1.81996300	-1.50711300
H	4.08896200	1.31486400	1.18421500
C	5.00893200	-0.48973000	-0.57271300
N	6.11950200	-0.66214800	-0.87383800



Ar = C₆H₄CN

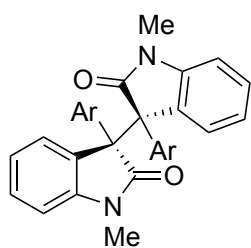
H: -800.802792 Hartrees

G: -800.862476 Hartrees

0 2

C	-1.45385200	-0.69544800	0.05282900
C	-2.71079800	-0.00969400	-0.02952300
C	-3.92415200	-0.68780000	-0.01382400
C	-3.89338400	-2.08074700	0.10658000
C	-2.67792200	-2.77725400	0.22572900
C	-1.46559300	-2.09900000	0.20701200
C	-0.42523300	0.29010200	0.01474000

C	-1.10616900	1.61161700	-0.05518800
H	-4.86730600	-0.15539000	-0.08425300
H	-4.82944600	-2.63183500	0.12230800
H	-2.68808900	-3.85654200	0.34355800
H	-0.53964400	-2.64731600	0.33807000
C	-3.48868400	2.38929300	-0.18225200
H	-4.09175100	2.28307900	-1.09140100
H	-4.15138500	2.36309600	0.69077500
H	-2.96319600	3.34533300	-0.20801600
N	-2.48347700	1.35079000	-0.10252500
O	-0.62391800	2.74028700	-0.08613500
C	1.01251900	0.13488500	-0.00292700
C	1.61986900	-1.06505300	-0.44746600
C	1.86230400	1.19036400	0.41296800
C	2.99698700	-1.21782200	-0.45058700
H	1.00324300	-1.86587000	-0.83762300
C	3.23990800	1.03881700	0.41568500
H	1.41959900	2.12559000	0.73031700
C	3.82411200	-0.16880000	-0.00898600
H	3.44493100	-2.14097900	-0.80409200
H	3.87658700	1.85245600	0.74807600
C	5.24661900	-0.32709000	-0.00352900
N	6.40327900	-0.45823700	0.00163900



Ar = C₆H₄CN

H: -1601.62277 Hartrees

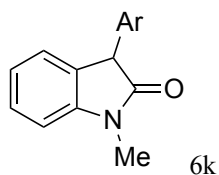
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0 1

C	-4.05345400	0.66859600	-1.97833500
C	-2.68299900	0.55895100	-1.76618700
C	-2.11021600	0.63365500	-0.48414700
C	-2.94700700	0.81410300	0.61382600
C	-4.33201700	0.92750900	0.42014400
C	-4.87532200	0.85643400	-0.86186700
H	-4.47376100	0.60596300	-2.97678200
H	-2.54392400	0.86886200	1.61864000

H	-4.98112800	1.07265400	1.27854600
H	-5.94913000	0.94609100	-1.00115900
C	-0.44467800	0.24734600	-2.15894300
O	0.58679900	0.06822200	-2.78203500
C	0.21504800	1.72816400	-0.24920200
C	1.55949100	1.84715800	-0.64792900
C	-0.36070800	2.79926300	0.45232500
C	2.30572200	2.97775100	-0.33183100
H	2.01288500	1.06529200	-1.24127200
C	0.37720800	3.93464100	0.77427700
H	-1.40166600	2.75882200	0.74659800
C	1.72292500	4.03062200	0.39066900
H	3.34051300	3.05172200	-0.65047900
H	-0.08775500	4.75072500	1.31811000
C	-0.10556400	-0.83977800	0.20789400
C	-0.40716500	-0.73647300	1.70238300
C	-1.25259300	-1.79969200	2.06606200
C	-0.59335700	0.46557400	-0.61003900
C	1.35613700	-1.29149200	-0.05096600
C	2.38531300	-0.97440100	0.85005200
C	1.68825600	-2.06550800	-1.17715300
C	3.69500700	-1.39340900	0.63738500
H	2.17379800	-0.40345400	1.74396000
C	2.99212300	-2.49486600	-1.39757500
H	0.92175700	-2.33980000	-1.88793700
C	4.01103800	-2.15989800	-0.49313100
H	4.47197300	-1.13426900	1.34934500
H	3.22454500	-3.09199000	-2.27332400
C	-1.04380400	-2.01904900	-0.20534100
O	-1.26644700	-2.41213400	-1.33939600
C	-1.69114400	-1.99159600	3.37137700
C	-1.27534200	-1.07236800	4.34170900
H	-1.60487300	-1.19835000	5.36917500
C	-0.45235900	0.00095100	4.00233700
C	-0.01388900	0.17174500	2.68009800
H	0.61202700	1.02116100	2.43104800
H	-0.14473400	0.71164200	4.76343300
H	-2.34217400	-2.82008300	3.63130200
N	-1.58455500	-2.56011600	0.93862300
N	-1.69241700	0.36593000	-2.72908700
C	-2.51237200	-3.67397300	0.92357600
H	-2.59344000	-4.01684200	-0.10865300
H	-2.14390700	-4.49072900	1.55375400
H	-3.50016900	-3.36149100	1.28184900

C	-1.92848700	0.17488400	-4.14590100
H	-2.44449100	1.04259100	-4.57146400
H	-0.95598100	0.05786000	-4.62525000
H	-2.53037600	-0.72478700	-4.31819200
C	5.35626400	-2.60369700	-0.71521000
N	6.44796200	-2.96428800	-0.89352000
C	2.48867400	5.19585300	0.72517500
N	3.10798500	6.14100400	1.00212700



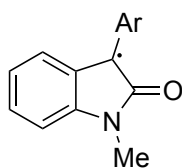
Ar = C₆H₄CF₃

H: -1046.19765 Hartrees

G: -1046.26326 Hartrees

0 1			
C	3.24353300	-0.03726600	0.21487600
C	2.32692700	-1.96855300	-0.90998200
C	3.40030000	-2.72873900	-0.42098900
C	4.37796300	-2.13363500	0.37721800
C	4.31600100	-0.77325100	0.70749600
C	1.81885800	1.70966700	-0.26962200
H	1.56376100	-2.43141700	-1.53030600
H	3.46956900	-3.78423300	-0.66669700
H	5.20516400	-2.73093200	0.75082100
H	5.08145500	-0.31479100	1.32571300
C	1.25211800	0.44577300	-0.97588700
H	1.31501600	0.65434800	-2.05327300
C	2.24855900	-0.62195300	-0.58738700
C	3.77922400	2.24744400	1.17105100
H	3.83587900	1.92969600	2.21879900
H	4.79524000	2.31374100	0.76447500
H	3.30062100	3.22635800	1.11369000
O	1.35414600	2.83287100	-0.29634800
N	2.97221400	1.32717600	0.39633600
C	-0.21165300	0.22778600	-0.62263900
C	-1.18426800	1.03196400	-1.23284700
C	-0.61733600	-0.71628900	0.32756900
C	-2.53097400	0.88851800	-0.91258100
H	-0.88007100	1.78611200	-1.95231100

C	-1.96492900	-0.86511000	0.65102900
H	0.12202100	-1.34223100	0.81661200
C	-2.92552100	-0.06482000	0.03004700
H	-3.27463300	1.51935200	-1.38819900
H	-2.26807900	-1.59817400	1.39158100
C	-4.38399000	-0.27263400	0.33060500
F	-4.58307700	-0.68334800	1.60374300
F	-5.10467700	0.85666700	0.15074700
F	-4.93152100	-1.21714700	-0.47251400



Ar = C₆H₄CF₃

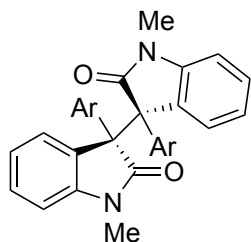
H: -1045.58844 Hartrees

G: -1045.65402 Hartrees

0 2

C	2.19680300	-0.69437900	-0.05644100
C	3.46772500	-0.03594700	0.03469100
C	4.66601500	-0.74041500	0.02210000
C	4.60559700	-2.13219300	-0.10341500
C	3.37591700	-2.80178900	-0.23002200
C	2.17836800	-2.09728600	-0.21440800
C	1.18894400	0.31164100	-0.02015700
C	1.89517100	1.61757800	0.05943600
H	5.62023200	-0.22883300	0.09872800
H	5.52963400	-2.70337200	-0.11684700
H	3.36330000	-3.88077100	-0.35101700
H	1.24025000	-2.62368500	-0.34981100
C	4.29269300	2.34634600	0.20184000
H	4.88949700	2.22407700	1.11321100
H	4.95928200	2.31225400	-0.66806300
H	3.78542300	3.31217000	0.23015800
N	3.26789000	1.32853900	0.11204000
O	1.43622800	2.75609800	0.09280700
C	-0.25407400	0.18372500	-0.01297300
C	-0.88659000	-0.99654500	0.44287200
C	-1.07924500	1.24576500	-0.45531400
C	-2.26941500	-1.12044600	0.43516800
H	-0.28827500	-1.80462900	0.84711200

C	-2.46141600	1.11586900	-0.46654900
H	-0.61736200	2.16632600	-0.78815700
C	-3.06494700	-0.06780000	-0.02813000
H	-2.73518100	-2.03305900	0.79213600
H	-3.07749800	1.93389700	-0.82580600
C	-4.56385400	-0.17877500	0.01087000
F	-5.07305600	0.31599700	1.16421400
F	-4.97712100	-1.46306600	-0.08008400
F	-5.14543500	0.50762200	-0.99810800



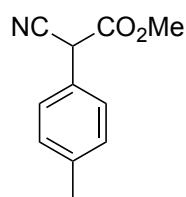
Ar = C₆H₄CF₃

H: -2091.19509 Hartrees

G: -2091.2994 Hartrees

0 1			
C	-4.57008400	-0.49825300	-2.10496100
C	-3.20759400	-0.35336600	-1.86394300
C	-2.69621900	-0.04330200	-0.59120600
C	-3.58616700	0.11725300	0.46704800
C	-4.96429500	-0.02409000	0.24390600
C	-5.44703800	-0.32740500	-1.02830800
H	-4.94267000	-0.74060200	-3.09501100
H	-3.22884200	0.35080000	1.46339800
H	-5.65547000	0.10608800	1.07137000
H	-6.51602200	-0.43426300	-1.19126100
C	-0.93604800	-0.32935600	-2.18651200
O	0.12888800	-0.40197600	-2.77332100
C	-0.58572700	1.43599600	-0.44158800
C	0.73523300	1.72913400	-0.82603500
C	-1.34916600	2.46884400	0.12280200
C	1.27673400	2.99602600	-0.62365100
H	1.32910600	0.97322300	-1.32084300
C	-0.80948500	3.73763900	0.32852700
H	-2.38189200	2.29467500	0.39712400
C	0.50960900	4.00487200	-0.03735700
H	2.29522600	3.20177100	-0.93680800
H	-1.42172600	4.52140700	0.76233400
C	-0.50567600	-1.08677700	0.29060300

C	-0.87633500	-0.87636000	1.75800400
C	-1.55298100	-2.01859700	2.22133900
C	-1.16846100	0.02708100	-0.67451300
C	1.01960600	-1.31421100	0.11385300
C	1.94705400	-0.73905900	0.99579800
C	1.51765500	-2.13219400	-0.91499300
C	3.31624300	-0.95627000	0.85466600
H	1.61205300	-0.11789600	1.81530600
C	2.88412500	-2.35573000	-1.05727800
H	0.83490300	-2.59872800	-1.61076600
C	3.79163400	-1.76681500	-0.17515400
H	4.01062700	-0.49201700	1.54710500
H	3.24337300	-2.98522100	-1.86490800
C	-1.22250500	-2.44230800	-0.00680200
O	-1.33360200	-2.98856200	-1.09283700
C	-2.00502700	-2.13895300	3.53075000
C	-1.77930600	-1.06571800	4.40069600
H	-2.12349400	-1.13321700	5.42894800
C	-1.12672700	0.08504000	3.96002400
C	-0.67146300	0.18308700	2.63598500
H	-0.18046100	1.09166000	2.30655900
H	-0.96607900	0.91385900	4.64293600
H	-2.52472300	-3.03022100	3.86774800
N	-1.71420900	-2.93931900	1.17958300
N	-2.16836000	-0.48293700	-2.78445200
C	-2.44496200	-4.18748500	1.27094700
H	-2.42313500	-4.65093000	0.28380100
H	-1.97568900	-4.85632500	2.00078100
H	-3.48561900	-4.00821100	1.56573700
C	-2.32283600	-0.86605600	-4.17273500
H	-2.95531700	-0.14637500	-4.70436700
H	-1.32803000	-0.87691900	-4.61954400
H	-2.76763800	-1.86491900	-4.25013300
C	5.26135900	-2.05895800	-0.29817700
C	1.11749200	5.35222800	0.23837400
F	5.60333200	-3.19440500	0.35765500
F	5.63548600	-2.22705100	-1.58624200
F	6.02001900	-1.06626400	0.21874200
F	2.03504900	5.69260700	-0.69325700
F	1.75064100	5.37744800	1.43659600
F	0.18606900	6.33175700	0.26908300



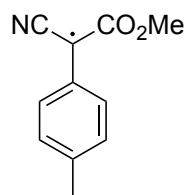
4a

H: -630.772806 Hartrees

G: -630.831018 Hartrees

0 1

C	0.34962600	0.33918300	-0.48538500
C	1.07062000	-0.66920100	-1.13699200
C	2.39293000	-0.92611200	-0.78618000
C	3.03359500	-0.18723100	0.21924600
C	2.29886000	0.81226500	0.86625400
C	0.97142400	1.07534000	0.52413000
H	0.58994600	-1.26133700	-1.91143500
H	2.93743000	-1.71274500	-1.30364000
H	2.76921600	1.39835200	1.65218000
H	0.42627700	1.86037600	1.03989800
C	-1.11598200	0.56485300	-0.88261100
H	-1.19861400	0.51755600	-1.97394900
C	-1.64098900	1.86425700	-0.44981300
N	-2.05274500	2.89977100	-0.12660000
C	-1.96616200	-0.61208800	-0.36270600
O	-2.18239300	-1.60518200	-1.01787900
O	-2.36713500	-0.41550600	0.89913000
C	-3.11453600	-1.49682200	1.48986900
H	-2.50233700	-2.40117000	1.53003900
H	-4.01696700	-1.69657700	0.90727100
H	-3.36925700	-1.15659900	2.49307400
C	4.47812500	-0.45131800	0.57359300
H	5.15571000	-0.02192400	-0.17606200
H	4.73938500	-0.01205300	1.54151900
H	4.68959300	-1.52553700	0.62087500

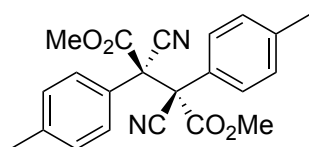


H: -630.162150 Hartrees

G: -630.219362 Hartrees

0 2

C	-0.45498300	0.18295200	-0.00442700
C	-1.37614200	1.26902600	-0.00500400
C	-2.74106900	1.04897900	-0.00833200
C	-3.27180800	-0.25463000	-0.00896700
C	-2.36721500	-1.33025000	-0.01317900
C	-0.99573500	-1.13260200	-0.00977800
H	-0.99739200	2.28606400	-0.00599700
H	-3.41691300	1.90071300	-0.01163800
H	-2.75243300	-2.34709100	-0.02036600
H	-0.32051400	-1.97702800	-0.01416900
C	0.95920100	0.44798600	-0.00183600
C	1.40709100	1.79215800	0.00059900
N	1.73598300	2.91337900	0.00241700
C	2.00867100	-0.60043000	0.00048200
O	1.82245500	-1.80492000	-0.00061900
O	3.24056400	-0.04696200	0.00432800
C	4.33523700	-0.97611600	0.00726800
H	4.30238700	-1.60976900	-0.88306800
H	4.29744300	-1.60989200	0.89733100
H	5.23484900	-0.36090800	0.00983400
C	-4.76022400	-0.48516900	0.02098800
H	-5.02429000	-1.46331600	-0.39326100
H	-5.14015400	-0.45337100	1.05155100
H	-5.29717100	0.28457000	-0.54369400



10

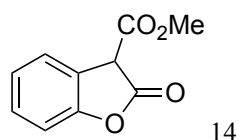
H: -1260.345072 Hartrees

G: -1260.434631 Hartrees

0 1

C	-1.60361900	-0.75892800	-0.03185000
C	-2.47137100	-1.28366600	-0.99949500
C	-3.77569000	-0.80822200	-1.11442700
C	-4.26156400	0.19793900	-0.27087200
C	-3.38668600	0.71973200	0.68884700
C	-2.07796100	0.25571600	0.81159200
H	-2.13262200	-2.06549600	-1.67060200
H	-4.42539200	-1.23190200	-1.87648900
H	-3.73037200	1.50683600	1.35606400
H	-1.42858200	0.68440600	1.56496800
C	-0.02903100	-2.59768200	-0.54763200
N	0.07461100	-3.61478100	-1.09588500
C	0.24107200	-1.37727500	1.57818400
O	0.45951300	-0.43110000	2.29941400
O	0.20550800	-2.64726900	1.98962500
C	0.53143300	-2.85960200	3.37585800
H	-0.16212700	-2.31165800	4.01831600
H	1.55287800	-2.52571400	3.57256400
H	0.43862200	-3.93407800	3.53025500
C	0.88582800	-0.30269800	-0.72881000
C	-0.14731100	-1.26528600	0.07734900
C	0.91505700	1.17697300	-0.28539200
C	0.08511000	2.11933000	-0.90436200
C	1.79481700	1.61658000	0.71309300
C	0.12958100	3.46080500	-0.52774700
H	-0.59189200	1.81400400	-1.69494600
C	1.83662600	2.95923900	1.07717200
H	2.44265000	0.91279900	1.22238500
C	1.00338600	3.90729500	0.46923100
H	-0.52359500	4.17134200	-1.02856700
H	2.53182200	3.27402600	1.85193700
C	0.49995000	-0.36647700	-2.15101300
N	0.16730800	-0.40867000	-3.26158700
C	2.31140800	-0.89835400	-0.57337400
O	2.66353200	-1.54191800	0.39055300
O	3.09380800	-0.57310100	-1.60155100
C	4.45214300	-1.05563800	-1.53514700
H	4.46034800	-2.14523000	-1.46091000
H	4.91762800	-0.72512400	-2.46268600
H	4.96188100	-0.62619200	-0.66922200

C	1.03635800	5.35691200	0.89090300
H	0.40168900	5.52683500	1.77089700
H	2.05020000	5.67404000	1.15813700
H	0.67317200	6.01468300	0.09469800
C	-5.68766000	0.68315500	-0.37745000
H	-6.04270900	0.65904900	-1.41322500
H	-6.36545800	0.05167900	0.21236700
H	-5.79172400	1.70786100	-0.00590100

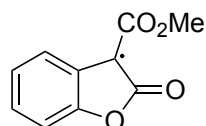


H: -686.611 Hartrees

G: -686.663 Hartrees

0 1

C	1.41468200	0.76523400	0.20166700
C	0.78355900	-0.24849700	-0.51806300
C	1.42950100	-1.46243100	-0.71507900
C	2.71286100	-1.63002900	-0.17960200
C	3.32694800	-0.59770800	0.53626500
C	2.68319500	0.62917100	0.74023900
C	-0.56160100	1.69677800	-0.35143900
C	-0.56905200	0.27090400	-0.93969900
H	0.94868400	-2.26293800	-1.27041600
H	3.23576300	-2.57085700	-0.32284000
H	4.32323700	-0.74557000	0.94313100
H	3.14744600	1.43897000	1.29247300
C	-1.72817500	-0.57975000	-0.42093600
O	-2.34697300	-1.36559200	-1.09986000
O	-1.92743900	-0.37410300	0.89171100
O	-1.40835700	2.53870300	-0.42340400
C	-2.98039300	-1.15260100	1.49132800
H	-2.75524900	-2.21918200	1.41254500
H	-3.01244100	-0.84038500	2.53478300
H	-3.93217200	-0.94674100	0.99600200
H	-0.68769900	0.33422600	-2.02616100
O	0.64067900	1.90924800	0.30310400

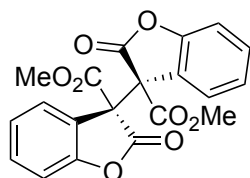


H: -685.999 Hartrees

G: -686.051 Hartrees

0 2

C	-1.67108700	0.80429000	0.00004000
C	-0.81653300	-0.33734800	-0.00006100
C	-1.38763400	-1.63332100	-0.00006000
C	-2.76793900	-1.73843000	-0.00002100
C	-3.58883300	-0.58765400	0.00004500
C	-3.05097500	0.70436900	0.00009500
C	0.41977900	1.62468000	-0.00036200
C	0.50037500	0.15636500	-0.00009700
H	-0.73938400	-2.50116400	-0.00011200
H	-3.23383800	-2.71914300	-0.00003500
H	-4.66838700	-0.70837000	0.00008900
H	-3.67721000	1.58960900	0.00019400
C	1.71778600	-0.66618300	-0.00000800
O	1.69790000	-1.88683600	0.00018900
O	2.84438500	0.06646300	-0.00007500
O	1.25361400	2.49204100	-0.00006600
C	4.06758500	-0.68672900	0.00005300
H	4.12880000	-1.31888800	-0.88992700
H	4.86337100	0.05785800	-0.00001600
H	4.12875000	-1.31867000	0.89019200
O	-0.96305400	1.96314900	0.00018500



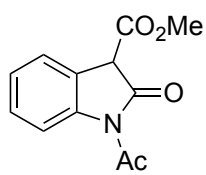
H: -1372.03 Hartrees

G: -1372.11 Hartrees

0 1

C	-2.02748200	1.72020100	-0.51137800
C	-1.62084300	0.74660300	0.40140500
C	-2.15374200	0.76121500	1.68881700
C	-3.03872300	1.78859500	2.03572700
C	-3.40336700	2.76923500	1.10813900
C	-2.90317600	2.74565500	-0.19808800
C	-0.68482200	0.42348200	-1.75543900
C	-0.72719400	-0.23423200	-0.34372400

H	-1.87542300	0.00066300	2.40607100
H	-3.45010400	1.81877500	3.04020500
H	-4.09324500	3.55668700	1.39818000
H	-3.18663000	3.48284400	-0.94129700
C	-1.43698800	-1.60461200	-0.34847900
O	-1.38544600	-2.36895600	0.58835900
O	-2.16428400	-1.78608900	-1.45333300
O	-0.04031900	0.08773600	-2.70742400
C	-2.87047500	-3.04144200	-1.53512200
H	-3.57664000	-3.13297200	-0.70641700
H	-3.39258000	-3.01505100	-2.49086500
H	-2.15721600	-3.86776900	-1.50375900
C	0.75881500	-0.43965900	0.12912700
C	1.62924700	0.79803100	0.07917900
C	1.48405700	-1.35879900	-0.90551500
C	2.69442000	0.53004200	-0.78073500
C	1.56403400	2.02001000	0.74102000
C	3.70277100	1.44344700	-1.03738600
C	2.56829400	2.96418100	0.49523500
H	0.76088100	2.22779900	1.43969100
C	3.61864200	2.67778000	-0.38245000
H	4.51376400	1.20373100	-1.71622000
H	2.53254400	3.92684800	0.99622000
H	4.38914200	3.42293000	-0.55913200
O	1.15095300	-2.43828600	-1.29723600
C	0.84886000	-1.03011500	1.55513300
O	0.38659100	-0.48563600	2.53254500
O	1.59421100	-2.13818100	1.58716900
C	1.75734900	-2.74166100	2.88469600
H	2.40472700	-3.60257600	2.72119800
H	2.21571500	-2.03352400	3.57922200
H	0.78494600	-3.05589300	3.27063800
O	2.63512900	-0.73399100	-1.33641700
O	-1.48032700	1.54337300	-1.77050100

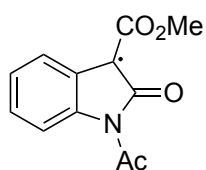


15

H: -819.353417 Hartrees

G: -819.413508 Hartrees

0 1			
C	-0.28680300	1.13879300	-0.53960300
C	0.99107600	0.82483100	-0.05789600
C	1.83273200	1.81865800	0.43923900
C	1.35260400	3.13375700	0.44454000
C	0.07915900	3.45261900	-0.03004100
C	-0.75385900	2.44562900	-0.52817000
C	-0.97009300	-0.11939900	-1.01348500
C	0.08286500	-1.20644200	-0.75956900
H	2.81856600	1.57662200	0.80642500
H	1.99527600	3.92078100	0.82925100
H	-0.26628300	4.48213600	-0.01357900
H	-1.74975700	2.67376800	-0.89805700
N	1.21932100	-0.58378100	-0.18588100
C	2.41207800	-1.23875200	0.21446600
O	3.32668700	-0.59227200	0.68995500
C	-2.28650800	-0.37300900	-0.28108600
O	-3.37220800	-0.07902300	-0.72519500
O	-2.07445000	-0.90345400	0.93571200
C	-3.25551800	-1.13033800	1.72821000
H	-3.93157800	-1.81665400	1.21278700
H	-2.89904000	-1.56711200	2.66078900
H	-3.77339300	-0.18643100	1.91562600
C	2.49671100	-2.73595100	0.03308500
H	1.69683800	-3.25165400	0.57086900
H	2.39251100	-3.01847400	-1.01784000
H	3.47177900	-3.04402200	0.41373000
O	-0.03631100	-2.38099500	-1.02478100
H	-1.20658100	-0.09892500	-2.08250800

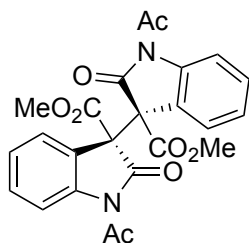


H: -818.740571 Hartrees

G: -818.800364 Hartrees

0 2			
C	0.00440900	1.15011300	0.00008200
C	1.32356200	0.58700500	0.00018000
C	2.45030000	1.40091600	0.00025500

C	2.24881900	2.78665900	0.00014900
C	0.96055000	3.35941500	-0.00005700
C	-0.16546200	2.55655900	-0.00007600
C	-0.92842300	0.09647000	0.00006000
C	-0.18769900	-1.17451600	-0.00010200
H	3.44135700	0.97295800	0.00030000
H	3.11886900	3.43743100	0.00026300
H	0.85551000	4.44019100	-0.00024300
H	-1.16840800	2.96446200	-0.00018500
N	1.21396000	-0.81574800	0.00013700
C	2.31541300	-1.70493600	-0.00002600
O	3.44977100	-1.26252200	-0.00012800
C	-2.39019800	0.26260400	-0.00017900
O	-2.94249800	1.35189500	-0.00060300
O	-3.05400300	-0.90658800	0.00031500
C	-4.48602200	-0.79814100	0.00042600
H	-4.83123800	-0.26441400	-0.88921700
H	-4.85167800	-1.82490600	0.00040500
H	-4.83107200	-0.26462900	0.89029900
C	2.03324000	-3.18878100	0.00003600
H	1.44926100	-3.48522100	0.87517500
H	1.44879500	-3.48533300	-0.87472500
H	3.00068000	-3.69338500	-0.00012300
O	-0.60336100	-2.31867400	-0.00050900



H: -1637.51725 Hartrees

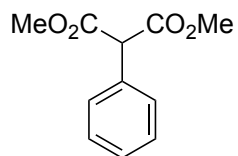
G: -1637.61228 Hartrees

0 1

C	-0.93340900	-0.51693500	1.33881700
C	-2.07227300	-1.22725700	0.92976400
C	-2.52429300	-2.33187500	1.65057900
C	-1.80481300	-2.70375000	2.79179500
C	-0.67915600	-1.99388400	3.21237100
C	-0.23988600	-0.88225200	2.48704500
C	-0.69403400	0.64770500	0.40123300
C	-1.81655000	0.45303600	-0.65885300

H	-3.40039500	-2.87610600	1.33280700
H	-2.14294900	-3.56409200	3.36288000
H	-0.14594200	-2.29842400	4.10807200
H	0.61515000	-0.30279800	2.81639000
N	-2.61518700	-0.63831800	-0.25317700
C	-3.72805100	-1.15481400	-0.96428300
O	-4.32876300	-2.12004800	-0.53016400
C	-0.91806000	1.95038900	1.20453000
O	-0.19928300	2.31236300	2.10859800
O	-2.06103400	2.55729600	0.86459600
C	-2.35939700	3.76438600	1.59087600
H	-1.58348600	4.51008700	1.40335600
H	-3.32065800	4.10227600	1.20453100
H	-2.41885700	3.56040100	2.66268300
C	-4.12629800	-0.47504400	-2.25240500
H	-4.36134100	0.58084700	-2.09615100
H	-3.31178800	-0.50658700	-2.98099300
H	-4.99938900	-1.00813700	-2.63219200
O	-1.96835800	1.12708300	-1.65051800
C	0.69693700	0.62172700	-0.34698900
C	1.98319800	0.64553800	0.46641000
C	0.80408300	-0.74863700	-1.06972000
C	2.71961700	-0.52382900	0.21982500
C	2.52475900	1.65771300	1.25413600
C	3.96929900	-0.73202100	0.80057000
C	3.77638500	1.46064400	1.84375000
H	1.97534800	2.57514600	1.41456900
C	4.48000800	0.27630300	1.62374800
H	4.52083600	-1.64006700	0.61190500
H	4.20062900	2.23831000	2.47197300
H	5.45210800	0.13049300	2.08677100
C	0.75589600	1.81561100	-1.32097500
O	0.46508800	2.94349600	-0.99224700
O	1.25629100	1.46857900	-2.51198400
C	2.46200600	-2.63869700	-1.13455000
O	3.51239500	-3.08361300	-0.71382400
O	-0.04057000	-1.22429600	-1.79727900
C	1.61071900	-3.39660700	-2.12535500
H	0.62517500	-3.62535600	-1.71134900
H	1.43712600	-2.81659600	-3.03542800
H	2.14706000	-4.31811800	-2.35711000
C	1.38280200	2.54229100	-3.46625300
H	2.05065100	3.31589300	-3.07980700
H	1.79815300	2.08329400	-4.36296000

H	0.40076000	2.97474700	-3.66961100
N	2.00929400	-1.36461900	-0.69313200

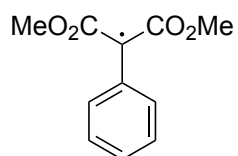


16

H: -727.071953 Hartrees

G: -727.131914 Hartrees

0 1			
C	2.73340000	-0.03887200	-1.34360200
C	3.69654600	-0.11400700	-0.33474600
C	3.29439400	-0.17359500	0.99961300
C	1.93608200	-0.15930800	1.32110800
C	0.96613300	-0.07916900	0.31556300
C	1.37669400	-0.02060700	-1.02311300
H	3.03901000	0.00582600	-2.38563400
H	4.75322300	-0.12800800	-0.58813800
H	4.03510200	-0.23489800	1.79245600
H	1.62710800	-0.21057500	2.36253200
H	0.63079900	0.04152000	-1.80876900
C	-0.51032600	-0.06371200	0.70031300
H	-0.60903800	-0.35071300	1.74928500
C	-1.21469200	1.29385900	0.58156100
O	-2.07893800	1.65316500	1.35066400
C	-1.29188500	-1.08654500	-0.12946100
O	-1.82107900	-0.86284500	-1.19610700
O	-0.78825800	2.01370400	-0.46573900
O	-1.28533800	-2.28886300	0.47483600
C	-1.46587100	3.26577400	-0.66874500
H	-1.34818300	3.91039000	0.20598300
H	-0.99389800	3.71257000	-1.54379900
H	-2.53033600	3.09534500	-0.84845000
C	-1.94083800	-3.34538400	-0.25036500
H	-1.84641600	-4.23072200	0.37842700
H	-2.99250100	-3.09866000	-0.41588200
H	-1.45378700	-3.50397300	-1.21601300

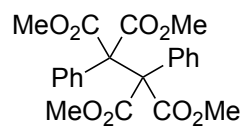


H: -726.44804 Hartrees

G: -726.508101 Hartrees

0 2

C	3.36041000	-1.20435700	-0.10097900
C	4.06690500	0.00000300	0.00001100
C	3.36041900	1.20437000	0.10099400
C	1.97430600	1.21344100	0.10342400
C	1.23095700	0.00001500	-0.00001400
C	1.97429700	-1.21341700	-0.10342900
H	3.89871400	-2.14482700	-0.18105100
H	5.15341100	-0.00000400	0.00002000
H	3.89872700	2.14483600	0.18107700
H	1.44403800	2.15080700	0.20305300
H	1.44401800	-2.15077700	-0.20306200
C	-0.20407600	0.00001400	-0.00001700
C	-0.98568900	1.25833400	0.14193100
O	-0.68589500	2.21345600	0.83518000
C	-0.98567400	-1.25832200	-0.14195100
O	-0.68588000	-2.21341700	-0.83524000
O	-2.09131000	1.23642800	-0.63680300
O	-2.09125100	-1.23646100	0.63682400
C	-2.93659500	2.39245500	-0.53529200
H	-2.39246500	3.29449000	-0.82782100
H	-3.76623400	2.20628500	-1.21778400
H	-3.29980500	2.51323300	0.48893500
C	-2.93651000	-2.39251800	0.53534000
H	-3.76603400	-2.20644700	1.21799900
H	-3.29989600	-2.51319100	-0.48883700
H	-2.39228400	-3.29455600	0.82767200



H: -1452.93448 Hartrees

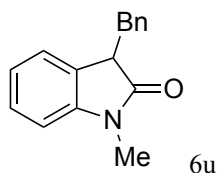
G: -1453.02481 Hartrees

0 1

C	-2.12222200	3.27619900	-0.72204000
C	-1.52671100	2.03513200	-0.95493300
C	-1.46615800	1.06267400	0.05389600
C	-2.01224100	1.38085700	1.30784500

C	-2.60284200	2.62138300	1.53930700
C	-2.66543300	3.57688500	0.52449200
C	-0.79023600	-0.31288100	-0.18813400
C	0.78993100	-0.31355900	0.18808000
C	1.46703300	1.06140700	-0.05405300
C	1.52873500	2.03371600	0.95485700
C	2.12528700	3.27427500	0.72191900
C	2.66841800	3.57459200	-0.52473300
C	2.60468400	2.61924400	-1.53962600
C	2.01304000	1.37922500	-1.30812800
C	0.92933500	-0.66509100	1.69755900
C	1.49497400	-1.44810600	-0.60501000
C	-1.49623300	-1.44671000	0.60512900
C	-0.93000900	-0.66443400	-1.69757900
O	-0.26953700	-0.15737200	-2.57930700
O	-1.90957900	-1.54718100	-1.93327600
C	-2.06293000	-1.94106700	-3.30795400
O	0.91837600	-2.37517500	-1.13106900
O	2.82797200	-1.30546700	-0.62466000
C	3.54969000	-2.37851900	-1.24990700
O	1.90856900	-1.54815100	1.93346000
O	0.26906900	-0.15755800	2.57918000
C	2.06164000	-1.94194800	3.30819400
O	-0.92036800	-2.37395300	1.13168600
O	-2.82913200	-1.30311600	0.62451500
C	-3.55171000	-2.37541800	1.25005800
H	-2.15377200	4.00808000	-1.52490100
H	-1.09833300	1.83654900	-1.92882100
H	-1.96237000	0.66605400	2.11783300
H	-3.01580200	2.83794200	2.52116700
H	-3.12916500	4.54304300	0.70585800
H	1.10047400	1.83540000	1.92884800
H	2.15771000	4.00605200	1.52483900
H	3.13296800	4.54034900	-0.70614100
H	3.01756300	2.83553600	-2.52157900
H	1.96229800	0.66455800	-2.11817800
H	-2.88969700	-2.65141000	-3.31343400
H	-2.29357200	-1.07377700	-3.93128600
H	-1.14406200	-2.41232700	-3.66466800
H	4.59975900	-2.09072400	-1.19500100
H	3.37675100	-3.31458100	-0.71220300
H	3.23502200	-2.49927800	-2.28961300
H	2.88818000	-2.65255200	3.31383200
H	2.29248300	-1.07467000	3.93146600

H	1.14257800	-2.41288200	3.66484100
H	-4.60156300	-2.08688100	1.19491300
H	-3.37938800	-3.31180200	0.71271500
H	-3.23726300	-2.49602900	2.28984700

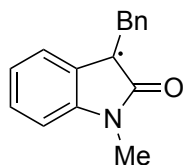


H: -748.45383 Hartrees

G: -748.513055 Hartrees

0 1			
C	-2.26713700	0.46688400	-0.06364500
C	-0.88109700	0.53993700	-0.29633900
C	-0.27709800	1.78064800	-0.44199800
C	-1.06096300	2.94097200	-0.34086200
C	-2.43237600	2.84933100	-0.10374200
C	-3.06045500	1.60437700	0.03673300
C	-1.58710600	-1.73291000	-0.12498600
H	0.78962200	1.85510500	-0.62892700
H	-0.59472100	3.91579400	-0.45111400
H	-3.02899500	3.75453600	-0.02885300
H	-4.12911400	1.53651000	0.21587900
C	-0.33276400	-0.86753100	-0.35707900
H	0.04373400	-1.10403400	-1.36166300
O	-1.63724200	-2.94949200	-0.06761200
N	-2.66496500	-0.87590600	0.03357200
C	-4.01374000	-1.33693300	0.28418200
H	-4.38625500	-0.95500600	1.24227900
H	-4.69317400	-1.01398200	-0.51358600
H	-3.98255800	-2.42739600	0.31543600
C	0.76612400	-1.24627800	0.67079500
H	0.43069000	-0.94850800	1.67098300
H	0.82970700	-2.34109300	0.66739700
C	2.12424700	-0.64371000	0.37997100
C	2.64155200	0.39352700	1.16639800
C	2.89865300	-1.11695300	-0.68997100
C	3.89354400	0.94825300	0.89073100
H	2.05790200	0.76923900	2.00351700
C	4.14819800	-0.56530500	-0.97016300
H	2.52103500	-1.93212400	-1.30421900

C	4.65024100	0.47172800	-0.17998200
H	4.27699800	1.75083900	1.51551400
H	4.73354800	-0.94923100	-1.80170600
H	5.62533600	0.90041100	-0.39530700



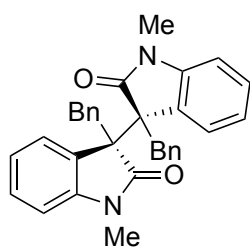
H: -747.836892 Hartrees

G: -747.896836 Hartrees

0 2

C	-1.21125200	-0.67300600	0.41869200
C	-2.29788600	0.02139900	-0.21786500
C	-3.38315300	-0.66182200	-0.75369900
C	-3.38841500	-2.05861800	-0.65665600
C	-2.33576600	-2.76140800	-0.03843100
C	-1.25078100	-2.08229800	0.49830400
C	-0.28866900	0.29474800	0.86038700
C	-0.81720800	1.61073300	0.47281800
H	-4.20224600	-0.13481800	-1.23321800
H	-4.22699200	-2.61244300	-1.06970700
H	-2.37690900	-3.84524800	0.01531400
H	-0.43705000	-2.62418400	0.97175100
C	1.02144700	0.13114600	1.56630400
H	1.18806100	1.02310300	2.18187600
H	0.97551200	-0.73119300	2.24172200
N	-2.04520900	1.37884900	-0.17822300
C	-2.88133900	2.43268200	-0.70934200
H	-3.01825300	2.32105800	-1.79155200
H	-3.86535800	2.43976700	-0.22536500
H	-2.37428200	3.37790800	-0.50652000
O	-0.32534200	2.72377100	0.65789200
C	2.19706000	-0.04104800	0.60650100
C	2.84801900	-1.27256500	0.48018300
C	2.63646300	1.03991200	-0.17088700
C	3.91982800	-1.42603000	-0.40222200
H	2.52098700	-2.11764400	1.08266800
C	3.70666300	0.88810800	-1.05184400
H	2.13198300	1.99847400	-0.07942700
C	4.35179600	-0.34553200	-1.17145600

H	4.41713400	-2.38914100	-0.48490000
H	4.03930400	1.73598700	-1.64523500
H	5.18644800	-0.46213300	-1.85769900

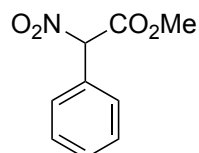


H: -1495.7157 Hartrees

G: -1495.80848 Hartrees

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C	1.40185900	2.24665400	-0.00839500
C	2.06244900	3.23693000	0.73519200
C	2.71367300	2.91005300	1.92452900
C	2.73004800	1.59274600	2.39885500
C	1.24864700	-1.39563800	0.93614100
H	0.89984600	2.51093200	-0.93365300
H	2.06585400	4.26299800	0.37881600
H	3.22207400	3.68447400	2.49276400
H	3.24511700	1.33774700	3.31959200
C	0.78962600	-0.33955100	-0.11516000
O	1.06758100	-2.60279700	0.89075700
N	1.97875500	-0.74472100	1.90692900
C	2.53267500	-1.41773300	3.06191200
H	3.62019100	-1.28708400	3.10348600
H	2.08597600	-1.02970800	3.98455700
H	2.29625900	-2.47804700	2.96339800
C	1.40200300	-0.73805100	-1.49634300
H	0.94728900	-1.68436600	-1.80376000
H	1.10853400	0.02332800	-2.22438300
C	2.91306200	-0.89013500	-1.52852000
C	3.51694300	-2.12110900	-1.23135000
C	3.73627100	0.18613500	-1.88742900
C	4.90383200	-2.26696800	-1.28316100
H	2.89347500	-2.96480000	-0.95005900
C	5.12319300	0.04283500	-1.94039900
H	3.28651000	1.14596500	-2.12774100
C	5.71226800	-1.18555000	-1.63721600

H	5.35176300	-3.23006300	-1.05179500
H	5.74222600	0.89061800	-2.22267800
H	6.79219300	-1.30049600	-1.68190300
C	-0.80426000	-0.26632500	-0.16702500
C	-1.34541800	0.87755000	-1.01282000
C	-2.02791200	1.77891600	-0.17616600
C	-1.32888100	1.11191800	-2.38237200
C	-2.65335200	2.92015800	-0.66642700
C	-1.94937400	2.26074300	-2.89848100
H	-0.85078700	0.41246500	-3.06160200
C	-2.59744800	3.15417300	-2.04593400
H	-3.17445400	3.60574300	-0.00567600
H	-1.92924800	2.44783100	-3.96809800
H	-3.07689400	4.03972900	-2.45409000
C	-1.45486900	-1.63533800	-0.56637600
H	-1.21331500	-1.82414300	-1.61793400
H	-0.96933000	-2.41706300	0.02070500
C	-2.95977900	-1.71414100	-0.38589500
C	-3.50743400	-2.14398600	0.83270700
C	-3.83637900	-1.39584700	-1.43267800
C	-4.88916700	-2.24158900	1.00104900
H	-2.84139300	-2.39709700	1.65238600
C	-5.21878400	-1.49378600	-1.26773700
H	-3.43229000	-1.07127200	-2.38815700
C	-5.75045800	-1.91614800	-0.04841700
H	-5.29219600	-2.58024400	1.95222600
H	-5.87932600	-1.24497900	-2.09456100
H	-6.82670600	-1.99766500	0.08056400
O	-1.09487200	-0.46966500	2.28989300
N	-1.97802500	1.33265000	1.14861900
C	-2.58642100	1.99636300	2.28221100
H	-2.16124000	2.99706800	2.42161100
H	-3.67059900	2.08276600	2.14532200
H	-2.37881700	1.38721600	3.16320600
C	-1.28684100	0.14203200	1.25119000



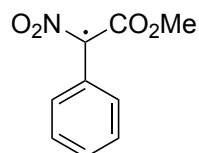
17

H: -703.73795 Hartrees

G: -703.793045 Hartrees

0 1

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C	-1.42014300	-0.51988100	0.96087100
C	-0.99837200	0.00167700	-0.26980800
C	-1.93543500	0.21981100	-1.28616200
C	-3.28068500	-0.08842300	-1.08281300
H	-4.74430400	-0.84877000	0.30446900
H	-3.08689800	-1.22630300	2.11768100
H	-0.69796100	-0.68608700	1.75168100
H	-1.61200300	0.63164900	-2.23898400
H	-3.99983600	0.08154600	-1.87907000
C	0.44446600	0.36423900	-0.51421600
N	0.81814300	1.58285300	0.34470800
O	0.71885700	2.68198200	-0.18041900
O	1.14847100	1.36195600	1.50602900
C	1.46777500	-0.73949000	-0.20398600
O	1.22100700	-1.81767300	0.27784300
O	2.68846000	-0.32502400	-0.58147700
C	3.76751600	-1.23948700	-0.30511400
H	3.60881200	-2.18312400	-0.83272000
H	4.66779500	-0.74147500	-0.66385200
H	3.83228000	-1.43105500	0.76858800
H	0.59330200	0.70999800	-1.53754000



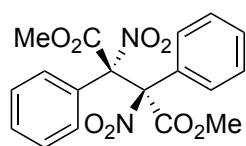
H: -703.109589 Hartrees

G: -703.164893 Hartrees

0 2

C	-3.78338500	-0.54318100	0.00540800
C	-3.29492300	0.76959900	-0.01260500
C	-1.93156000	1.01268300	-0.02042000
C	-0.99918900	-0.06589300	-0.00709800
C	-1.51509900	-1.39452600	0.01128100
C	-2.88379200	-1.61570800	0.01614400
H	-4.85398600	-0.72670000	0.01067000
H	-3.98585500	1.60756100	-0.02341600
H	-1.57609600	2.03596700	-0.05049400
H	-0.82123100	-2.22375300	0.02801100

H	-3.25613400	-2.63610700	0.03026500
C	0.40376600	0.18410500	0.00546100
N	0.84651600	1.58642300	0.04846200
O	1.31519100	1.98089400	1.11114700
O	0.69859300	2.26332200	-0.96641300
C	1.49111800	-0.80643900	0.00832000
O	1.34000000	-2.01340900	0.09643500
O	2.69449100	-0.21367400	-0.13166300
C	3.82339100	-1.10271500	-0.13794800
H	3.74867600	-1.80909300	-0.96879400
H	4.69486500	-0.45906600	-0.25462000
H	3.87598400	-1.65838500	0.80183100

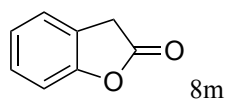


H: -1406.26367 Hartrees

G: -1406.34454 Hartrees

0 1			
C	4.47151400	-0.63117500	-0.42095700
C	3.86640300	-0.13848500	0.73204500
C	2.48439900	-0.23295300	0.90376700
C	1.67527800	-0.82776500	-0.07776900
C	2.29776700	-1.32201200	-1.23831000
C	3.67743300	-1.22230000	-1.40397900
H	5.54759700	-0.55852900	-0.55360800
H	4.46419800	0.32791000	1.51021200
H	2.03998300	0.17298100	1.80180700
H	1.71665600	-1.79835300	-2.01334200
H	4.12928500	-1.61782700	-2.30928900
C	0.14546100	-0.89400600	0.10671700
N	-0.42410300	-2.20766400	-0.53354000
O	-1.59433500	-2.19143200	-0.89756300
O	0.30406200	-3.18304600	-0.55549800
C	-0.21415300	-1.02114200	1.62849200
O	0.00870600	-0.15430700	2.43976700
O	-0.73254100	-2.21394800	1.91692700
C	-1.14554400	-2.39402700	3.28572700
H	-1.93228000	-1.67572100	3.52650500
H	-1.52006100	-3.41556400	3.33807600
H	-0.29729500	-2.25328400	3.95921100

C	-0.65047600	0.35622400	-0.48723200
N	-0.48193600	0.41765900	-2.04725300
O	-0.73403000	1.48428300	-2.58009200
O	-0.15044600	-0.60353000	-2.63657800
C	-2.17145100	0.16476300	-0.21898600
O	-2.59460900	-0.11131200	0.88304200
O	-2.92431200	0.41091400	-1.28440700
C	-4.34183800	0.21614500	-1.10339700
H	-4.71790400	0.88018700	-0.32193200
H	-4.78715900	0.45832300	-2.06737400
H	-4.53925000	-0.82307400	-0.83127300
C	-0.16546200	1.70441200	0.06903900
C	1.01027400	2.28046900	-0.43858100
C	-0.86826500	2.38622000	1.06982500
C	1.46339600	3.50772600	0.03745400
H	1.57459000	1.78261000	-1.21897800
C	-0.41131400	3.61640600	1.54393800
H	-1.76150500	1.95499800	1.50250200
C	0.75326800	4.18308600	1.03093600
H	2.37262600	3.93558800	-0.37504500
H	-0.97294200	4.12673300	2.32125800
H	1.10563300	5.14255400	1.39965200



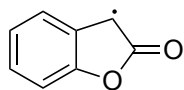
H: -458.791443 Hartrees

G: -458.831274 Hartrees

0 1

C	0.12852000	-0.62972700	-0.00006700
C	0.18174900	0.76511500	0.00002000
C	1.41769700	1.39983300	-0.00005400
C	2.57863700	0.61541800	-0.00022100
C	2.49621900	-0.77994600	-0.00030600
C	1.25729500	-1.43256800	-0.00023400
C	-2.04899300	-0.03555800	0.00021800
C	-1.23586200	1.26345100	0.00018900
H	1.48681200	2.48440000	0.00000700
H	3.55193500	1.09725200	-0.00028300
H	3.40667300	-1.37260300	-0.00043100
H	1.17570300	-2.51412900	-0.00029300
H	-1.50801300	1.85707700	-0.88084500

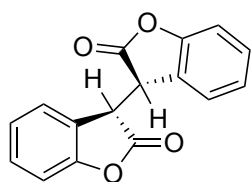
O	-1.17043700	-1.11279400	0.00003900
O	-3.23666800	-0.18784800	0.00037000
H	-1.50783500	1.85703400	0.88130400



H: -458.168985 Hartrees

G: -458.208927 Hartrees

0 2			
C	-0.08500600	-0.64626200	0.00003800
C	-0.13917700	0.78186900	-0.00003700
C	-1.40201500	1.42174200	0.00005200
C	-2.54273200	0.63528400	0.00022300
C	-2.45446600	-0.77383800	0.00029500
C	-1.22048400	-1.43627700	0.00019500
C	2.04774700	0.04592300	-0.00010700
C	1.19043100	1.21861200	-0.00021900
H	-1.46749200	2.50564700	-0.00001200
H	-3.52203900	1.10432100	0.00029500
H	-3.36807500	-1.36128900	0.00042200
H	-1.14957600	-2.51848000	0.00024000
H	1.57796900	2.22764200	-0.00038200
O	1.19612700	-1.09819100	-0.00009700
O	3.24930200	-0.08182800	-0.00030300



H: -916.399506 Hartrees

G: -916.457685 Hartrees

0 1			
C	-2.62626400	0.26776500	-0.17178000
C	-1.30207000	0.53772500	-0.52116300
C	-0.83643500	1.84754600	-0.47246200
C	-1.71573900	2.85859300	-0.06412100
C	-3.03638400	2.55848900	0.28235200
C	-3.51923800	1.24531300	0.23176900

C	-1.82350200	-1.76687200	-0.68774900
C	-0.66670200	-0.77096600	-0.91002100
H	0.18772100	2.08434500	-0.74522900
H	-1.36711900	3.88595100	-0.01730100
H	-3.70384200	3.35573900	0.59684000
H	-4.54029700	0.99516900	0.49827500
O	-2.94697900	-1.07673100	-0.28252900
O	-1.81381800	-2.95441000	-0.84823200
H	-0.42439900	-0.80641300	-1.98108600
C	0.59866300	-1.22454500	-0.14218600
C	1.86883300	-0.46144400	-0.40500600
C	0.43677500	-1.05934800	1.37889200
C	2.35026000	-0.01154000	0.82522700
C	2.58647900	-0.18059900	-1.56230900
C	3.52285200	0.71242100	0.96258200
C	3.77507800	0.55336100	-1.45730100
H	2.23739400	-0.52428800	-2.53273500
C	4.23393400	0.99113400	-0.21102400
H	3.86520800	1.04432100	1.93675200
H	4.34658800	0.78104200	-2.35208700
H	5.15876700	1.55730600	-0.14760200
O	1.52747500	-0.36846500	1.88180200
O	-0.46128800	-1.43249500	2.07830600
H	0.71762300	-2.29856800	-0.34478400

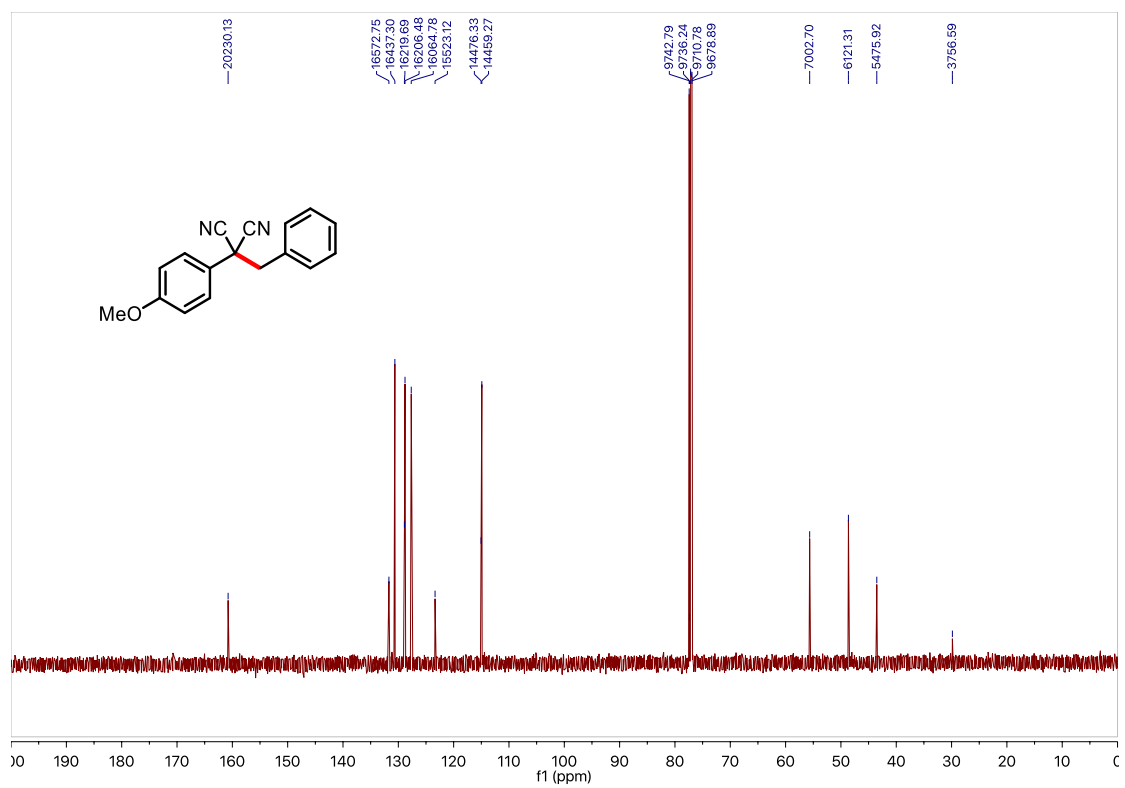
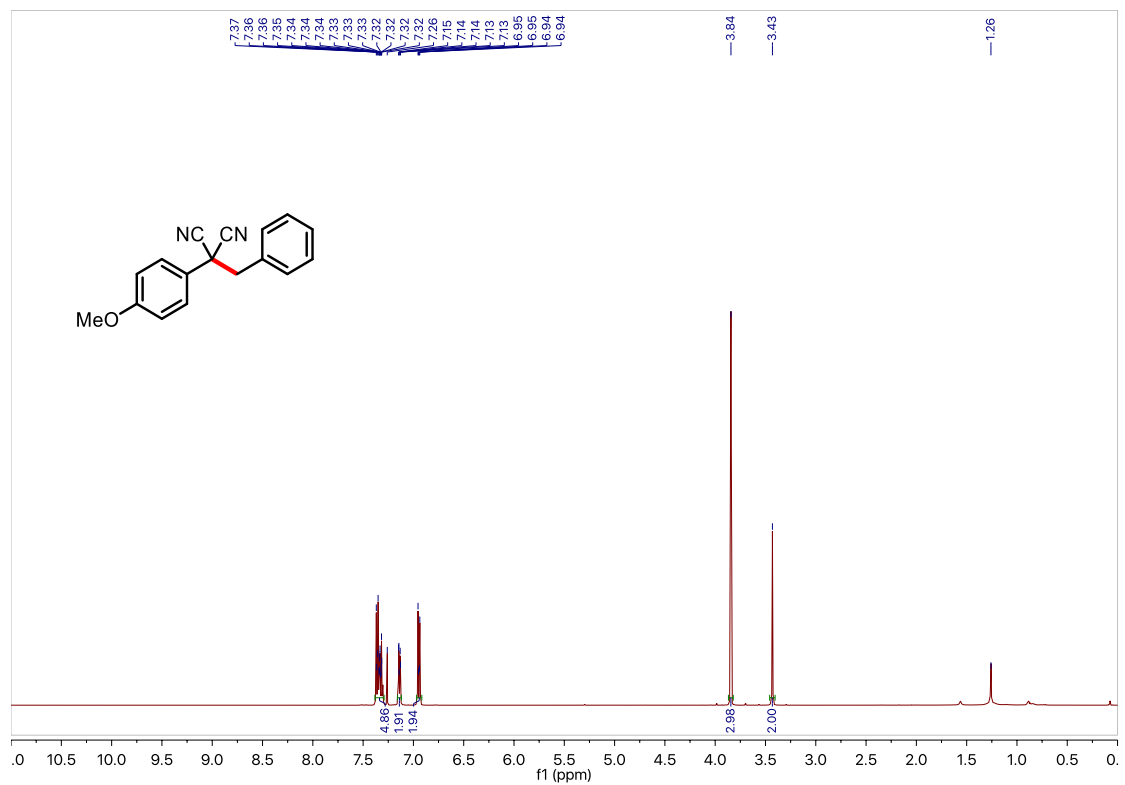
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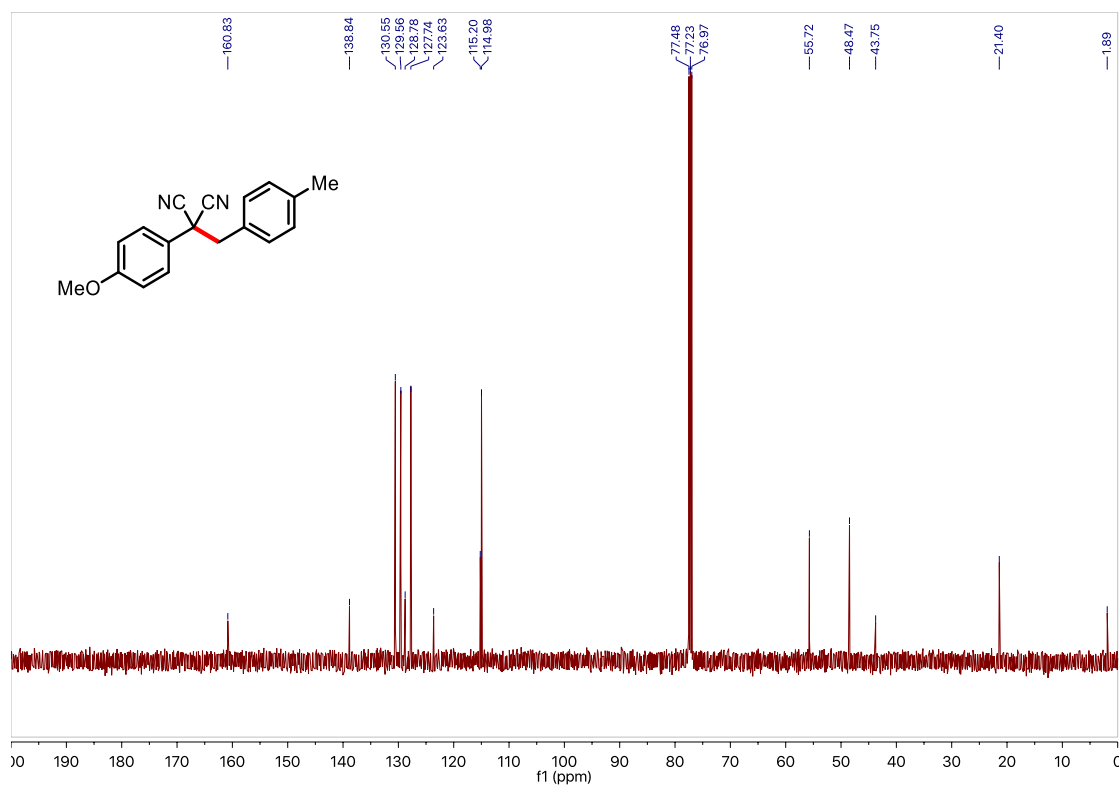
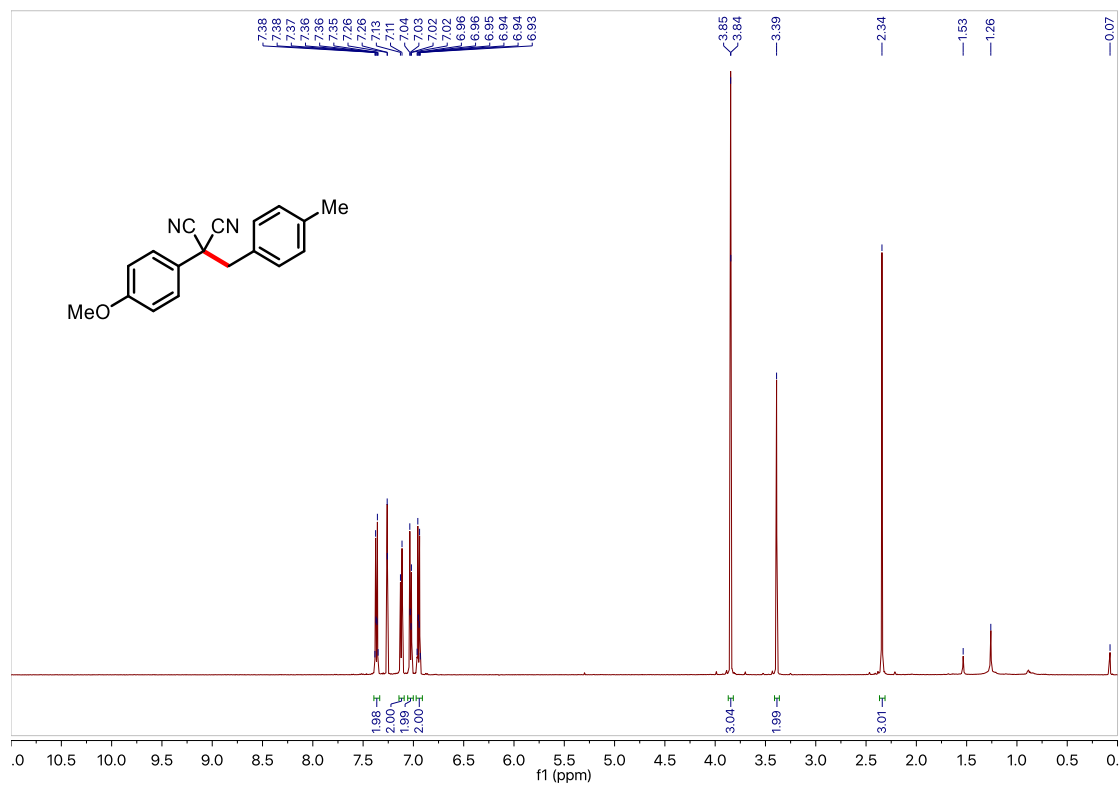
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8. ¹H NMR, ¹³C NMR Spectra of Products.

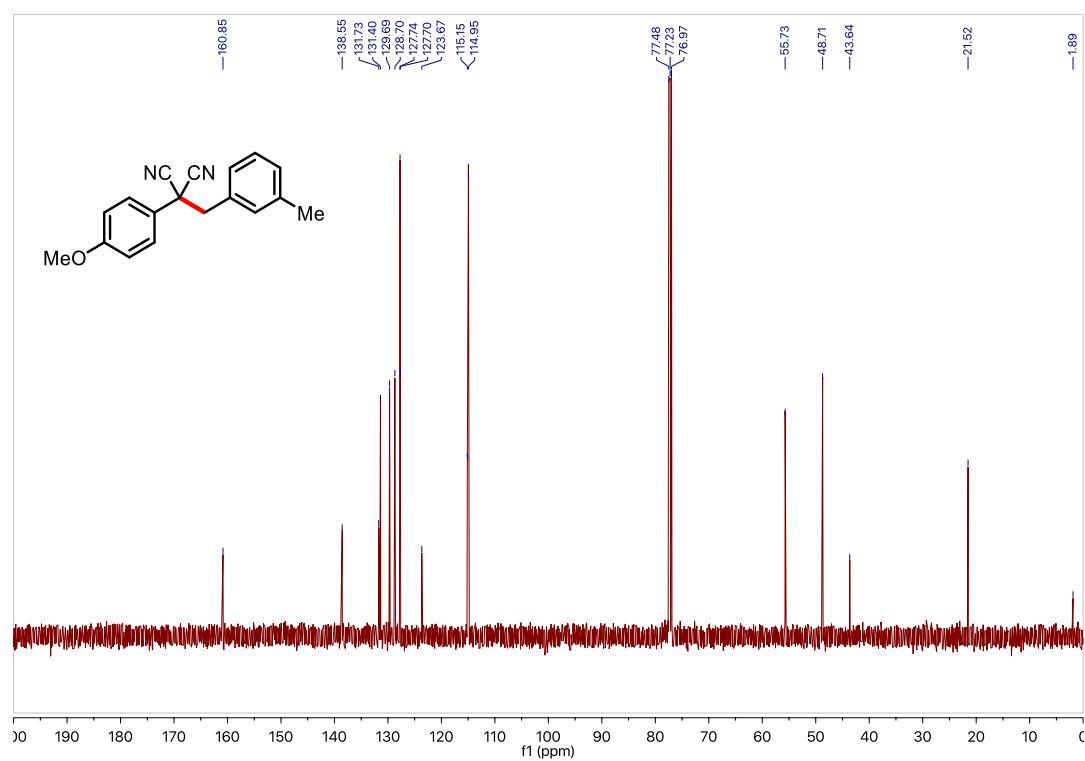
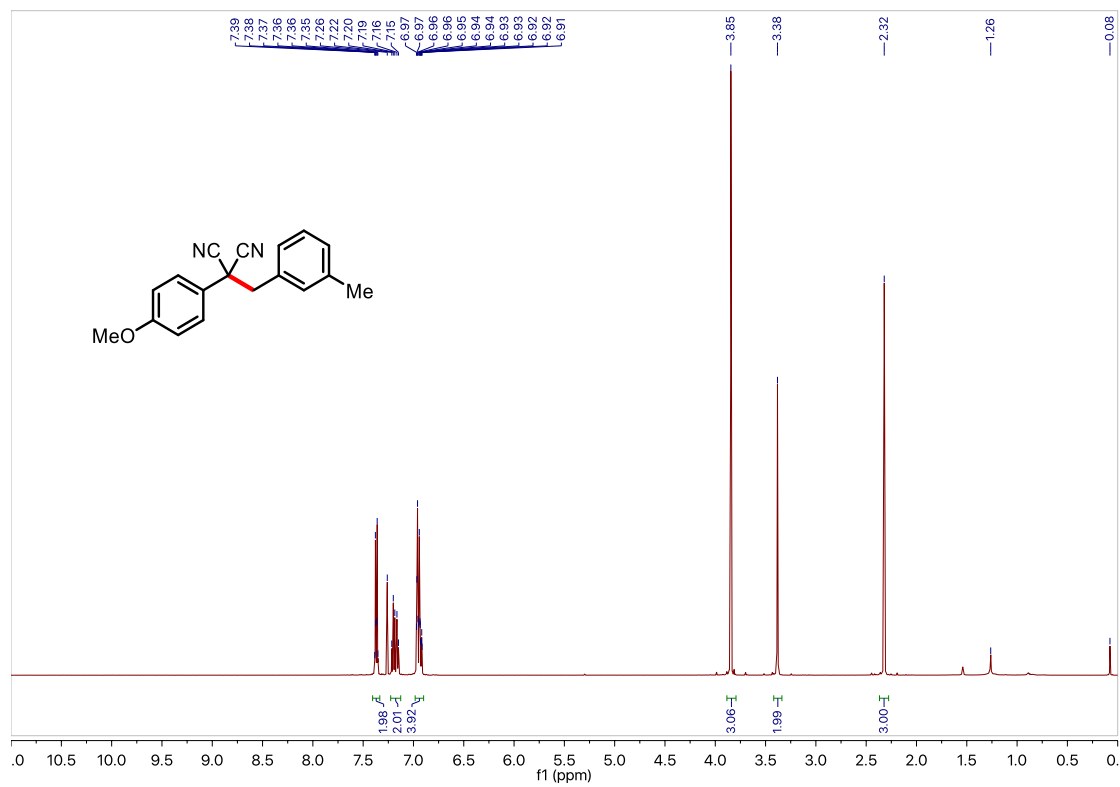
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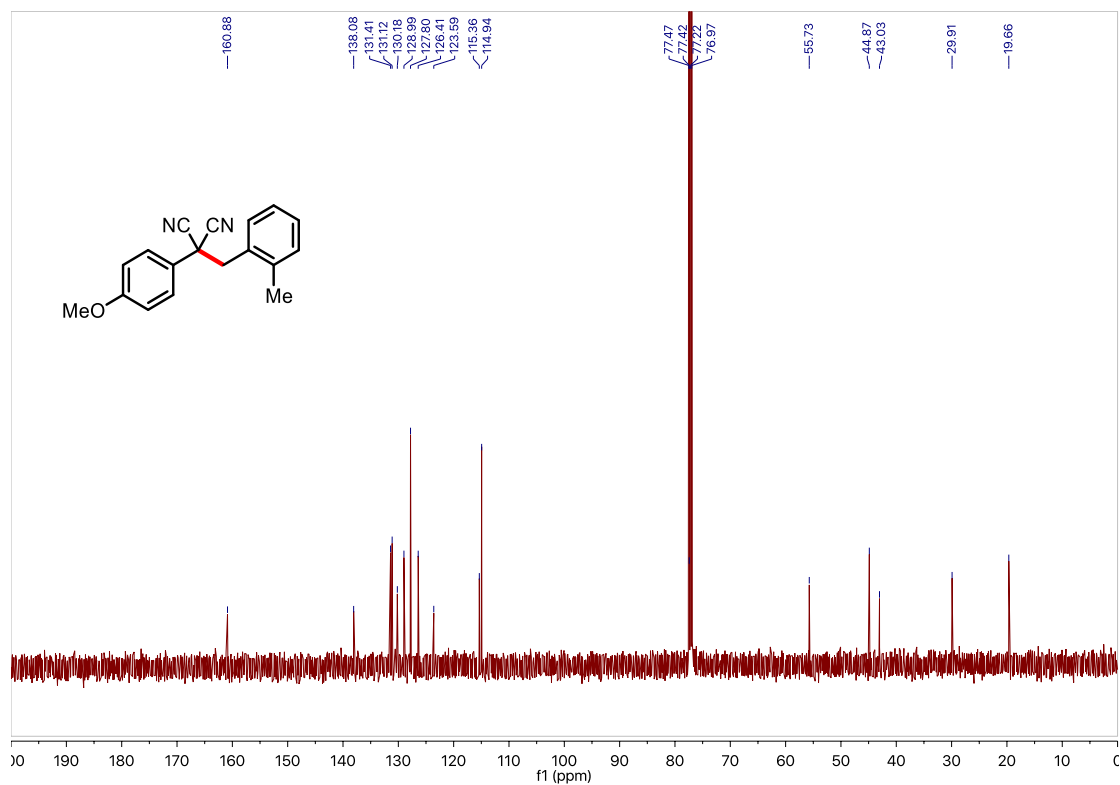
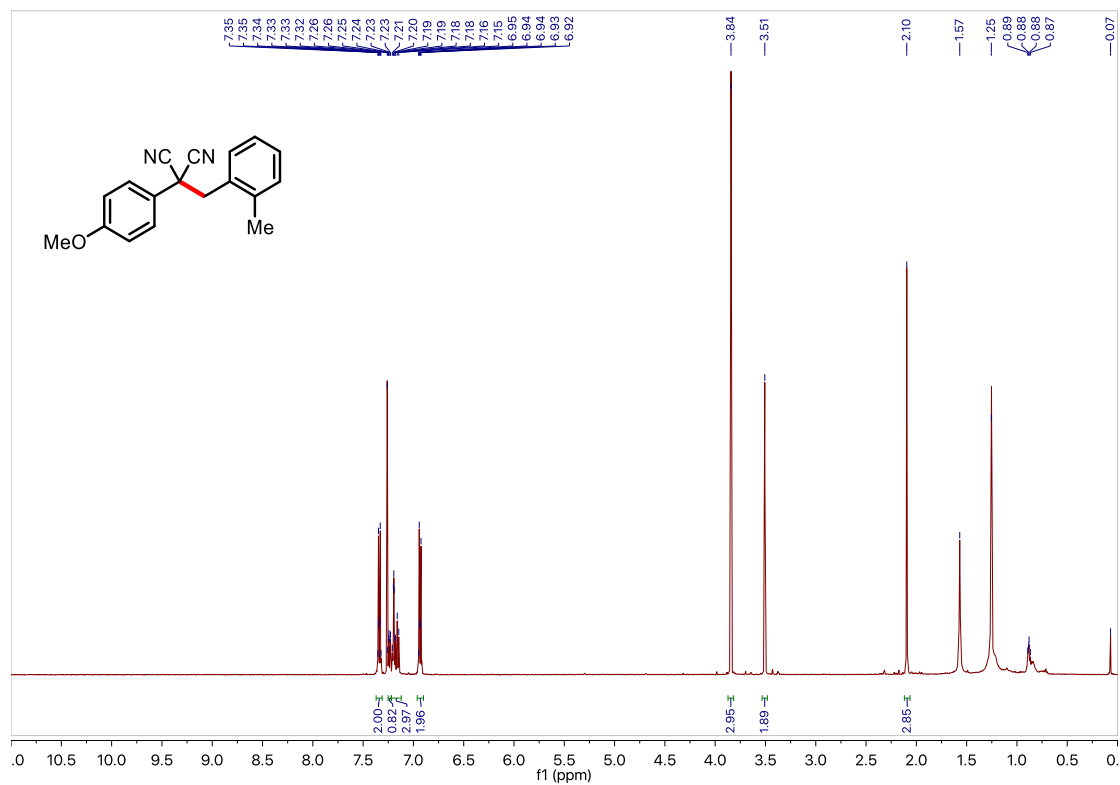
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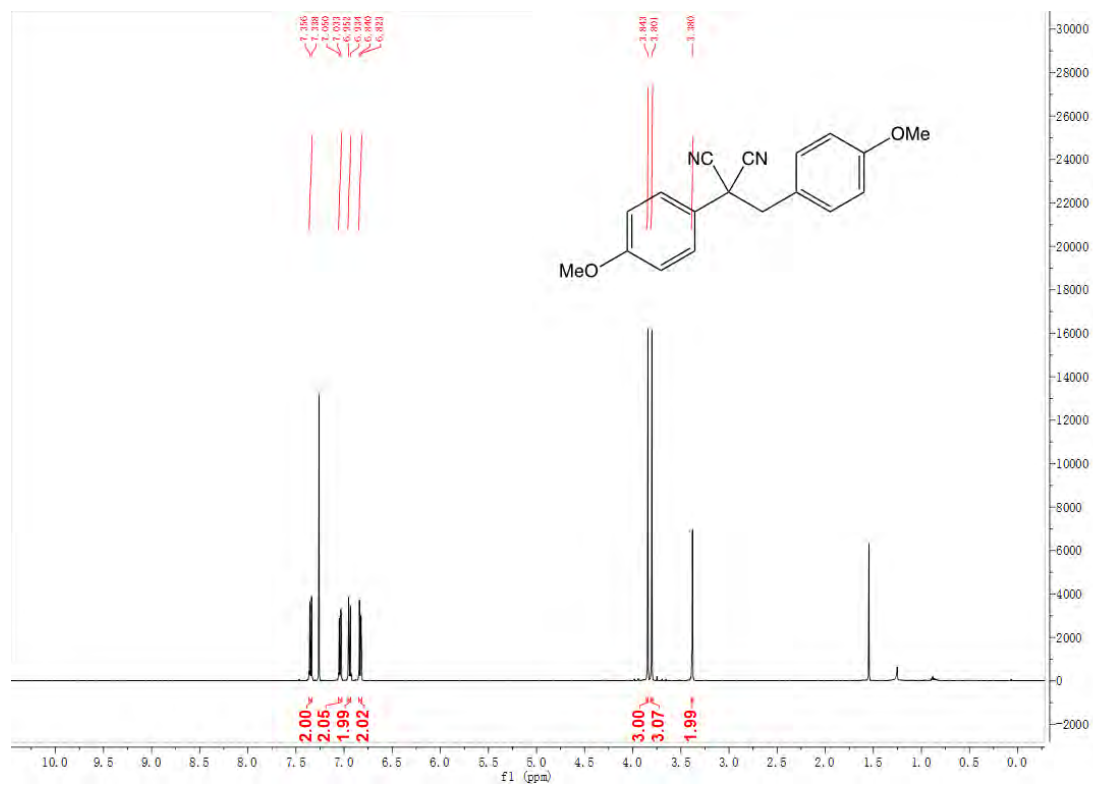
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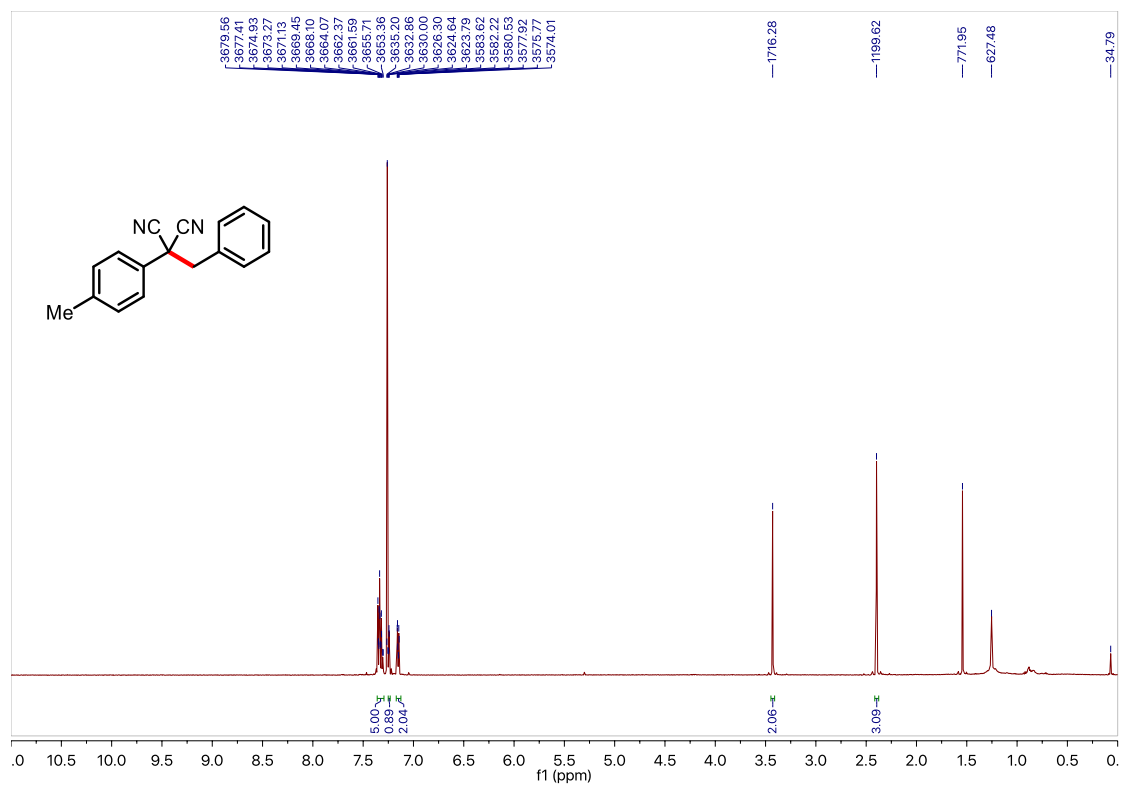
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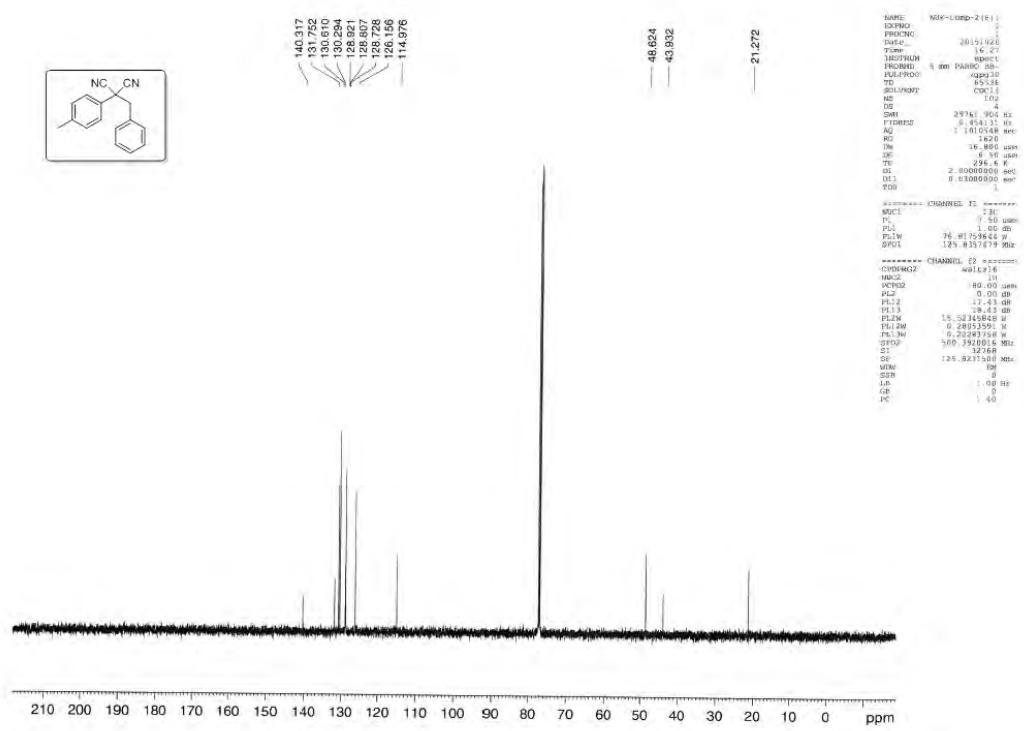


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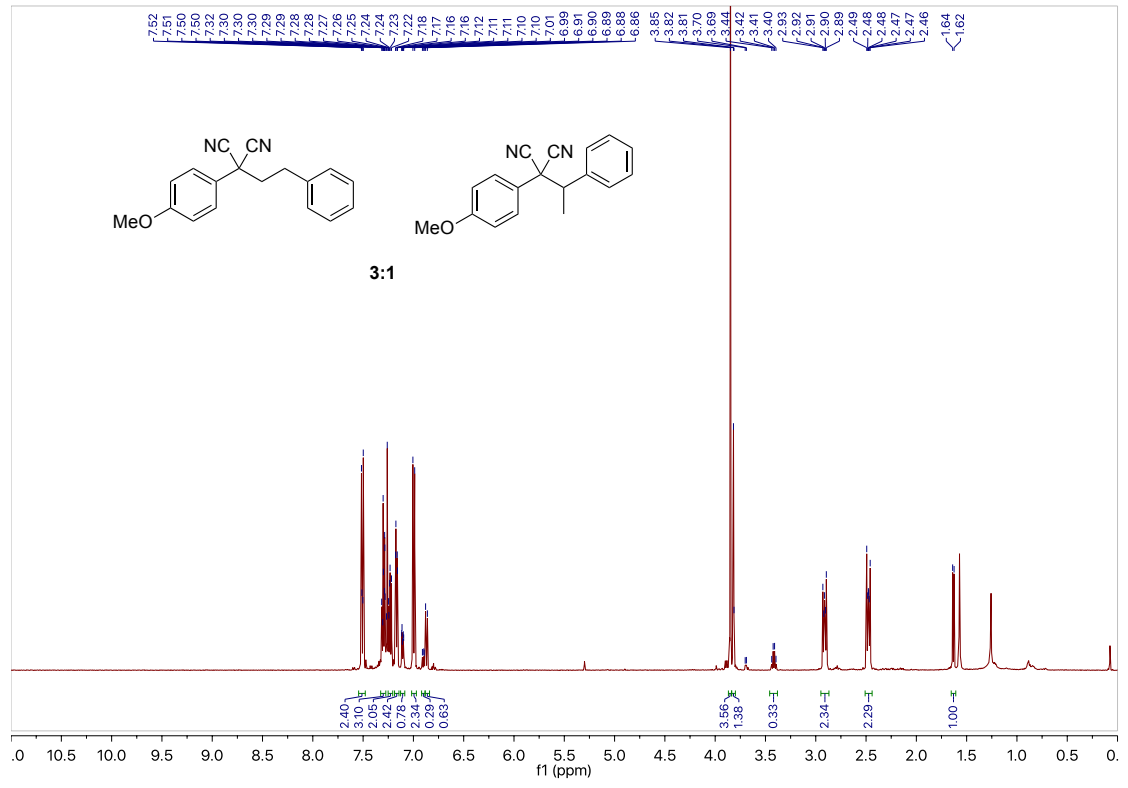


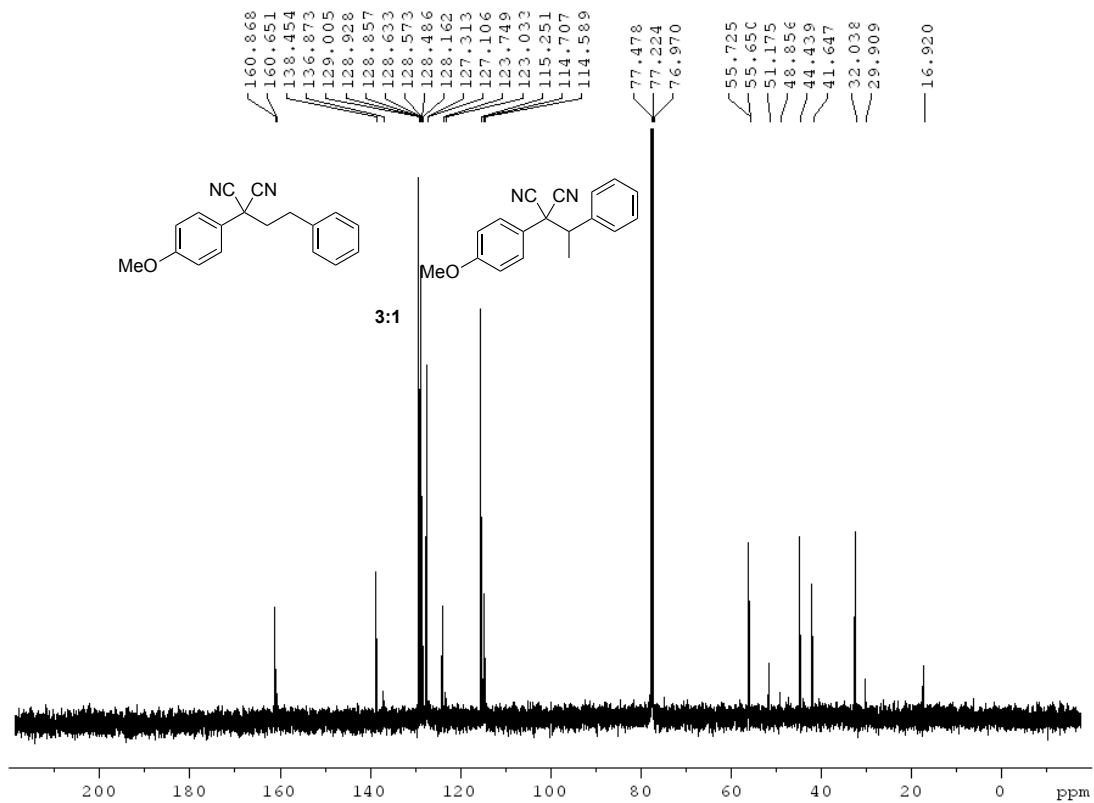
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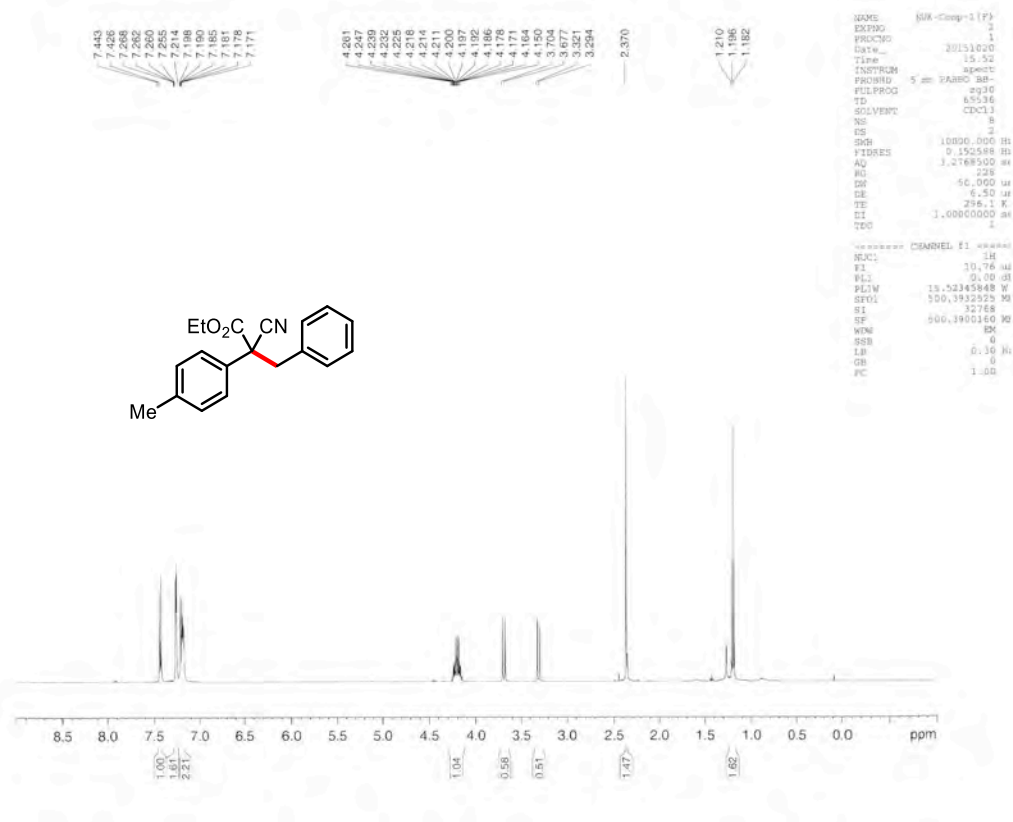


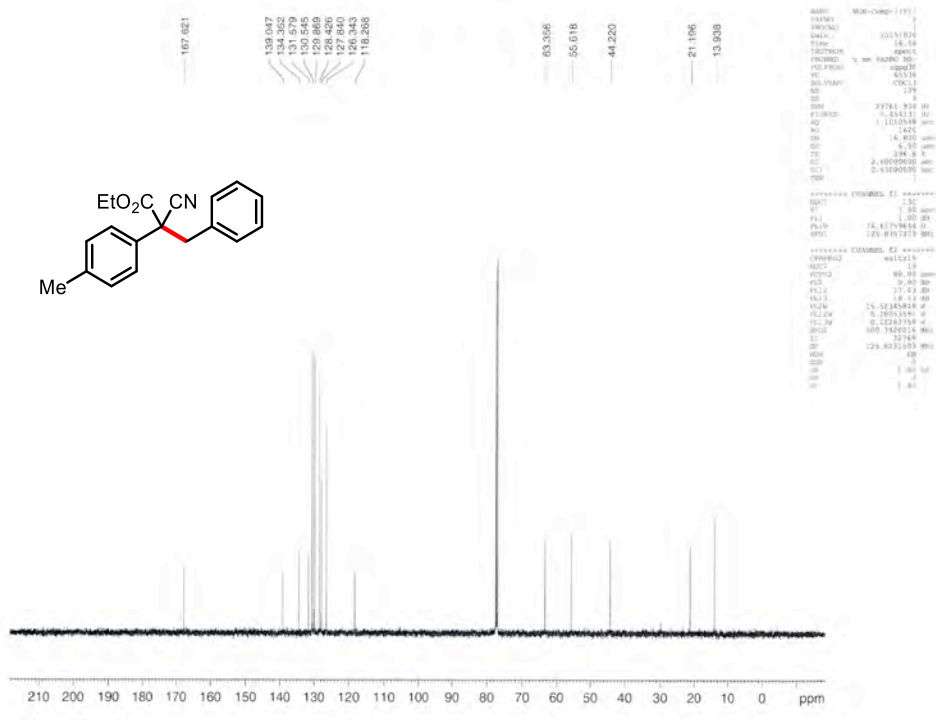
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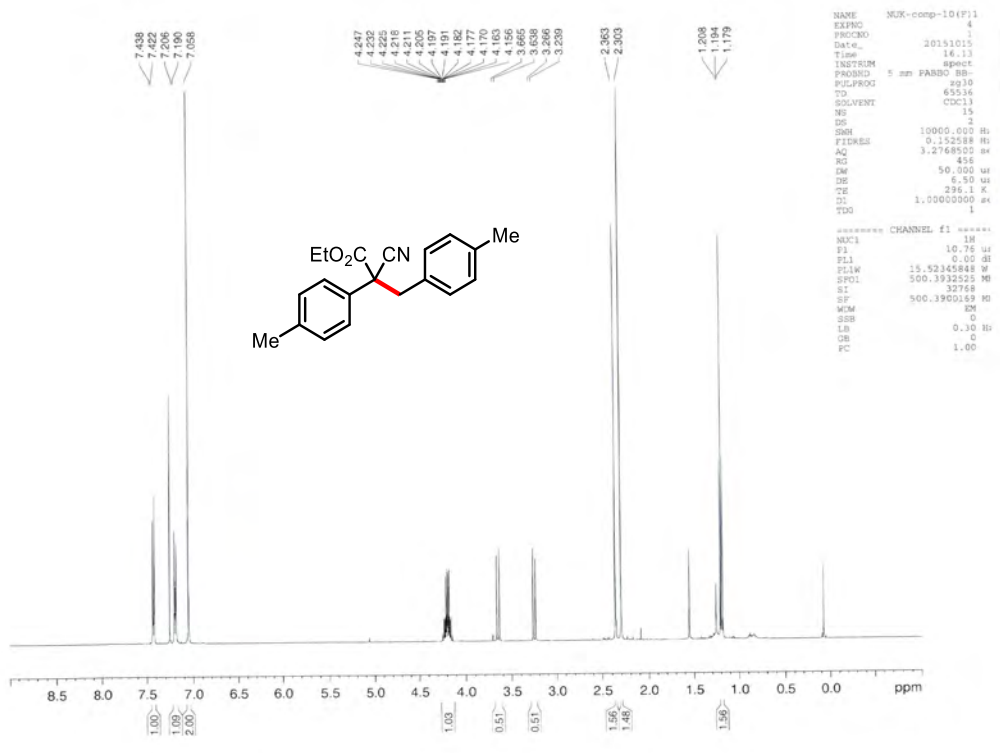


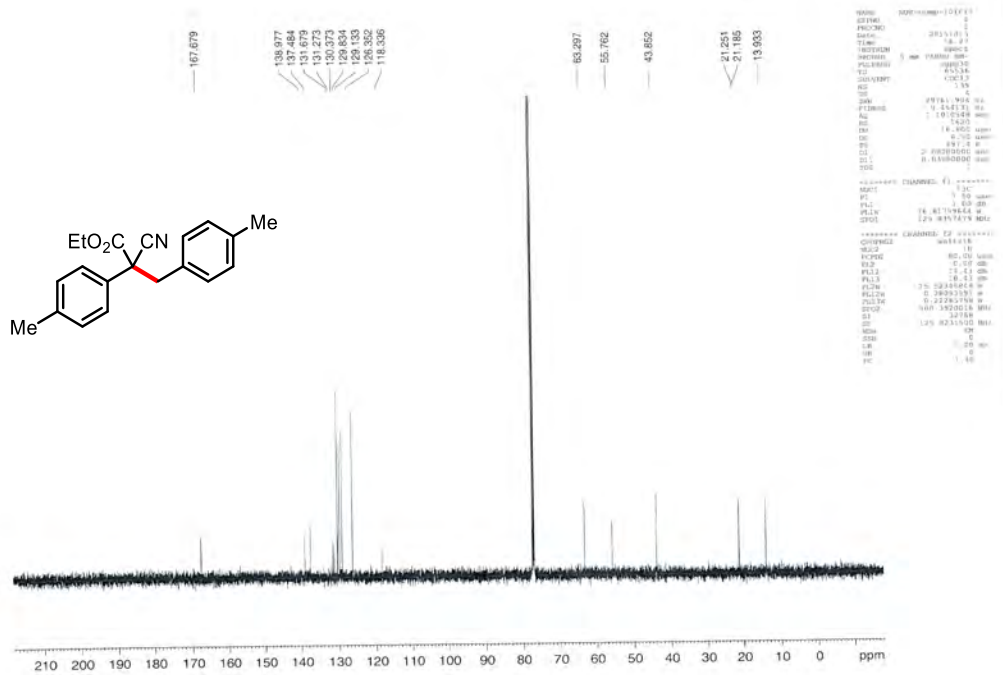
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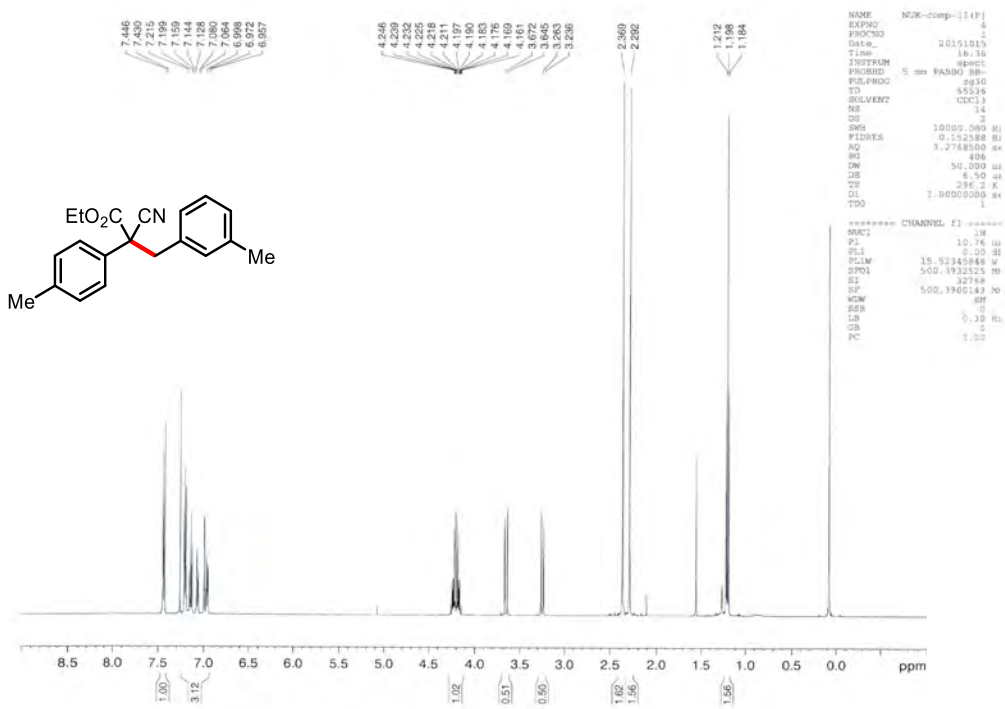


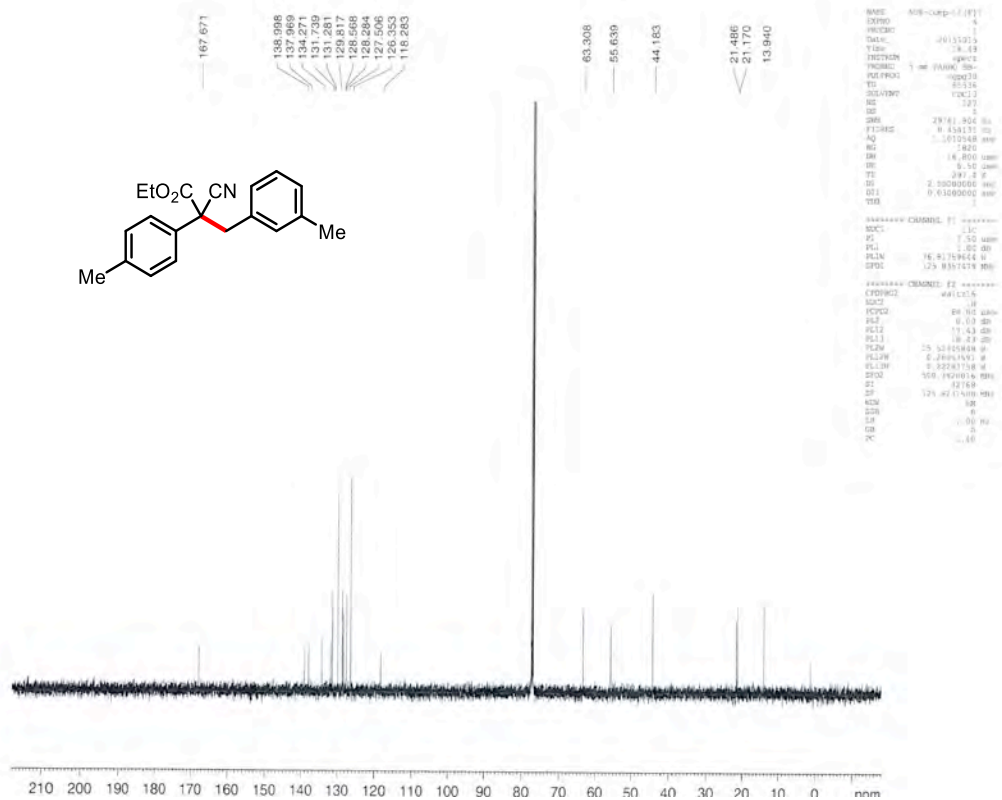
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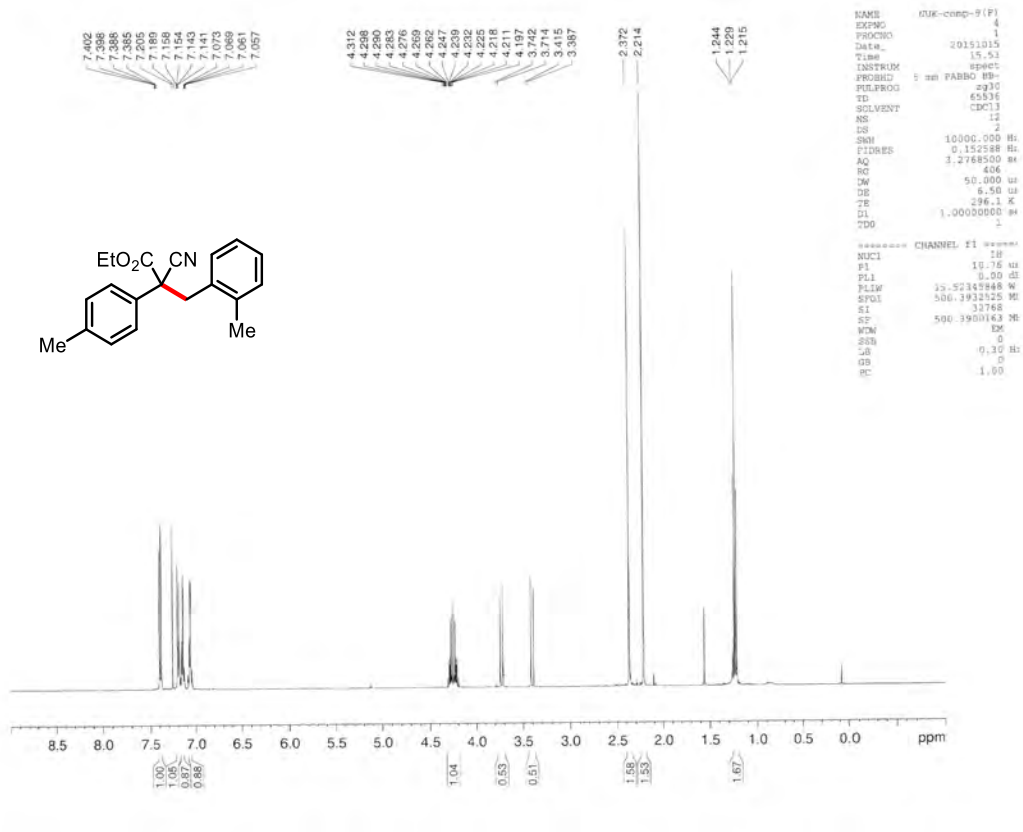


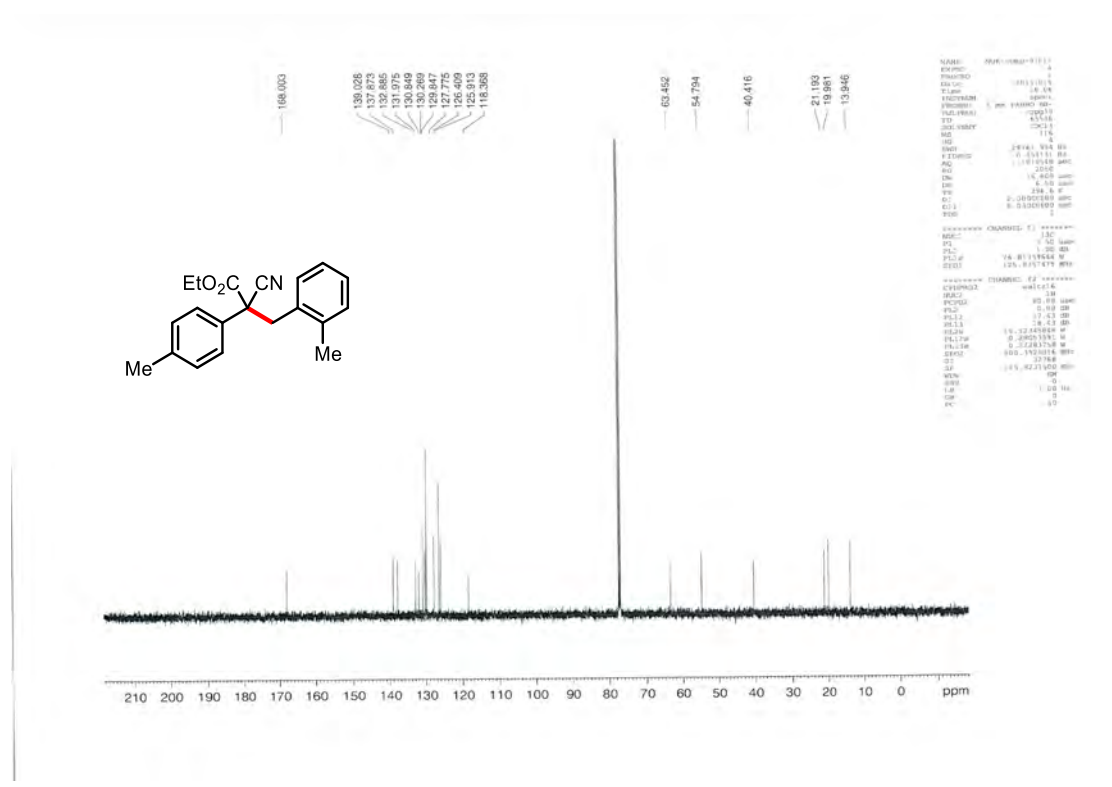
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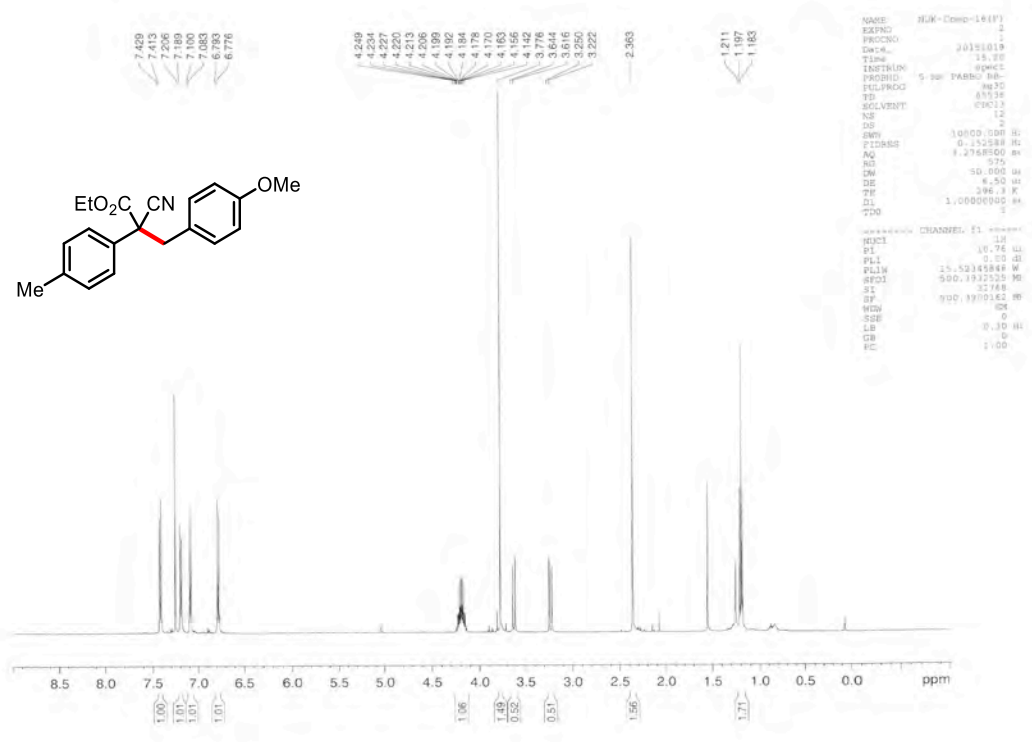


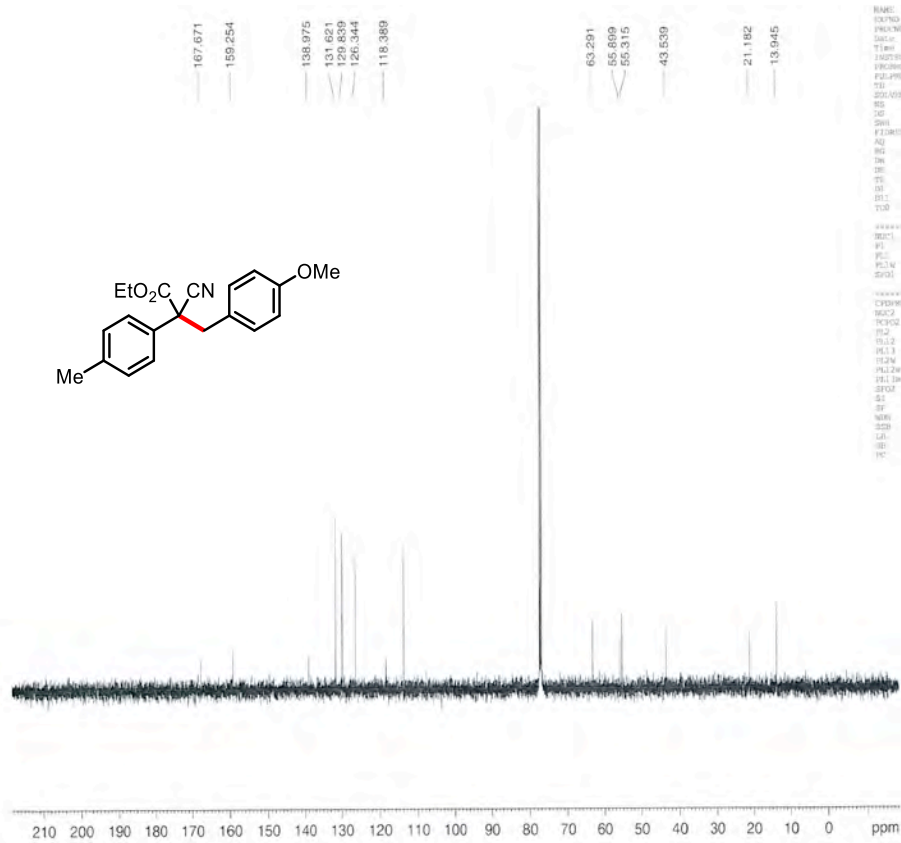
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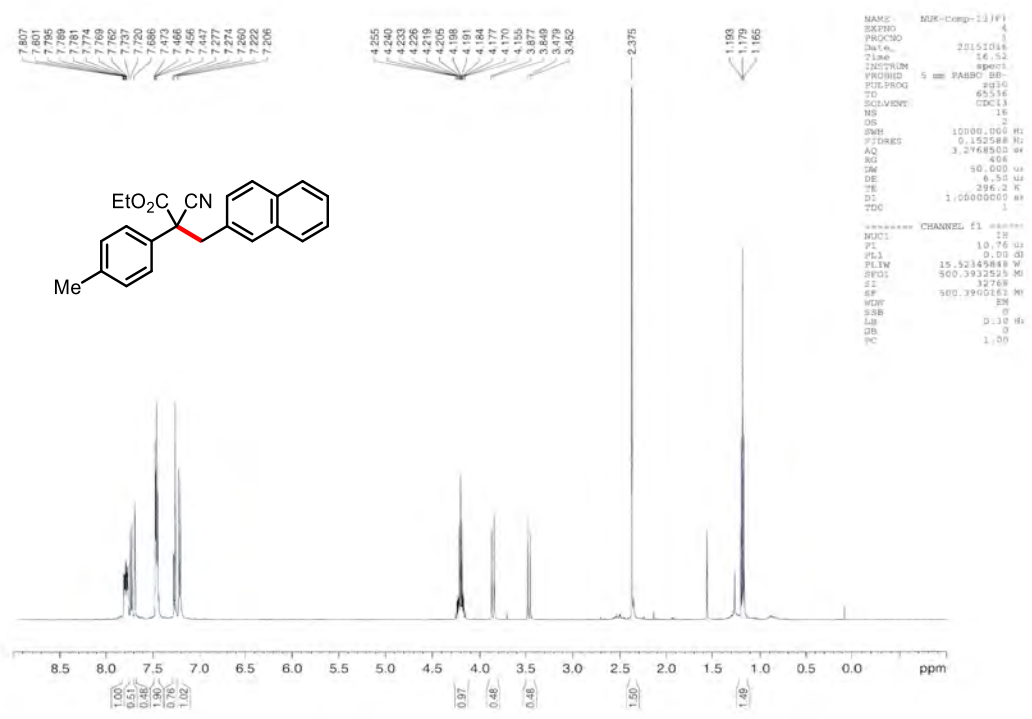


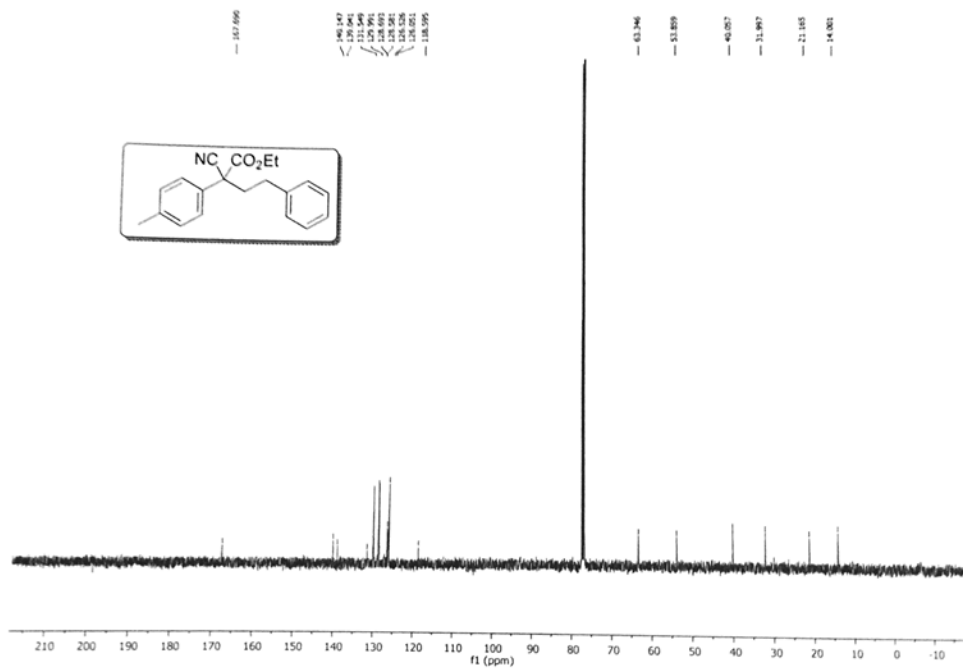
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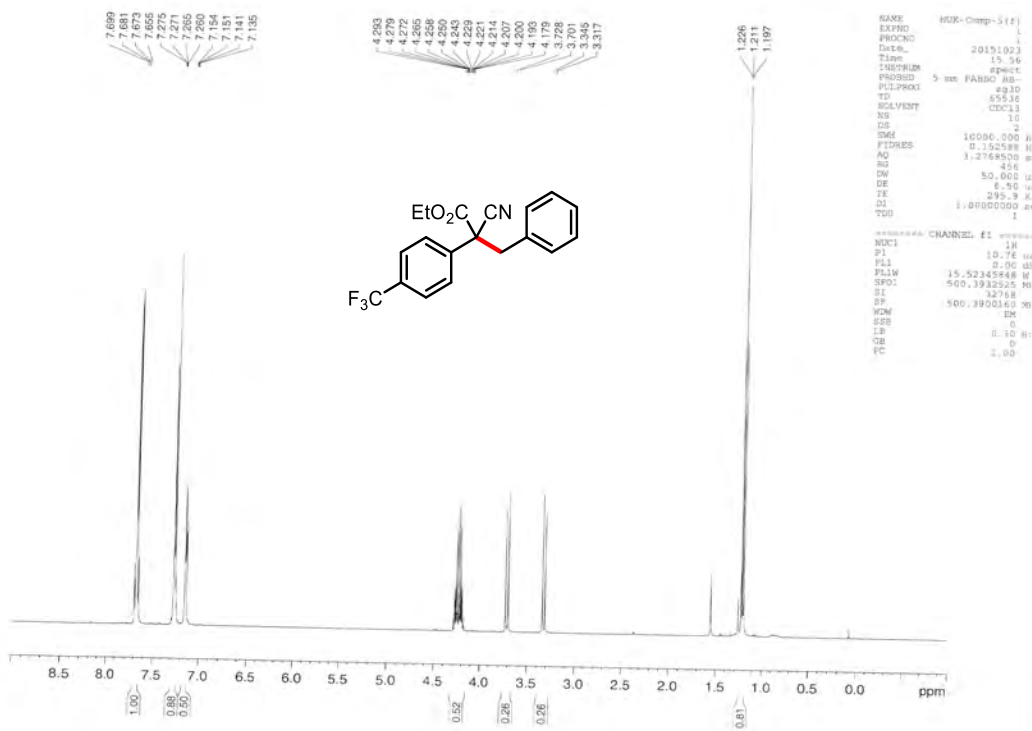


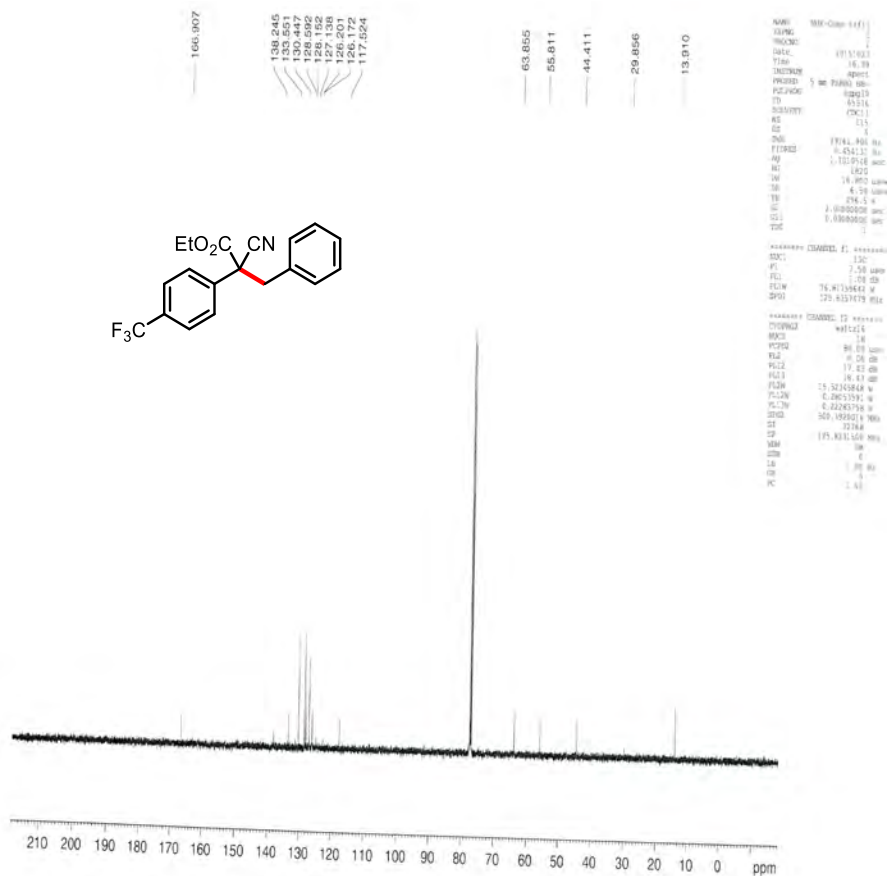
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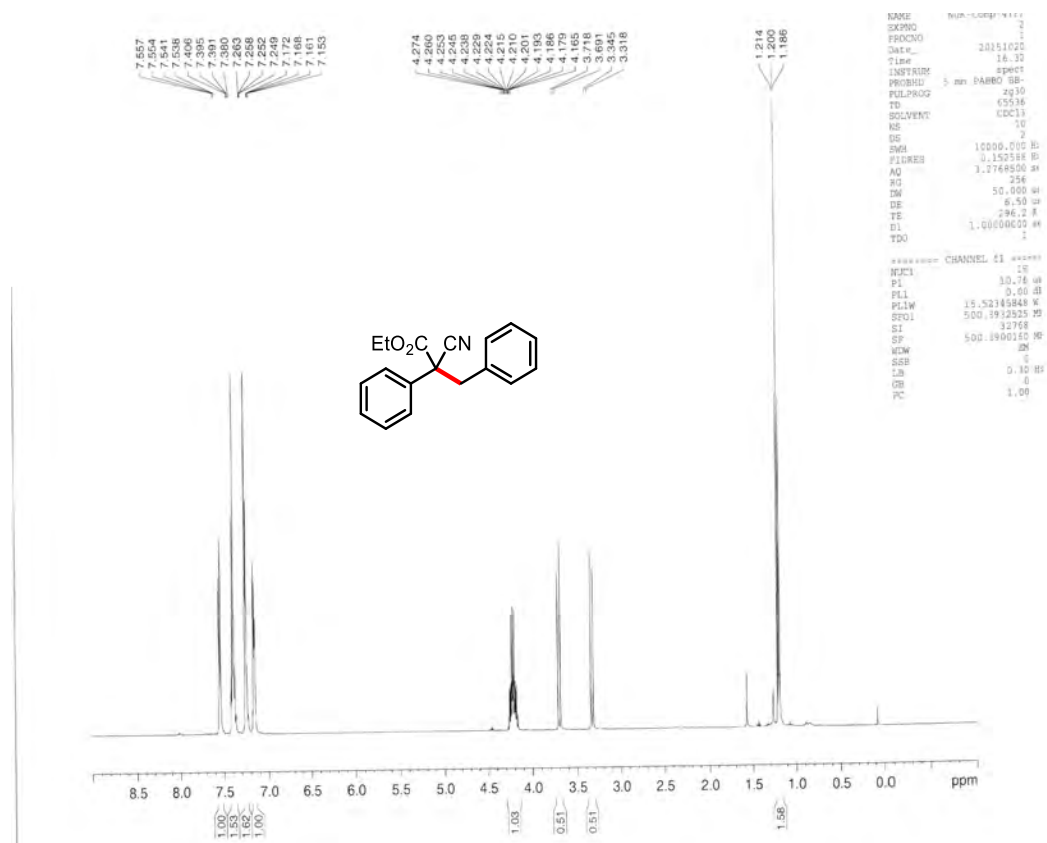


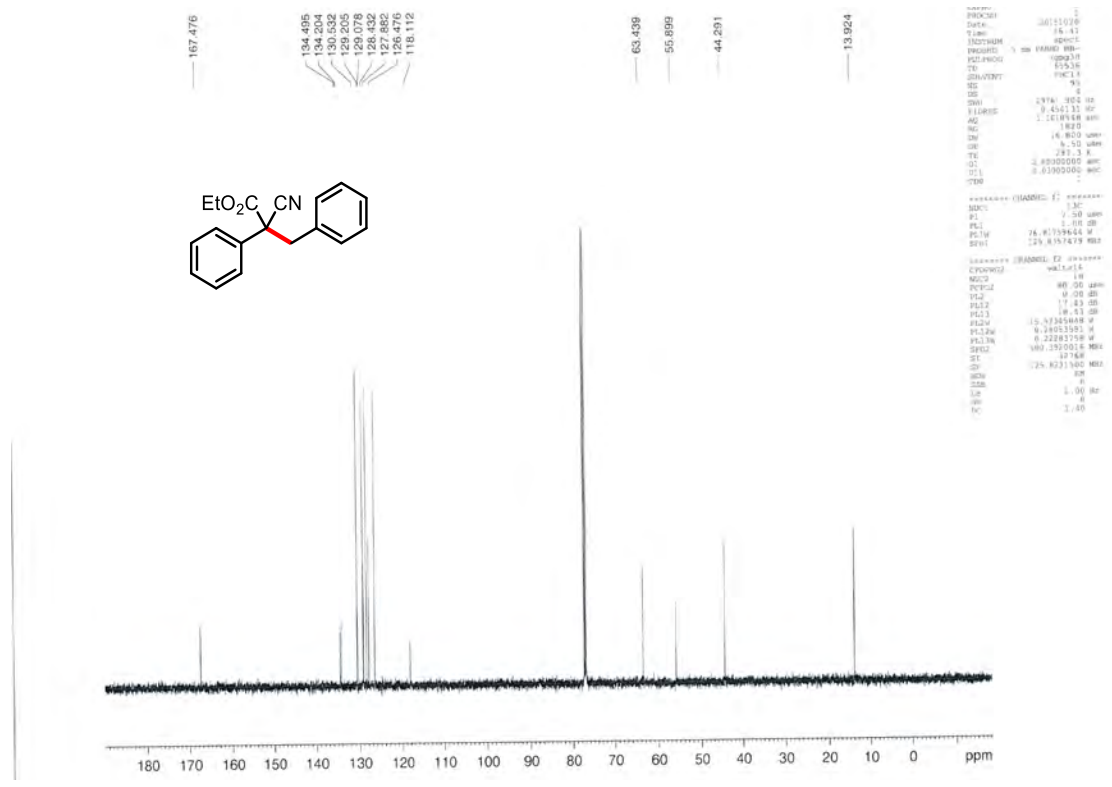
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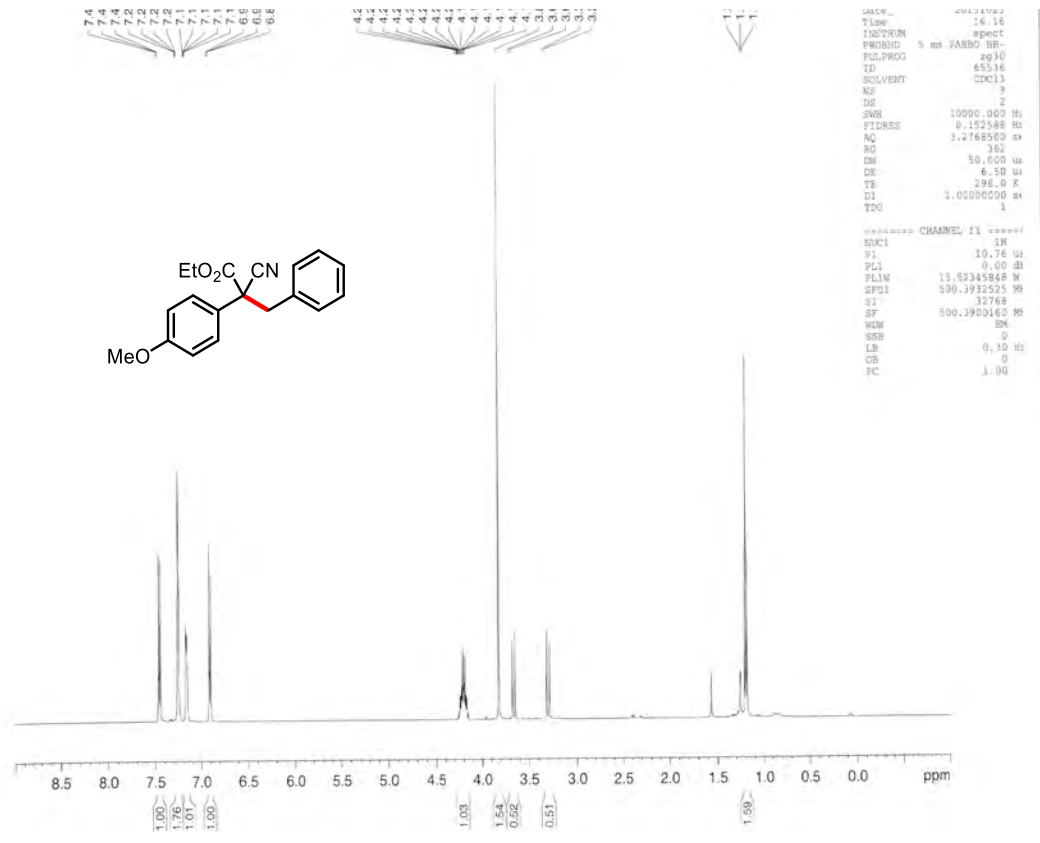


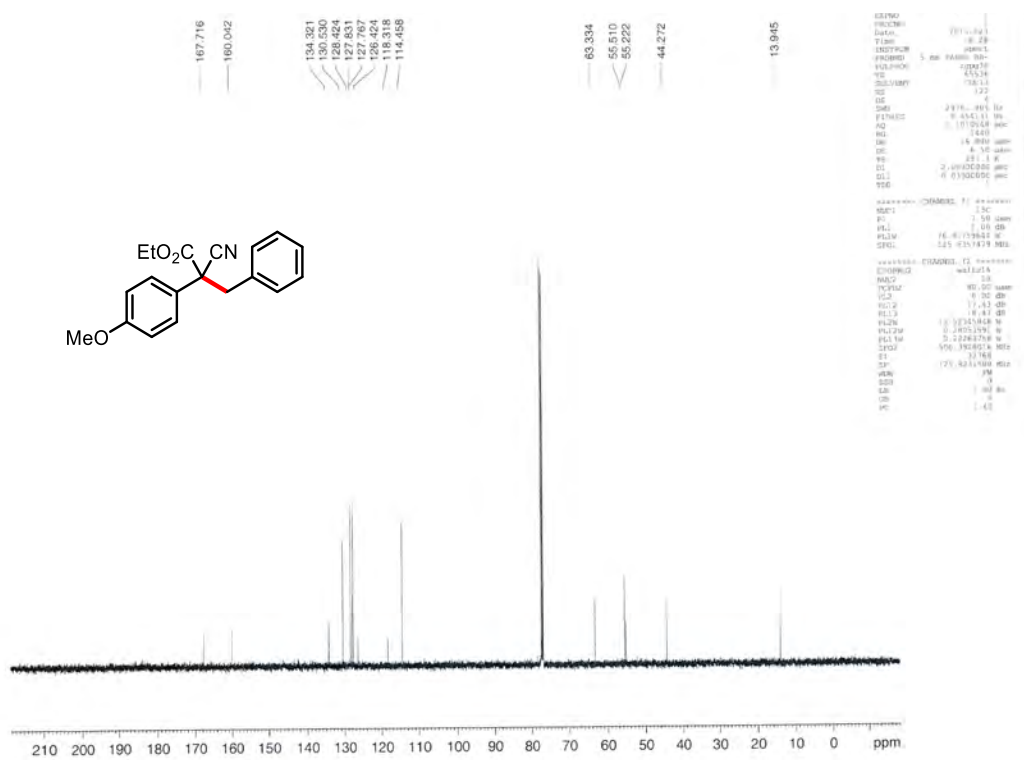
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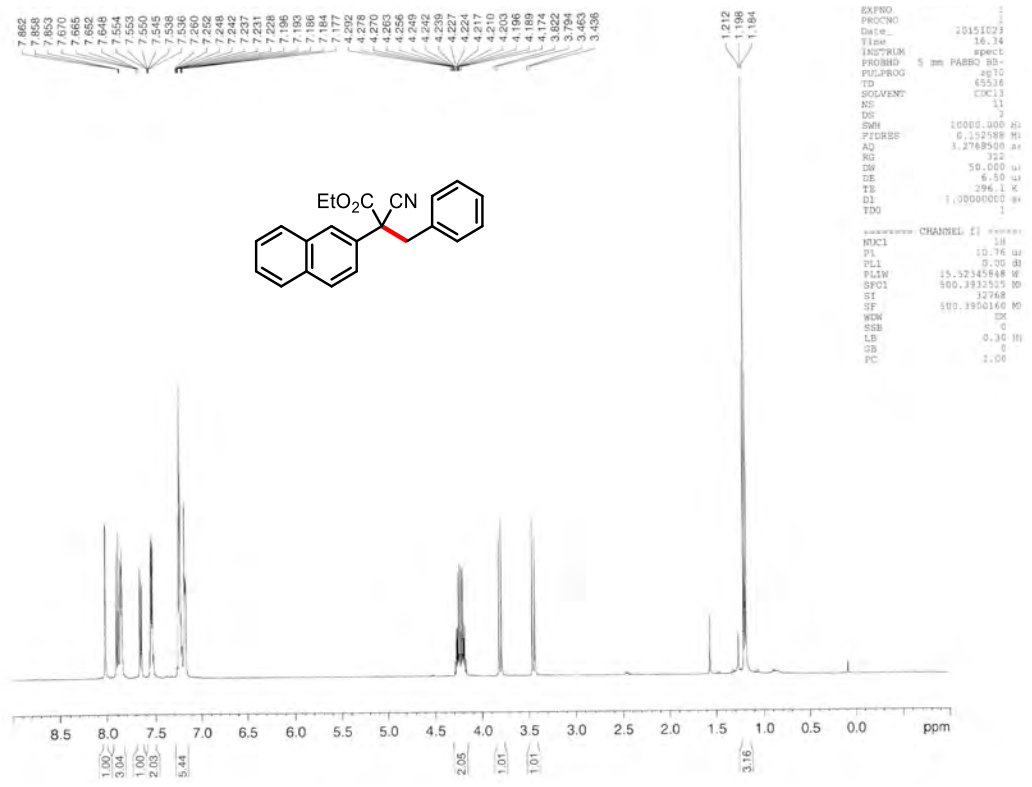


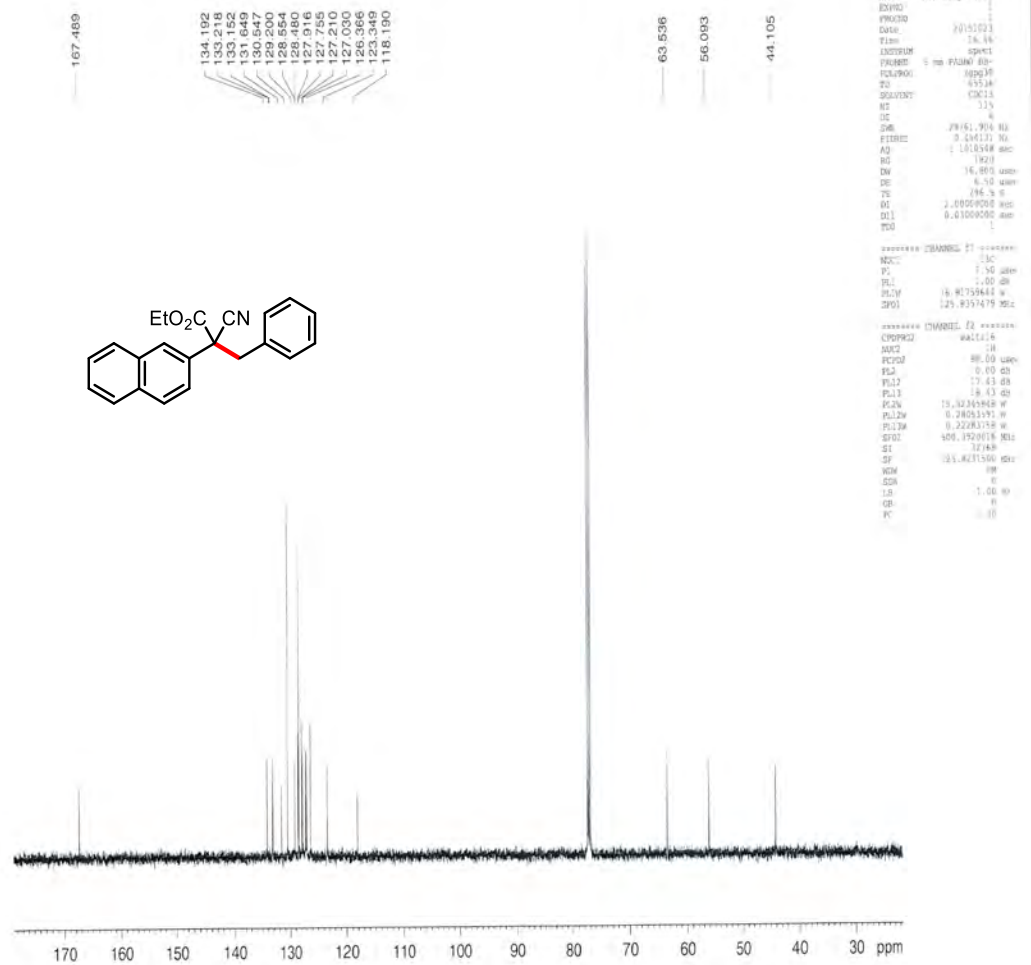
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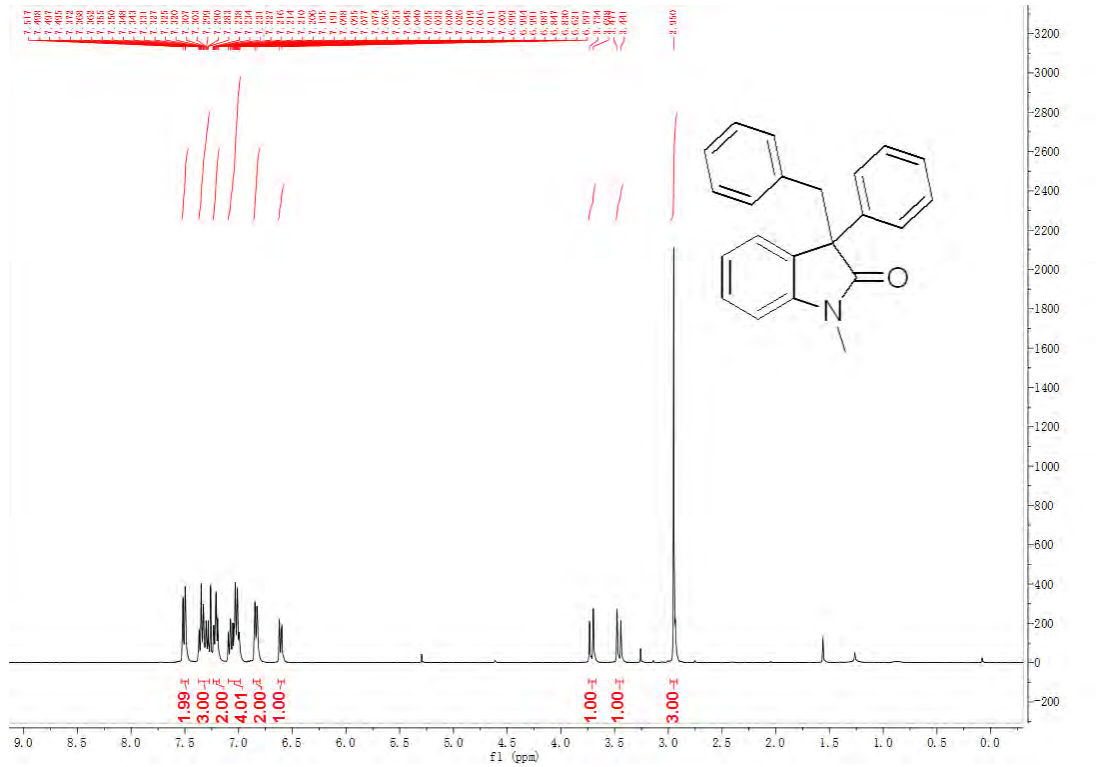


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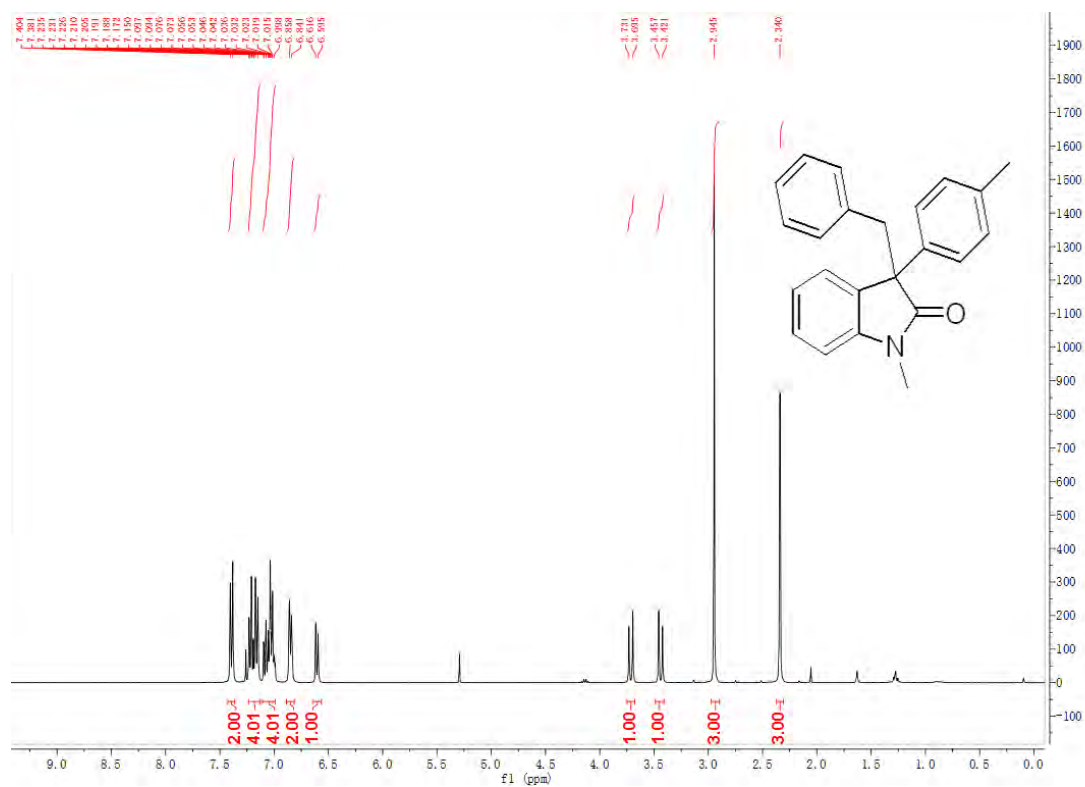




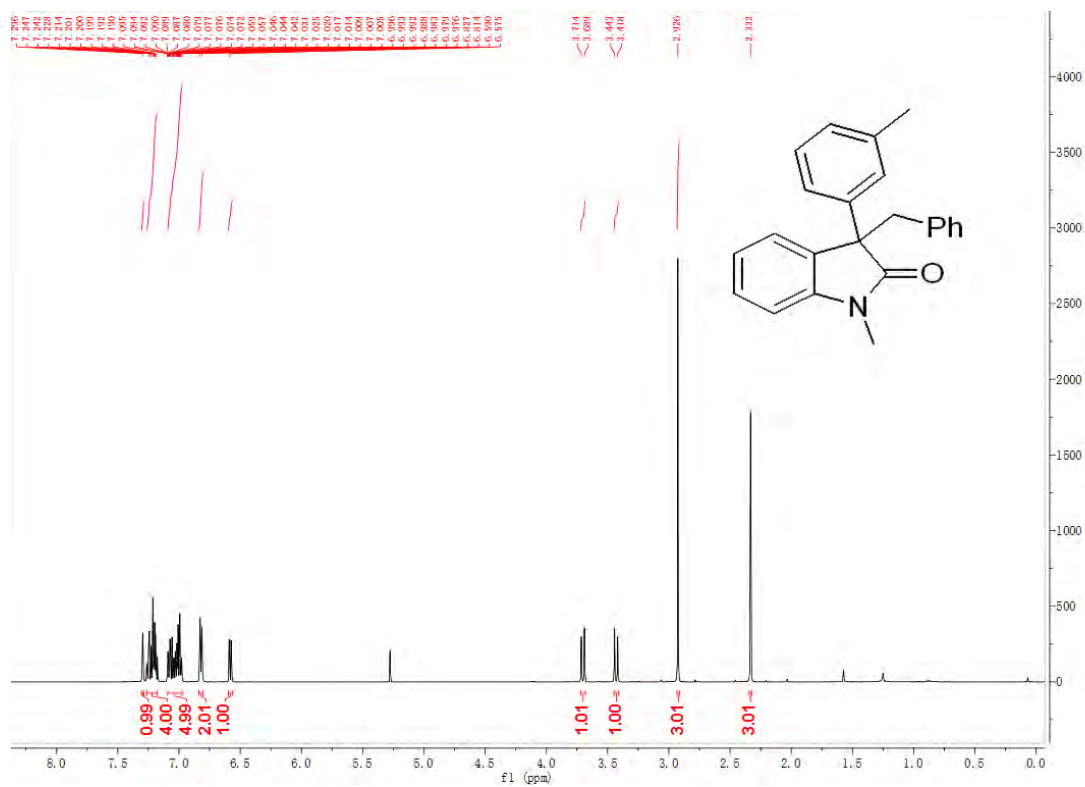
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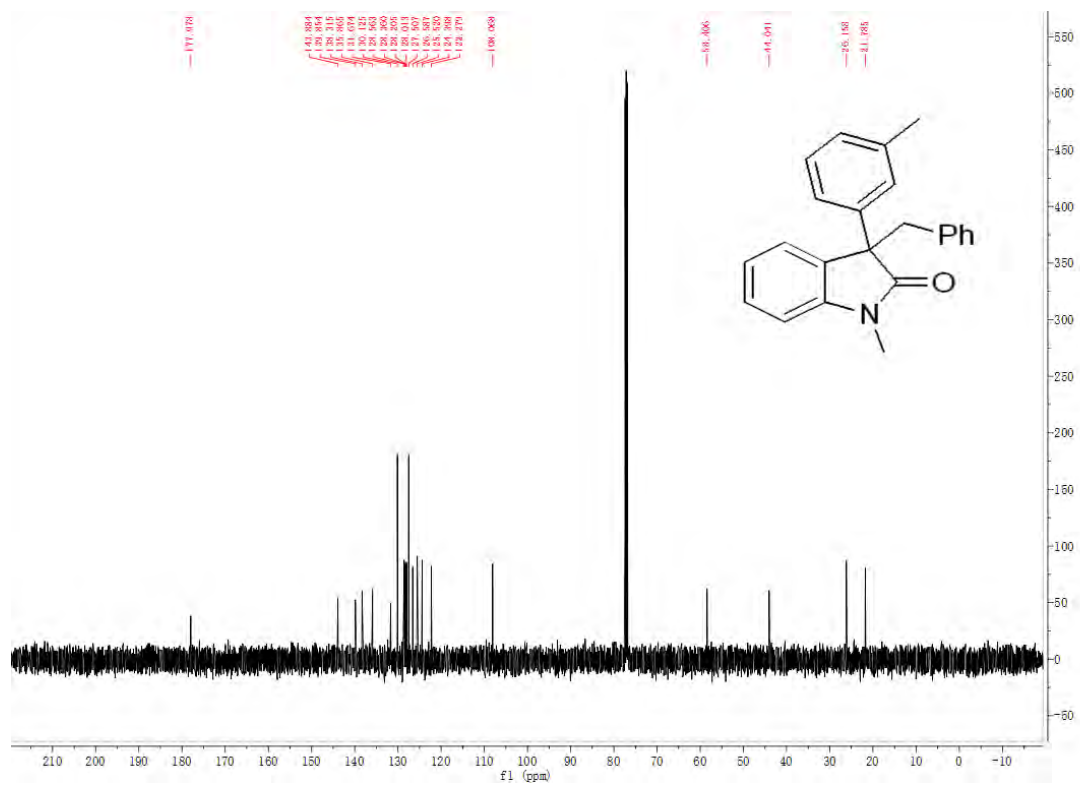


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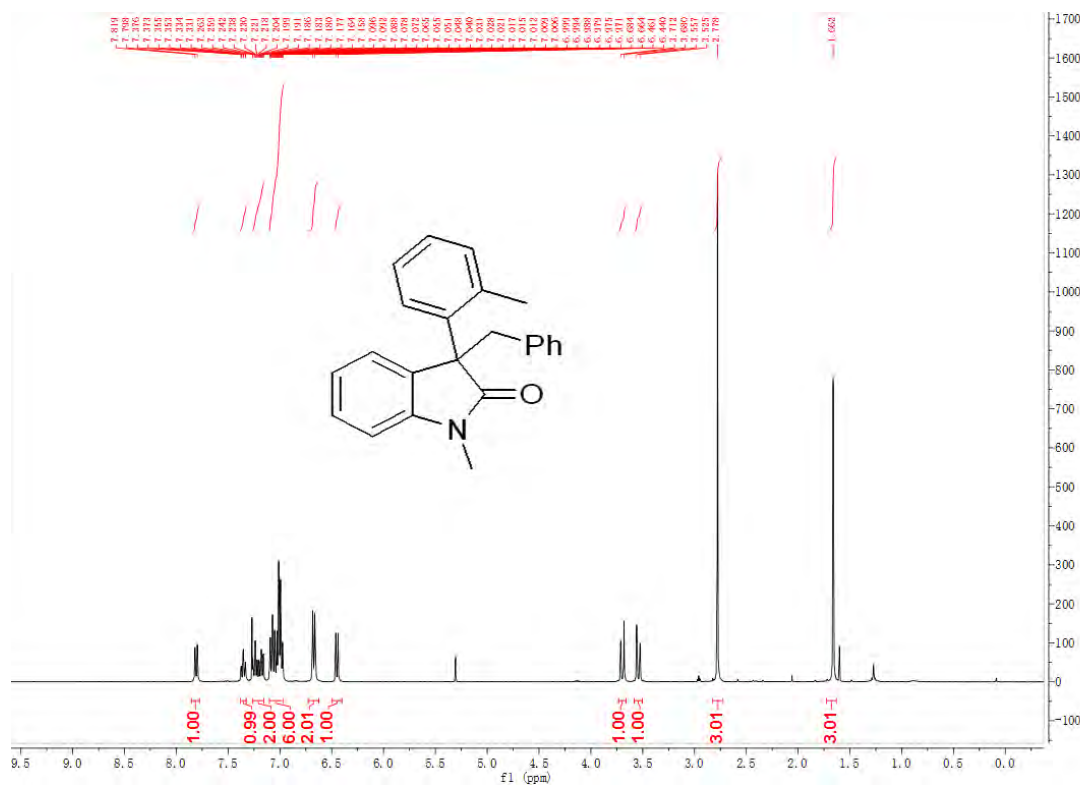


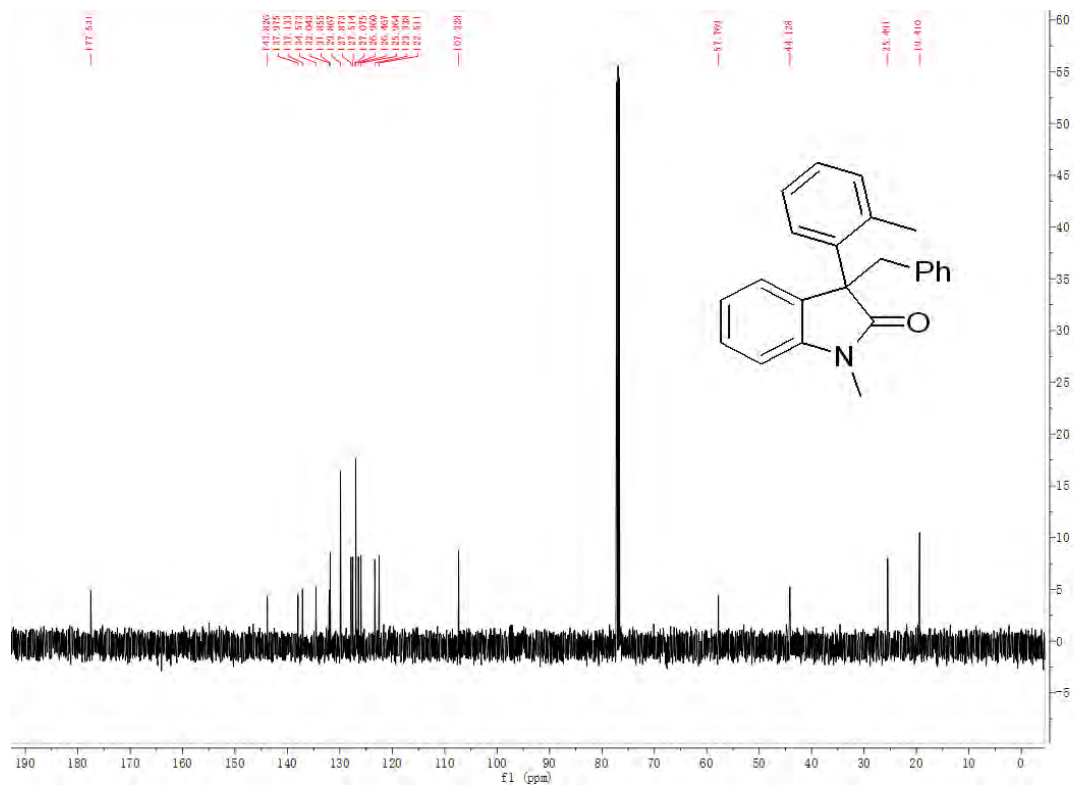
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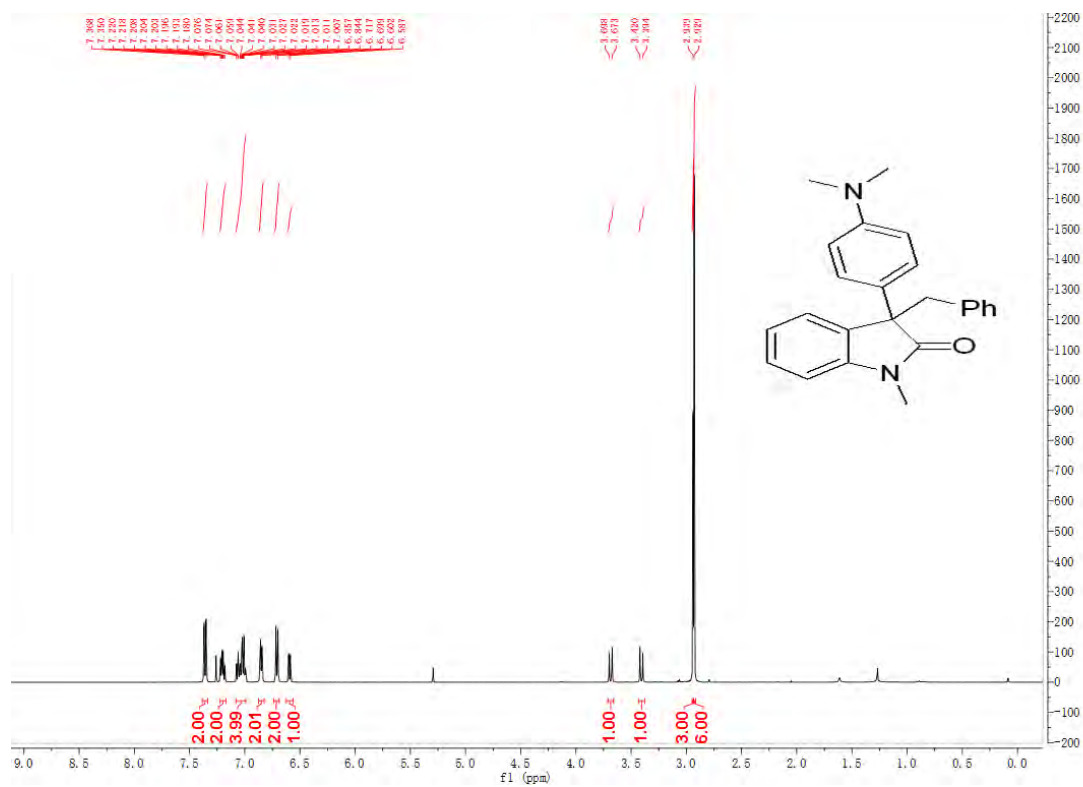


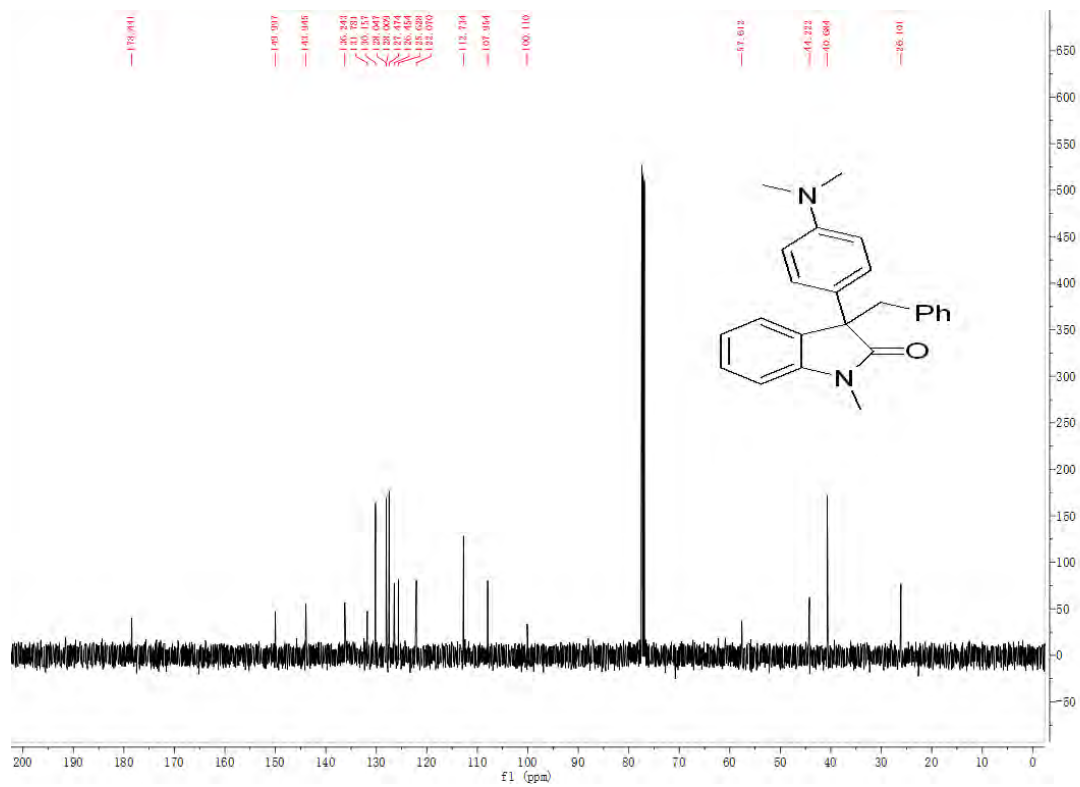
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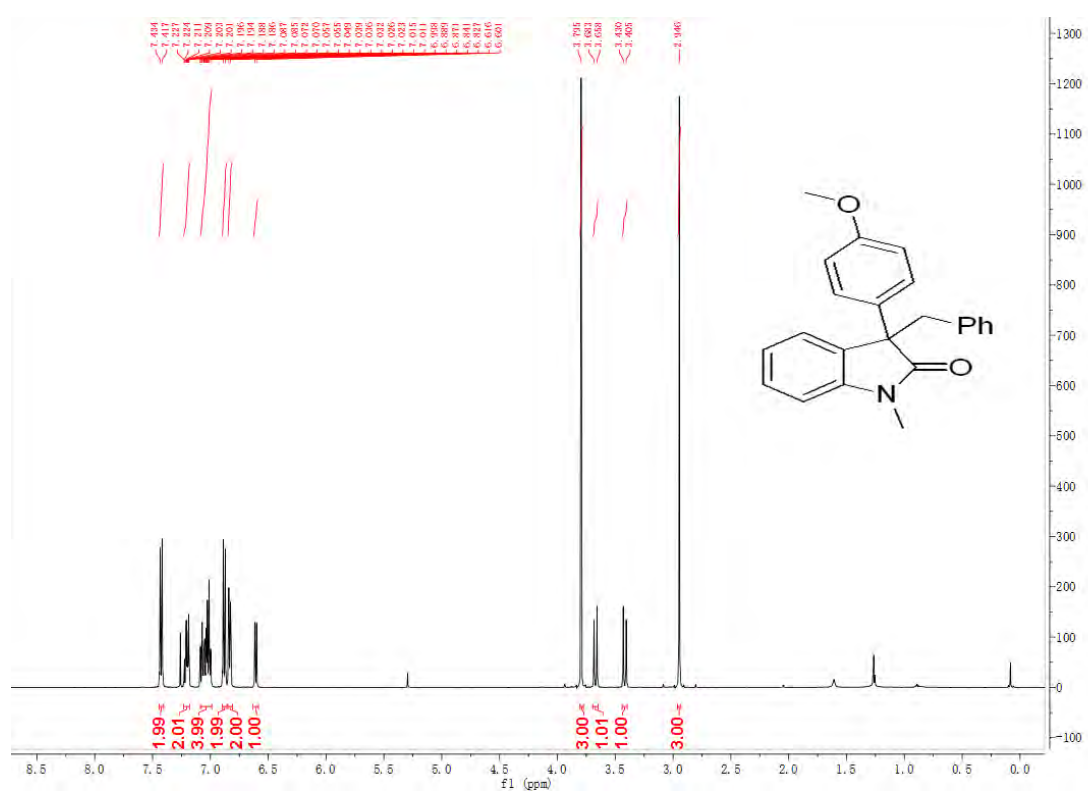


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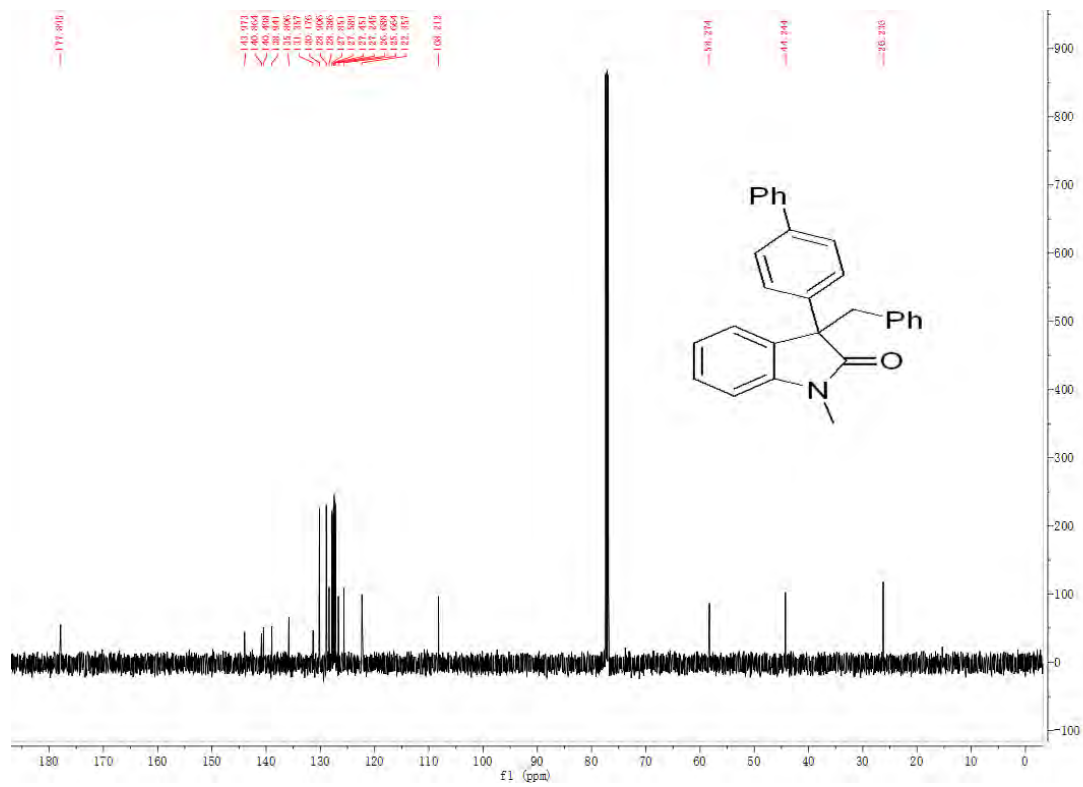
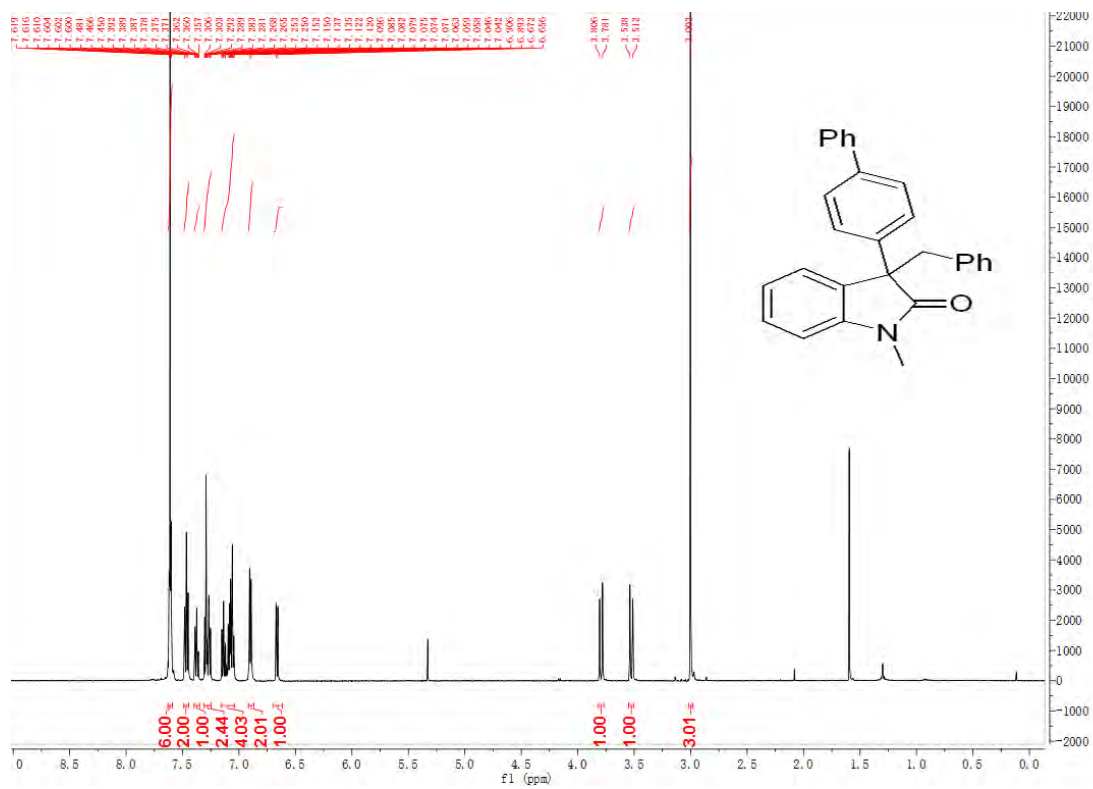




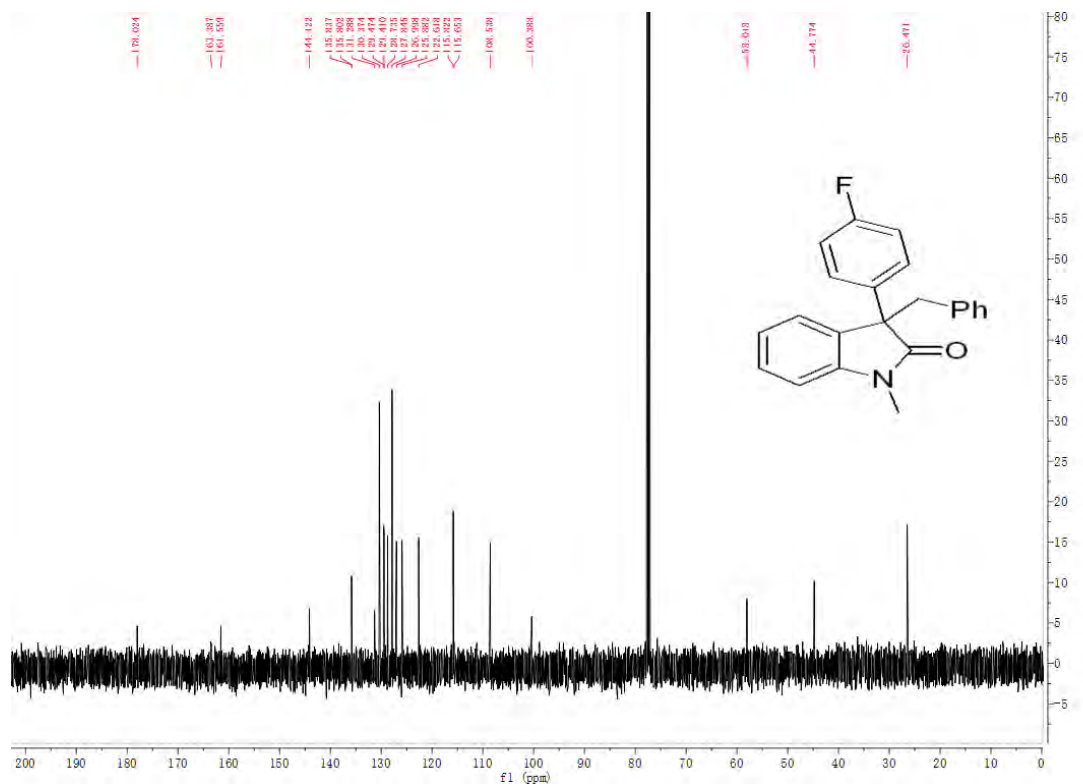
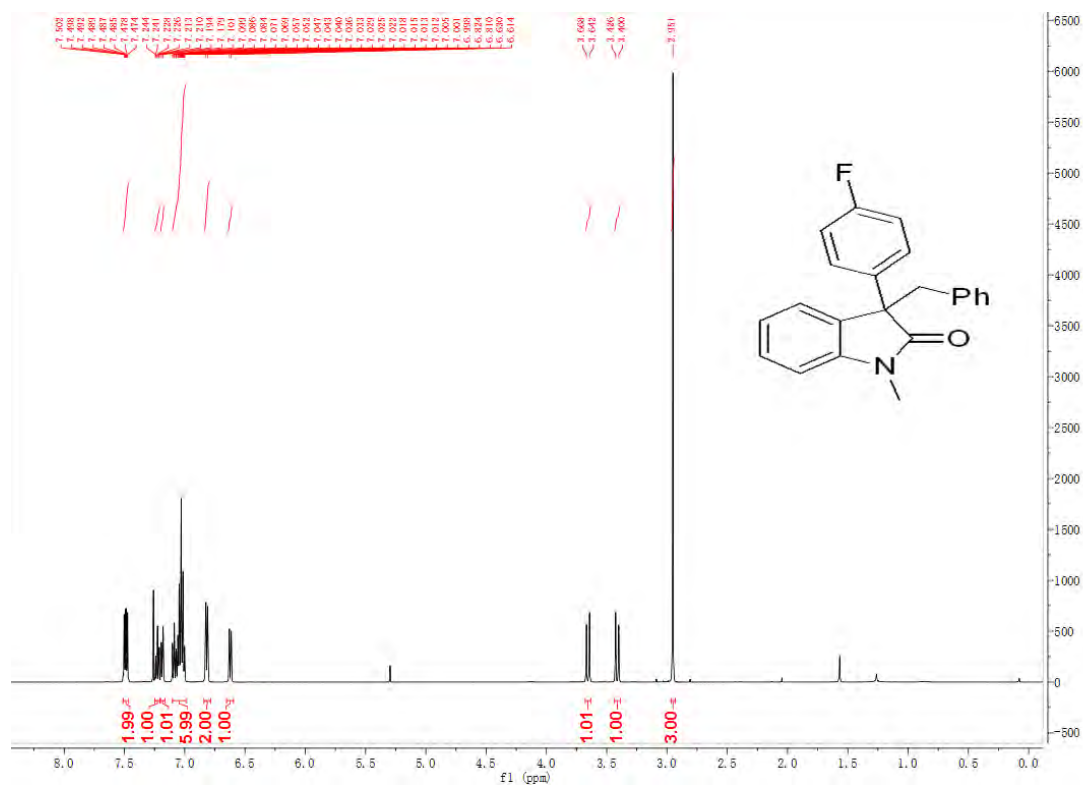
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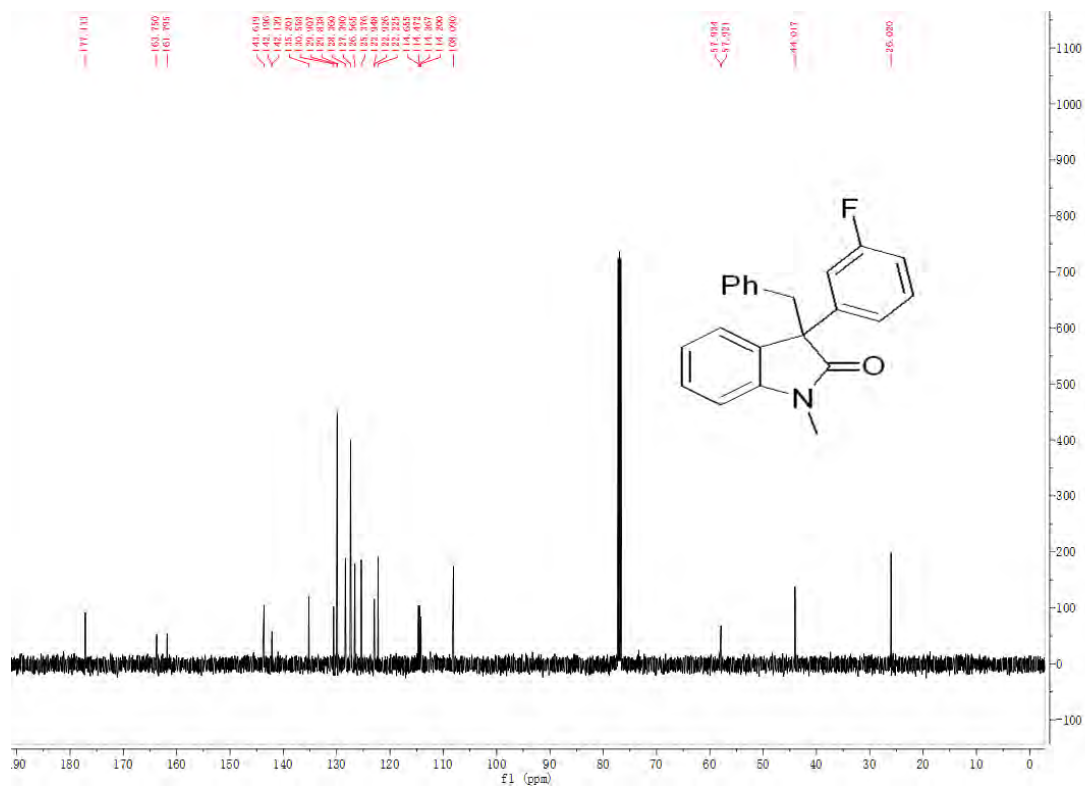
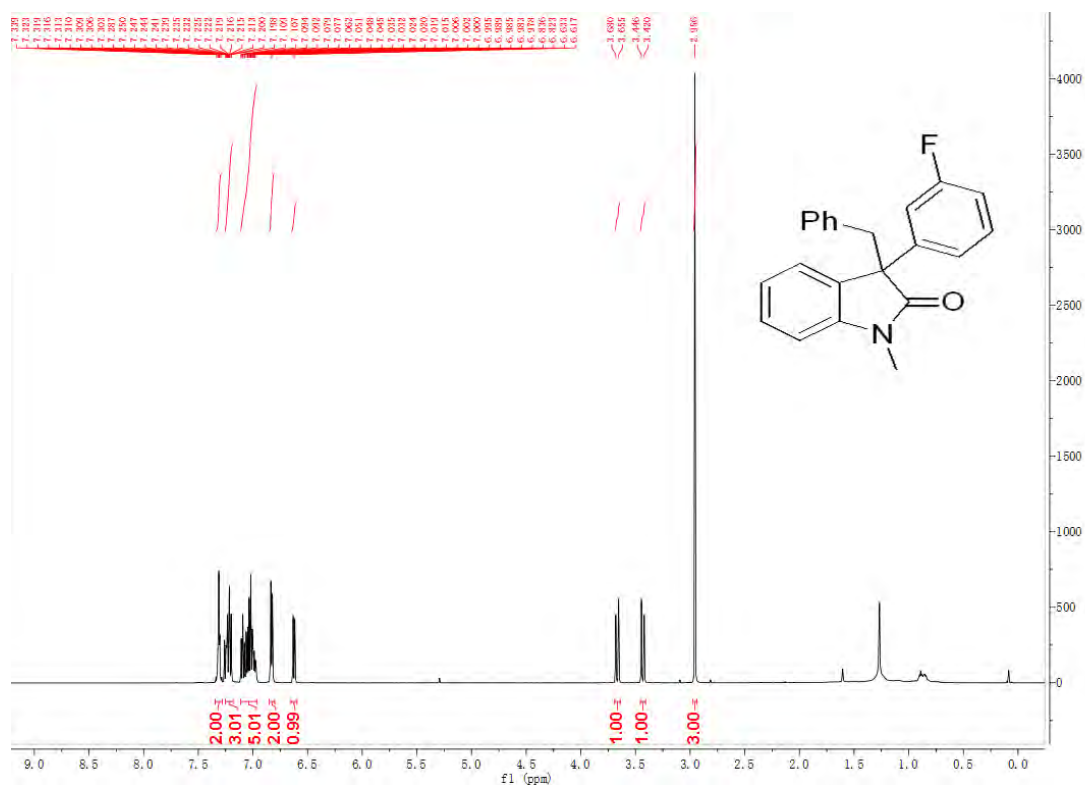
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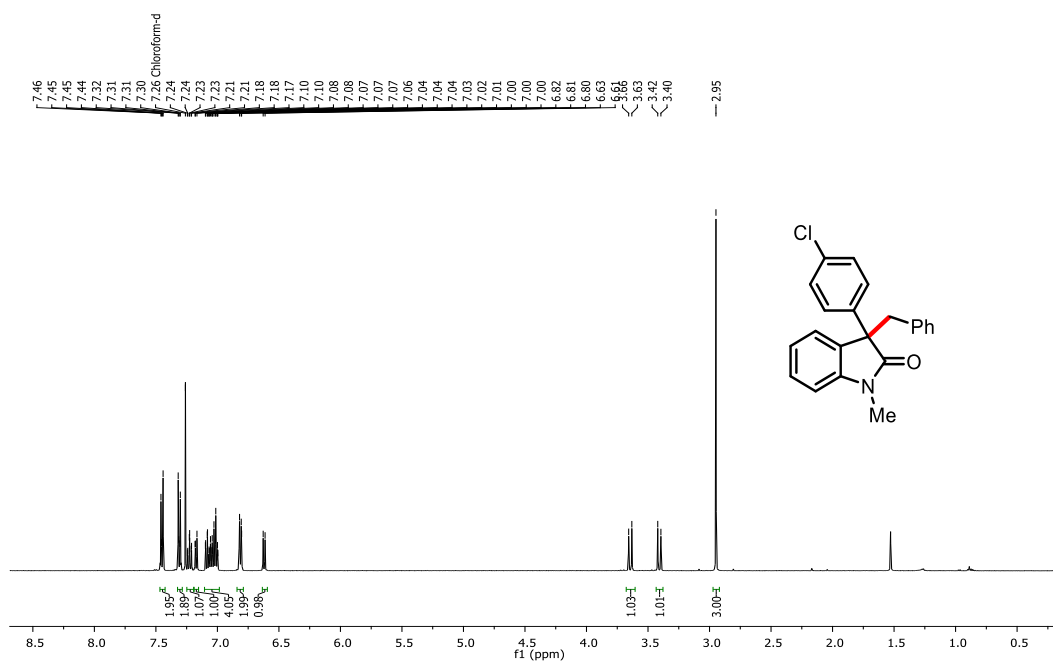
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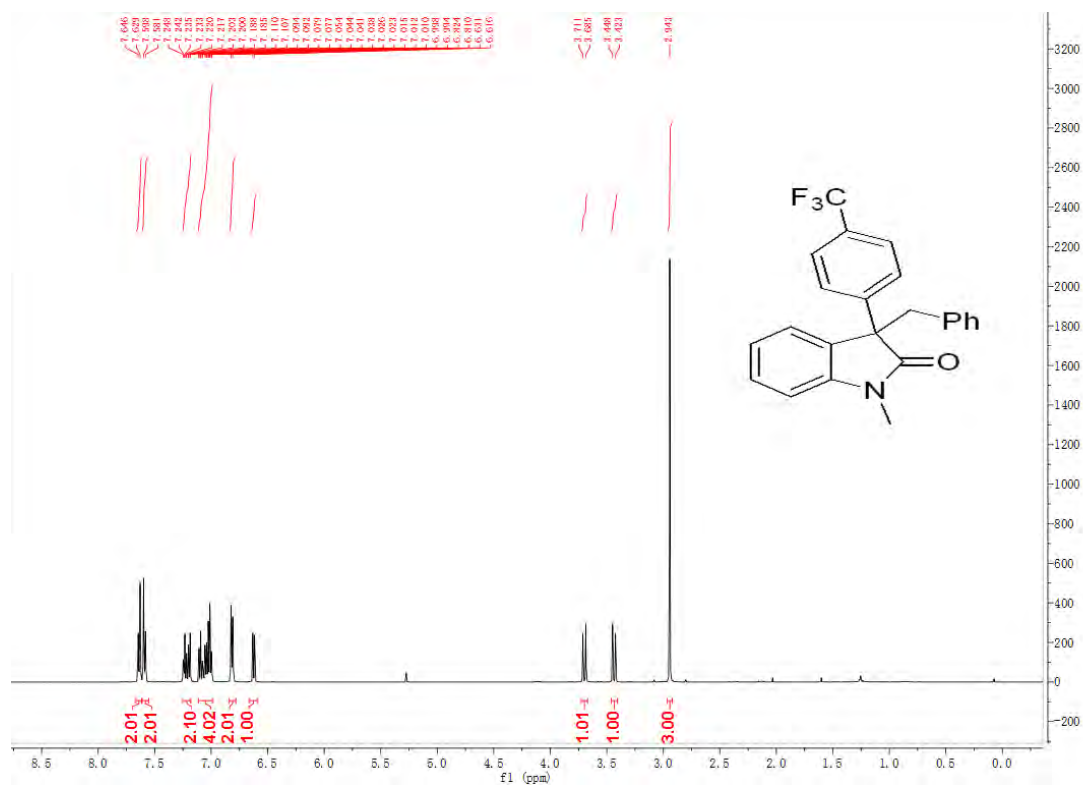
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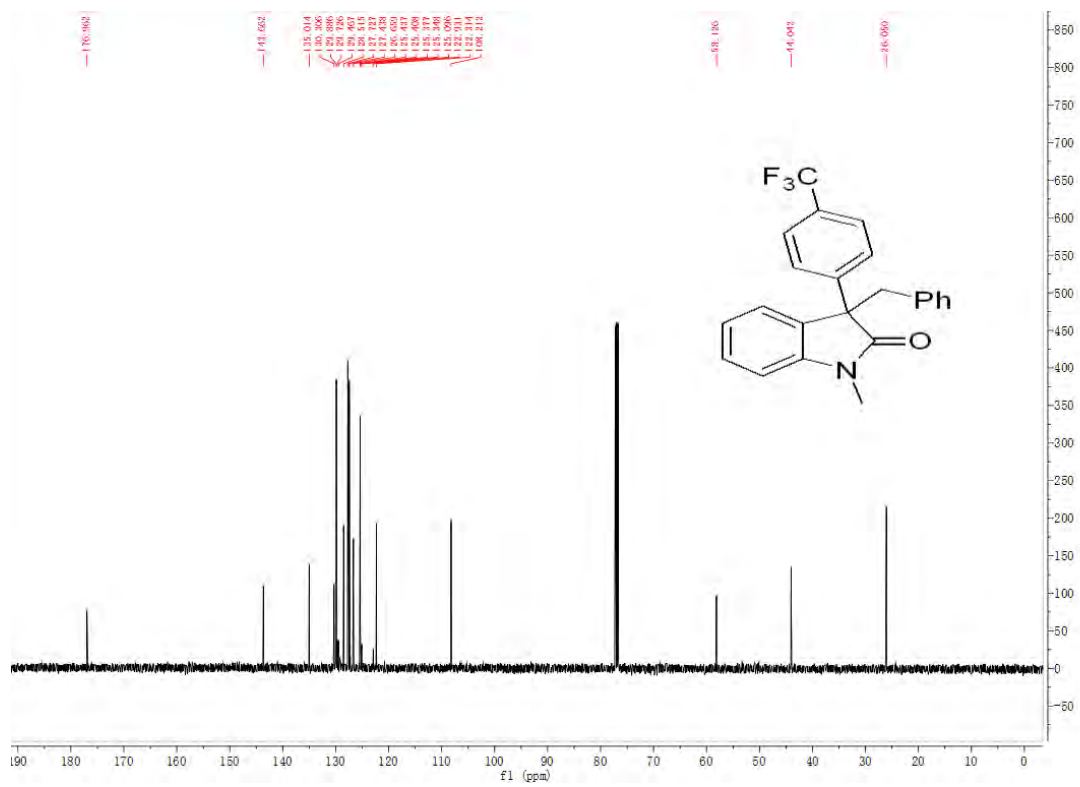


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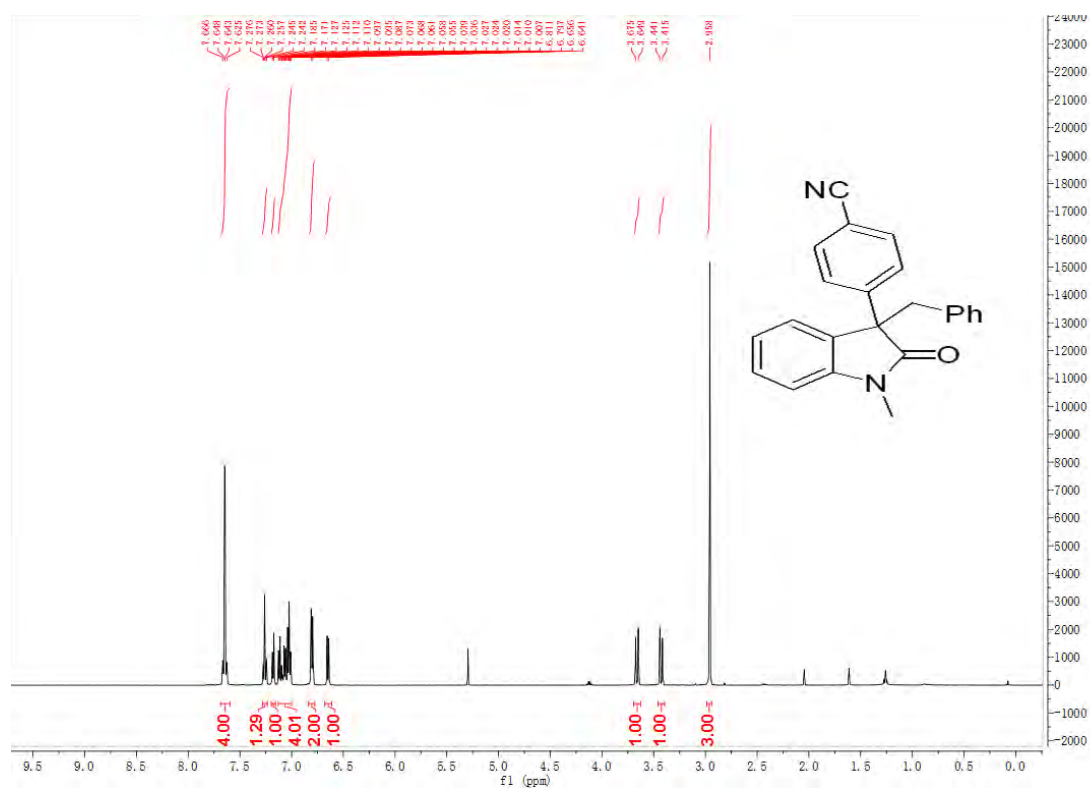


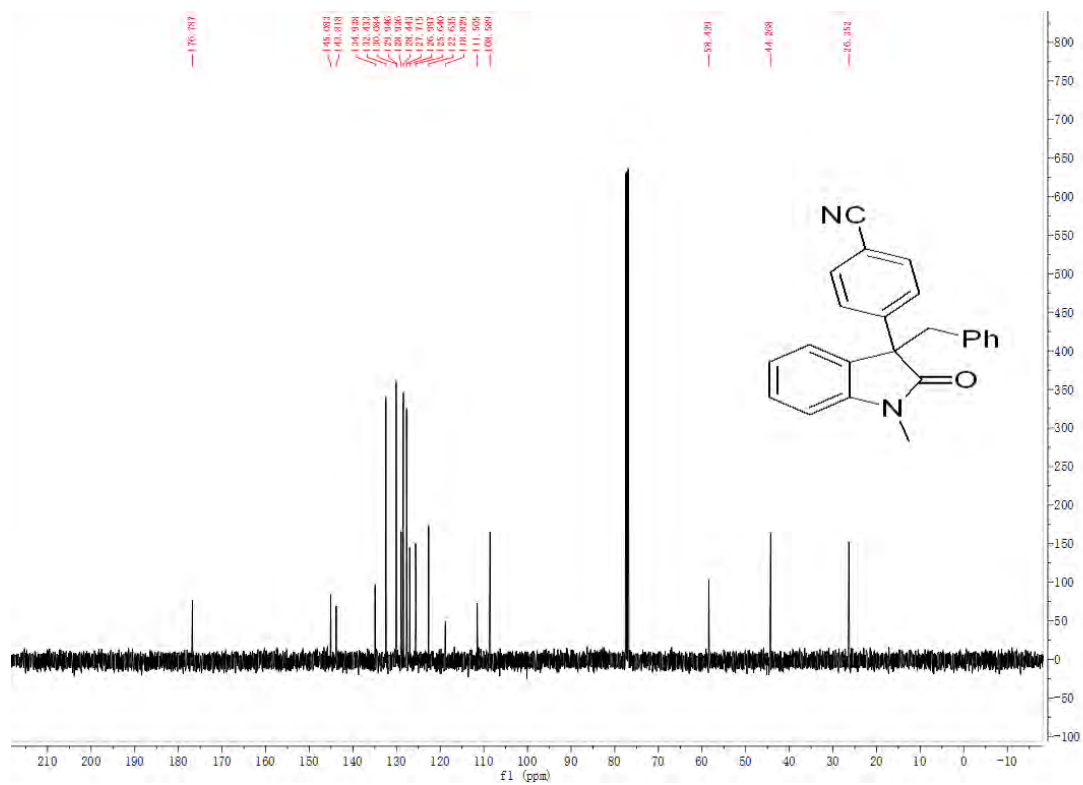
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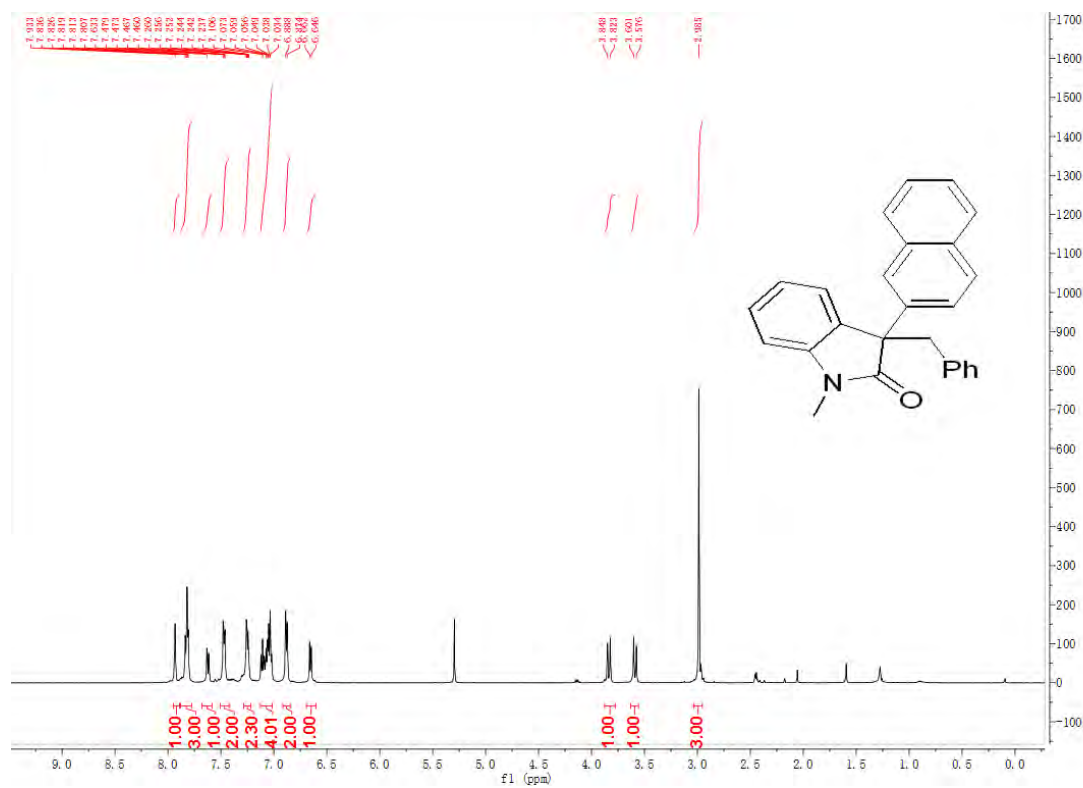


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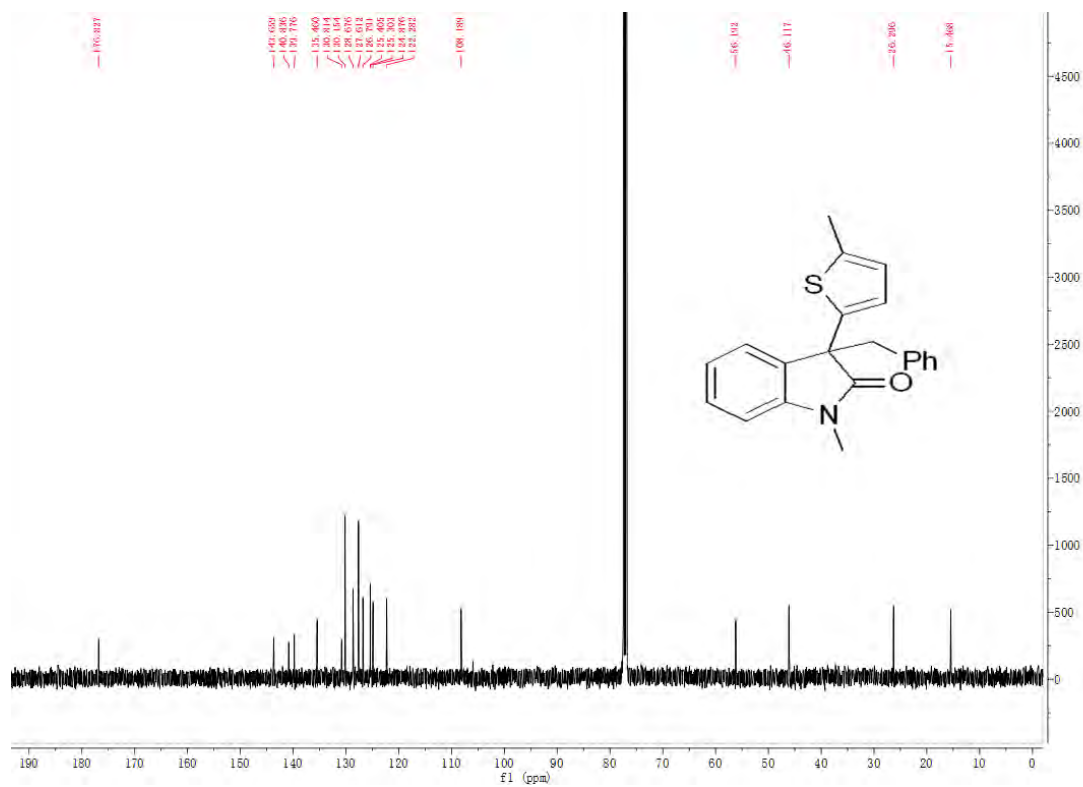
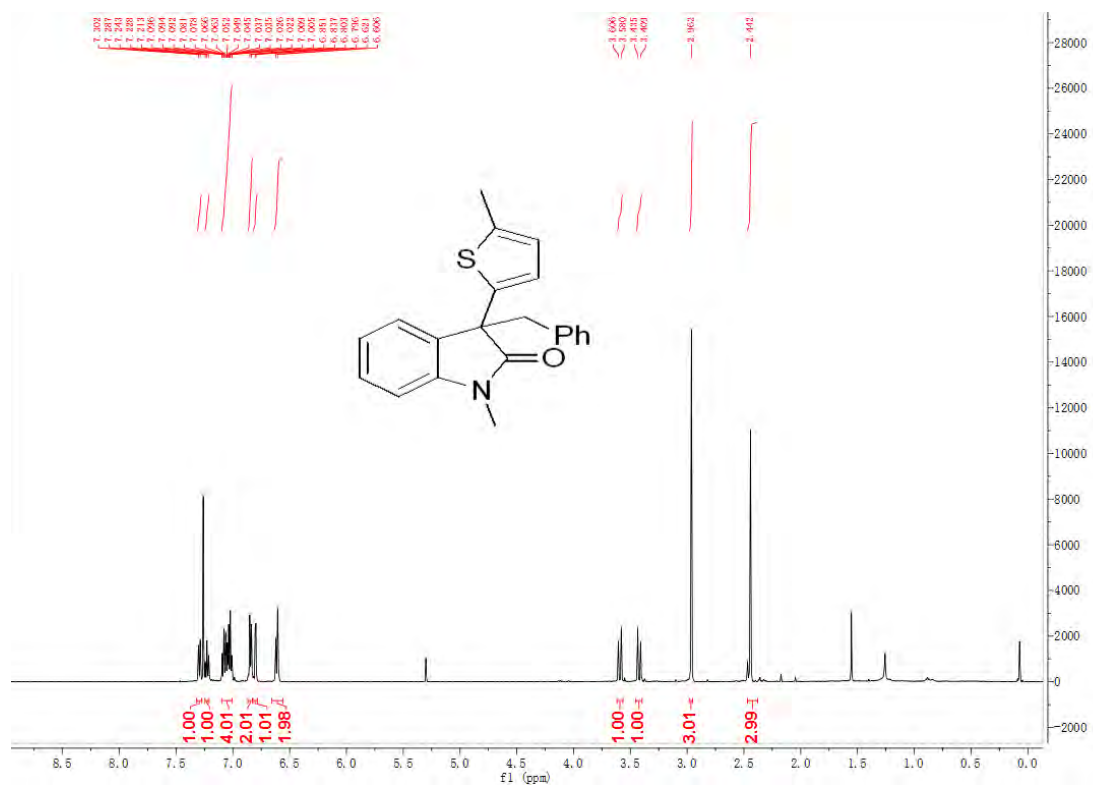




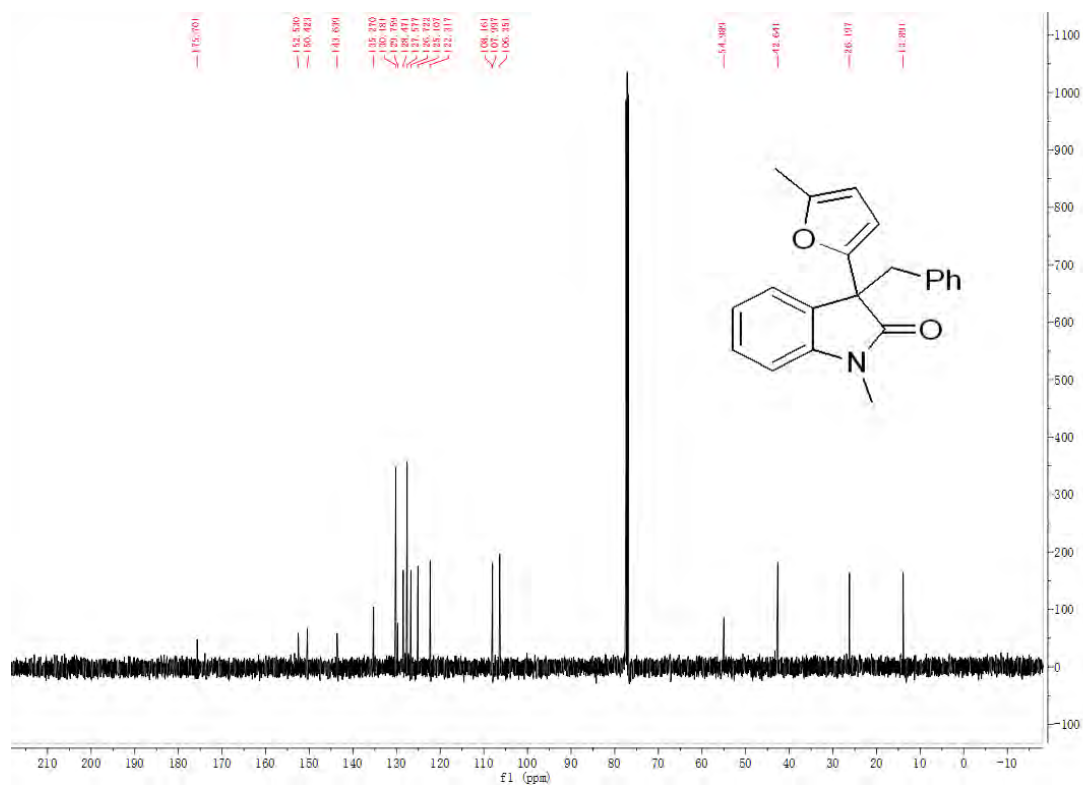
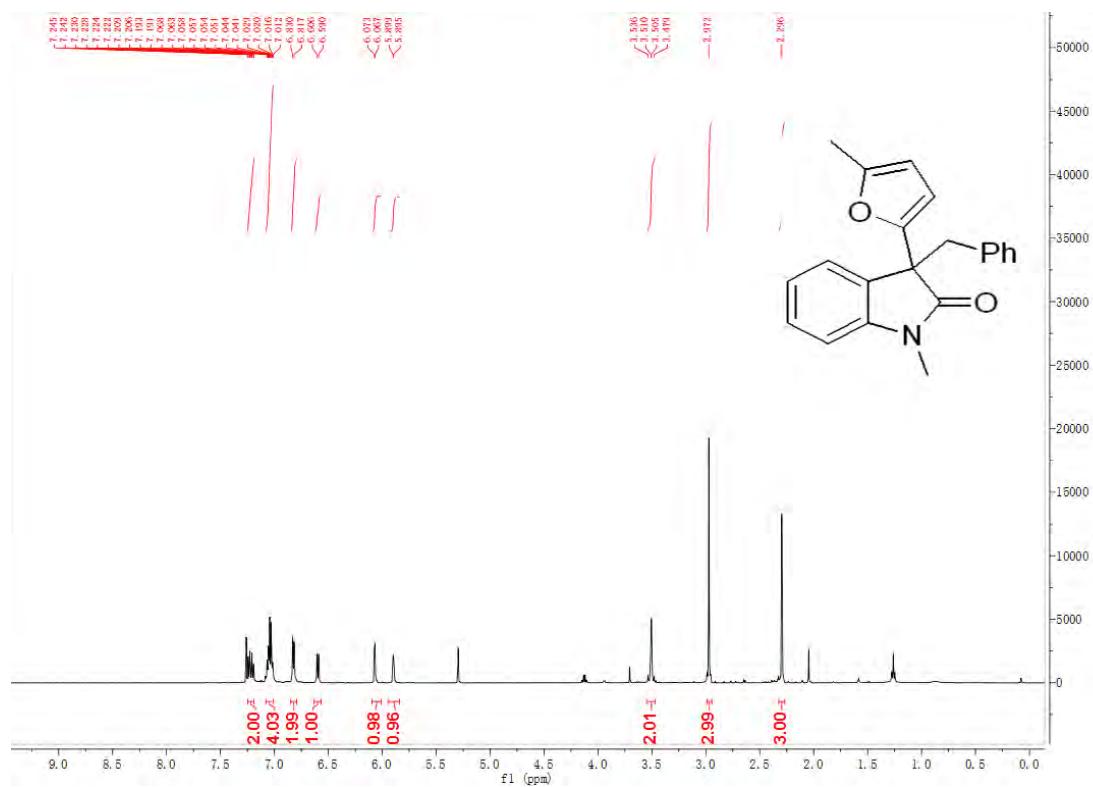
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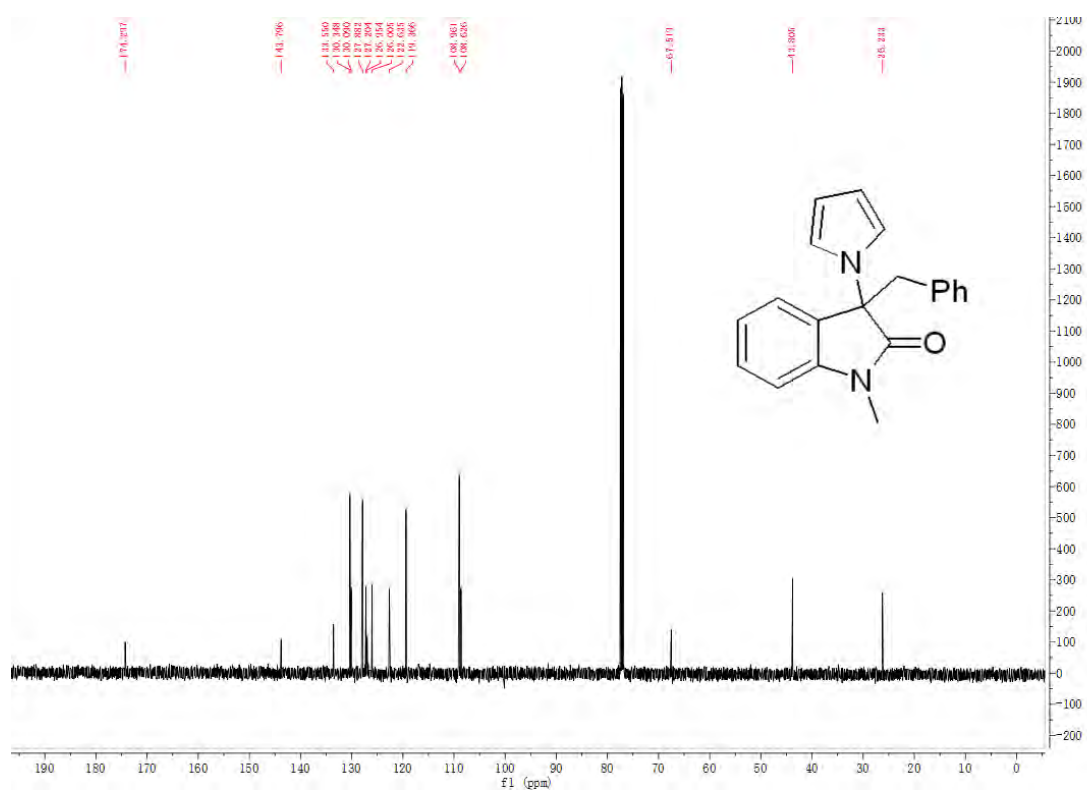
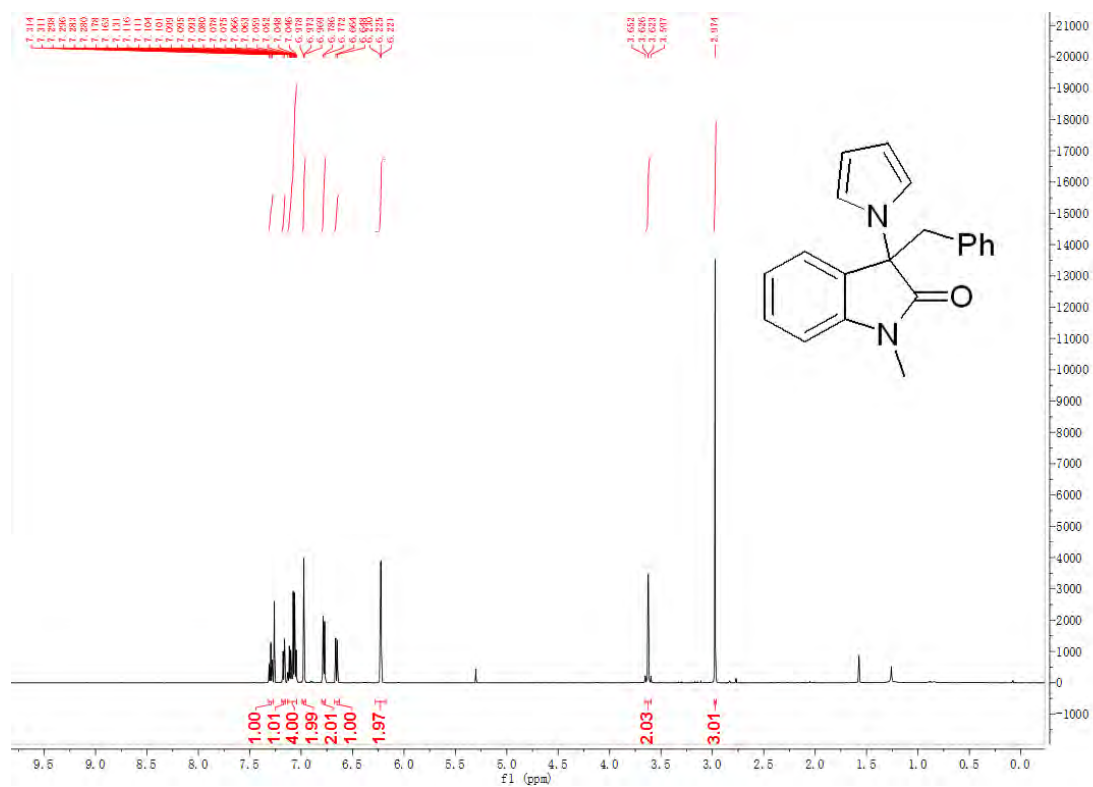
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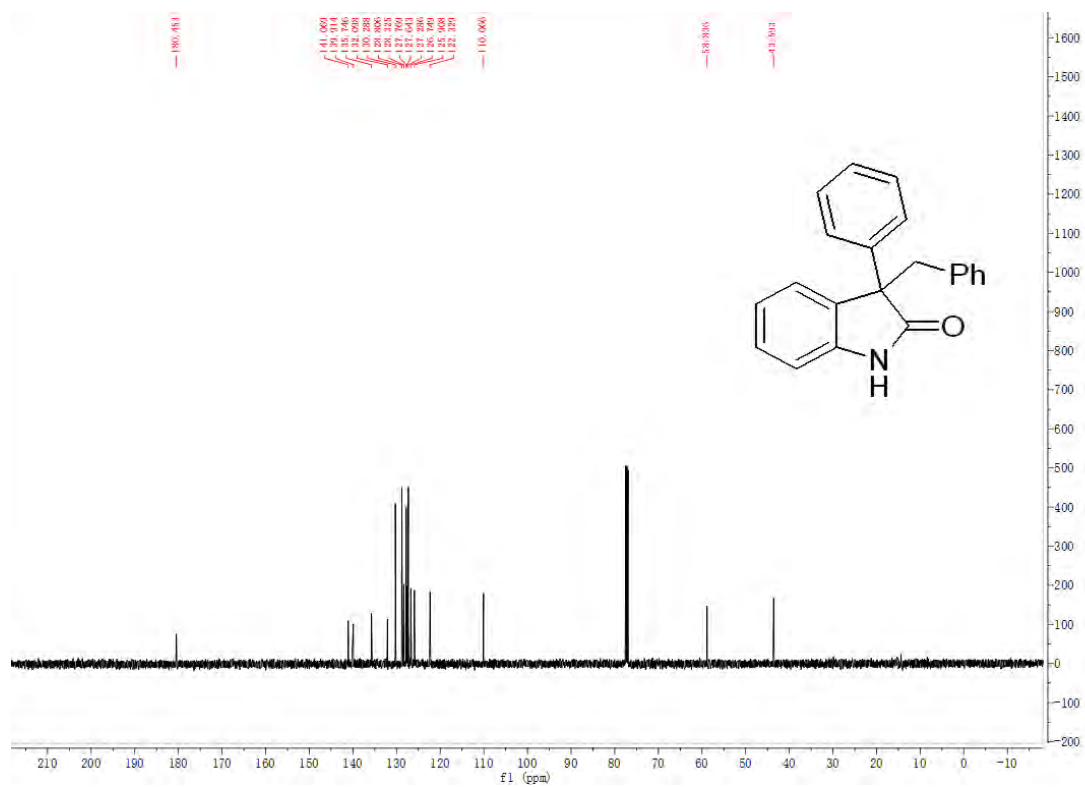
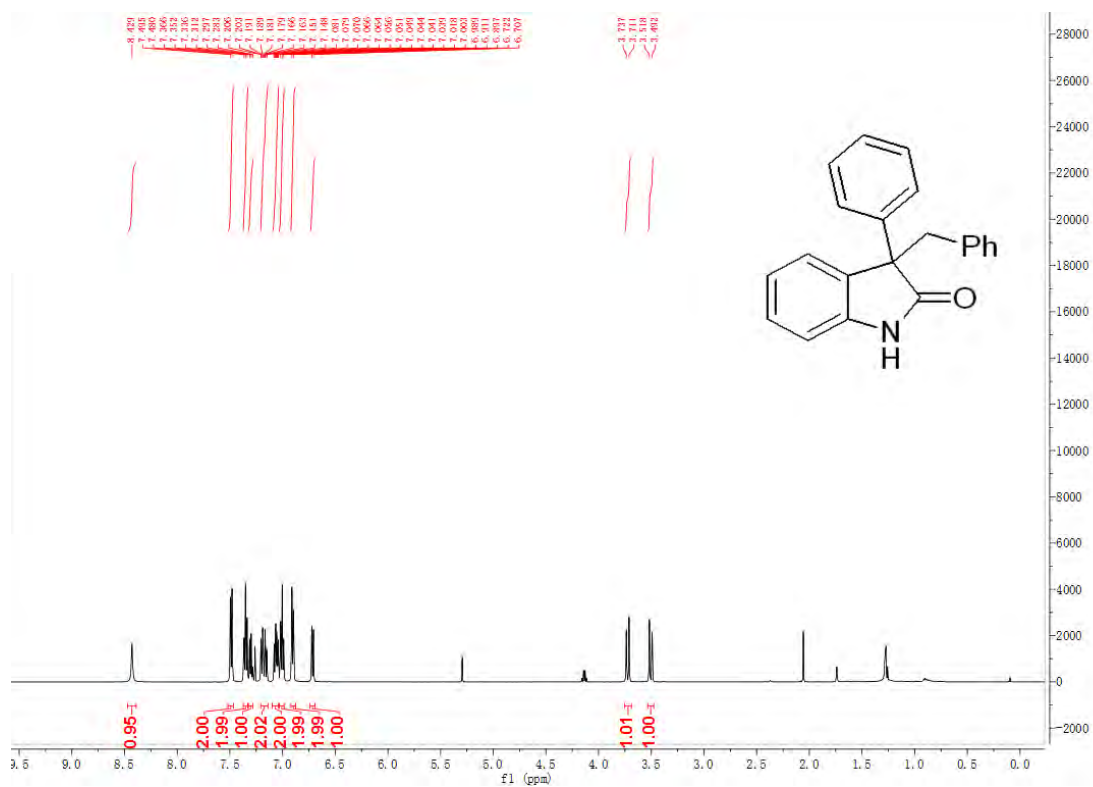
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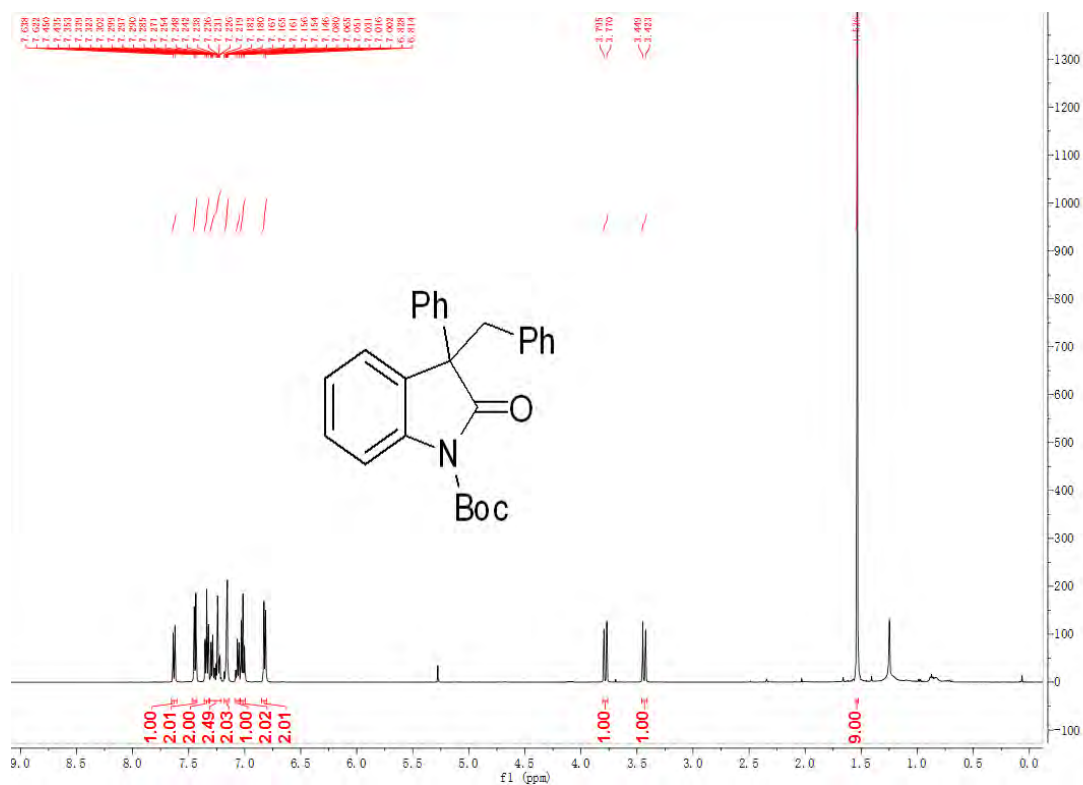
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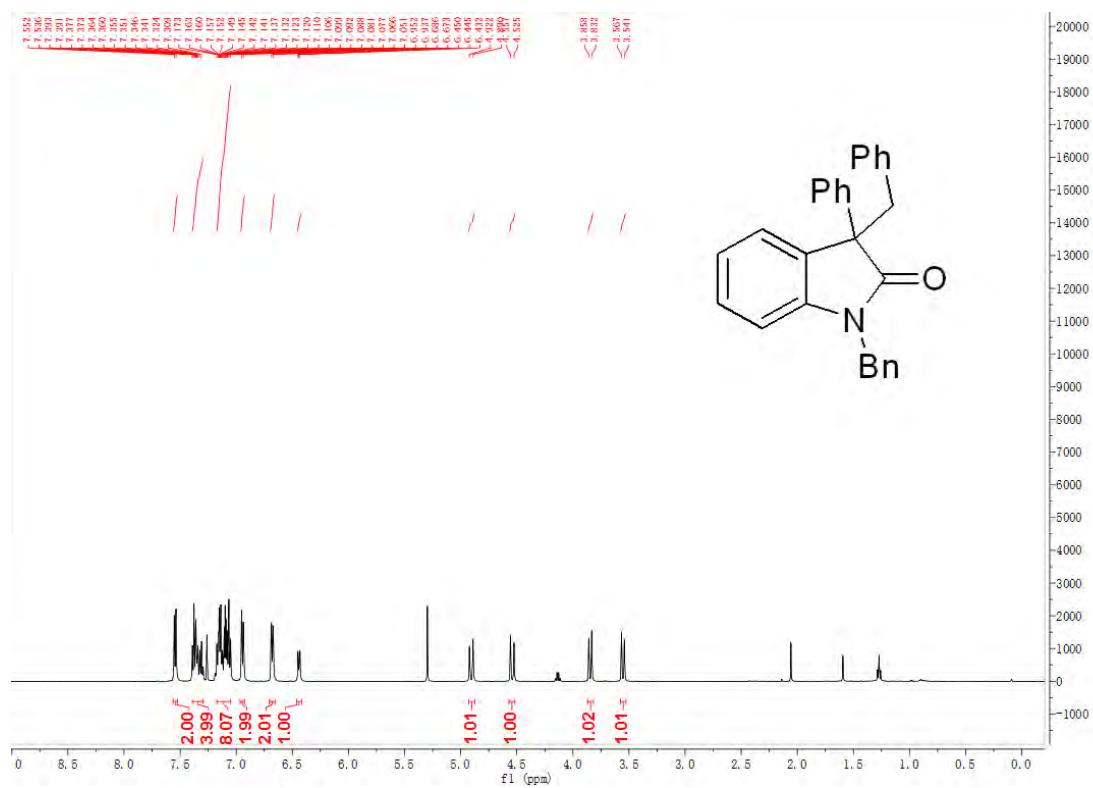
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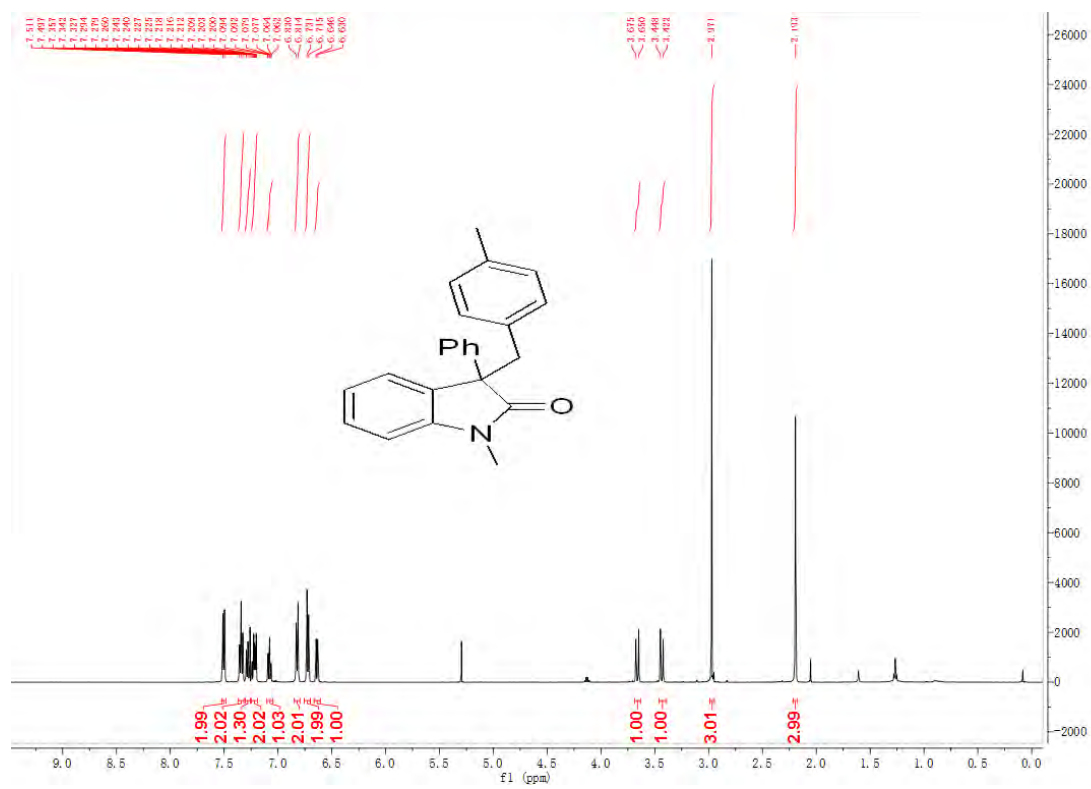
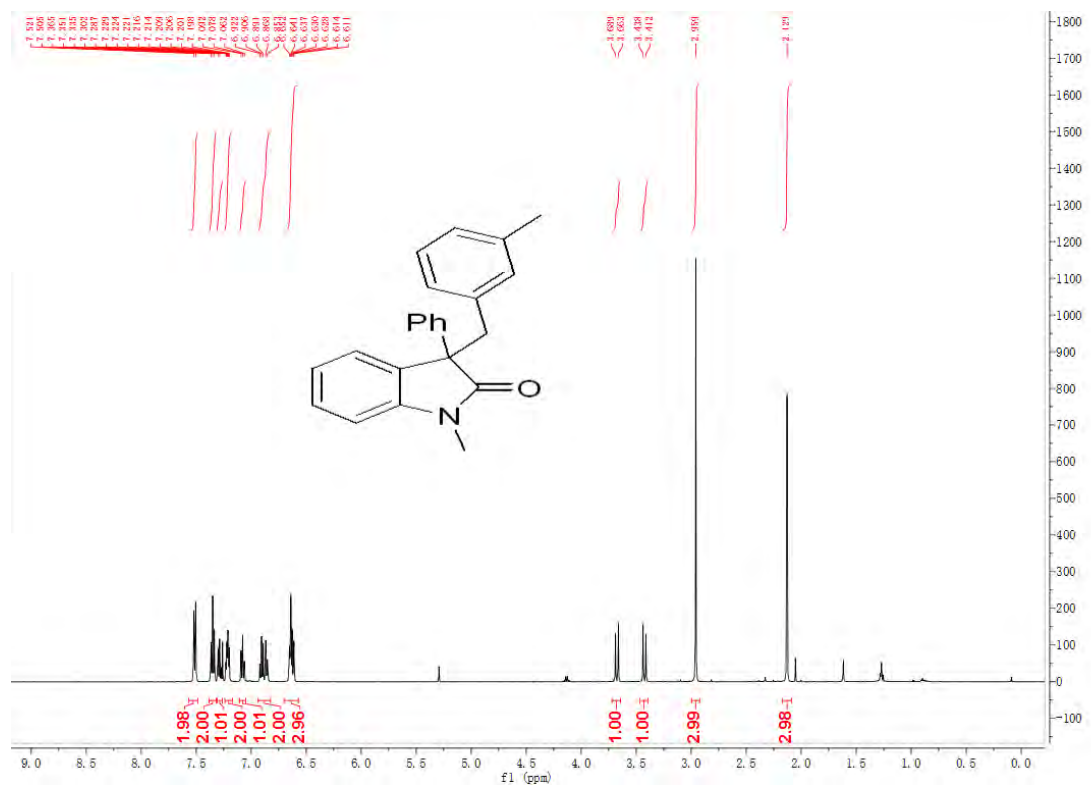


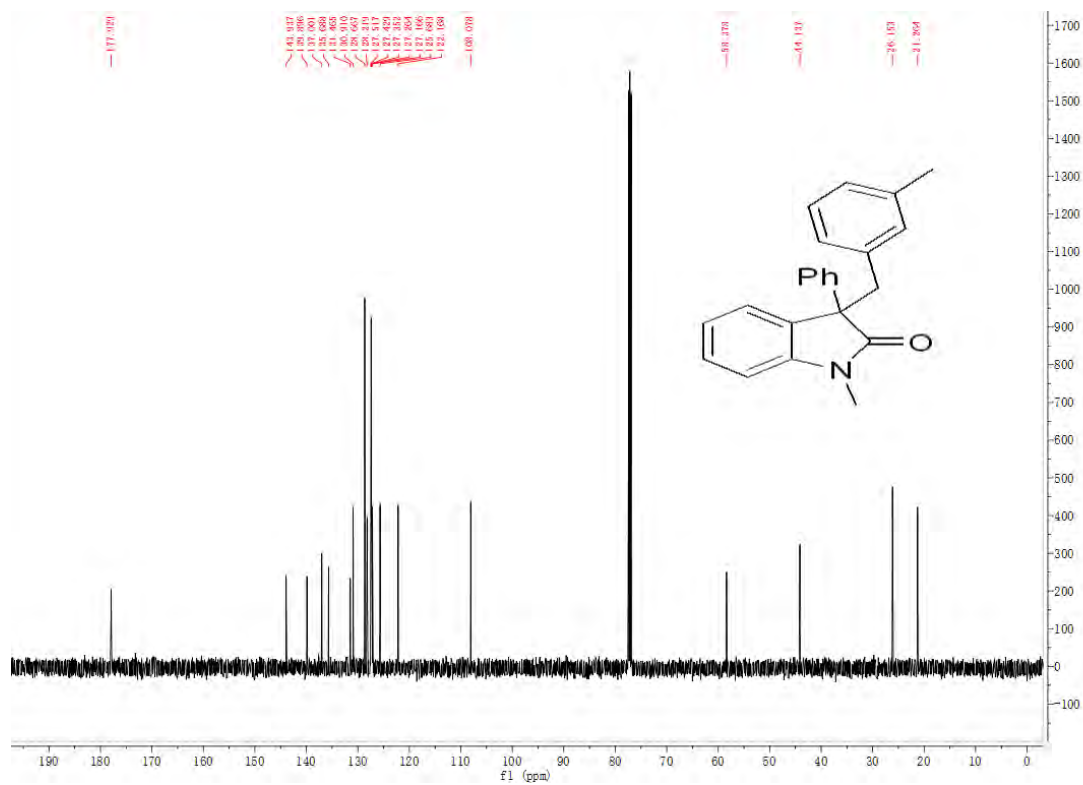
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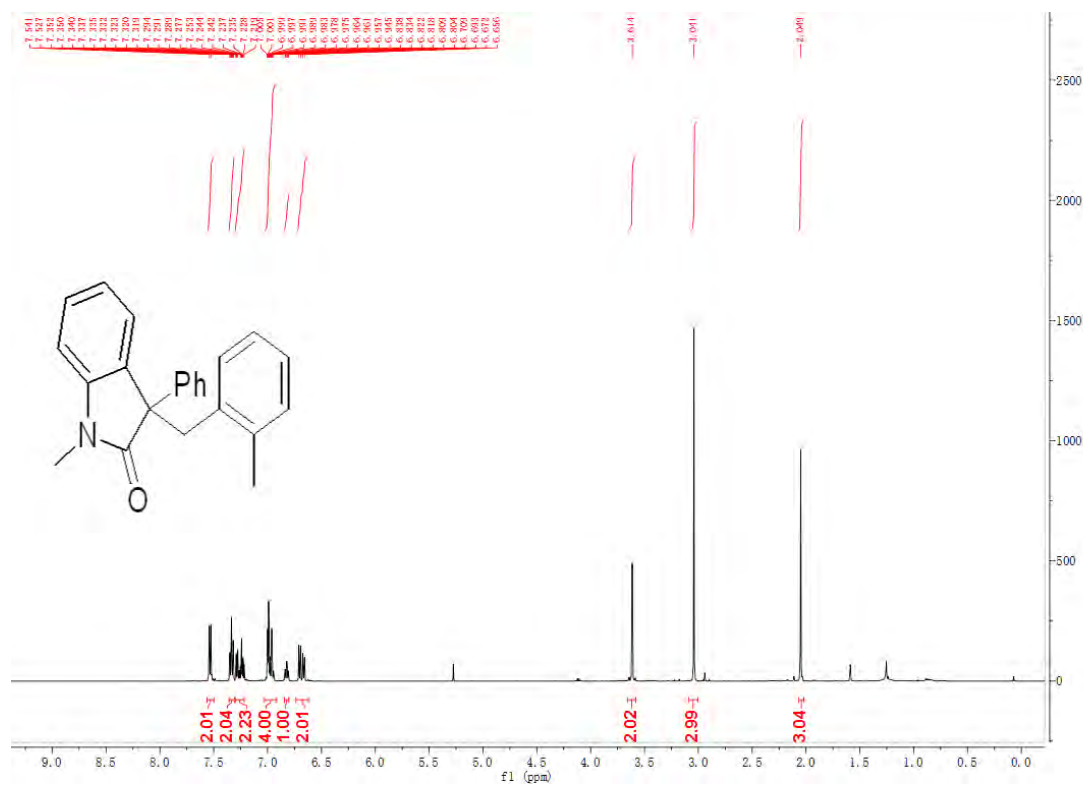
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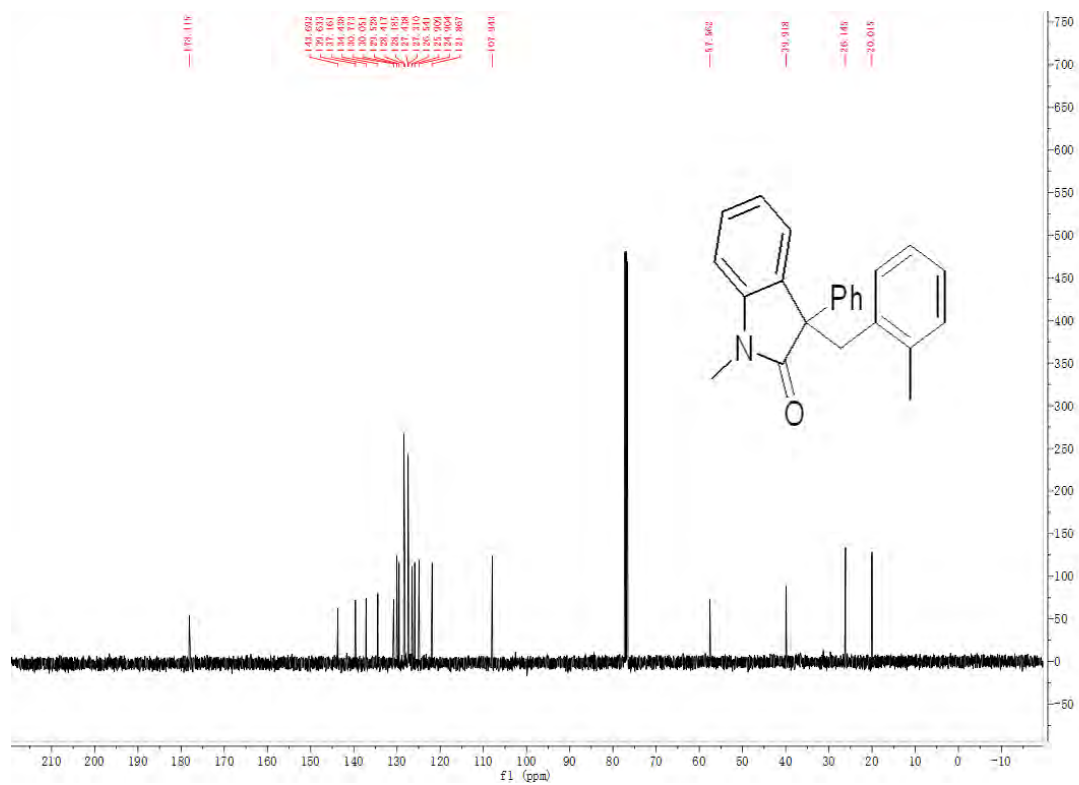


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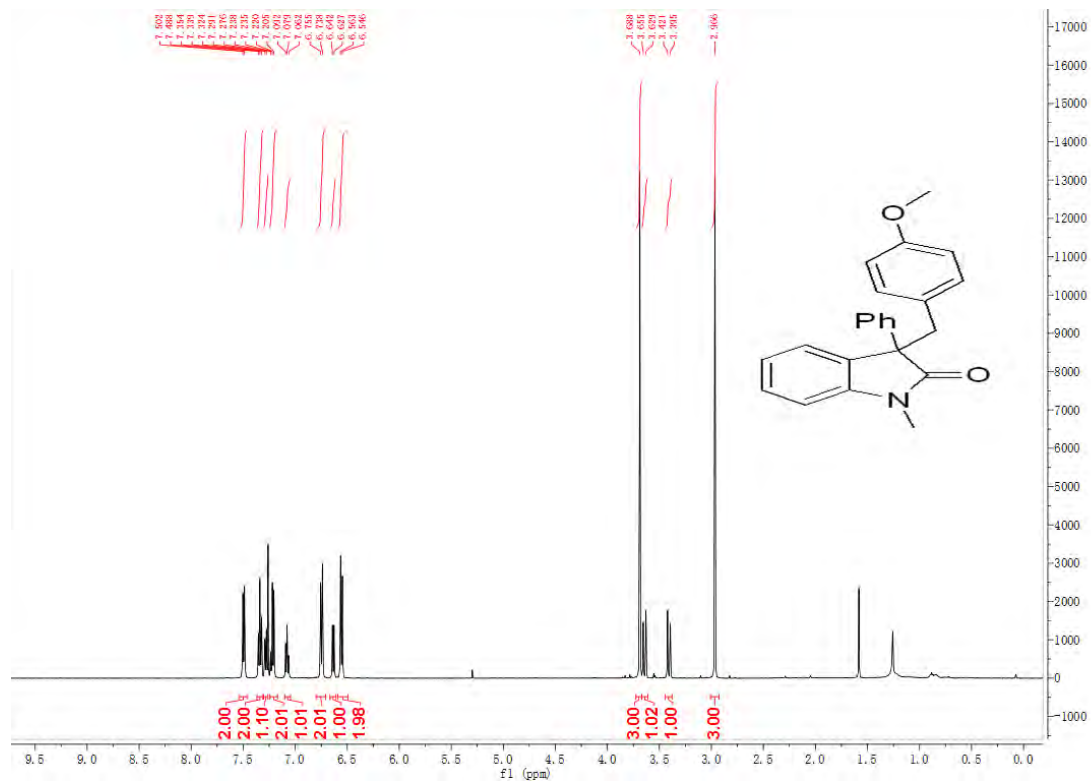


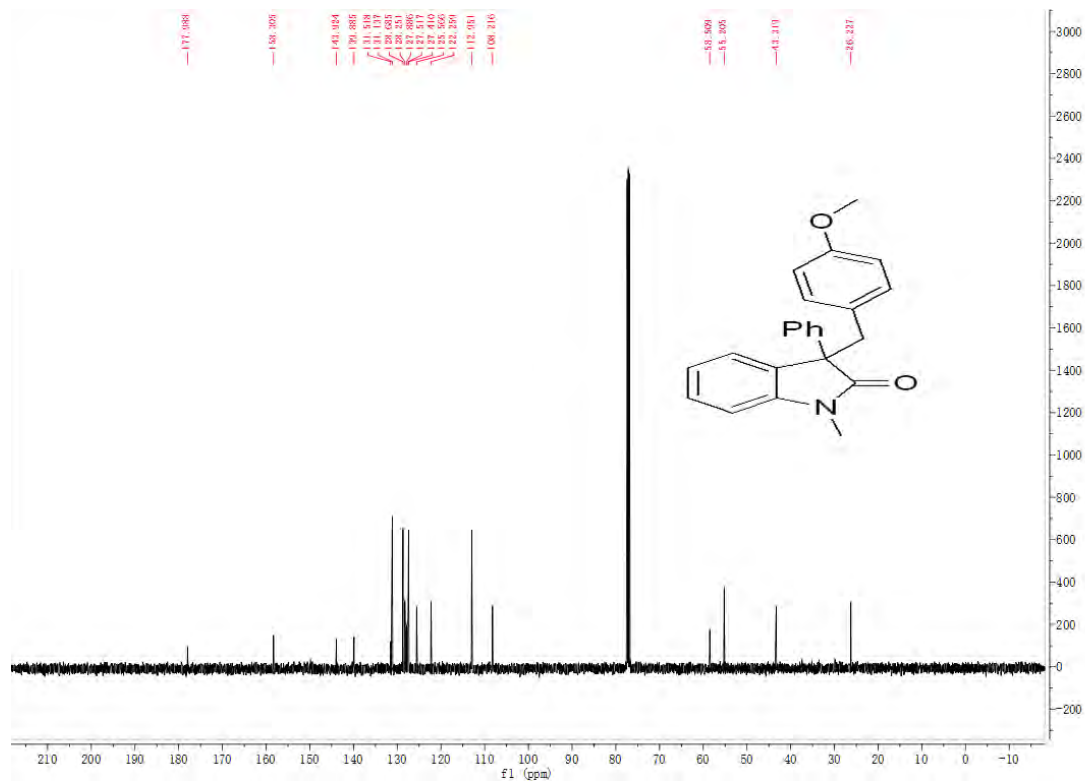
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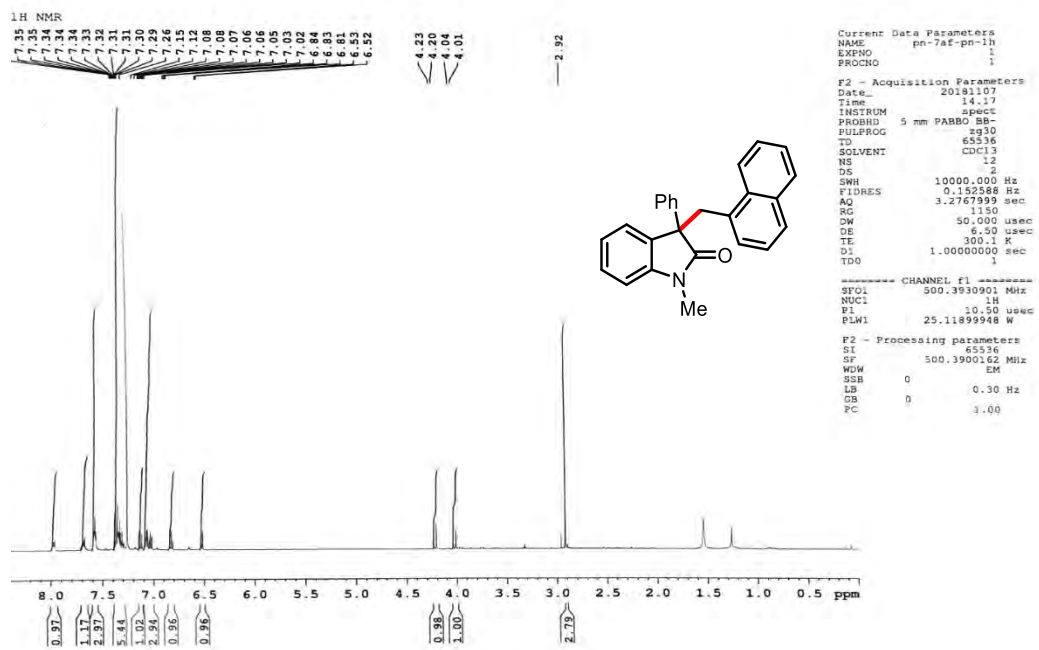


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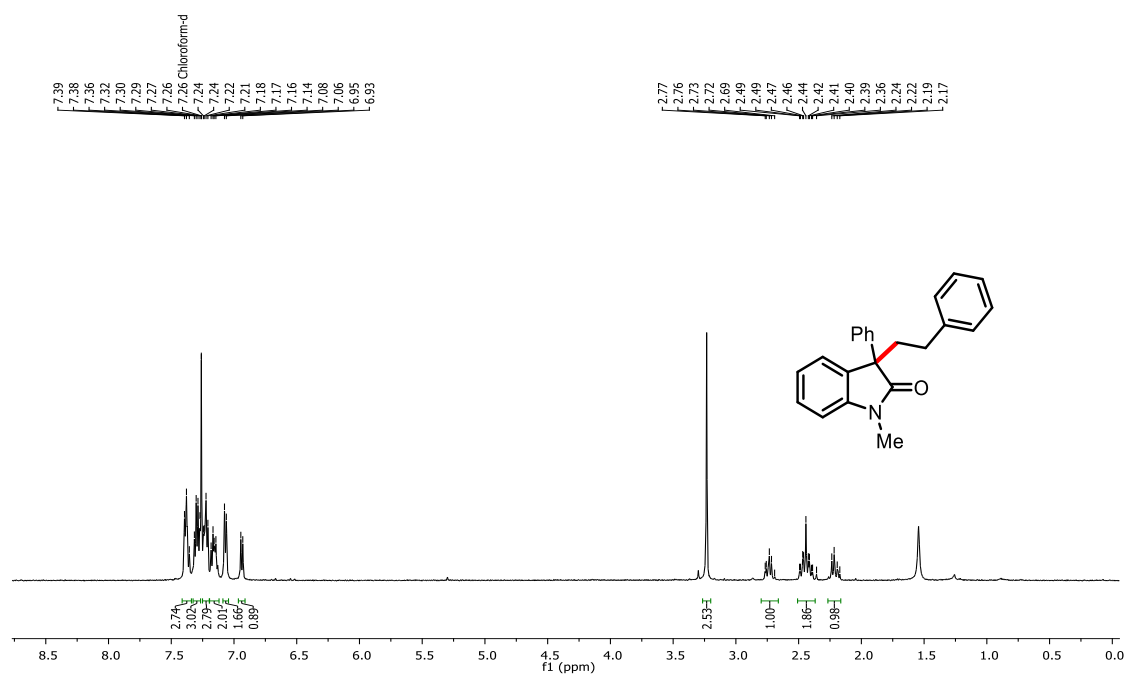




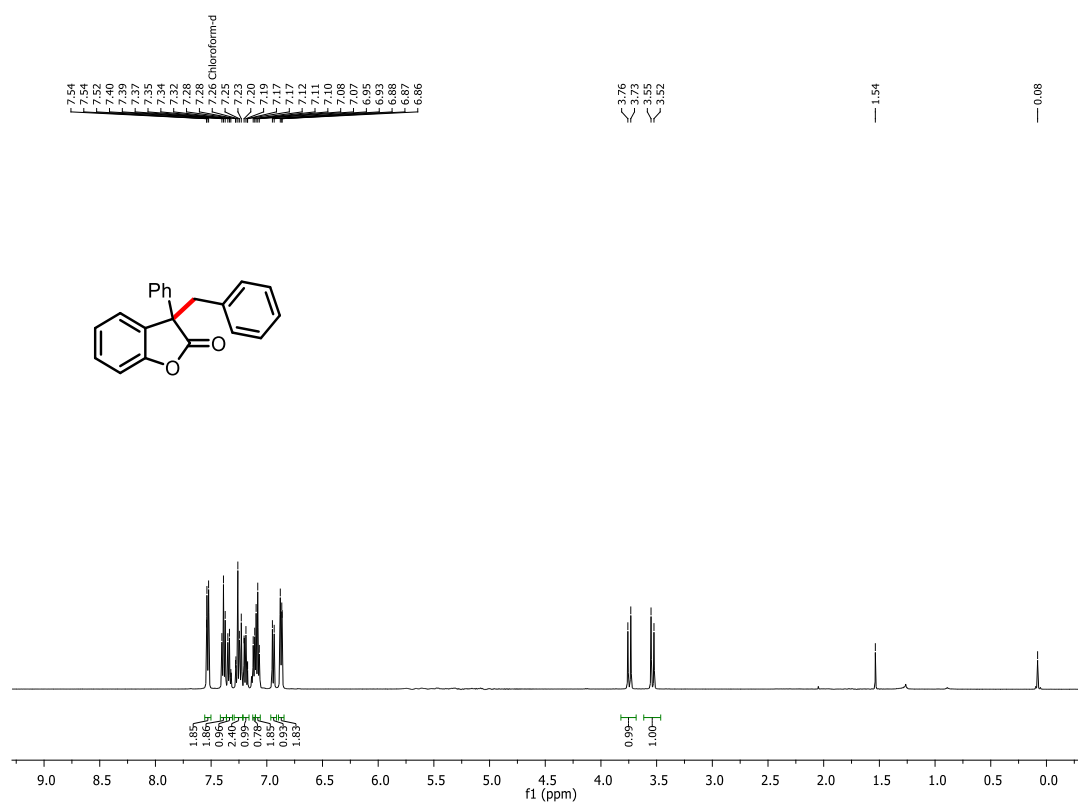
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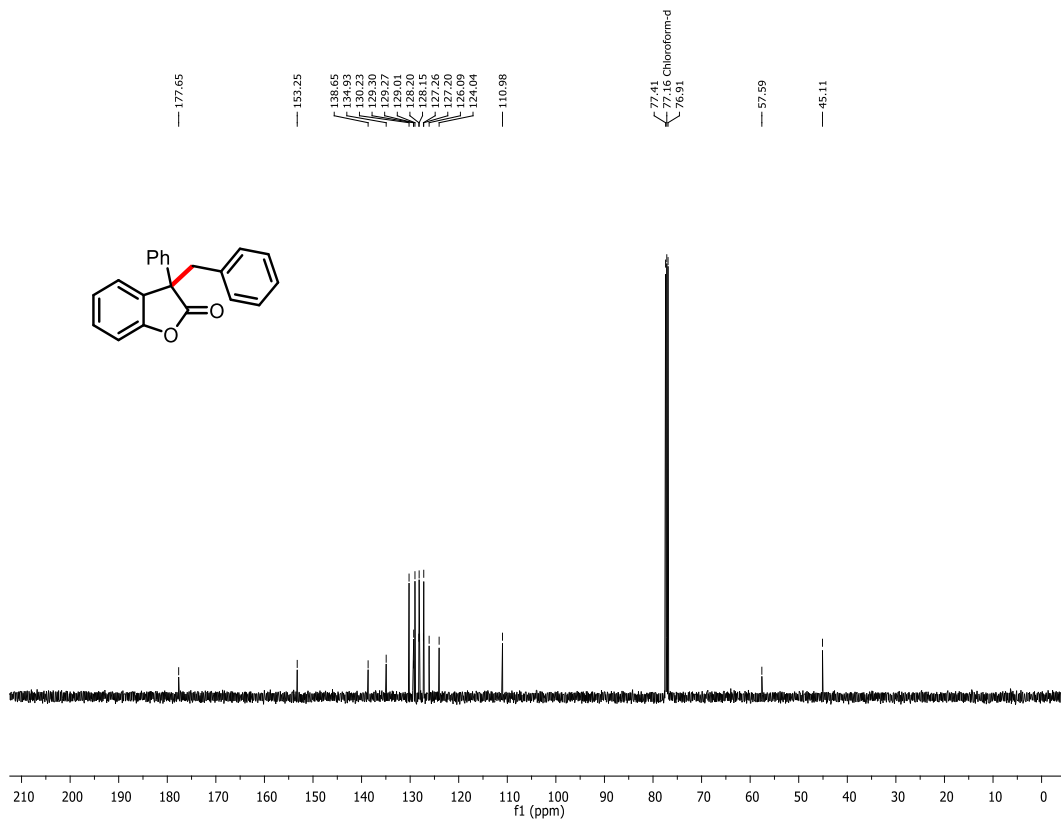


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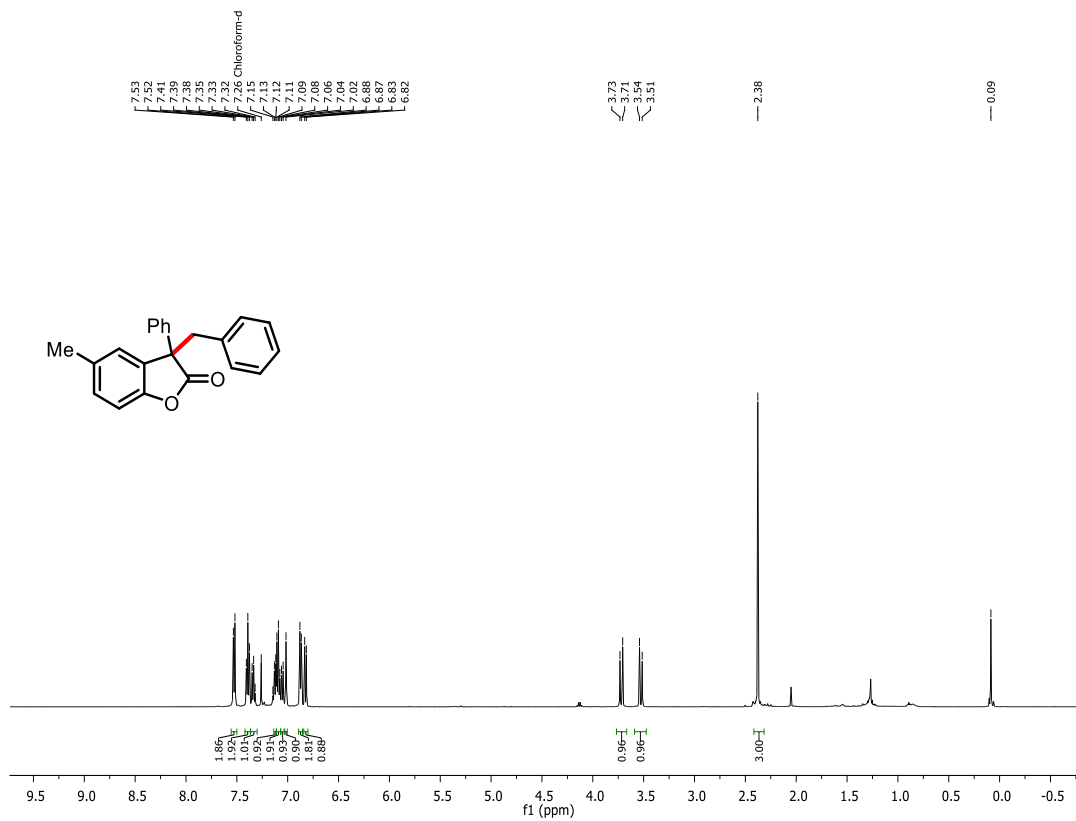


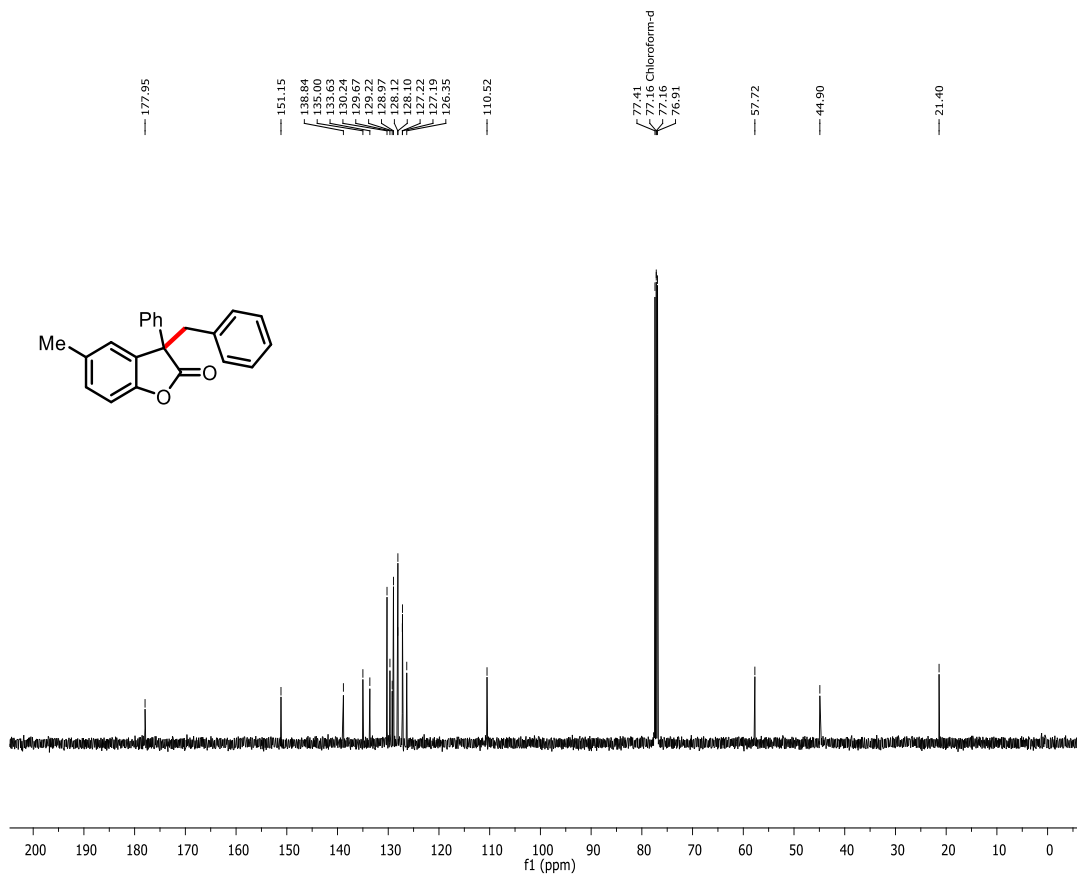
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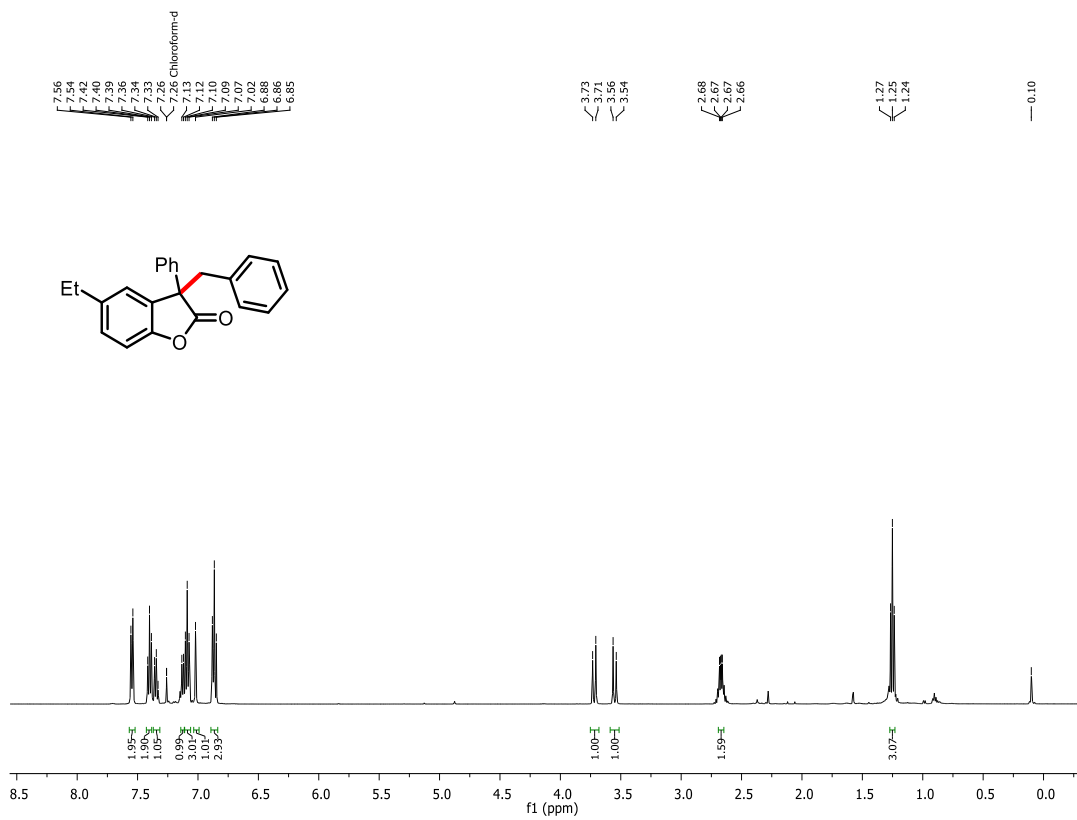


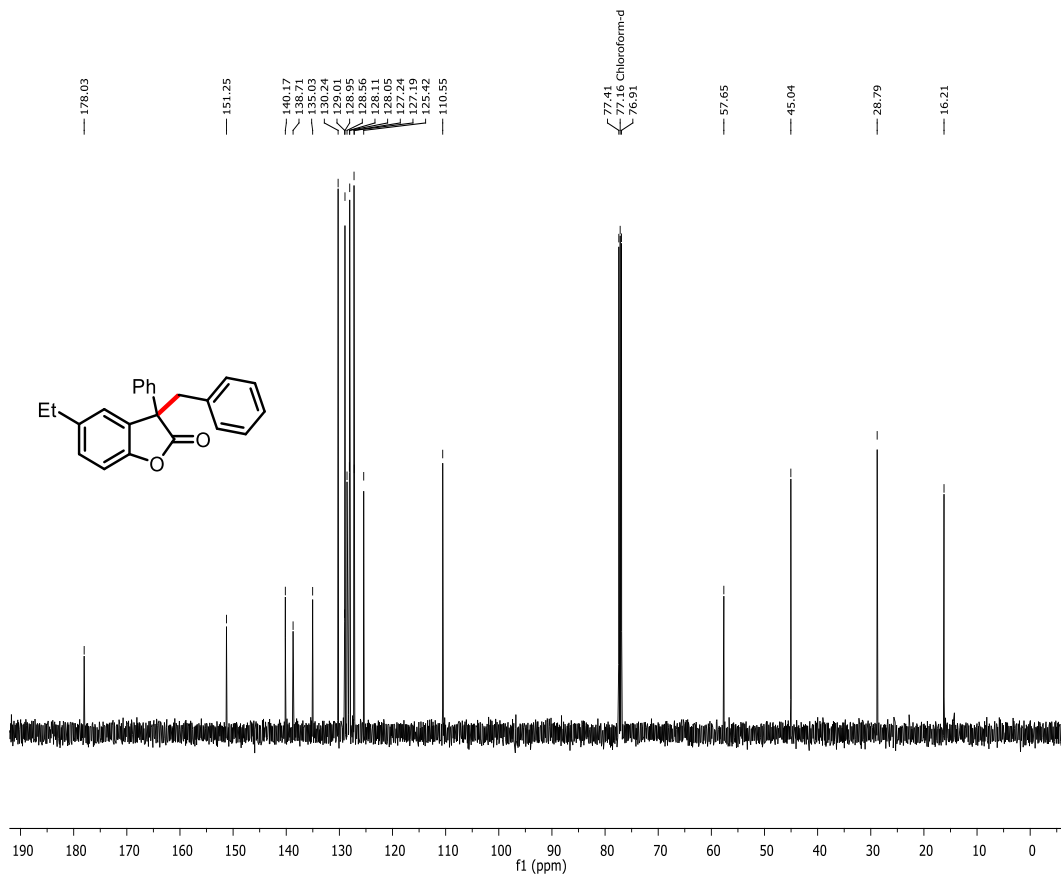
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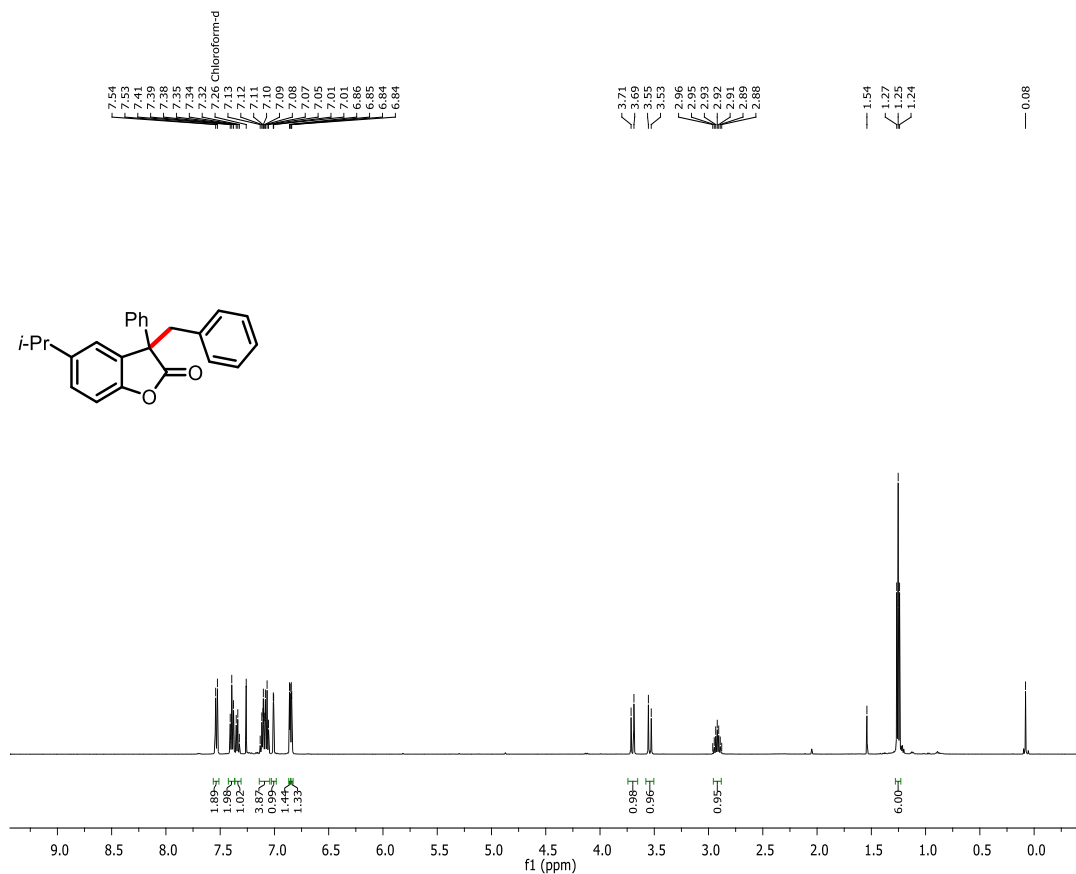


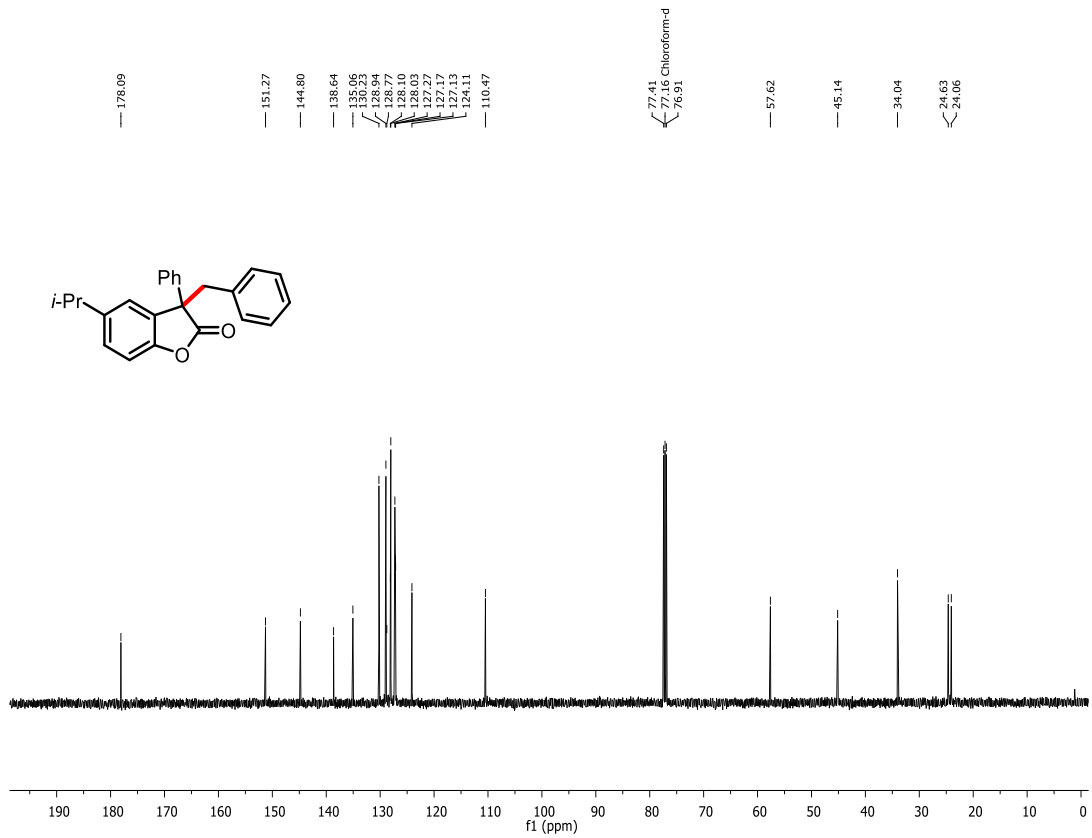
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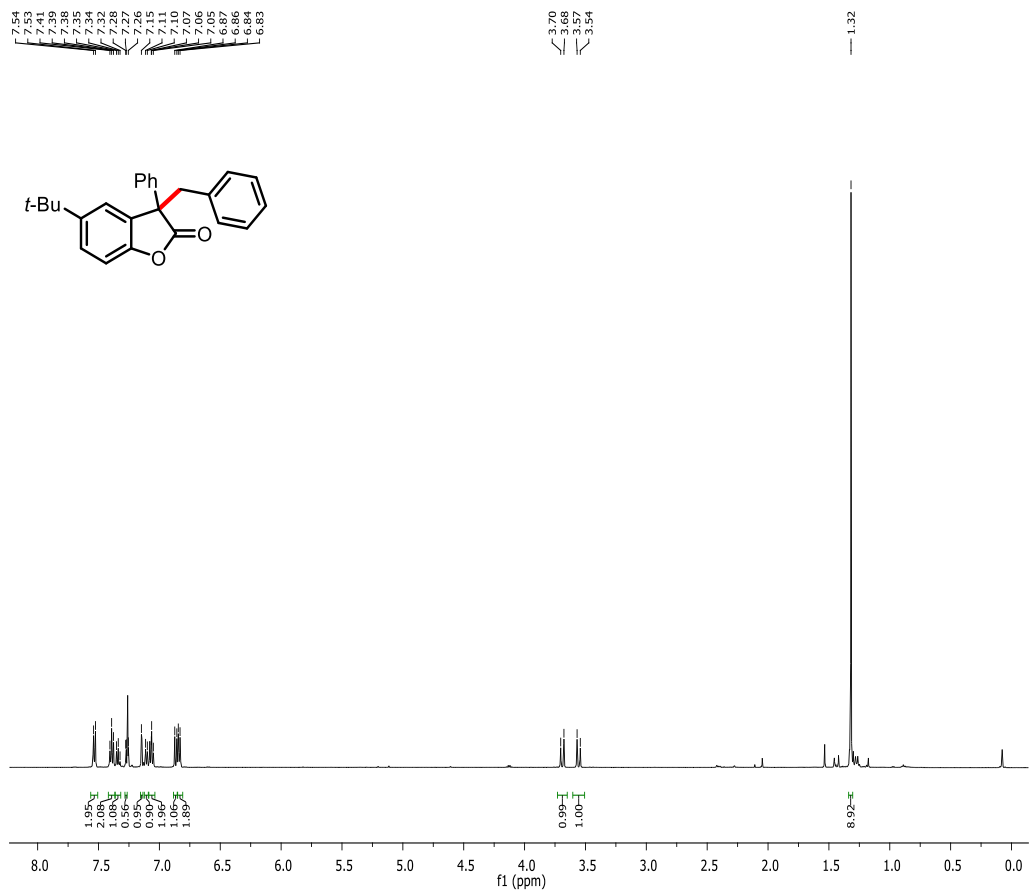


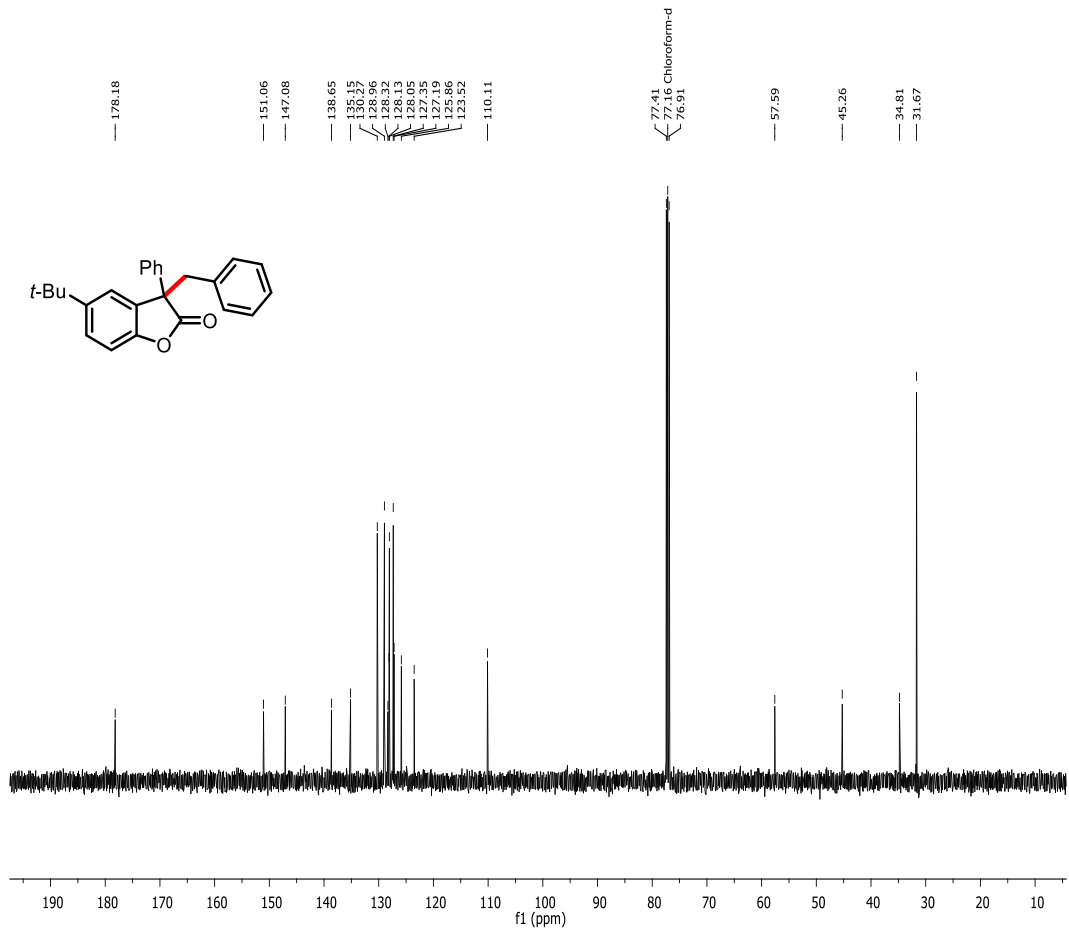
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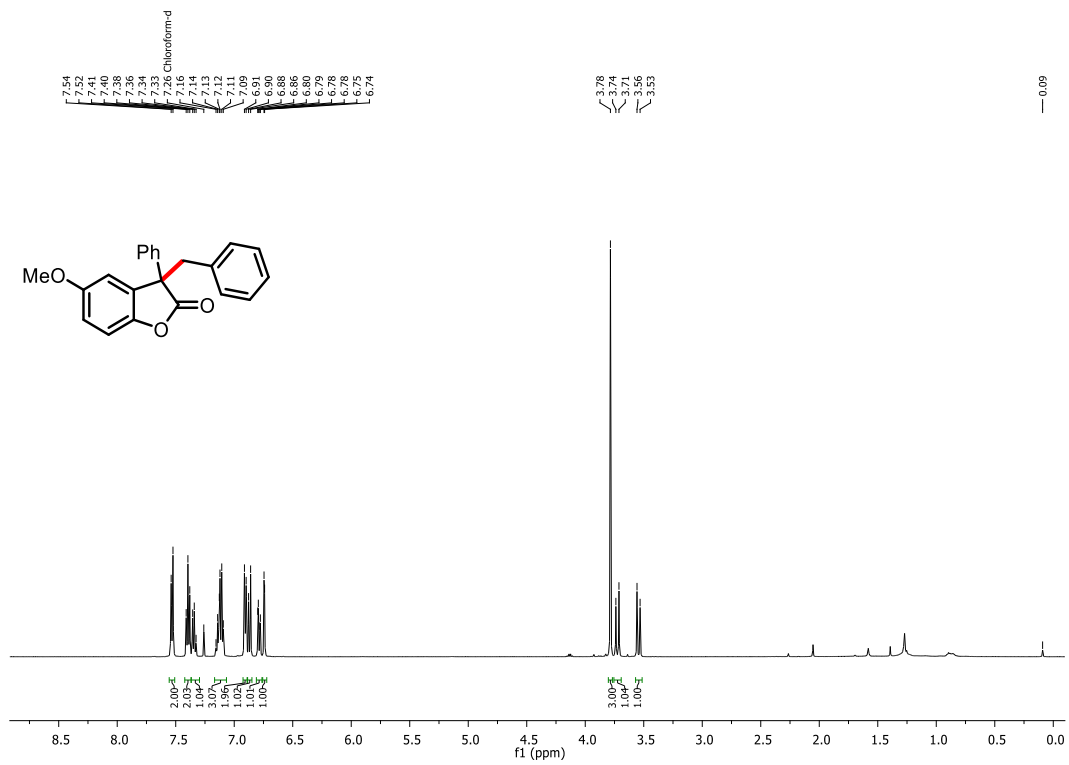


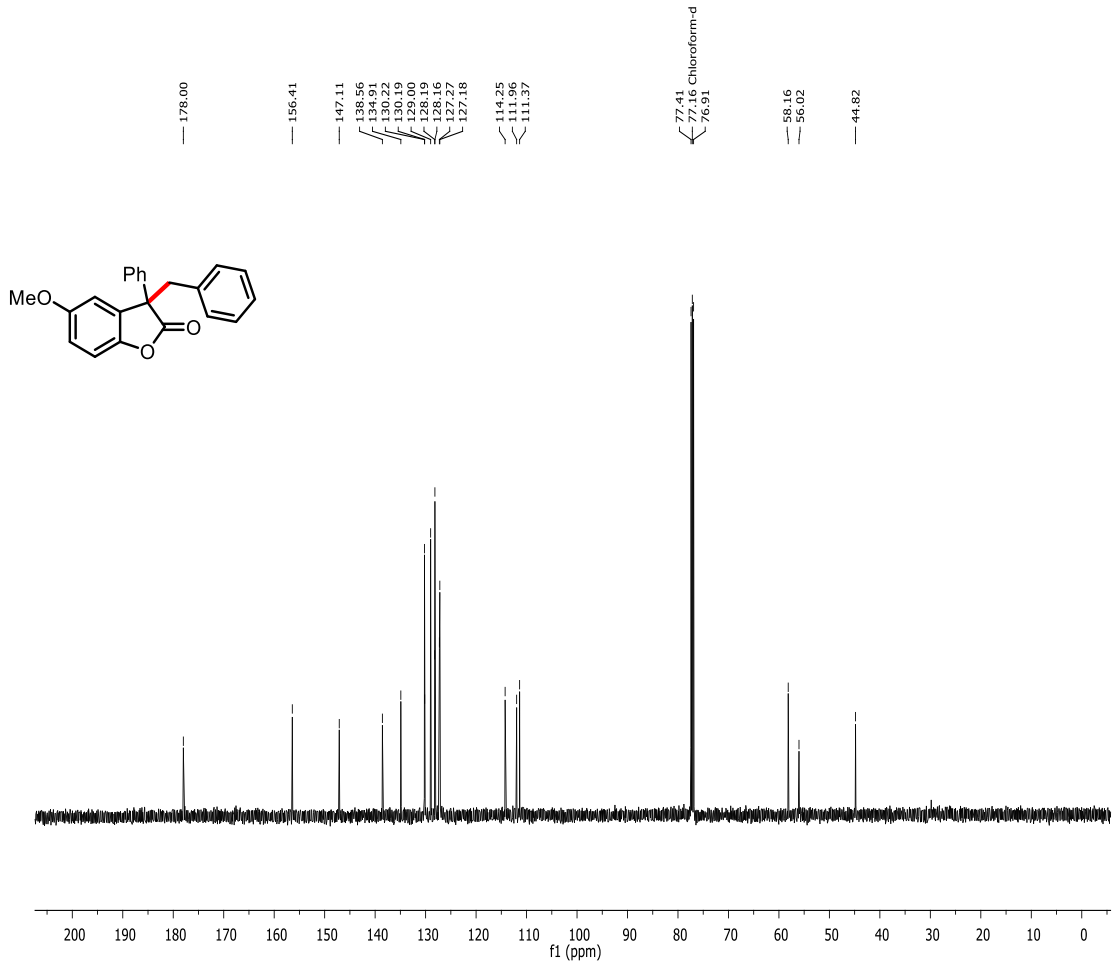
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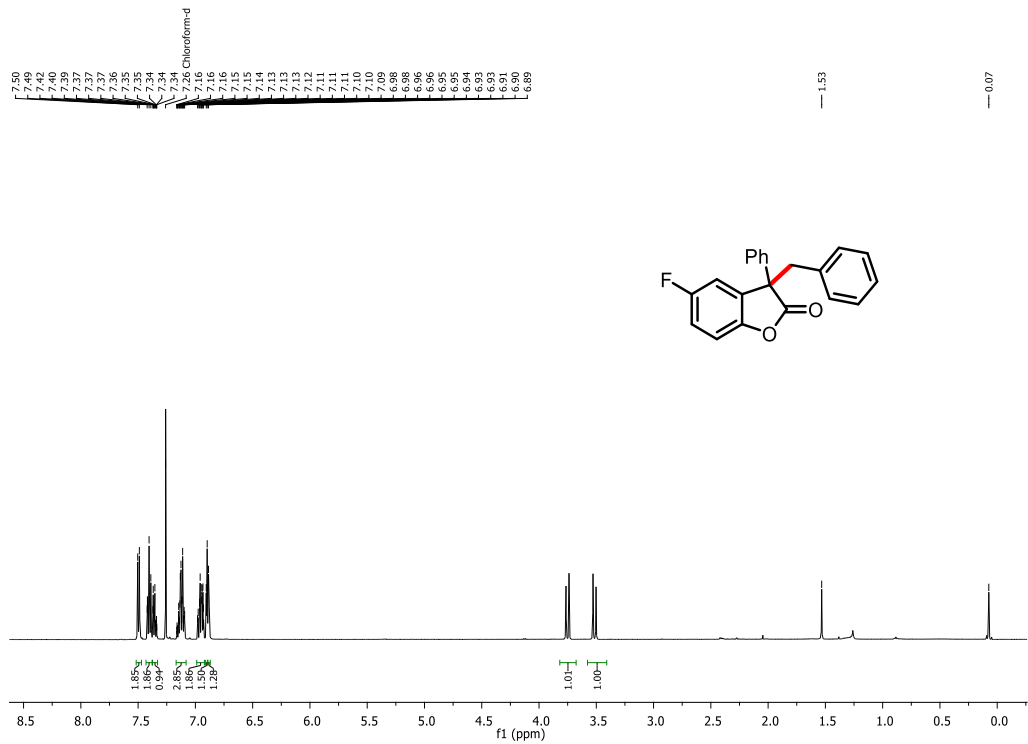


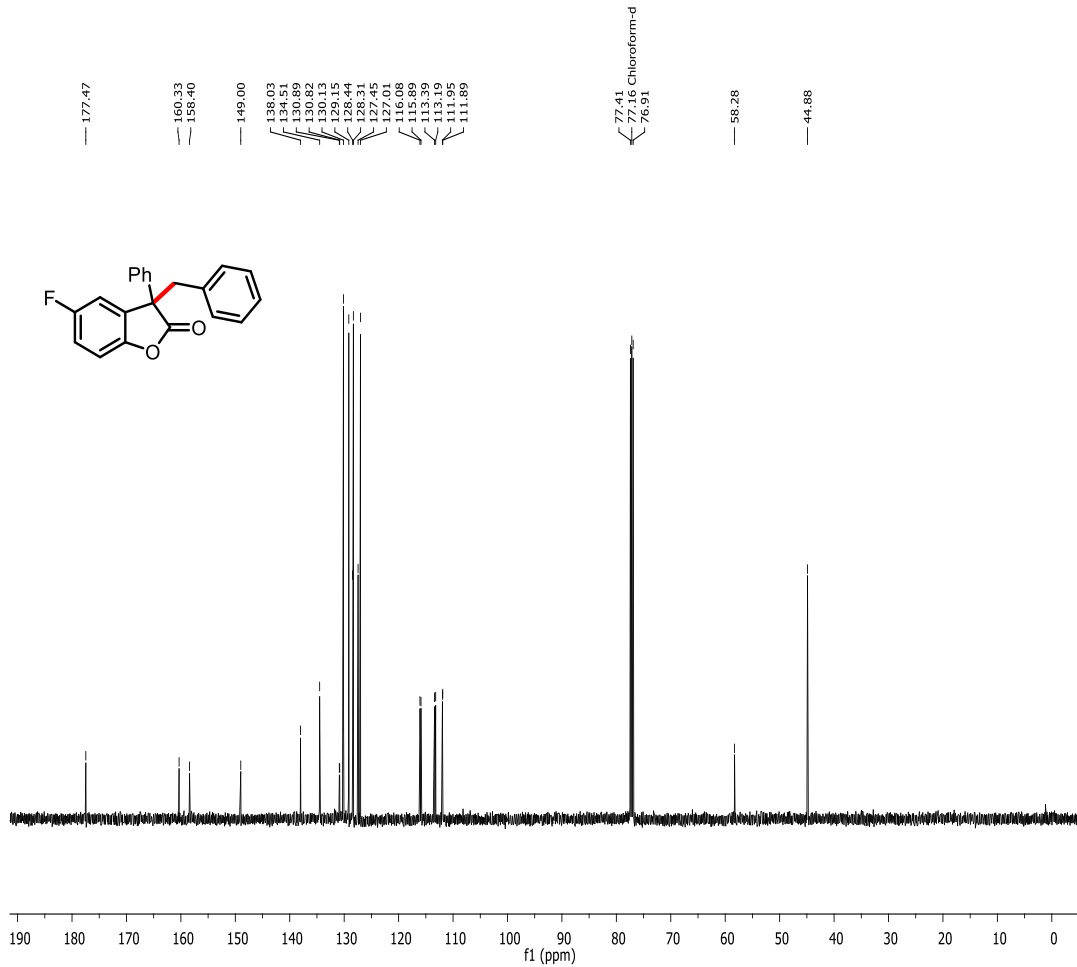
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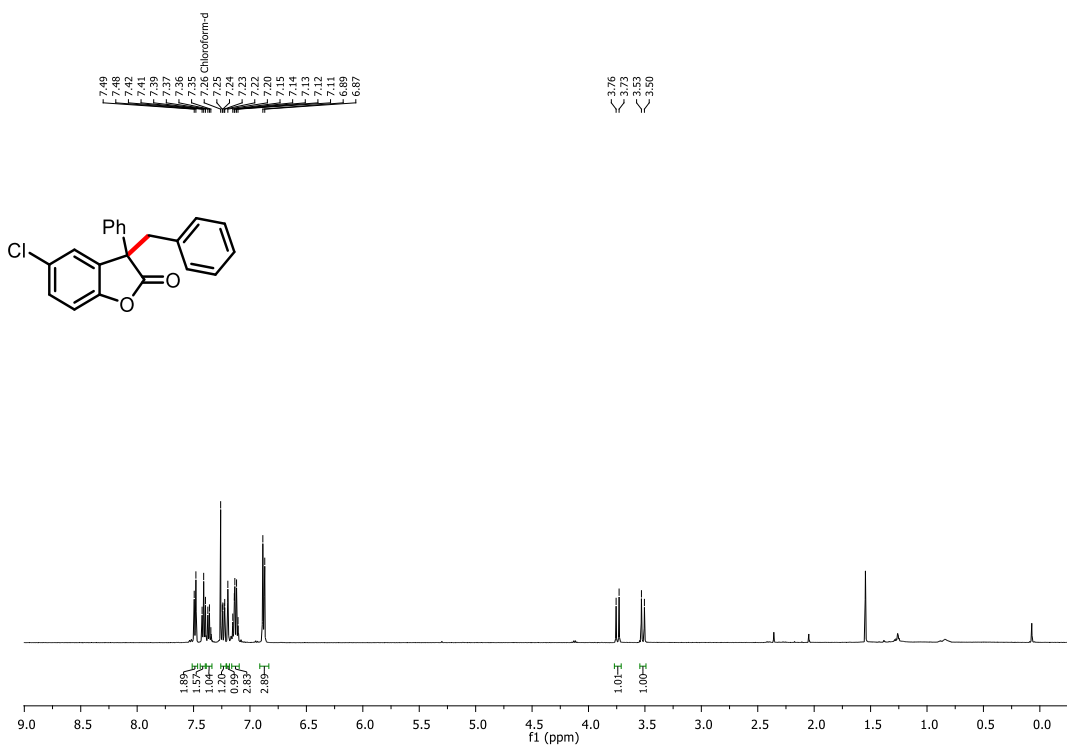


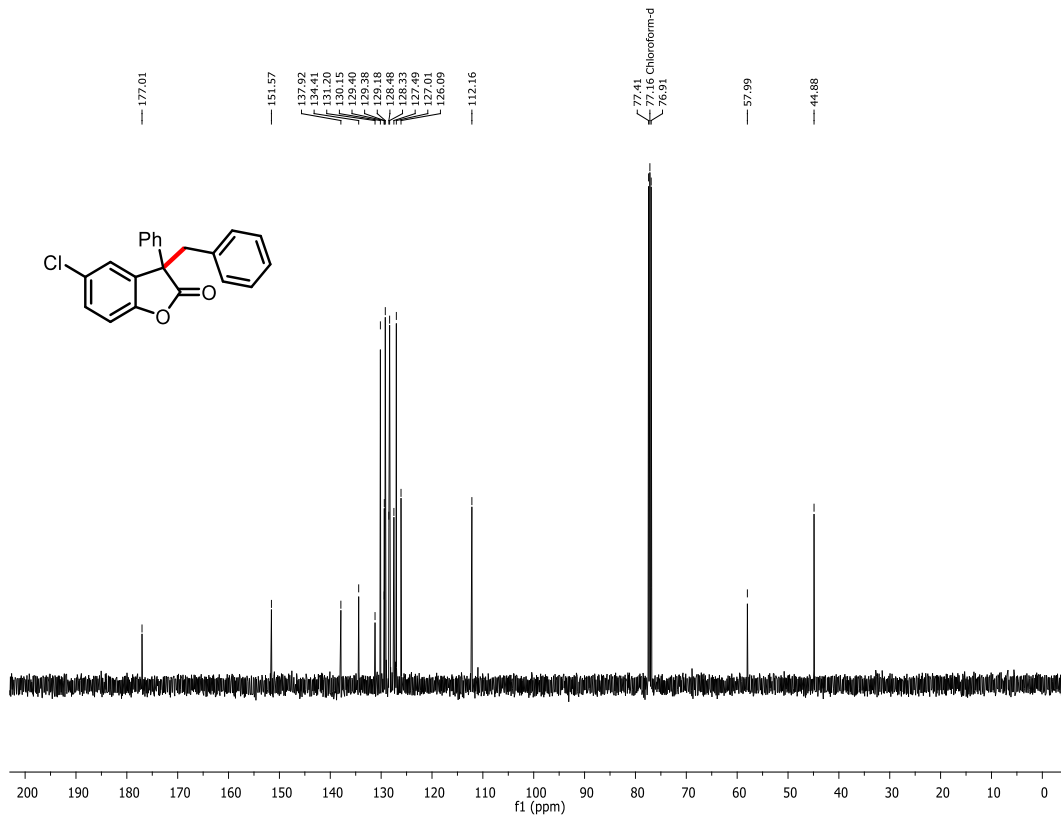
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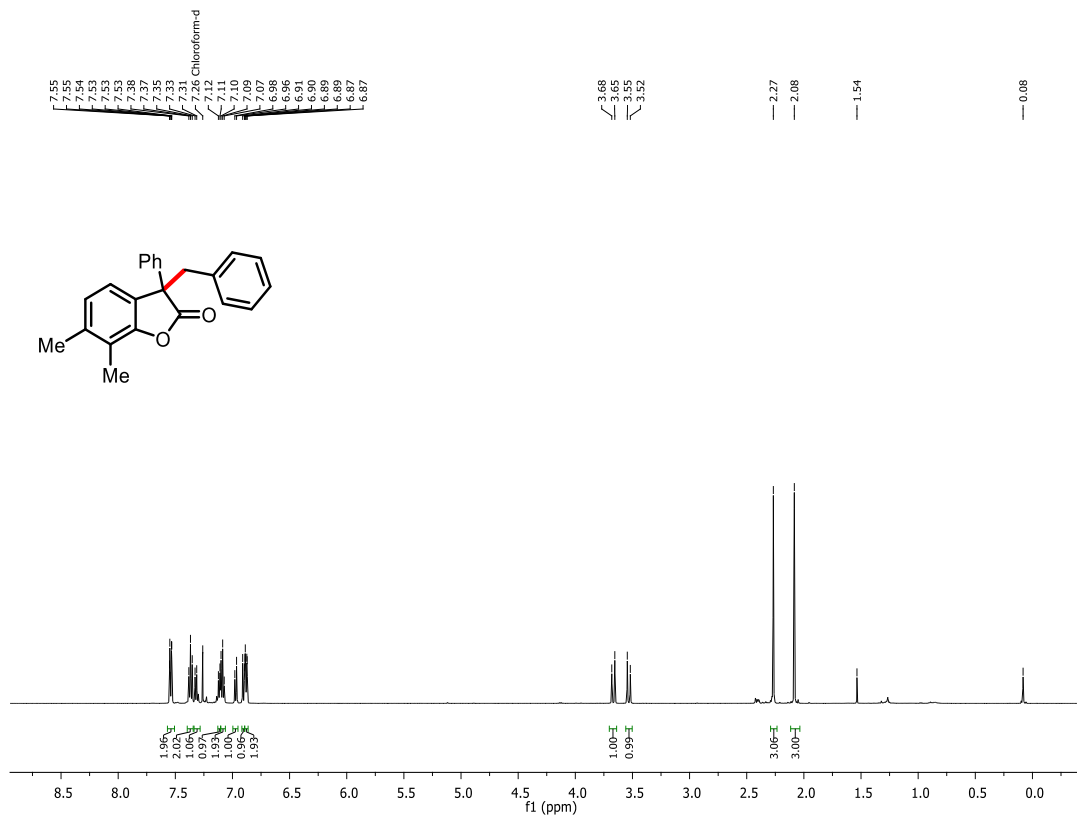


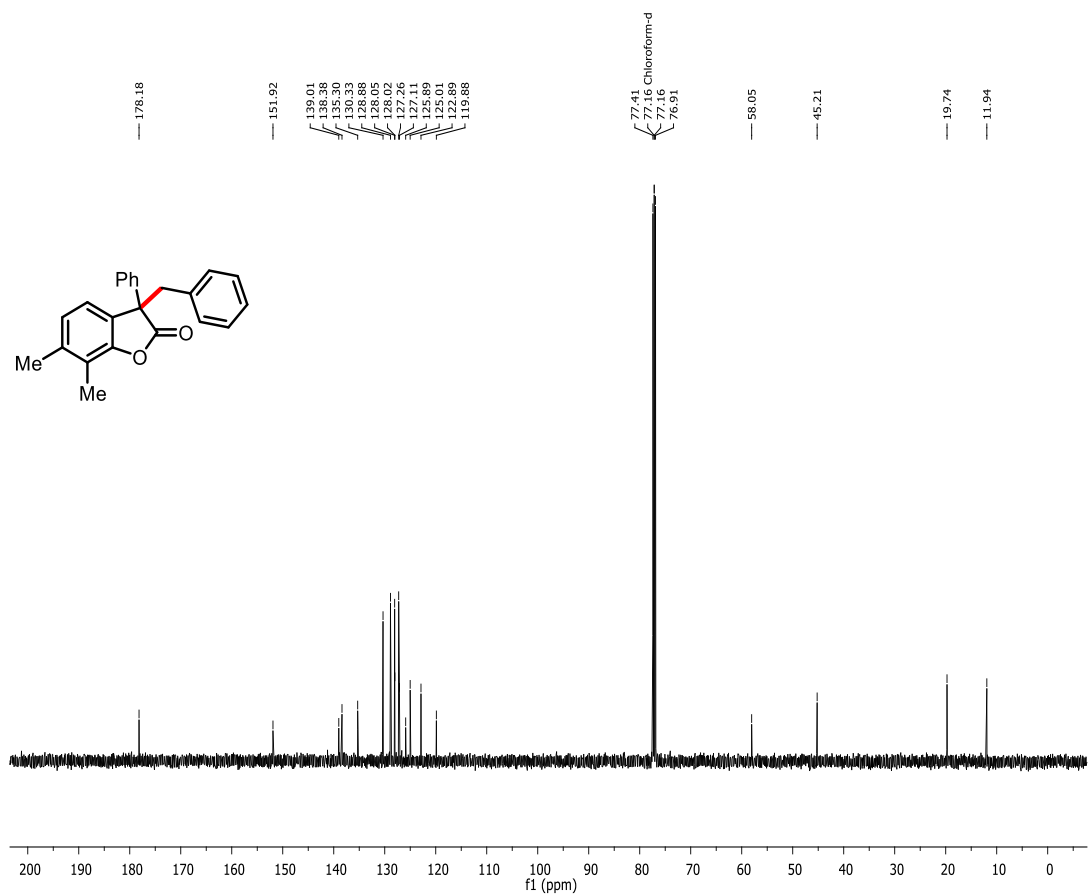
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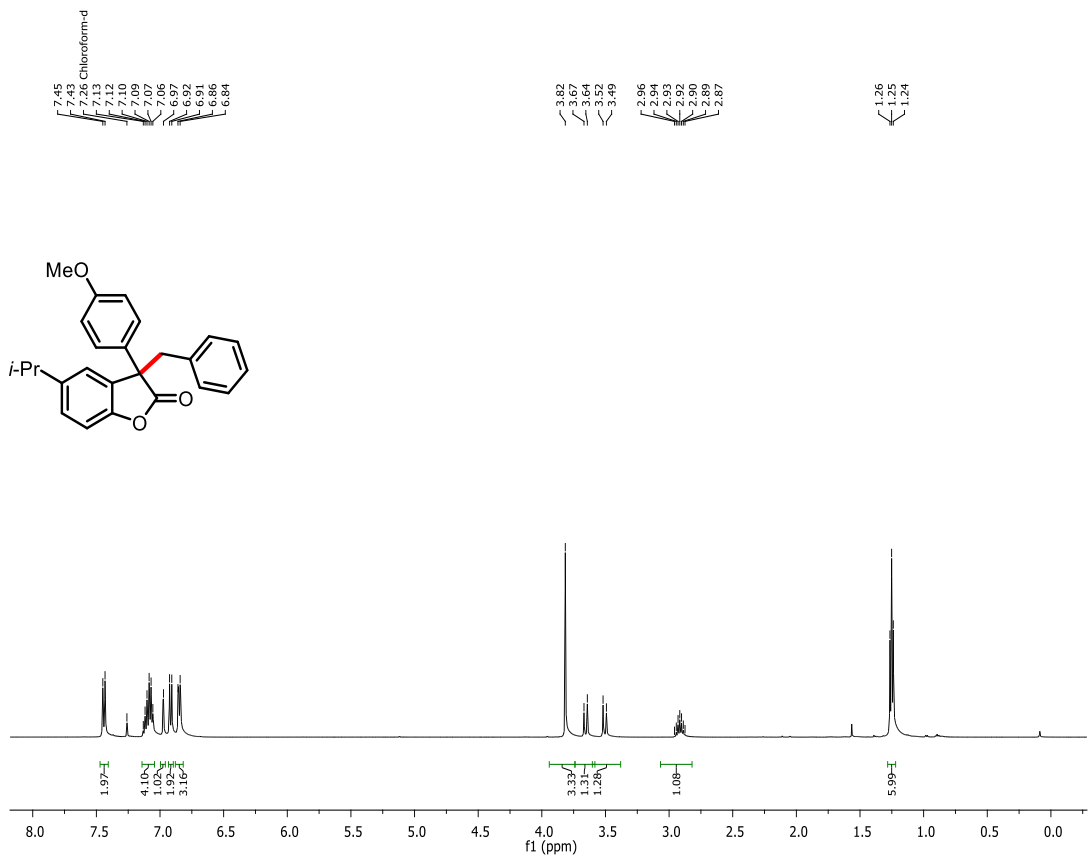


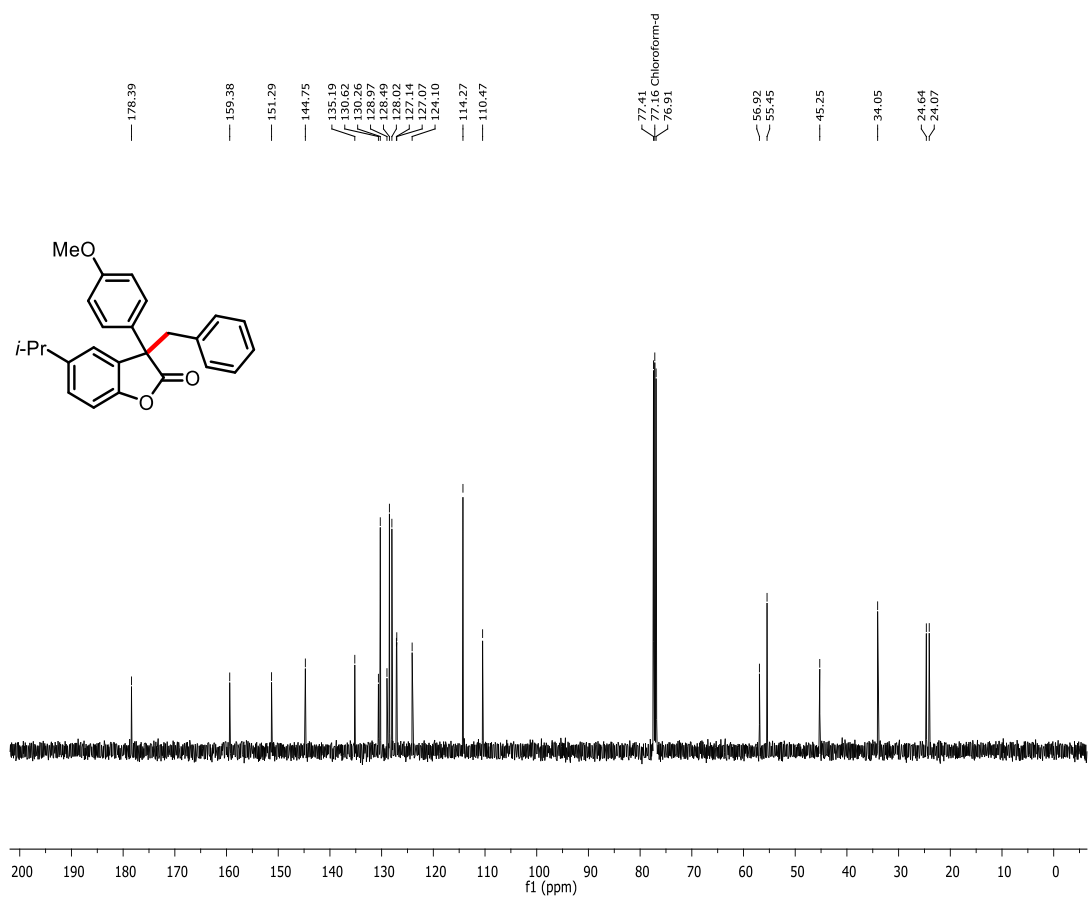
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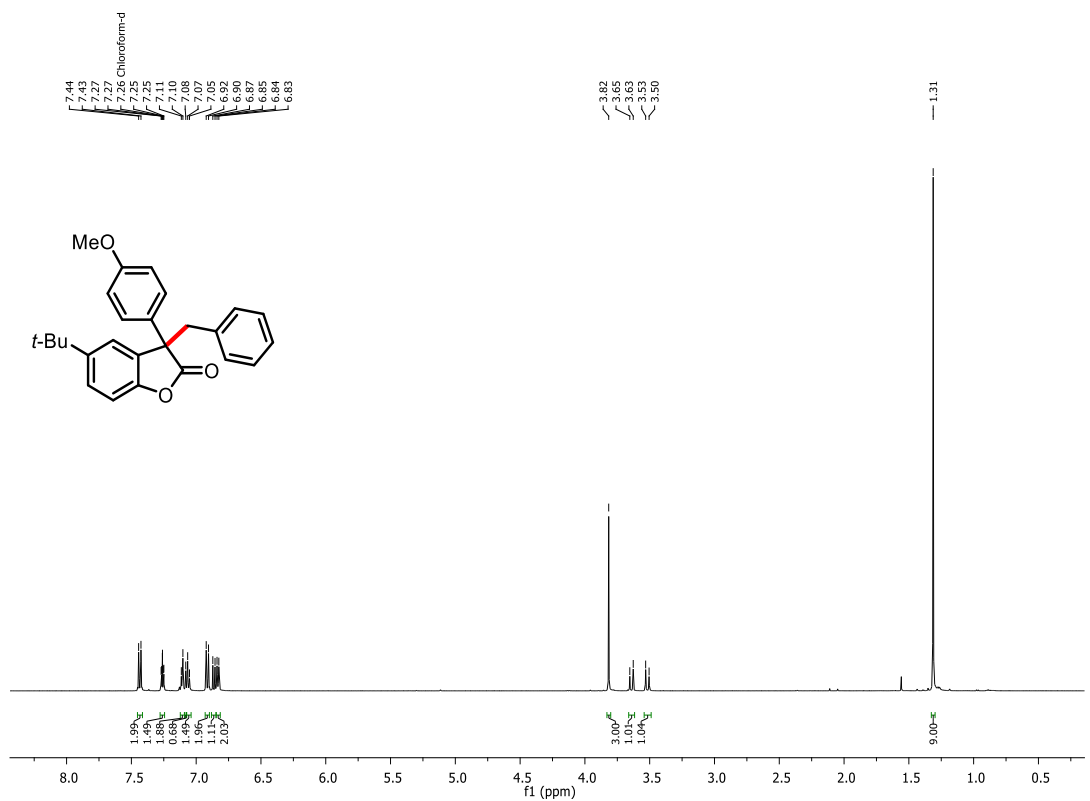


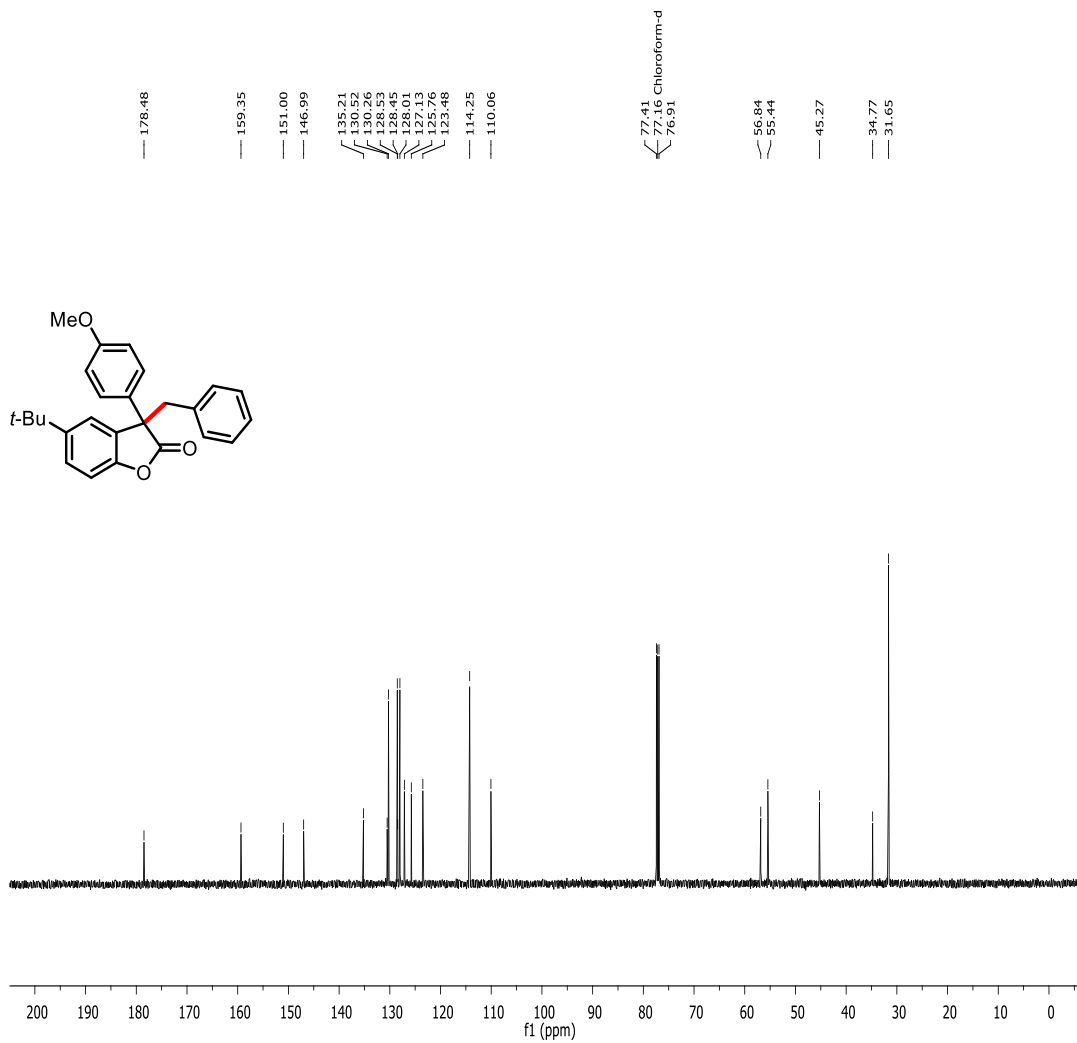
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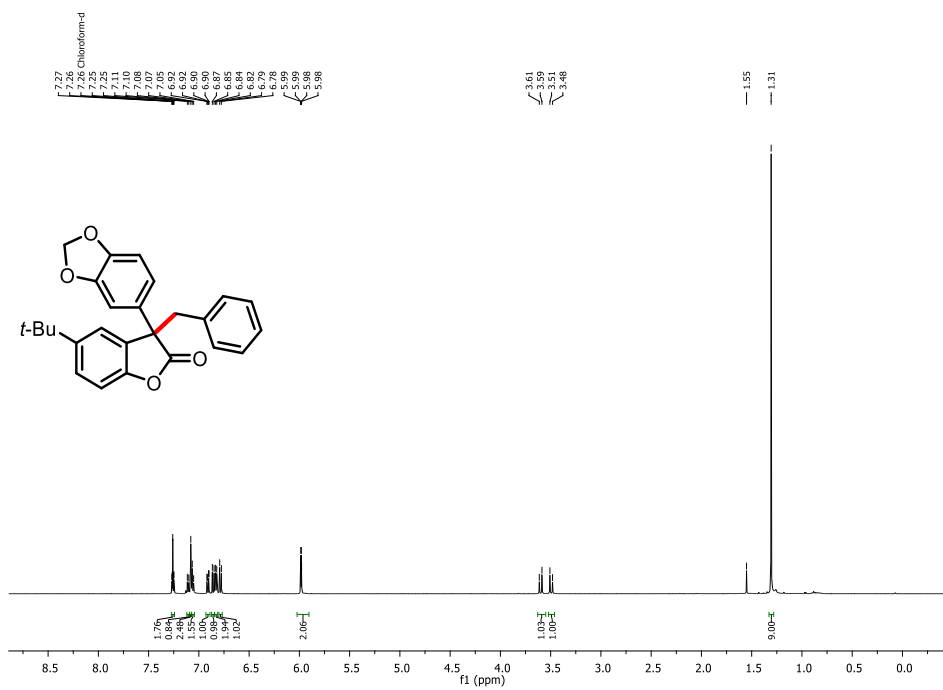


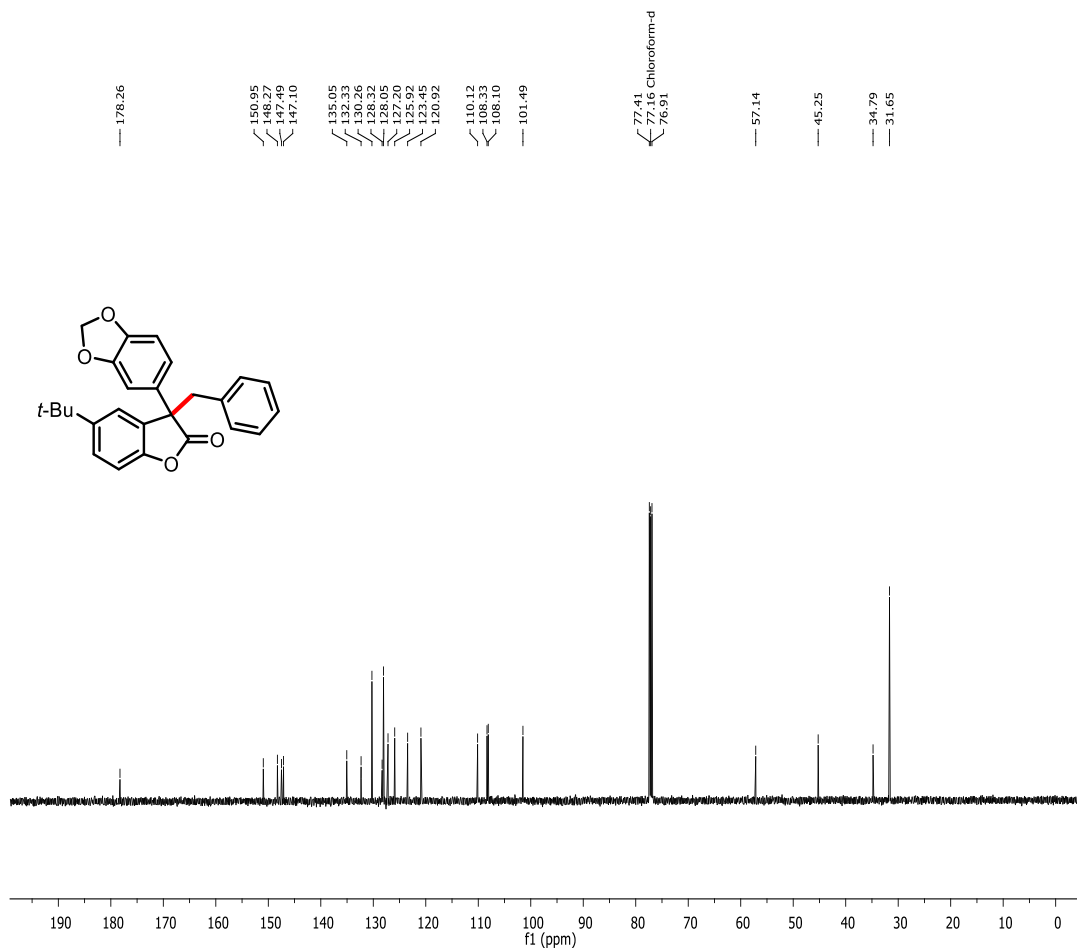
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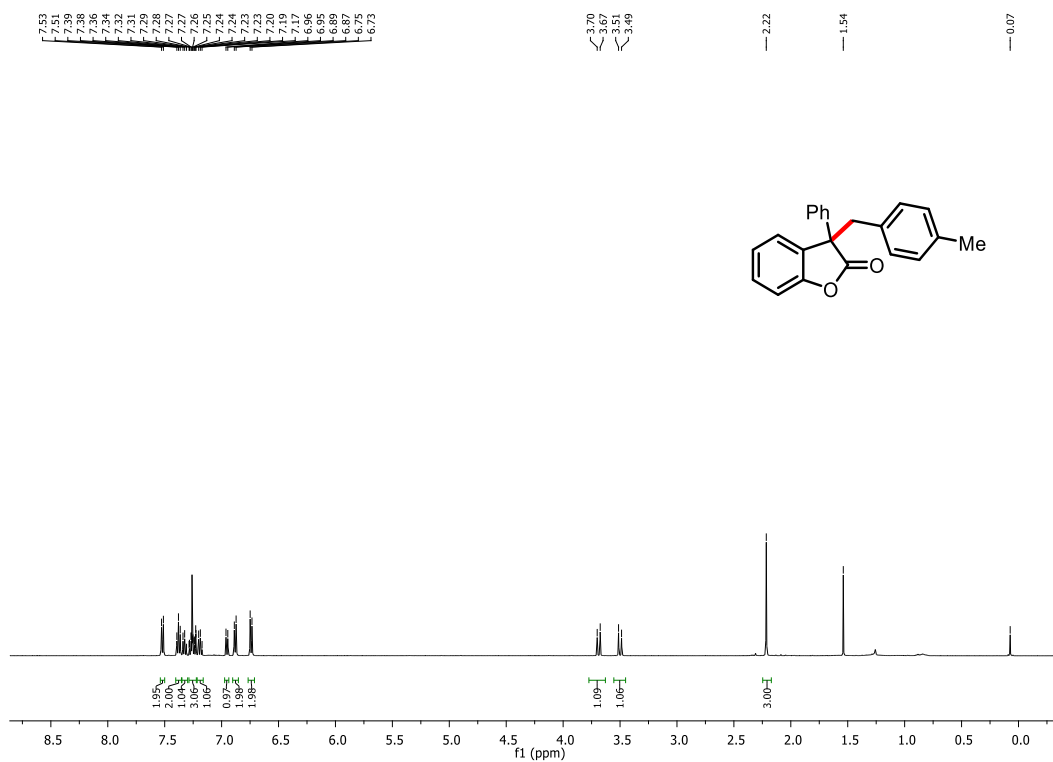


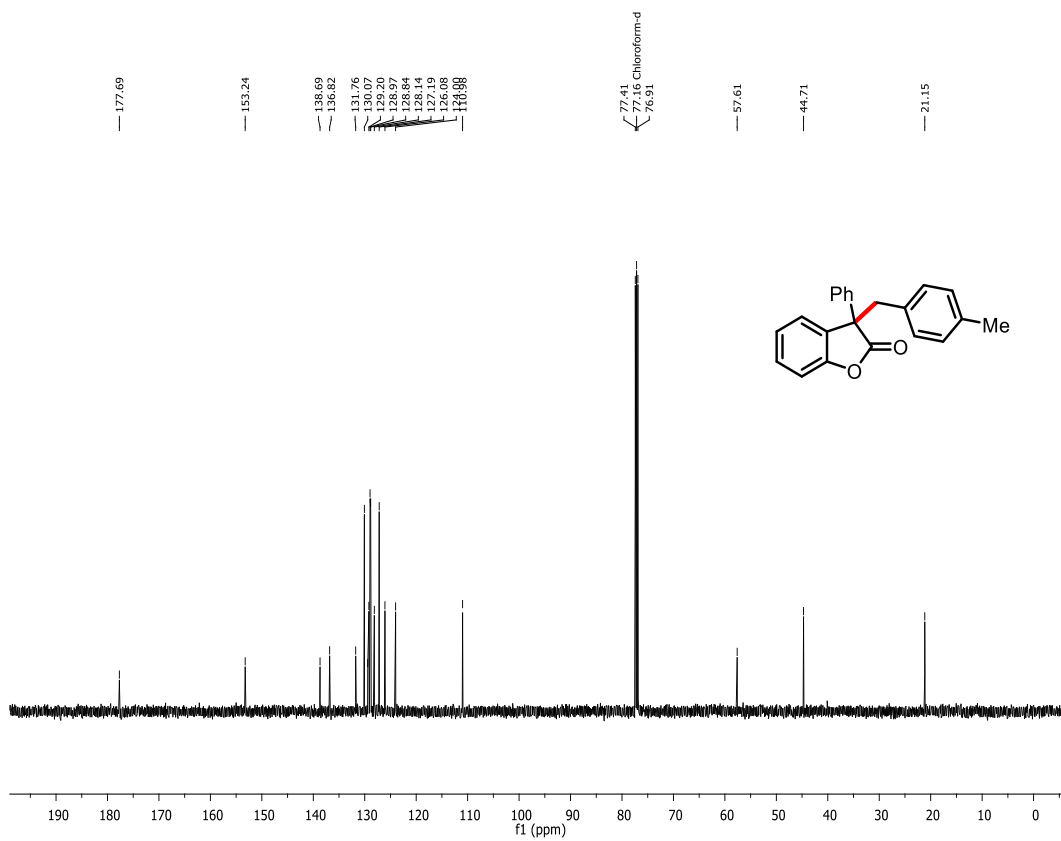
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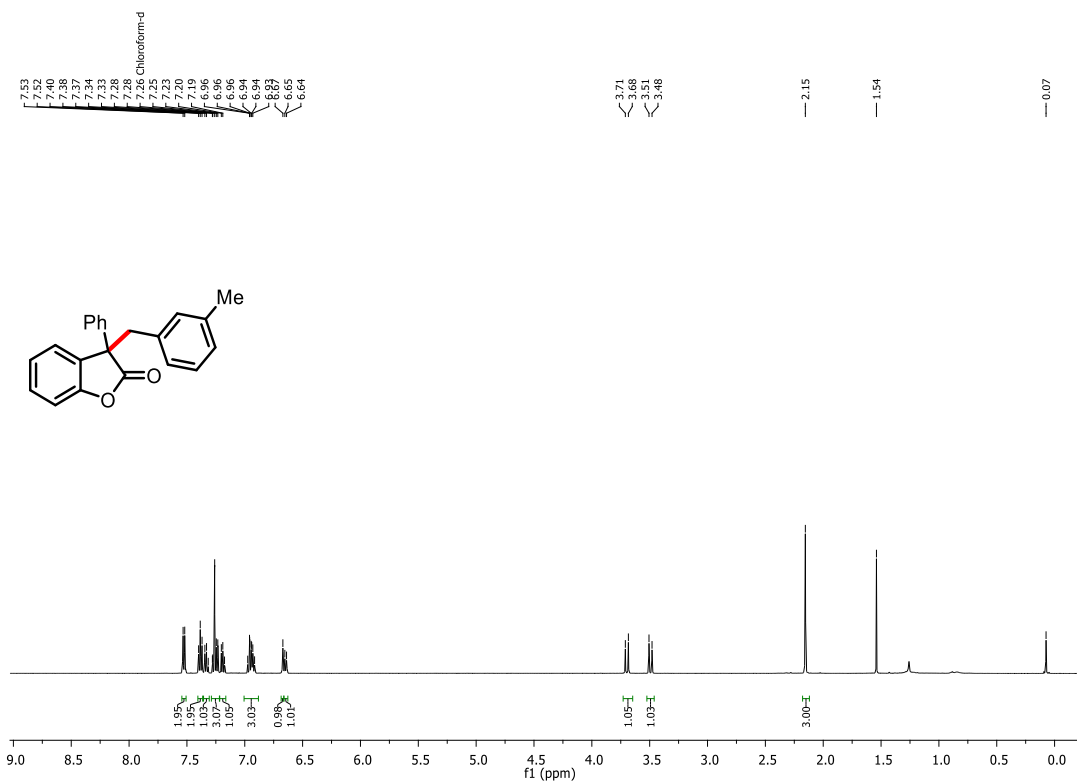


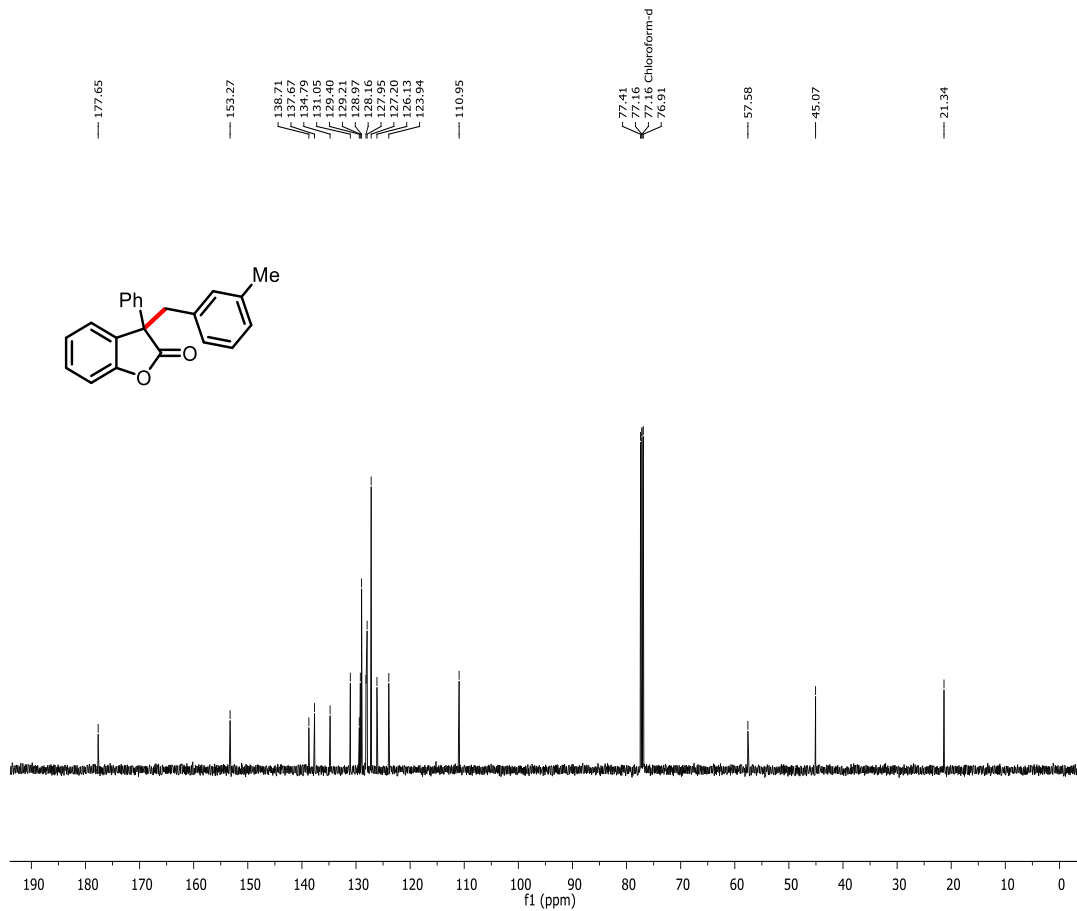
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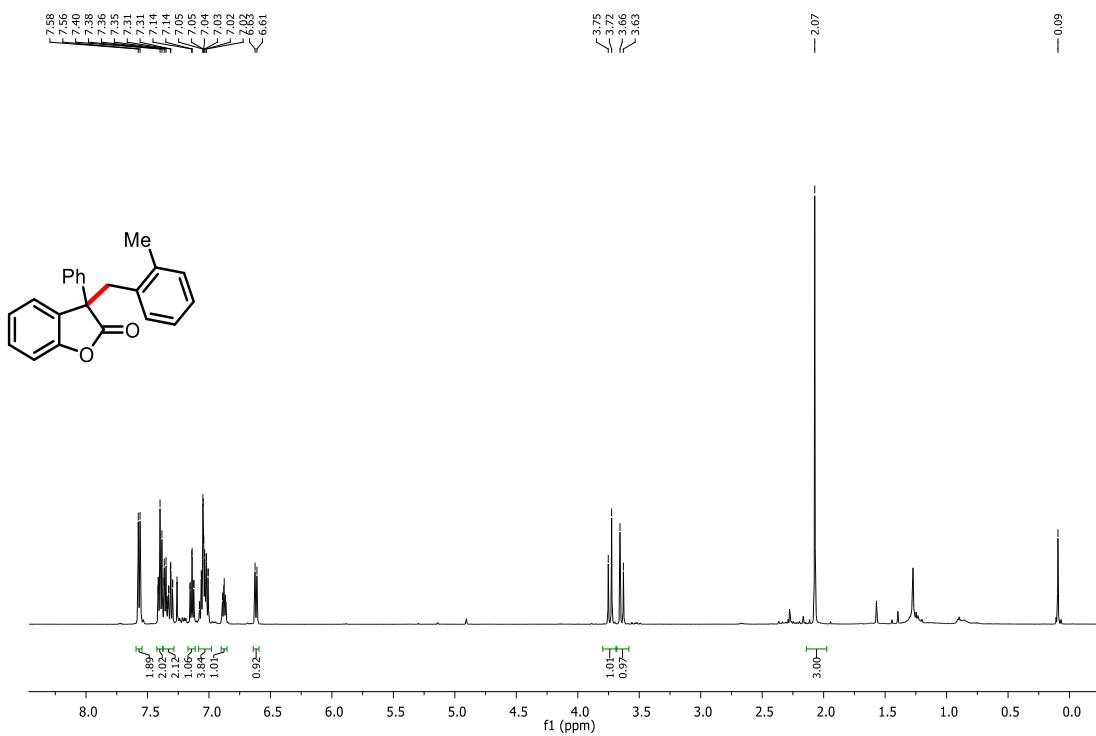


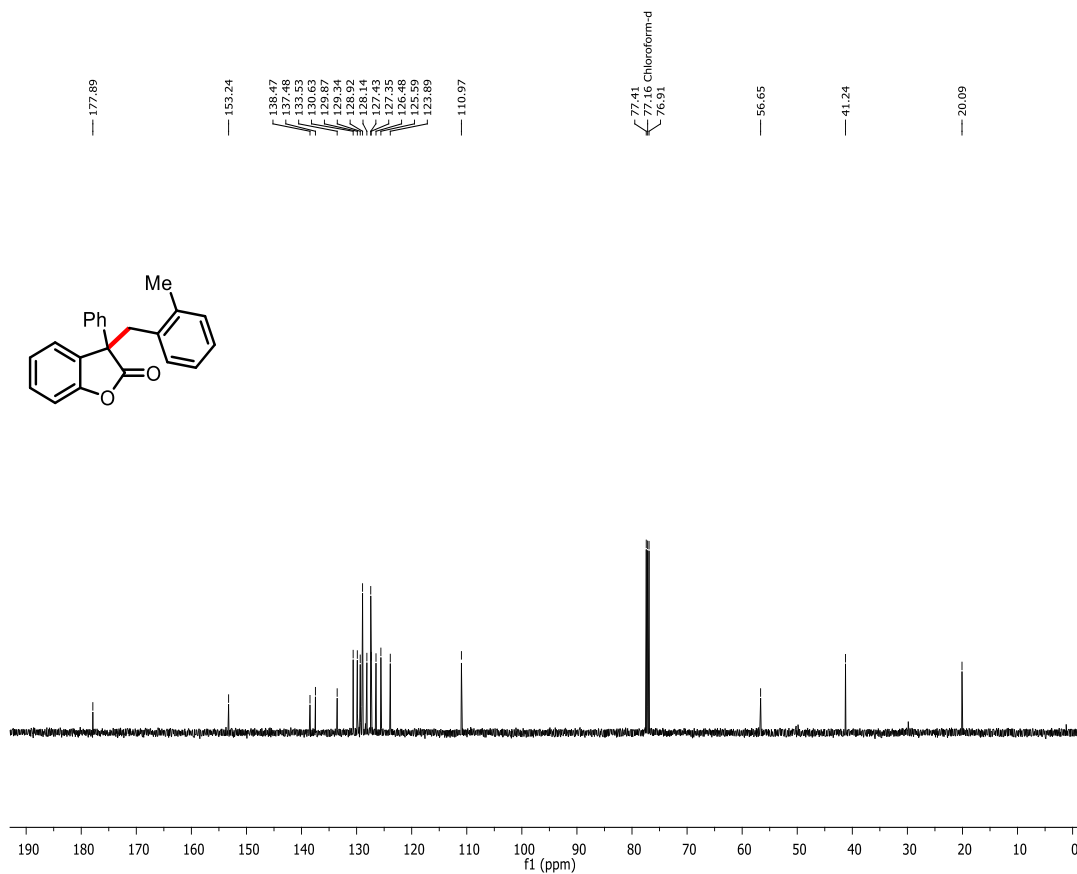
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9ad





9be

