# Supporting Information

# Ir(III)-Catalyzed Oxidative Coupling of NH Isoquinolones with Benzoquinone

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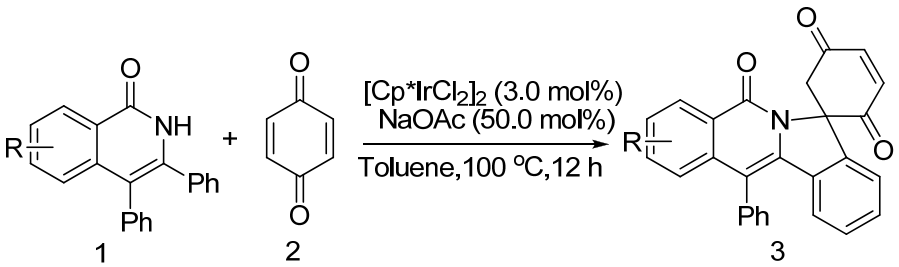
## Contents

## Experimental Section:

**General Considerations.** All reactions were carried out under argon atmosphere using standard Schlenk technique. $^{1}H$ NMR (400 MHz), $^{19}F$ (376 MHz), and $^{13}C$ NMR (100MHz) were recorded on Bruker AV400 NMR spectrometer with $CDCl_3$ as solvent. Chemical shifts of $^{1}H$, $^{19}F$, and $^{13}C$ NMR spectra are reported in parts per million (ppm). The residual solvent signals were used as references and the chemical shifts converted to the TMS scale ($CDCl_3$: $\delta_H$ = 7.26 ppm, $\delta_C$ = 77.00 ppm). All coupling constants (*J* values) were reported in Hertz (Hz). Multiplicities are reported as follows: singlet (s), doublet (d), doublet of doublets (dd), triplet (t), quartet (q), and multiplet (m). Column chromatography was performed on silica gel 200-300 mesh. Analytical thin-layer chromatography (TLC) was performed on pre-coated, glass-backed silica gel plates. Visualization of the developed chromatogram was performed by UV absorbance (254 nm). IR spectra were recorded as KBr disks on a Nicolet 380 FT-IR spectrometer. High-resolution mass spectrometry (HRMS) were done on Varian 7.0 T FTICR-mass spectrometer. $[Cp^*IrCl_2]_2$ was prepared from $IrCl_3.xH_2O$ following a literature procedure.[1] Unless otherwise noted below, all other compounds have been reported in the literature or are commercially available from Alfa Aesar China (Tianjin) Chemical Co., Ltd. without any further purification. The substrates **1a-q**,[2] **2c**,[3] were prepared according to the known procedures.

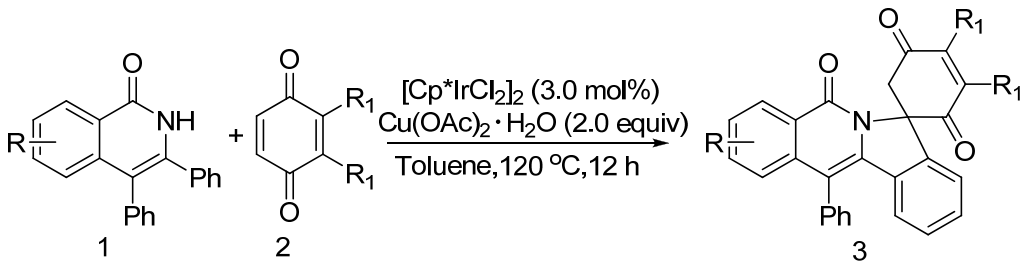
**General Procedure for the Ir(III)-Catalyzed Cascade Synthesis (A)**




A mixture of substituted isoquinolone (**1**) (0.2 mmol, 1 equiv), benzoquinone (**2**) (0.44 mmol, 2.2 equiv), $[Cp^*IrCl_2]_2$ (4.8 mg, 0.006 mmol, 3.0 mol %), and NaOAc (8.2 mg, 0.1 mmol, 0.5 equiv) were weighted in a Schlenk tube equipped with a stir bar. Dry toluene (1.0 mL) was added and the mixture was stirred at 100 °C for 12 h under Ar atmosphere. Afterwards, it was diluted with $CH_2Cl_2$ and transferred to a round bottom flask. Silica was

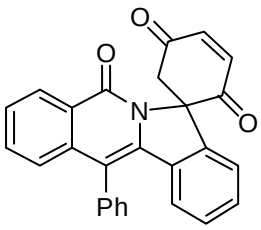
added to the flask and volatiles were evaporated under reduced pressure. The purification was performed by flash column chromatography on silica gel with EtOAc/petroleum ether.

**General Procedure for the Ir(III)-Catalyzed Cascade Synthesis (B)**




A mixture of substituted isoquinolone (**1**) (0.2 mmol, 1 equiv), benzoquinone (**2**) (0.24 mmol, 1.2 equiv), $[Cp^*IrCl_2]_2$ (4.8 mg, 0.006 mmol, 3.0 mol %), and $Cu(OAc)_2 \cdot H_2O$ (80 mg, 0.40 mmol, 2.0 equiv.) were weighted in a Schlenk tube equipped with a stir bar. Dry toluene (1.0 mL) was added and the mixture was stirred at 120 °C for 12 h under Ar atmosphere. Afterwards, it was diluted with $CH_2Cl_2$ and transferred to a round bottom flask. Silica was added to the flask and volatiles were evaporated under reduced pressure. The purification was performed by flash column chromatography on silica gel with EtOAc/petroleum ether.

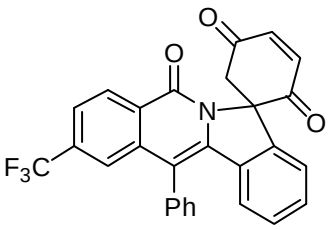
**Preparation and Characterization of Products 3**



**12'-Phenyl-5'H-spiro[cyclohex[3]ene-1,7'-isoindolo[2,1-b]isoquinoline]-2,5,5'-trione (3aa)**

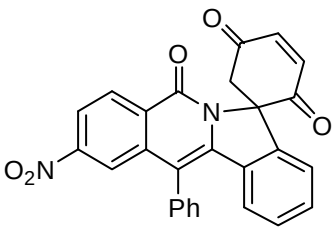
The title compound was isolated by column chromatography (eluent: EtOAc/petroleum ether = 1/5 to 1/2) as a yellow solid in 99% yield (80.1 mg, 0.198 mmol) following the general procedure A. Mp: 252-254 °C. **$^1$H NMR ($CDCl_3$, 400 MHz):** δ 8.56 (d, *J* = 7.7 Hz, 1H), 7.68 (m, 5H), 7.60 (d, *J* = 7.2 Hz, 1H), 7.57–7.51 (m, 2H), 7.39–7.28 (m, 4H), 7.22 (t, *J* = 7.6 Hz, 1H), 6.51 (d, *J* = 7.9 Hz, 1H), 5.01 (d, *J* = 16.1 Hz, 1H), 3.07 (d, *J* = 16.1 Hz, 1H). **$^{13}$C NMR ($CDCl_3$, 100 MHz):** δ 195.1, 189.1, 160.3, 142.8, 141.4, 140.0, 138.9, 136.9, 134.5, 133.2, 132.7, 130.9, 130.8, 129.8, 129.7, 129.6, 129.5, 128.7, 127.5, 126.9, 125.6, 125.1, 124.9, 121.0, 115.3, 74.5, 45.9. **HRMS (ESI):** Calcd for $C_{27}H_{18}NO_3$ $[M+H]^+$ 404.1281, found: 404.1289. **IR (cm$^{-1}$):** ν 3060, 2915, 1798, 1693, 1652, 1599, 1473, 1414, 1350, 1322, 1269, 1216, 1190, 1087, 1027, 912, 886, 835, 760, 696,

595, 550, 499, 445.



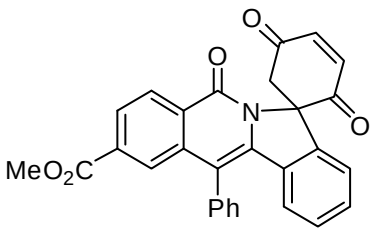
**12'-Phenyl-2'-(trifluoromethyl)-5'H-spiro[cyclohex[3]ene-1,7'-isoindolo[2,1-b]isoquinoline]-2,5,5'-trione (3ba)**

The title compound was isolated by column chromatography (eluent: EtOAc/petroleum ether = 1/5 to 1/2) as a yellow solid in 99% yield (93.5 mg, 0.198 mmol) following the general procedure A. Mp: 190-193 °C. **$^{1}$H NMR ($CDCl_3$, 400 MHz):** δ 8.58 (d, *J* = 8.3 Hz, 1H), 7.71 (d, *J* = 8.3 Hz, 1H), 7.63 (s, 3H), 7.48-7.44 (m, 3H), 7.31 (t, *J* = 7.5 Hz, 1H), 7.23 (d, *J* = 7.7 Hz, 1H), 7.20–7.11 (m, 3H), 6.41 (d, *J* = 7.9 Hz, 1H), 4.88 (d, *J* = 16.1 Hz, 1H), 2.98 (d, *J* = 16.0 Hz, 1H). **$^{13}$C NMR ($CDCl_3$, 100 MHz):** δ 194.7, 188.7, 159.5, 142.9, 141.2, 140.1, 139.0, 138.5, 134.3 (q, *J* = 32.3 Hz), 133.4, 132.7, 130.8, 130.7, 130.3, 129.9, 129.8, 129.8, 129.2, 128.7, 127.2, 125.3, 123.6 (q, *J* = 271.5 Hz), 122.8, 122.7, 121.0, , 114.8, 74.8, 45.6. **$^{19}$F NMR ($CDCl_3$, 376 MHz):** δ -62.97 (s). **HRMS (ESI):** Calcd for $C_{28}H_{17}F_3NO_3$ $[M+H]^+$ 472.1155, found: 472.1163. **IR (cm$^{-1}$):** ν 3049, 2920, 1694, 1654, 1619, 1560, 1489, 1467, 1432, 1374, 1354, 1338, 1313, 1269, 1222, 1165, 1128, 1091, 1047, 1024, 970, 890, 842, 792, 772, 751, 702, 698, 553, 504.



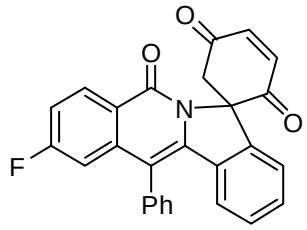
**2'-Nitro-12'-phenyl-5'H-spiro[cyclohex[3]ene-1,7'-isoindolo[2,1-b]isoquinoline]-2,5,5'-trione (3ca)**

The title compound was isolated by column chromatography (eluent: EtOAc/petroleum ether = 1/5 to 1/2) as a yellow solid in 99% yield (89.0 mg, 0.198 mmol) following the general procedure A. Mp: 275-277 °C. **$^{1}$H NMR ($CDCl_3$, 400 MHz):** δ 8.62 (d, *J* = 8.8 Hz, 1H), 8.25 (d, *J* = 8.8 Hz, 1H), 8.07 (s, 1H), 7.66 (s, 3H), 7.45 (s, 2H), 7.34 (m, 1H), 7.25 – 7.12 (m, 4H), 6.44 (d, *J* = 7.9 Hz, 1H), 4.86 (d, *J* = 16.2 Hz, 1H), 3.00 (d, *J* = 16.1 Hz, 1H). **$^{13}$C NMR ($CDCl_3$, 100 MHz):** δ 194.5 , 188.4, 159.1, 150.6, 143.1, 141.2, 140.1, 139.8, 133.0, 132.4, 130.8, 130.7, 130.2, 130.0, 129.7, 129.5, 128.5, 125.5, 121.1, 120.9, 120.4, 114.8, 75.0, 45.5. **HRMS (ESI):** Calcd for $C_{27}H_{17}N_2O_5$ $[M+H]^+$ 449.1132, found: 449.1138. **IR (cm$^{-1}$):** ν 3055, 1699, 1656, 1619, 1522, 1463, 1344, 1268, 1212, 1148, 1082, 884, 833, 769, 745, 715.



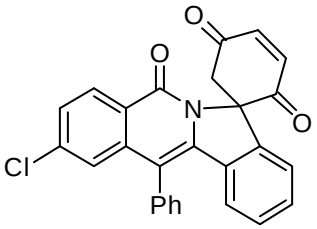

**Methyl 2,5,5'-trioxo-12'-phenyl-5'H-spiro[cyclohex[3]ene-1,7'-isoindolo[2,1-b]isoquinoline]-2'-carboxylate (3da)**

The title compound was isolated by column chromatography (eluent: EtOAc/petroleum ether = 1/5 to 1/2) as a yellow solid in 99% yield (91.6 mg, 0.198 mmol) following the general procedure A. Mp: 239-240 °C. **$^{1}$H NMR ($CDCl_3$, 400 MHz):** δ 8.52 (d, *J* = 8.3 Hz, 1H), 8.11 (d, *J* = 8.3 Hz, 1H), 7.92 (s, 1H), 7.62 (m, 3H), 7.44 (m, 2H), 7.29 (t, *J* = 7.7 Hz, 1H), 7.24 – 7.10 (m, 4H), 6.39 (d, *J* = 7.8 Hz, 1H), 4.88 (d, *J* = 16.0 Hz, 1H), 3.89 (s, 3H), 2.98 (d, *J* = 16.1 Hz, 1H). **$^{13}$C NMR ($CDCl_3$, 100 MHz):** δ 194.9, 188.9, 166.3, 159.8, 142.9, 141.3, 140.0, 138.8, 137.9, 133.82, 133.8, 132.9, 130.9, 130.8, 130.1, 129.9, 129.7, 129.0, 128.0, 127.8, 127.3, 126.9, 125.2, 121.0, 116.1, 115.4, 74.7, 52.5, 45.7. **HRMS (ESI):** Calcd for $C_{29}H_{20}NO_5$ $[M+H]^+$ 462.1336, found: 462.1343. **IR ($cm^{-1}$):** ν 3052, 2948, 2363, 1712, 1696, 1651, 1616, 1551, 1498, 1466, 1434, 1439, 1296, 1270, 1248, 1185, 1092, 979, 954, 914, 880, 815, 759, 732, 708, 605, 504



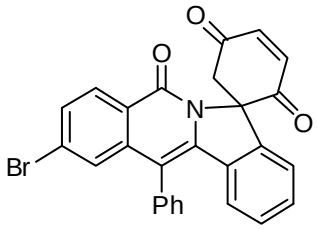

**2'-Fluoro-12'-phenyl-5'H-spiro[cyclohex[3]ene-1,7'-isoindolo[2,1-b]isoquinoline]-2,5,5'-trione (3ea)**

The title compound was isolated by column chromatography (eluent: EtOAc/petroleum ether = 1/5 to 1/2) as a yellow solid in 99% yield (83.6 mg, 0.198 mmol) following the general procedure A. M.p: 251-253 °C. **$^{1}$H NMR ($CDCl_3$, 400 MHz):** δ 8.46 (dd, *J* = 8.8, 5.8 Hz, 1H), 7.65 – 7.58 (m, 3H), 7.47 – 7.38 (m, 2H), 7.29 (t, *J* = 7.6 Hz, 1H), 7.24 – 7.10 (m, 5H), 6.84 (dd, *J* = 10.3, 2.4 Hz, 1H), 6.42 (d, *J* = 8.0 Hz, 1H), 4.88 (d, *J* = 16.1 Hz, 1H), 2.97 (d, *J* = 16.1 Hz, 1H). **$^{13}$C NMR ($CDCl_3$, 100 MHz):** δ 194.9, 189.0, 165.6 (d, *J* = 250 Hz), 159.6, 142.9, 141.5(d, *J* = 9.8 Hz), 141.3, 140.2, 138.3, 133.9, 132.9, 130.8, 130.7, 130.6, 130.2, 129.8, 129.8, 129.7, 129.0, 125.1, 121.7, 121.0, 115.6, 115.3, 114.6, 110.9, 110.7, 74.6, 45.9. **$^{19}$F NMR ($CDCl_3$, 376 MHz):** δ -104.76 (dd, *J* = 14.3, 9.9 Hz). **HRMS (ESI):** Calcd for $C_{27}H_{17}FNO_3$ $[M+H]^+$ 422.1187, found: 422.1194. **IR ($cm^{-1}$):** ν 3037, 2912, 1692, 1662, 1617, 1481, 1463, 1416, 1371, 1343, 1292, 1221, 1188, 1126, 1092, 1024, 981, 939, 881, 864, 831, 759, 744, 696, 673, 584.



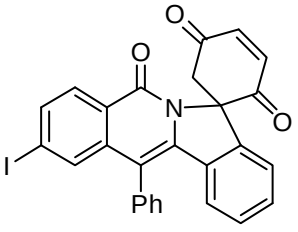

**2'-Chloro-12'-phenyl-5'H-spiro[cyclohex[3]ene-1,7'-isoindolo[2,1-b]isoquinoline]-2,5,5'-trione (3fa)**

The title compound was isolated by column chromatography (eluent: EtOAc/petroleum ether = 1/5 to 1/2) as a yellow solid in 99% yield (86.9 mg, 0.198 mmol) following the general procedure A. Mp: 223-225°C. **$^1$H NMR ($CDCl_3$, 400 MHz):** δ 8.38 (d, *J* = 8.6 Hz, 1H), 7.66 – 7.59 (m, 3H), 7.47 – 7.39 (m, 3H), 7.29 (t, *J* = 7.6 Hz, 1H), 7.24 – 7.10 (m, 5H), 6.39 (d, *J* = 7.9 Hz, 1H), 4.87 (d, *J* = 16.1 Hz, 1H), 2.97 (d, *J* = 16.1 Hz, 1H). **$^{13}$C NMR ($CDCl_3$, 100 MHz):** δ 194.8, 188.9, 159.6 , 142.9, 141.2, 140.1, 139.5, 138.3, 133.7, 132.8, 130.8, 130.7, 130.2, 129.8, 129.8, 129.7, 129.2, 129.0, 127.3, 125.1, 124.9, 123.4, 121.0, 114.3, 74.6, 45.8. **HRMS (ESI):** Calcd for $C_{27}H_{17}ClNO_3$ $[M+H]^+$ 438.0891, found: 438.0893. **IR (cm$^{-1}$):** ν 3063, 2920, 1698, 1653, 1620, 1594, 1545, 1492, 1461, 1418, 1322, 1284, 1255, 1182, 1085, 1063, 1001, 975, 929, 889, 836, 766, 726, 701, 681, 596, 560.



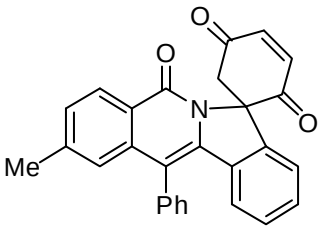

**2'-Bromo-12'-phenyl-5'H-spiro[cyclohex[3]ene-1,7'-isoindolo[2,1-b]isoquinoline]-2,5,5'-trione(3ga)**

The title compound was isolated by column chromatography (eluent: EtOAc/petroleum ether = 1/5 to 1/2) as a yellow solid in 99% yield (95.7 mg, 0.198 mmol) following the general procedure A. Mp: 207-209 °C. **$^1$H NMR ($CDCl_3$, 400 MHz):** δ 8.30 (d, *J* = 8.5 Hz, 1H), 7.61 (m, 4H), 7.43 (m, 2H), 7.34 (s, 1H), 7.29 (t, *J* = 7.8 Hz, 1H), 7.24 – 7.10 (m, 4H), 6.35 (dd, *J* = 23.9, 7.6 Hz, 1H), 4.87 (d, *J* = 16.1 Hz, 1H), 2.97 (d, *J* = 16.1 Hz, 1H). **$^{13}$C NMR ($CDCl_3$, 100 MHz):** δ 194.9, 188.9, 142.9, 141.3, 140.4, 140.1, 138.3, 133.7, 132.9, 130.9, 130.8, 130.2, 129.9, 129.8, 129.7, 129.3, 129.1, 128.3, 128.0, 125.2, 123.8, 121.0, 114.2, 74.6, 45.8. **HRMS (ESI):** Calcd for $C_{27}H_{17}BrNO_3$ $[M+H]^+$ 482.0386, found: 482.0389. **IR (cm$^{-1}$):** ν 3049, 2918, 1698, 1654, 1616, 1591, 1543, 1506, 1461, 1413, 1344, 1322, 1267, 1219, 1186, 1087, 898, 834, 767, 712, 674.



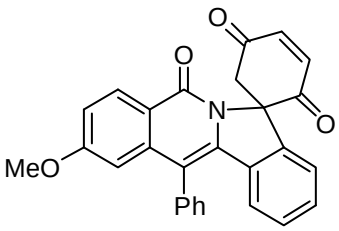

**2'-Iodo-12'-phenyl-5'H-spiro[cyclohex[3]ene-1,7'-isoindolo[2,1-b]isoquinoline]-2,5,5'-trione (3ha)**

The title compound was isolated by column chromatography (eluent: EtOAc/petroleum ether = 1/5 to 1/2) as a yellow solid in 99% yield (105.0 mg, 0.198 mmol) following the general procedure A. Mp: 173-175°C. **$^1$H NMR ($CDCl_3$, 400 MHz):** δ 8.13 (d, *J* = 8.4 Hz, 1H), 7.81 (d, *J* = 8.4 Hz, 1H), 7.67 – 7.59 (m, 3H), 7.56 (s, 1H), 7.42 (dd, *J* = 10.3, 4.8 Hz, 2H), 7.28 (m, 1H), 7.24 – 7.08 (m, 4H), 6.32 (dd, *J* = 24.1, 7.8 Hz, 1H), 4.86 (d, *J* = 16.1 Hz, 1H), 2.97 (d, *J* = 16.1 Hz, 1H). **$^{13}$C NMR ($CDCl_3$, 100 MHz):** δ 194.9, 188.8, 160.0, 142.88, 141.3, 140.3, 140.1, 138.1, 135.9, 134.3, 133.7, 132.9, 130.9, 130.8, 130.2, 129.9, 129.8, 129.7, 129.0, 129.0, 125.2, 124.3, 121.0, 114.0, 101.2, 74.6 (s), 45.8 (s). **HRMS (ESI):** Calcd for $C_{27}H_{17}INO_3$ $[M+H]^+$ 530.0248, found: 530.0249. **IR (cm$^{-1}$):** ν 3394, 3046, 2916, 1699, 1651, 1614, 1585, 1539, 1492, 1459, 1407, 1344, 1320, 1267, 1187, 1088, 889, 834, 768, 708, 673, 553.




**2'-Methyl-12'-phenyl-5'H-spiro[cyclohex[3]ene-1,7'-isoindolo[2,1-b]isoquinoline]-2,5,5'-trione (3ia)**

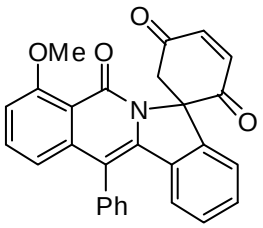
The title compound was isolated by column chromatography (eluent: EtOAc/petroleum ether = 1/5 to 1/2) as a yellow solid in 99% yield (82.9 mg, 0.198 mmol) following the general procedure A. Mp: 245-246 °C. **$^1$H NMR ($CDCl_3$, 400 MHz):** δ 8.35 (d, *J* = 8.1 Hz, 1H), 7.65 – 7.57 (m, 3H), 7.47 – 7.40 (m, 2H), 7.33 (d, *J* = 8.1 Hz, 1H), 7.26 – 7.24 (m, 1H), 7.21 – 7.08 (m, 4H), 6.98 (s, 1H), 6.37 (d, *J* = 7.9 Hz, 1H), 4.91 (d, *J* = 16.1 Hz, 1H), 2.96 (d, *J* = 16.1 Hz, 1H), 2.37 (s, 3H): **$^{13}$C NMR ($CDCl_3$, 100 MHz):** δ 195.2, 189.2, 160.2, 143.4, 142.7, 141.3, 140.0, 138.9, 137.0, 134.6, 133.3, 130.9, 130.8, 129.7, 129.6, 129.4, 128.6,128.5, 127.5, 125.3, 124.9, 123.0, 120.9, 115.2, 77.3, 46.0, 22.0. **HRMS (ESI):** Calcd for $C_{28}H_{20}NO_3$ $[M+H]^+$ 418.1438, found: 438.1447. **IR (cm$^{-1}$):** ν 3048, 2917, 1695, 1649, 1601, 1491, 1463, 1373, 1341, 1271, 1217, 1161, 1091, 1026, 885, 834, 769, 747, 703, 676, 551.




**2'-Methoxy-12'-phenyl-5'H-spiro[cyclohex[3]ene-1,7'-isoindolo[2,1-b]isoquinoline]-2,5,5'-trione (3ja)**

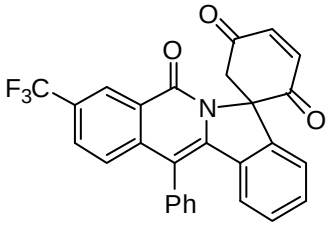
The title compound was isolated by column chromatography (eluent: EtOAc/petroleum ether = 1/5 to 1/2) as a yellow solid in

99% yield (86.0 mg, 0.198 mmol) following the general procedure A. Mp: 245-246 °C. **$^1$H NMR ($CDCl_3$, 400 MHz):** δ 8.38 (d, *J* = 8.8 Hz, 1H), 7.58 – 7.57 (m, 3H), 7.44 – 7.40 (m, 2H), 7.24 – 7.22 (m, 1H), 7.18 – 7.05 (m, 5H), 6.57 (s, 1H), 6.38 (d, *J* = 7.9 Hz, 1H), 4.91 (d, *J* = 16.1 Hz, 1H), 3.73 (s, 3H), 2.96 (d, *J* = 16.1 Hz, 1H). **$^{13}$C NMR ($CDCl_3$, 100 MHz):** δ 195.2, 189.3, 163.1, 159.9, 142.8, 141.3, 141.1, 140.2, 137.5, 134.5, 133.3 , 130.9, 130.7, 129.8,129.6, 129.5, 128.7, 124.9, 120.9, 119.0, 116.0, 115.4, 114.9, 107.6, 74.3, 55.3, 46.1. **HRMS (ESI):** Calcd for $C_{28}H_{20}NO_4$ $[M+H]^+$ 434.1387, found: 434.1393. **IR ($cm^{-1}$):** ν 3314, 2973, 1701, 1641, 1607, 1584, 1518, 1487, 1462, 1376, 1351, 1273, 1230, 1083, 1030, 836, 767, 744, 704, 684, 633, 595.




**4'-Methoxy-12'-phenyl-5'H-spiro[cyclohex[3]ene-1,7'-isoindolo[2,1-b]isoquinoline]-2,5,5'-trione (3ka)**

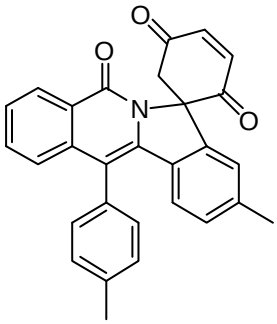
The title compound was isolated by column chromatography (eluent: EtOAc/petroleum ether = 1/5 to 1/2) as a yellow solid in 58% yield (50.3 mg, 0.116 mmol) following the general procedure A. Mp: 256-259 °C. **$^1$H NMR ($CDCl_3$, 400 MHz):** δ 7.61 – 7.54 (m, 3H), 7.50 – 7.44 (m, 1H), 7.43 – 7.37 (m, 2H), 7.22 (dd, *J* = 9.0, 8.2 Hz, 1H), 7.18 – 7.04 (m, 4H), 6.93 (d, *J* = 8.0 Hz, 1H), 6.78 – 6.71 (m, 1H), 6.31 (d, *J* = 7.9 Hz, 1H), 4.93 (d, *J* = 16.1 Hz, 1H), 4.01 (s, 3H), 2.92 (d, *J* = 16.1 Hz, 1H). **$^{13}$C NMR ($CDCl_3$, 100 MHz):** δ 195.4, 189.1, 161.3, 159.0, 142.4, 142.0, 141.5, 140.5, 137.6, 135.0, 133.2, 133.1, 131.0, 130.9, 129.8, 129.6, 129.5, 129.4, 128.5, 124.9, 120.8, 118.0, 114.6, 114.4, 108.3, 74.3, 56.2, 45.77. **HRMS (ESI):** Calcd for $C_{28}H_{19}NNaO_4$ $[M+Na]^+$ 456.1206, found: 456.1212. **IR (cm-1):** ν 3359, 3065, 2909, 2835, 1690, 1653, 1618, 1599, 1555, 1475, 1369, 1271, 1218, 1184, 1091, 1039, 1020, 989, 884, 810, 768, 739, 708, 685, 551, 498.




**12'-Phenyl-3'-(trifluoromethyl)-5'H-spiro[cyclohex[3]ene-1,7'-isoindolo[2,1-b]isoquinoline]-2,5,5'-trione (3la)**

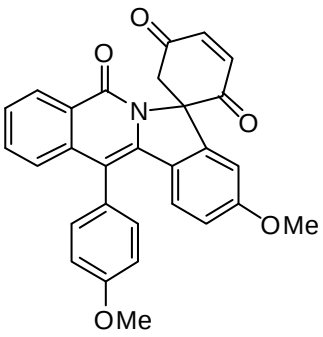
The title compound was isolated by column chromatography (eluent: EtOAc/petroleum ether = 1/5 to 1/2) as a yellow solid in 99% yield (93.5 mg, 0.198 mmol) following the general procedure A. Mp: 214-216 °C. **$^1$H**

**NMR ($CDCl_3$, 400 MHz):** δ 8.76 (s, 1H), 7.77 (dd, *J* = 8.6, 1.8 Hz, 1H), 7.67 – 7.56 (m, 3H), 7.45-7.42 (m, 2H), 7.36 – 7.29 (m, 2H), 7.23 (d, *J* = 7.7 Hz, 1H), 7.20 – 7.12 (m, 3H), 6.44 (d, *J* = 8.0 Hz, 1H), 4.87 (d, *J* = 16.1 Hz, 1H), 2.99 (d, *J* = 16.0 Hz, 1H). **$^{13}$C NMR ($CDCl_3$, 100 MHz):** δ 194.7, 188.6, 159.6, 143.0, 141.3, 141.1, 140.2, 139.2, 133.7, 132.6, 130.8, 130.7, 130.5, 129.8, 129.7, 129.0, 128.8, 128.6, 128.4, 126.4, 125.3, 125.2, 124.8, 122.4, 121.1, 114.5, 74.7, 45.6. **HRMS (ESI):** Calcd for $C_{27}H_{17}F_3NO_3$ $[M+Na]^+$ 494.0974, found: 494.0978. **IR ($cm^{-1}$):** ν 3743, 3057, 1701, 1661, 1621, 1551, 1500, 1466, 1421, 1375, 1326, 1265, 1233, 1170, 1123, 1088, 1071, 1025, 966, 927, 876, 744, 770, 749, 701, 624, 553, 504.



**9'-Methyl-12'-p-tolyl-5'H-spiro[cyclohex[3]ene-1,7'-isoindolo[2,1-b]isoquinoline]-2,5,5'-trione (3ma)**

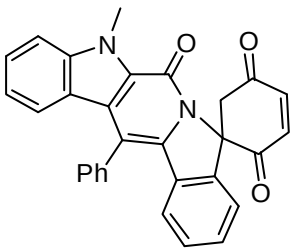
The title compound was isolated by column chromatography (eluent: EtOAc/petroleum ether = 1/5 to 1/2) as a yellow solid in 99% yield (85.6 mg, 0.198 mmol) following the general procedure A. Mp: 245-246 °C. **$^1$H NMR ($CDCl_3$, 400 MHz):** δ 8.44 (dd, *J* = 8.0, 1.0 Hz, 1H), 7.60 – 7.55 (m, 1H), 7.51 – 7.46 (m, 1H), 7.41 – 7.39 (m, 2H), 7.35 – 7.27 (m, 2H), 7.25 – 7.23 (m, 1H), 7.17 (s, 2H), 6.96 – 6.94 (m, 2H), 6.37 (d, *J* = 8.7 Hz, 1H), 4.89 (d, *J* = 16.1 Hz, 1H), 2.96 (d, *J* = 16.1 Hz, 1H), 2.52 (s, 3H), 2.29 (s, 3H). **$^{13}$C NMR ($CDCl_3$, 100 MHz):** δ 195.4, 189.4, 160.3, 142.75, 141.5, 140.4, 140.3, 139.2, 138.3, 137.1, 132.6, 131.5, 130.8, 130.7, 130.3, 130.1, 127.5, 126.6, 125.5, 125.0, 124.8, 121.3, 114.6, 74.3, 45.9, 21.6, 21.5. **HRMS (ESI):** Calcd for $C_{29}H_{22}NO_3$ $[M+H]^+$ 432.1594, found: 432.1603. **IR ($cm^{-1}$):** ν 3043, 2911, 1694, 1654, 1604, 1551, 1514, 1478, 1412, 1371,1346, 1273, 1216, 1184, 1138, 1088, 1043, 1023, 886, 834, 812, 770, 750, 700, 512.



**9'-Methoxy-12'-(4-methoxyphenyl)-5'H-spiro[cyclohex[3]ene-1,7'-isoindolo[2,1-b]isoquinoline]-2,5,5'-trione (3na)**

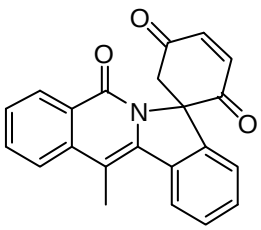
The title compound was isolated by column chromatography (eluent: EtOAc/petroleum ether = 1/5 to 1/2) as a yellow solid in 62% yield (57.3 mg, 0.123 mmol) following the general procedure A. Mp: 214-215 °C. **$^1$H NMR ($CDCl_3$, 400 MHz):** δ 8.42 (d, *J* =

7.9 Hz, 1H), 7.59 – 7.55 (m, 1H), 7.46 (t, *J* = 7.5 Hz, 1H), 7.35 – 7.31 (m, 2H), 7.25 – 7.23 (m, 1H), 7.18 – 7.08 (m, 4H), 6.70 – 6.66 (m, 2H), 6.44 (d, *J* = 8.6 Hz, 1H), 4.86 (d, *J* = 16.1 Hz, 1H), 3.94 (s, 3H), 3.72 (s, 3H), 2.96 (d, *J* = 16.1 Hz, 1H). **$^{13}$C NMR ($CDCl_3$, 100 MHz):** δ 195.1, 189.1, 160.9, 160.3, 159.7, 142.7, 141.7, 141.4, 139.4, 137.3, 132.6, 132.2, 132.0, 127.4, 126.6, 126.4, 126.2, 125.8, 125.2, 124.5, 116.1, 115.3, 114.9, 113.3, 106.9, 74.2, 55.6, 55.3, 45.9.**HRMS (ESI):** Calcd for $C_{29}H_{22}NO_5$ $[M+H]^+$ 464.1492, found: 464.1502. **IR (cm$^{-1}$):** ν 3034, 2966, 2839, 1696, 1649, 1607, 1513, 1481, 1371, 1248, 1217, 1180, 1090, 1029, 890, 820, 775, 699, 564.




**9'-Methyl-15'-phenylspiro[cyclohex[3]ene-1,5'-indol[1,2-g]isoindolo[2,1-b]isoquinoline]-2,5,7'(9'H)-trione (3oa)**

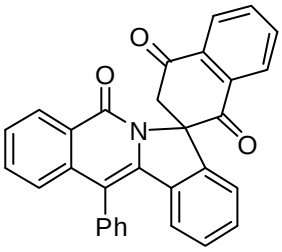
The title compound was isolated by column chromatography (eluent: EtOAc/petroleum ether = 1/5 to 1/2) as a yellow solid in 99% yield (90.4 mg, 0.198 mmol) following the general procedure A. Mp: 280-283°C. **$^1$H NMR ($CDCl_3$, 400 MHz):** δ 7.68 – 7.62 (m, 3H), 7.61 – 7.54 (m, 2H), 7.47 – 7.39 (m, 2H), 7.23 – 7.14 (m, 4H), 7.13 – 7.09 (m, 1H), 7.00 – 6.91 (m, 1H), 6.76 (d, *J* = 8.2 Hz, 1H), 6.54 (d, *J* = 7.9 Hz, 1H), 5.02 (d, *J* = 16.1 Hz, 1H), 4.348 (s, 3H), 3.00 (dd, *J* = 16.1, 1.0 Hz, 1H). **$^{13}$C NMR ($CDCl_3$, 100 MHz):** δ 195.3, 189.5, 154.2, 142.8, 141.5, 139.3, 135.3, 133.8, 133.7, 130.3, 130.1, 129.7, 129.6, 129.5, 128.8, 128.5, 126.8, 126.3, 123.4, 122.7, 121.9, 120.8, 120.2, 114.3, 110.0, 74.5, 45.8, 31.4. **HRMS (ESI):** Calcd for $C_{30}H_{20}N_2NaO_3$ $[M+Na]^+$ 479.1366, found: 479.1370. **IR (cm$^{-1}$):** ν 3743, 3050, 2923, 2364, 1686, 1652, 1583, 1491, 1463, 1419, 1396, 1341, 1313, 1259, 1213, 1158, 1132, 1070, 971, 894, 864, 806, 741, 699, 571, 542, 456.




**12'-Methyl-5'H-spiro[cyclohex[3]ene-1,7'-isoindolo[2,1-b]isoquinoline]-2,5,5'-trione (3pa)**

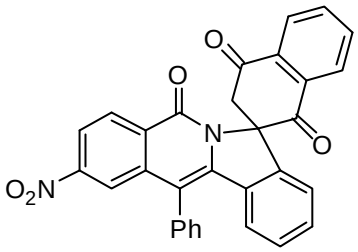
The title compound was isolated by column chromatography (eluent: EtOAc/petroleum ether = 1/5 to 1/2) as a yellow solid in 99% yield (67.8 mg, 0.198 mmol) following the general procedure A. Mp: 261-263 °C. **$^1$H NMR ($CDCl_3$, 400 MHz):** δ 8.45 (dd, *J* = 8.0, 1.0 Hz, 1H), 8.06 (d, *J* = 8.0 Hz, 1H), 7.89 (m, 1H), 7.82 – 7.74 (m, 1H), 7.58 – 7.48 (m, 2H), 7.40 (t, *J* = 7.3 Hz, 1H), 7.27 (d, *J* = 6.5 Hz, 1H),

7.16 (s 2H), 4.86 (d, *J* = 16.1 Hz, 1H), 2.91 (d, *J* = 16.1 Hz, 1H), 2.73 (s, 3H). **$^{13}$C NMR ($CDCl_3$, 100 MHz):** δ 195.3, 189.5, 160.0, 142.8, 141.4, 140.2, 138.7, 136.7, 134.1, 132.8, 130.0, 129.5, 127.9, 126.9, 125.4, 125.3, 123.5, 121.3, 109.3, 74.2, 46.1, 12.5. **HRMS (ESI):** Calcd for $C_{22}H_{16}NO_3$ $[M+H]^+$ 342.1125, found: 342.1128. **IR (cm$^{-1}$):** ν 3742, 3057, 2914, 1694, 1645, 1598, 1522, 1468, 1354, 1321, 1257, 1215, 1084, 1033, 885, 840, 764, 691.




**12-Phenyl-1'H,5H-spiro[isoindolo[2,1-b]isoquinoline-7,2'-naphthalene]-1',4',5(3'H)-trione (3ab)**

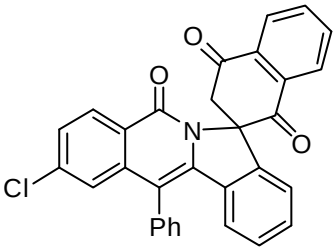
The title compound was isolated by column chromatography (eluent: EtOAc/petroleum ether = 1/5 to 1/2) as a yellow solid in 99% yield (90.0 mg, 0.198 mmol) following the general procedure B. Mp: 271-272 °C. **$^{1}$H NMR ($CDCl_3$, 400 MHz):** δ 8.49 (d, *J* = 7.9 Hz, 1H), 8.29 (m, 2H), 7.93 – 7.83 (m, 2H), 7.67 – 7.56 (m, 4H), 7.55 – 7.41 (m, 3H), 7.25 – 7.24 (m, 1H), 7.16-7.06 (m, 2H), 6.90 (d, *J* = 7.5 Hz, 1H), 6.42 (d, *J* = 7.9 Hz, 1H), 5.19 (d, *J* = 15.8 Hz, 1H), 3.15 (d, *J* = 15.8 Hz, 1H). **$^{13}$C NMR ($CDCl_3$, 100 MHz):** δ 193.6, 188.2, 188.2, 160.4, 140.4, 138.9, 137.2, 136.3, 135.1, 134.7, 134.1, 133.4, 132.6, 131.0, 130.9, 129.7, 129.6, 129.5, 129.4, 129.1, 128.6, 127.6, 126.8, 125.5, 125.3, 124.8, 121.4, 115.2, 46.3. **HRMS (ESI):** Calcd for $C_{31}H_{20}NO_3$ $[M+H]^+$ 454.1438, found: 454.1447. **IR (cm$^{-1}$):** ν 3050, 2898, 1690, 1650, 1621, 1596, 1470, 1419, 1352, 1325, 1282, 1256, 1158, 1061, 992, 970, 915, 859, 764, 731, 699, 594, 541, 509, 451.




**2-Nitro-12-phenyl-1'H,5H-spiro[isoindolo[2,1-b]isoquinoline-7,2'-naphthalene]-1',4',5(3'H)-trione (3cb)**

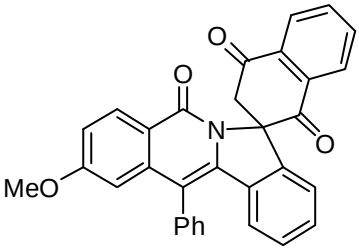
The title compound was isolated by column chromatography (eluent: EtOAc/petroleum ether = 1/5 to 1/2) as a yellow solid in 99% yield (98.9 mg, 0.198 mmol) following the general procedure B. Mp: 285-286 °C. **$^{1}$H NMR ($CDCl_3$, 400 MHz):** δ 8.64 (d, *J* = 8.7 Hz, 1H), 8.36 – 8.22 (m, 3H), 8.09 (d, *J* = 1.8 Hz, 1H), 7.96 – 7.86 (m, 2H), 7.67 (s, 3H), 7.48 (s, 2H), 7.20 (t, *J* = 7.6 Hz, 1H), 7.13 (t, *J* = 7.6 Hz, 1H), 6.93 (d, *J* = 7.7 Hz, 1H), 6.44 (d, *J* = 7.9 Hz, 1H), 5.13 (d, *J* = 15.8 Hz, 1H), 3.17 (d, *J* = 15.8 Hz, 1H). **$^{13}$C NMR ($CDCl_3$, 100 MHz):** δ 193.1,

187.6, 159.3, 150.6, 140.6, 139.8, 139.6, 136.2, 135.4, 134.9, 133.9, 133.1, 132.5, 130.8, 130.7, 130.6, 130.1, 130.0, 129.8, 129.7, 129.4, 129.1, 128.7, 127.0, 125.3, 121.5, 120.9, 120.3, 114.7, 75.8, 45.9. **HRMS (ESI):** Calcd for $C_{31}H_{19}N_2O_5$ $[M+H]^+$ 499.1288, found: 499.1297. **IR ($cm^{-1}$):** ν 3075, 2925, 1697, 1659, 1617, 1594, 1526, 1462, 1408, 1347, 1289, 1259, 1176, 1147, 1066, 1000, 940, 899, 935, 770, 738, 724, 699, 596, 499, 446.




**2-Chloro-12-phenyl-1'H,5H-spiro[isoindolo[2,1-b]isoquinoline-7,2'-naphthalene]-1',4',5(3'H)-trione (3fb)**

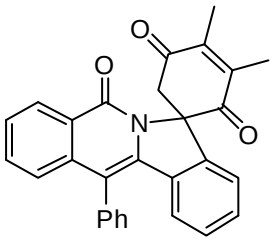
The title compound was isolated by column chromatography (eluent: EtOAc/petroleum ether = 1/5 to 1/2) as a yellow solid in 99% yield (96.6 mg, 0.198 mmol) following the general procedure B. Mp: 276-277 °C. **$^1$H NMR ($CDCl_3$, 400 MHz):** δ 8.40 (d, *J* = 8.6 Hz, 1H), 8.29 – 8.27 (m, 2H), 7.91 – 7.85 (m, 2H), 7.65 – 7.62 (m, 3H), 7.49 – 7.41 (m, 3H), 7.19-7.07 (m, 3H), 6.90 (d, *J* = 7.6 Hz, 1H), 6.40 (d, *J* = 7.9 Hz, 1H), 5.15 (d, *J* = 15.8 Hz, 1H), 3.15 (d, *J* = 15.8 Hz, 1H). **$^{13}$C NMR ($CDCl_3$, 100 MHz):** δ 193.4, 188.0, 159.9, 140.6, 140.3, 139.4, 138.6, 136.2, 135.2, 134.7, 134.0, 133.9, 133.0, 130.9, 130.8, 130.1, 129.8, 129.7, 129.6, 129.4, 129.1, 129.0, 127.3, 126.9, 125.1, 124.8, 123.6, 121.4, 114.2, 75.5, 46.2. **HRMS (ESI):** Calcd for $C_{31}H_{19}ClNO_3$ $[M+H]^+$ 488.0975, found: 488.1053. **IR ($cm^{-1}$):** ν 3063, 2920, 1698, 1653, 1620, 1594, 1545, 1492, 1461, 1418, 1322, 1284, 1255, 1182, 1085, 1063, 1001, 975, 929, 889, 836, 766, 726, 701, 681, 596, 560.




**2-Methoxy-12-phenyl-1'H,5H-spiro[isoindolo[2,1-b]isoquinoline-7,2'-naphthalene]-1',4',5(3'H)-trione (3jb)**

The title compound was isolated by column chromatography (eluent: EtOAc/petroleum ether = 1/5 to 1/2) as a yellow solid in 99% yield (95.9 mg, 0.198 mmol) following the general procedure B. Mp: 274-276 °C. **$^1$H NMR ($CDCl_3$, 400 MHz):** δ 8.40 (d, *J* = 8.9 Hz, 1H), 8.32 – 8.22 (m, 2H), 7.92 – 7.82 (m, 2H), 7.65 – 7.54 (m, 3H), 7.52 – 7.42 (m, 2H), 7.18 – 7.02 (m, 3H), 6.89 (d, *J* = 7.6 Hz, 1H), 6.59 (d, *J* = 2.4 Hz, 1H), 6.39 (d, *J* = 7.8 Hz, 1H), 5.19 (d, *J* = 15.8 Hz, 1H), 3.74 (s, 3H), 3.15 (d, *J* = 15.8 Hz, 1H). **$^{13}$C NMR ($CDCl_3$, 100 MHz):** δ 193.7,

188.4, 163.0, 160.1, 141.1, 140.6, 137.8, 136.3, 135.0, 134.7, 134.6, 134.1, 133.4, 130.9, 130.8, 129.7, 129.6, 129.6, 129.5, 129.4, 129.1, 128.6, 126.8, 124.86, 121.35, 119.23, 115.31, 114.86, 107.55, 75.21, 55.30, 46.49. **HRMS (ESI):** Calcd for $C_{32}H_{22}NO_4$ $[M+H]^+$ 484.1543, found: 484.1554. **IR ($cm^{-1}$):** ν 3552, 3415, 3066, 2965, 2919, 1701, 1649, 1601, 1489, 1463, 1380, 1344, 1315, 1281, 1257, 1230, 1139, 1103, 1061, 1019, 979, 949, 903, 848, 762, 732, 697, 593, 499.

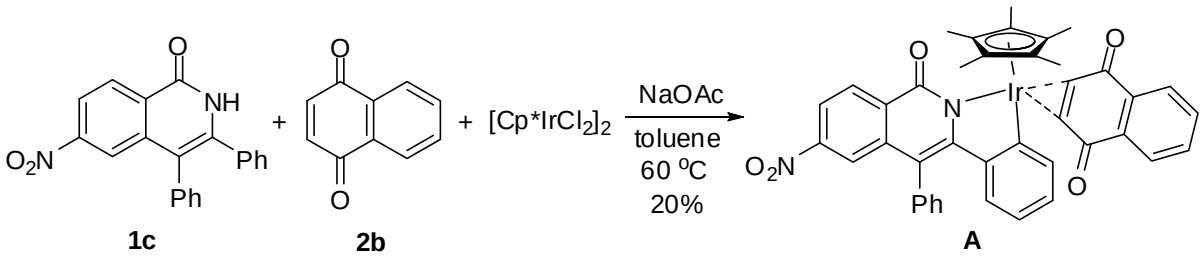



**3,4-Dimethyl-12'-phenyl-5'H-spiro[cyclohex[3]ene-1,7'-isoindolo[2, 1-b]isoquinoline]-2,5,5'-trione (3ac)**

The title compound was isolated by column chromatography (eluent: EtOAc/petroleum ether = 1/5 to 1/2) as a yellow solid in 99% yield (85.4 mg, 0.198 mmol) following the general procedure B. Mp: 250-251 °C. **$^1$H NMR ($CDCl_3$, 400 MHz):** δ 8.47 (dd, *J* = 8.0, 1.0 Hz, 1H), 7.64 – 7.55 (m, 4H), 7.52 – 7.47 (m, 1H), 7.45-7.42 (m, 2H), 7.25 – 7.19 (m, 2H), 7.13 – 7.03 (m, 2H), 6.40 (d, *J* = 7.9 Hz, 1H), 4.90 (d, *J* = 15.6 Hz, 1H), 2.98 (d, *J* = 15.6 Hz, 1H), 2.25 (d, *J* = 1.0 Hz, 3H), 2.16 (t, *J* = 4.5 Hz, 3H). **$^{13}$C NMR ($CDCl_3$, 100 MHz):** δ 194.9, 189.3, 160.3, 148.5, 146.5, 140.5, 138.8, 137.1, 134.6, 133.2, 132.6, 131.0, 130.8, 129.7, 129.6, 129.4, 128.6, 127.5, 126.8, 125.5, 125.2, 124.8, 120.9, 115.1, 74.7, 45.4, 13.7, 13.6. **HRMS (ESI):** Calcd for $C_{29}H_{21}NO_3$ $[M+H]^+$ 432.1600, found: 432.1598. **IR ($cm^{-1}$):** ν 3743, 3069, 2915, 1684, 1653, 1615, 1473, 1374, 1348, 1287, 1252, 1070, 1035, 762, 702, 601.

**Mechanism Research:**

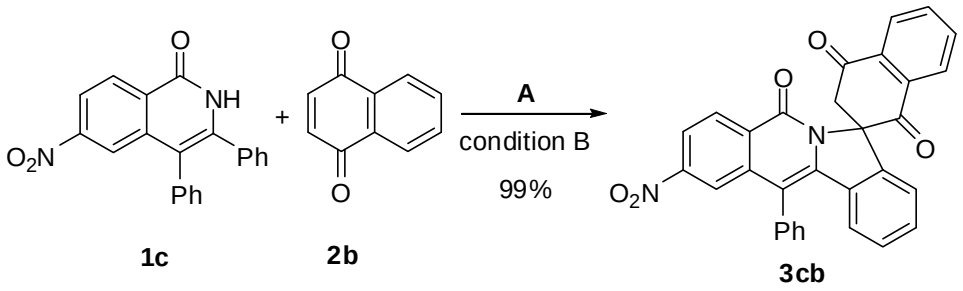
**Preparation and Characterzation of A.**




**1c** **2b** **A**

A mixture of **1c** (0.2 mmol, 68 mg), **2b** (0.4 mmol, 63 mg), $[Cp^*IrCl_2]_2$ (0.1 mmol, 80 mg), and NaOAc (0.4 mmol, 33 mg) were weighted in a Schlenk tube equipped with a stir bar. Dry toluene (4.0 mL) was added and the mixture was stirred at 60 °C for 12 h under Ar atmosphere. Afterwards, it was diluted with $CH_2Cl_2$ and transferred to a round bottom flask. Silica was added to the flask and volatiles were evaporated under reduced pressure. The purification was performed by flash column chromatography on silica gel (eluent: EtOAc/petroleum ether = 1/5 to pure EtOAc) compound **A** was isolated as a red solid in 20% yield (33.0 mg, 0.04 mmol). Mp: 250-251 °C. **$^1$H NMR ($CDCl_3$, 400 MHz):** δ 8.56 (d, *J* = 8.8 Hz, 1H), 8.02 (d, *J* = 8.5 Hz, 1H), 7.69 (s, 1H), 7.50-7.48 (m, 1H), 7.48 – 7.37 (m, 2H), 7.11 (t, *J* = 7.3 Hz, 1H), 7.057-6.966 (m, 3H), 6.91 – 6.81 (m, 3H), 6.78 (d, *J* = 7.5 Hz, 1H), 6.40 (t, *J* = 7.5 Hz, 1H), 5.75 (d, *J* = 8.1 Hz, 1H), 5.28 (d, *J* = 7.5 Hz, 1H), 4.58 (d, *J* = 7.6 Hz, 1H), 1.62 (s, 15H). **$^{13}$C NMR ($CDCl_3$, 100 MHz):** δ 193.5, 192.7, 165.4, 152.2, 149.1, 148.6, 139.4, 138.8, 137.0, 136.7, 133.4, 132.8, 132.1, 131.9, 131.2, 130.8, 129.9, 129.6, 128.9, 128.7, 128.2, 128.0, 125.9, 124.5, 124.3, 123.9, 120.2, 118.7, 116.8, 104.8, 53.6, 53.4, 9.0. **HRMS (ESI):** Calcd for $C_{31}H_{28}IrN_2O_3$ $[M+H-C_{10}H_6O_2]^+$ 669.1724. found: 669.1729. **IR (cm$^{-1}$):** ν 3050, 3020, 2910, 1661, 1623, 1597, 1570, 1519, 1487, 1466, 1415, 1376, 1362, 1341, 1322, 1285, 1248, 1224, 1160, 1136, 1121, 1079, 1027, 1009, 975, 925, 902, 837, 813, 787, 777, 745, 734, 707, 671, 654, 559.

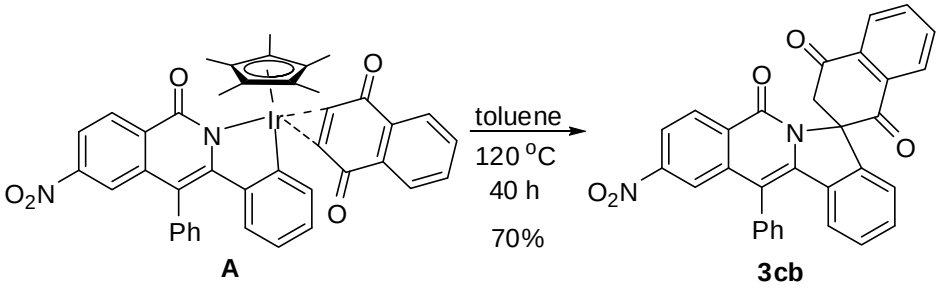
**Reaction Catalyzed by Intermediate A.**




**1c** **2b** **3cb**

A mixture of **1c** (0.2 mmol, 1.0 equiv), **2b** (0.24 mmol, 1.2 equiv), and intermediate **A** (6.0 mol %) were weighted in a Schlenk tube equipped with a stir bar. Dry toluene (1.0 mL) was added and the mixture was stirred at 120 °C for 12 h under Ar. Afterwards, it was transferred to a round bottom flask. Silica was added to the flask and volatiles were evaporated under reduced pressure. After purification by flash column chromatography on silica gel the desired product **3cb** was obtained in 99% yield (98.9 mg, 0.198 mmol).

**Transformation Reaction of Intermediate A.**




**A** **3cb**

Intermediate **A** (83.0 mg, 0.1 mmol) and dry toluene (4.0 mL) were weighted in a Schlenk tube equipped with a stir bar. The reaction was stirred at 120 °C for 40 h. Afterwards, it was diluted with $CH_2Cl_2$ and transferred to a round bottom flask and volatiles were evaporated under reduced pressure. After purification by flash column chromatography on silica gel (eluent: EtOAc/petroleum ether = 1/5 to 1/2) the desired product **3cb** was obtained in 70% yield (35.1 mg, 0.07 mmol).

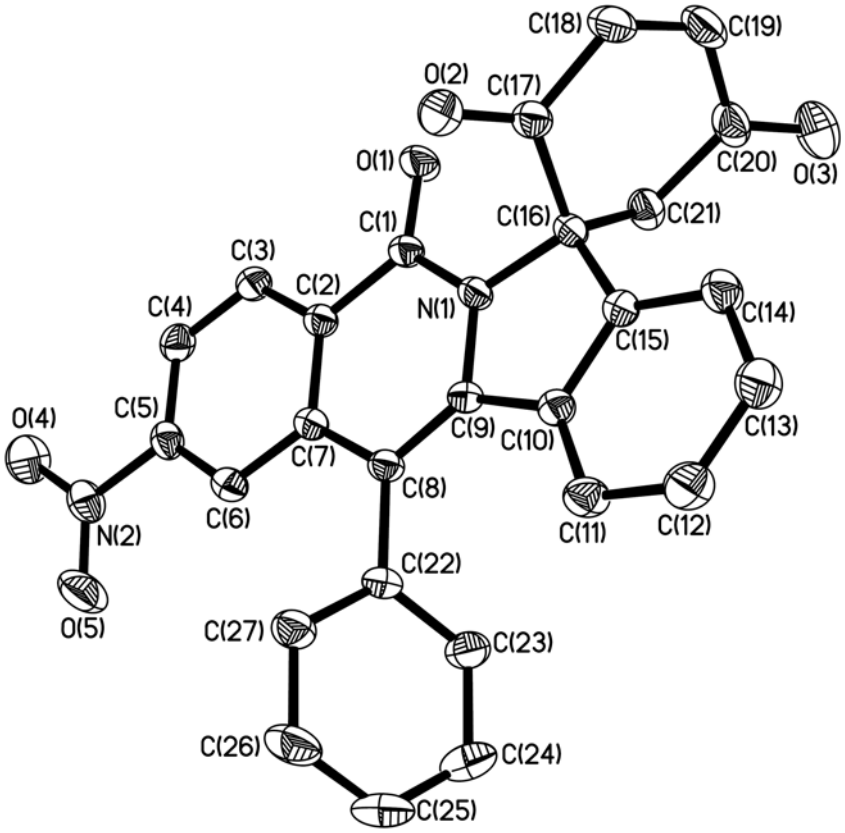
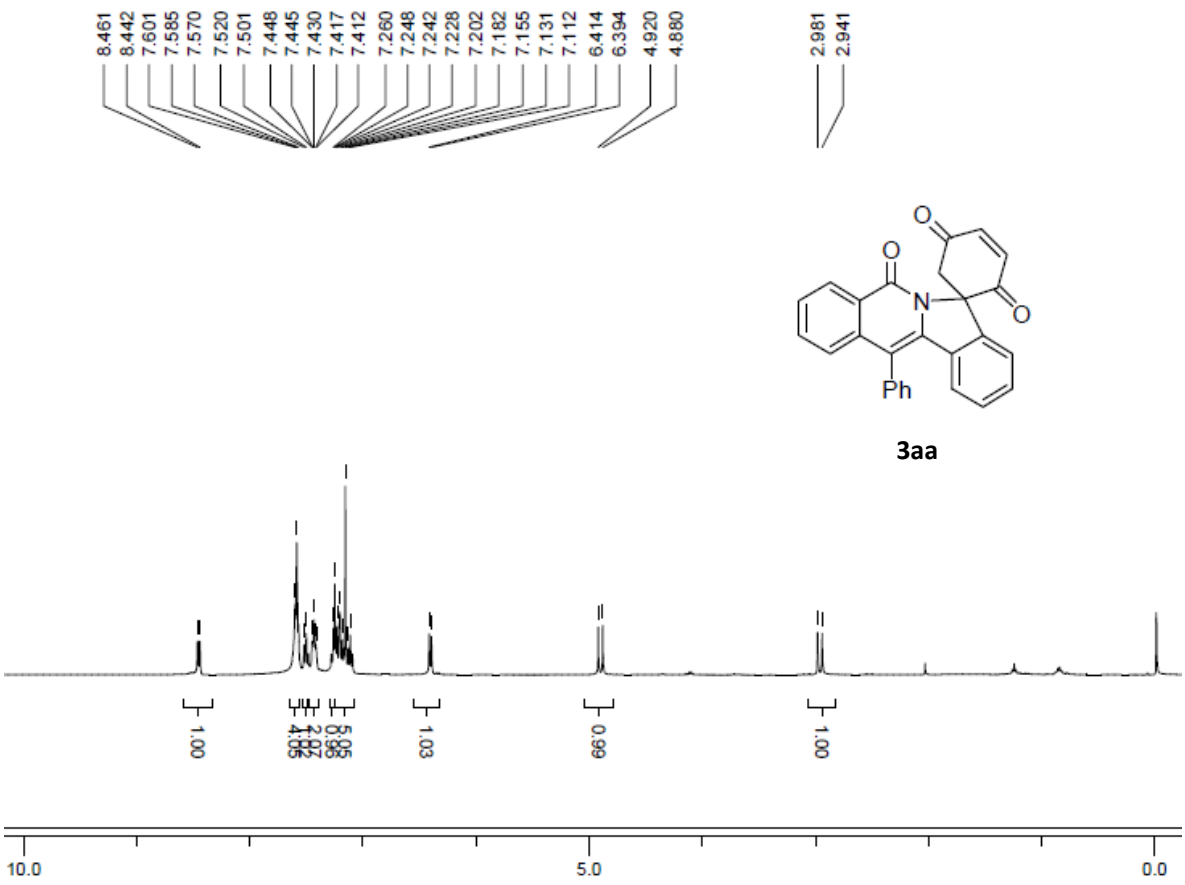



**Figure S1.** The molecular structure of **3ac**. Thermal ellipsoids are shown at the 30% level. Hydrogen atoms have been omitted for clarity.

# Spectral Copies of $^{1}H$, $^{13}C$, and $^{19}F$ NMR of Compounds Obtained in This Study

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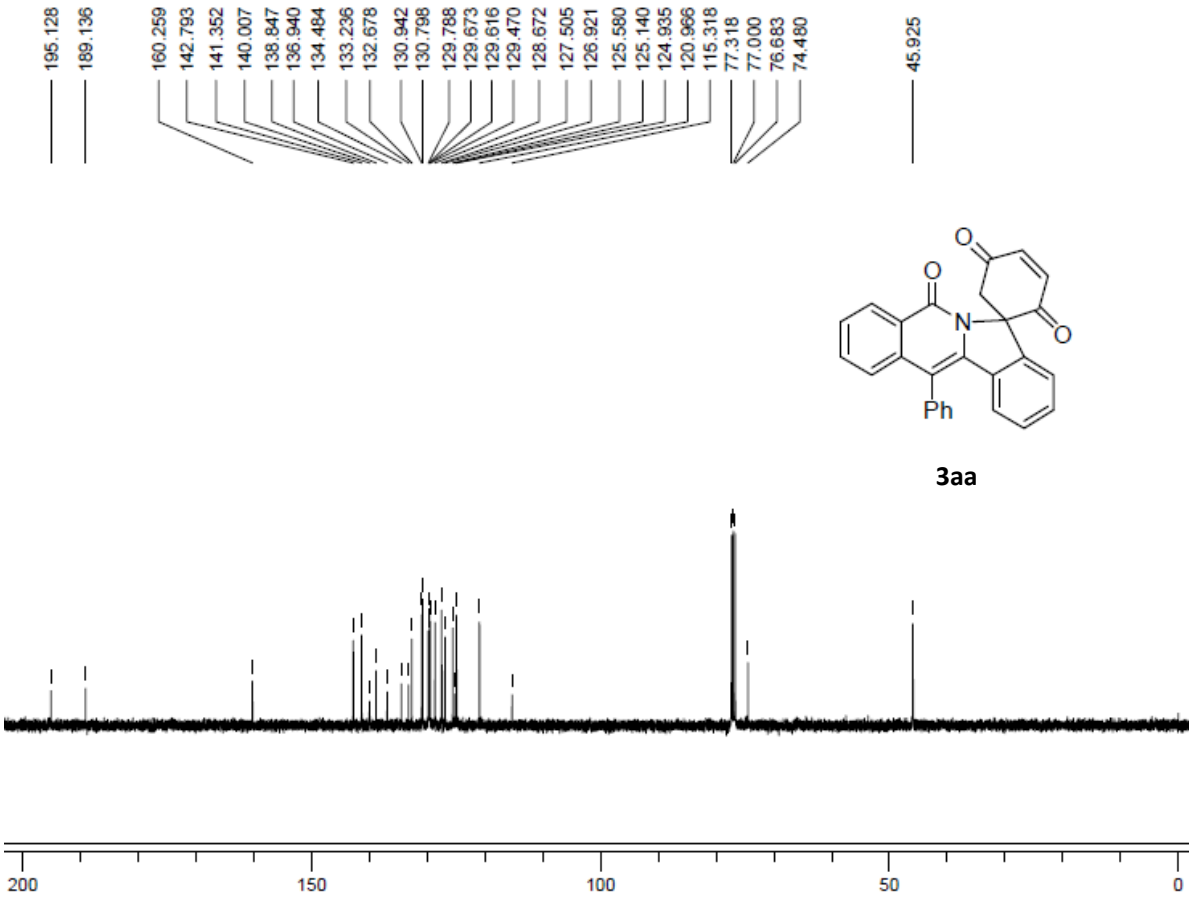
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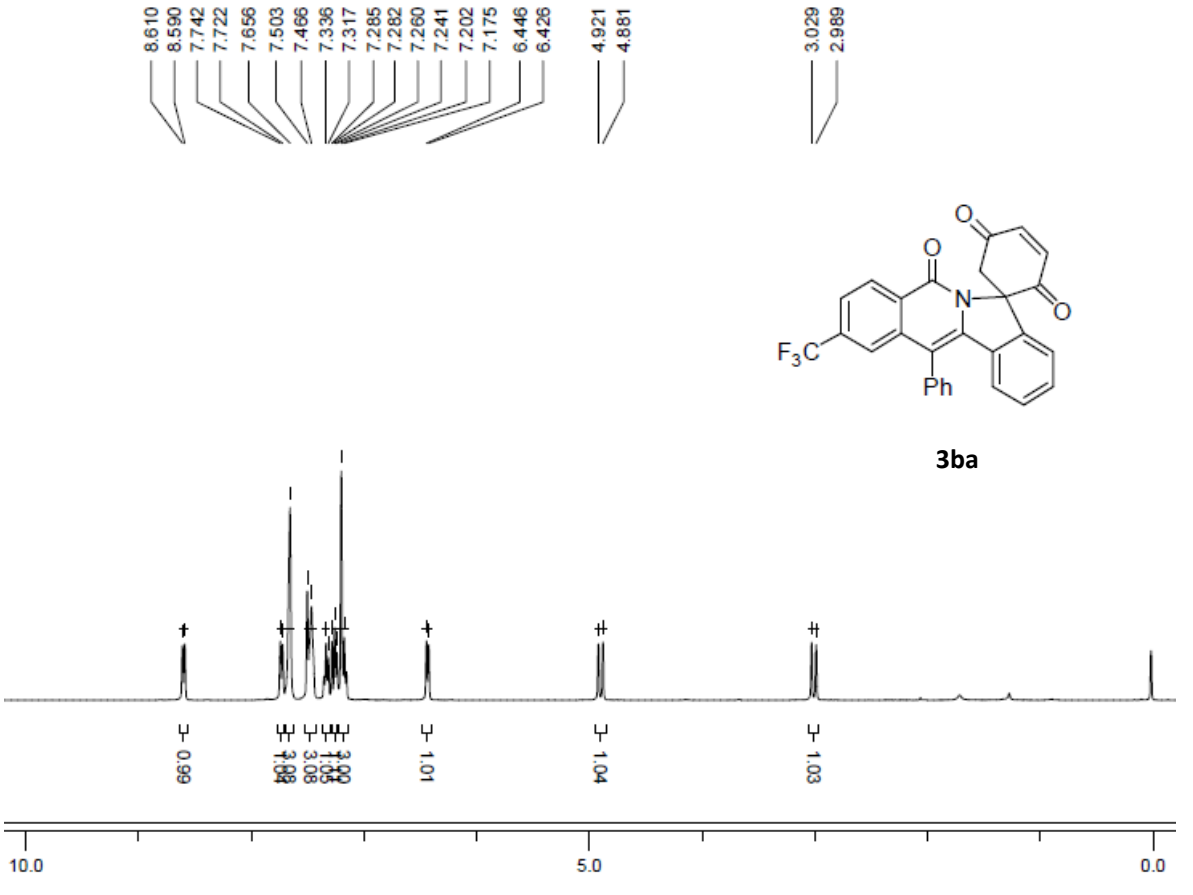
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7.175
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1.03
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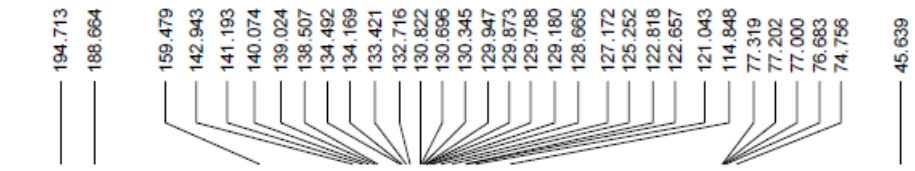
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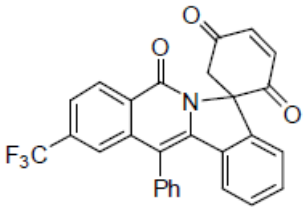
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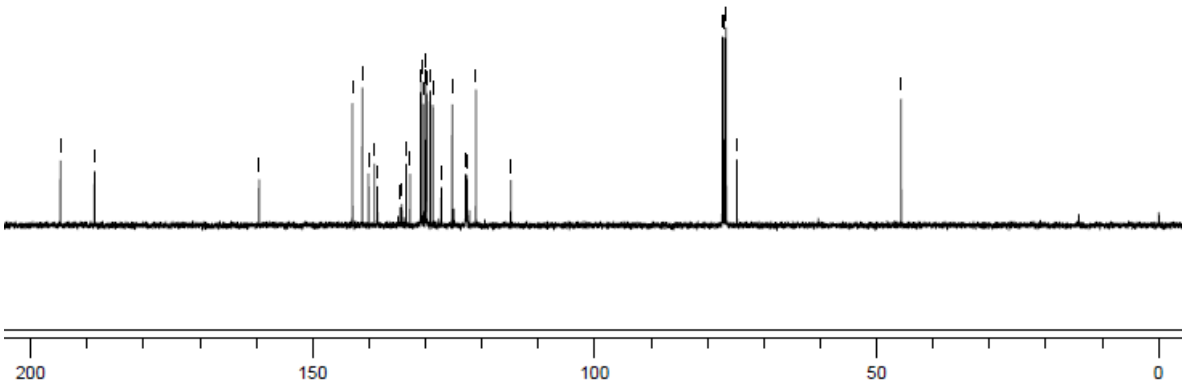
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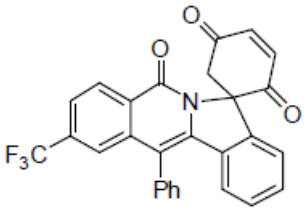
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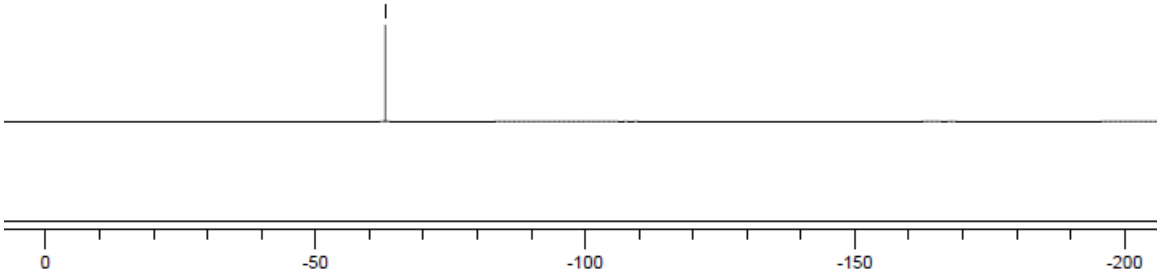
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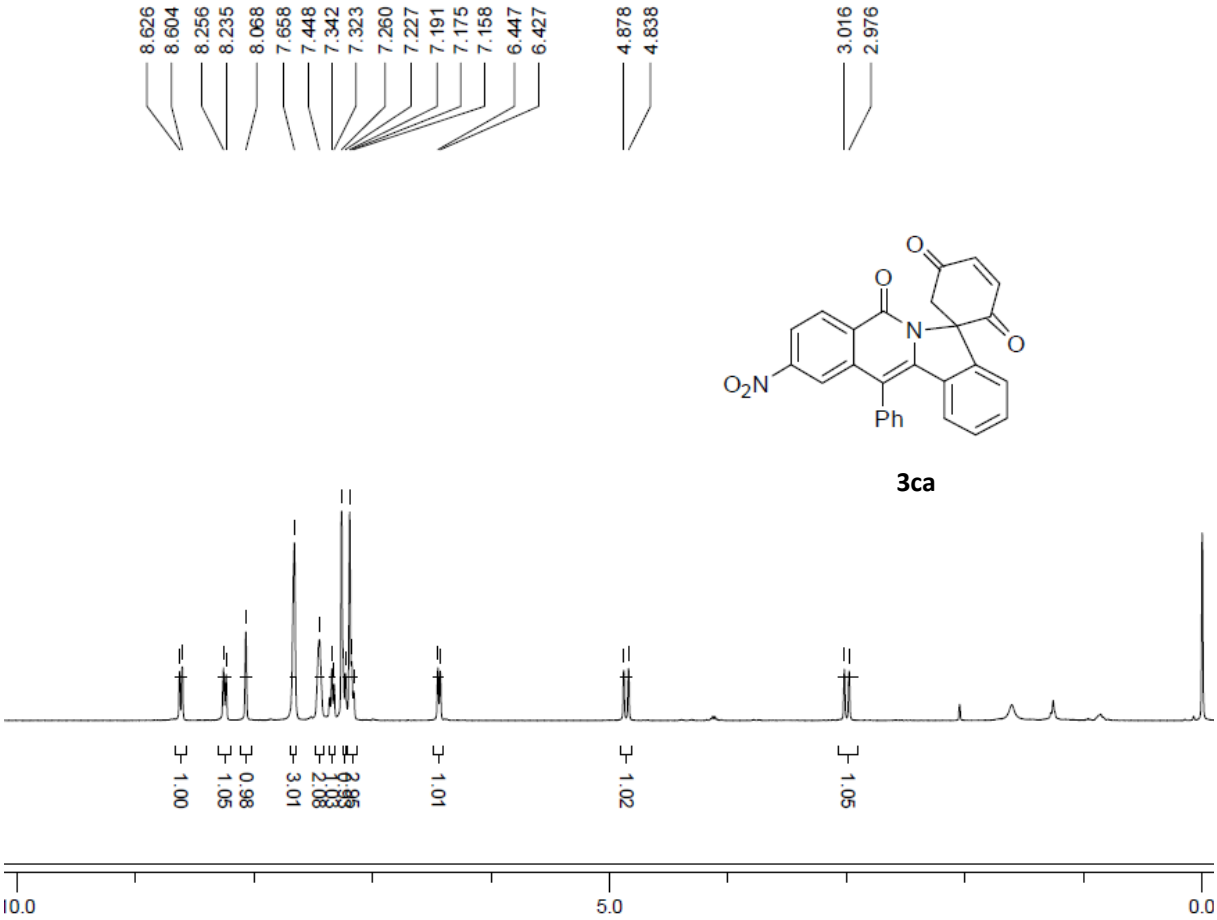
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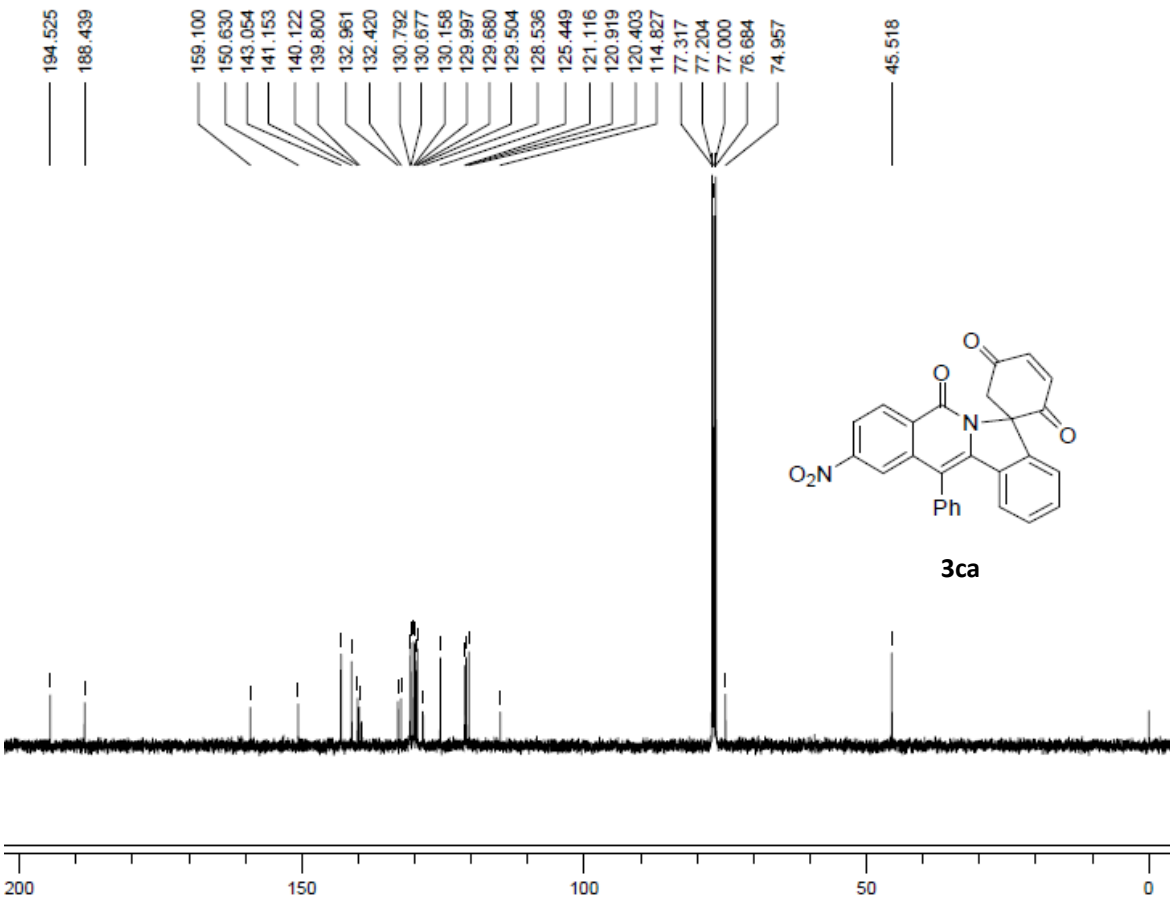
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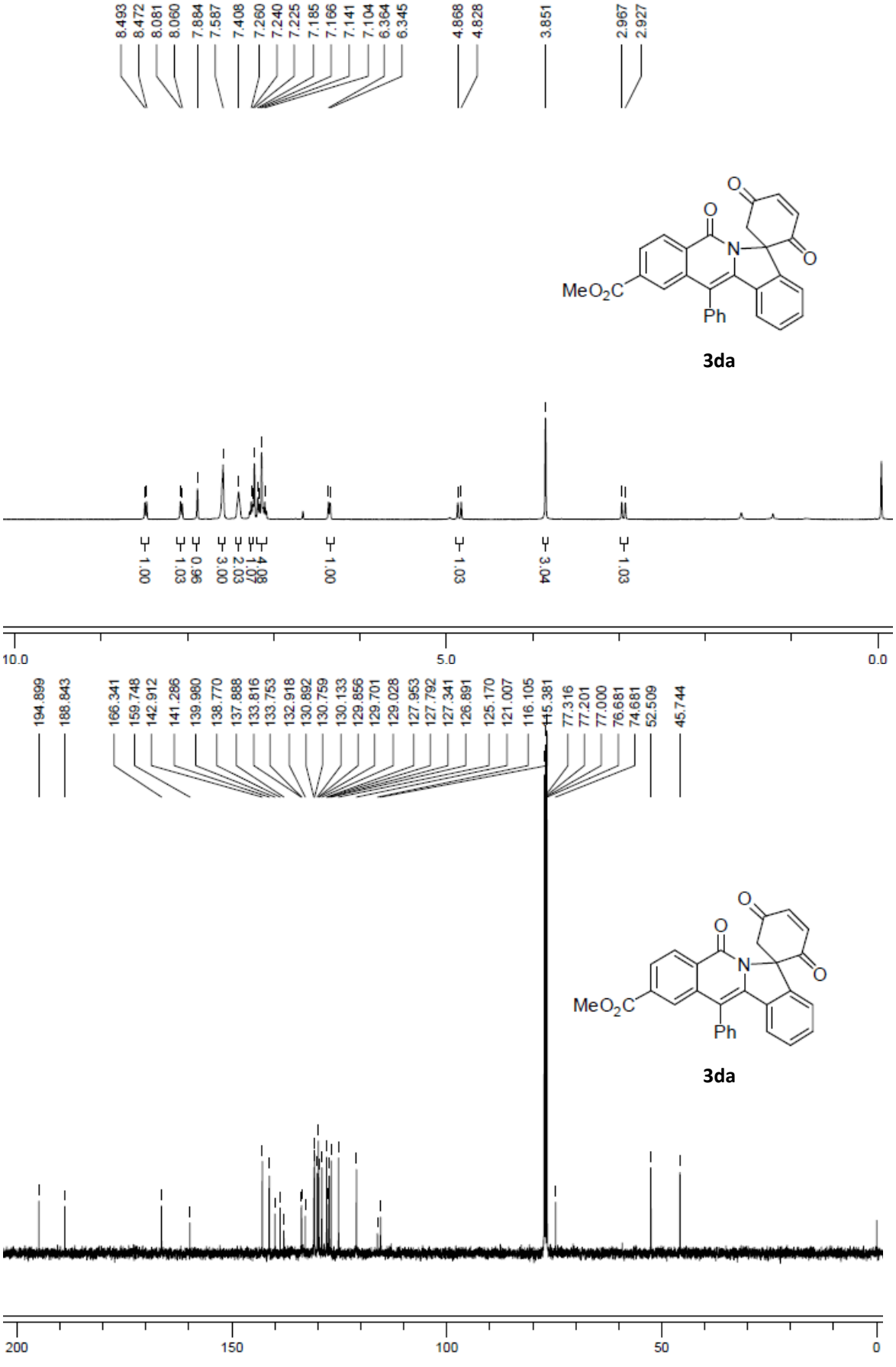
**3ca**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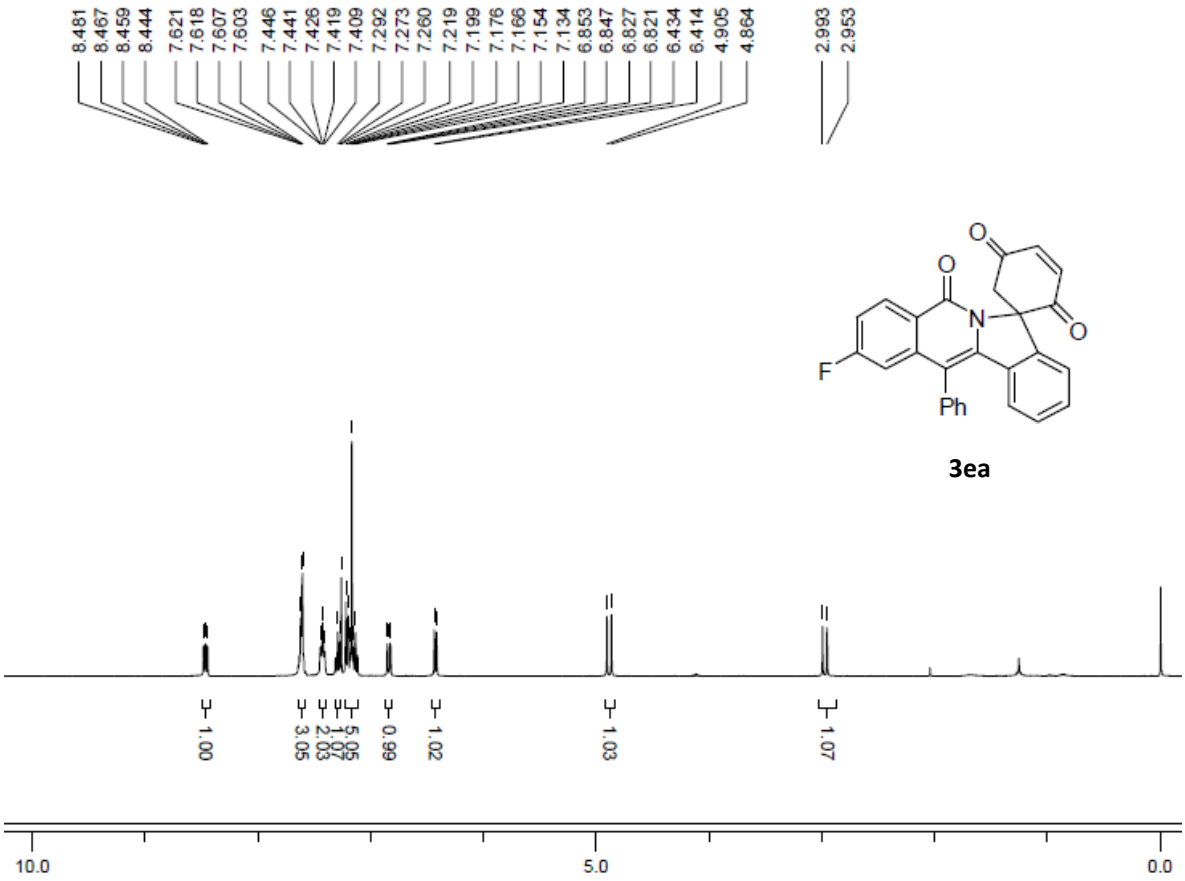
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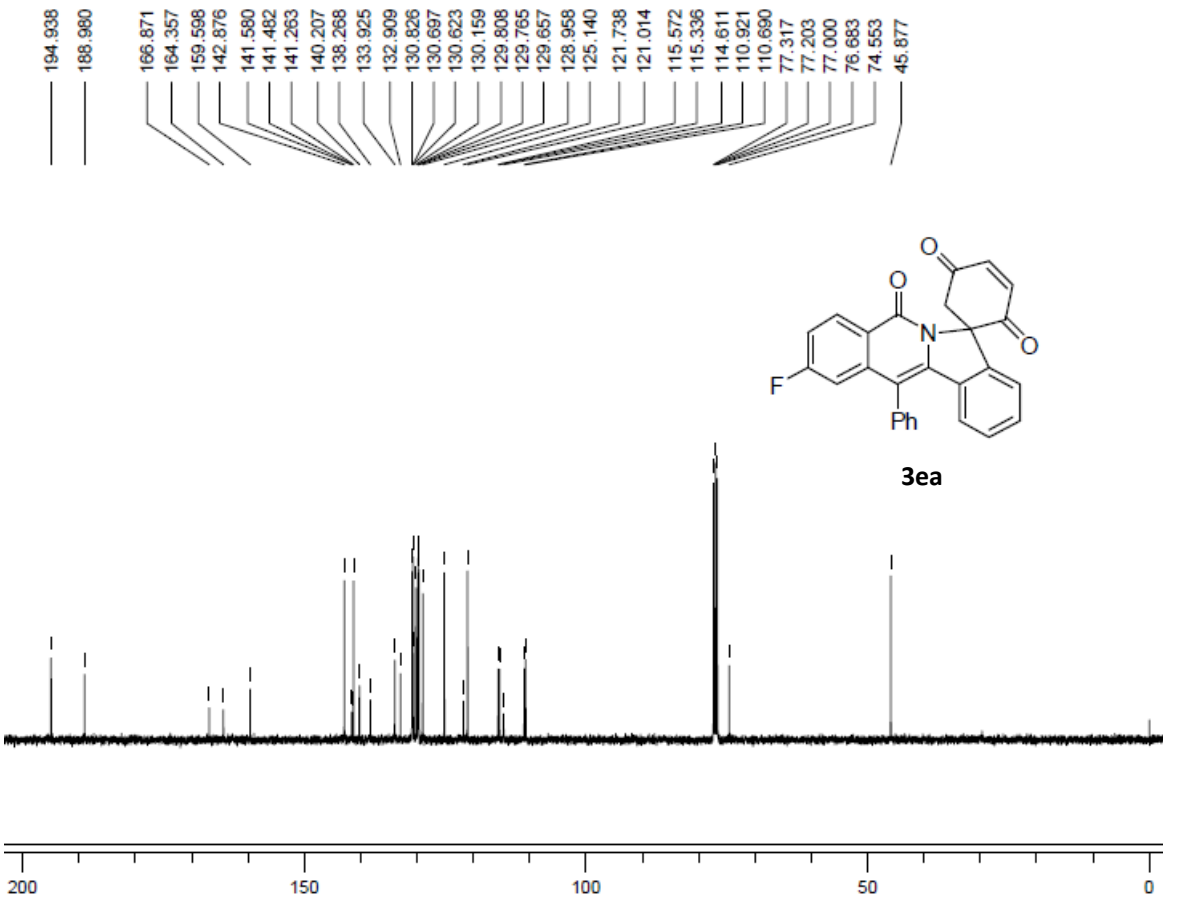
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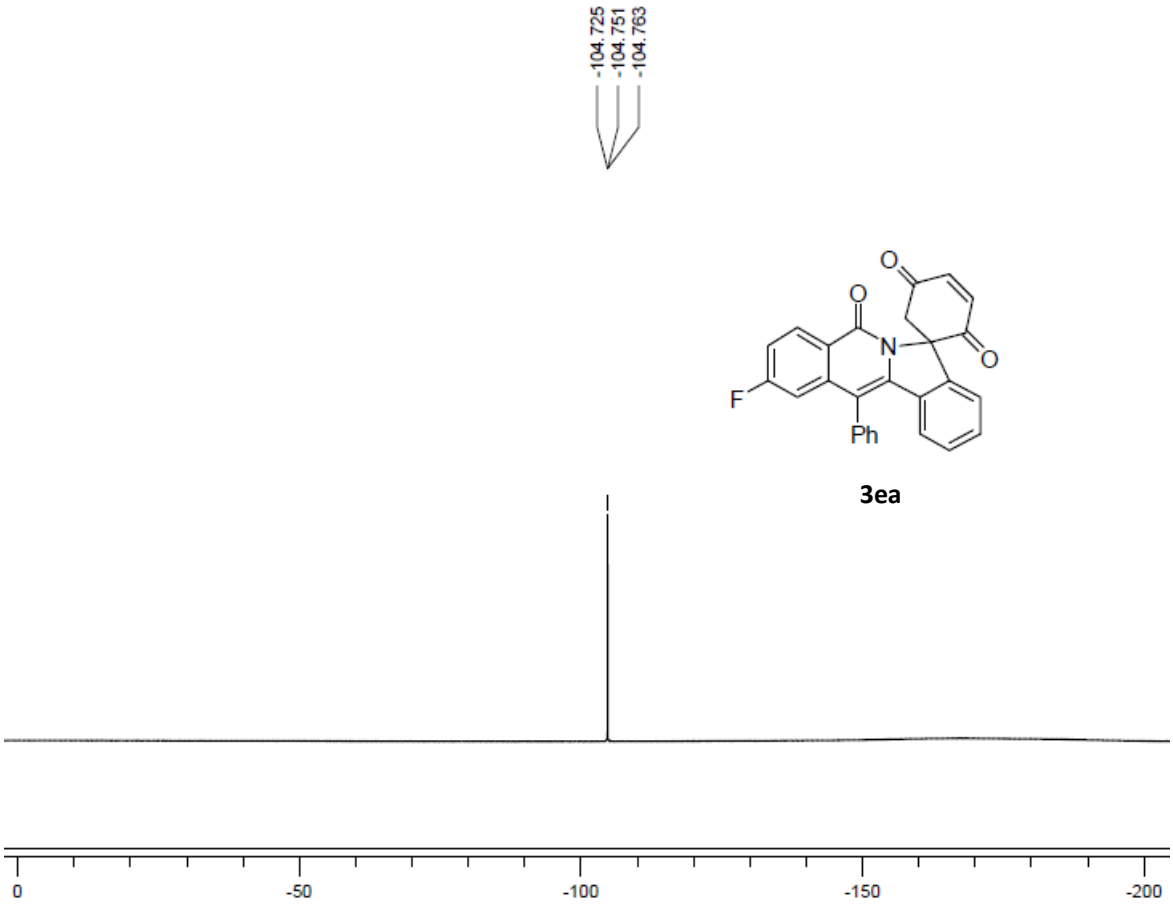
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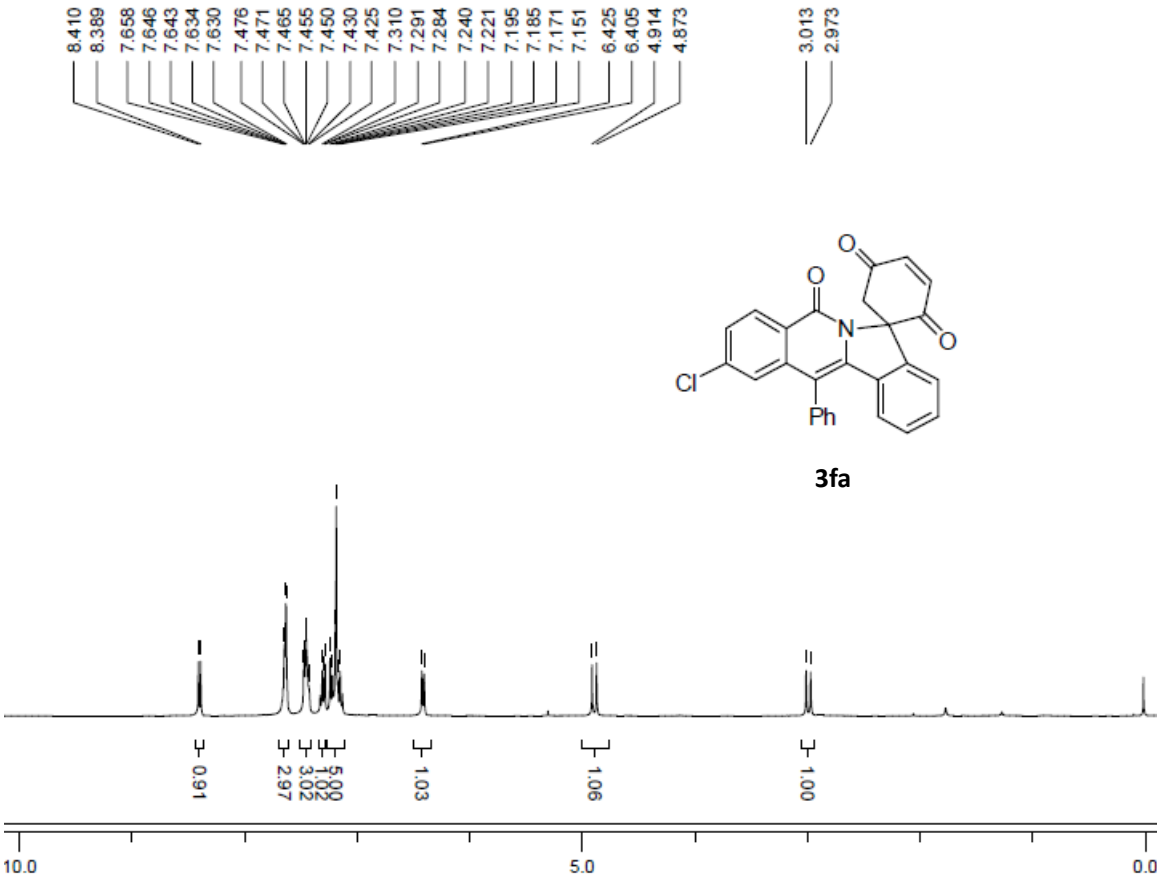
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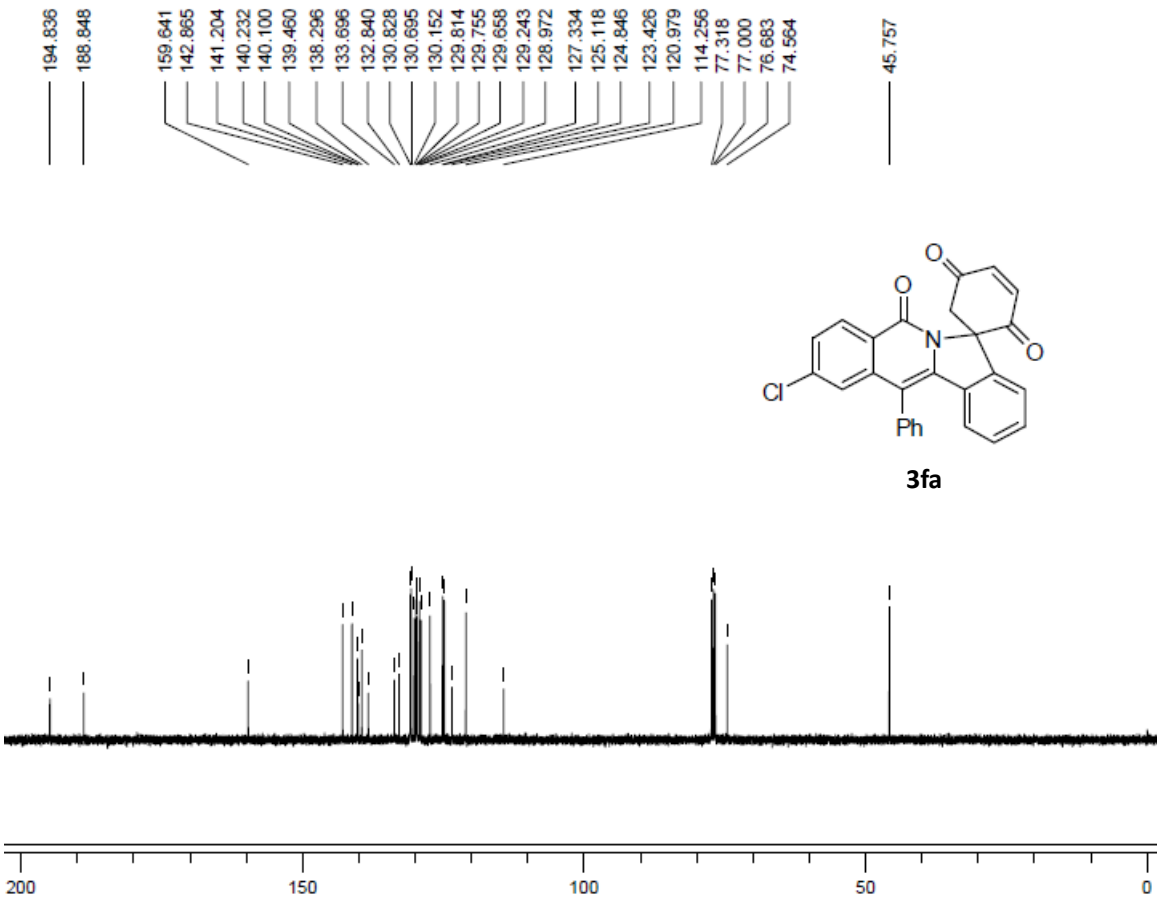
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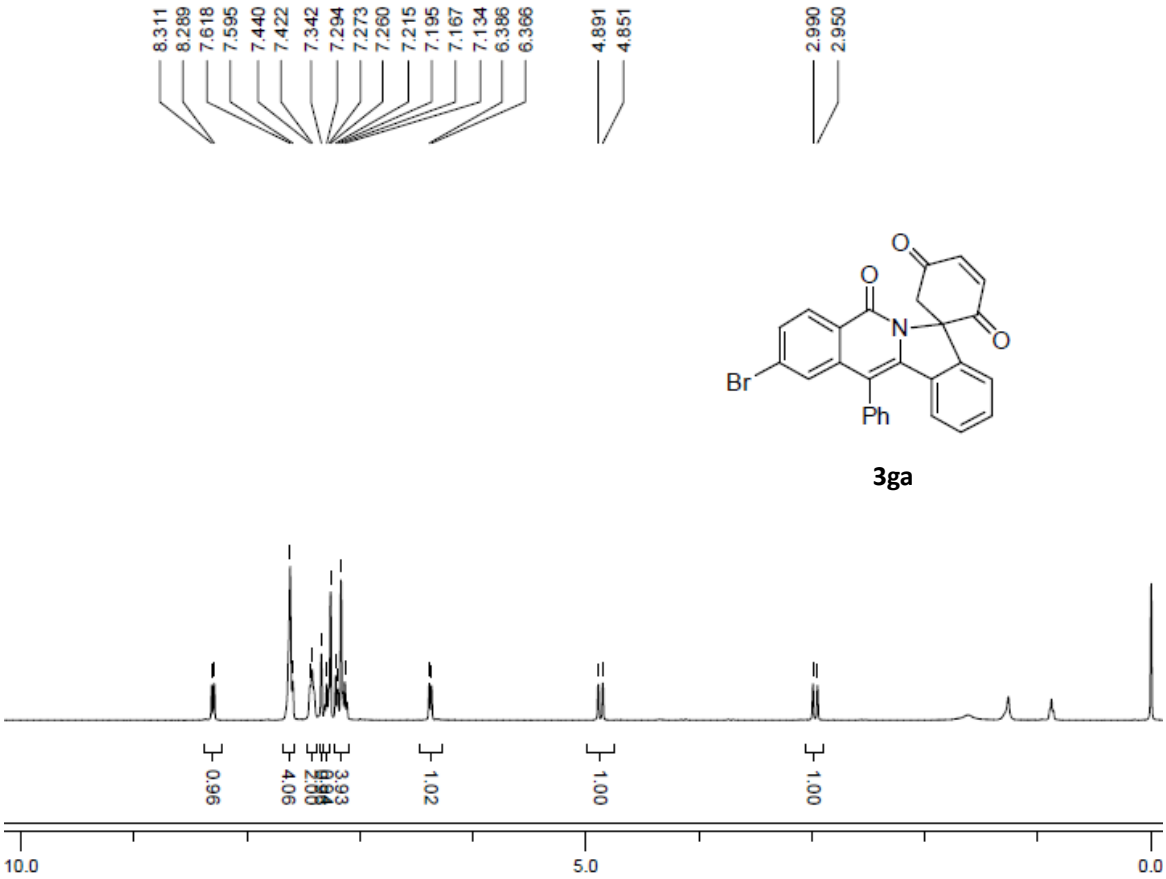
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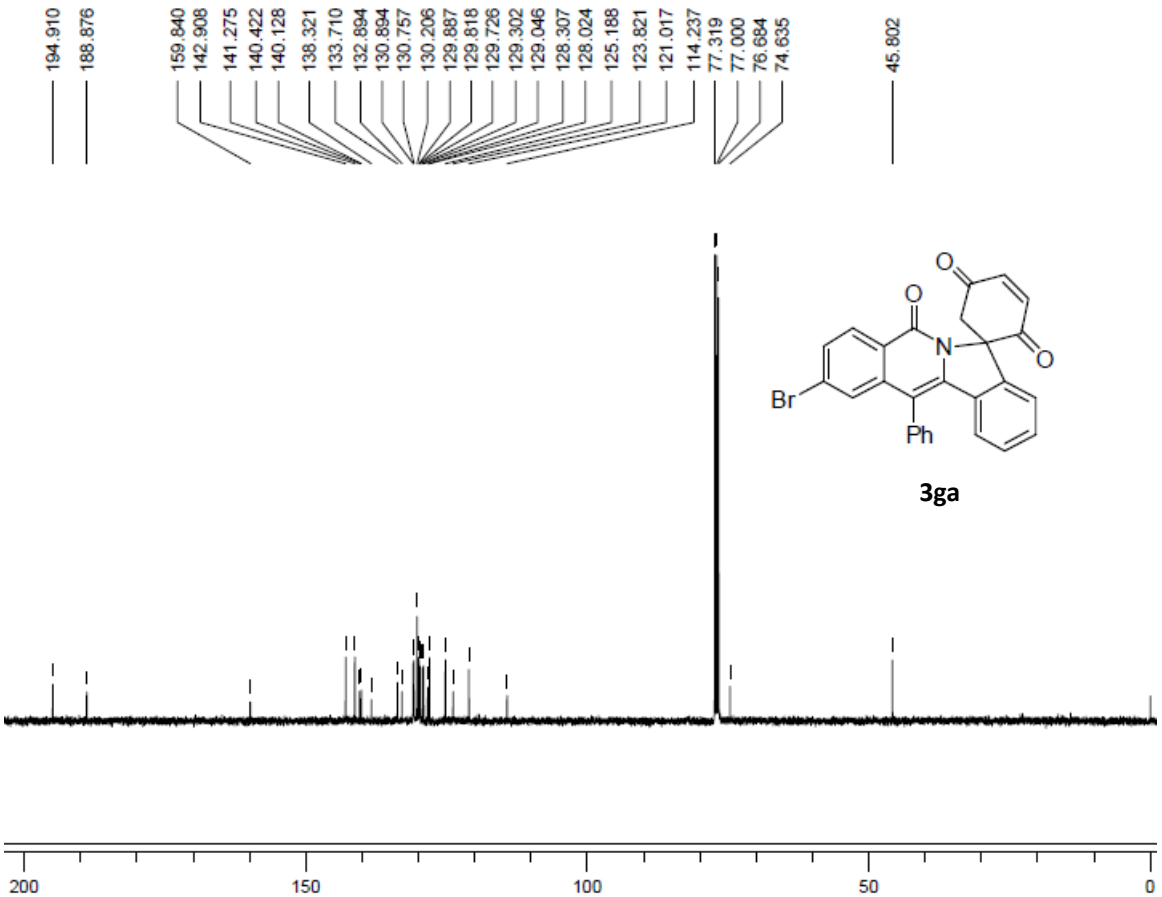
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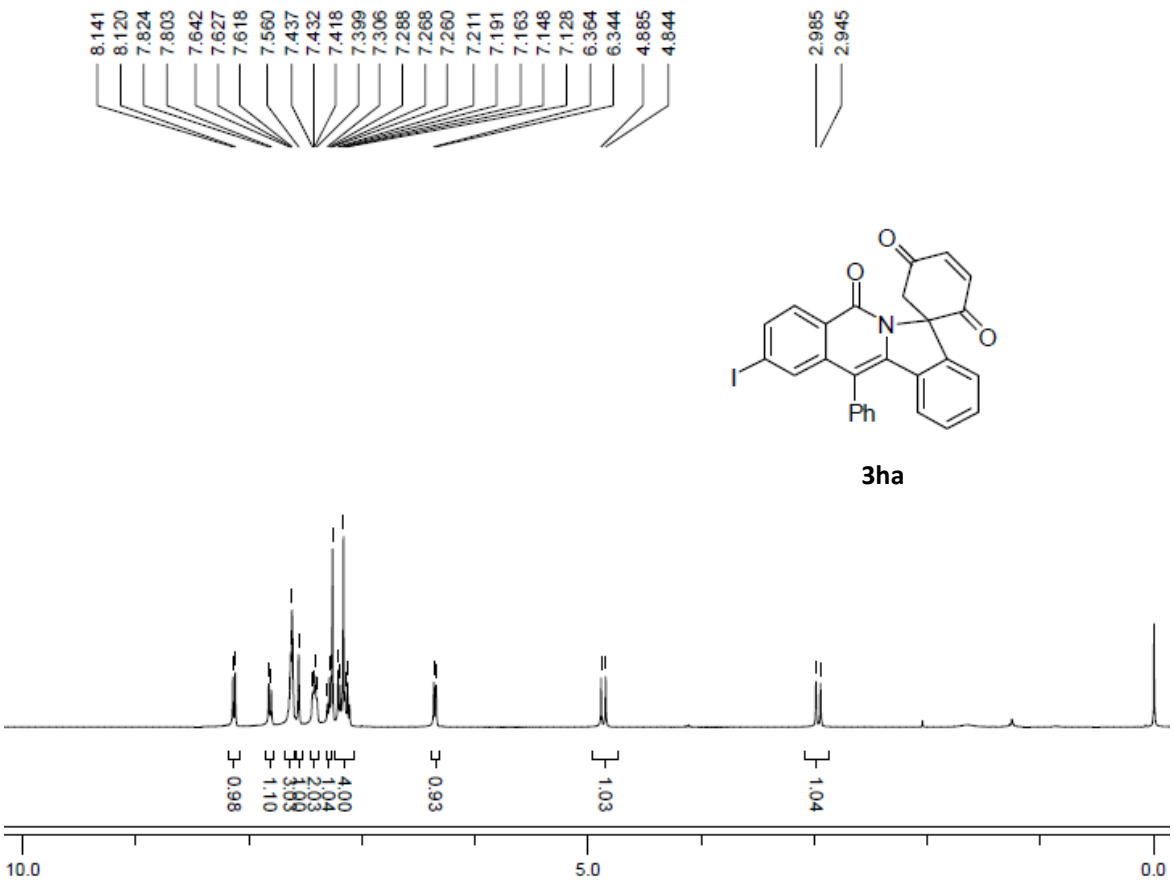
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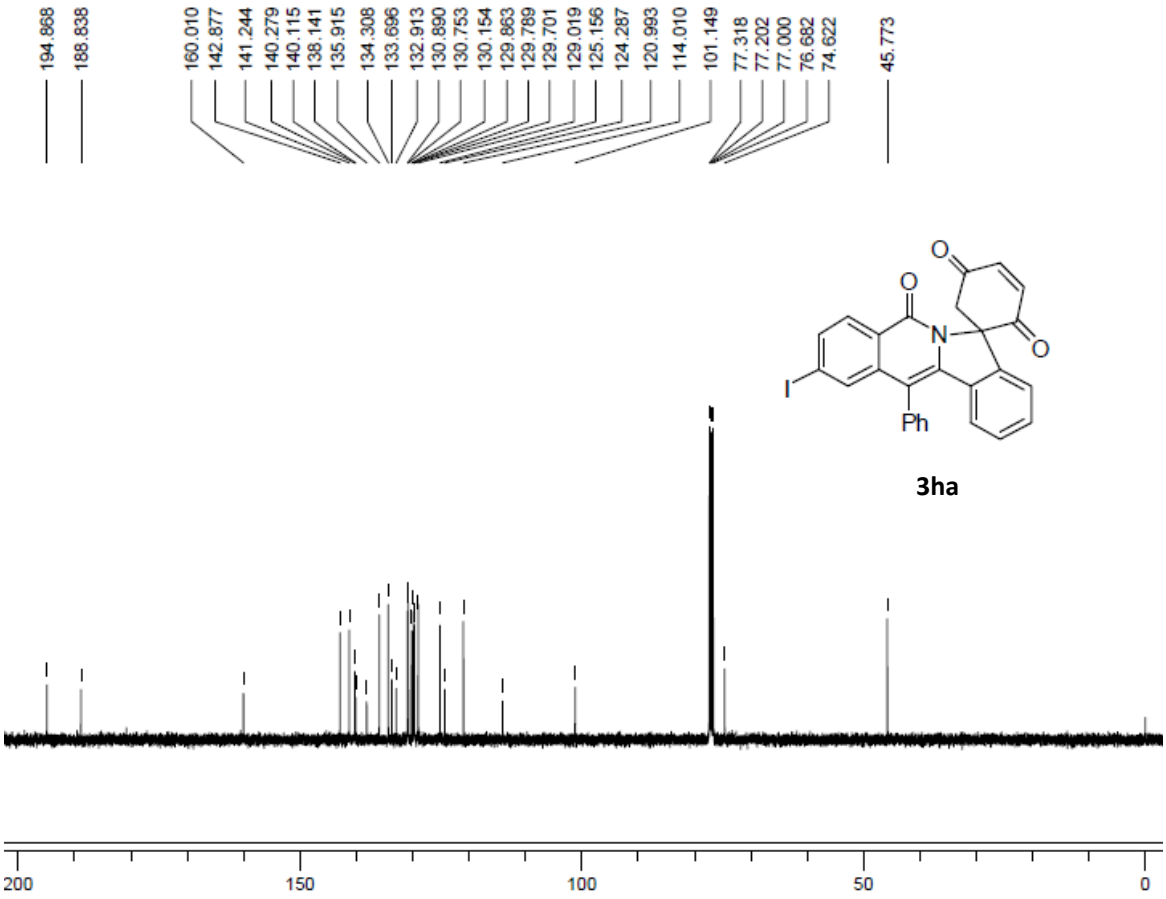
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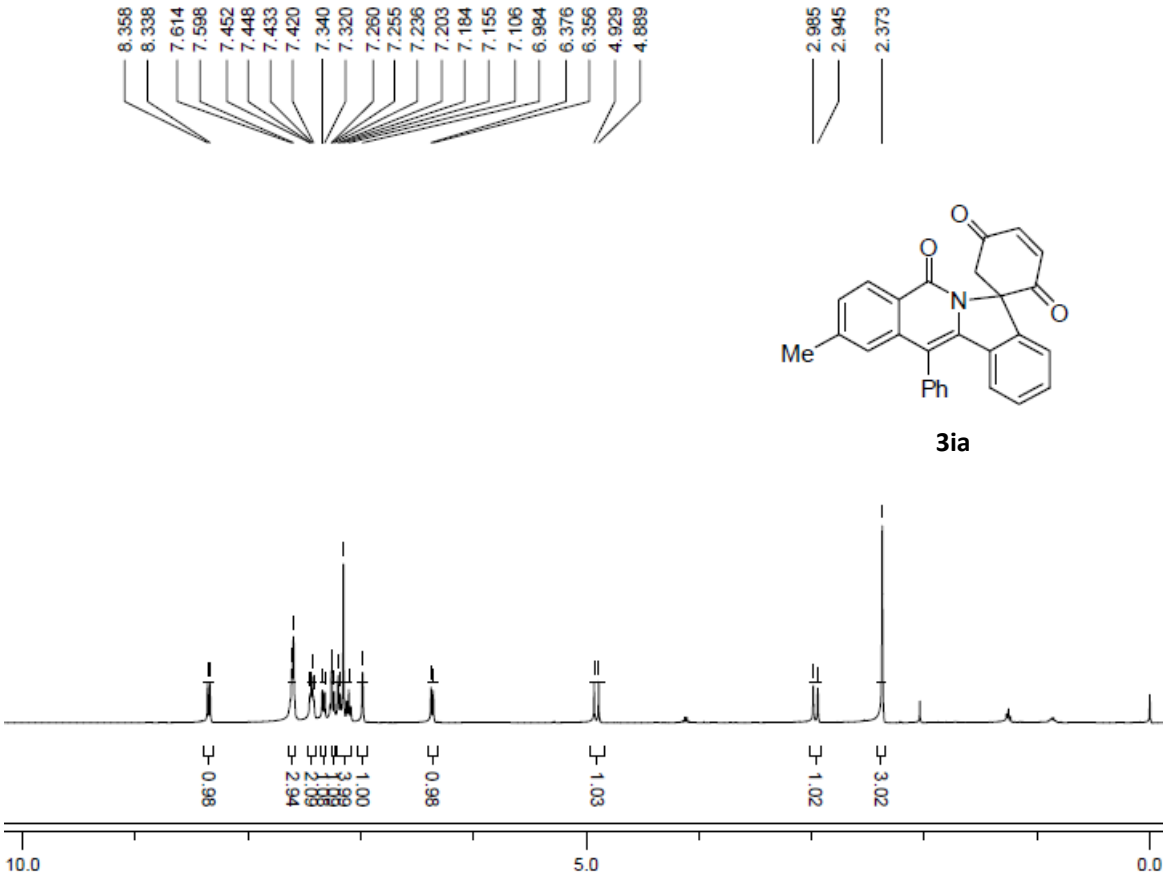
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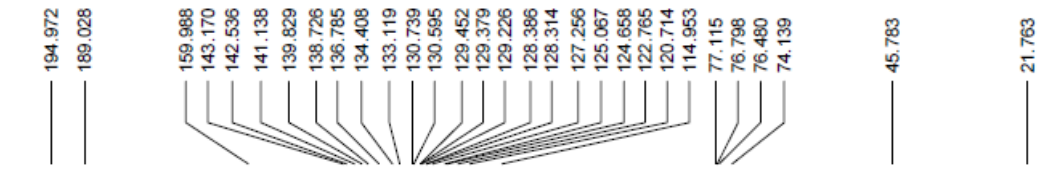
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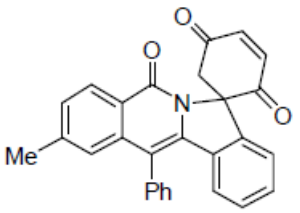
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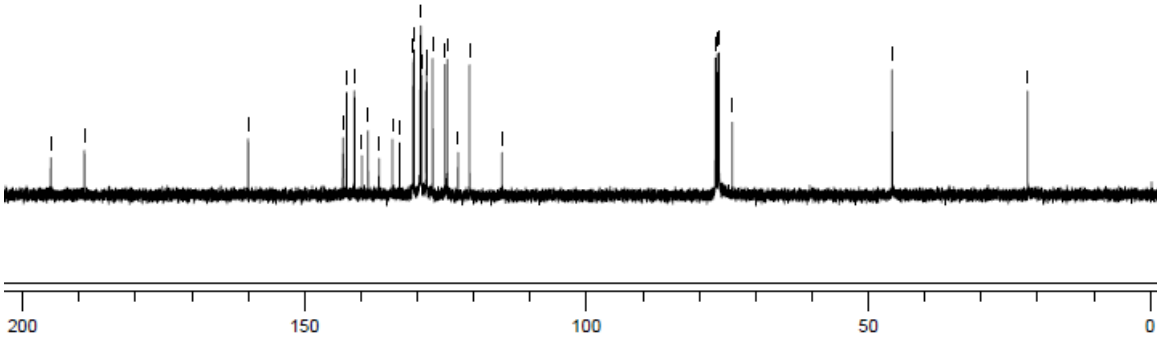
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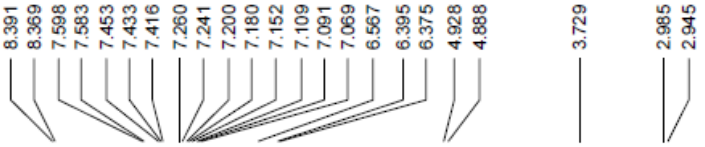
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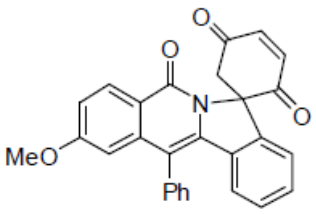
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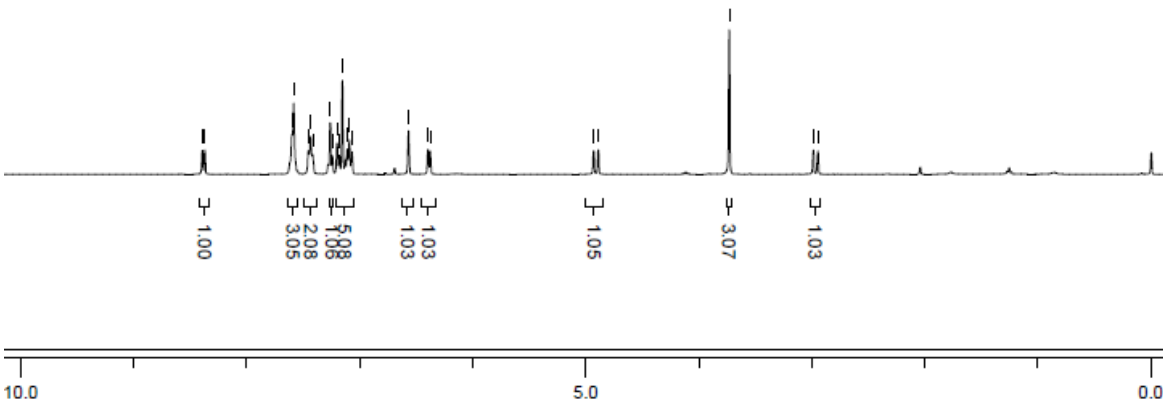
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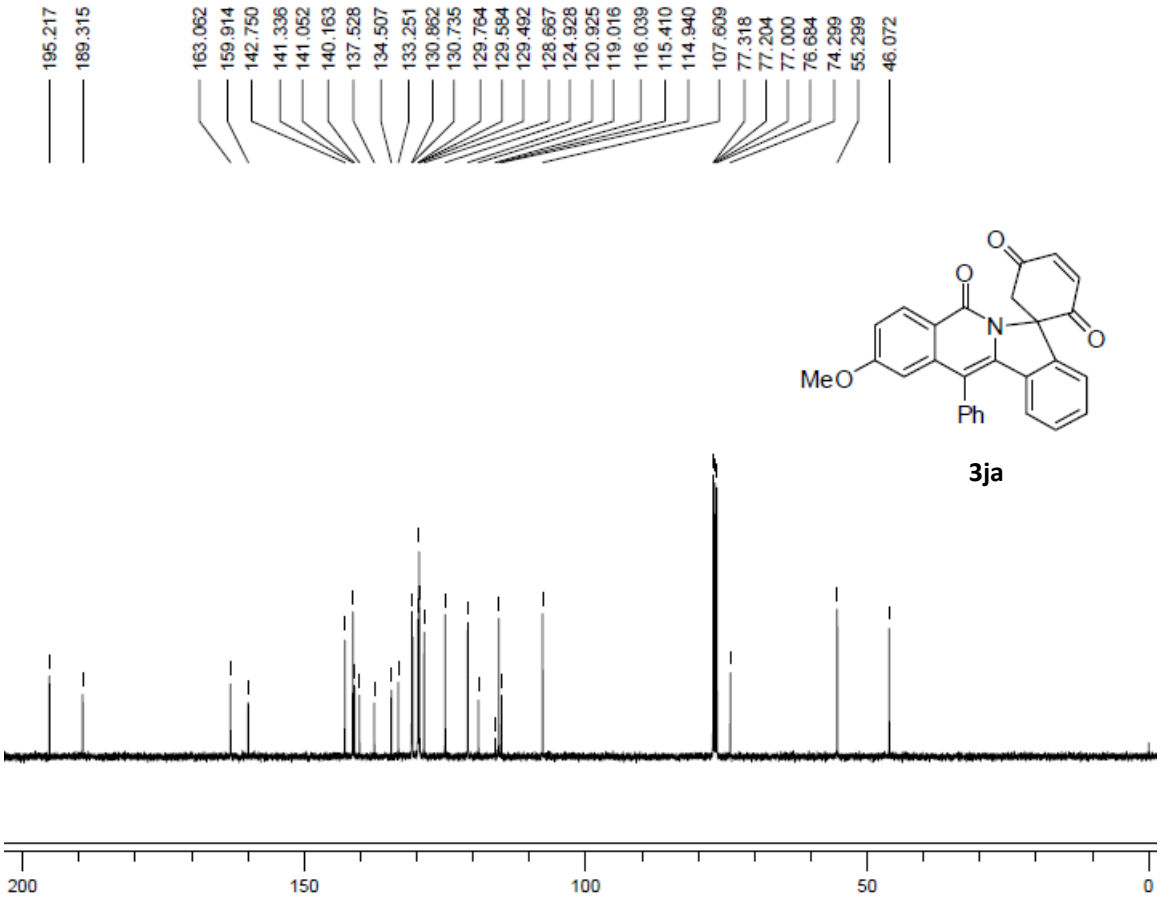
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Ph
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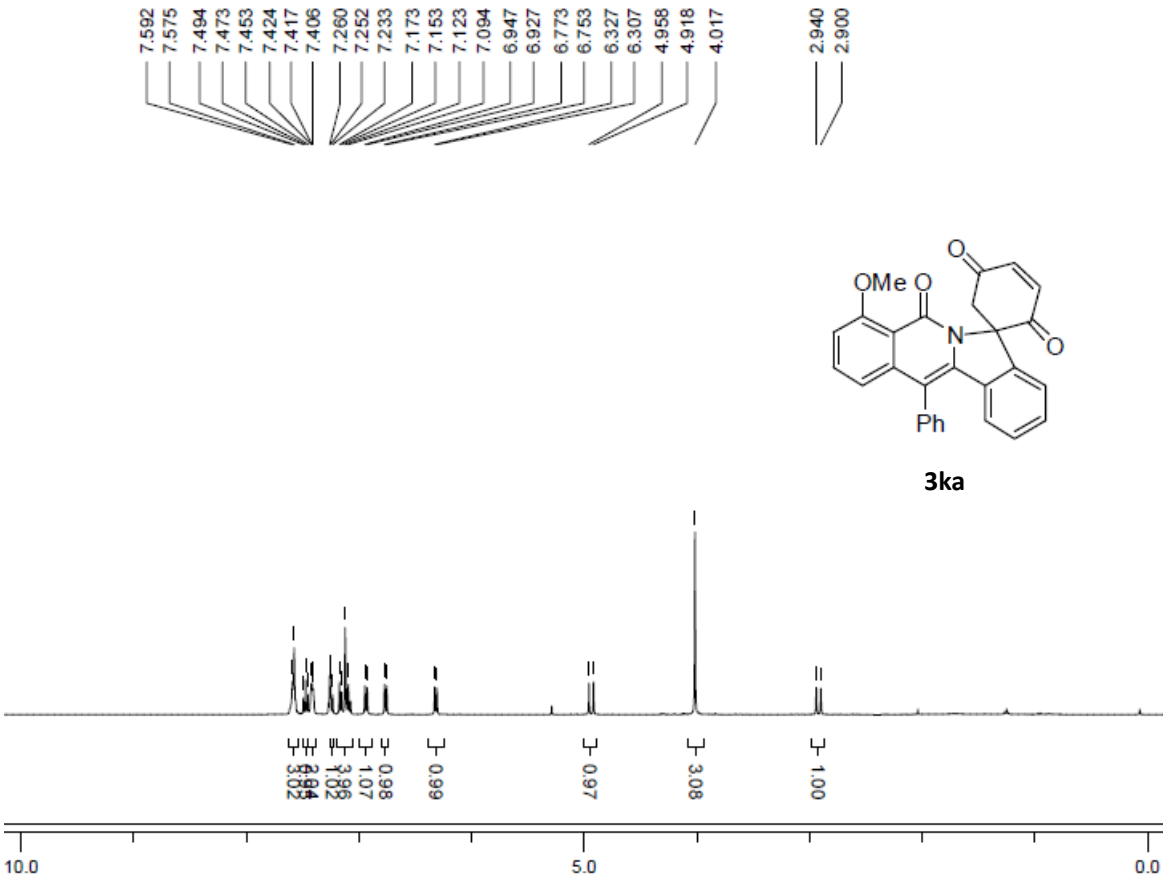
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2.900
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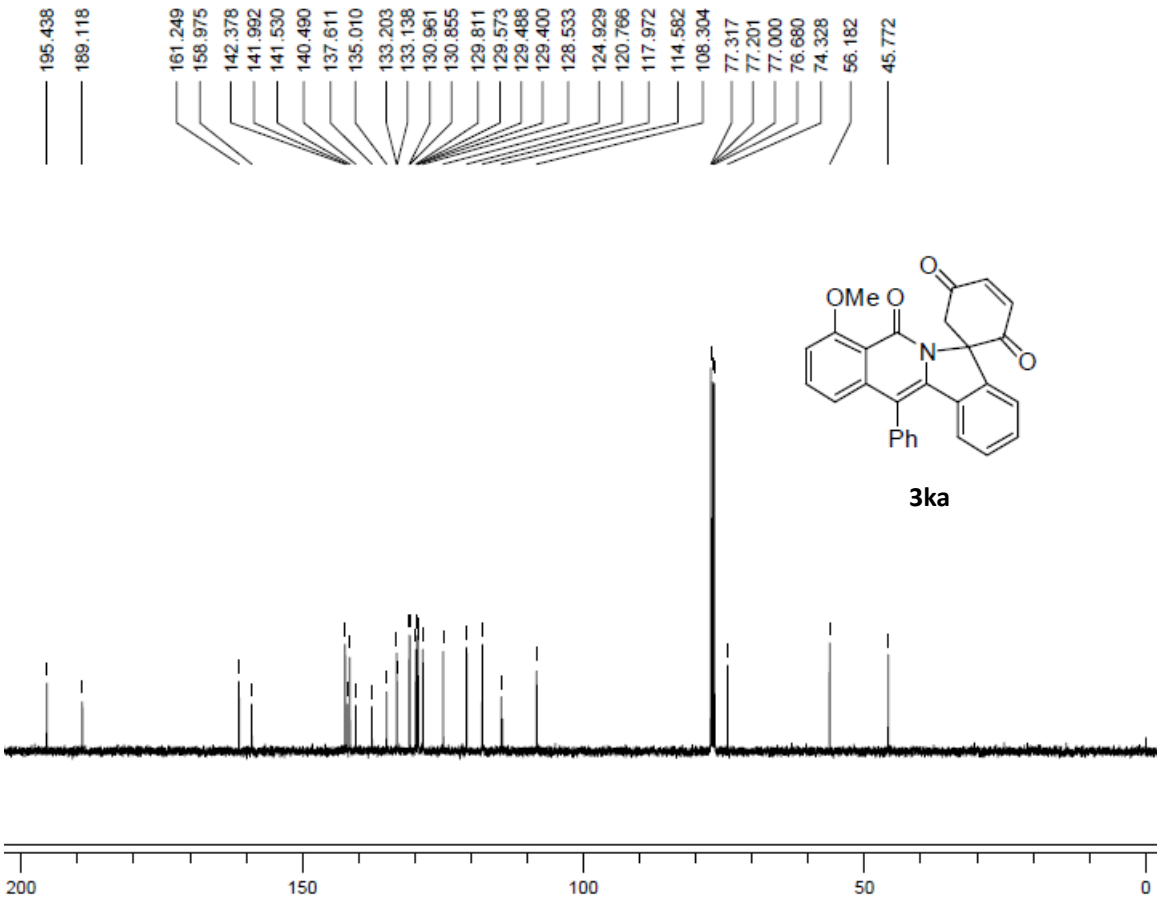
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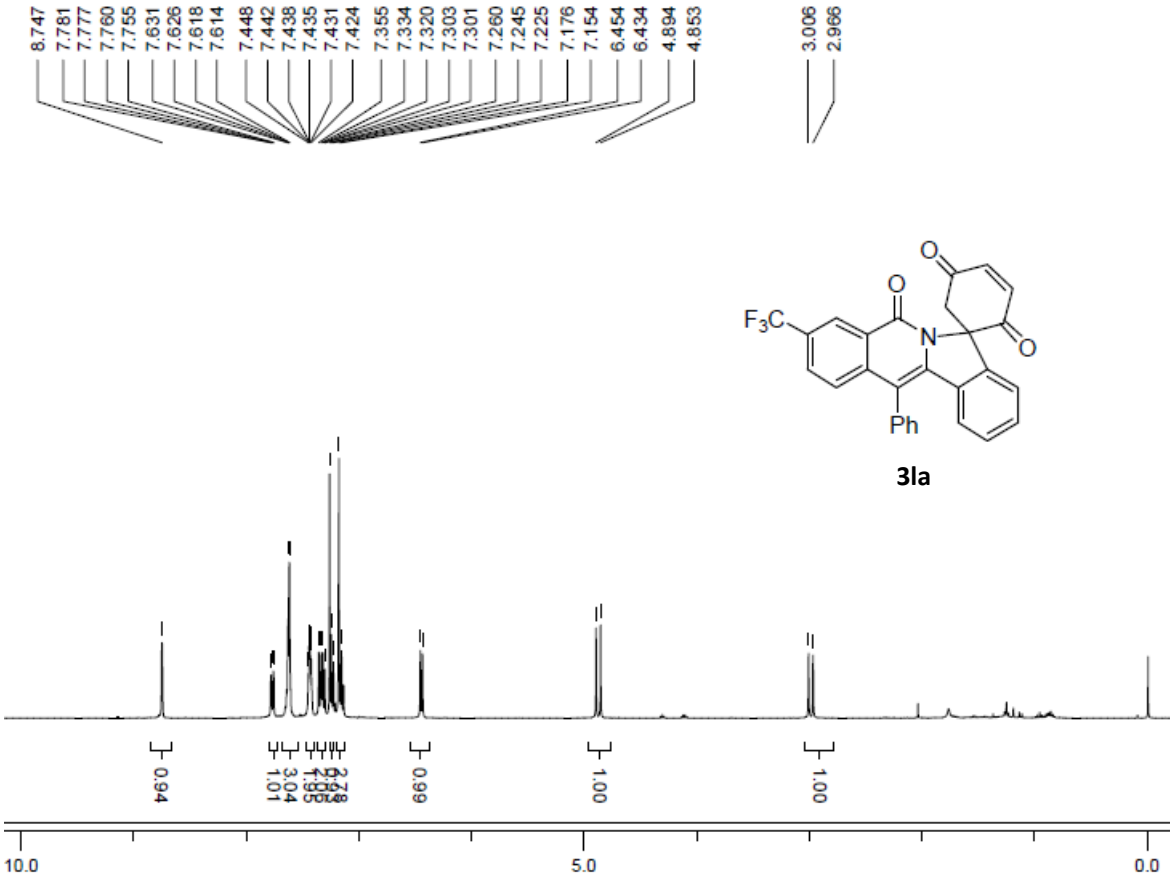
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7.245
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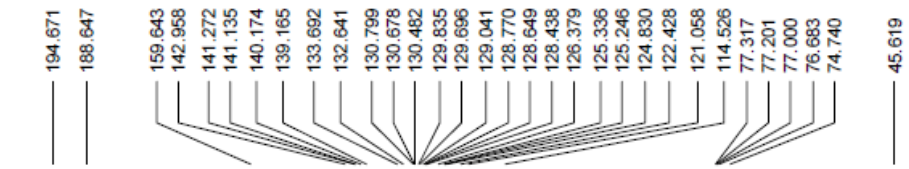
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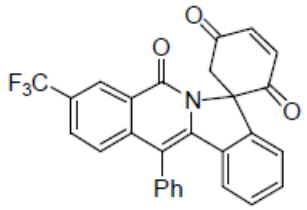
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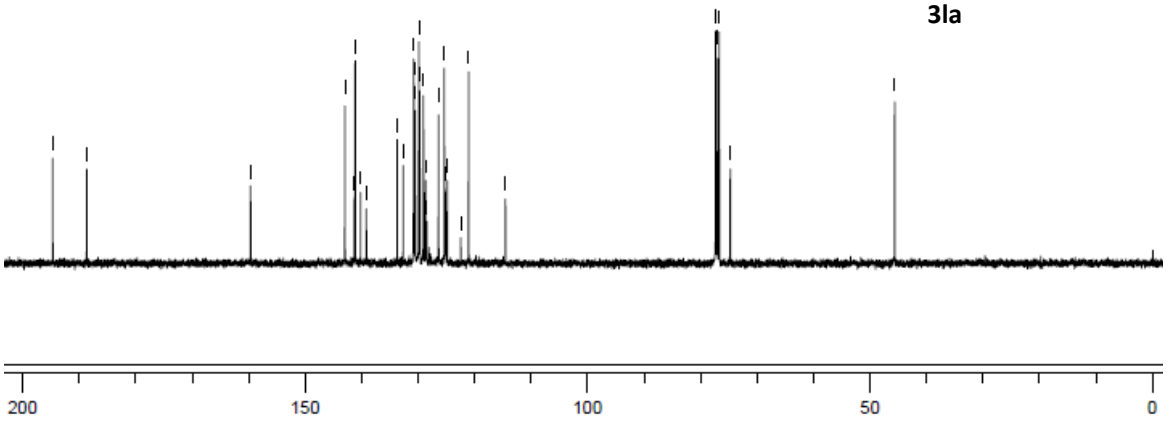
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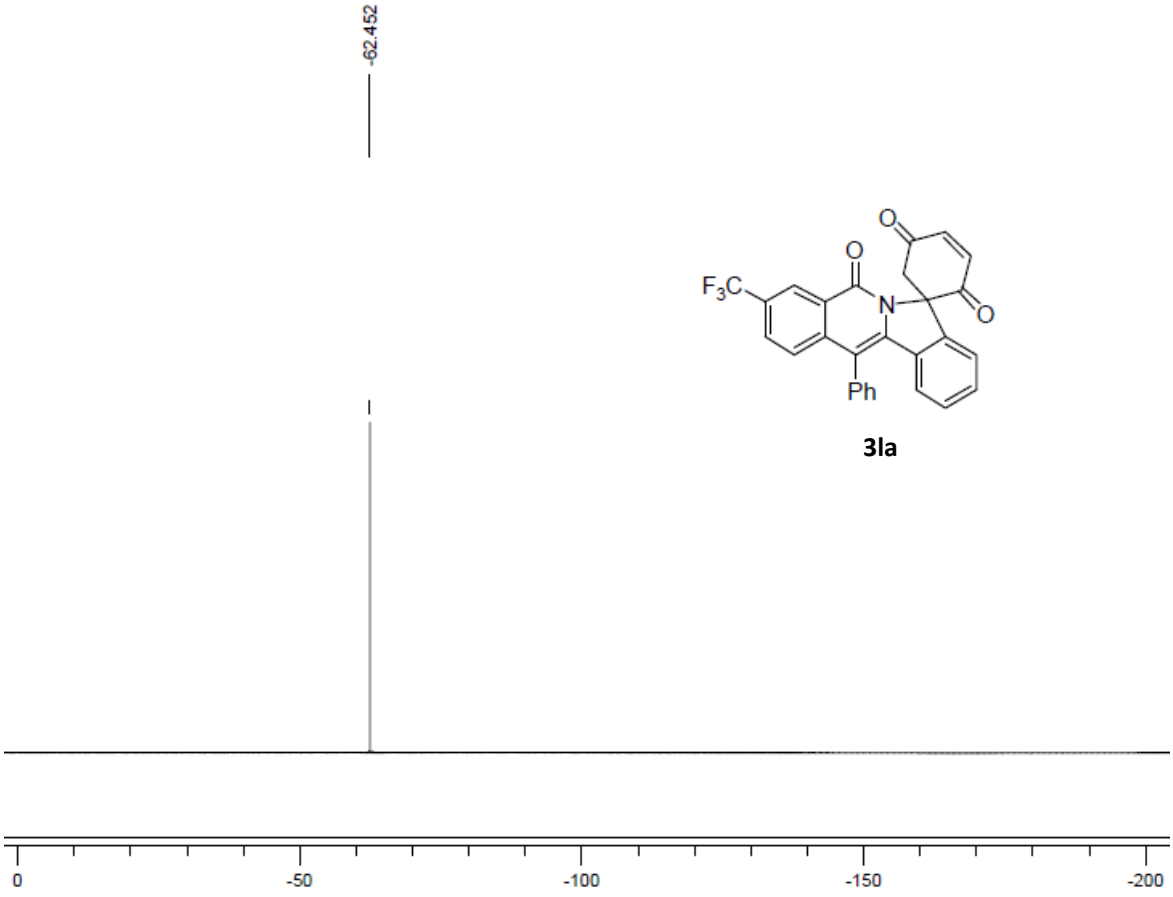
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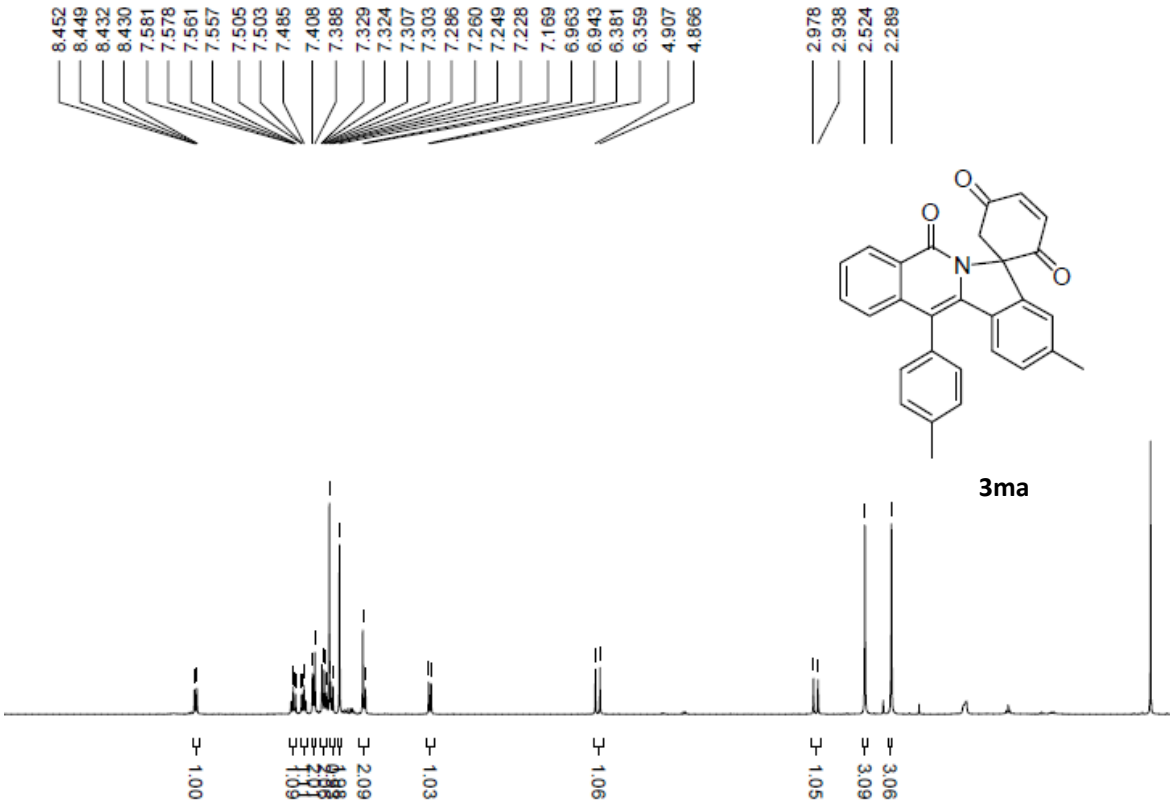
**3la**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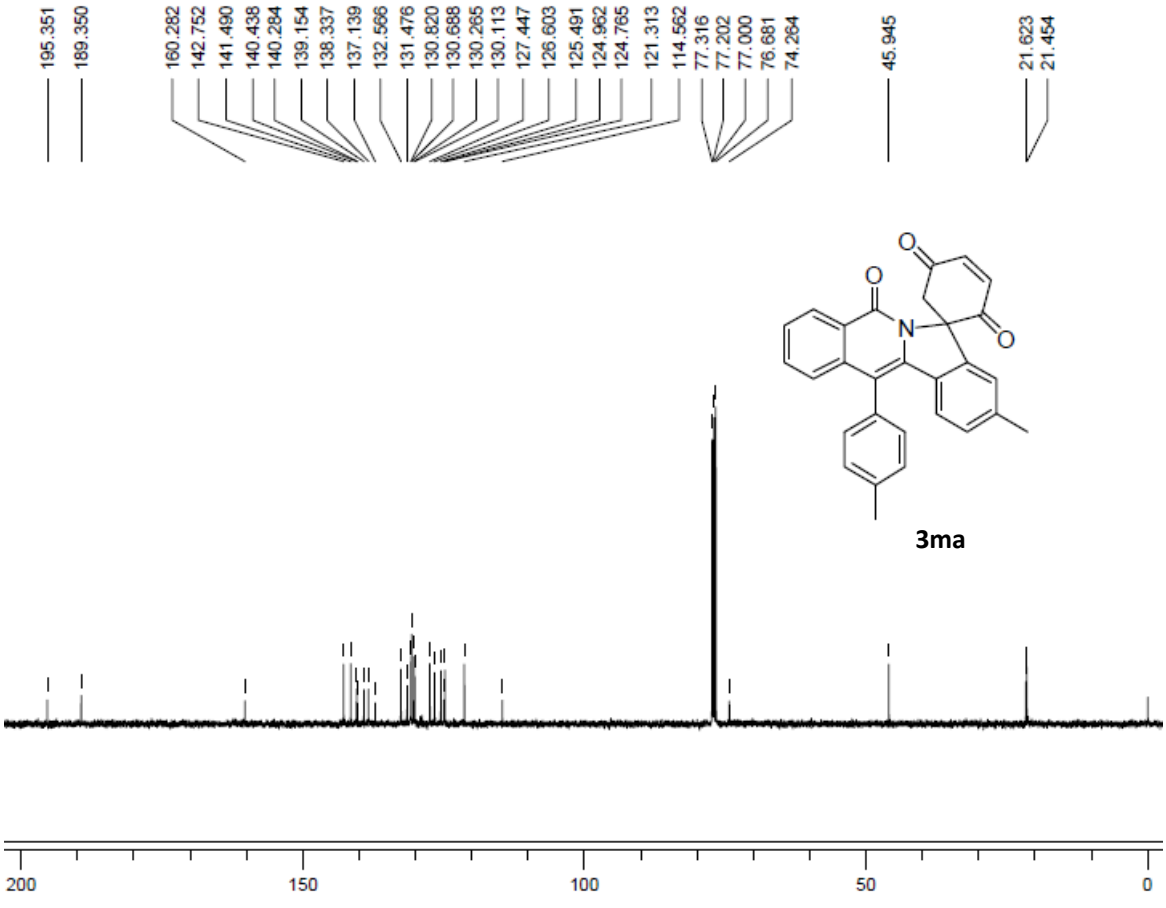
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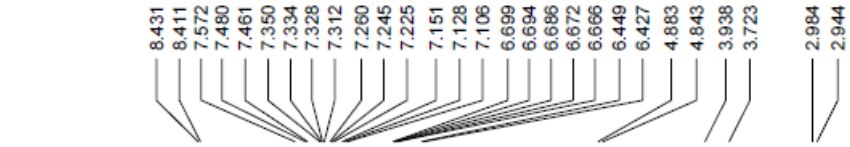
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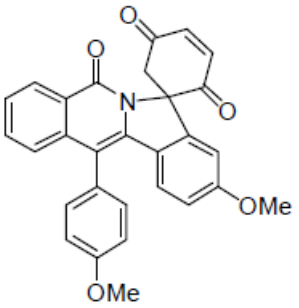
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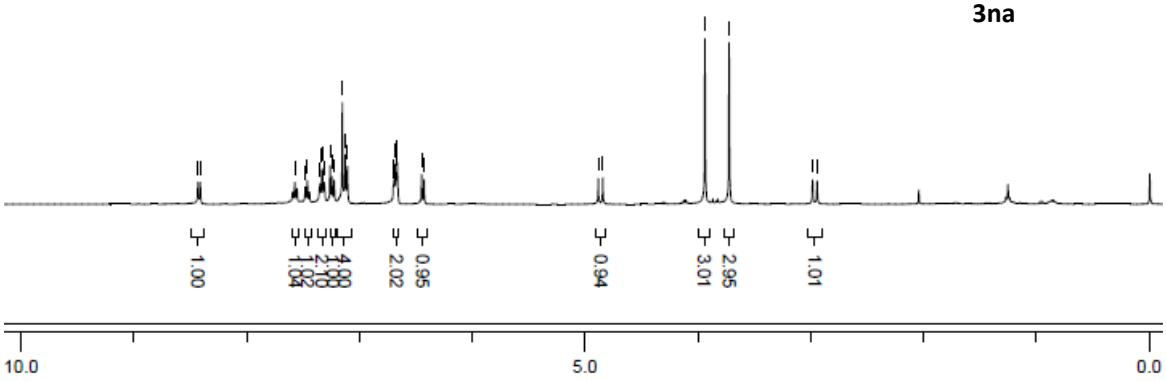
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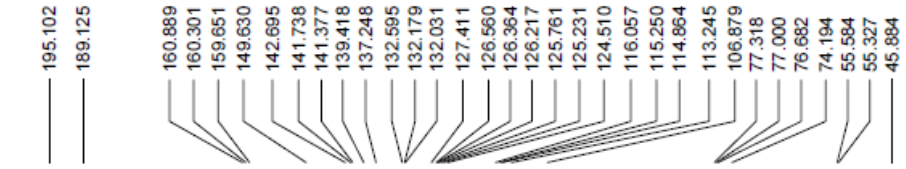
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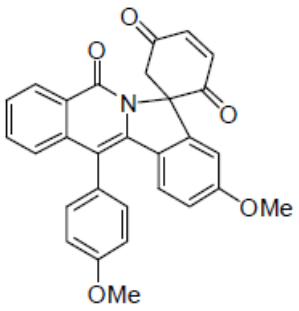
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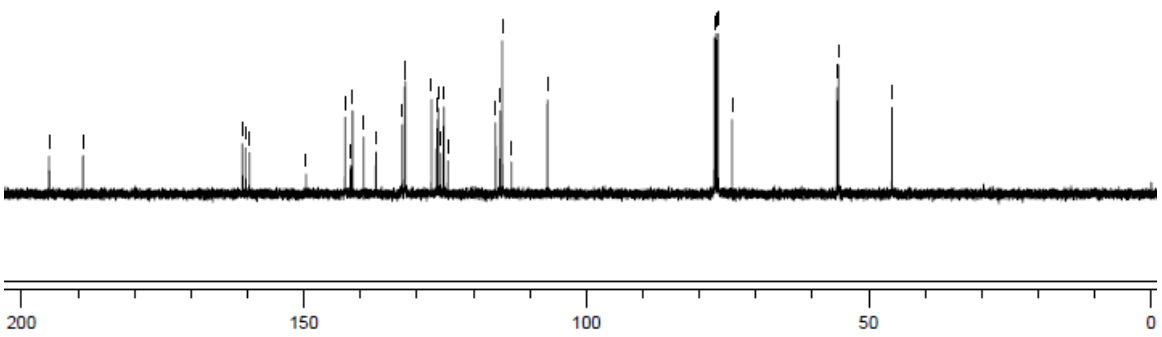
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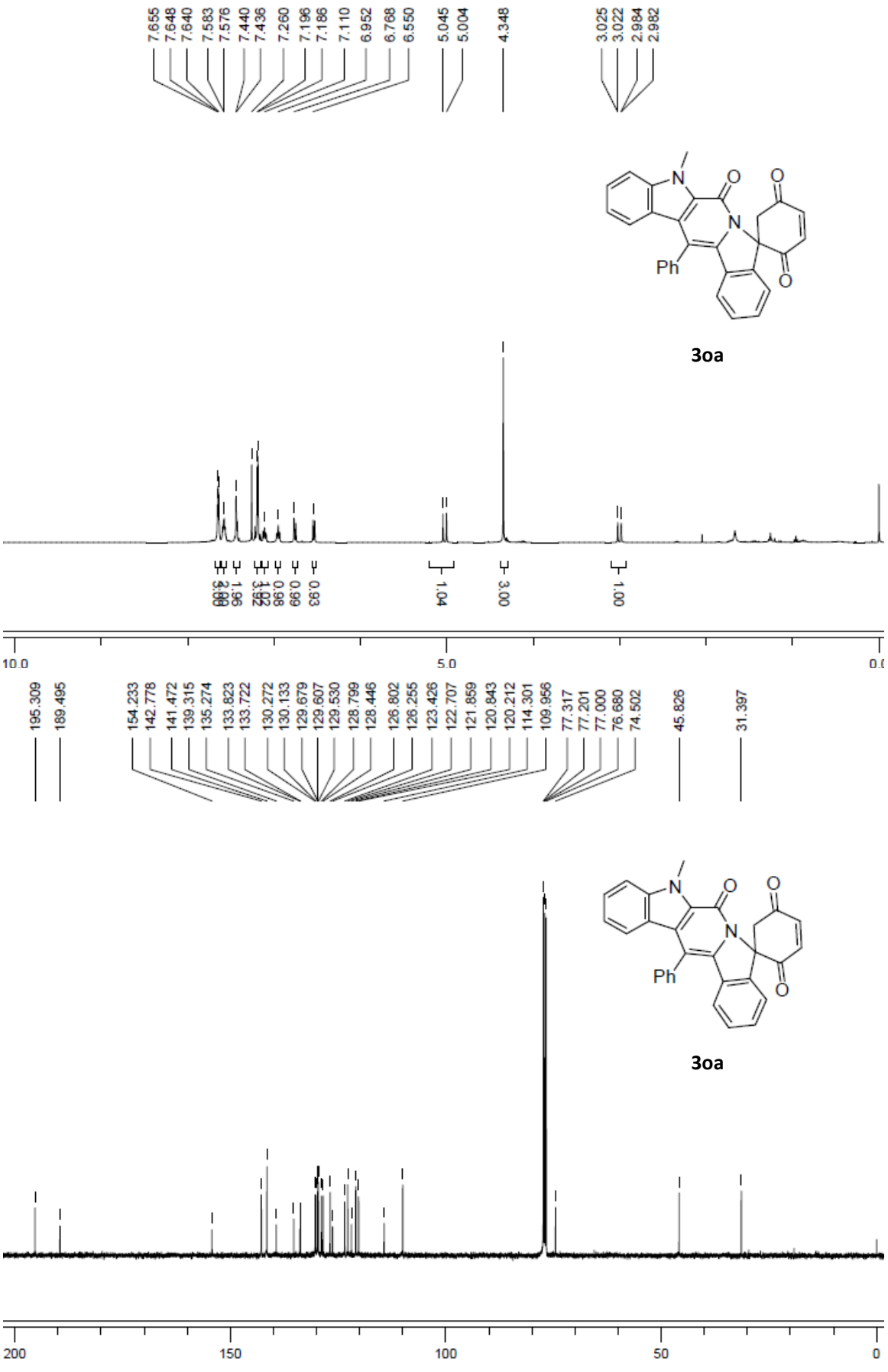
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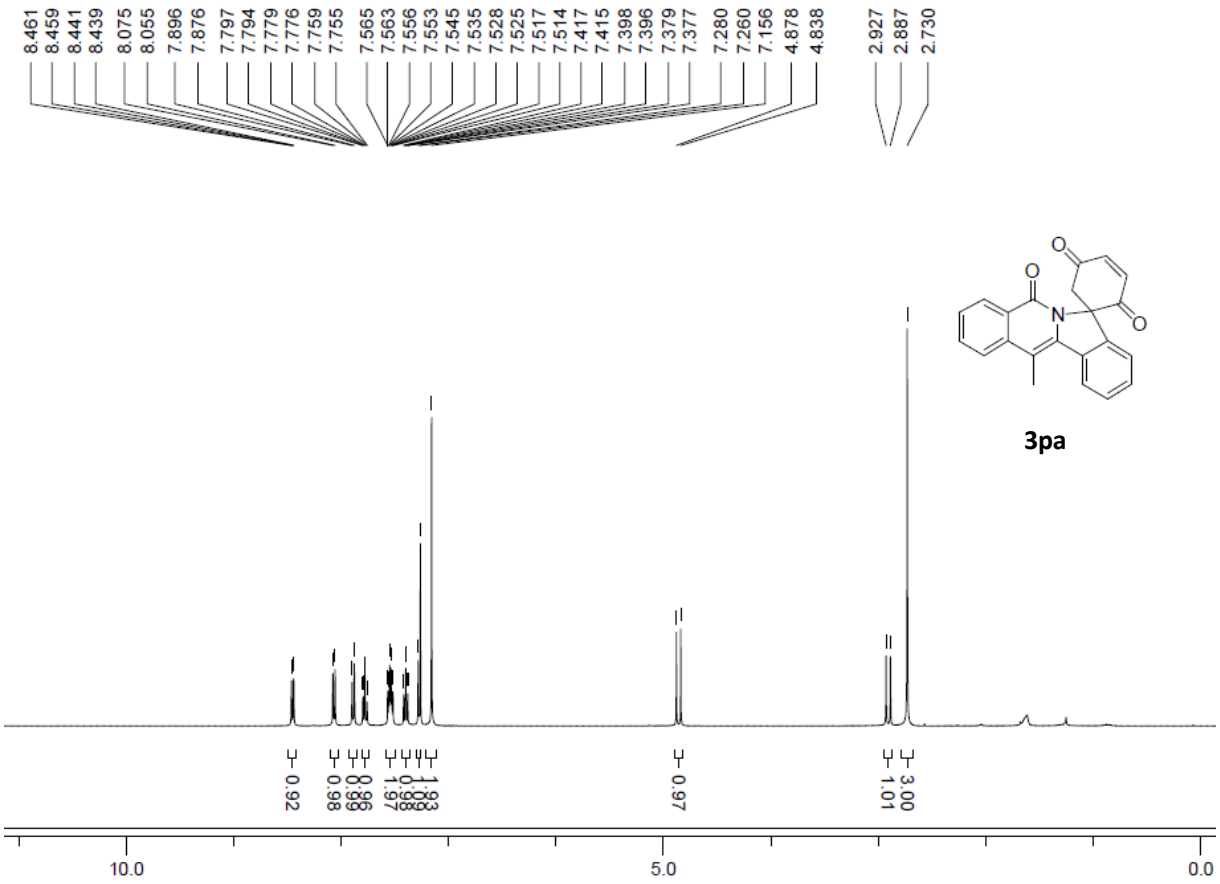
**3oa**

**3oa**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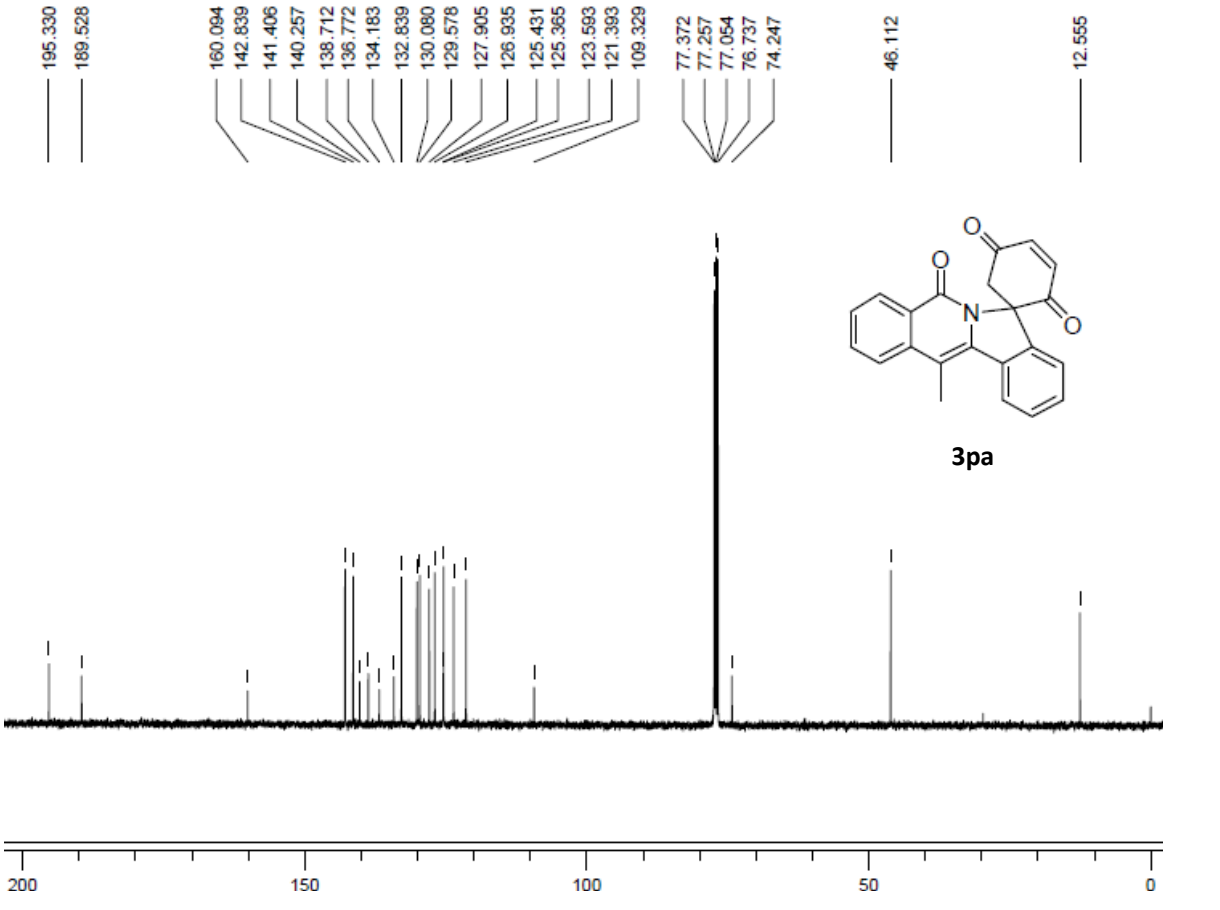
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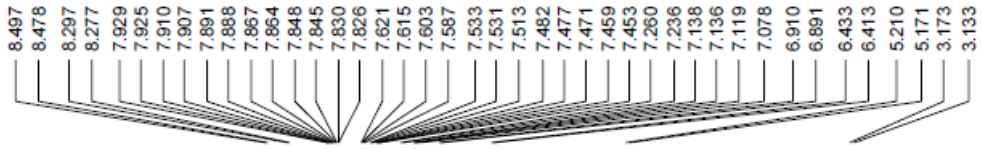
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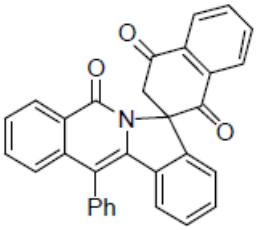
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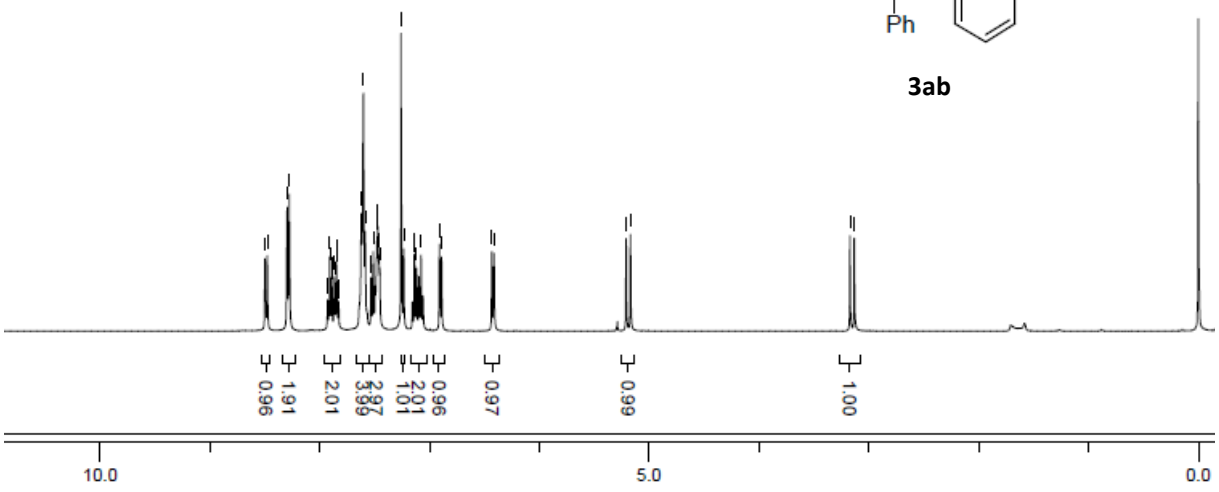
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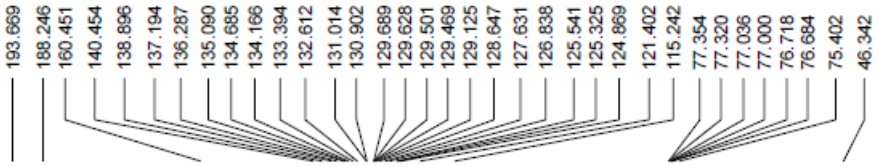
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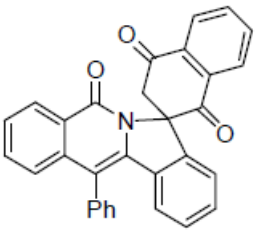
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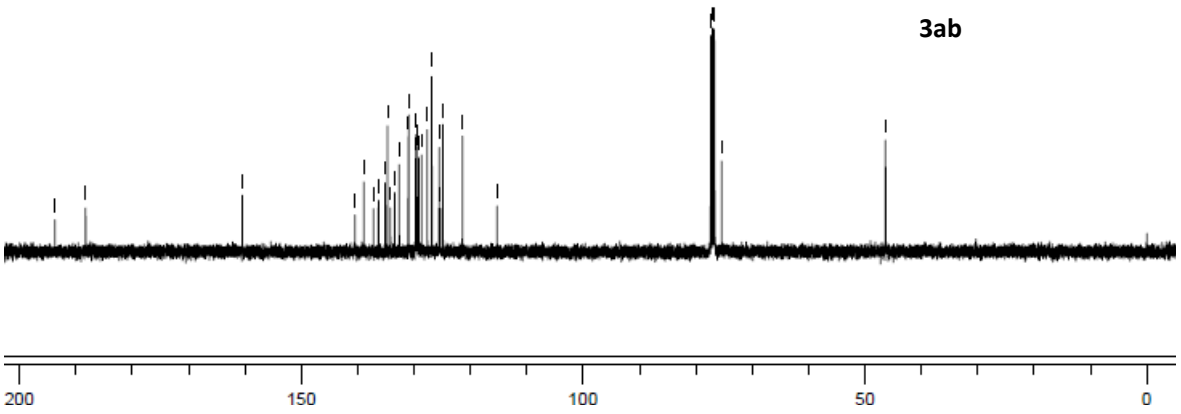
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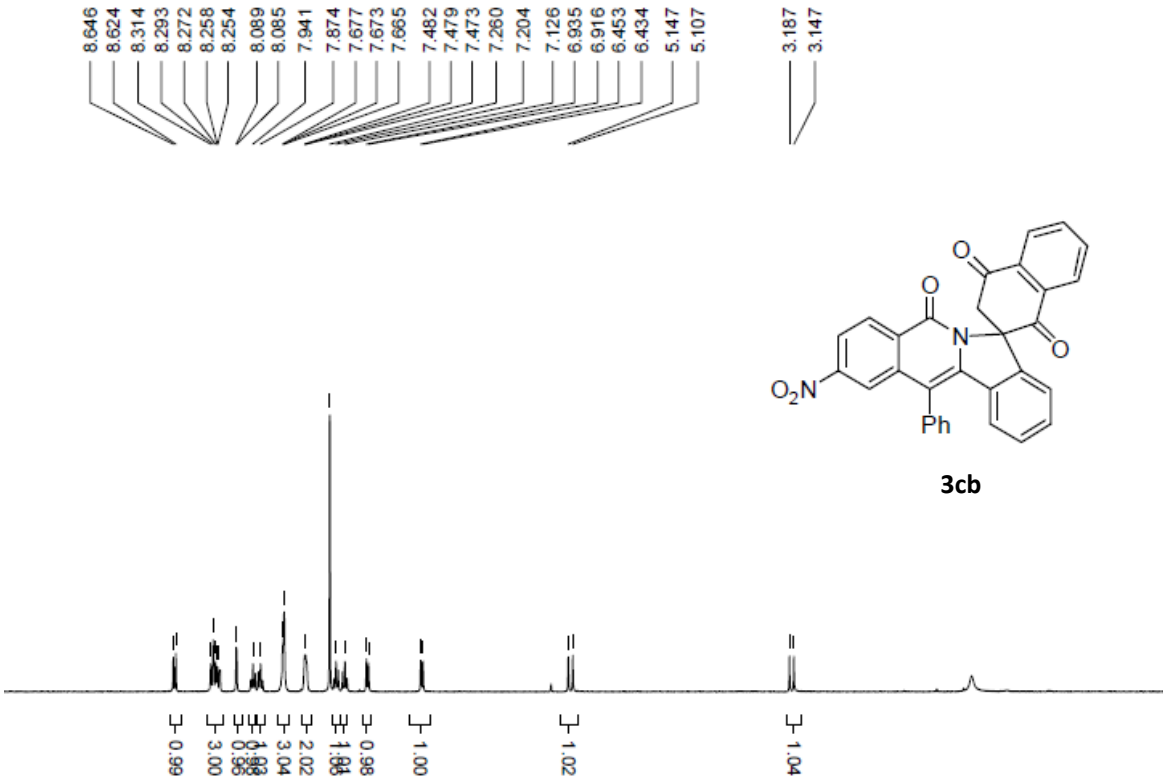
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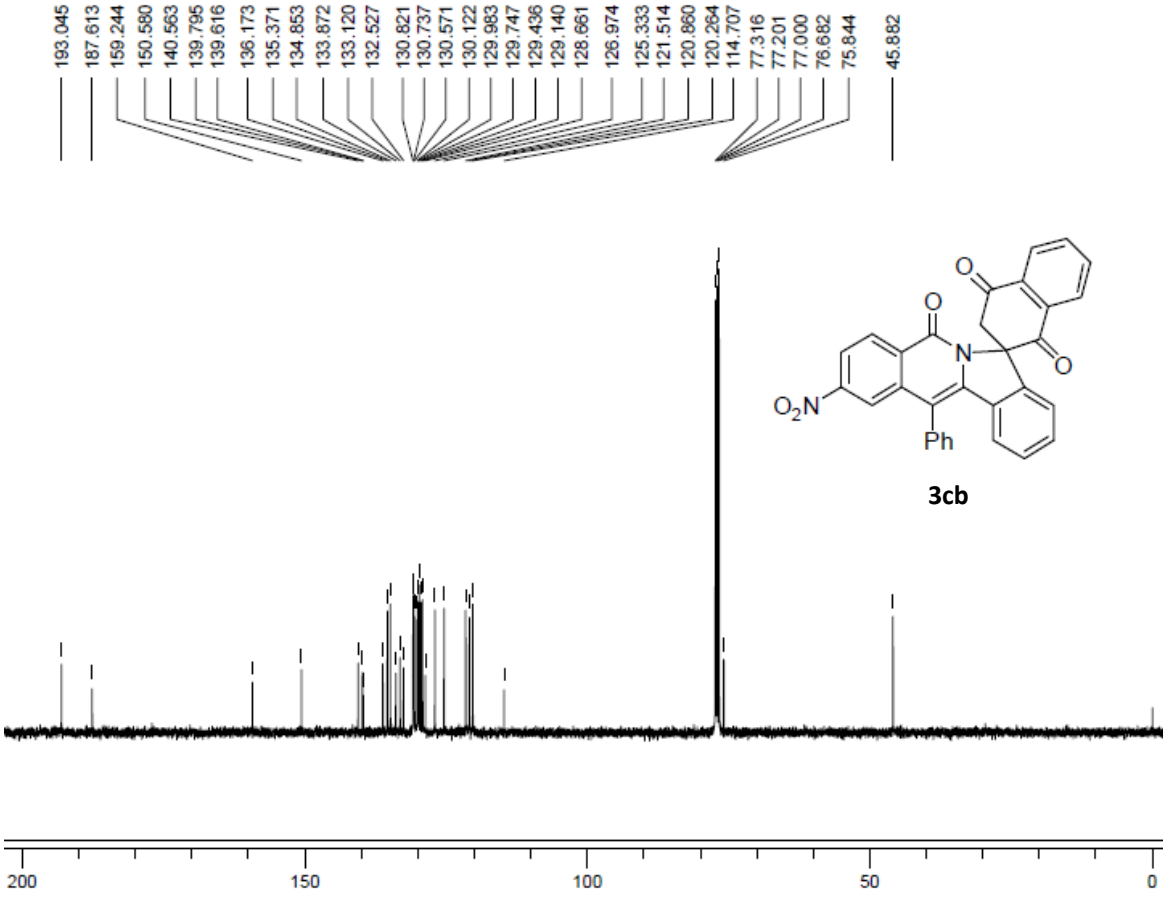
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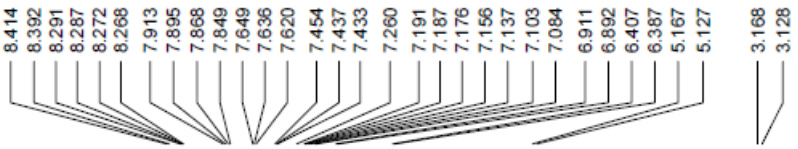
**3cb**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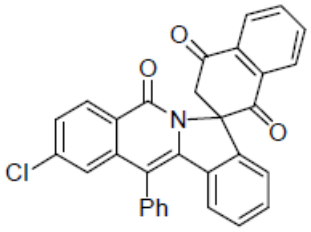
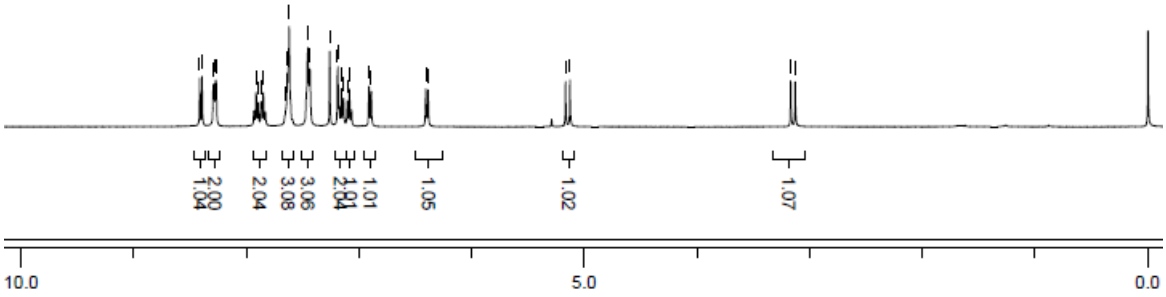
7.895
7.868
7.849
7.649
7.636
7.620
7.454
7.437
7.433
7.260
7.191
7.187
7.176
7.156
7.137
7.103
7.084
6.911
6.892
6.407
6.387
5.167
5.127
3.168
3.128


O
O
N
O
Cl
Ph

**3fb**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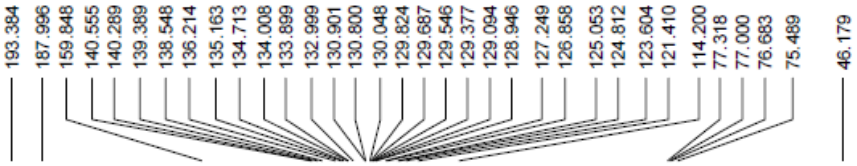
2.04
3.08
3.06
2.01
1.01
1.05
1.02
1.07
10.0
5.0
0.0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187.996
159.848
140.555
140.289
139.389
138.548
136.214
135.163
134.713
134.008
133.899
132.999
130.901
130.800
130.048
129.824
129.687
129.546
129.377
129.094
128.946
127.249
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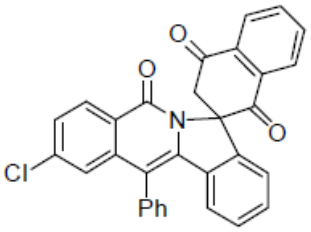
125.053
124.812
123.604
121.410
114.200
77.318
77.000
76.683
75.489
46.179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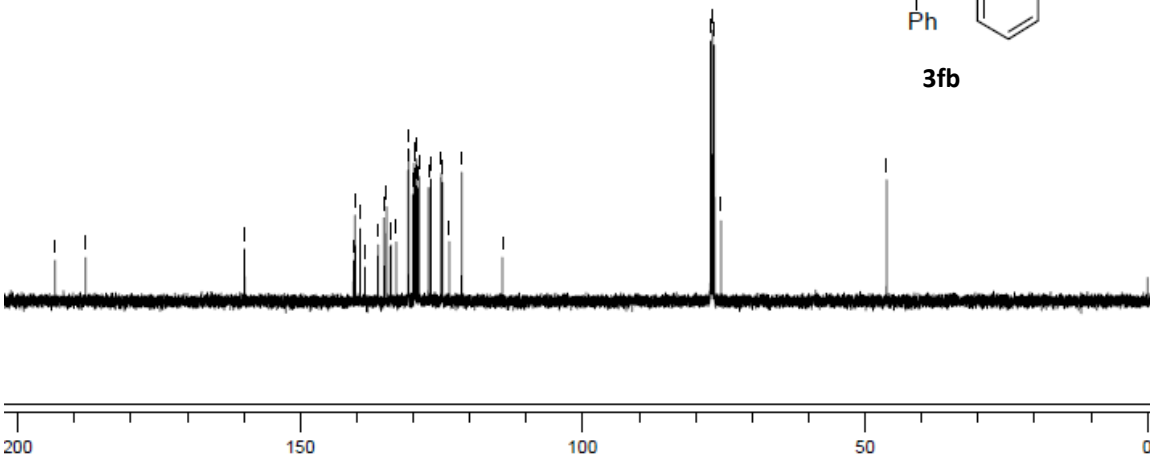
N
O
Cl
Ph

**3fb**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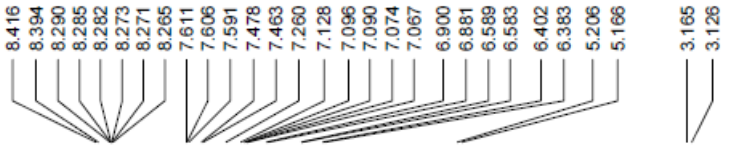
150
100
50
0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8.290
8.285
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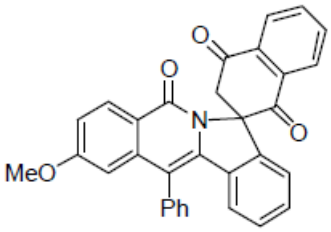
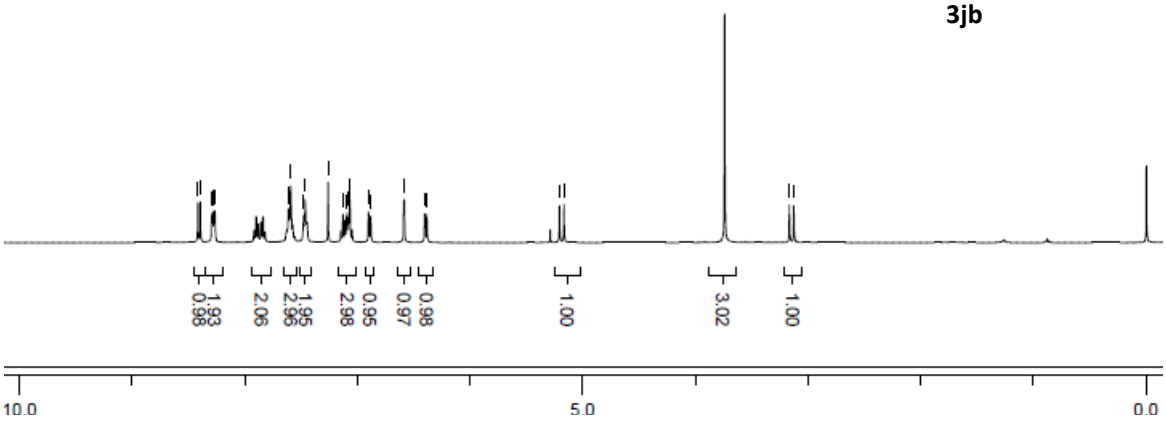
8.273
8.271
8.265
7.611
7.606
7.591
7.478
7.463
7.260
7.128
7.096
7.090
7.074
7.067
6.900
6.881
6.589
6.583
6.402
6.383
5.206
5.166
3.165
3.126


O
O
N
O
MeO
Ph

**3jb**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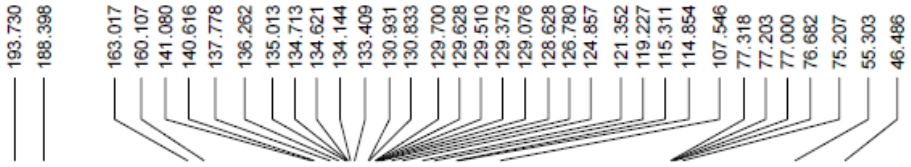
1.00
10.0
5.0
0.0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140.616
137.778
136.262
135.013
134.713
134.621
134.144
133.409
130.931
130.833
129.700
129.628
129.510
129.373
129.076
128.628
126.780
124.857
121.352
119.227
115.311
114.854
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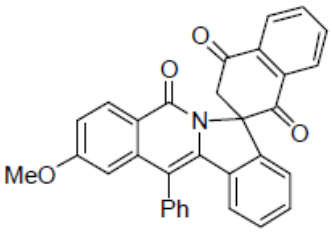
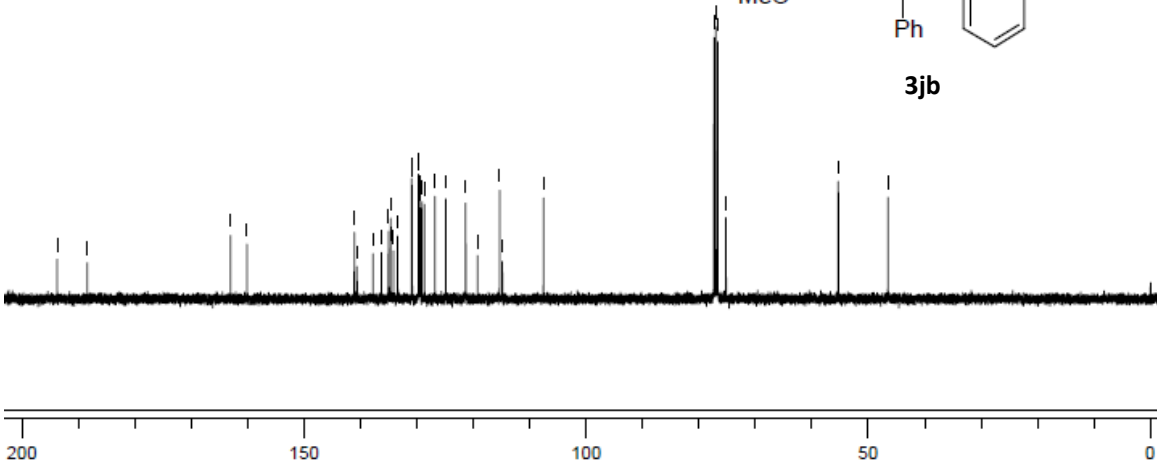
77.318
77.203
77.000
76.682
75.207
55.303
46.486


O
O
N
O
MeO
Ph

**3jb**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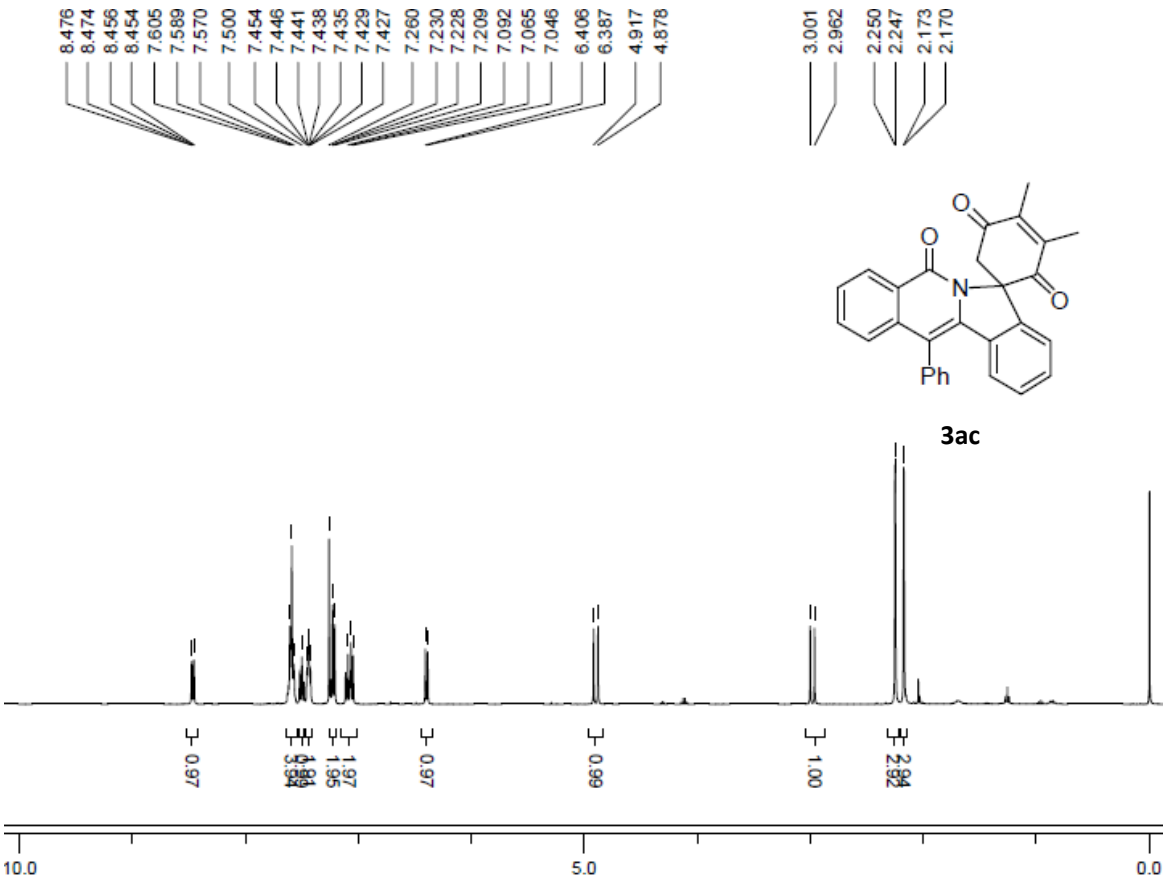
150
100
50
0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8.456
8.454
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7.589
7.570
7.500
7.454
7.446
7.441
7.438
7.435
7.429
7.427
7.260
7.230
7.228
7.209
7.092
7.065
7.046
6.406
6.387
4.917
4.878
3.001
2.962
2.250
2.247
2.173
2.170
O
O
N
O
Ph
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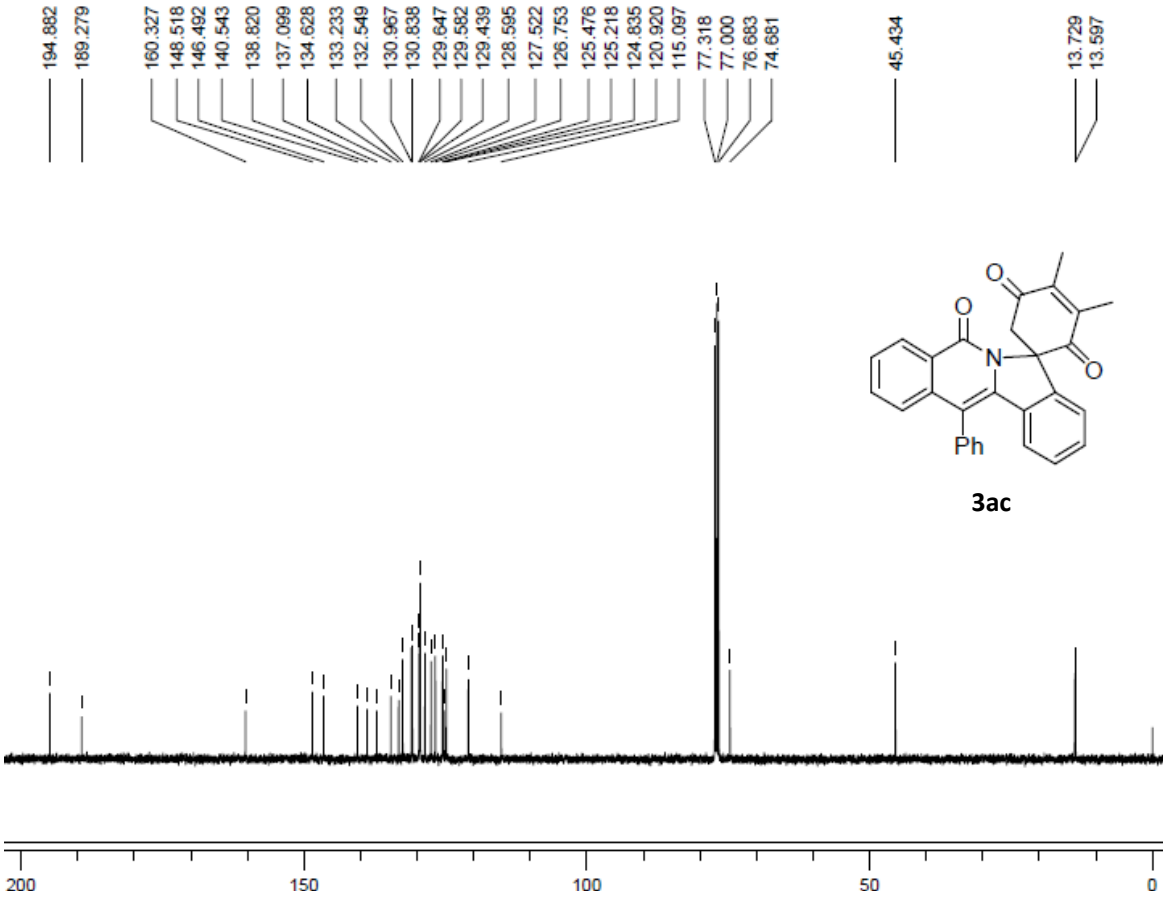
3.96
1.97
0.97
0.99
1.00
2.92
10.0
5.0
0.0

**3ac**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160.327
148.518
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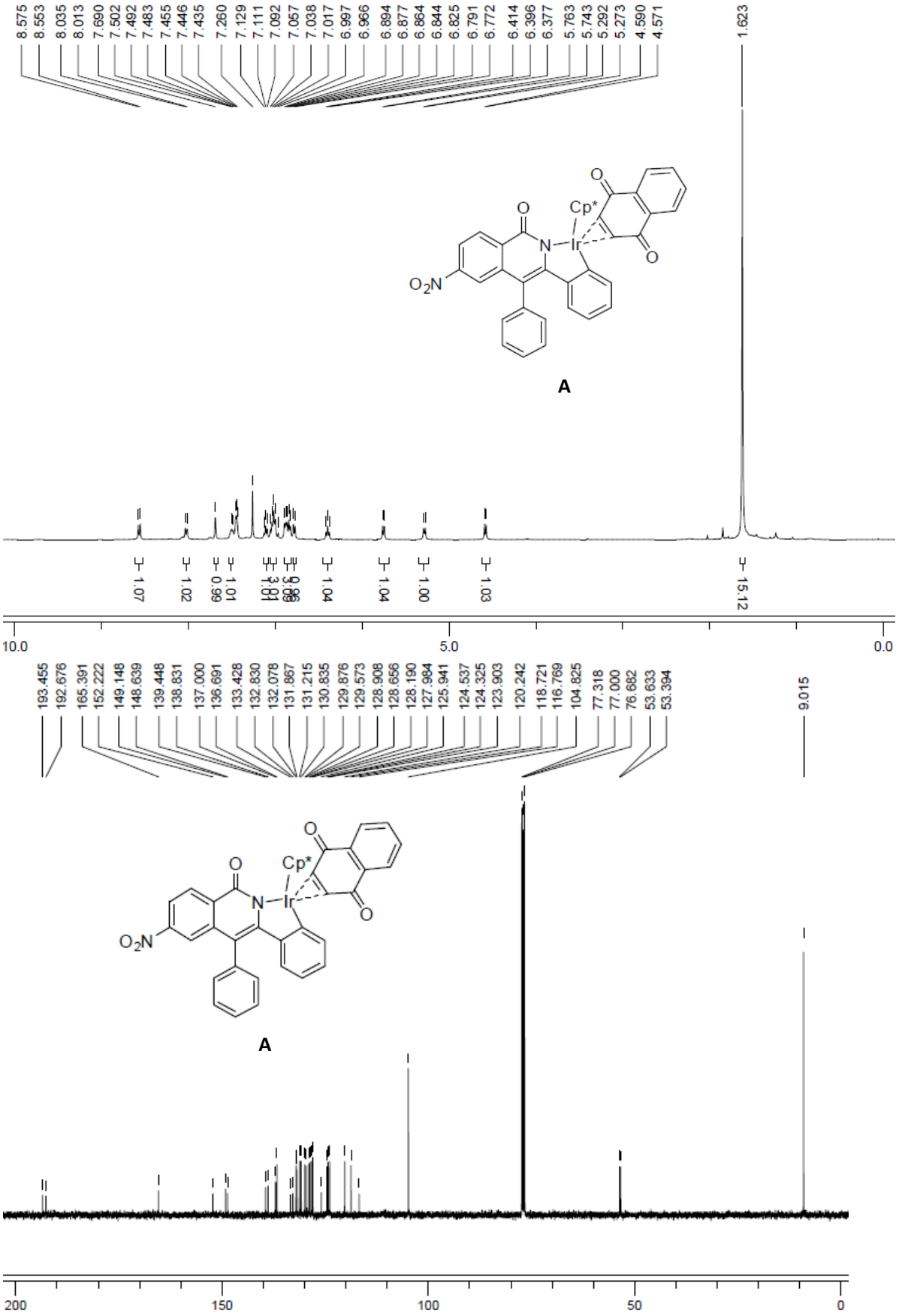
140.543
138.820
137.099
134.628
133.233
132.549
130.967
130.838
129.647
129.582
129.439
128.595
127.522
126.753
125.476
125.218
124.835
120.920
115.097
77.318
77.000
76.683
74.681
45.434
13.729
13.597
O
O
N
O
Ph
200
150
100
50
0

**3ac**


8.575
8.553
8.035
8.013
7.690
7.502
7.492
7.483
7.455
7.446
7.435
7.260
7.129
7.111
7.092
7.057
7.038
7.017
6.997
6.966
6.894
6.877
6.864
6.844
6.825
6.791
6.772
6.414
6.396
6.377
5.763
5.743
5.292
5.273
4.590
4.571
1.623
O
Cp*
N
Ir
O
O
O2N
A
1.07
1.02
0.99
1.01
1.04
1.04
1.00
1.03
15.12
10.0
5.0
0.0
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192.676
165.391
152.222
149.148
148.639
139.448
138.831
137.000
136.691
133.428
132.830
132.078
131.867
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128.908
128.656
128.190
127.984
125.941
124.537
124.325
123.903
120.242
118.721
116.769
104.825
77.318
77.000
76.682
53.633
53.394
9.015
O
Cp*
N
Ir
O
O
O2N
A
200
150
100
50
0

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1. White, C.; Yates, A.; Maitlis, P. M. *Inorg. Syn.* **1992**, *29*, 228.

2. Li, B.; Feng, H.; Xu, S.; Wang, B. *Chem. Eur. J.* **2011**, *17*, 12573.

3. Hu, P.; Huang, S.; Xu, J.; Shi, Z.-J.; Su, W. *Angew. Chem., Int. Ed.* **2011**, *50*, 9926.