Electronic Supplementary Material (ESI) for ChemComm.

Supporting Information

Selective C-H Acylation of Indoles with α-Oxocarboxylic Acids at the C4 Position by Pd Catalysis

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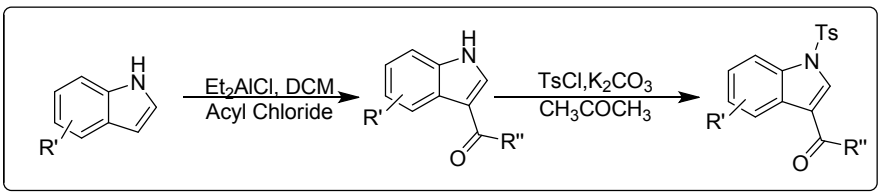
General Information and Procedure for the Reaction

1. General information:

All commercial materials were used as received unless otherwise noted. Commercial reagents were purchased from Alfa Aesar, TCI, Energy Chemical, and used without further purification. Starting materials α-oxocarboxylic acids were prepared according to the reported procedure.[1] All of other commercially available compounds were used without further purification. ^{1}H NMR spectra were recorded at 400 MHz or 500 MHz and NMR spectrometers using TMS as an internal standard, ^{13}C NMR spectra were recorded at 100 MHz or 125 MHz NMR spectrometers using TMS as an internal standard. ^{19}F NMR spectra were recorded at a 376 MHz NMR spectrometer using TMS as an internal standard and were fully decoupled by broad band proton decoupling. The multiplicities are reported as follows: singlet (s), doublet (d), doublet of doublets (dd), multiplet (m), triplet (t) and broad resonances (br). IR spectra were measured as potassium bromide pellets or as liquid films between two potassium bromide pellets. Melting points were measured on a hot-stage microscope (XT4-A) and are uncorrected. High resolution mass spectra (HRMS) were obtained on an APEXM Fourier transform mass spectrometry (ESI). The X-ray diffraction spectrum was carried out with a SMART APEX II X-ray Single-crystal diffract meter.

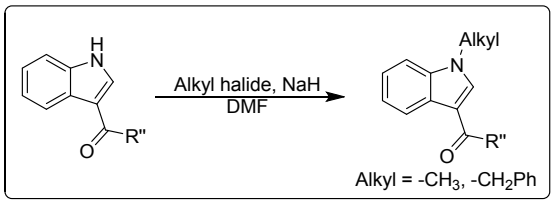
2. General procedure for the preparation of indoles



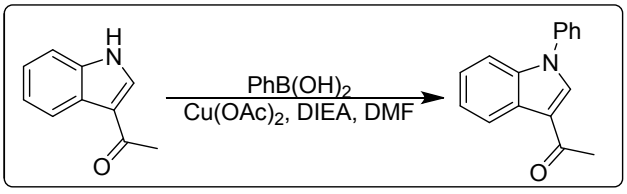
General Procedure A for the preparation of 1a, 1e, 1f, 1h-1s[2]: To a solution of indole derivative (5 mmol, 1.0 equiv) in DCM (10 mL), Et_2AlCl (7.5 mmol, 1.5 equiv) (0.98 mol/L in hexane) was added at 0 °C and the mixture was stirred at this temperature for 30 min. To this solution was added drop-wise a DCM solution (10 mL) of acyl chloride (6 mmol, 1.2 equiv) at 0 ºC. The mixture was warmed to room temperature and stirred until

completion of the reaction (monitored by TLC). Then the mixture was quenched with saturated aqueous NH_4Cl, extracted with CH_2Cl_2 (15 mL x 3), the combined organic phases were dried over anhydrous Na_2SO_4, filtered and concentrated under reduced pressure. The crude product was purified by flash column chromatography to give the 3-acylindole derivatives.

To a 100 mL round bottom flask and stir bar was added 3-acylindole derivatives (5 mmol), 20 mL acetone, K_2CO_3 (10 mmol), and TsCl (6 mmol). The reaction was stirred at room temperature and monitored by TLC. Upon completion, the mixture was filtered through Celite®, and the filter cake was rinsed with EtOAc. The combined organic was removed in vacuo and purified using flash chromatography to give **1a**, **1e**, **1f**, **1h-1s** (60-95% yield).



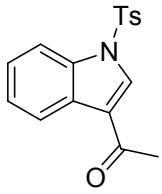
General Procedure B for the preparation of 1b, 1c, 1g[3]: To a solution of 3-acylindole (5 mmol) in *N,N*-dimethylformamide (15 mL) was added NaH (1.2 equiv) under ice cooled conditions. Alkyl halide (1.2 equiv) was added dropwise to this solution and allowed to stir at room temperature for appropriate time. After completion of the reaction it was quenched with water and extracted by Et_2O. The organic layer was dried over anhydrous Na_2SO_4 and filtered, concentrated under pressure and then purified by silica gel flash column chromatography to afford **1b**, **1c**, **1g**.



General Procedure C for the preparation of 1d[4]: In a sealed (glass cap and parafilm) oven-dried 25 mL flask, a mixture of 3-acetylindole (1.0 mmol), $PhB(OH)_2$ (2.5 mmol), anhydrous $Cu(OAc)_2$ (2.5 mmol), *N,N*-Diisopropylethylamine (2.5 mmol) in dry DMF (2

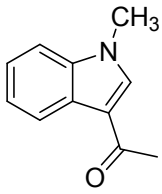
mL) was stirred at room temperature for 5 days. After quenching with saturated aqueous NH_4Cl and extracted with Et_2O (3 x 10 mL). The organic layers were combined and washed with brine (20 mL), dried over Na_2SO_4, filtered and was purified by flash column chromatography on silica to afford **1d**.

3. Analytical data for indoles



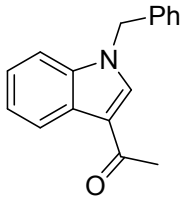
1-(1-tosyl-1*H*-indol-3-yl)ethanone (1a)

^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.34-8.32 (m, 1H), 8.22 (s, 1H), 7.94-7.91 (m, 1H), 7.83 (d, J = 8.4 Hz, 2H), 7.39-7.31 (m, 2H), 7.27 (d, J = 8.0 Hz, 2H), 2.57 (s, 3H), 2.35 (s, 3H). **^{13}C NMR** (100 MHz, Chloroform-*d*) δ 193.6, 146.0, 134.9, 134.5, 132.3, 130.3, 127.5, 127.2, 125.8, 124.8, 123.1, 121.6, 113.1, 27.9, 21.7. **HRMS** (ESI) m/z calcd for $C_{17}H_{16}NO_3S$ $(M+H)^+$: 314.0845, found: 314.0843.



1-(1-methyl-1*H*-indol-3-yl)ethanone (1b)

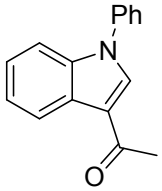
^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.38-8.35 (m, 1H), 7.63 (s, 1H), 7.30-7.27 (m, 3H), 3.77 (s, 3H), 2.48 (s, 3H). **^{13}C NMR** (100 MHz, Chloroform-*d*) δ 193.0, 137.4, 135.9, 126.2, 123.3, 122.6, 122.5, 116.8, 109.7, 33.5, 27.6. **HRMS** (ESI) m/z calcd for $C_{11}H_{12}NO$ $(M+H)^+$: 174.0913, found: 174.0910.



1-(1-benzyl-1*H*-indol-3-yl)ethanone (1c)

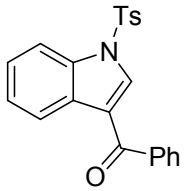
^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.41 (d, J = 7.5 Hz, 1H), 7.73 (s, 1H), 7.32-7.22 (m, 6H), 7.15-

7.13 (m, 2H), 5.31 (s, 2H), 2.49 (s, 3H). **^{13}C NMR** (100 MHz, Chloroform-*d*) δ 193.2, 137.1, 135.8, 135.2, 129.1, 128.2, 127.0, 126.4, 123.5, 122.8, 122.7, 117.5, 110.2, 50.7, 27.7. **HRMS** (ESI) m/z calcd for $C_{17}H_{16}NO$ $(M+H)^+$: 250.1226, found: 250.1224.



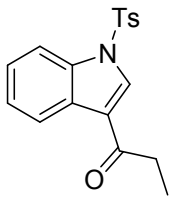
1-(1-phenyl-1*H*-indol-3-yl)ethanone (1d)

^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.47 (d, J = 7.8 Hz, 1H), 7.93 (s, 1H), 7.58-7.55 (m, 2H), 7.51-7.46 (m, 4H), 7.36-7.27 (m, 2H), 2.57 (s, 3H). **^{13}C NMR** (100 MHz, Chloroform-*d*) δ 193.4, 138.4, 137.0, 134.7, 129.9, 128.1, 126.6, 125.0, 124.0, 123.1, 122.8, 118.6, 110.9, 27.8. **HRMS** (ESI) m/z calcd for $C_{16}H_{14}NO$ $(M+H)^+$: 236.1070, found: 236.1071.



phenyl(1-tosyl-1*H*-indol-3-yl)methanone (1e)

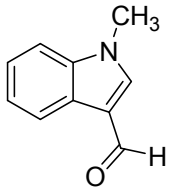
^{1}H NMR (500 MHz, Chloroform-*d*) δ 8.32-8.30 (m, 1H), 8.03 (s, 1H), 8.00-7.98 (m, 1H), 7.88-7.86 (m, 2H), 7.81-7.79 (m, 2H), 7.65-7.62 (m, 1H), 7.56-7.53 (m, 2H), 7.43-7.36 (m, 2H), 7.27 (m, 1H), 7.26-7.25 (m, 1H), 2.36 (s, 3H). **^{13}C NMR** (125 MHz, Chloroform-*d*) δ 191.3, 146.4, 139.6, 135.4, 134.8, 134.0, 132.8, 130.6, 129.4, 129.1, 128.9, 127.5, 126.4, 125.3, 123.4, 120.8, 113.6, 22.1. **HRMS** (ESI) m/z calcd for $C_{22}H_{18}NO_3S$ $(M+H)^+$: 376.1002, found: 376.1003.



1-(1-tosyl-1*H*-indol-3-yl)propan-1-one (1f)

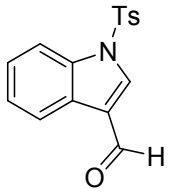
^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.35-8.33 (m, 1H), 8.24 (s, 1H), 7.9-7.92(m, 1H), 7.83 (d, J =8.4 Hz, 2H), 7.3-7.31 (m, 2H), 7.26 (d, J = 8.0 Hz, 2H), 2.94 (q, J = 7.3 Hz, 2H), 2.35 (s, 3H), 1.24 (t, J =

7.3 Hz, 3H). **^{13}C NMR** (100 MHz, Chloroform-*d*) δ 196.8, 145.9, 134.9, 134.5, 131.5, 130.3, 127.7, 127.1, 125.7, 124.8, 123.1, 121.0, 113.1, 33.2, 21.7, 8.4. **HRMS** (ESI) m/z calcd for $C_{18}H_{18}NO_3S$ $(M+H)^+$: 328.1002, found: 328.1004.



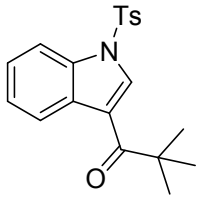
1-methyl-1*H*-indole-3-carbaldehyde (1g)

^{1}H NMR (400 MHz, Chloroform-*d*) δ 9.93 (s, 1H), 8.29-8.27 (m, 1H), 7.60-7.58 (m, 1H), 7.32-7.30 (m, 3H), 3.81 (s, 3H). **^{13}C NMR** (100 MHz, Chloroform-*d*) δ 184.5, 139.5, 137.9, 125.2, 124.0, 122.9, 122.0, 118.0, 110.0, 33.7. **HRMS** (ESI) m/z calcd for $C_{10}H_{10}NO$ $(M+H)^+$: 160.0757, found: 160.0754.



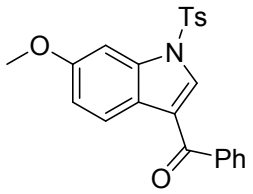
1-tosyl-1*H*-indole-3-carbaldehyde (1h)

^{1}H NMR (400 MHz, Chloroform-*d*) δ 10.09 (s, 1H), 8.26-8.24 (m, 2H), 7.96-7.94 (m, 1H), 7.86-7.84 (m, 2H), 7.43-7.33 (m, 2H), 7.28 (d, J = 8.0 Hz, 2H), 2.35 (s, 3H). **^{13}C NMR** (100 MHz, Chloroform-*d*) δ 185.4, 146.2, 136.3, 135.2, 134.3, 130.4, 127.3, 126.4, 126.3, 125.1, 122.6, 122.3, 113.3, 21.7. **HRMS** (ESI) m/z calcd for $C_{16}H_{14}NO_3S$ $(M+H)^+$: 300.0689, found: 300.0685.



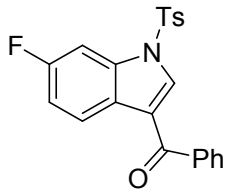
2,2-dimethyl-1-(1-tosyl-1*H*-indol-3-yl)propan-1-one (1i)

^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.33-8.31 (m, 1H), 8.25 (s, 1H), 7.94-7.92 (m, 1H), 7.81 (d, J = 8.4 Hz, 2H), 7.38-7.30 (m, 2H), 7.26 (d, J = 8.0 Hz, 2H), 2.35 (s, 3H), 1.42 (s, 9H). **^{13}C NMR** (100 MHz, Chloroform-*d*) δ 202.7, 145.9, 134.5, 134.1, 130.2, 130.1, 129.6, 127.1, 125.6, 124.7, 123.5, 117.8, 112.9, 44.7, 28.4, 21.7. **HRMS** (ESI) m/z calcd for $C_{20}H_{22}NO_3S$ $(M+H)^+$: 356.1315, found: 356.1317.



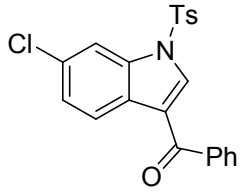
(6-methoxy-1-tosyl-1*H*-indol-3-yl)(phenyl)methanone (1k)

^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.18 (d, J = 8.8 Hz, 1H), 7.92 (s, 1H), 7.87-7.85 (m, 2H), 7.78 (d, J = 8.4 Hz, 2H), 7.65-7.60 (m, 1H), 7.55-7.51 (m, 2H) , 7.49 (d, J = 2.2 Hz, 1H), 7.26 (d, J = 8.0 Hz, 2H), 7.00 (dd, J = 2.3, 8.8 Hz, 1H), 3.89 (s, 3H), 2.36 (s, 3H). **^{13}C NMR** (100 MHz, Chloroform-*d*) δ 190.9, 158.7, 146.0, 139.2, 136.1, 134.4, 132.6, 132.4, 130.3, 129.0, 128.7, 127.1, 123.6, 122.2, 120.5, 113.7, 97.4, 55.8, 21.7. **HRMS** (ESI) m/z calcd for $C_{23}H_{20}NO_4S$ $(M+H)^+$: 406.1108, found: 406.1104.



(6-fluoro-1-tosyl-1*H*-indol-3-yl)(phenyl)methanone (1l)

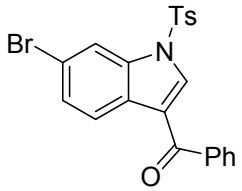
^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.27 (dd, J = 5.5, 8.8 Hz, 1H), 8.00 (s, 1H), 7.87-7.84 (m, 2H), 7.80 (d, J = 8.4 Hz, 2H), 7.71 (dd, J = 2.3, 9.4 Hz, 1H), 7.66-7.62 (m, 1H), 7.54 (t, J = 7.7 Hz, 2H), 7.29 (d, J = 8.1 Hz, 2H), 7.13 (td, J = 9.0, 2.3 Hz, 1H), 2.37 (s, 3H). **^{13}C NMR** (100 MHz, Chloroform-*d*) δ 190.7, 161.4 (d, J = 242.7 Hz), 146.3, 138.9, 135.2 (d, J = 12.5 Hz), 134.1, 133.7 (d, J = 3.4 Hz), 132.6, 130.4, 129.0, 128.8, 127.2, 124.8 (d, J = 1.6 Hz), 124.2 (d, J = 9.7 Hz), 120.1, 113.4 (d, J = 23.7. Hz), 100.6 (d, J = 28.2 Hz), 21.7. **HRMS** (ESI) m/z calcd for $C_{22}H_{17}FNO_3S$ $(M+H)^+$: 394.0908, found: 394.0906.



(6-chloro-1-tosyl-1*H*-indol-3-yl)(phenyl)methanone (1m)

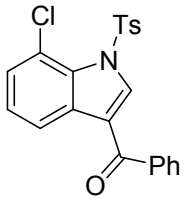
^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.23 (d, J = 8.6 Hz, 1H) , 8.01-8.00 (m, 2H), 7.86-7.84 (m, 2H), 7.80 (d, J = 8.4 Hz, 2H), 7.67-7.63 (m, 1H), 7.55 (t, J = 7.7 Hz, 2H), 7.36 (dd, J = 1.9, 8.6 Hz, 1H), 7.30

(d, J = 8.0 Hz, 2H), 2.38 (s, 3H). **^{13}C NMR** (100 MHz, Chloroform-*d*) δ 190.5, 146.4, 138.8, 135.3, 134.1, 133.8, 132.6, 132.0, 130.5, 129.0, 128.8, 127.2, 127.0, 125.6, 123.9, 120.1, 113.4, 21.8. **HRMS** (ESI) m/z calcd for $C_{22}H_{17}ClNO_3S$ $(M+H)^+$: 410.0612, found: 410.0615.



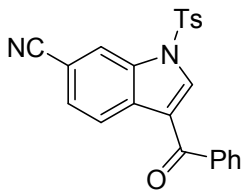
(6-bromo-1-tosyl-1*H*-indol-3-yl)(phenyl)methanone (1n)

^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.18-8.16 (m, 2H), 8.00 (s, 1H), 7.85-7.83 (m, 2H), 7.79 (d, J = 8.44 Hz, 2H), 7.64-7.61 (m, 1H), 7.53 (t, J = 7.8 Hz, 2H), 7.47 (dd, J = 1.6, 8.6 Hz, 1H), 7.28 (d, J = 8.2 Hz, 2H), 2.36 (s, 3H). **^{13}C NMR** (100 MHz, Chloroform-*d*) δ 190.5, 146.4, 138.8, 135.6, 134.1, 133.7, 132.6, 130.5, 129.0, 128.8, 128.3, 127.4, 127.2, 124.2, 120.1, 119.8, 116.3, 21.8. **HRMS** (ESI) m/z calcd for $C_{22}H_{17}BrNO_3S$ $(M+H)^+$: 454.0107, found: 454.0106.



(7-chloro-1-tosyl-1*H*-indol-3-yl)(phenyl)methanone (1o)

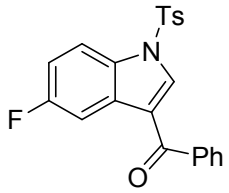
^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.39 (s, 1H), 8.36 (dd, J = 2.0, 7.0 Hz, 1H), 7.92-7.90 (m, 2H), 7.70 (d, J = 8.4 Hz, 2H), 7.67-7.63 (m, 1H), 7.57 (t, J = 7.7 Hz, 2H), 7.32-7.29 (m, 4H), 2.42 (s, 3H). **^{13}C NMR** (100 MHz, Chloroform-*d*) δ 190.7, 145.6, 139.0, 137.7, 136.0, 132.6, 132.4, 132.3, 130.0, 129.1, 128.8, 128.2, 127.5, 125.8, 121.6, 118.7, 118.6, 21.8. **HRMS** (ESI) m/z calcd for $C_{22}H_{17}ClNO_3S$ $(M+H)^+$: 410.0612, found: 410.0610.



3-benzoyl-1-tosyl-1*H*-indole-6-carbonitrile (1p)

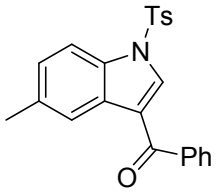
^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.43 (d, J = 8.3 Hz, 1H), 8.32 (s, 1H), 8.18 (s, 1H), 7.87-7.82 (m,

4H), 7.68 (t, *J* = 7.4 Hz, 1H), 7.64 (dd, *J* = 1.3 Hz, 8.3 Hz, 1H), 7.57 (t, *J* = 7.8 Hz, 2H), 7.34 (d, *J* = 8.2 Hz, 2H), 2.41 (s, 3H). **^{13}C NMR** (100 MHz, Chloroform-*d*) δ 190.1, 146.8, 138.5, 135.8, 134.0, 133.8, 132.9, 131.9, 130.7, 129.0, 128.9, 127.9, 127.3, 124.1, 119.9, 119.1, 117.6, 109.1, 21.8. **HRMS** (ESI) m/z calcd for $C_{23}H_{17}N_2O_3S$ $(M+H)^+$: 401.0954, found: 401.0952.



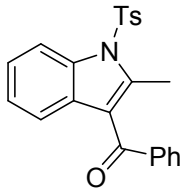
(5-fluoro-1-tosyl-1*H*-indol-3-yl)(phenyl)methanone (1q)

^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.06 (s, 1H), 8.01 (dd, *J* = 2.5, 9.0 Hz, 1H), 7.93 (dd, *J* = 4.3, 9.1 Hz, 1H), 7.87-7.84 (m, 2H), 7.79-7.78 (m, 2H), 7.67-7.62 (m, 1H), 7.57-7.53 (m, 2H), 7.28 (d, *J* = 8.0 Hz, 2H), 7.14 (td, *J* = 9.0, 2.6 Hz, 1H), 2.37 (s, 3H). **^{13}C NMR** (100 MHz, Chloroform-*d*) δ 190.5, 160.6 (d, *J* = 240.4 Hz), 146.3, 138.9, 134.8, 134.2, 132.6, 131.3, 130.4, 129.7 (d, *J* = 10.8 Hz), 129.0, 128.8, 127.1, 120.1 (d, *J* = 4.2 Hz), 114.4, 114.2 (d, *J* = 16.2 Hz), 108.9 (d, *J* = 25.2 Hz), 21.7. **HRMS** (ESI) m/z calcd for $C_{22}H_{17}FNO_3S$ $(M+H)^+$: 394.0908, found: 394.0909.



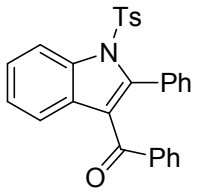
(5-methyl-1-tosyl-1*H*-indol-3-yl)(phenyl)methanone (1r)

^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.12 (s, 1H), 7.97 (s, 1H), 7.87-7.85 (m, 3H), 7.78 (d, *J* = 8.4 Hz, 2H), 7.66-7.62 (m, 1H), 7.54 (t, *J* = 7.7 Hz, 2H), 7.26 (s, 1H), 7.24-7.22 (m, 2H), 2.46 (s, 3H), 2.36 (s, 3H). **^{13}C NMR** (100 MHz, Chloroform-*d*) δ 191.0, 145.9, 139.2, 134.8, 134.4, 133.8, 133.2, 132.4, 130.2, 129.1, 128.8, 128.7, 127.4, 127.1, 122.7, 120.2, 112.8, 21.7, 21.5. **HRMS** (ESI) m/z calcd for $C_{23}H_{20}NO_3S$ $(M+H)^+$: 390.1158, found: 390.1157.



(2-methyl-1-tosyl-1*H*-indol-3-yl)(phenyl)methanone (1s)

^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.27 (d, J = 8.5 Hz, 1H), 7.77-7.74 (m, 4H), 7.60-7.55 (m, 1H), 7.45-7.41 (m, 2H), 7.34,-7.24 (m, 4H), 7.19-7.15 (m, 1H), 2.63 (s, 3H), 2.36 (s, 3H). **^{13}C NMR** (100 MHz, Chloroform-*d*) δ 193.0, 145.6, 141.2, 139.0, 136.0, 135.9, 133.2, 130.2, 129.6, 128.6, 128.1, 126.6, 124.8, 124.0, 120.7, 120.3, 114.4, 21.7, 14.7. **HRMS** (ESI) m/z calcd for $C_{23}H_{20}NO_3S$ $(M+H)^+$: 390.1158, found: 390.1157.

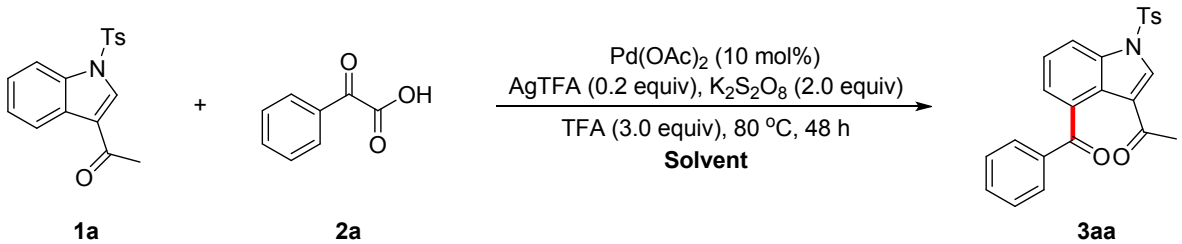


phenyl(2-phenyl-1-tosyl-1*H*-indol-3-yl)methanone (1t)

^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.42 (d, J = 8.3 Hz, 1H), 7.61 (d, J = 7.6 Hz, 1H) 7.49-7.43 (m, 3H), 7.35-7.29 (m, 2H), 7.25-7.20 (m, 5H), 7.16-7.13 (m, 4H), 7.05 (d, J = 7.7 Hz, 2H), 2.31 (s, 3H). **^{13}C NMR** (100 MHz, Chloroform-*d*) δ 193.2, 145.3, 142.7, 137.5, 137.0, 134.8, 132.6, 132.1, 129.8, 129.5, 129.4, 129.2, 128.0, 127.1, 127.0, 125.8, 125.0, 123.1, 120.9, 116.2, 21.6. **HRMS** (ESI) m/z calcd for $C_{28}H_{22}NO_3S$ $(M+H)^+$: 452.1315, found: 452.1314.

4. Optimization of Reaction Conditions

Screening of Solvent

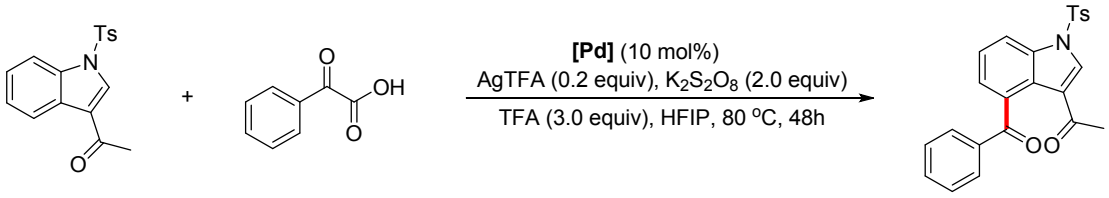


1a **2a** **3aa**

Entry[a]	Solvent	Yield (%)[b]
1	MeOH	trace
2	toluene	trace
3	1,4-dioxane	trace
4	DCE	22
5	TFE	35
6	HFIP	65

[a] Reactions conditons: **1a** (0.2 mmol), **2a** (0.3 mmol), $Pd(OAc)_2$ (0.02 mmol), AgTFA (0.04 mmol), $K_2S_2O_8$ (0.4 mmol), TFA (3.0 equiv), solvent (1.0 mL), Air, 80 °C, 48 h. [b] Isolated yield by flash column chromatography.

Screening of Catalyst

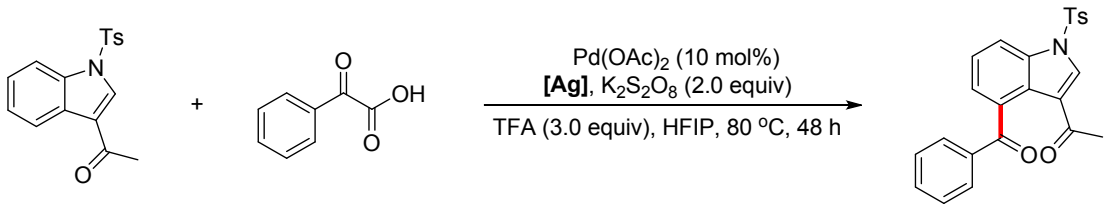


1a **2a** **3aa**

Entry[a]	[Pd]	Yield (%)[b]
1	$Pa(OAc)_2$	62
2	$Pd(TFA)_2$	51
3	$PdCl_2$	40
4	$Pd(CH_3CN)_2Cl_2$	43

[a] Reactions conditons: **1a** (0.2 mmol), **2a** (0.3 mmol), [Pd] (0.02 mmol), AgTFA (0.04 mmol), $K_2S_2O_8$ (0.4 mmol), TFA (3.0 equiv), HFIP (1.0 mL), Air, 80 °C, 48 h. [b] Isolated yield by flash column chromatography.

Screening of [Ag]



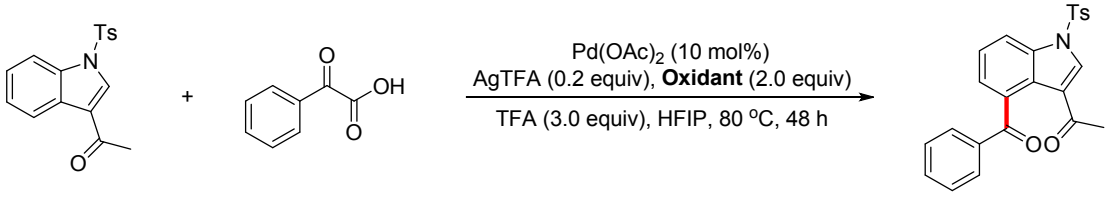
1a **2a** **3aa**

Entry[a]	[Ag]	Yield (%)[b]
1	AgTFA	62
2	AgOAc	47
3	Ag_2CO_3	53
4	Ag_2O	50

5[c]	AgTFA	Trace
6[d]	AgTFA	46
7[e]	AgTFA	50
8[f]	AgTFA	65
9[g]	AgTFA	60
10[h]	AgTFA	55
11[i]	AgTFA	55
12	$Cu(OAc)_2$	Nr
13		45
14[j]	AgTFA	52

[a] Reactions conditons: **1a** (0.2 mmol), **2a** (0.3 mmol), $Pd(OAc)_2$ (0.02 mmol), [Ag] (0.04 mmol), $K_2S_2O_8$ (0.4 mmol), TFA (3.0 equiv), HFIP (1.0 mL), Air, 80 °C, 48 h. [b] Isolated yield by flash column chromatography. [c]AgTFA instead of $K_2S_2O_8$. [d]AgTFA (0.1 equiv). [e]AgTFA (0.25 equiv). [f]AgTFA (0.3 equiv). [g]AgTFA (0.35 equiv). [h]AgTFA (0.4 equiv). [i]AgTFA (0.5 equiv). [j]Ar.

Screening of Oxidant

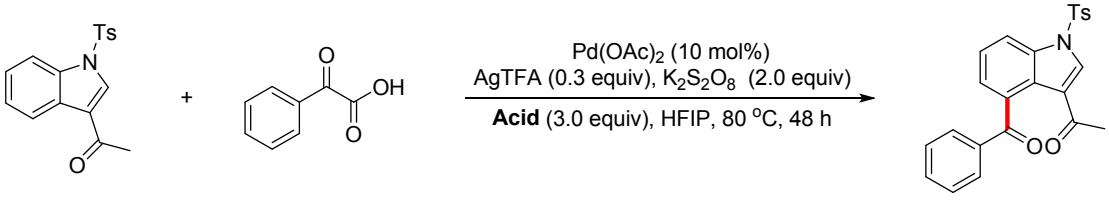


1a **2a** **3aa**

Entry[a]	Oxidant	Yield (%)[b]
1	$K_2S_2O_8$	62
2	$Na_2S_2O_8$	39
3	$(NH_4)_2S_2O_8$	35
4	Oxone	30

[a] Reactions conditons: **1a** (0.2 mmol), **2a** (0.3 mmol), $Pd(OAc)_2$ (0.02 mmol), AgTFA (0.04 mmol), Oxidant (0.4 mmol), TFA (3.0 equiv), HFIP (1.0 mL), Air, 80 °C, 48 h. [b] Isolated yield by flash column chromatography.

Screening of Acid

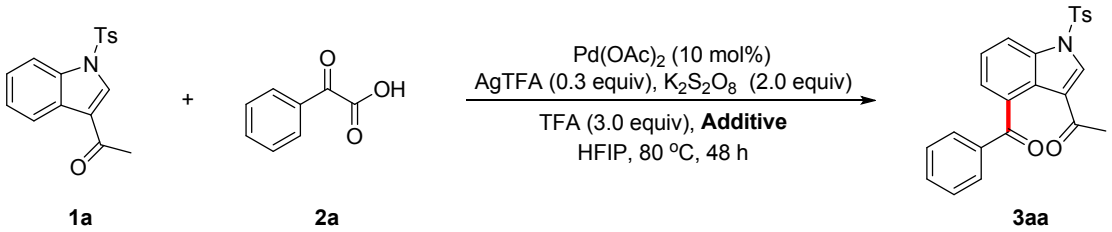


1a **2a** **3aa**

Entry[a]	Acid	Yield (%)[b]
1	TFA	65
2	TfOH	Nd
3	AcOH	32
4	TsOH • H_2O	Nd
5	PivOH	31
6[c]	TFA	41
7[d]	TFA	54

[a] Reactions conditons: **1a** (0.2 mmol), **2a** (0.3 mmol), $Pd(OAc)_2$ (0.02 mmol), AgTFA (0.06 mmol), $K_2S_2O_8$ (0.4 mmol), Acid (3.0 equiv), HFIP (1.0 mL), Air, 80 °C, 48 h. [b] Isolated yield by flash column chromatography. [c]TFA (2.0 equiv). [d]TFA (5.0 equiv).

Screening of Additive

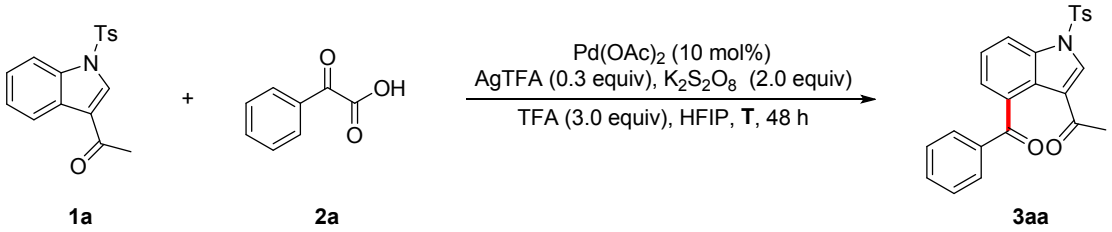


1a **2a** **3aa**

Entry[a]	Additive	Yield (%)[b]
1	TBAB (1.0 equiv)	Nr
2	H_2O (3.0 equiv)	43
3	DMSO (50 uL)	46
4	4Å MS (50 mg)	54
5		65

[a] Reactions conditons: **1a** (0.2 mmol), **2a** (0.3 mmol), $Pd(OAc)_2$ (0.02 mmol), AgTFA (0.04 mmol), $K_2S_2O_8$ (0.4 mmol), TFA (3.0 equiv), HFIP (1.0 mL), Air, 80 °C, 48 h. [b] Isolated yield by flash column chromatography.

Screening of Temperature



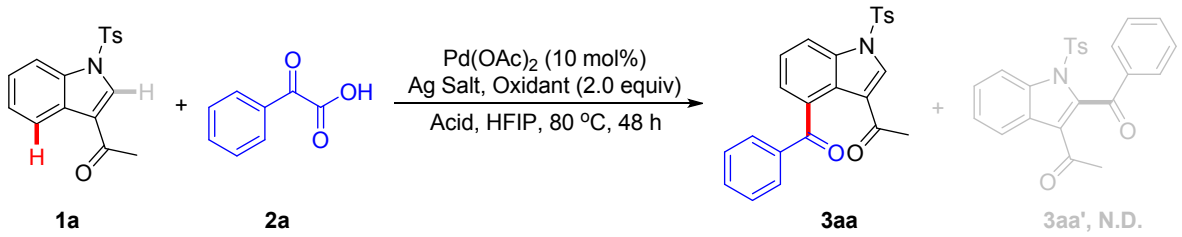
1a **2a** **3aa**

Entry[a]	T (°C)	Yield (%)[b]
1	60	53

2	80	65
4	100	43

[a]Reactions conditons: **1a** (0.2 mmol), **2a** (0.3 mmol), $Pd(OAc)_2$ (0.02 mmol), AgTFA (0.04 mmol), $K_2S_2O_8$ (0.4 mmol), TFA (3.0 equiv), HFIP (1.0 mL), Air, 48 h. [b]Isolated yield by flash column chromatography.

Table S1 Optimization of reaction conditions[a]

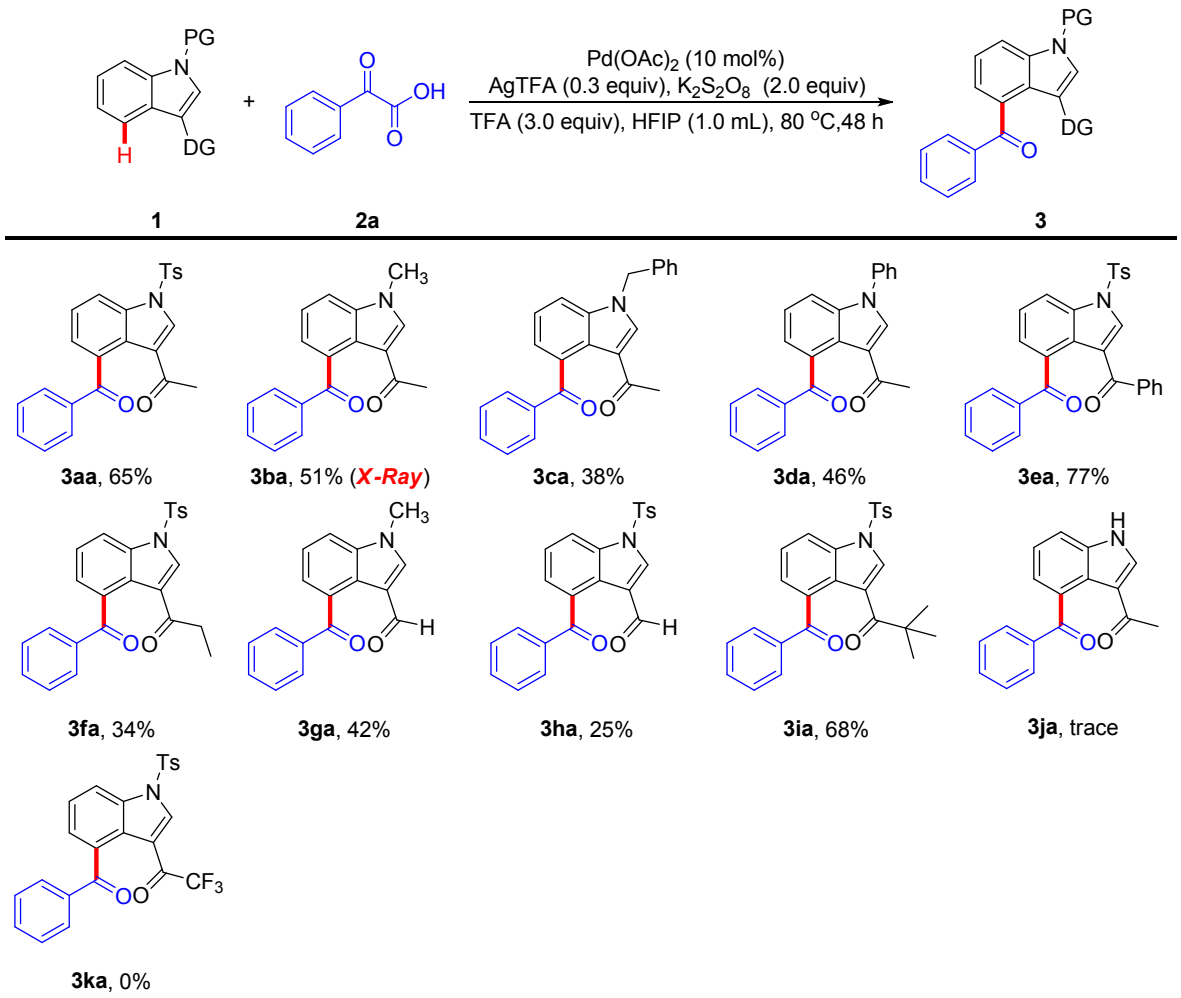


1a **2a** **3aa** **3aa', N.D.**

Entry	Ag salt	oxidant	acid	yield (%)[b]
1	AgOAc	$K_2S_2O_8$	TFA	47
2	Ag_2CO_3	$K_2S_2O_8$	TFA	53
3	Ag_2O	$K_2S_2O_8$	TFA	50
4	AgTFA	$K_2S_2O_8$	TFA	62
5	AgTFA	$Na_2S_2O_8$	TFA	39
6	AgTFA	$(NH_4)_2S_2O_8$	TFA	35
7	AgTFA	Oxone	TFA	30
8[c]	AgTFA	$K_2S_2O_8$	TFA	52
9[d]	AgTFA	$K_2S_2O_8$	TFA	65
10[d]	AgTFA	$K_2S_2O_8$	MsOH	nd
11[d]	AgTFA	$K_2S_2O_8$	$TsOH·H_2O$	nd
12[d]	AgTFA	$K_2S_2O_8$	AcOH	32
13[d]	AgTFA	$K_2S_2O_8$	PivOH	31

[a]Reaction conditions: **1a** (0.2 mmol), **2a** (0.3 mmol), $Pd(OAc)_2$ (0.02 mmol), Ag salt (0.04 mmol), Oxidant (0.4 mmol), Acid (3.0 equiv), HFIP (1.0 mL), Air, 80 °C, 48 h. [b]Isolated yield by flash column chromatography. [c]Ar. [d]AgTFA (0.06 mmol).

Screening of Auxiliary Groups



5. General procedure for palladium-catalyzed C4-acylation of indole

A mixture of indole substrates (**1**, 0.2 mmol), α-oxocarboxylic acids (**2**, 0.3 mmol), $Pd(OAc)_2$ (0.02 mmol), AgTFA(0.06 mmol), $K_2S_2O_8$ (0.4 mmol), TFA (0.6 mmol) and HFIP (1.0 mL) was added to a 15 mL sealed tube. The tube was stirred at 80 °C for 48 h. Then, the reaction mixture was cooled to room temperature. The mixture was filtered through Celite®, and the filter cake was rinsed with EtOAc. The combined organic was removed in vacuo. Then the mixture was subjected to column chromatography on silica gel to give the desired product.

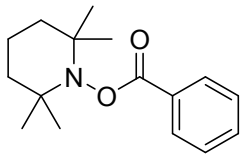
6. Gram-scale preparation of 3ea

A 15 mL Schlenk tube was charged with indole substrates **1e** (5 mmol), **2a** (7.5 mmol), and

$Pd(OAc)_2$ (10 mol%), AgTFA (30 mol%), $K_2S_2O_8$ (2.0 equiv) to a 15 mL sealed tube. The mixture was dissolved in 5 mL HFIP followed by addition of TFA (3.0 equiv).The reaction mixture was stirred for 48 hours at 80 °C. After that it was filtered through a short pad of Celite® and washed with ethyl acetate. The solvent was then evaporated under reduced pressure and the crude was purified by column chromatography on silica gel to afford the pure product **3ea** (1.50 g, 63% isolated yield).

7. Radical trapping experiments

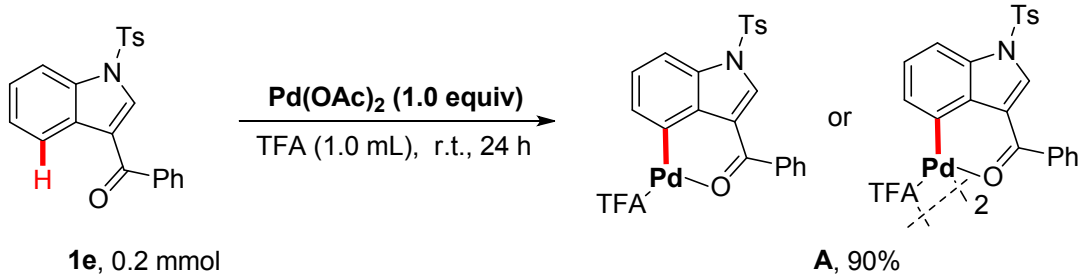
A mixture of **1e** (0.2 mmol), **2a** (0.3 mmol), TEMPO (0.6 mmol), $Pd(OAc)_2$ (10 mol%), AgTFA(30 mol%), $K_2S_2O_8$ (2.0 equiv) was dissolved in HFIP (1 mL). The mixture was sealed in an 8 mL sealed tube and was heated in an 80 ^oC oil bath for 3 h. After the reaction, the reaction mixture was cooled to room temperature and concentrated in vacuo. The crude product was purified by flash column chromatography, and 56% of **4** was isolated.



2,2,6,6-tetramethylpiperidin-1-yl benzoate (6)

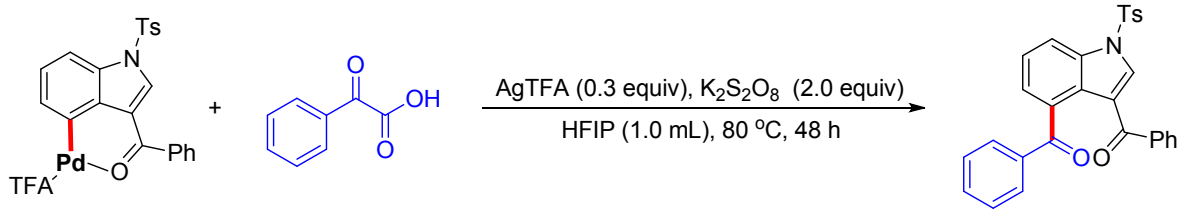
White solid. Melting point: 88-89 °C. **^{1}H NMR** (500 MHz, Chloroform-*d*) δ 8.09-8.07 (m, 2H), 7.59-7.56 (m, 1H), 7.48-7.45 (m, 2H), 1.81-1.68 (m, 3H), 1.66-1.58 (m, 2H), 1.48-1.44 (m, 1H), 1.28 (s, 6H), 1.12 (s, 6H). **^{13}C NMR** (125 MHz, Chloroform-*d*) δ 166.7, 133.2, 130.1, 129.9, 128.8, 60.8, 39.4, 32.3, 21.2, 17.4.

8. Mechanistic studies



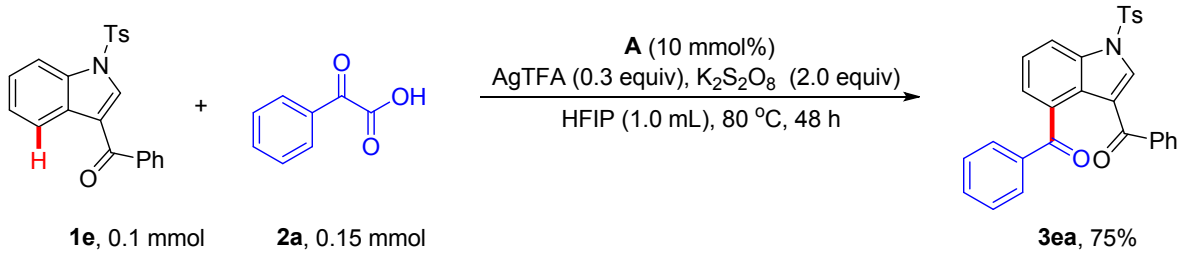
1e, 0.2 mmol **A**, 90%

To a 15 ml sealed-tube were added phenyl(1-tosyl-1*H*-indol-3-yl)methanone (75 mg, 0.20 mmol), $Pd(OAc)_2$ (46 mg, 0.20 mmol) and 1 mL TFA. The tube was sealed and stirred at r.t. for 24 h. Then the reaction mixture was filtered and washed with hexane to give the desired palladacycle product as an orange solid (115.4 mg, 90%).[5] ^{1}H NMR (500 MHz, DMSO-d_6) δ (ppm) 8.43 (s, 1H), 8.06 (d, J = 8.4 Hz, 2H), 8.01 (d, J = 7.3 Hz, 2H), 7.88 (t, J = 7.3 Hz,1H), 7.70-7.65 (m, 3H), 7.57 (d, J = 7.8 Hz, 1 H), 7.41 (d, J = 8.3 Hz, 2H), 7.22 (t, J = 8.0 Hz, 1H), 2.32 (s, 3H); ^{13}C NMR (125 MHz, DMSO-d_6) δ (ppm) 190.7, 147.2, 137.2, 133.9, 133.4, 132.4, 131.0, 130.3, 130.1, 129.7, 129.5, 128.6, 128.2, 125.6, 122.1, 110.8, 21.6; ^{19}F NMR (376 MHz, DMSO-d_6) δ (ppm) -73.56.



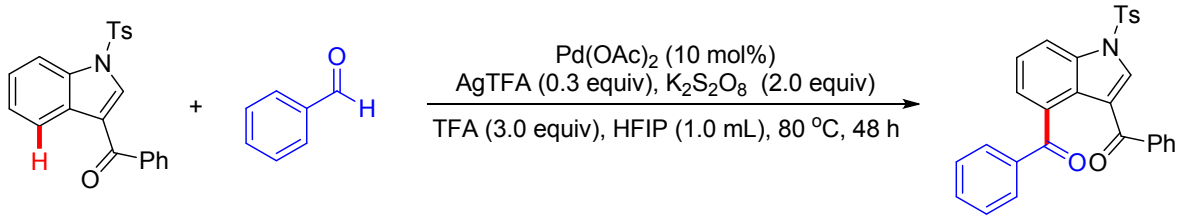
A, 0.1 mmol **2a**, 0.15 mmol **3ea**, 93%

A mixture of **A** (0.1 mmol), α-oxocarboxylic acids (**2a**, 0.15 mmol), AgTFA (0.06 mmol), $K_2S_2O_8$ (0.4 mmol) and HFIP (1.0 mL) was added to a 15 mL sealed tube. The tube was stirred at 80 °C for 48 h. Then, the reaction mixture was cooled to room temperature. The mixture was filtered through Celite®, and the filter cake was rinsed with EtOAc. The combined organic was removed in vacuo. Then the mixture was subjected to column chromatography on silica gel to give the desired product in 93% yield.



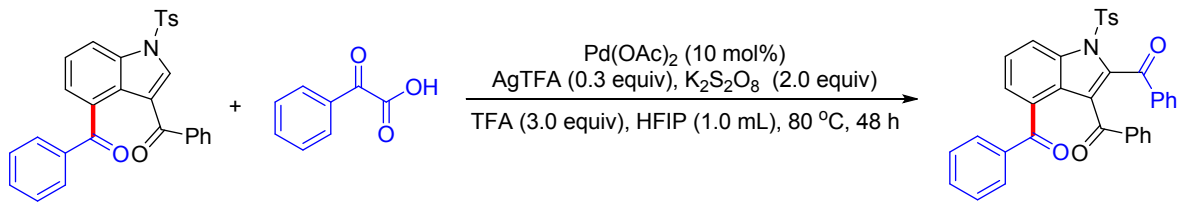
1e, 0.1 mmol **2a**, 0.15 mmol **3ea**, 75%

A mixture of indole substrates (**1e**, 0.1 mmol), α-oxocarboxylic acids (**2a**, 0.15 mmol), **A** (0.01 mmol), AgTFA (0.06 mmol), $K_2S_2O_8$ (0.4 mmol) and HFIP (1.0 mL) was added to a 15 mL sealed tube. The tube was stirred at 80 °C for 48 h. Then, the reaction mixture was cooled to room temperature. The mixture was filtered through Celite®, and the filter cake was rinsed with EtOAc. The combined organic was removed in vacuo. Then the mixture was subjected to column chromatography on silica gel to give the desired product in 75% yield.



1e, 0.2 mmol **7**, 0.30 mmol **3ea**, 0%

A mixture of indole substrates (**1e**, 0.2 mmol), aldehyde (**7**, 0.3 mmol), $Pd(OAc)_2$ (0.02 mmol), AgTFA (0.06 mmol), $K_2S_2O_8$ (0.4 mmol), TFA (0.6 mmol) and HFIP (1.0 mL) was added to a 15 mL sealed tube. The tube was stirred at 80 °C for 48 h. Then, the reaction mixture was cooled to room temperature. And the reaction was monitored by TLC.

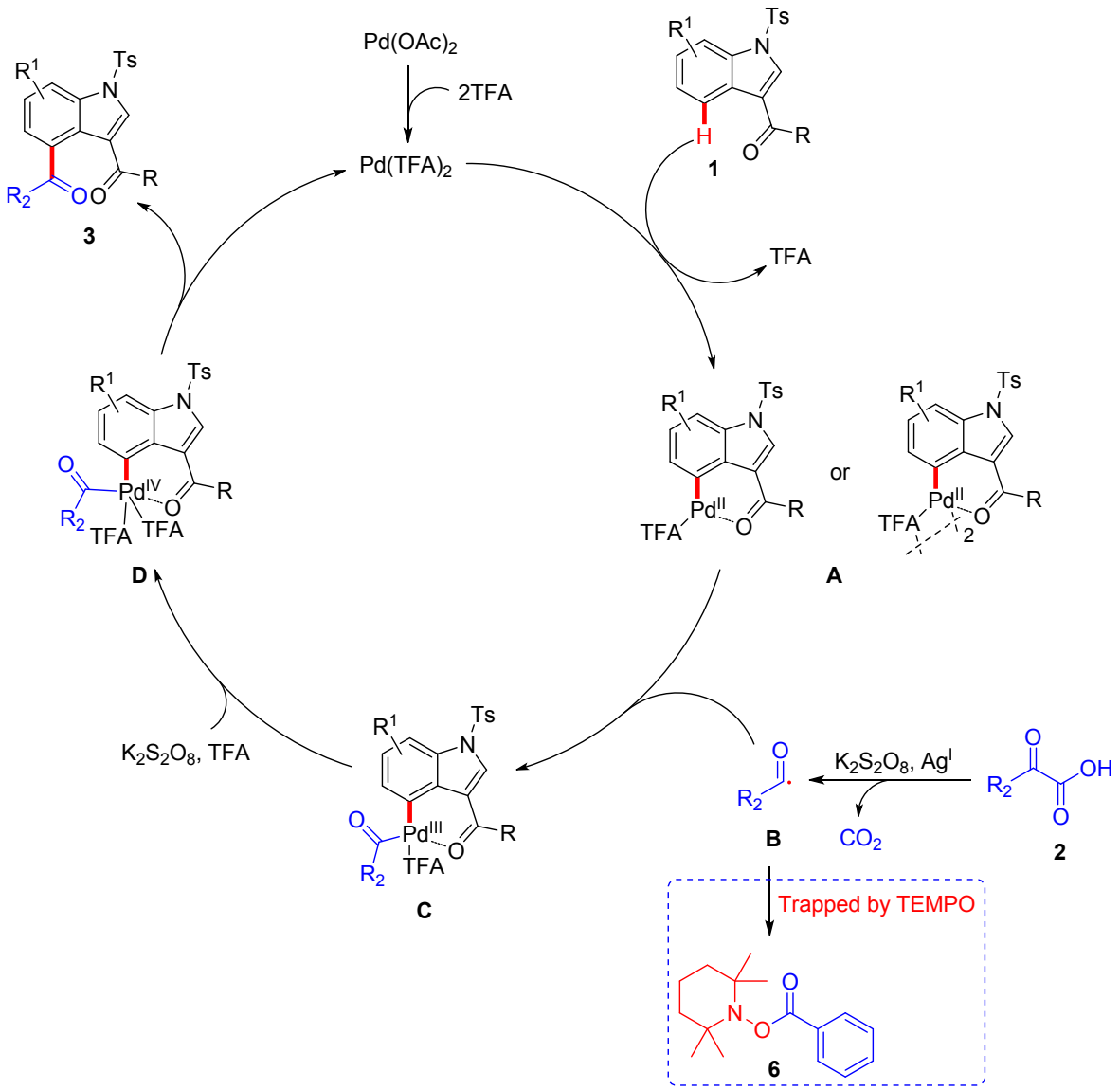


3ea, 0.1 mmol **2a**, 0.15 mmol **3eaa**, 0%

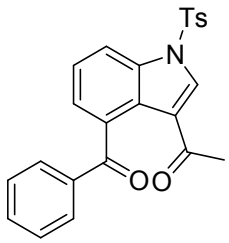
A mixture of indole substrates (**3ea**, 0.1 mmol), α-oxocarboxylic acids (**2a**, 0.15 mmol), $Pd(OAc)_2$ (0.01 mmol), AgTFA (0.06 mmol), $K_2S_2O_8$ (0.4 mmol), TFA (0.6 mmol) and HFIP (1.0 mL) was added to a 15 mL sealed tube. The tube was stirred at 80 °C for 48 h.

Then, the reaction mixture was cooled to room temperature. And the reaction was monitored by TLC.

9. Proposed mechanism

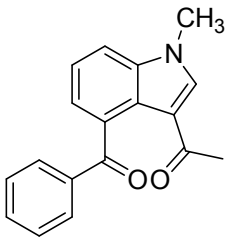


Analytic Data of Products



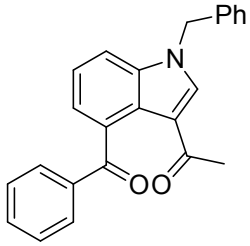
1-(4-benzoyl-1-tosyl-1*H*-indol-3-yl)ethanone (3aa)

White solid. Melting point: 173-174 °C. Isolated yield: 65%. **^{1}H NMR** (500 MHz, Chloroform-*d*) δ 8.24 (s, 1H), 8.08 (d, J = 8.4 Hz, 1H), 7.85 (d, J = 8.5 Hz, 2H), 7.82-7.80 (m, 2H), 7.54-7.51 (m, 1H), 7.45-7.39 (m, 3H), 7.33-7.29 (m, 3H), 2.41 (s, 3H), 2.39 (s, 3H). **^{13}C NMR** (125 MHz, Chloroform-*d*) δ 195.7, 192.1, 146.7, 138.2, 135.8, 135.4, 134.7, 133.2, 132.9, 130.8, 130.3, 128.7, 127.6, 125.7, 124.7, 124.0, 122.5, 115.0 27.9 22.1 **IR** (KBr, ν, cm^{-1}): 1678, 1666, 1597, 1531, 1489, 1446, 1384, 1172, 840, 748, 667. **HRMS** (ESI) m/z calcd for $C_{24}H_{20}NO_4S$ $(M+H)^+$: 418.1108, found: 418.1110.



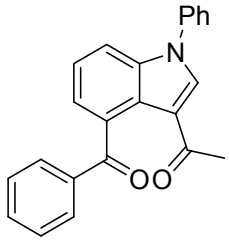
1-(4-benzoyl-1-methyl-1*H*-indol-3-yl)ethanone (3ba)

White solid. Melting point: 165-167 °C. Isolated yield: 51%. **^{1}H NMR** (500 MHz, Chloroform-*d*) δ 7.84-7.82 (m, 2H), 7.71 (s, 1H), 7.49-7.44 (m, 2H), 7.39-7.36 (m, 3H), 7.24 (dd, J = 0.9, 7.2 Hz, 1H), 3.89 (s, 3H), 2.28 (s, 3H). **^{13}C NMR** (125 MHz, Chloroform-*d*) δ 196.7, 191.0, 139.1, 138.3, 137.0, 134.9, 132.6, 130.1, 128.5, 123.4, 122.3, 122.2, 117.3, 111.5, 34.1, 27.2. **IR** (KBr, ν, cm^{-1}): 1658, 1639, 1597, 1573, 1527, 1450, 756, 713. **HRMS** (ESI) m/z calcd for $C_{18}H_{16}NO_2$ $(M+H)^+$: 278.1176, found: 278.1179.



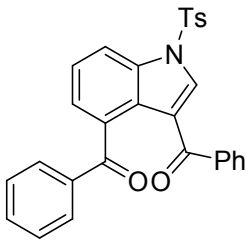
1-(4-benzoyl-1-benzyl-1*H*-indol-3-yl)ethanone (3ca)

White solid. Melting point: 182-183 °C. Isolated yield: 38%. **^{1}H NMR** (500 MHz, Chloroform-*d*) δ 7.89-7.87 (m, 2H), 7.77 (s, 1H), 7.51-7.48 (m, 1H), 7.43-7.31 (m, 7H), 7.23 (dd, J = 0.8, 7.3 Hz, 1H), 7.20-7.18 (m, 2H), 5.42 (s, 2H), 2.31 (s, 3H). **^{13}C NMR** (125 MHz, Chloroform-*d*) δ 196.7, 191.3, 138.9, 138.0, 136.1, 135.9, 135.2, 132.7, 130.2, 129.5, 128.8, 128.6, 127.4, 123.6, 122.6, 122.5, 118.1, 112.0, 51.3, 27.4. **IR** (KBr, ν, cm^{-1}): 1666, 1643, 1597, 1523, 1446, 1435, 759, 721, 694. **HRMS** (ESI) m/z calcd for $C_{24}H_{20}NO_2$ $(M+H)^+$: 354.1489, found: 354.1485.



1-(4-benzoyl-1-phenyl-1*H*-indol-3-yl)ethanone (3da)

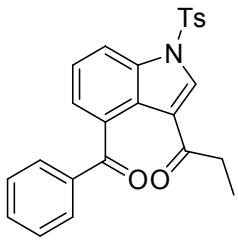
White solid. Melting point: 183-184 °C. Isolated yield: 46%. **^{1}H NMR** (500 MHz, Chloroform-*d*) δ 7.95 (s, 1H), 7.93-7.91 (m, 2H), 7.63-7.60 (m, 2H), 7.57-7.51 (m, 5H), 7.43 (t, J = 7.8 Hz, 2H), 7.38-7.34 (m, 1H), 7.29-7.28 (m, 1H), 2.39 (s, 3H). **^{13}C NMR** (125 MHz, Chloroform-*d*) δ 196.6, 191.5, 138.8, 138.5, 138.1, 135.8, 135.2, 132.8, 130.4, 130.3, 128.9, 128.6, 125.7, 124.0, 123.0, 122.6, 119.2, 112.7, 27.5. **IR** (KBr, ν, cm^{-1}): 1673, 1657, 1590, 1546, 1448, 1432, 748, 726, 695. **HRMS** (ESI) m/z calcd for $C_{23}H_{18}NO_2$ $(M+H)^+$: 340.1332, found: 340.1331.



(1-tosyl-1*H*-indole-3,4-diyl)bis(phenylmethanone) (3ea)

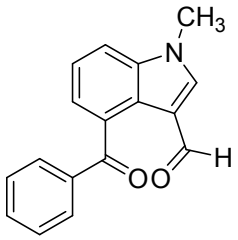
White solid. Melting point: 175-176 °C. Isolated yield: 77%. **^{1}H NMR** (500 MHz, Chloroform-*d*) δ 8.18 (dd, J = 0.8, 8.3 Hz, 1H), 7.96 (s, 1H), 7.83-7.81 (m, 2H), 7.79-7.76 (m, 4H), 7.51 (t, J = 7.4 Hz, 1H), 7.48-7.44 (m, 2H), 7.41-7.38 (m, 3H), 7.35 (t, J = 7.9 Hz, 2H), 7.29 (d, J = 8.4 Hz, 2H), 2.38 (s, 3H). **^{13}C NMR** (100 MHz, Chloroform-*d*) δ 195.2, 189.3, 146.2, 137.8, 137.2, 135.6, 134.3, 133.8, 133.0, 132.9, 132.7, 130.4, 130.2, 129.5, 128.5, 128.3, 127.2, 126.0, 125.3, 125.2, 121.5, 115.6, 21.7. **IR** (KBr, ν, cm^{-}

[1]): 1670, 1651, 1597, 1535, 1446, 1373, 1226, 875, 732, 702. **HRMS** (ESI) m/z calcd for $C_{29}H_{22}NO_4S$ $(M+H)^+$: 480.1264, found: 480.1263.



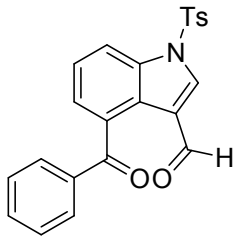
1-(4-benzoyl-1-tosyl-1*H*-indol-3-yl)propan-1-one (3fa)

Pale yellow solid. Melting point: 180-182 °C. Isolated yield: 65%. **^{1}H NMR** (500 MHz, Chloroform-*d*) δ 8.19 (s, 1H), 8.09 (dd, J = 1.0, 8.4 Hz, 1H), 7.85-7.83 (m, 2H), 7.79-7.77 (m, 2H), 7.53-7.50 (m, 1H), 7.45-7.41 (m, 2H), 7.39-7.38 (m, 1H), 7.33-7.31 (m, 3H), 2.72 (q, J = 7.4 Hz, 2H), 2.40 (s, 3H), 1.01 (t, J = 7.4 Hz, 3H). **^{13}C NMR** (125 MHz, Chloroform-*d*) δ 195.7, 195.6, 146.6, 138.3, 135.8, 135.1, 134.7, 133.1, 131.8, 130.8, 130.3, 128.7, 127.6, 125.7, 125.0, 124.5, 122.3, 115.2, 33.8, 22.1, 8.8. **IR** (KBr, ν, cm^{-1}): 1670, 1645, 1597, 1535, 1450, 1377, 1276, 813, 759, 709. **HRMS** (ESI) m/z calcd for $C_{25}H_{22}NO_4S$ $(M+H)^+$: 432.1264, found: 432.1267.



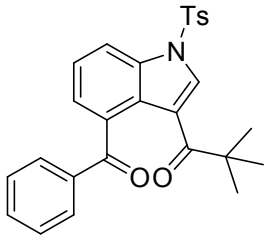
4-benzoyl-1-methyl-1*H*-indole-3-carbaldehyde (3ga)

White solid. Melting point: 172-173 °C. Isolated yield: 42%. **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 9.78 (s, 1H), 7.86-7.83 (m, 3H), 7.57-7.53 (m, 2H), 7.44-7.38 (m, 4H), 3.92 (s, 3H). **^{13}C NMR** (100 MHz, Chloroform-*d*) δ 197.3, 184.5, 138.3, 138.3, 138.2, 138.0, 133.0, 132.9, 130.1, 128.4, 123.6, 122.9, 117.7, 112.6, 34.0. **IR** (KBr, ν, cm^{-1}): 1693, 1670, 1597, 1535, 1450, 1280, 790, 759, 717. **HRMS** (ESI) m/z calcd for $C_{17}H_{14}NO_2$ $(M+H)^+$: 264.1019, found: 264.1023.



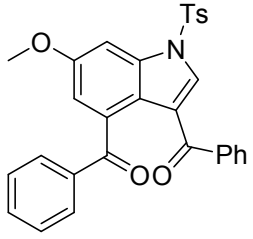
4-benzoyl-1-tosyl-1*H*-indole-3-carbaldehyde (3ha)

White solid. Melting point: 122-123 °C. Isolated yield: 25%. **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 9.87 (s, 1H), 8.36 (s, 1H), 8.16 (dd, *J* = 0.9, 8.3 Hz, 1H), 7.87 (d, 8.4 Hz, 2H), 7.83-7.81 (m, 2H), 7.59-7.55 (m, 1H), 7.50-7.42 (m, 3H), 7.41-7.39 (m, 1H), 7.33 (d, *J* = 8.1 Hz, 2H), 2.41 (s, 3H). **^{13}C NMR** (100 MHz, Chloroform-*d*) δ 196.2, 184.6, 146.5, 137.3, 135.6, 135.4, 134.0, 133.7, 133.3, 130.4, 130.2, 128.5, 127.3, 125.4, 125.2, 123.3, 122.1, 115.5, 21.7. **IR** (KBr, ν, cm^{-1}): 1684, 1674, 1584, 1573, 1447, 821, 785, 755, 728. **HRMS** (ESI) m/z calcd for $C_{23}H_{18}NO_4S$ $(M+H)^+$: 404.0951, found: 404.0948.



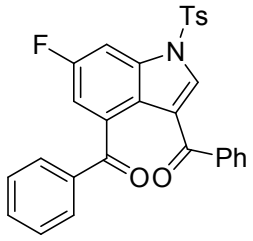
1-(4-benzoyl-1-tosyl-1*H*-indol-3-yl)-2,2-dimethylpropan-1-one (3ia)

White solid. Melting point: 117-119 °C. Isolated yield: 68%. **^{1}H NMR** (500 MHz, Chloroform-*d*) δ 8.11 (dd, *J* = 1.0, 8.3 Hz, 1H), 8.04 (s, 1H), 7.81 (d, *J* = 8.4 Hz, 2H), 7.76-7.74 (m, 2H), 7.54-7.51 (m, 1H), 7.42-7.38 (m, 3H), 7.35-7.34 (m, 1H), 7.30 (d, *J* = 8.0 Hz, 2H), 2.39 (s, 3H), 1.20 (s, 9H). **^{13}C NMR** (125 MHz, Chloroform-*d*) δ 203.7, 195.4, 146.4, 138.2, 135.1, 134.8, 134.0, 133.1, 130.7, 130.2, 128.6, 128.1, 127.4, 127.0, 125.6, 125.2, 120.9, 115.7, 44.7, 27.8, 22.0. **IR** (KBr, ν, cm^{-1}): 1674, 1648, 1597, 1535, 1473, 1450, 1369, 1281, 806, 759, 717. **HRMS** (ESI) m/z calcd for $C_{27}H_{26}NO_4S$ $(M+H)^+$: 460.1517, found: 460.1515.



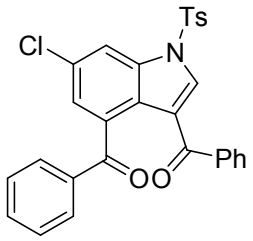
(6-methoxy-1-tosyl-1*H*-indole-3,4-diyl)bis(phenylmethanone) (3ka)

White solid. Melting point: 155-156 °C. Isolated yield: 53%. **^{1}H NMR** (500 MHz, Chloroform-*d*) δ 7.83 (s, 1H), 7.81-7.78 (m, 4H), 7.75-7.73 (m, 2H), 7.67 (d, J = 2.3 Hz, 1H), 7.53-7.50 (m, 1H), 7.47-7.44 (m, 1H), 7.40 (t, J = 7.9 Hz, 2H), 7.35 (t, J = 8.0 Hz, 2H), 7.31 (d, J = 8.1 Hz, 2H), 7.02 (d, J = 2.3 Hz, 1H), 3.90 (s, 3H), 2.41 (s, 3H). **^{13}C NMR** (125 MHz, Chloroform-*d*) δ 195.0, 189.6, 158.2, 146.5, 138.2, 137.4, 137.1, 134.8, 134.7, 133.2, 133.0, 132.1, 130.7, 130.4, 129.8, 128.7, 128.6, 127.5, 121.9, 120.0, 114.2, 100.0, 56.4, 22.0. **IR** (KBr, ν, cm^{-1}): 1670, 1651, 1597, 1577, 1489, 1446, 1373, 1234, 825, 763, 729, 705. **HRMS** (ESI) m/z calcd for $C_{30}H_{24}NO_5S$ $(M+H)^+$: 510.1370, found: 510.1375.



(6-fluoro-1-tosyl-1*H*-indole-3,4-diyl)bis(phenylmethanone) (3la)

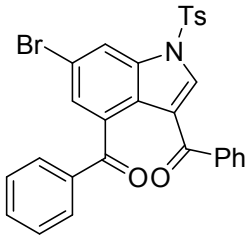
White solid. Melting point: 123-124 °C. Isolated yield: 81%. **^{1}H NMR** (500 MHz, Chloroform-*d*) δ 7.92 (s, 1H), 7.91 (dd, J = 2.3, 8.9 Hz, 1H), 7.83-7.81 (m, 2H), 7.80-7.75 (m, 4H), 7.55-7.52 (m, 1H), 7.50-7.47 (m, 1H), 7.43-7.40 (m, 2H), 7.39-7.36 (m, 2H), 7.34-7.32 (m, 2H), 7.17 (dd, J = 2.3, 9.0 Hz, 1H), 2.42 (s, 3H). **^{13}C NMR** (125 MHz, Chloroform-*d*) δ 194.1, 189.3, 160.7 (d, J = 244.7 Hz), 146.8, 138.0, 137.0, 136.3 (d, J = 11.9 Hz), 135.4 (d, J = 7.3 Hz), 134.5, 133.5, 133.3, 133.2, 130.8, 130.4, 129.8, 128.8, 128.7, 127.6, 122.7, 121.7, 114.0 (d, J = 24.8 Hz), 103.1 (d, J = 27.9 Hz), 22.1. **IR** (KBr, ν, cm^{-1}): 1701, 1654, 1597, 1558, 1489, 1450, 1373, 1261, 802, 705. **HRMS** (ESI) m/z calcd for $C_{29}H_{21}FNO_4S$ $(M+H)^+$: 498.1170, found: 498.1167.



(6-chloro-1-tosyl-1*H*-indole-3,4-diyl)bis(phenylmethanone) (3ma)

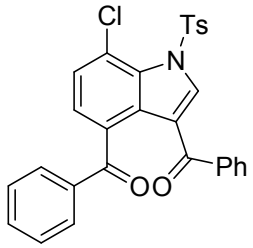
White solid. Melting point: 219-220 °C. Isolated yield: 72%. **^{1}H NMR** (500 MHz, Chloroform-*d*) δ 8.20 (d, J = 1.8 Hz, 1H), 7.93 (s, 1H), 7.83-7.81 (m, 2H), 7.78-7.77 (m, 2H), 7.75-7.73 (m, 2H), 7.54-7.51 (m, 1H), 7.50-7.47 (m, 1H), 7.42-7.36 (m, 5H), 7.33 (d, J = 8.1 Hz, 2H), 2.41 (s, 3H). **^{13}C NMR** (125 MHz,

Chloroform-*d*) δ 194.0, 189.2, 146.9, 137.9, 137.1, 136.4, 135.1, 134.5, 133.5, 133.3, 131.7, 130.9, 130.4, 129.8, 128.9, 128.8, 127.5, 125.7, 124.9, 121.6, 115.8, 22.1. **IR** (KBr, ν, cm^{-1}): 1670, 1643, 1597, 1531, 1446, 1381, 1226, 806, 759, 721, 702. **HRMS** (ESI) m/z calcd for $C_{29}H_{21}ClNO_4S$ $(M+H)^+$: 514.0874, found: 514.0873.



(6-bromo-1-tosyl-1*H*-indole-3,4-diyl)bis(phenylmethanone) (3na)

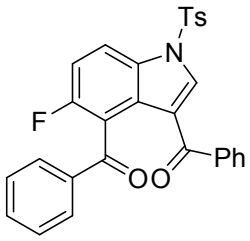
White solid. Melting point: 224-226 °C. Isolated yield: 71%. **^{1}H NMR** (500 MHz, Chloroform-*d*) δ 8.36 (d, J = 1.7 Hz, 1H), 7.91 (s, 1H), 7.83-7.81 (m, 2H), 7.78-7.76 (m, 2H), 7.75-7.73 (m, 2H), 7.55-7.51 (m, 2H), 7.50-7.47 (m, 1H), 7.42-7.33 (m, 6H), 2.42 (s, 3H). **^{13}C NMR** (125 MHz, Chloroform-*d*) δ 193.9, 189.2, 146.9, 137.9, 137.0, 136.6, 135.4, 134.4, 133.5, 133.3, 133.2, 130.9, 130.4, 129.8, 128.9, 128.8, 128.3, 127.5, 125.2, 121.7, 119.1, 118.7, 22.1. **IR** (KBr, ν, cm^{-1}): 1668, 1643, 1582, 1527, 1433, 1376, 1216, 802, 749, 718, 703. **HRMS** (ESI) m/z calcd for $C_{29}H_{21}BrNO_4S$ $(M+H)^+$: 558.0369, found: 558.0371.



(7-chloro-1-tosyl-1*H*-indole-3,4-diyl)bis(phenylmethanone) (3oa)

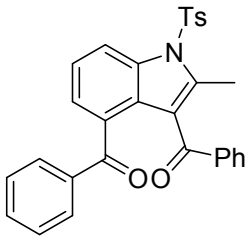
White solid. Melting point: 202-203 °C. Isolated yield: 73%. **^{1}H NMR** (500 MHz, Chloroform-*d*) δ 8.30 (s, 1H), 7.83-7.81 (m, 2H), 7.80-7.79 (m, 2H), 7.74 (d, J = 8.4 Hz, 2H), 7.55-7.52 (m, 1H), 7.50-7.47 (m, 1H), 7.42 (t, J = 7.9 Hz, 2H), 7.39-7.35 (m, 4H), 7.33-7.30 (m, 2H), 2.44 (s, 3H). **^{13}C NMR** (125 MHz, Chloroform-*d*) δ 194.7, 189.5, 146.1, 137.9, 137.4, 136.8, 136.5, 133.4, 133.3, 132.7, 130.5, 130.4, 130.3, 129.9, 128.9, 128.7, 127.8, 127.6, 126.4, 121.8, 120.4, 22.1. **IR** (KBr, ν, cm^{-1}): 1668, 1645, 1588, 1517, 1426, 1389, 1253, 805, 746, 718, 706. **HRMS** (ESI) m/z calcd for $C_{29}H_{21}ClNO_4S$ $(M+H)^+$: 514.0874,

found: 514.0872.



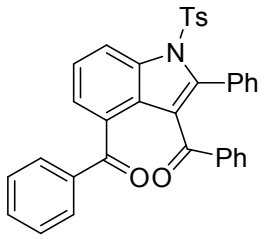
(5-fluoro-1-tosyl-1*H*-indole-3,4-diyl)bis(phenylmethanone) (3qa)

White solid. Melting point: 207-208 °C. Isolated yield: 71%. **^{1}H NMR** (500 MHz, Chloroform-*d*) δ 8.11 (dd, *J* = 4.2, 9.2 Hz, 1H), 7.98 (s, 1H), 7.86 (d, *J* = 7.5 Hz, 2H), 7.80 (d, *J* = 8.5 Hz, 2H), 7.74-7.72 (m, 2H), 7.56-7.51 (m, 2H), 7.43-7.39 (m, 4H), 7.32 (d, *J* = 8.0 Hz, 2H), 7.22 (t, *J* = 9.3 Hz, 1H), 2.41 (s, 3H). **^{13}C NMR** (125 MHz, Chloroform-*d*) δ 191.7, 189.1, 157.3 (d, *J* = 242.5 Hz), 146.8, 138.2 (d, *J* = 12.5 Hz), 134.7, 134.5, 133.6, 133.2, 132.2, 130.8, 129.9, 129.8, 128.9, 128.8, 127.5, 127.2 (d, *J* = 6.3 Hz), 121.4 (d, *J* = 33.8 Hz), 116.4 (d, *J* = 8.8 Hz), 114.7 (d, *J* = 26.3 Hz), 22.0. **IR** (KBr, ν, cm^{-1}): 1712, 1643, 1583, 1552, 1471, 1452, 1367, 1251, 808, 706. **HRMS** (ESI) m/z calcd for $C_{29}H_{21}FNO_4S$ $(M+H)^+$: 498.1170, found: 498.1171.



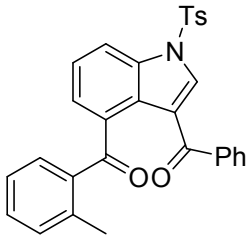
(2-methyl-1-tosyl-1*H*-indole-3,4-diyl)bis(phenylmethanone) (3sa)

White solid. Melting point: 158-159 °C. Isolated yield: 42%. **^{1}H NMR** (500 MHz, Chloroform-*d*) δ 8.49 (dd, *J* = 1.1, 8.4 Hz, 1H), 7.78-7.76 (m, 2H), 7.61-7.57 (m, 4H), 7.45-7.41 (m, 1H), 7.39-7.36 (m, 1H), 7.32 (dd, *J* = 1.1, 7.5 Hz, 1H), 7.29-7.26 (m, 5H), 7.22-7.19 (m, 2H), 2.54 (s, 3H), 2.41 (s, 3H). **^{13}C NMR** (125 MHz, Chloroform-*d*) δ 196.0, 192.8, 146.1, 141.6, 140.4, 138.7, 137.1, 136.1, 133.1, 133.0, 131.4, 130.7, 130.6, 129.6, 128.7, 128.3, 127.1, 127.0, 126.4, 124.0, 120.8, 117.7, 22.0, 14.6. **IR** (KBr, ν, cm^{-1}): 1677, 1658, 1597, 1450, 1427, 1377, 1234, 813, 759, 725, 705. **HRMS** (ESI) m/z calcd for $C_{30}H_{24}NO_4S$ $(M+H)^+$: 494.1421, found: 494.1423.



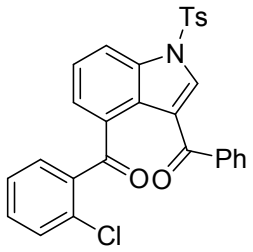
(2-phenyl-1-tosyl-1*H*-indole-3,4-diyl)bis(phenylmethanone) (3ta)

White solid. Melting point: 178-179 °C. Isolated yield: 40%. **^{1}H NMR** (500 MHz, Chloroform-*d*) δ 8.66 (dd, J = 1.0, 8.5 Hz, 1H), 7.64-7.62 (m, 2H), 7.51-7.47 (m, 1H), 7.43-7.39 (m, 4H), 7.32-7.26 (m, 4H), 7.22-7.18 (m, 3H), 7.17-7.11 (m, 5H), 7.05-7.02 (m, 2H), 2.36 (s, 3H). **^{13}C NMR** (125 MHz, Chloroform-*d*) δ 195.7, 192.7, 145.9, 142.2, 137.8, 137.4, 135.4, 133.1, 132.7, 132.2, 132.0, 130.6, 130.0, 129.8, 129.7, 129.6, 128.4, 128.1, 127.5, 127.4, 127.2, 126.8, 124.8, 123.6, 119.0, 22.0. **IR** (KBr, ν, cm^{-1}): 1673, 1646, 1594, 1455, 1417, 1327, 1221, 803, 739, 728, 706. **HRMS** (ESI) m/z calcd for $C_{35}H_{26}NO_4S$ $(M+H)^+$: 556.1577, found: 556.1576.



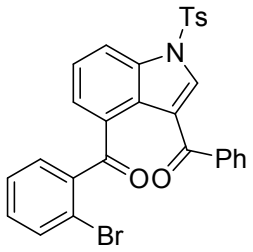
(3-benzoyl-1-tosyl-1*H*-indol-4-yl)(*o*-tolyl)methanone (3eb)

White solid. Melting point: 151-153 °C. Isolated yield: 58%. **^{1}H NMR** (500 MHz, Chloroform-*d*) δ 8.19 (dd, J = 0.9, 8.4 Hz, 1H), 7.94 (s, 1H), 7.84-7.81 (m, 4H), 7.56-7.53 (m, 1H), 7.44-7.40 (m, 3H), 7.34-7.33 (m, 1H), 7.32-7.29 (m, 3H), 7.27-7.24 (m, 1H), 7.16-7.14 (m, 1H), 7.09 (t, J = 7.5 Hz, 1H), 2.43 (s, 3H), 2.39 (s, 3H). **^{13}C NMR** (125 MHz, Chloroform-*d*) δ 197.3, 189.8, 146.5, 139.7, 138.1, 137.6, 136.0, 135.1, 134.8, 133.3, 132.1, 131.7, 131.6, 131.4, 130.7, 129.9, 128.8, 127.5, 126.6, 126.5, 125.5, 125.4, 122.4, 116.6, 22.0, 21.2. **IR** (KBr, ν, cm^{-1}): 1666, 1651, 1597, 1535, 1454, 1415, 1377, 1261, 813, 763, 729, 702. **HRMS** (ESI) m/z calcd for $C_{30}H_{24}NO_4S$ $(M+H)^+$: 494.1421, found: 494.1417.



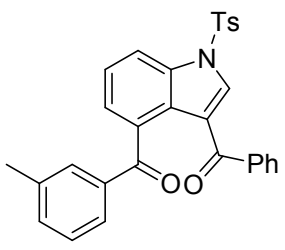
(3-benzoyl-1-tosyl-1*H*-indol-4-yl)(2-chlorophenyl)methanone (3ec)

White solid. Melting point: 133-134 °C. Isolated yield: 75%. **^{1}H NMR** (500 MHz, Chloroform-*d*) δ 8.24 (d, J = 8.3 Hz, 1H), 7.98 (s, 1H), 7.89 (d, J = 7.2 Hz, 2H), 7.83 (d, J = 8.3 Hz, 2H), 7.56 (t, J = 7.3 Hz, 1H), 7.46-7.42 (m, 3H), 7.41-7.30 (m, 6H), 7.25-7.23 (m, 1H), 2.40 (s, 3H). **^{13}C NMR** (125 MHz, Chloroform-*d*) δ 193.8, 189.9, 146.5, 138.3, 137.7, 136.1, 134.9, 133.3, 133.2, 133.1, 132.3, 132.1, 131.6, 130.8, 130.7, 130.0, 128.8, 127.5, 127.2, 126.8, 126.4, 125.4, 122.7, 117.6, 22.0. **IR** (KBr, ν, cm^{-1}): 1678, 1654, 1593, 1570, 1473, 1435, 1303, 1226, 813, 744, 713. **HRMS** (ESI) m/z calcd for $C_{29}H_{21}ClNO_4S$ $(M+H)^+$: 514.0874, found: 514.0876.



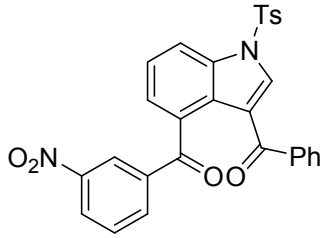
(3-benzoyl-1-tosyl-1*H*-indol-4-yl)(2-bromophenyl)methanone (3ed)

White solid. Melting point: 161-163 °C. Isolated yield: 64%. **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 8.25 (d, J = 10.2 Hz, 1H), 8.00 (s, 1H), 7.90-7.89 (m, 2H), 7.84-7.82 (m, 2H), 7.57-7.54 (m, 2H), 7.46-7.38 (m, 4H), 7.33-7.25 (m, 5H), 2.38 (s, 3H). **^{13}C NMR** (125 MHz, Chloroform-*d*) δ 194.4, 190.0, 146.5, 139.7, 138.3, 136.1, 134.9, 134.0, 133.3, 132.7, 132.2, 132.0, 131.5, 130.7, 130.0, 128.8, 127.6, 127.5, 127.3, 126.6, 125.4, 122.8, 121.3, 117.8, 22.0. **IR** (KBr, ν, cm^{-1}): 1667, 1647, 1592, 1577, 1422, 1371, 1219, 803, 729, 703. **HRMS** (ESI) m/z calcd for $C_{29}H_{21}BrNO_4S$ $(M+H)^+$: 558.0369, found: 558.0367.



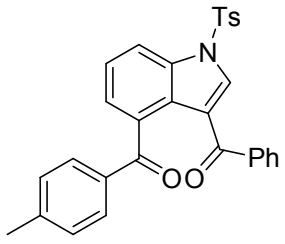
(3-benzoyl-1-tosyl-1*H*-indol-4-yl)(m-tolyl)methanone (3ee)

White solid. Melting point: 188-190 °C. Isolated yield: 60%. **^{1}H NMR** (500 MHz, Chloroform-*d*) δ 8.19-8.17 (m, 1H), 7.95 (s, 1H), 7.82 (d, J = 8.4 Hz, 2H), 7.79-7.78 (m, 2H), 7.63 (s, 1H), 7.57-7.52 (m, 2H), 7.48-7.45 (m, 1H), 7.43-7.40 (m, 3H), 7.31-7.30 (m, 2H), 7.28-7.26 (m, 1H), 7.25-7.22 (m, 1H), 2.40 (s, 3H), 2.31 (s, 3H). **^{13}C NMR** (125 MHz, Chloroform-*d*) δ 195.6, 189.6, 146.5, 138.4, 138.1, 137.5, 135.9, 134.7, 134.2, 134.0, 133.2, 132.9, 130.8, 130.7, 129.9, 128.7, 128.5, 127.9, 127.5, 126.4, 125.6, 125.5, 121.9, 115.9, 22.0, 21.6. **IR** (KBr, ν, cm^{-1}): 1693, 1670, 1593, 1535, 1446, 1415, 1373, 1280, 813, 748, 709. **HRMS** (ESI) m/z calcd for $C_{30}H_{24}NO_4S$ $(M+H)^+$: 494.1421, found: 494.1420.



(3-benzoyl-1-tosyl-1*H*-indol-4-yl)(3-nitrophenyl)methanone (3ef)

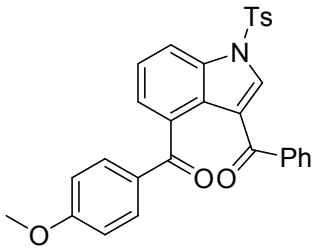
White solid. Melting point: 155-156 °C. Isolated yield: 72%. **^{1}H NMR** (500 MHz, Chloroform-*d*) δ 8.55-8.54 (m, 1H), 8.30-8.28 (m, 1H), 8.24 (dd, J = 0.9, 8.5 Hz, 1H), 8.21 (d, J = 7.7 Hz, 1H), 8.02 (s, 1H), 7.85-7.83 (m, 2H), 7.76-7.74 (m, 2H), 7.60-7.51 (m, 3H), 7.44-7.40 (m, 3H), 7.33 (d, J = 8.4 Hz, 2H), 2.41 (s, 3H). **^{13}C NMR** (125 MHz, Chloroform-*d*) δ 193.0, 189.7, 148.4, 146.8, 139.2, 137.9, 136.0, 135.7, 134.5, 133.8, 133.4, 132.8, 130.8, 130.0, 129.7, 129.0, 127.6, 127.4, 126.0, 125.9, 125.3, 125.1, 121.2, 116.6, 22.1. **IR** (KBr, ν, cm^{-1}): 1670, 1643, 1597, 1531, 1446, 1419, 1381, 1226, 810, 756, 717. **HRMS** (ESI) m/z calcd for $C_{29}H_{21}N_2O_6S$ $(M+H)^+$: 525.1115, found: 525.1118.



(3-benzoyl-1-tosyl-1*H*-indol-4-yl)(p-tolyl)methanone (3eg)

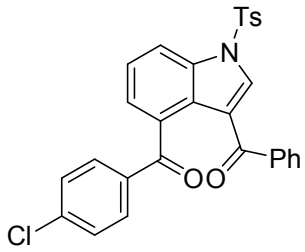
White solid. Melting point: 184-186 °C. Isolated yield: 71%. **^{1}H NMR** (500 MHz, Chloroform-*d*) δ 8.18-8.16 (m, 1H), 7.94 (s, 1H), 7.83-7.81(m, 2H)), 7.78-7.77 (m, 2H), 7.69-7.68 (m, 2H), 7.54-7.51 (m, 1H), 7.48-7.44 (m, 1H), 7.42-7.39 (m, 3H), 7.31-7.29 (m, 2H), 7.16-7.14 (m, 2H), 2.40 (s, 3H), 2.33 (s,

3H). **^{13}C NMR** (125 MHz, Chloroform-*d*) δ 195.2, 189.6, 146.5, 144.0, 138.2, 135.9, 135.1, 134.8, 134.4, 133.1, 132.9, 130.7, 130.6, 129.9, 129.3, 128.7, 127.5, 126.3, 125.5, 125.4, 121.9, 115.7, 22.1 22.0. **IR** (KBr, ν, cm^{-1}): 1666, 1647, 1600, 1573, 1446, 1373, 1276, 759, 729, 709. **HRMS** (ESI) m/z calcd for $C_{30}H_{24}NO_4S$ $(M+H)^+$: 494.1421, found: 494.1423.



(3-benzoyl-1-tosyl-1*H*-indol-4-yl)(4-methoxyphenyl)methanone (3eh)

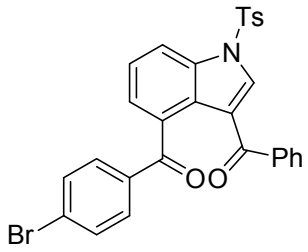
White solid. Melting point: 180-182 °C. Isolated yield: 72%. **^{1}H NMR** (500 MHz, Chloroform-*d*) δ 8.16 (dd, *J* = 0.9, 8.4 Hz, 1H), 7.95 (s, 1H), 7.83-7.81 (m, 2H), 7.79-7.77 (m, 4H), 7.54-7.51 (m, 1H), 7.48-7.45 (m, 1H), 7.42-7.38 (m, 3H), 7.31-7.29 (m, 2H), 6.85-6.83 (m, 2H), 3.80 (s, 3H), 2.40 (s, 3H). **^{13}C NMR** (125 MHz, Chloroform-*d*) δ 194.3, 189.6, 163.8, 146.5, 138.2, 135.9, 134.7, 134.5, 133.1, 132.9, 132.8, 130.7, 130.6, 129.9, 128.7, 127.5, 126.3, 125.5, 125.3, 121.9, 115.6, 113.9, 55.8, 22.0. **IR** (KBr, ν, cm^{-1}): 1668, 1643, 1573, 1527, 1485, 1465, 1388, 1242, 744, 694. **HRMS** (ESI) m/z calcd for $C_{30}H_{24}NO_5S$ $(M+H)^+$: 510.1370, found: 510.1369.



(3-benzoyl-1-tosyl-1*H*-indol-4-yl)(4-chlorophenyl)methanone (3ei)

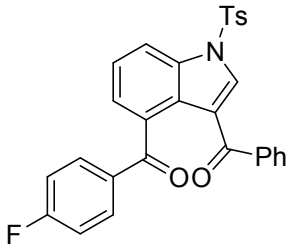
White solid. Melting point: 191-192 °C. Isolated yield: 73%. **^{1}H NMR** (500 MHz, Chloroform-*d*) δ 8.19 (dd, *J* = 0.8, 8.4 Hz, 1H), 7.97 (s, 1H), 7.83-7.82 (m, 2H), 7.79-7.77 (m, 2H), 7.75-7.73 (m, 2H), 7.57-7.54 (m, 1H), 7.50-7.46 (m, 1H), 7.45-7.42 (m, 2H), 7.39-7.37 (m, 1H), 7.34-7.30 (m, 4H), 2.41 (s, 3H). **^{13}C NMR** (125 MHz, Chloroform-*d*) δ 194.3, 189.6, 146.6, 139.7, 138.1, 136.1, 136.0, 134.7, 133.7, 133.3, 133.2, 131.8, 130.7, 129.8, 129.0, 128.9, 127.6, 126.1, 125.6, 125.3, 121.6, 116.0, 22.0. **IR** (KBr, ν, cm^{-1}): 1666, 1647, 1593, 1535, 1485, 1373, 1226, 790, 748, 709. **HRMS** (ESI) m/z calcd for

$C_{29}H_{21}ClNO_4S$ $(M+H)^+$: 514.0874, found: 514.0877.



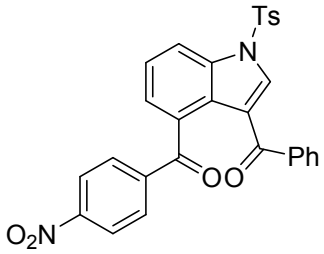
(3-benzoyl-1-tosyl-1*H*-indol-4-yl)(4-bromophenyl)methanone (3ej)

White solid. Melting point: 209-211 °C. Isolated yield: 80%. **^{1}H NMR** (500 MHz, Chloroform-*d*) δ 8.19 (dd, J = 0.9, 8.4 Hz, 1H), 7.98 (s, 1H), 7.83-7.82 (m, 2H), 7.79-7.77 (m, 2H), 7.67-7.66 (m, 2H), 7.57-7.54 (m, 1H), 7.51-7.49 (m, 2H), 7.48-7.42 (m, 3H), 7.38-7.37 (m, 1H), 7.32-7.30 (m, 2H), 2.40 (s, 3H). **^{13}C NMR** (125 MHz, Chloroform-*d*) δ 194.5, 189.6, 146.6, 138.0, 136.4, 135.9, 134.6, 133.6, 133.4, 133.3, 132.0, 131.9, 130.7, 129.8, 128.9, 128.5, 127.6, 126.1, 125.6, 125.3, 121.6, 116.1, 22.1. **HRMS** (ESI) m/z calcd for $C_{29}H_{21}BrNO_4S$ $(M+H)^+$: 558.0369, found: 558.0374.



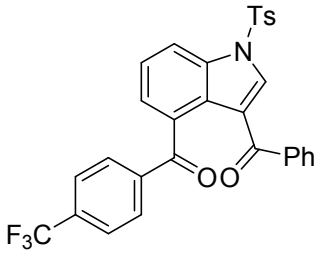
(3-benzoyl-1-tosyl-1*H*-indol-4-yl)(4-fluorophenyl)methanone (3ek)

White solid. Melting point: 140-141 °C. Isolated yield: 78%. **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 8.19 (dd, J = 0.9, 8.4 Hz, 1H), 7.98 (s, 1H), 7.85-7.82 (m, 4H), 7.79-7.77 (m, 2H), 7.57-7.53 (m, 1H), 7.50-7.46 (m, 1H), 7.45-7.41 (m, 2H), 7.40-7.38 (m, 1H), 7.32-7.30 (m, 2H), 7.06-7.02 (m, 2H), 2.40 (s, 3H). **^{13}C NMR** (100 MHz, Chloroform-*d*) δ 193.6, 189.3, 165.6 (d, J = 253.3 Hz), 146.2, 137.7, 135.6, 134.2, 133.7 (d, J = 2.3 Hz), 133.5, 132.9, 132.7, 132.6, 130.4, 129.5, 128.5, 127.2, 125.8, 125.2, 124.9, 121.3, 115.6 (d, J = 4.5 Hz), 115.3, 21.7. **IR** (KBr, ν, cm^{-1}): 1673, 1643, 1597, 1531, 1477, 1446, 1373, 1207, 748, 729, 713. **HRMS** (ESI) m/z calcd for $C_{29}H_{21}FNO_4S$ $(M+H)^+$: 498.1170, found: 498.1168.



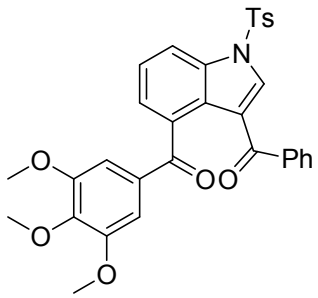
(3-benzoyl-1-tosyl-1*H*-indol-4-yl)(4-nitrophenyl)methanone (3el)

Pale yellow solid. Melting point: 239-241 °C. Isolated yield: 28%. **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 8.25-8.23 (m, 1H), 8.21-8.19 (m, 2H), 8.01 (s, 1H), 7.97-7.94 (m, 2H), 7.85-7.83 (m, 2H), 7.77-7.75 (m, 2H), 7.59-7.51 (m, 2H), 7.47-7.39 (m, 3H), 7.34-7.32 (m, 2H), 2.42 (s, 3H). **^{13}C NMR** (100 MHz, Chloroform-*d*) δ 193.2, 189.3, 149.9, 146.4, 142.2, 137.4, 135.5, 134.1, 133.3, 133.1, 132.6, 130.8, 130.4, 129.4, 128.6, 127.2, 125.6, 125.5, 124.9, 123.5, 120.8, 116.1, 21.7. **IR** (KBr, ν, cm^{-1}): 1666, 1646, 1593, 1539, 1477, 1446, 1377, 1238, 783, 759, 713. **HRMS** (ESI) m/z calcd for $C_{29}H_{21}N_2O_6S$ $(M+H)^+$: 525.1115, found: 525.1116.



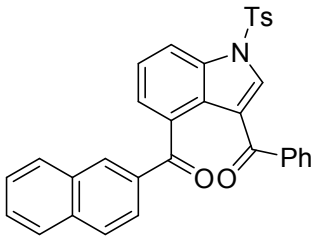
(3-benzoyl-1-tosyl-1*H*-indol-4-yl)(4-(trifluoromethyl)phenyl)methanone (3em)

White solid. Melting point: 169-170 °C. Isolated yield: 67%. **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 8.22 (d, J = 8.2 Hz, 1H), 8.00 (s, 1H), 7.92-7.90 (m, 2H), 7.85-7.82 (m, 2H), 7.78-7.76 (m, 2H), 7.63-7.61 (m, 2H), 7.57-7.54 (m, 1H), 7.52-7.48 (m, 1H), 7.45-7.39 (m, 3H), 7.32-7.30 (m, 2H), 2.40 (s, 3H). **^{13}C NMR** (100 MHz, Chloroform-*d*) δ 194.0, 189.3, 146.4, 140.1, 137.5, 135.6, 134.1, 134.0 (q, J = 32.4 Hz), 133.2, 133.1, 133.0, 130.4, 130.3, 129.4, 128.5, 127.2, 125.8, 125.3, 125.0, 123.6 (q, J = 271.1 Hz) 121.1, 116.0, 21.7. **^{19}F NMR** (471 MHz, Chloroform-*d*) δ -63.0. **IR** (KBr, ν, cm^{-1}): 1679, 1651, 1597, 1527, 1446, 1423, 1392, 1215, 756, 713, 698. **HRMS** (ESI) m/z calcd for $C_{30}H_{21}F_3NO_4S$ $(M+H)^+$: 548.1138, found: 548.1134.



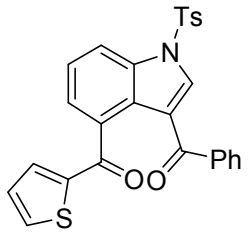
(3-benzoyl-1-tosyl-1*H*-indol-4-yl)(3,4,5-trimethoxyphenyl)methanone (3en)

Pale yellow solid. Melting point: 193-194 °C. Isolated yield: 36%. **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 8.20 (dd, *J* = 1.2, 8.1 Hz, 1H), 7.98 (s, 1H), 7.86-7.82 (m, 4H), 7.59-7.55 (m, 1H), 7.51-7.43 (m, 4H), 7.33-7.31 (m, 2H), 7.08 (s, 2H), 3.84 (s, 3H), 3.78 (s, 6H), 2.41 (s, 3H). **^{13}C NMR** (100 MHz, Chloroform-*d*) δ 193.9, 189.2, 152.8, 146.2, 142.4, 137.7, 135.6, 134.3, 133.5, 133.0, 132.5, 132.2, 130.4, 129.5, 128.5, 127.2, 126.1, 125.2, 125.1, 121.4, 115.6, 107.7, 60.8, 56.2, 21.7. **IR** (KBr, ν, cm^{-1}): 1674, 1658, 1581, 1535, 1454, 1411, 1373, 1230, 748, 729. **HRMS** (ESI) m/z calcd for $C_{32}H_{28}NO_7S$ $(M+H)^+$: 570.1581, found: 570.1578.



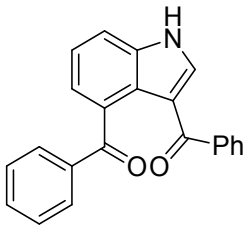
(4-(2-naphthoyl)-1-tosyl-1*H*-indol-3-yl)(phenyl)methanone (3eo)

White solid. Melting point: 176-178 °C. Isolated yield: 53%. **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 8.24-8.21 (m, 1H), 8.19 (s, 1H), 7.99-7.96 (m, 2H), 7.85-7.78 (m, 5H), 7.73-7.71 (m, 2H), 7.56-7.47 (m, 4H), 7.45-7.43 (m, 1H), 7.35-7.31 (m, 4H), 2.41 (s, 3H). **^{13}C NMR** (100 MHz, Chloroform-*d*) δ 195.1, 189.3, 146.2, 137.6, 135.6, 135.5, 134.6, 134.3, 133.9, 132.7, 132.5, 132.3, 132.2, 130.3, 129.5, 129.4, 128.3, 127.7, 127.2, 126.5, 126.1, 125.4, 125.3, 125.2, 121.5, 115.6, 21.7. **IR** (KBr, ν, cm^{-1}): 1683, 1666, 1572, 1535, 1447, 1401, 1373, 1218, 753, 739, 704. **HRMS** (ESI) m/z calcd for $C_{33}H_{24}NO_4S$ $(M+H)^+$: 530.1421, found: 530.1425.



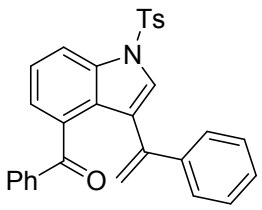
(3-benzoyl-1-tosyl-1*H*-indol-4-yl)(thiophen-2-yl)methanone (3ep)

White solid. Melting point: 175-177 °C. Isolated yield: 27%. **^{1}H NMR** (500 MHz, Chloroform-*d*) δ 8.19 (dd, J = 1.0, 8.4 Hz, 1H), 7.98 (s, 1H), 7.83-7.80 (m, 4H), 7.64-7.62 (m, 1H), 7.57-7.52 (m, 2H), 7.50-7.47 (m, 1H), 7.47-7.46 (m, 1H), 7.43-7.40 (m, 2H), 7.31-7.30 (m, 2H), 7.03- 7.01 (m, 1H), 2.40 (s, 3H). **^{13}C NMR** (125 MHz, Chloroform-*d*) δ 189.6, 187.6, 146.6, 144.8, 138.2, 136.0, 135.2, 135.1, 134.6, 133.8, 133.2, 133.1, 130.7, 129.9, 128.8, 128.2, 127.6, 125.9, 125.6, 125.2, 121.8, 116.1, 22.1. **IR** (KBr, ν, cm^{-1}): 1671, 1635, 1597, 1535, 1458, 1419, 1384, 1211, 748, 717, 698. **HRMS** (ESI) m/z calcd for $C_{27}H_{20}NO_4S_2$ $(M+H)^+$: 486.0828, found: 486.0827.



(1*H*-indole-3,4-diyl)bis(phenylmethanone) (4)

White solid. Melting point: 181-182 °C. Isolated yield: 86%. **^{1}H NMR** (500 MHz, Chloroform-*d*) δ 10.63 (s, 1H), 7.86 (d, J = 7.5 Hz, 2H), 7.46-7.45 (m, 2H), 7.41-7.36 (m, 2H), 7.30-7.23 (m, 6H), 7.19-7.16 (m, 1H), 7.07 (d, J = 2.9 Hz, 1H). **^{13}C NMR** (125 MHz, Chloroform-*d*) δ 198.0, 190.4, 139.6, 138.2, 137.7, 136.3, 133.2, 133.1, 131.9, 130.5, 129.4, 128.6, 128.5, 123.2, 123.0, 117.0, 115.0. **HRMS** (ESI) m/z calcd for $C_{22}H_{16}NO_2$ $(M+H)^+$: 326.1176, found: 326.1173.



phenyl(3-(1-phenylvinyl)-1-tosyl-1*H*-indol-4-yl)methanone (5)

White solid. Melting point: 155-157 °C. Isolated yield: 72%. **^{1}H NMR** (400 MHz, Chloroform-d) δ

8.19-8.17(m, 1H), 7.84 (m, 2H), 7.74 (s, 1H), 7.41-7.38 (m, 3H), 7.34-7.28 (m, 3H), 7.22-7.18 (m, 2H), 7.12-7.10 (m, 1H), 6.92-6.90 (m, 2H), 6.87-6.83 (m, 2H), 6.81-6.77 (m, 1H), 5.43 (d, *J* = 1.2 Hz, 1H), 5.33 (d, *J* = 1.2 Hz, 1H), 2.41 (s, 3H). **^{13}C NMR** (100 MHz, Chloroform-*d*) δ 194.9, 145.4, 141.4, 139.1, 136.1, 136.0, 134.9, 133.5, 132.6, 130.4, 130.0, 127.9, 127.5, 127.4, 127.2, 127.1, 127.0, 124.0, 123.9, 123.7, 115.8, 114.8, 21.6. **HRMS** (ESI) m/z calcd for $C_{30}H_{24}NO_3S$ $(M+H)^+$: 478.1471, found: 478.1469.

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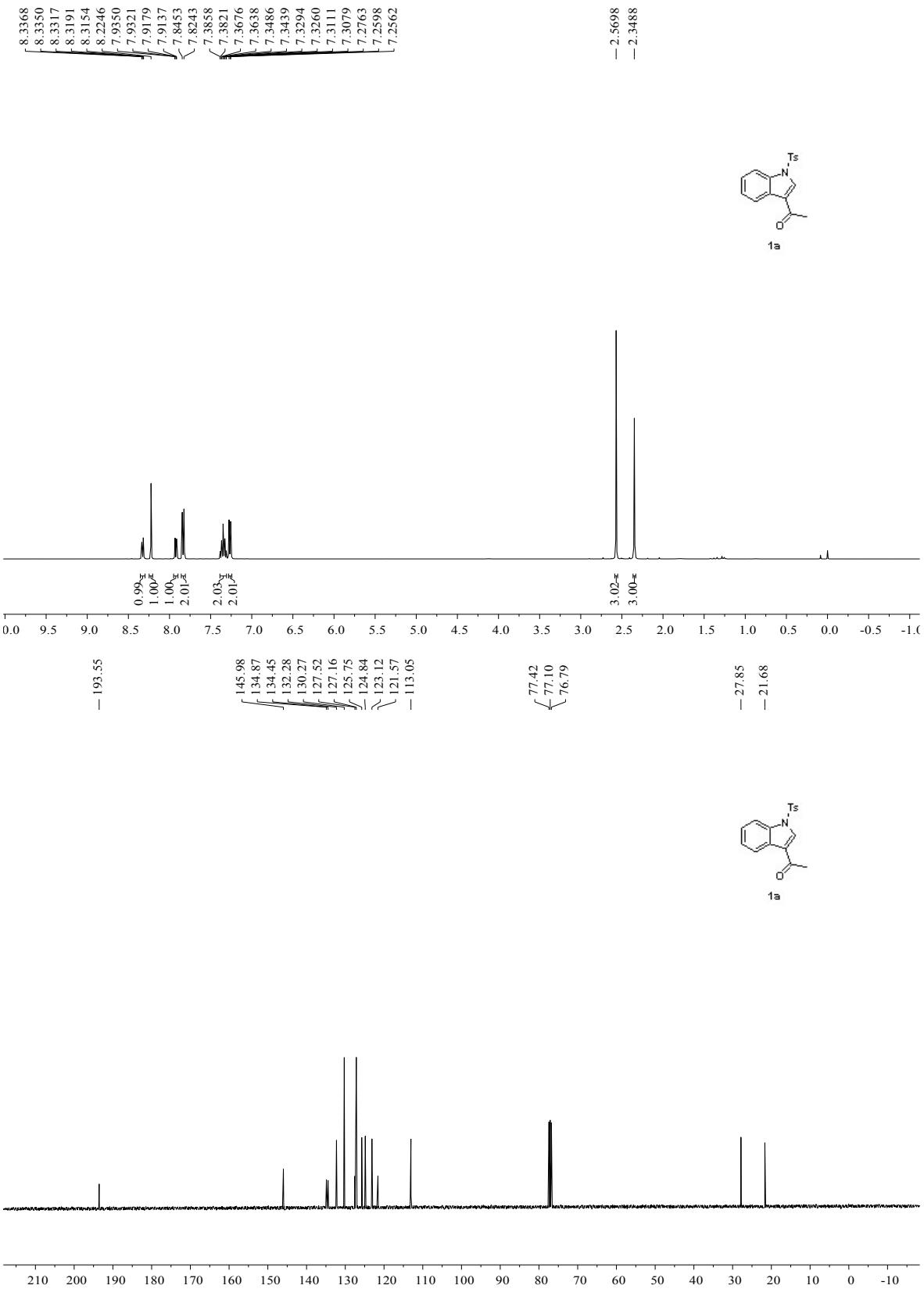
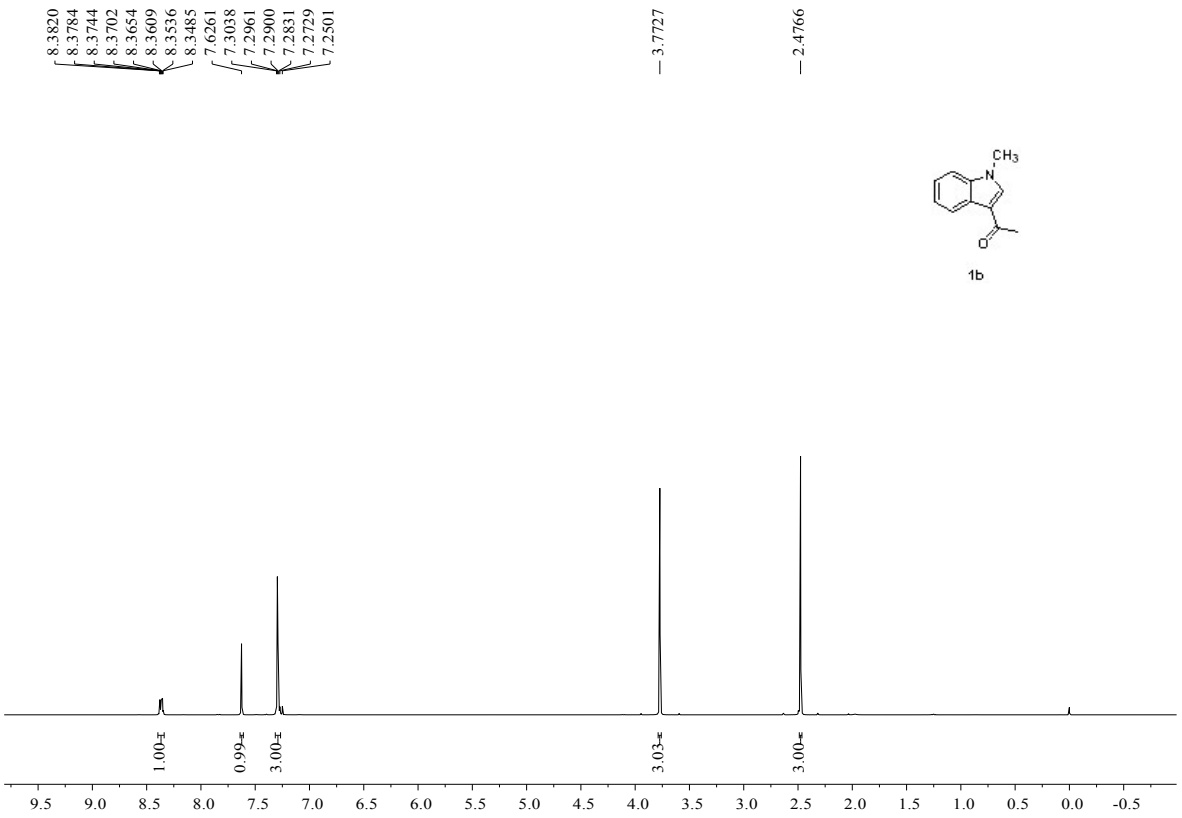
1. Wadhwa. K.; Yang C. X.; West P. R.; Deming K. C.; Chemburkar S. R.; Reddy. R. E. *Synth. Commun*. **2008**, *38*, 4434.
2. Okauchi, T.; Itonaga, M.; Minami, T.; Owa, T.; Kitoh, K.; Yoshino, H. *Org. Lett*. **2000**, *2*, 1485.
3. Borah. A. J.; Shi. Z. Z. *Chem. Commun*. **2017**, *53*, 3945.
4. Bekolo. H. *Can. J. Chem*. **2007**, *85*, 42.
5. G. Shan, X. Yang, L. Ma, and Y. Rao, *Angew. Chem. Int. Ed.,* **2012**, *51*, 13070.

Copies of ^{1}H, ^{13}C and ^{19}F NMR Spectra

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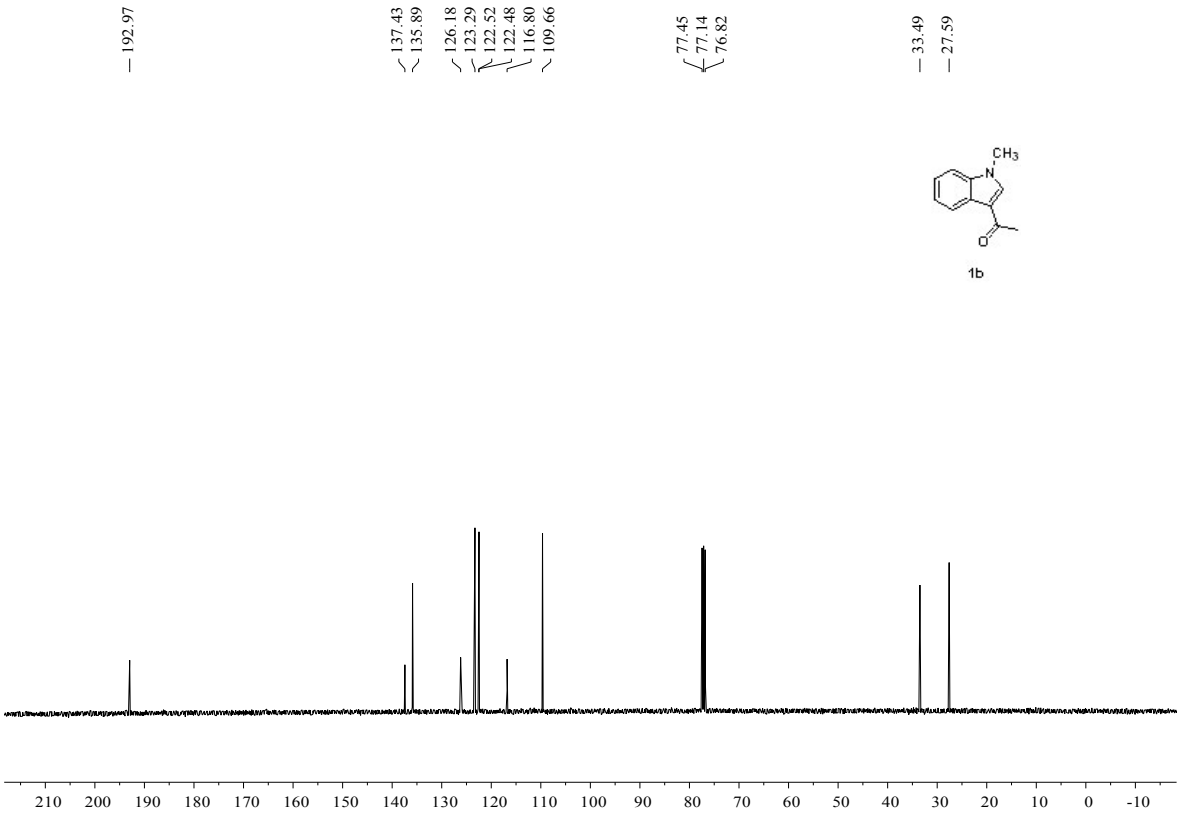
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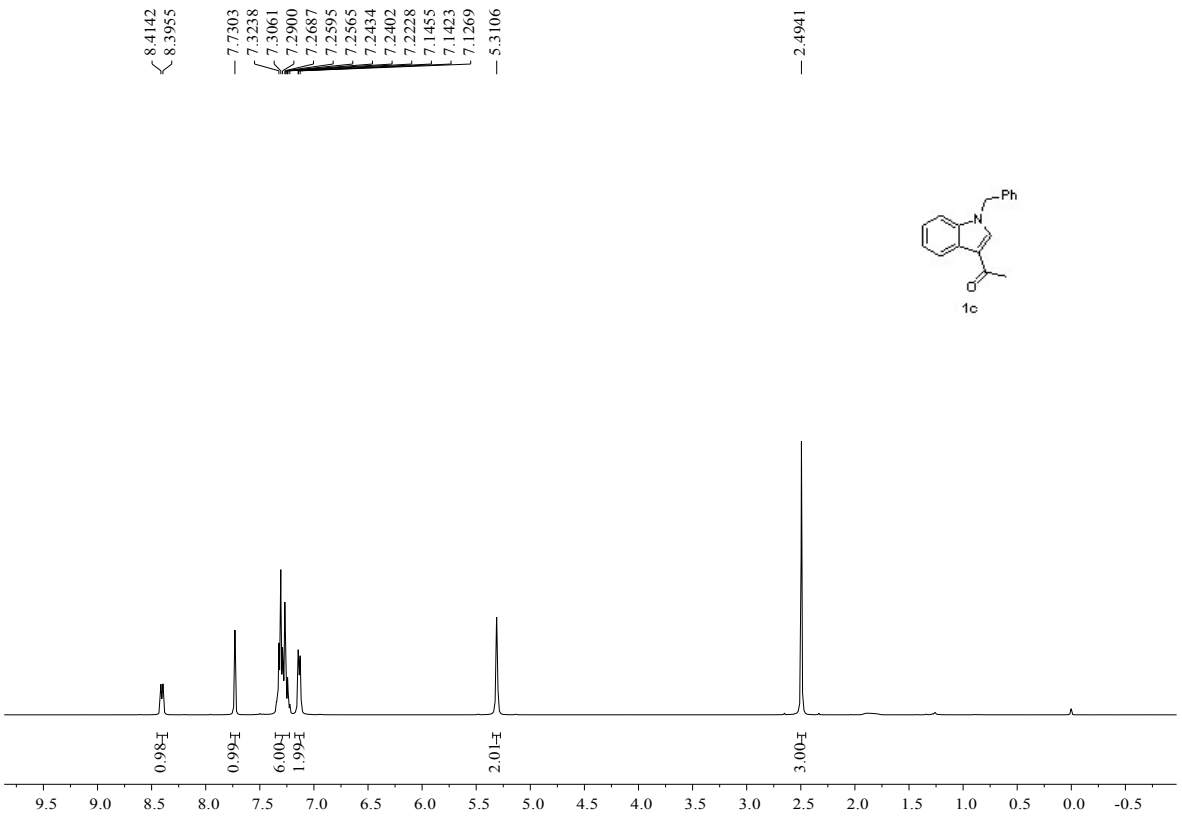
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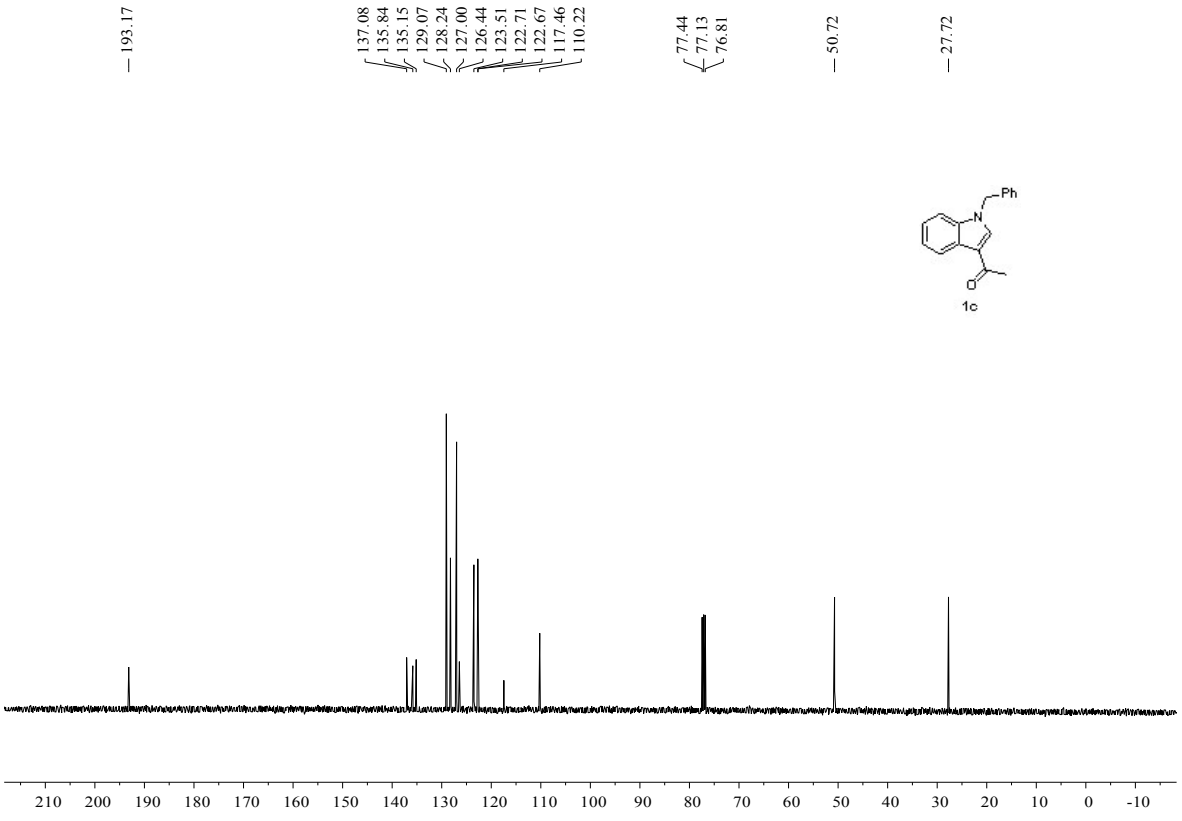
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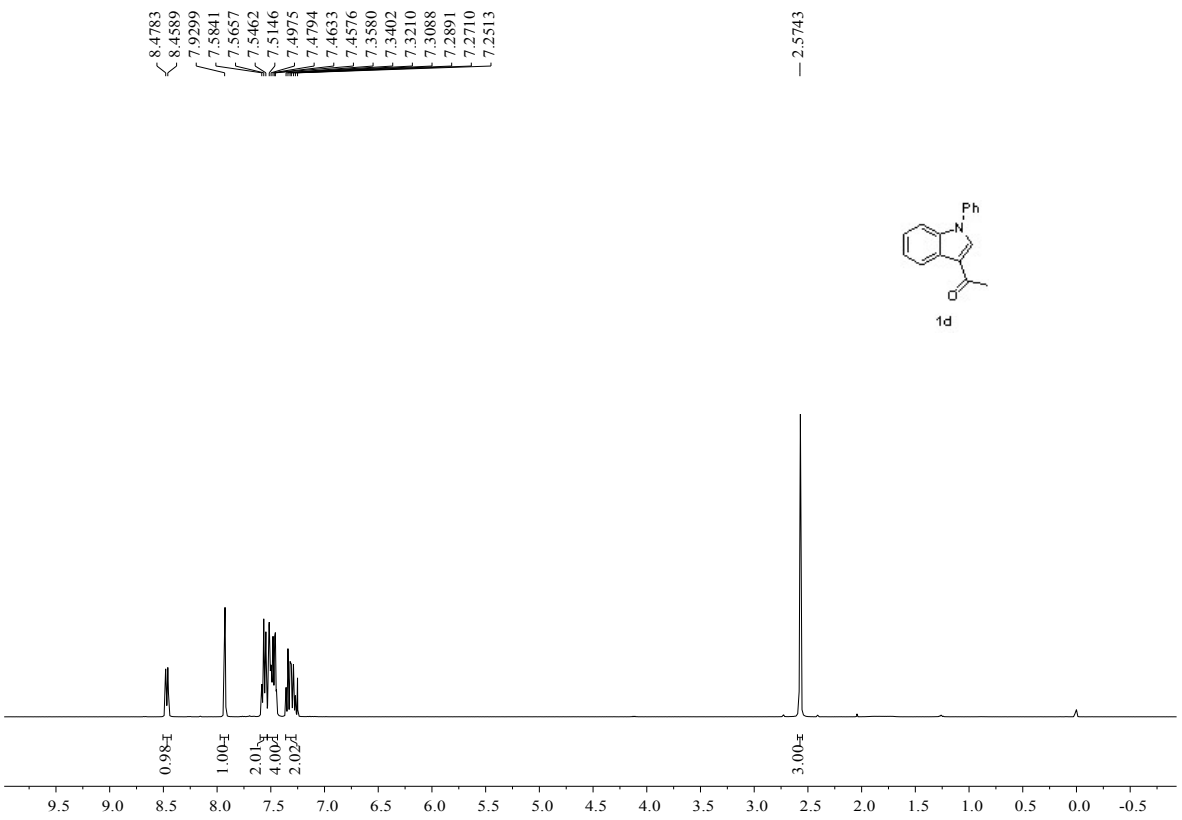
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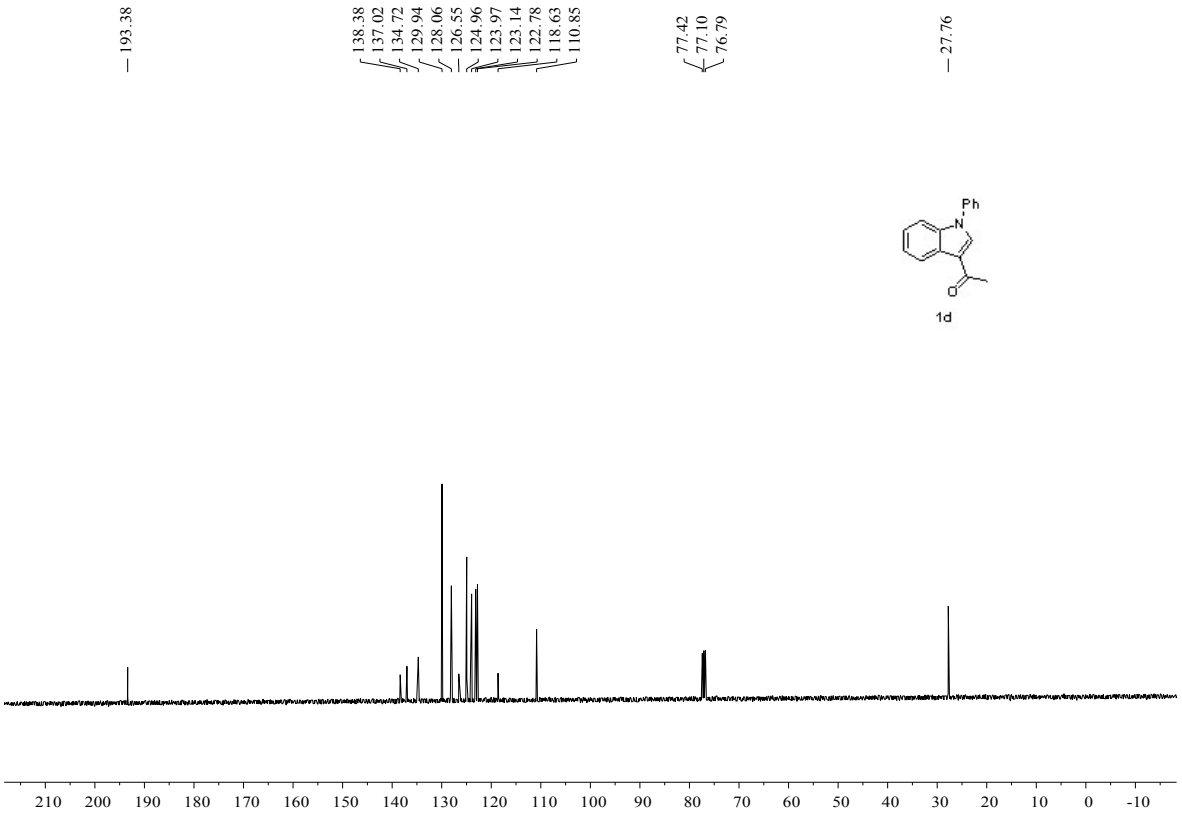
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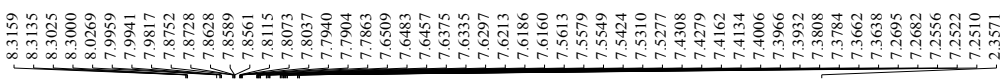
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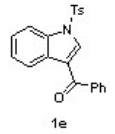
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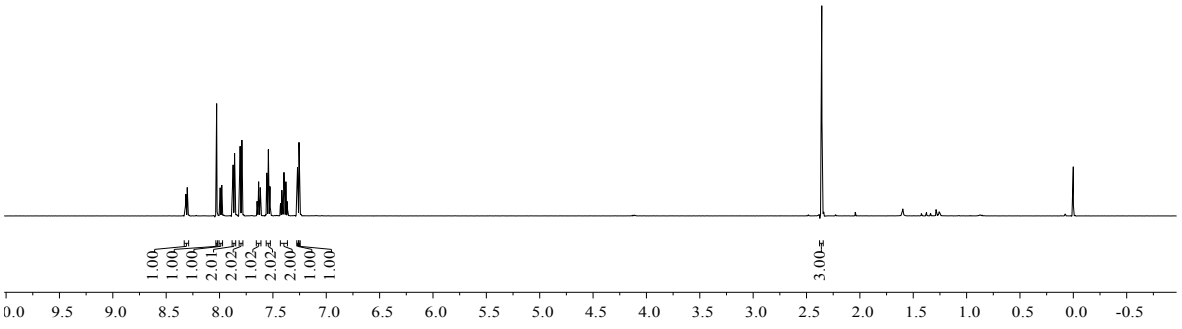
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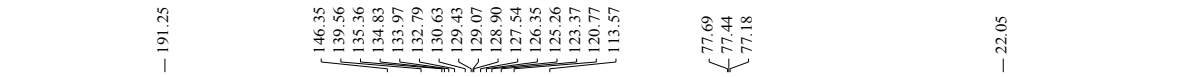
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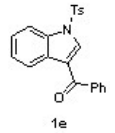
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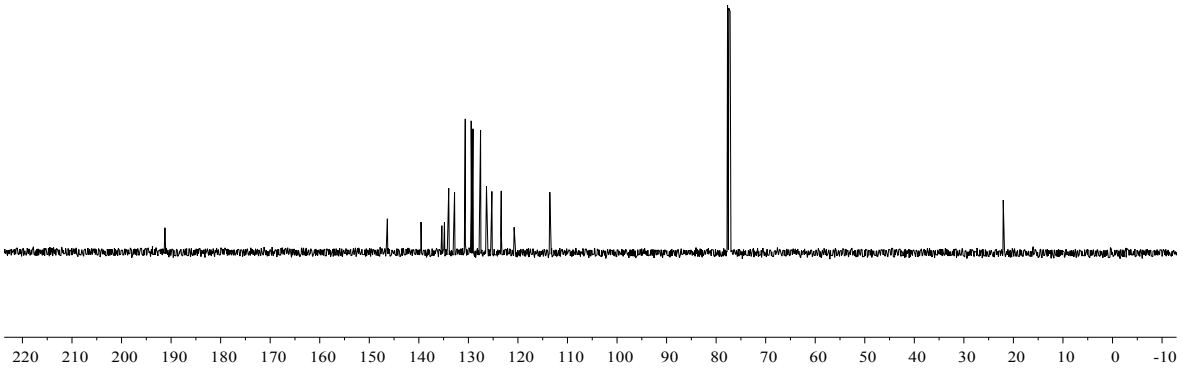
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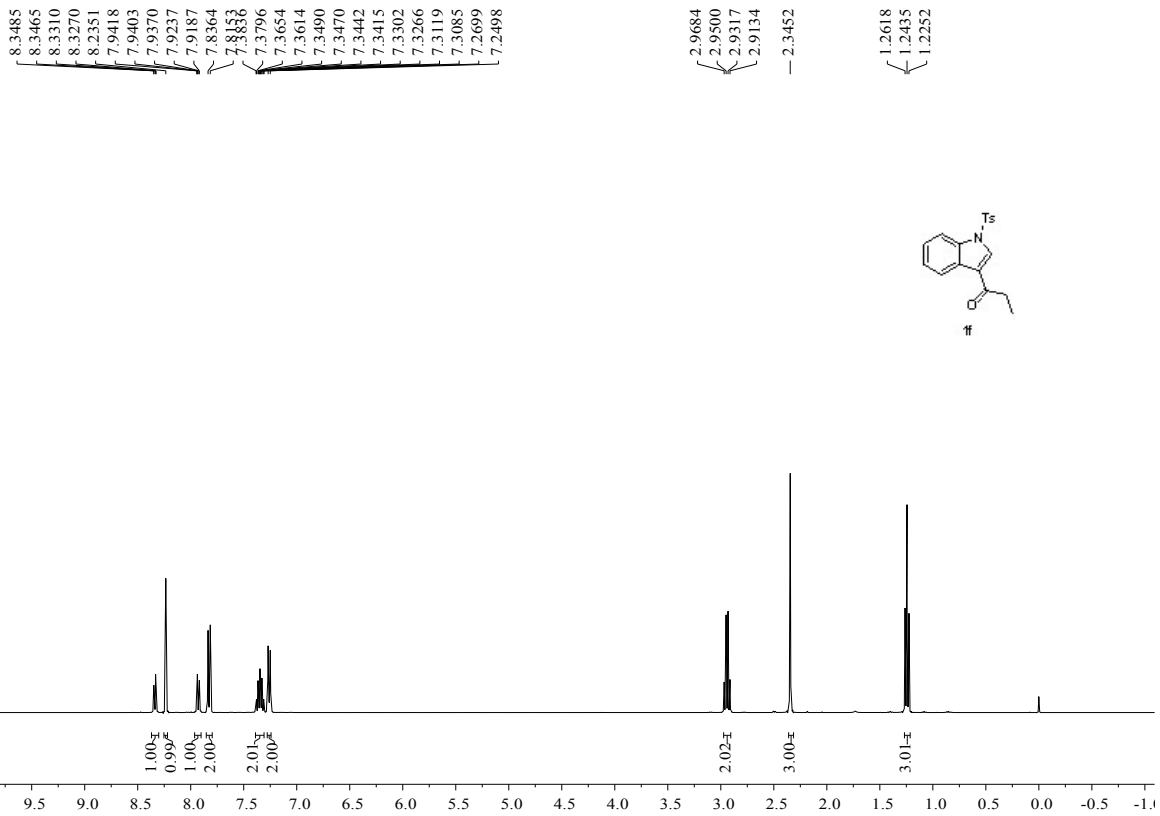
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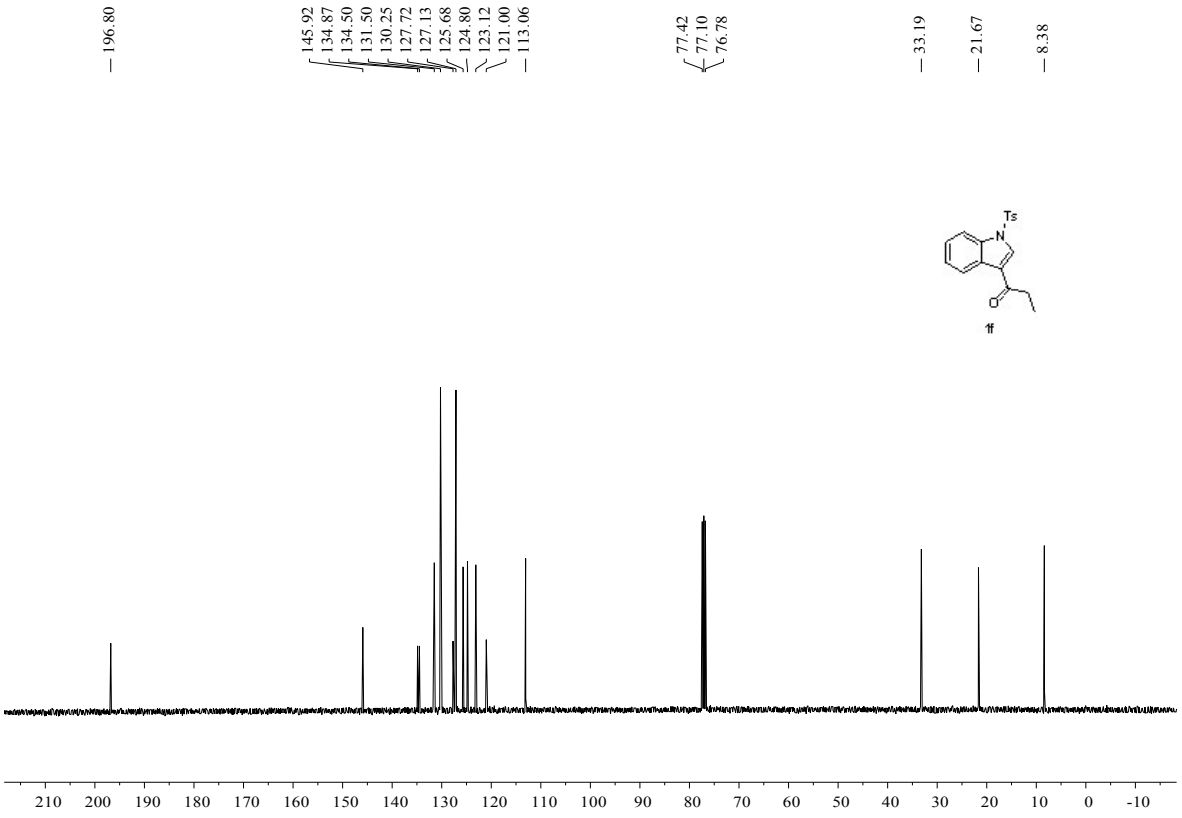
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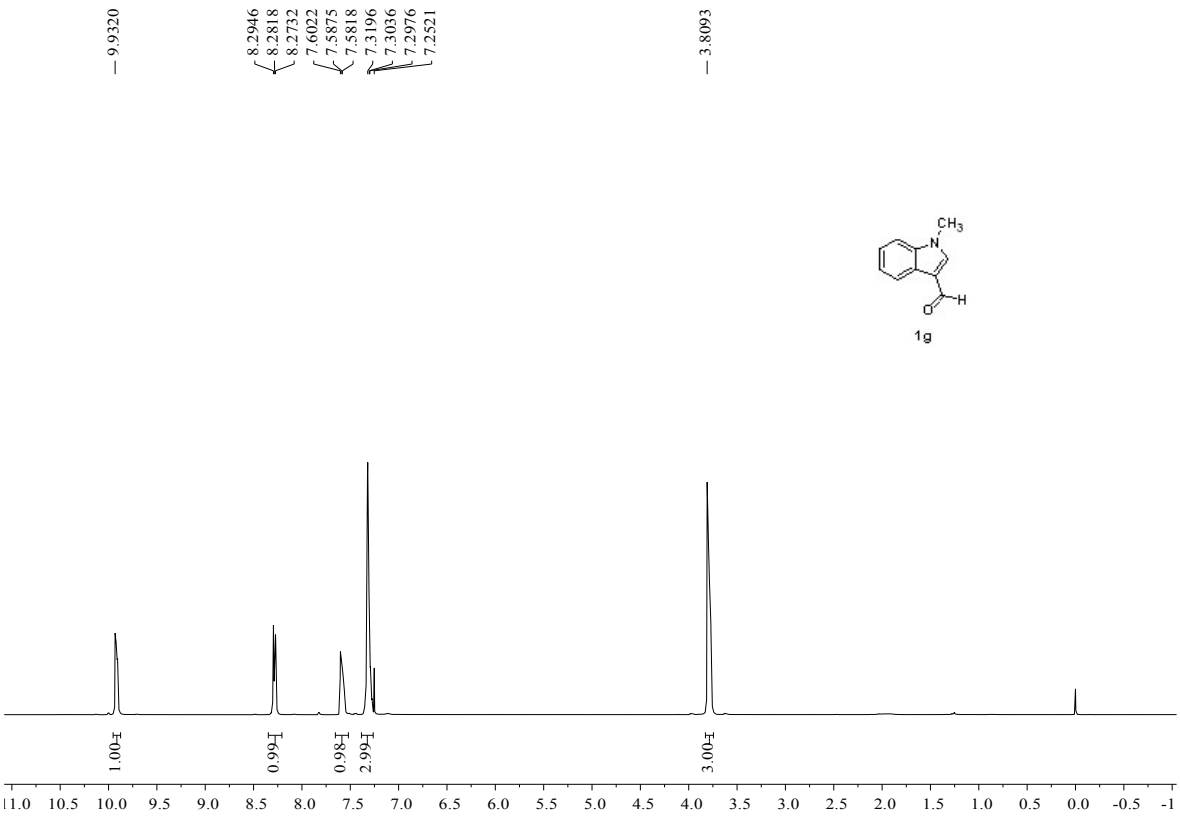
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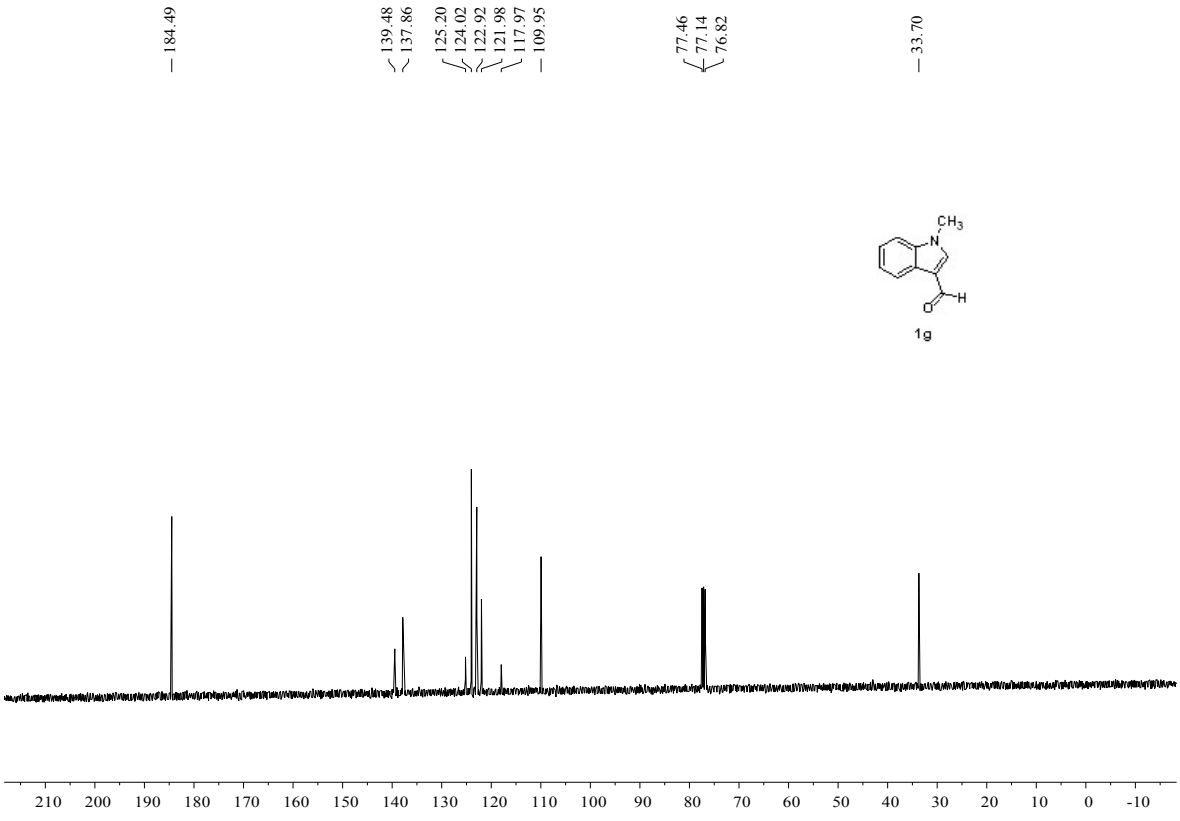
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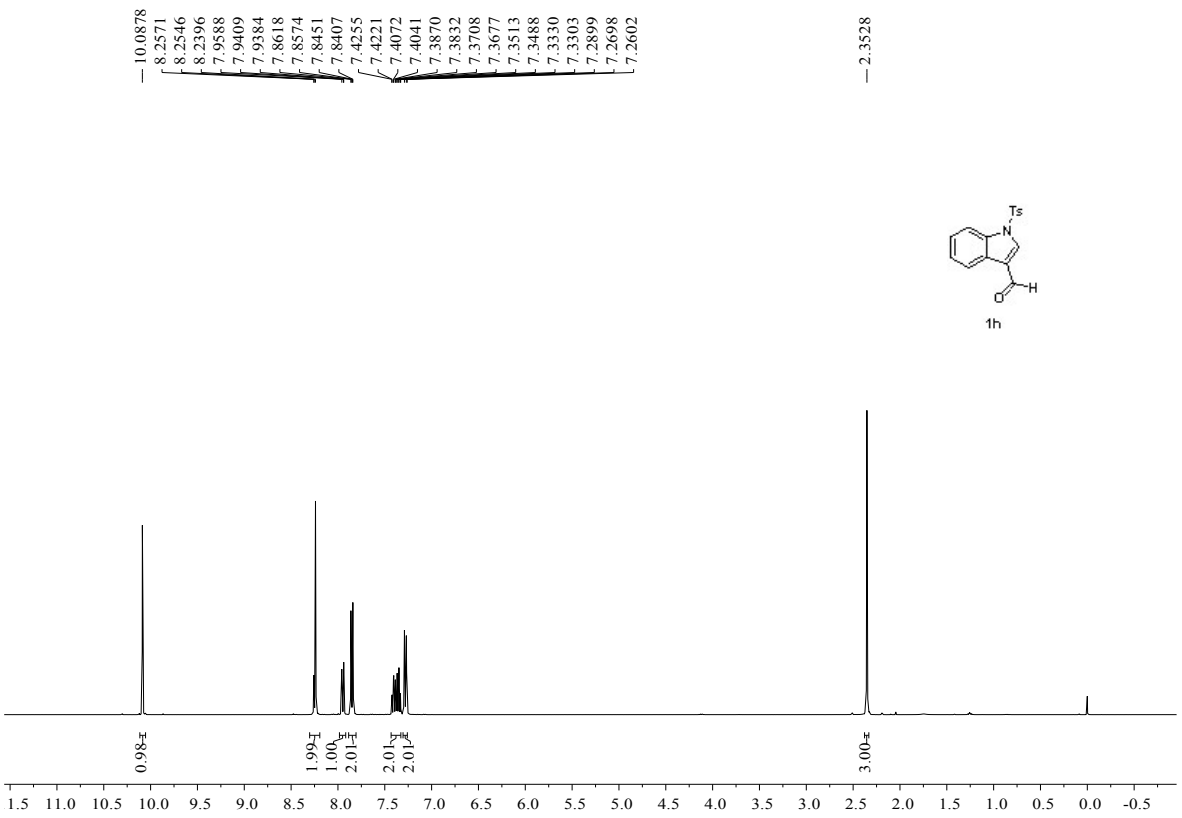
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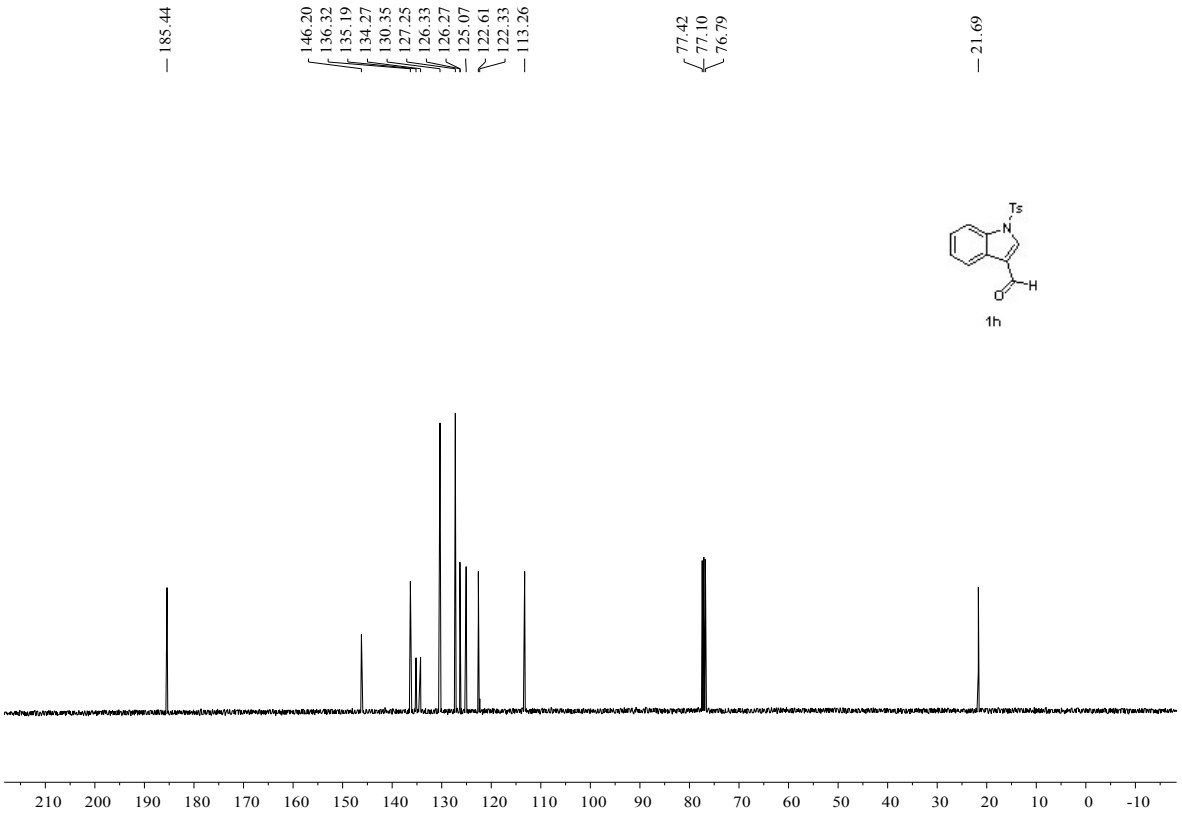
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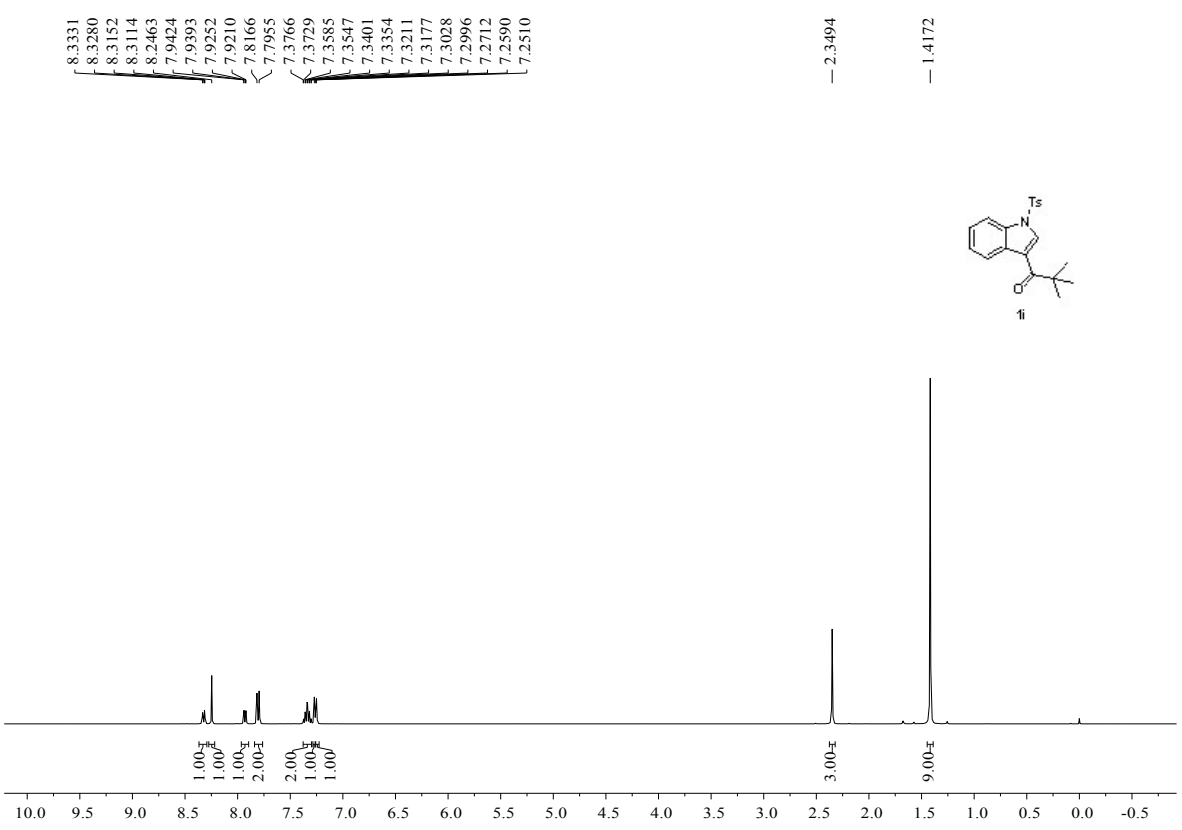
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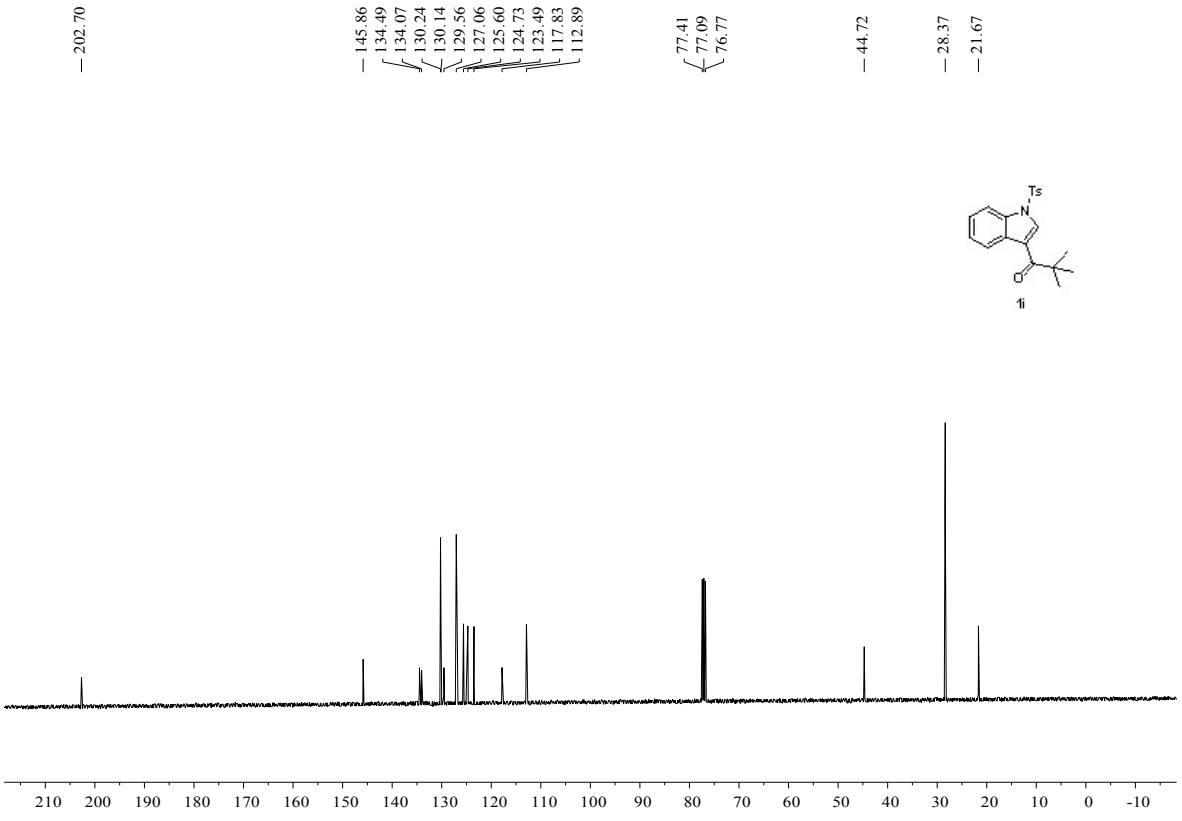
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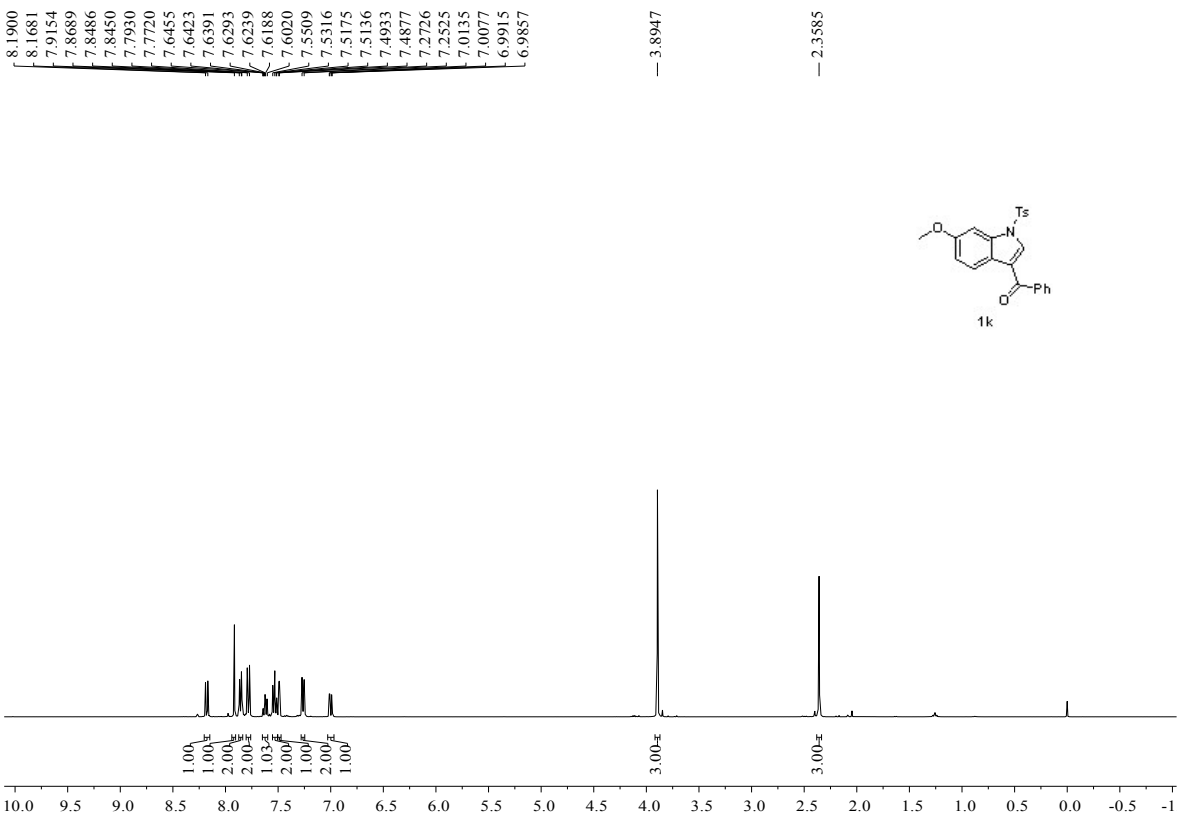
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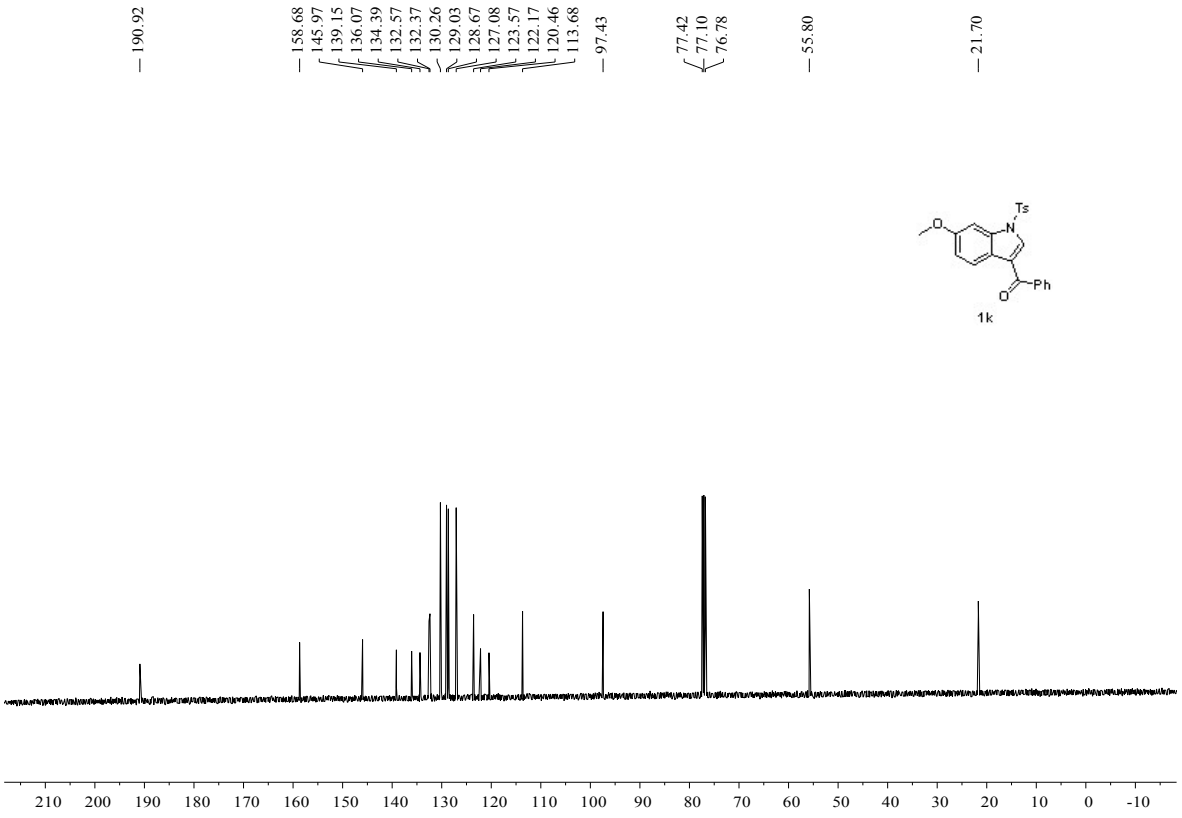
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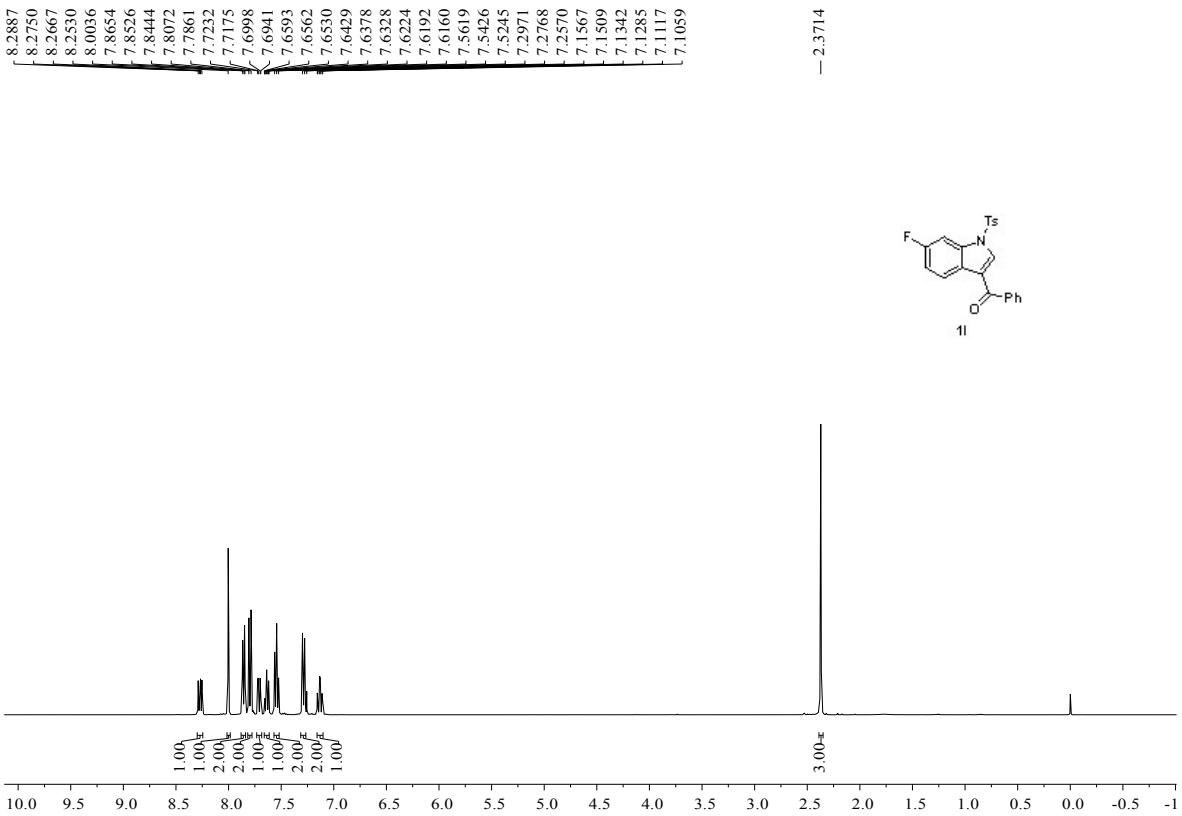
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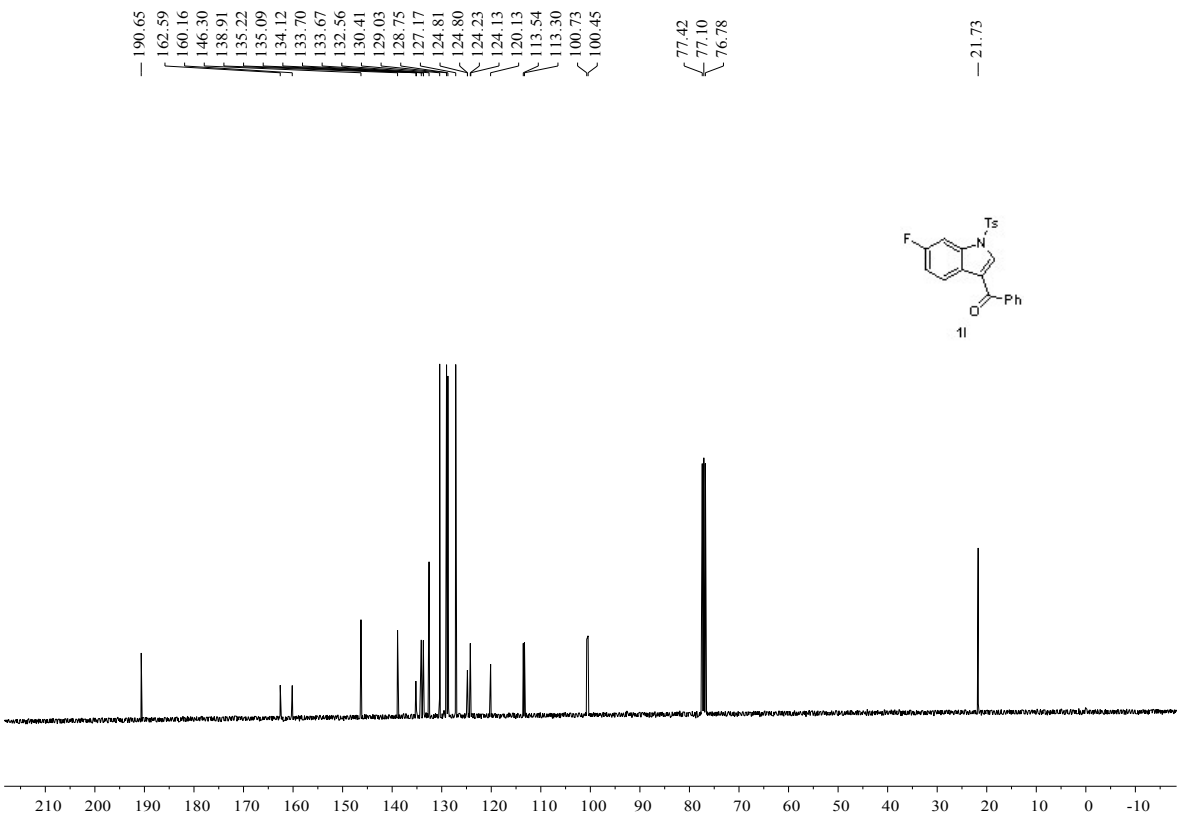
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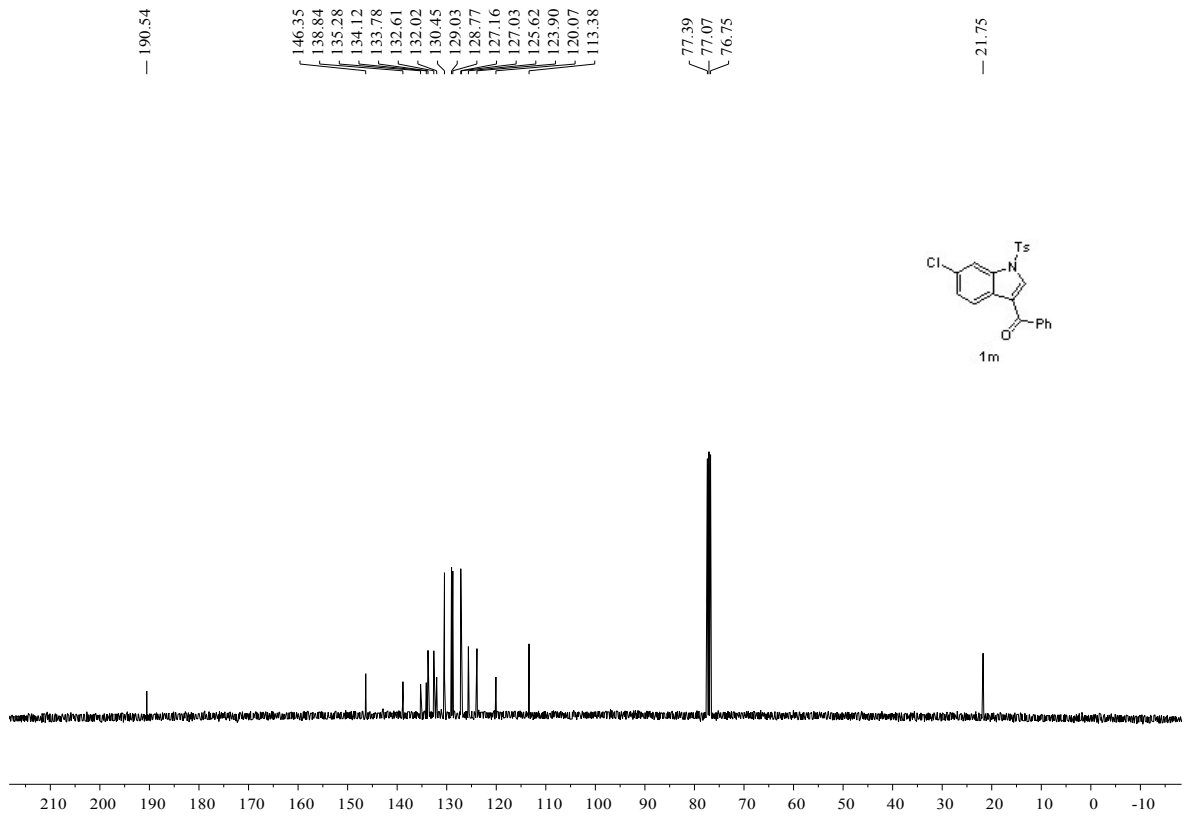
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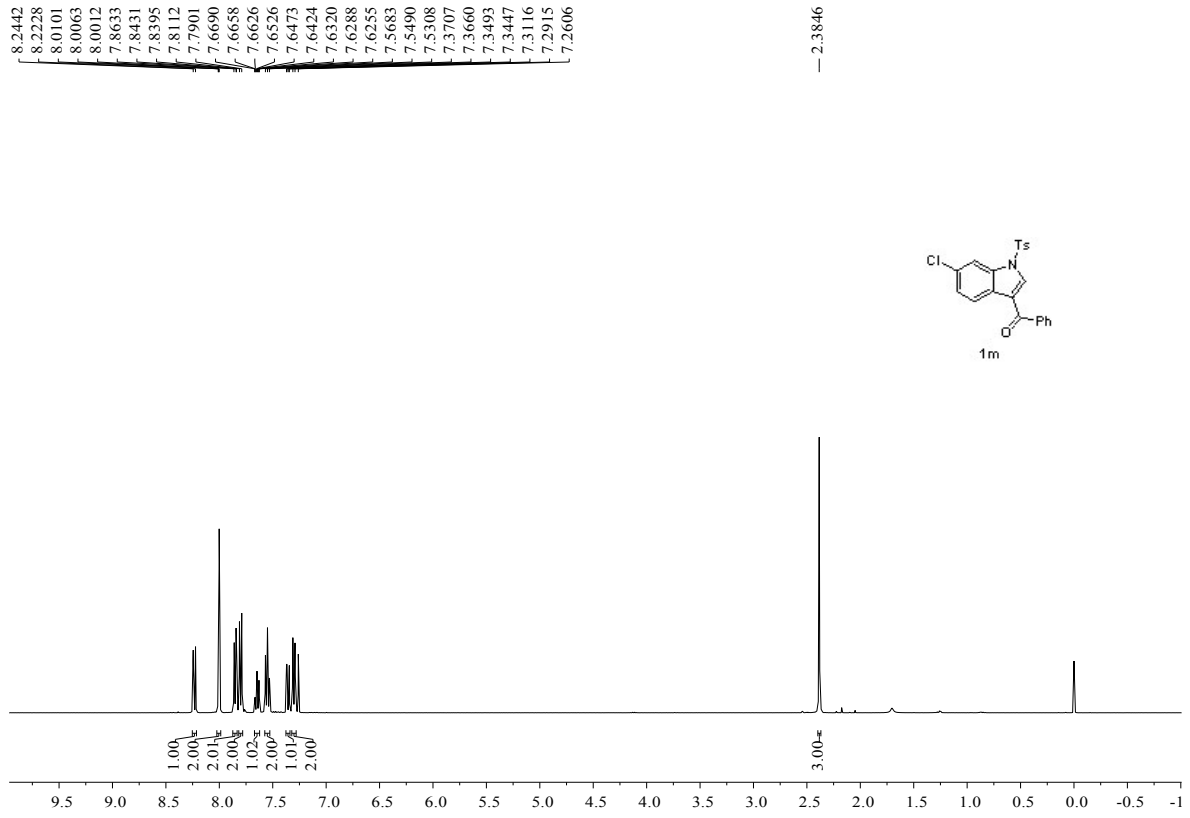
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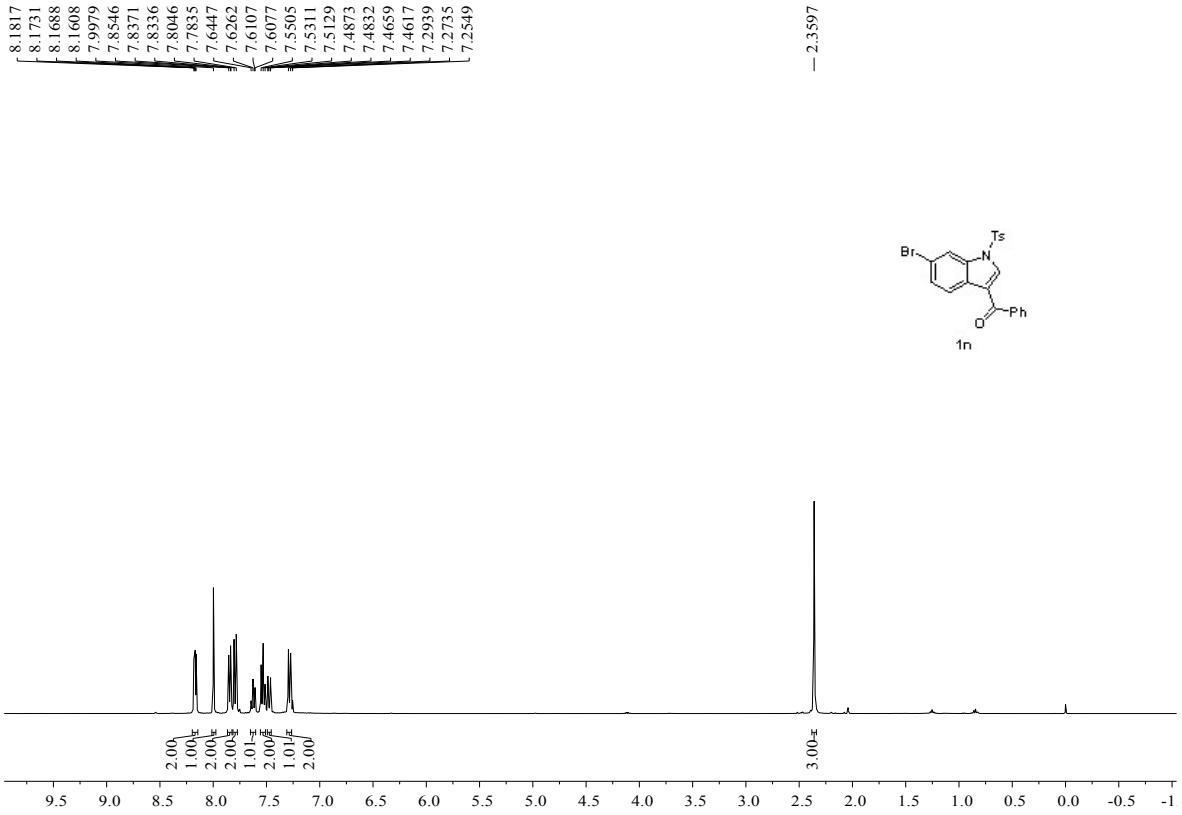
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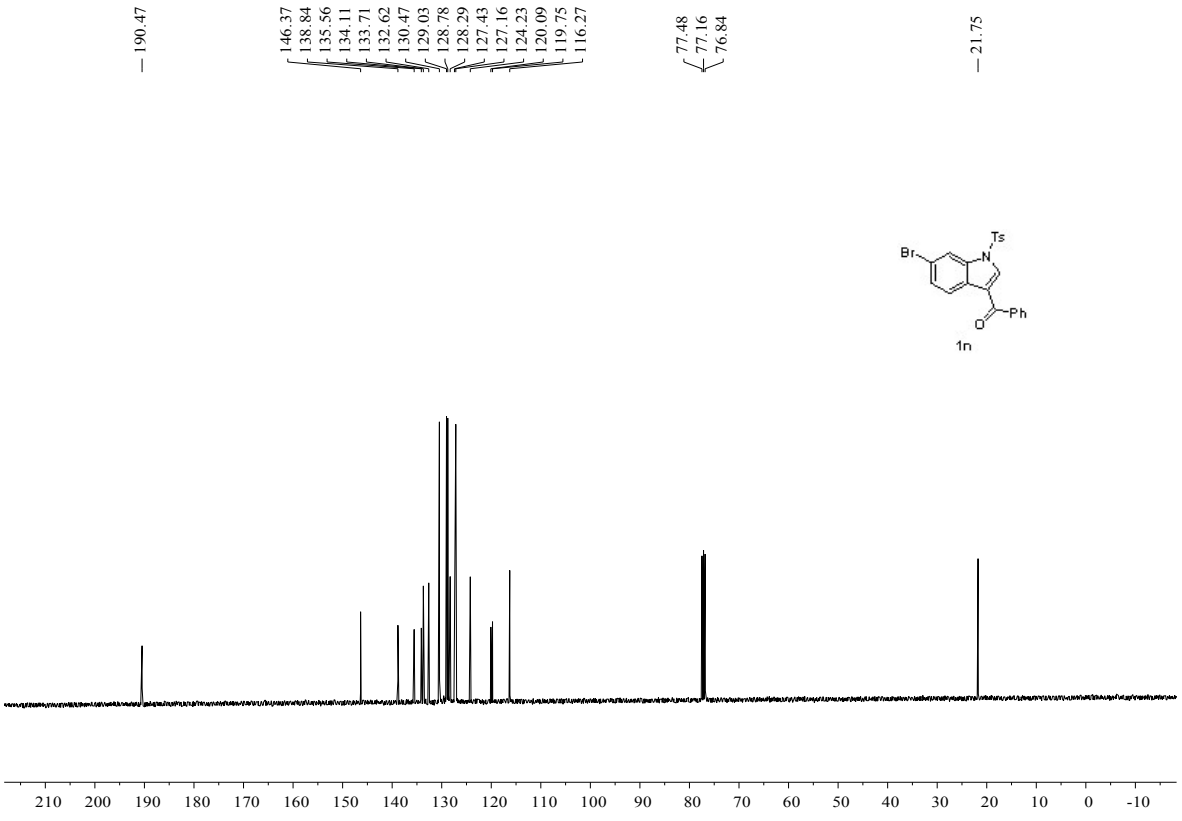
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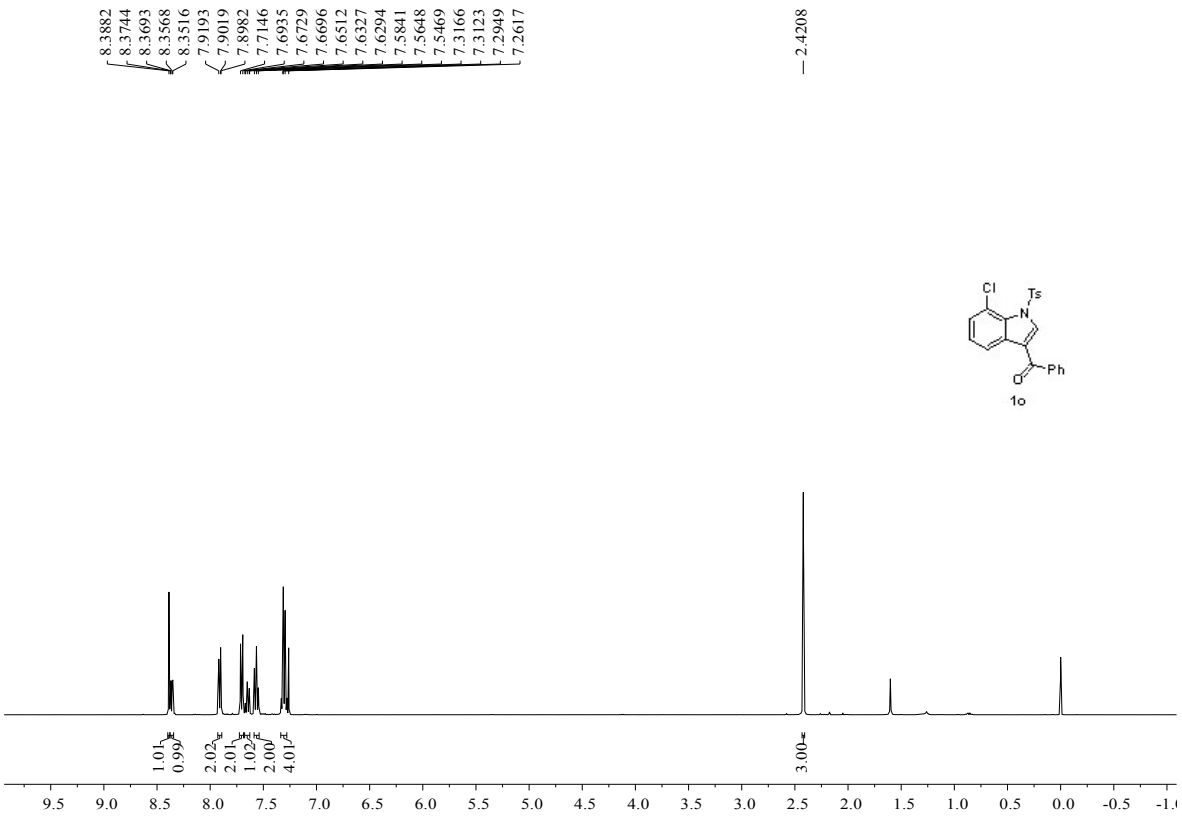
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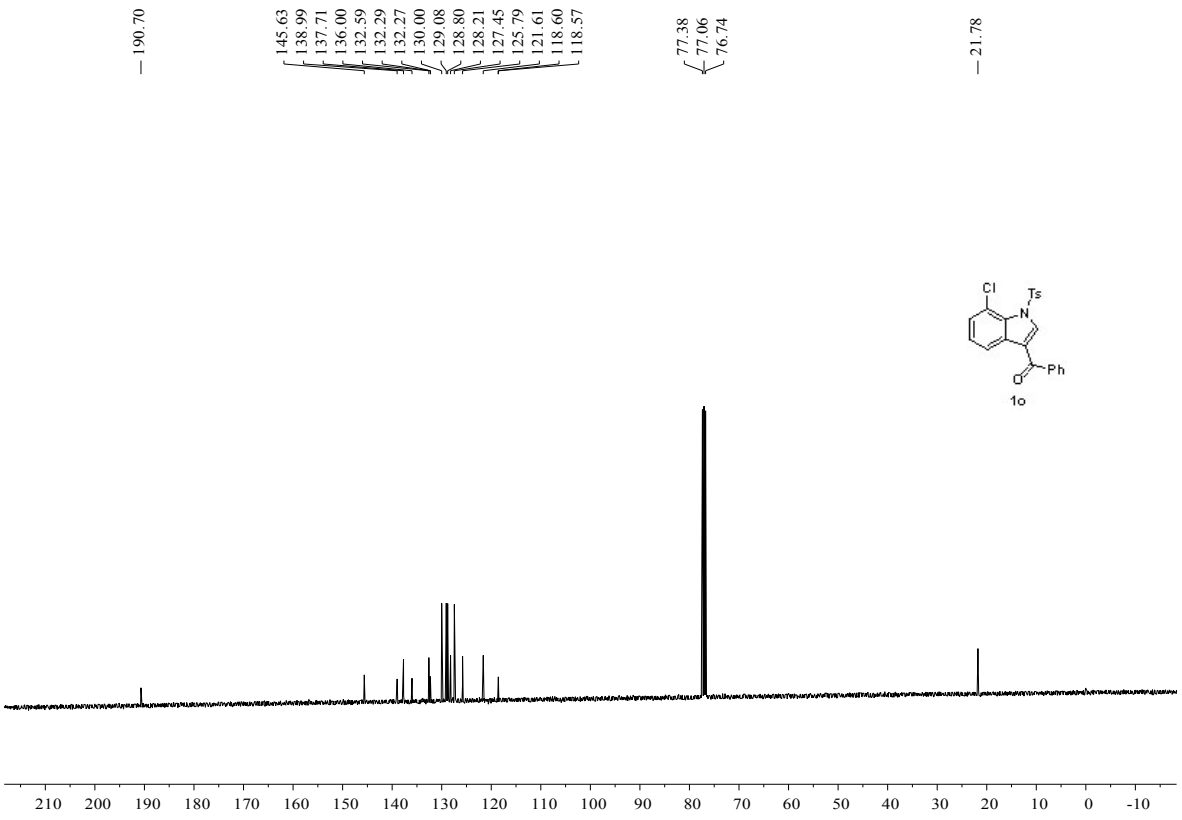
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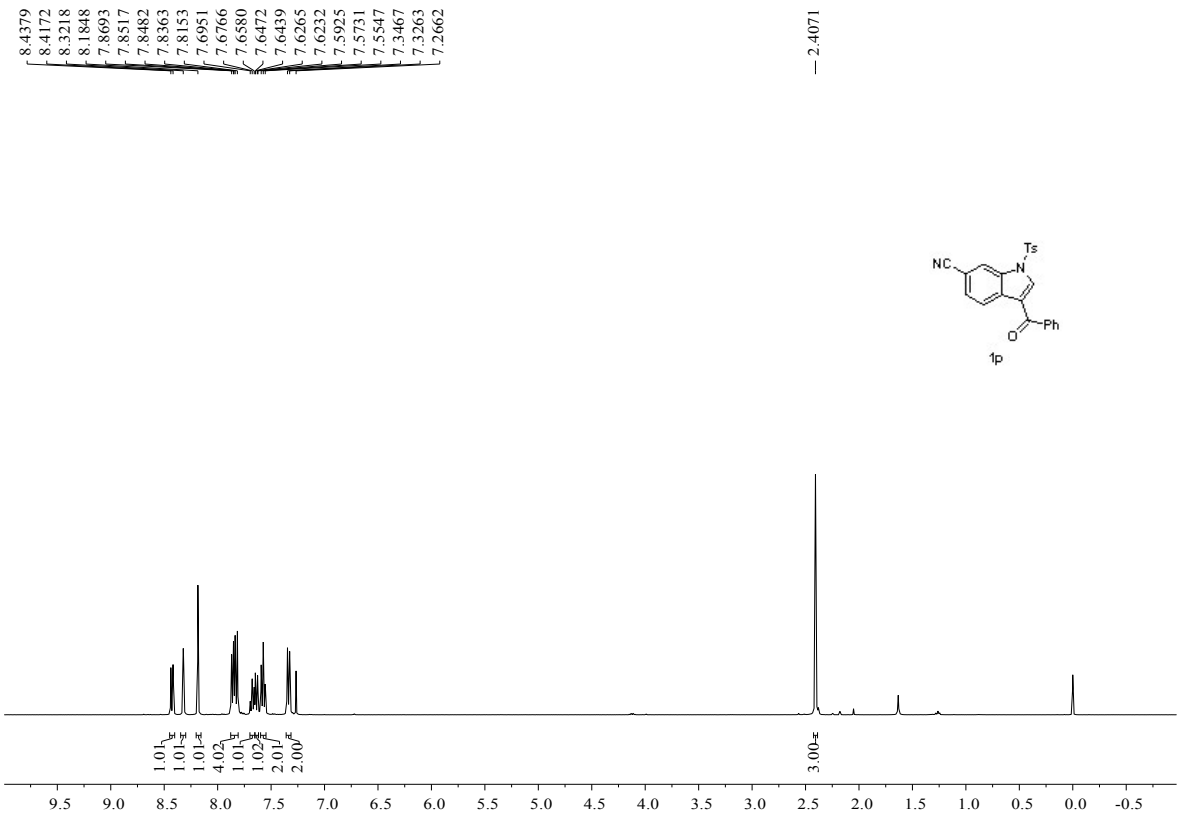
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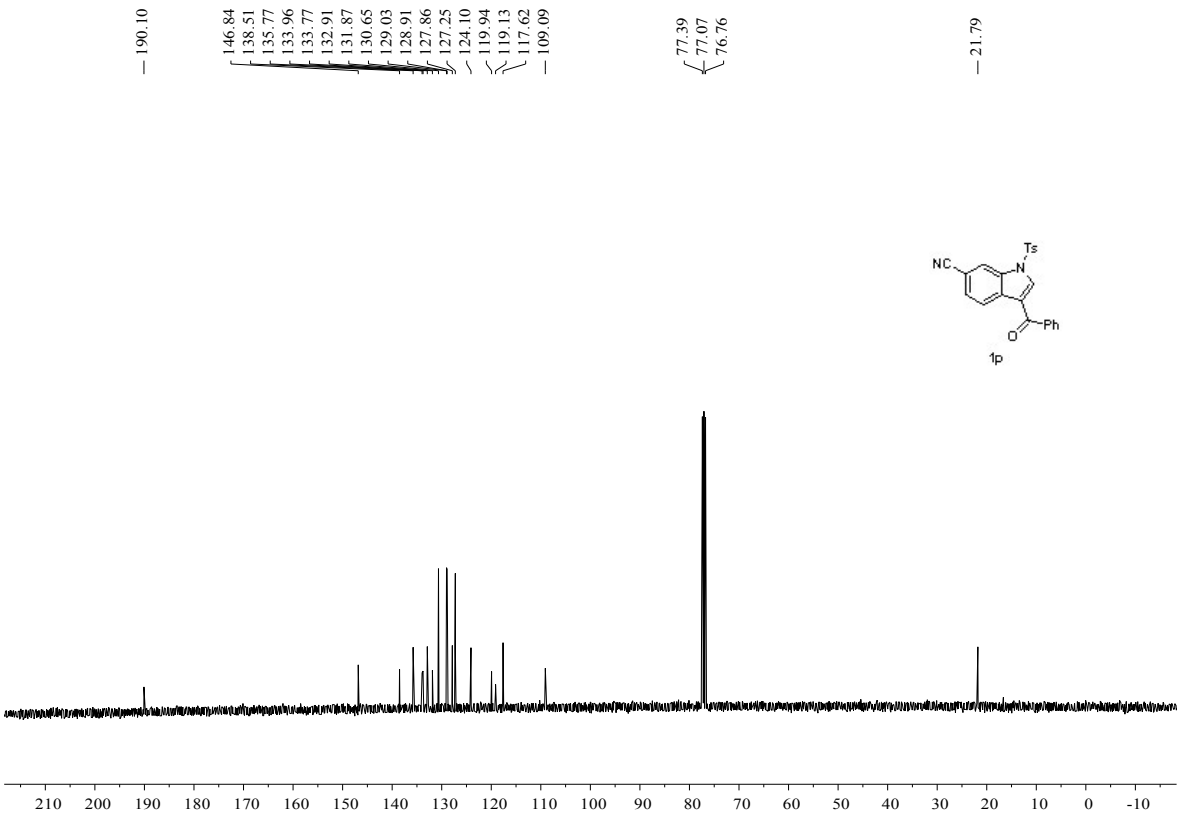
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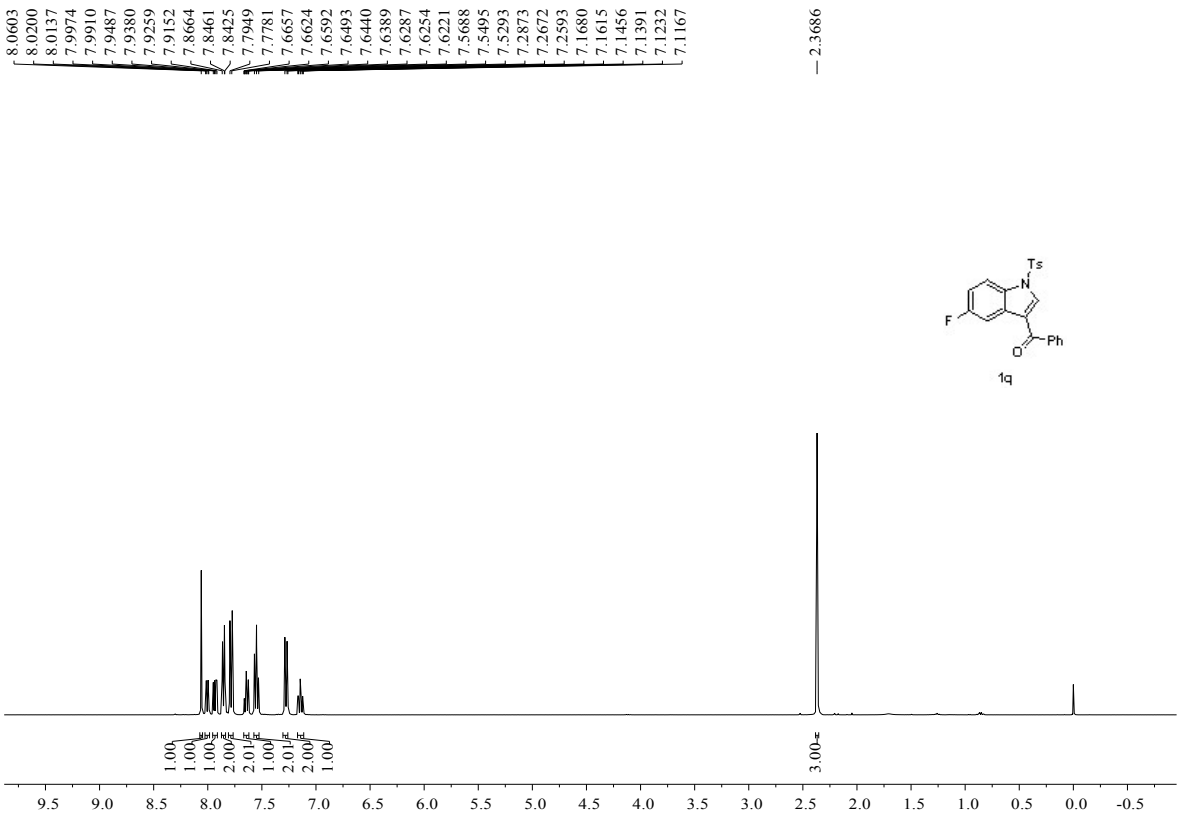
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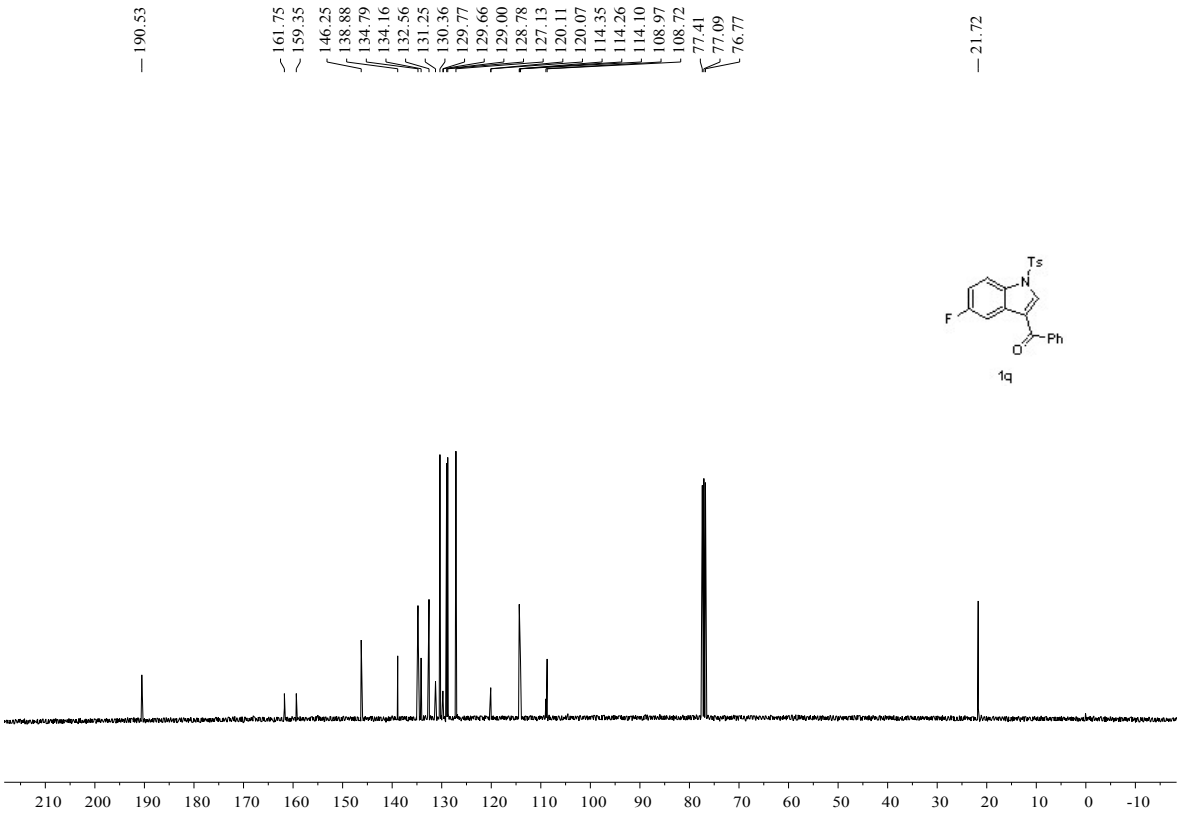
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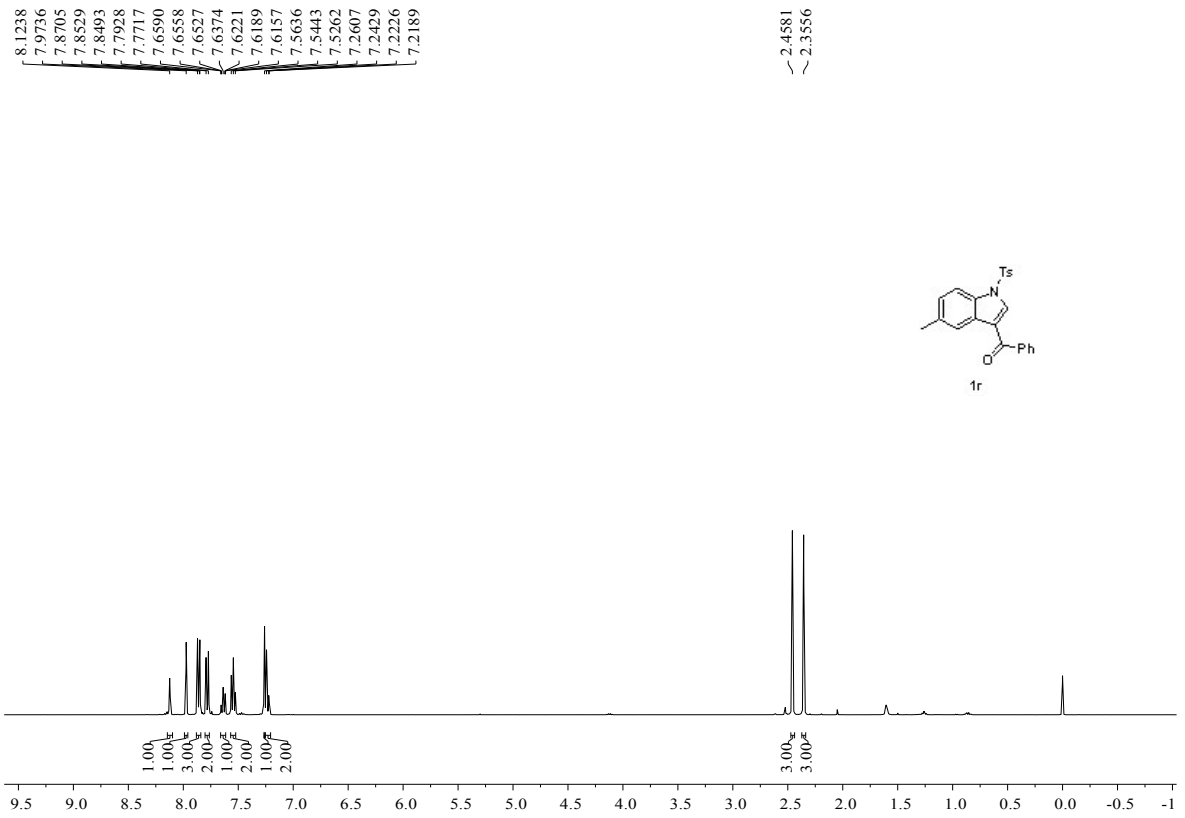
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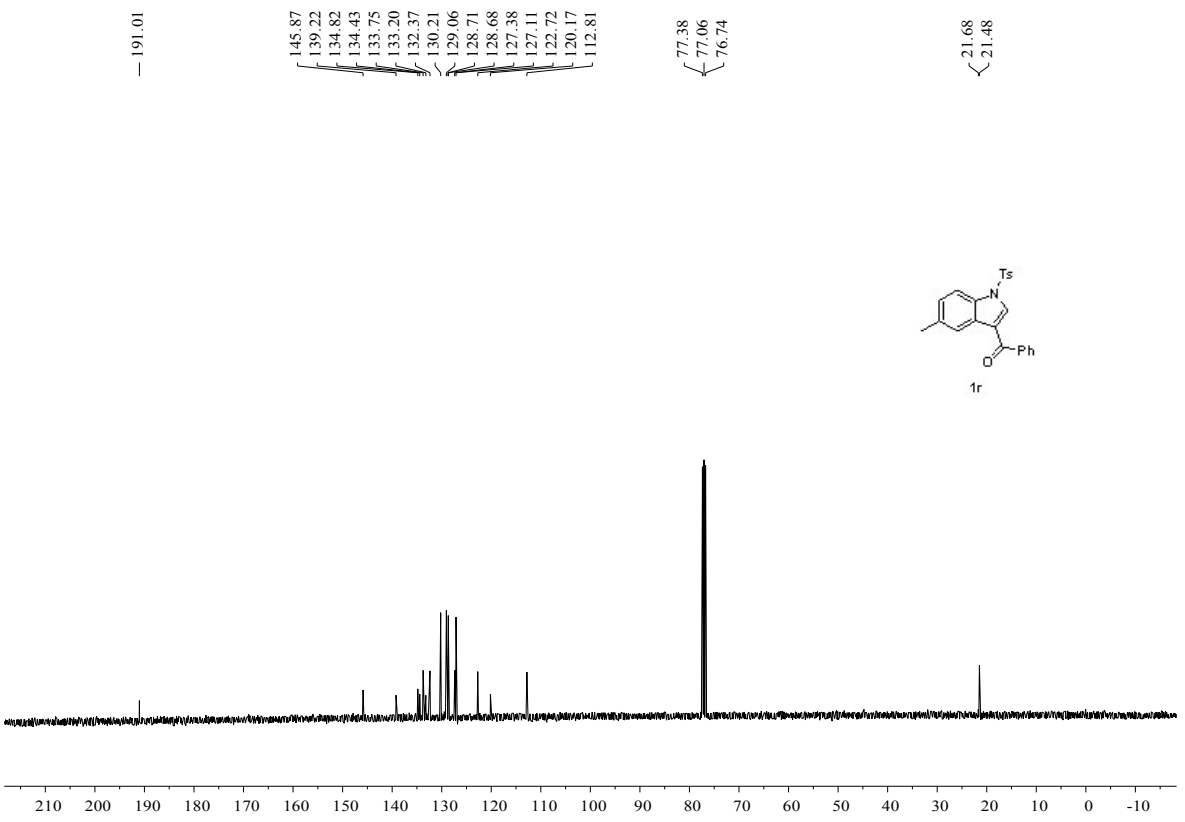
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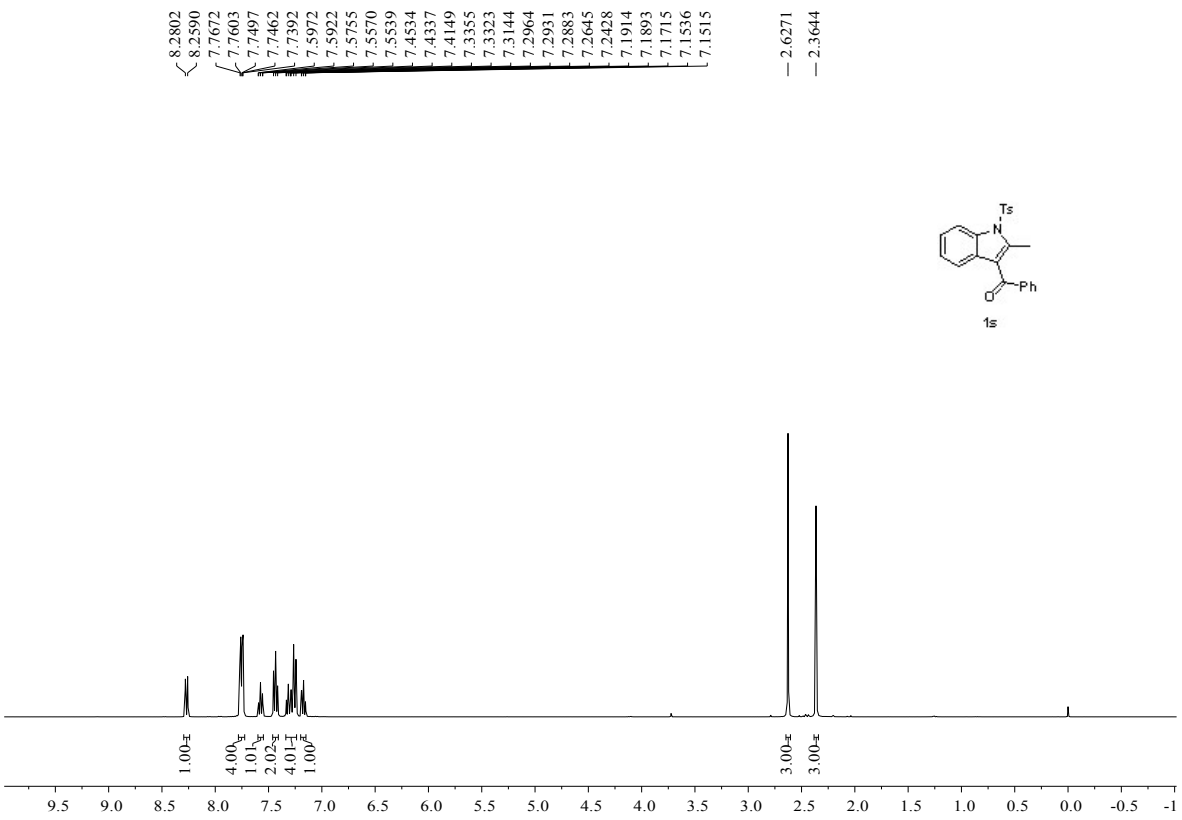
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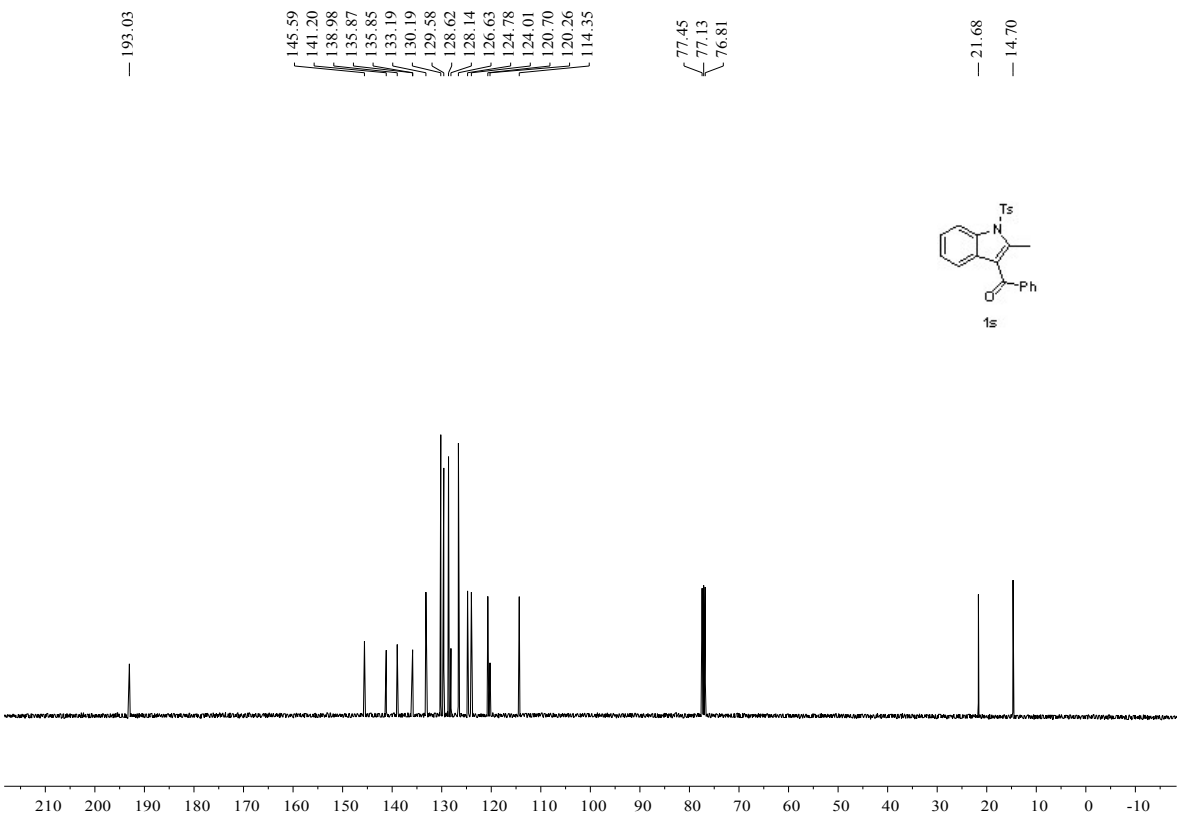
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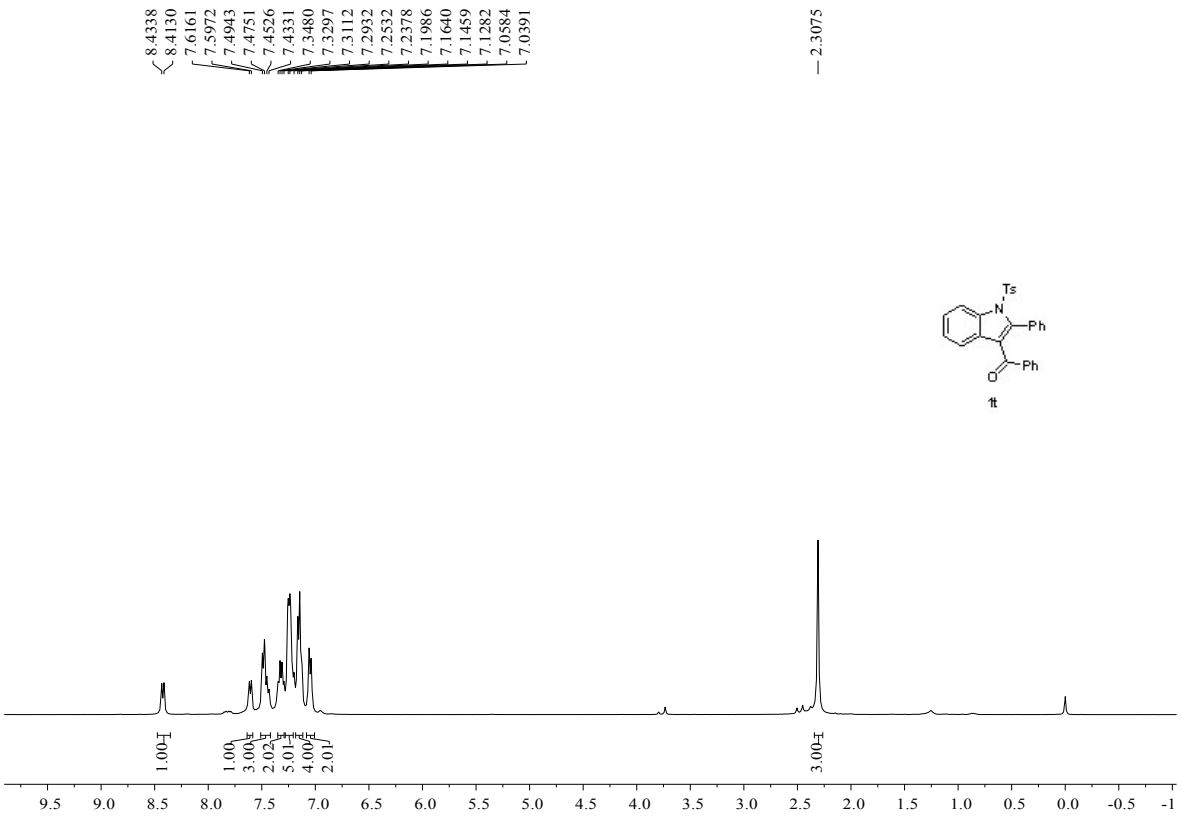
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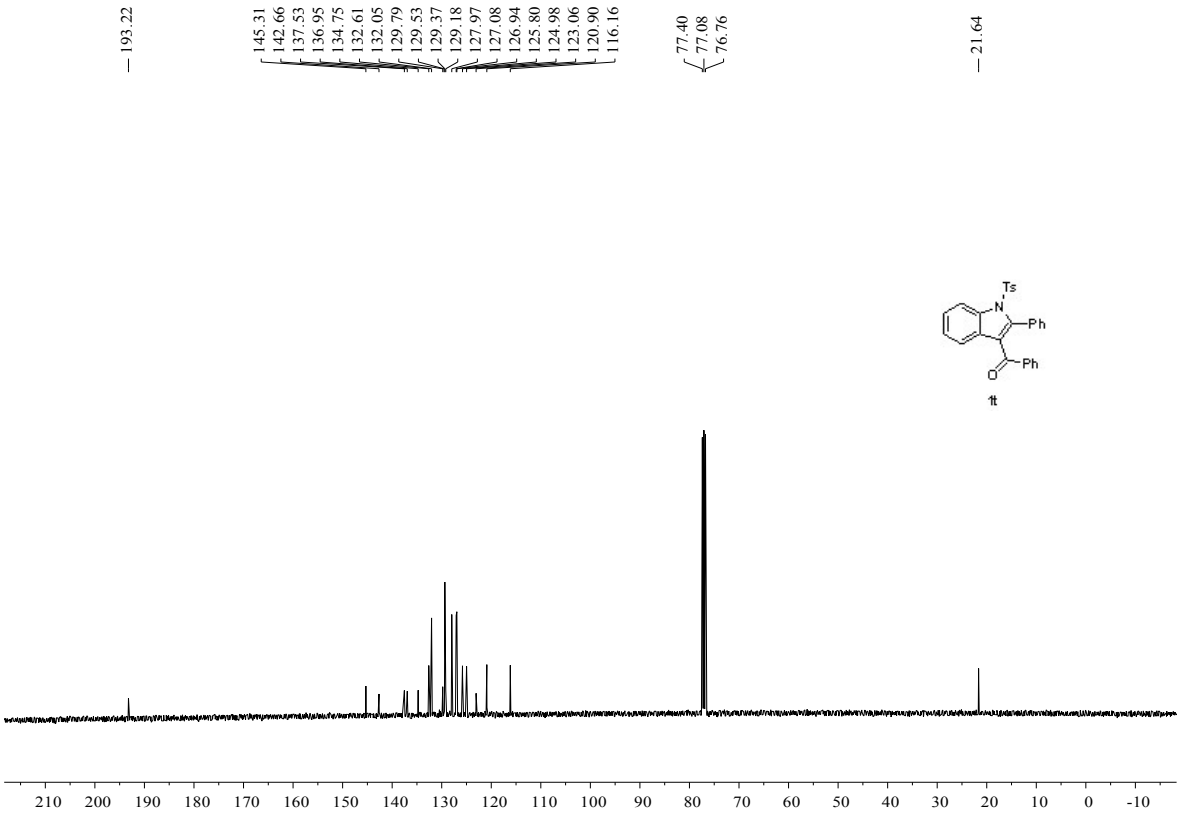
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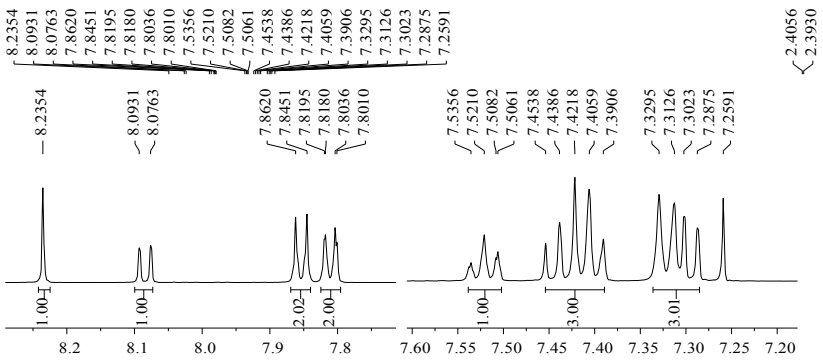
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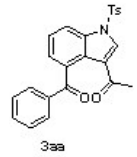
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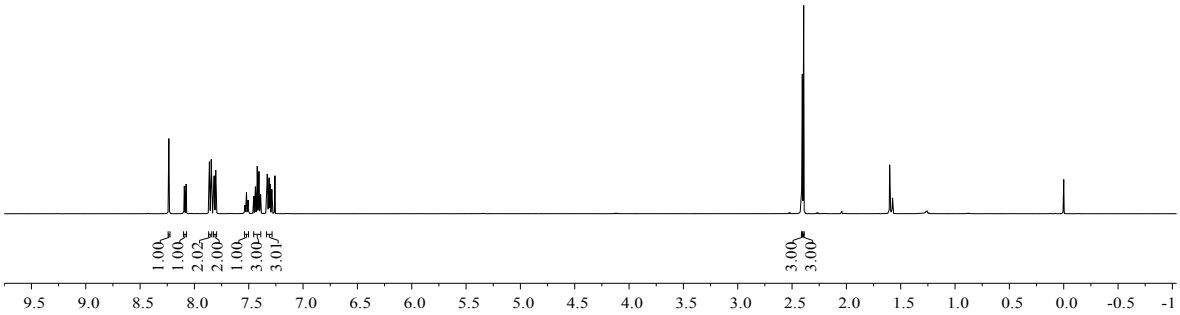

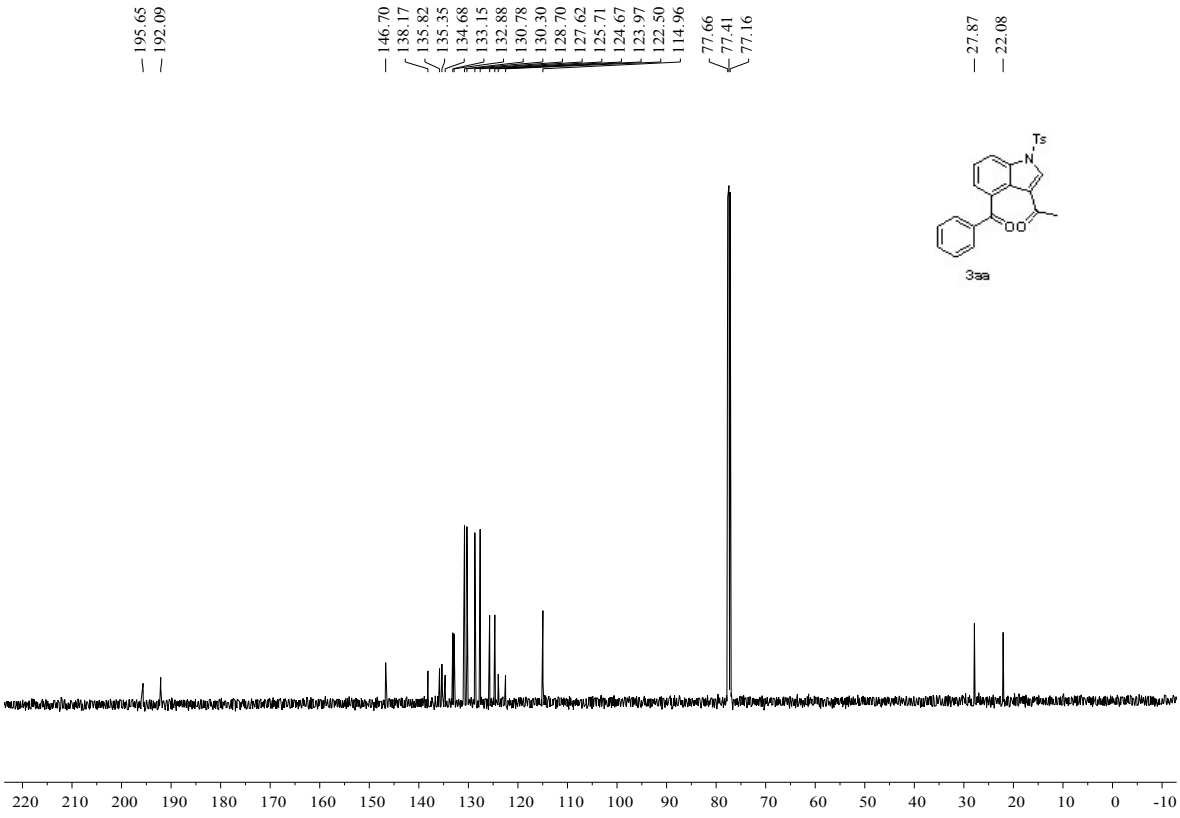
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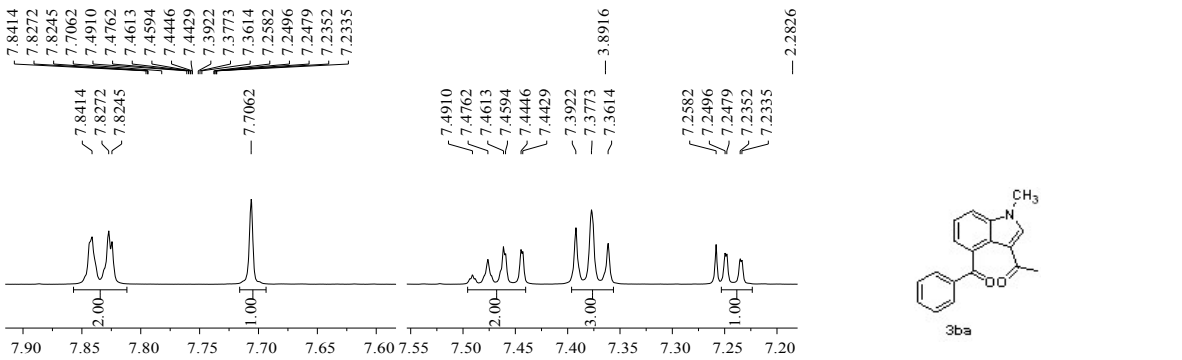
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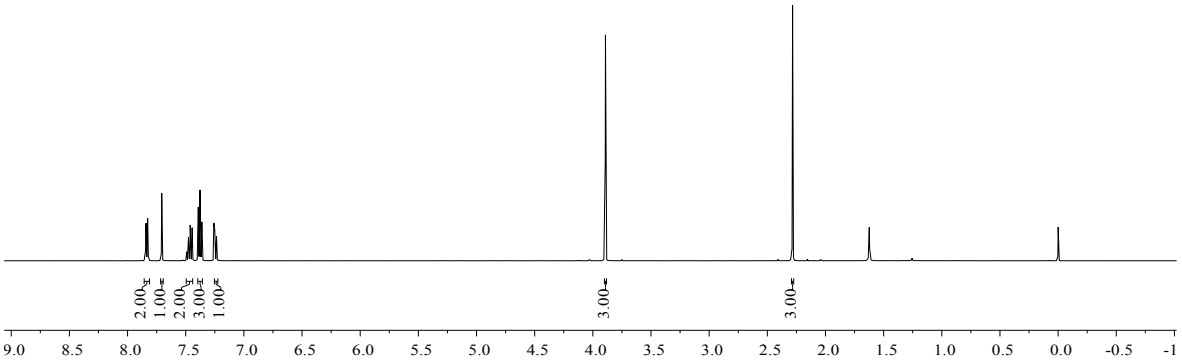
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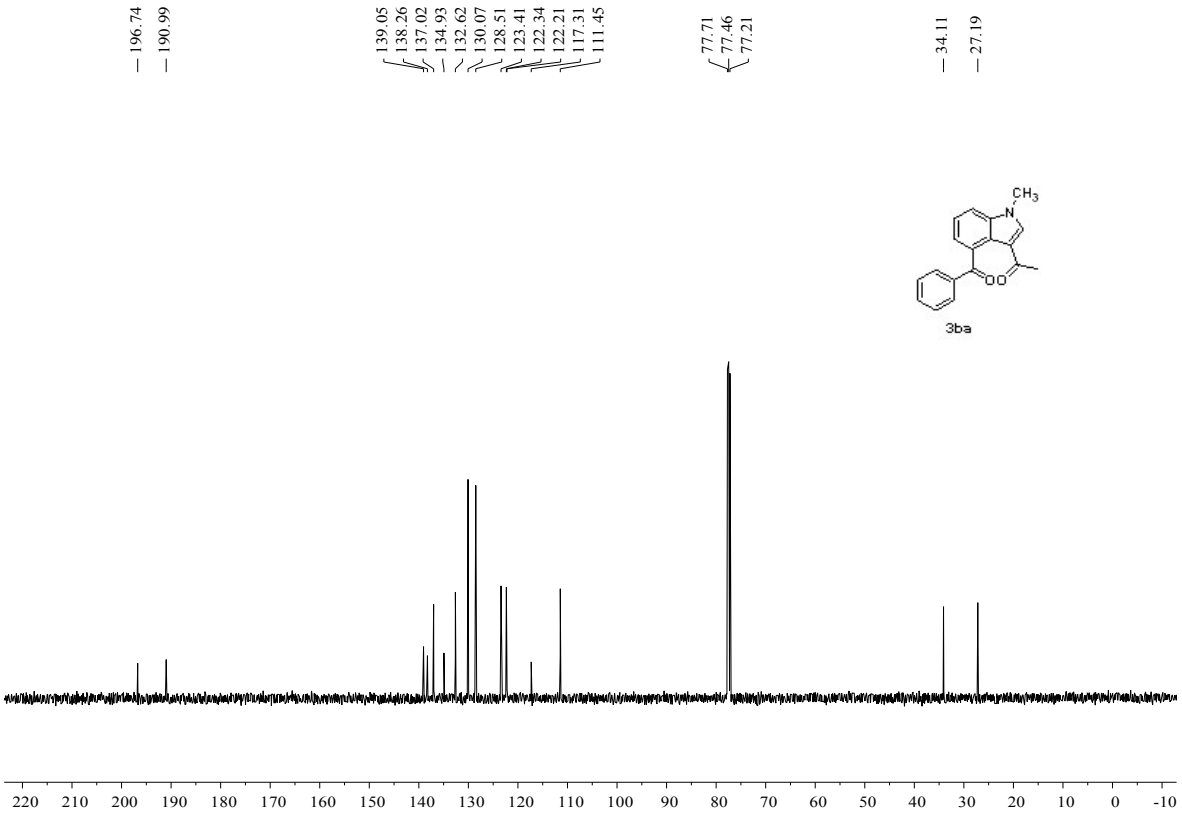
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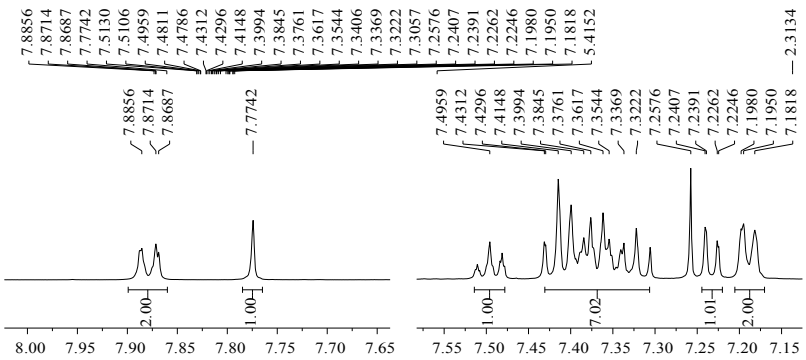
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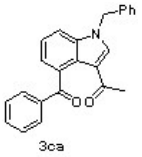
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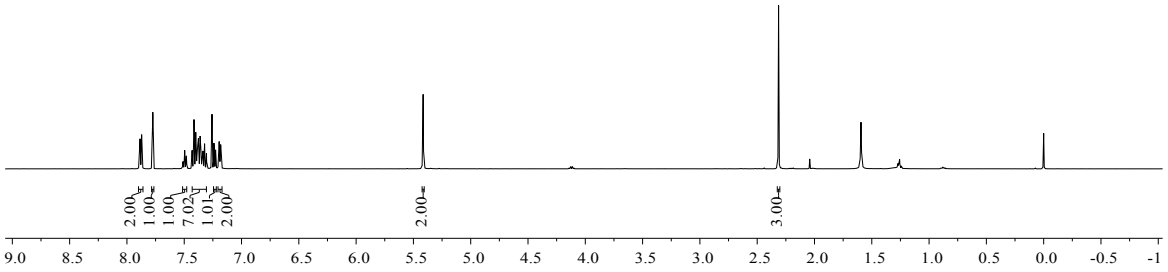
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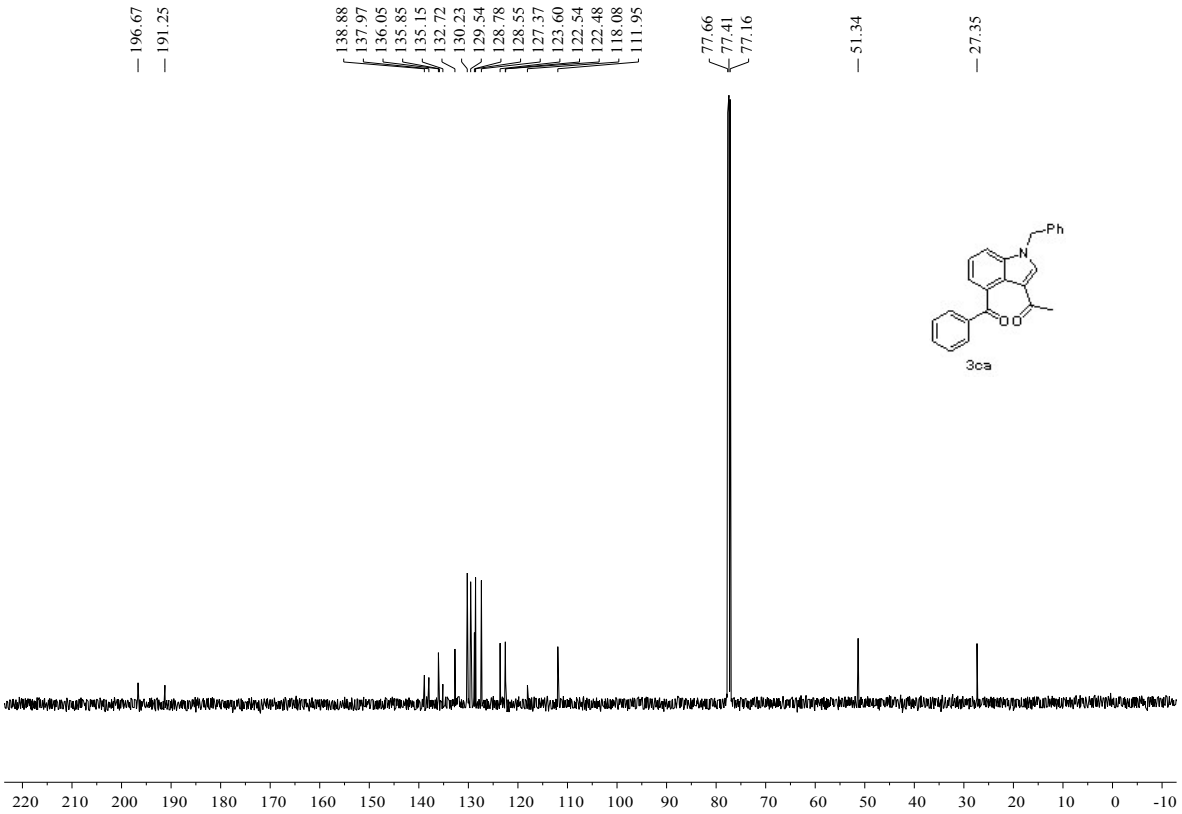
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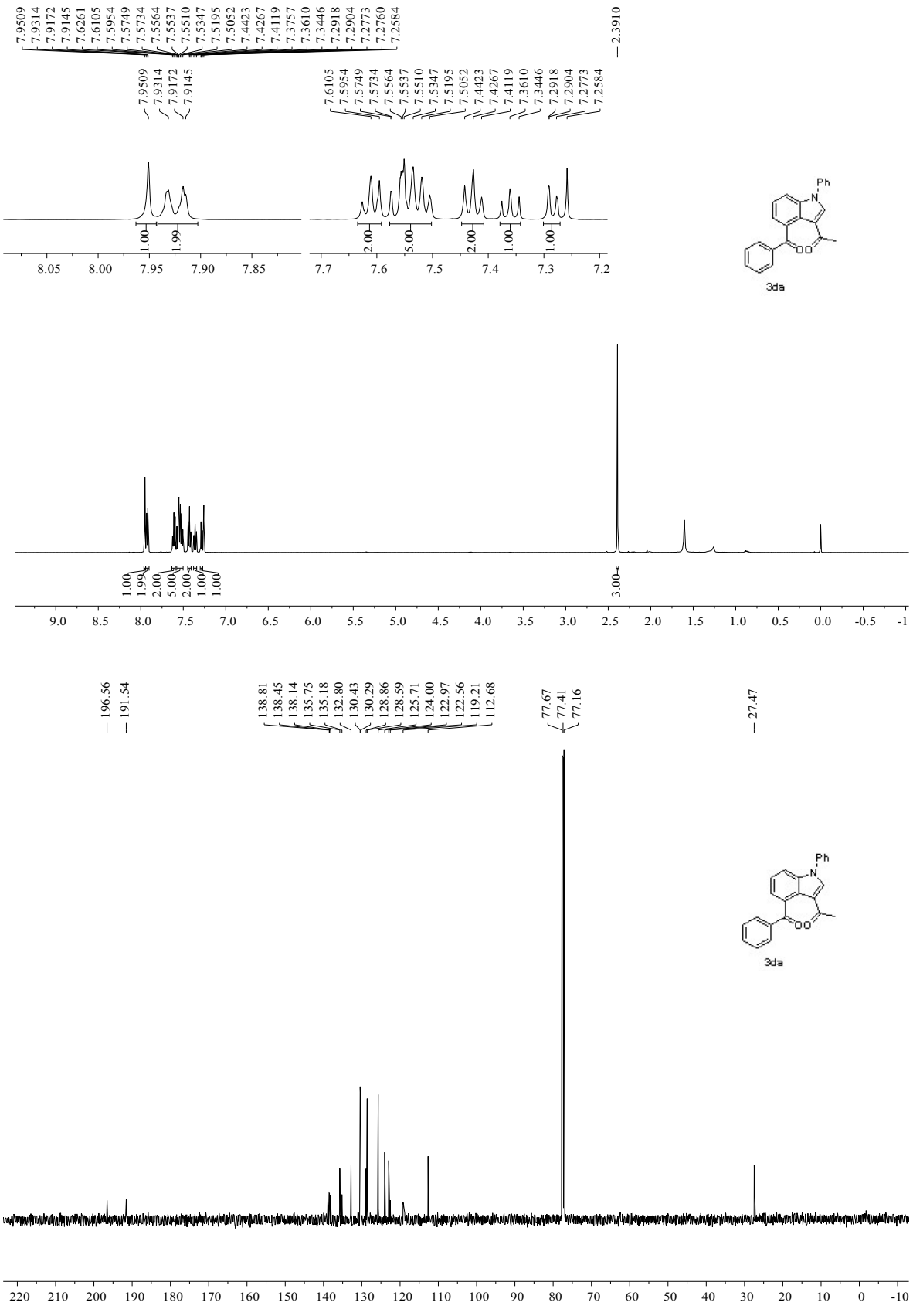
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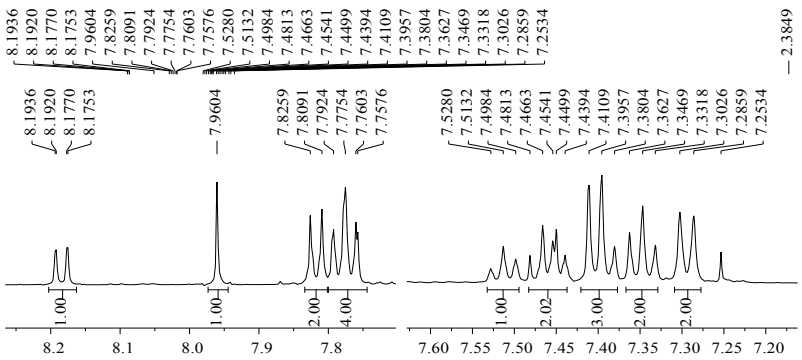
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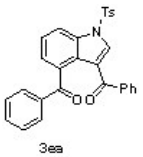
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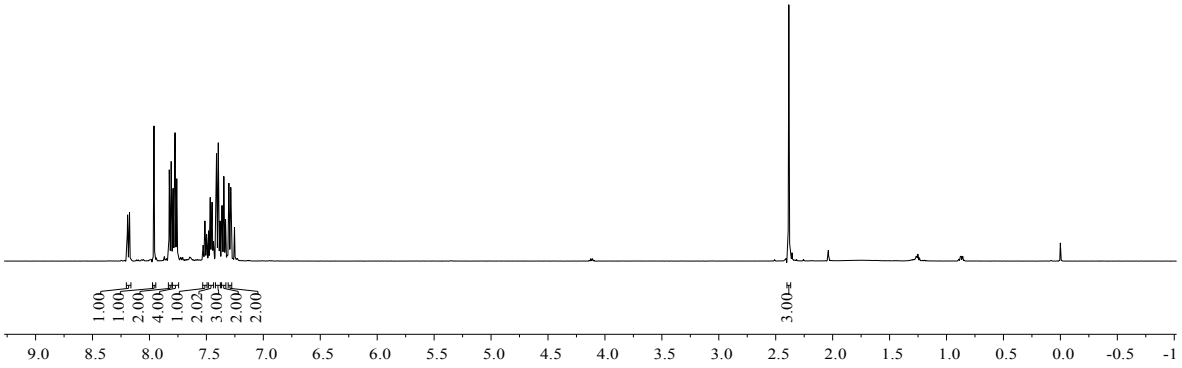
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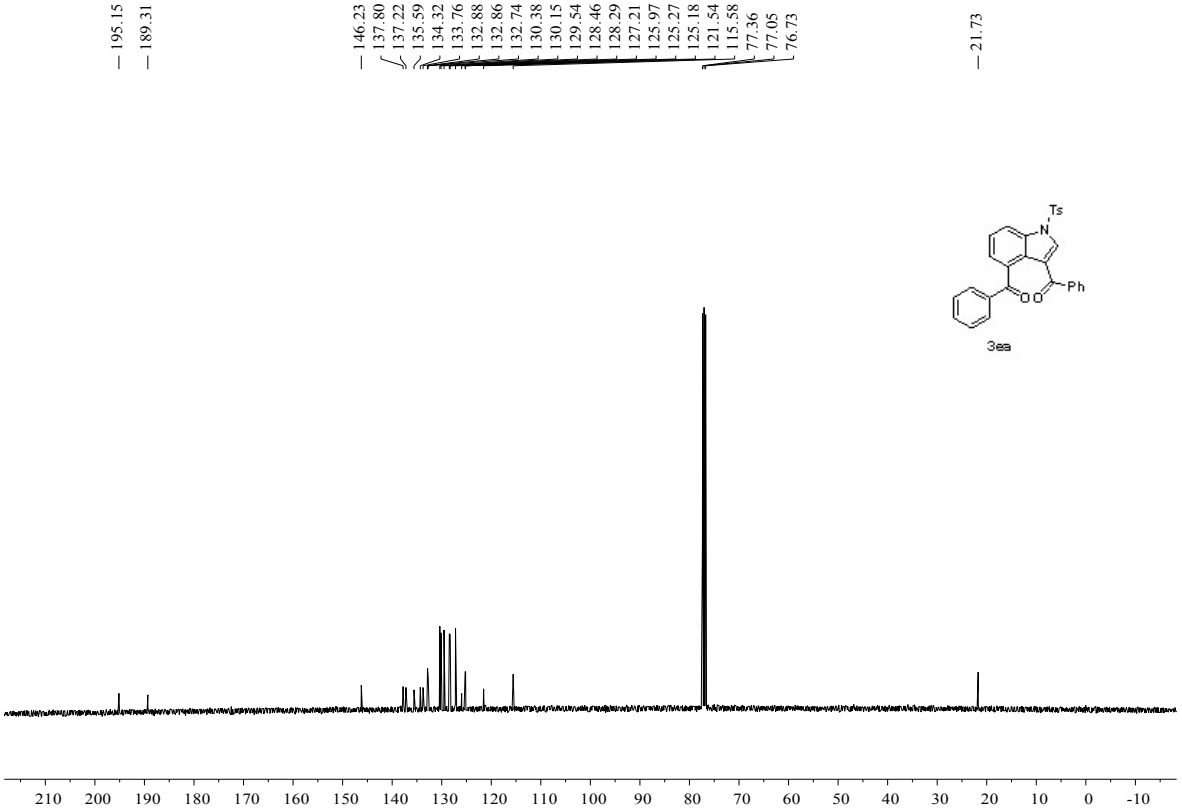
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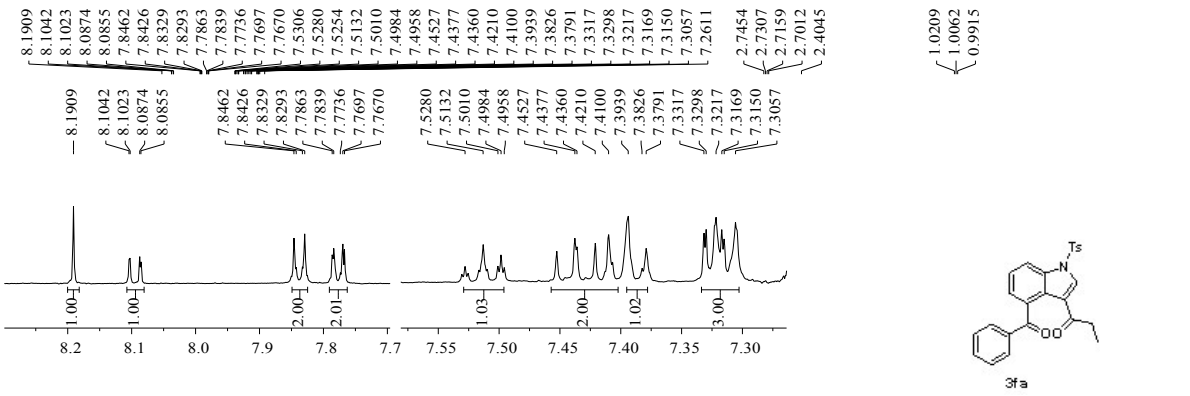
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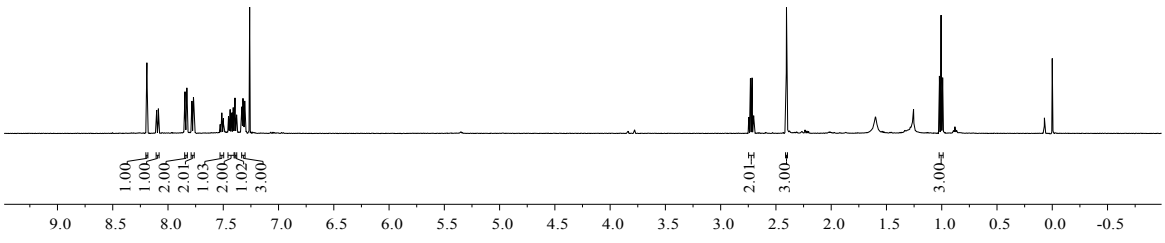
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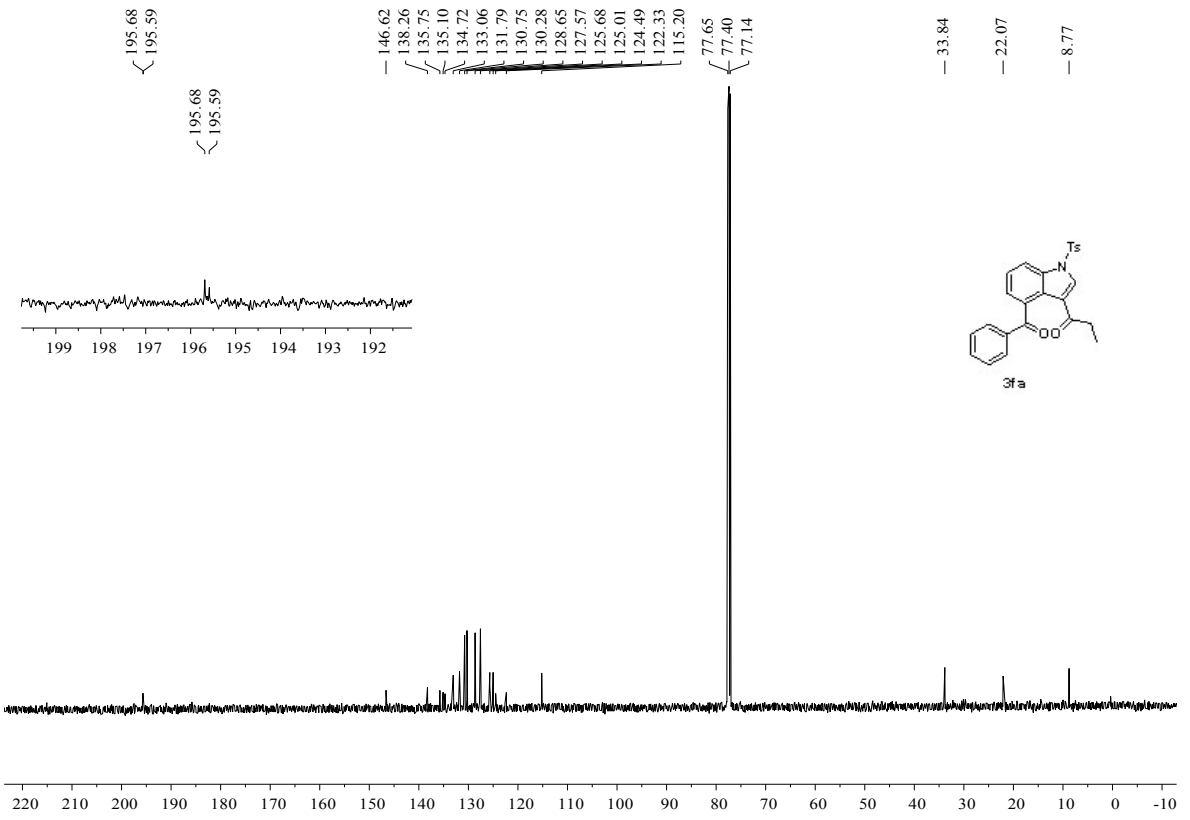
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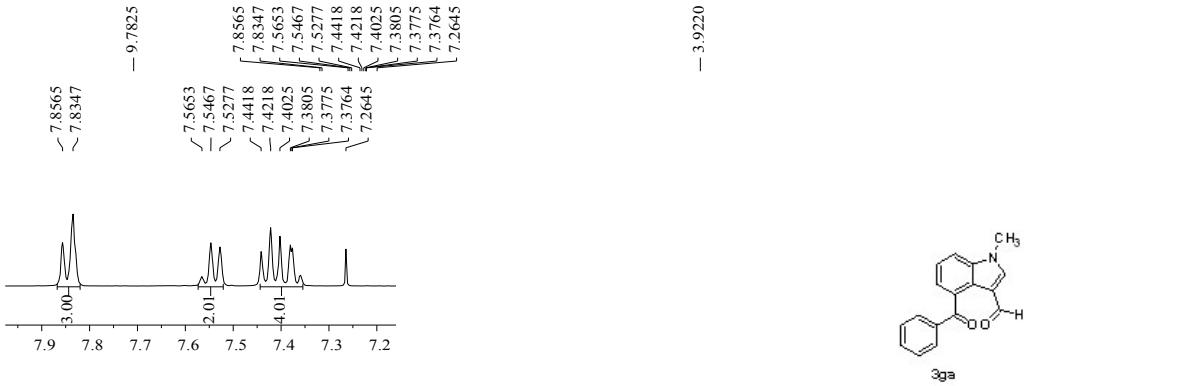
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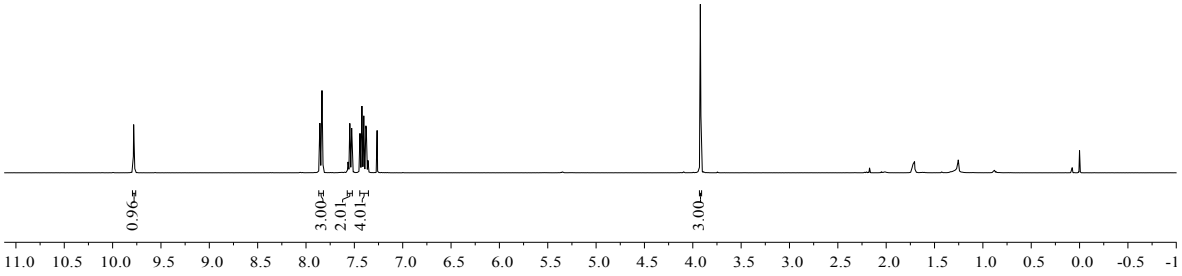
3ga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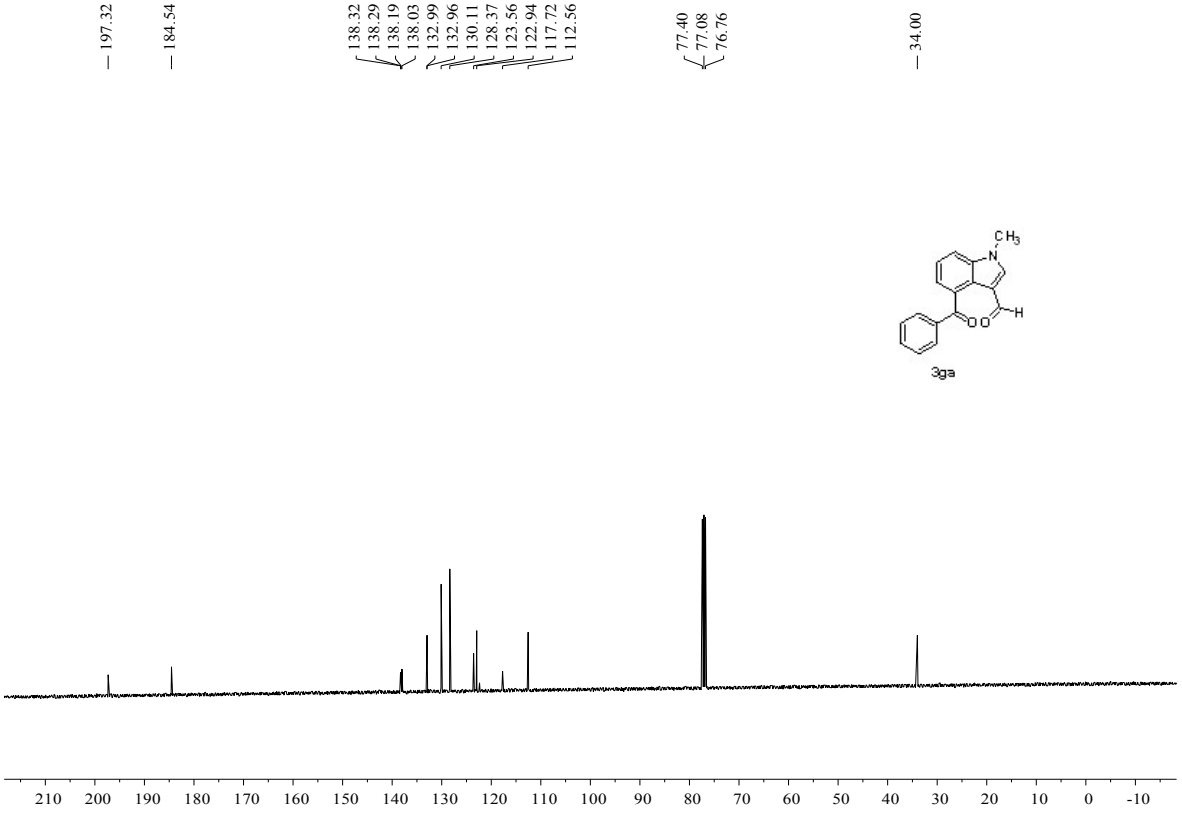
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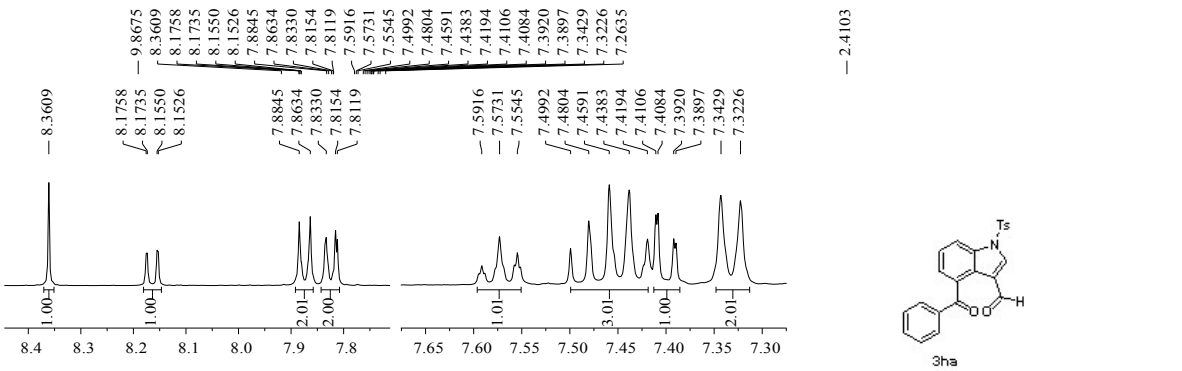
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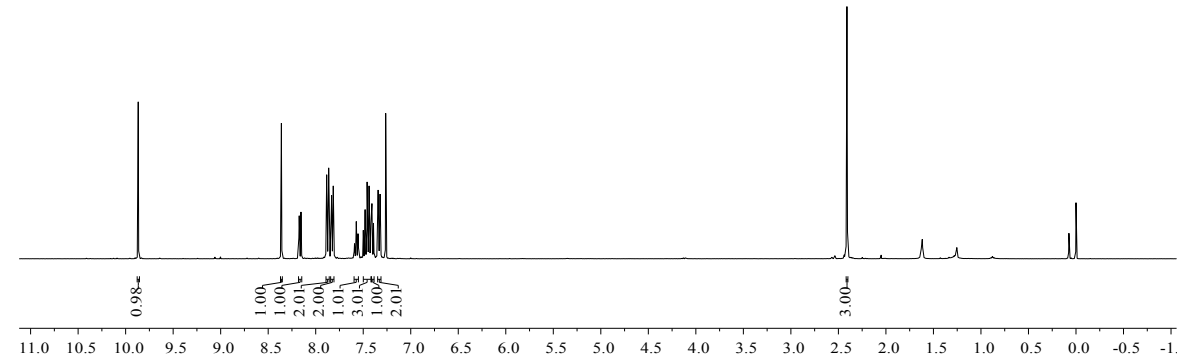
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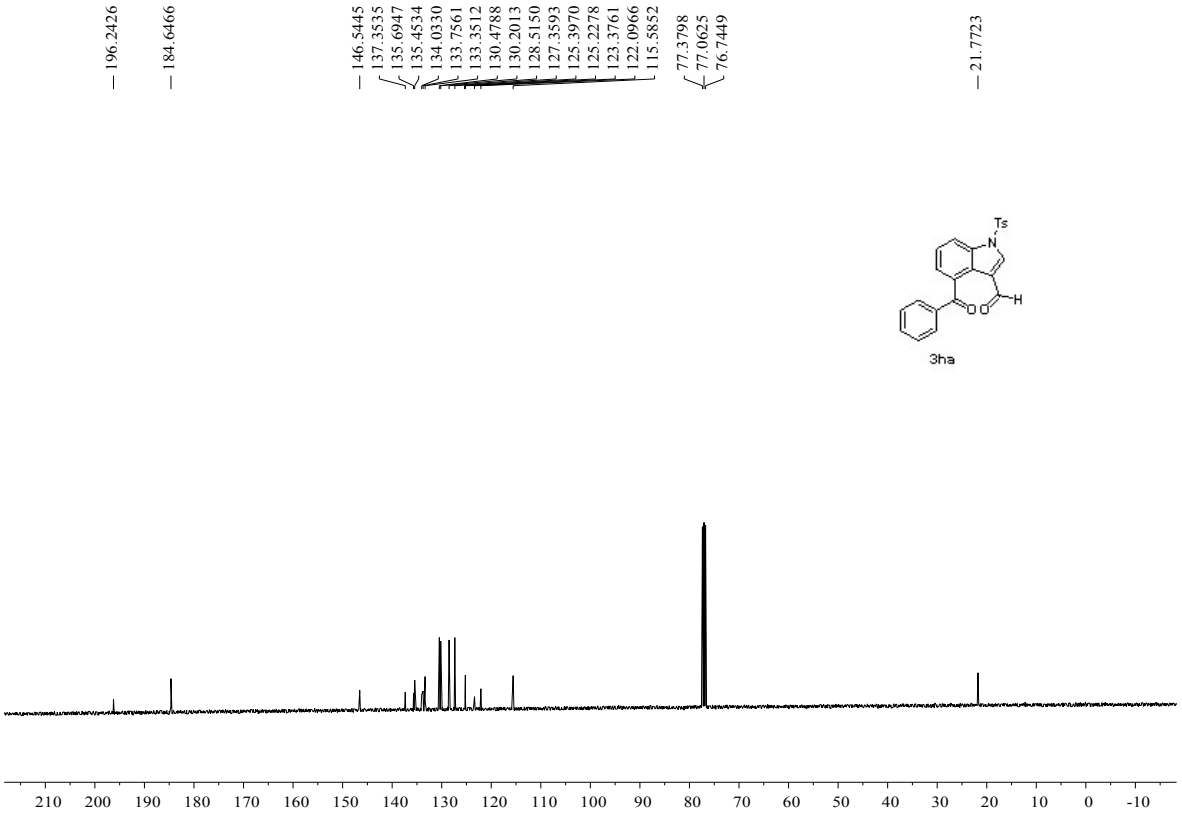
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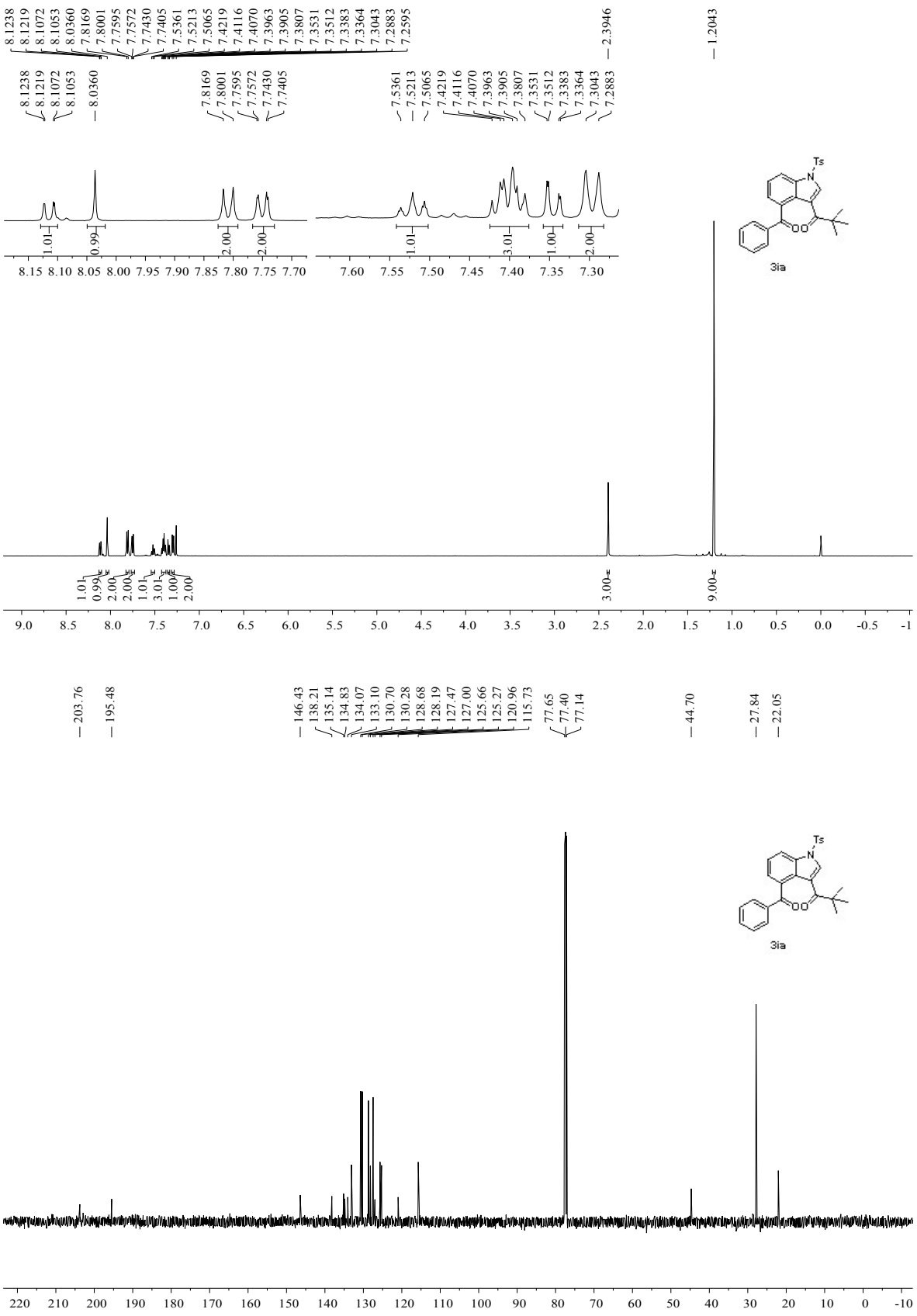
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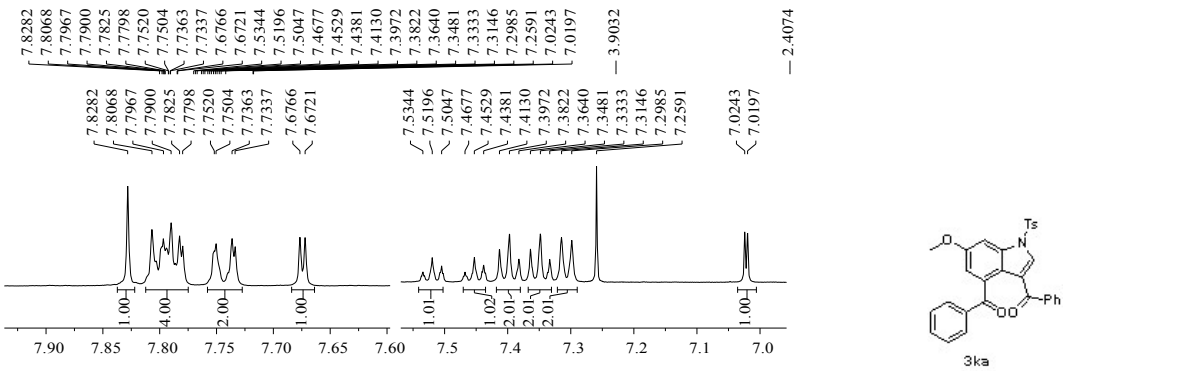
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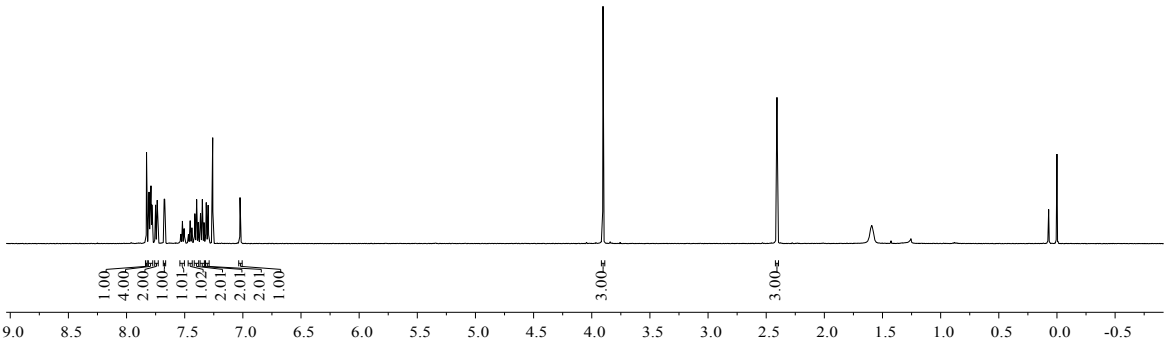
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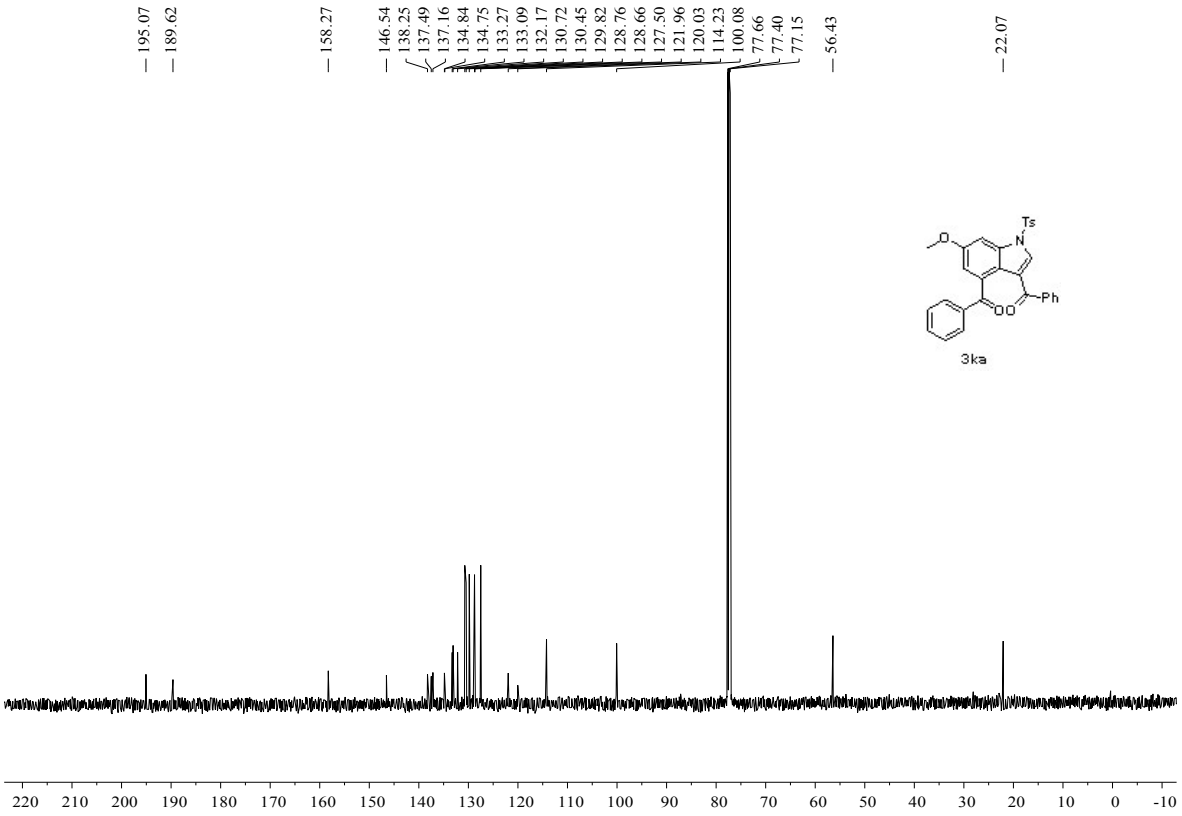
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Ph

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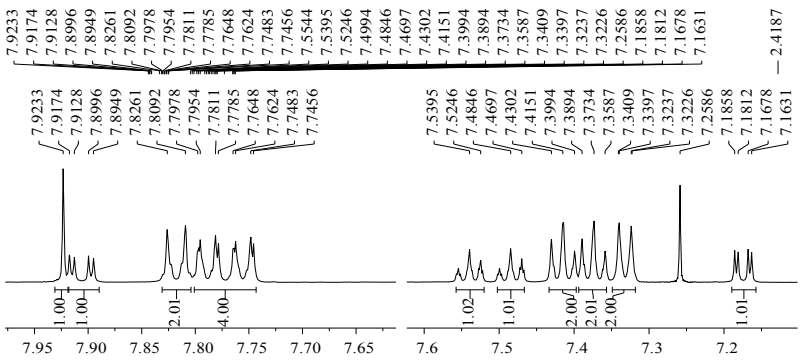
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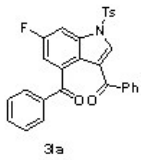
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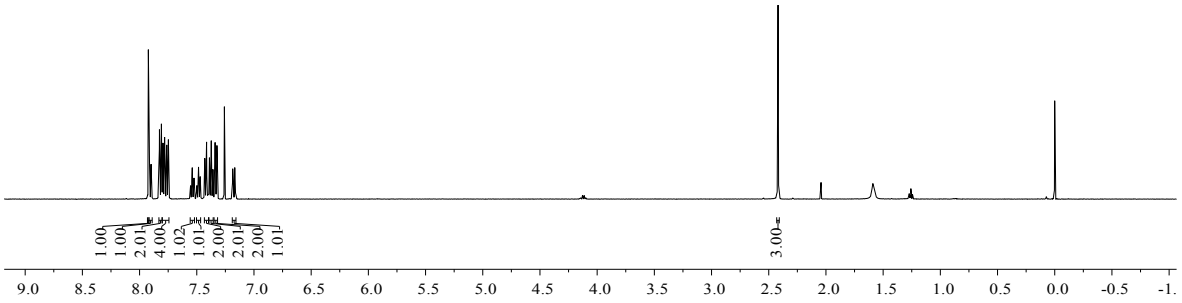
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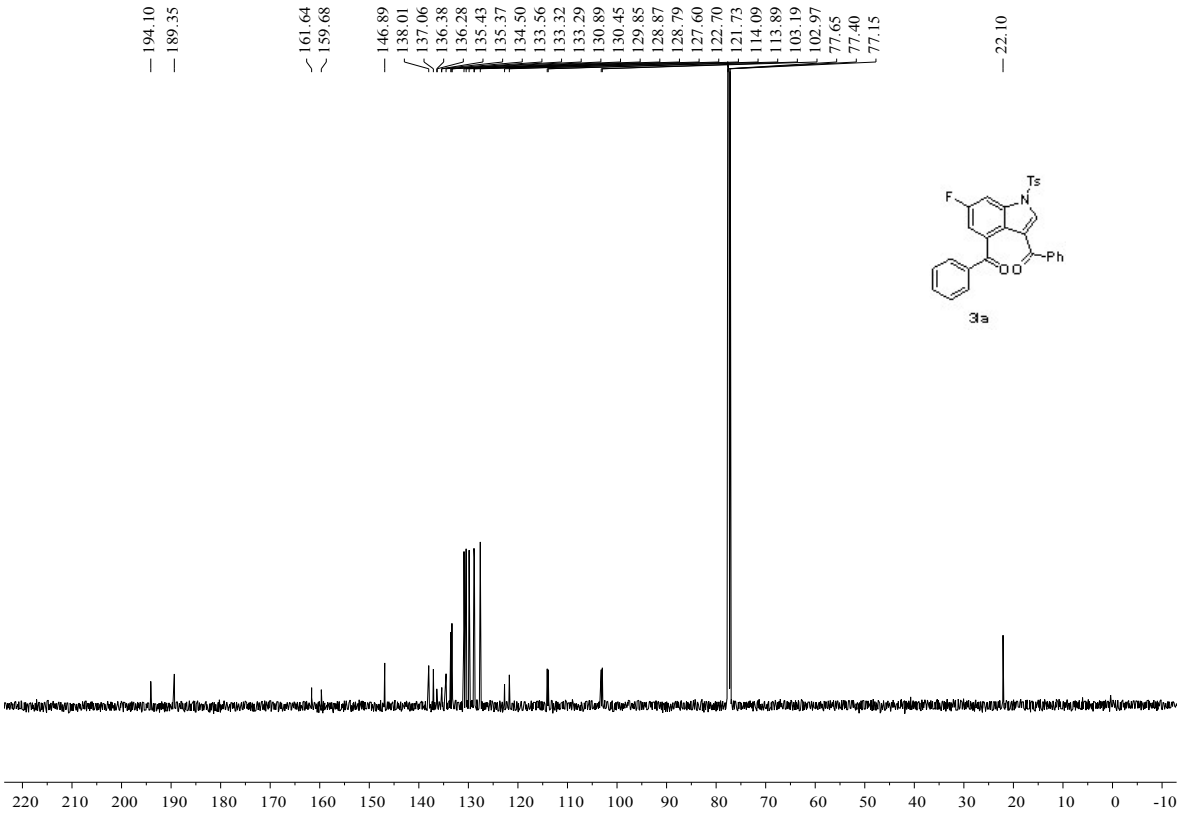
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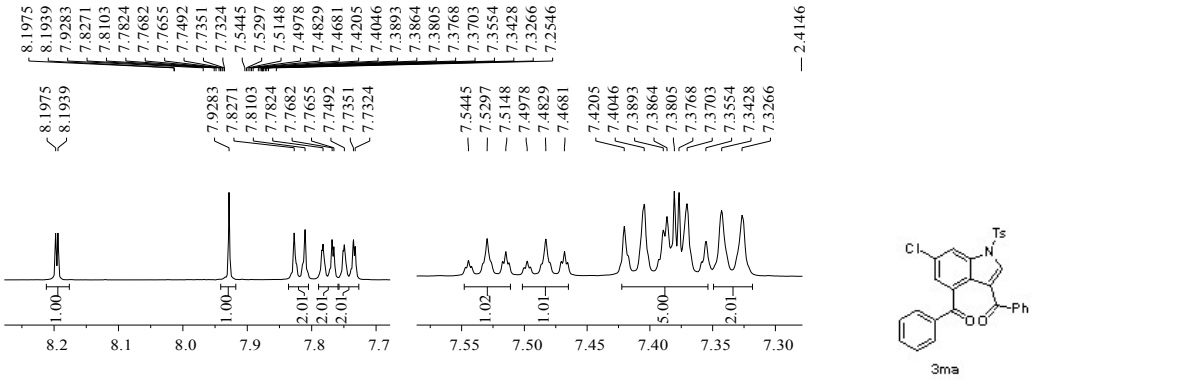
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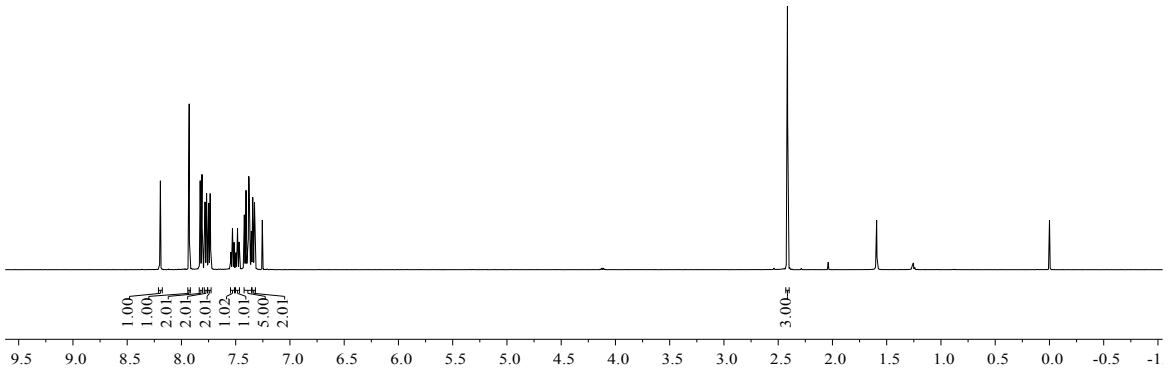
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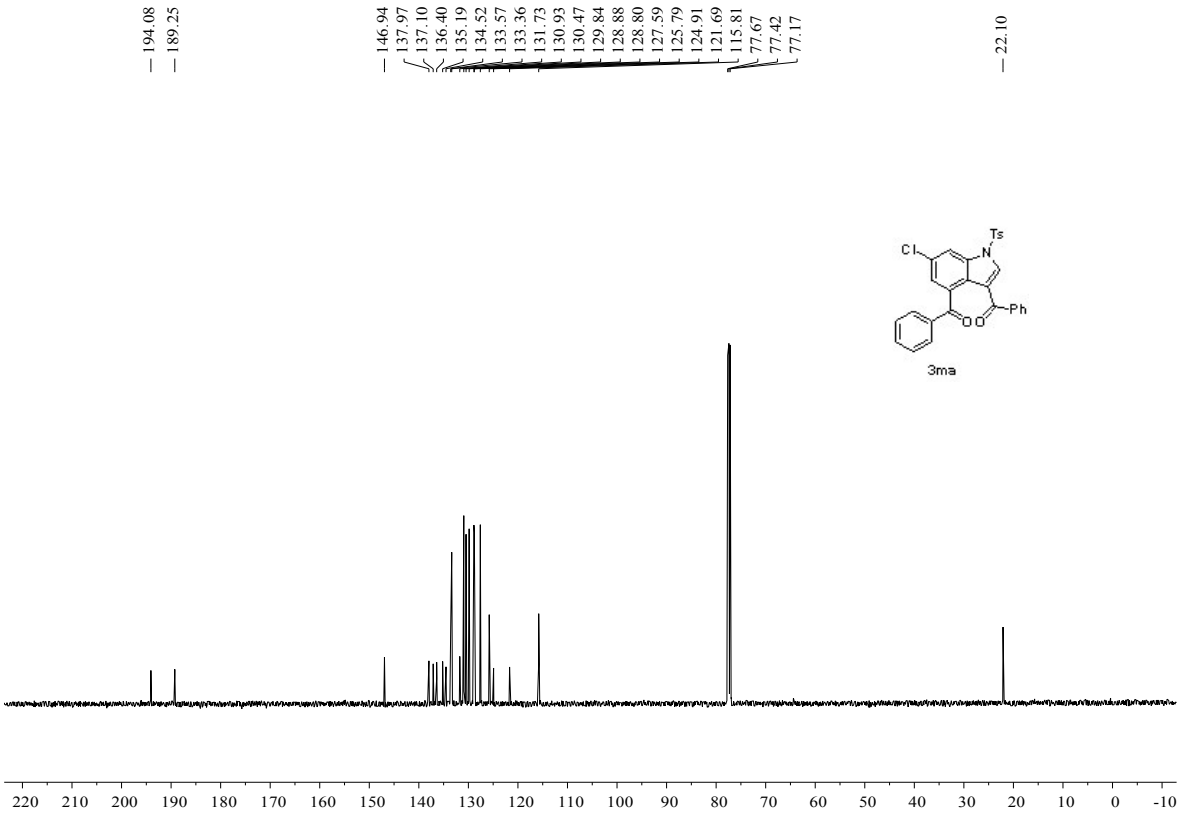
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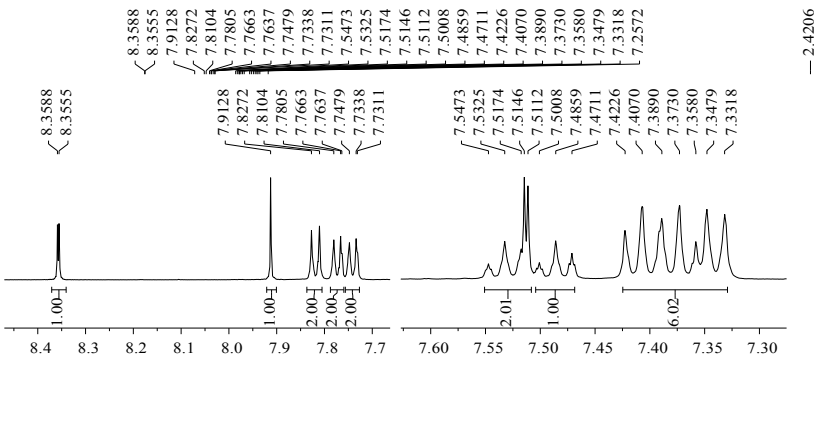
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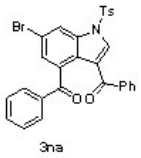
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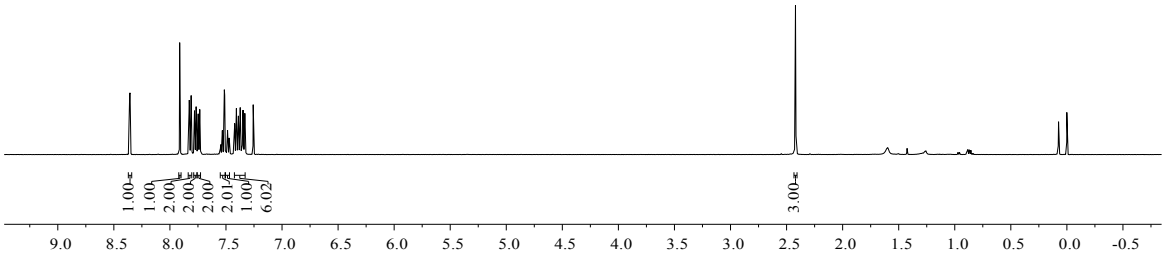
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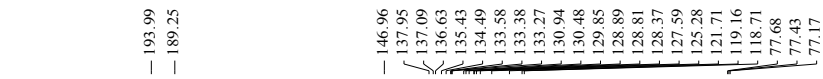
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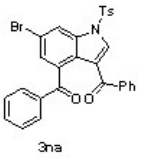
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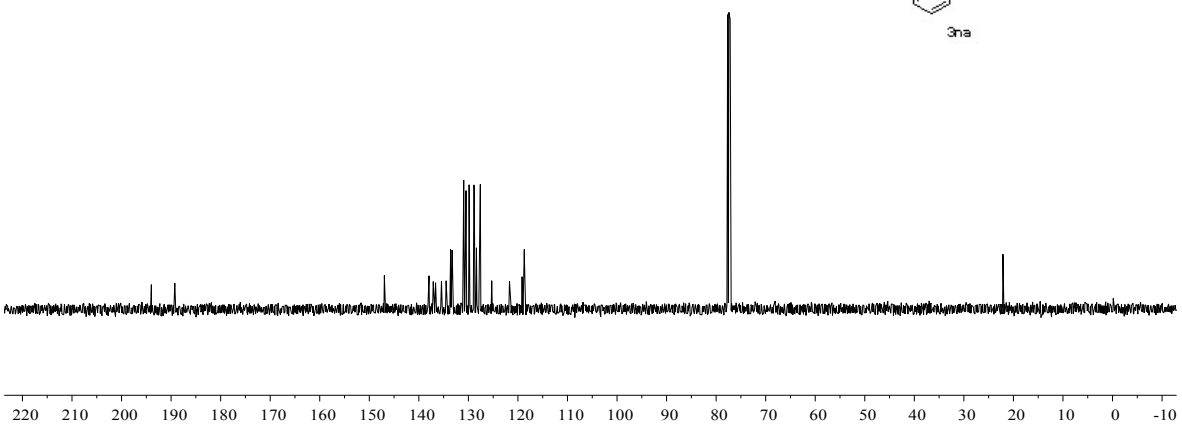

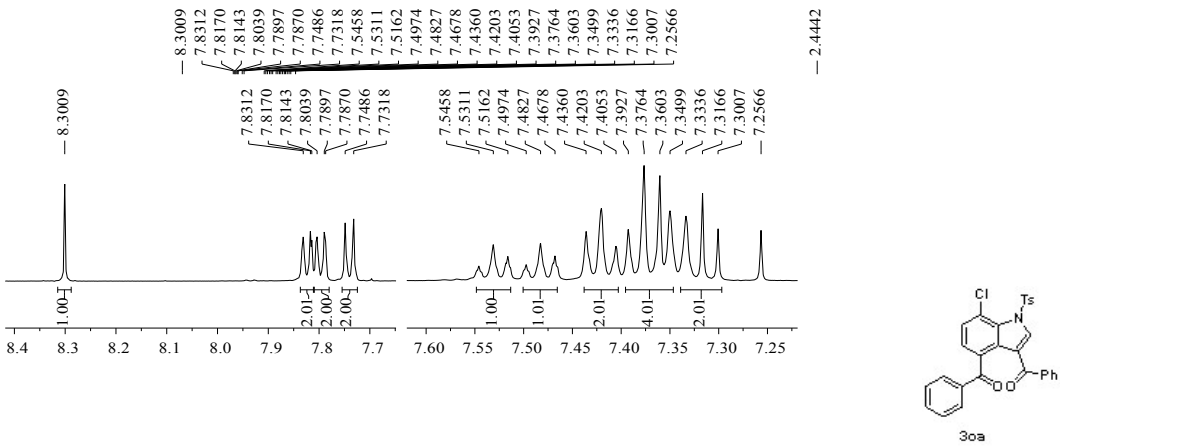
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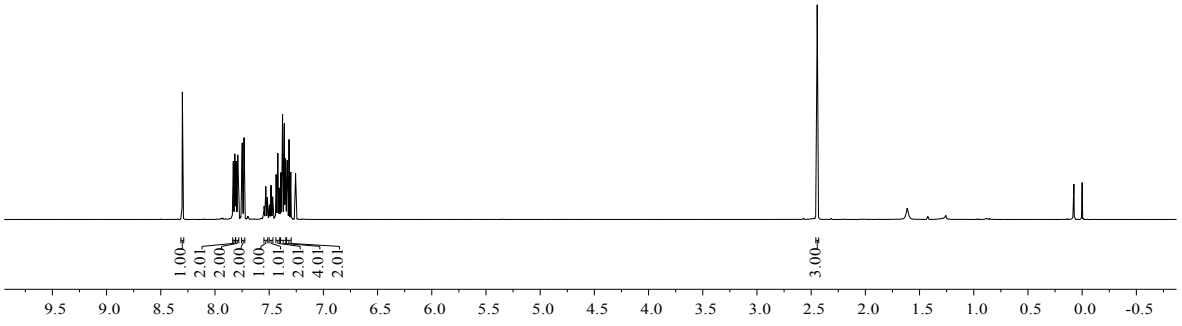
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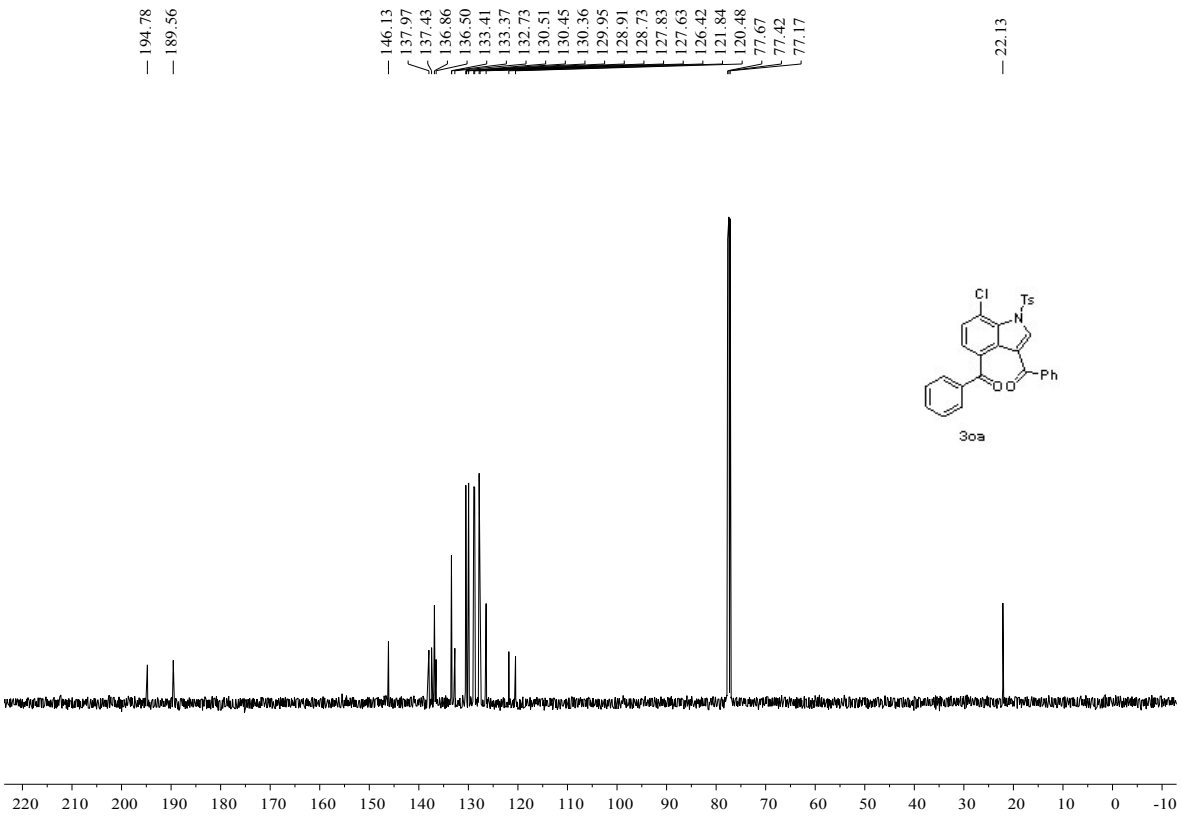
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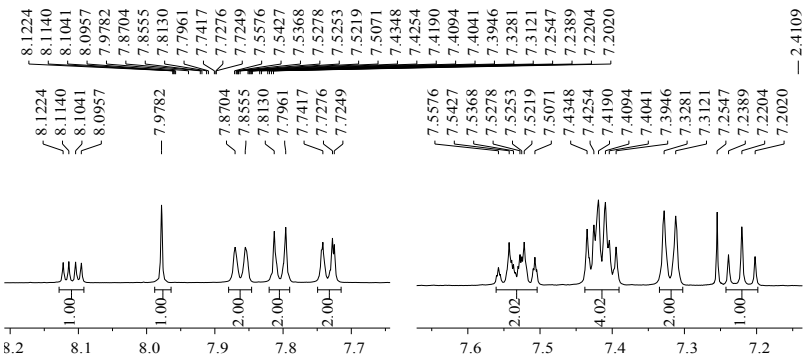
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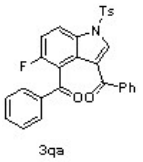
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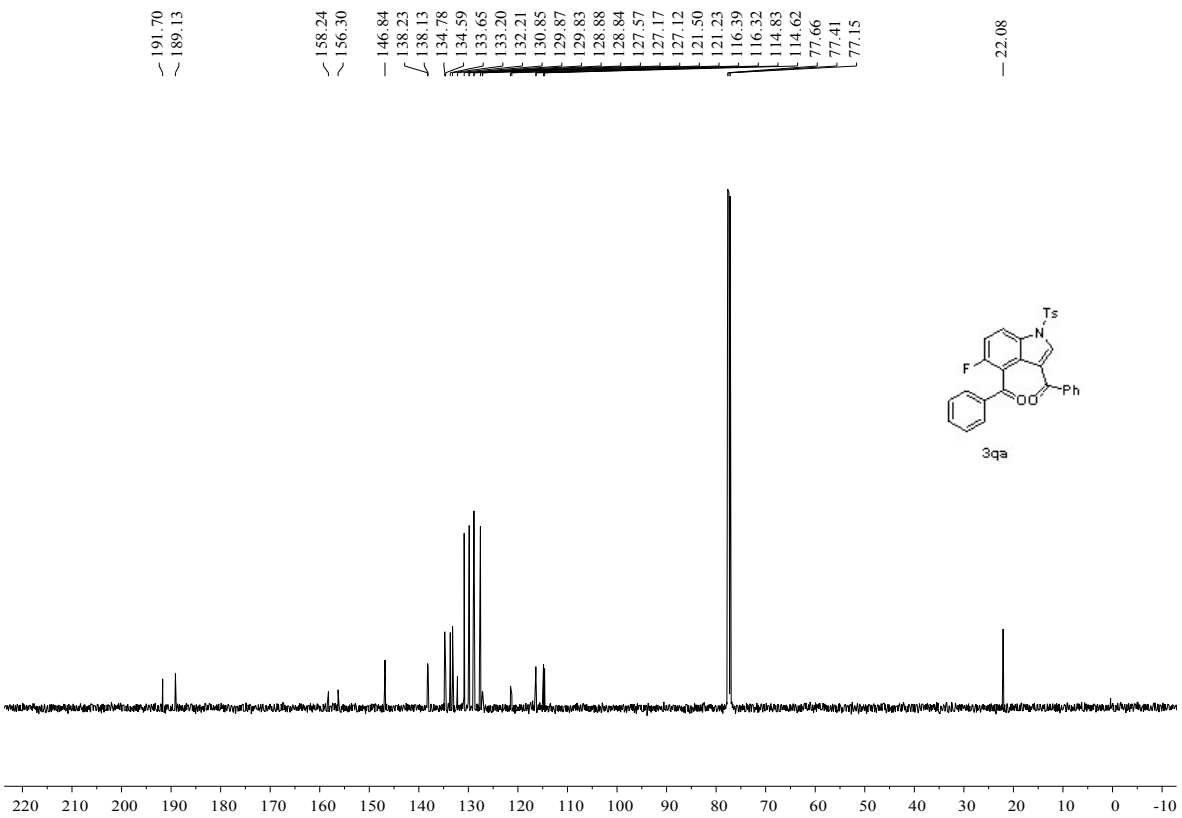
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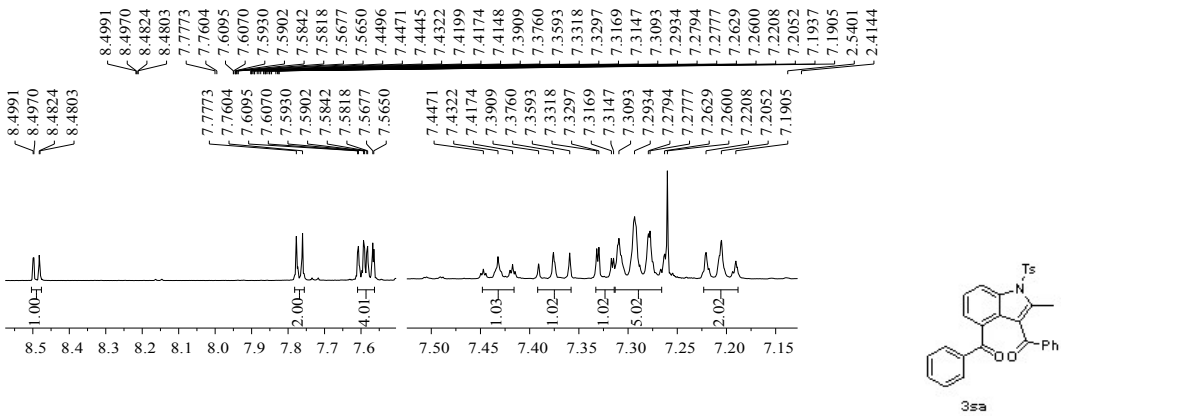
Ph

3qa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Ph
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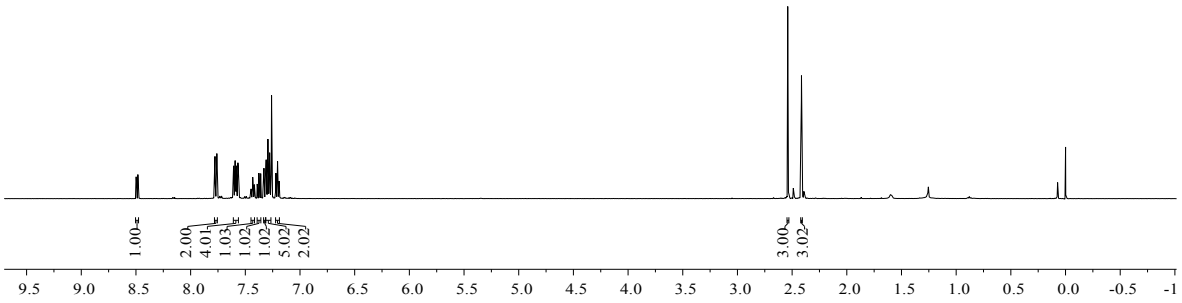
O

3sa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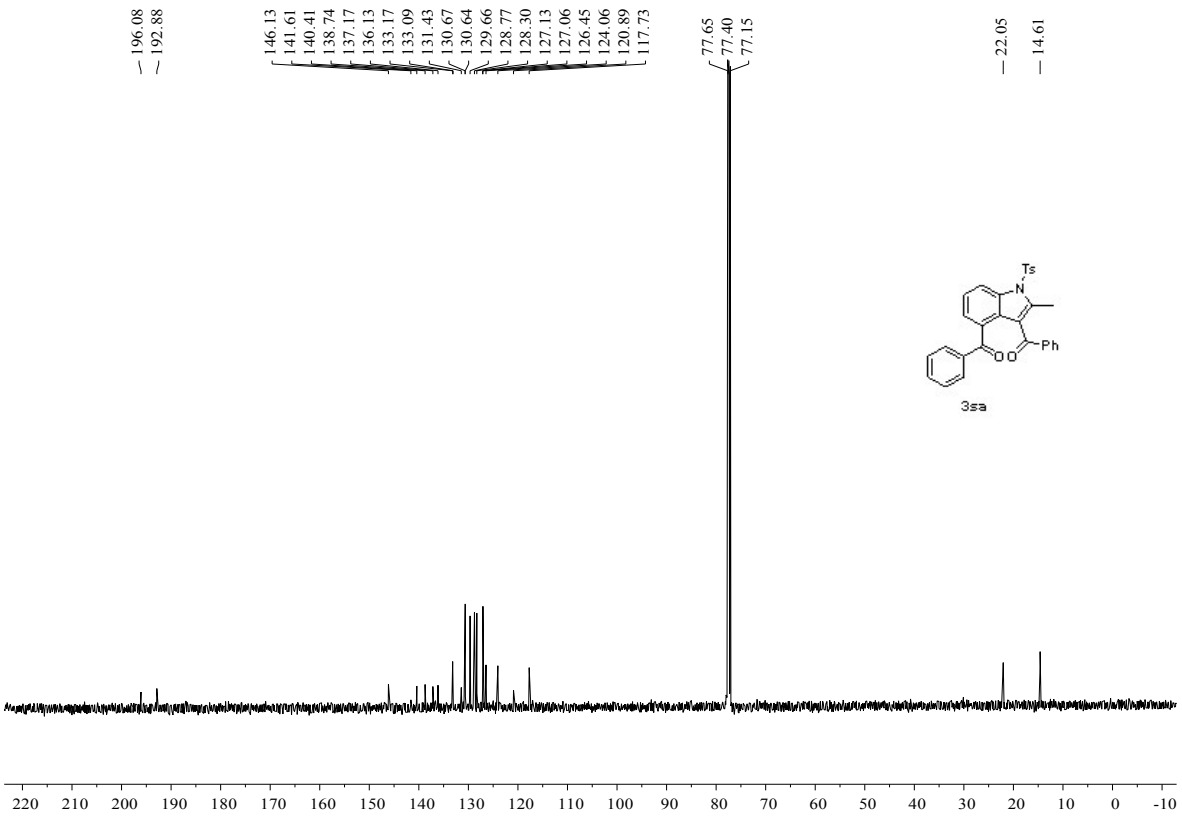
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Ts
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Ph
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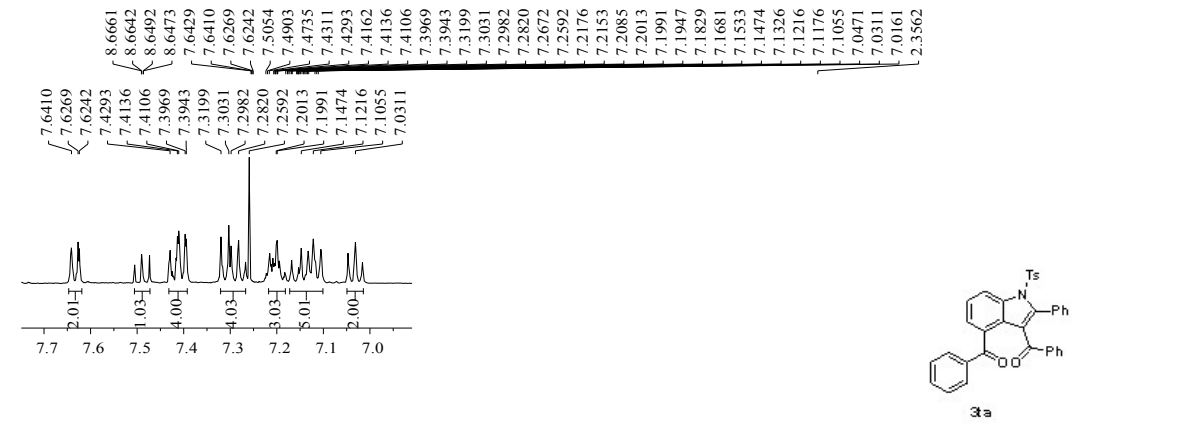
3sa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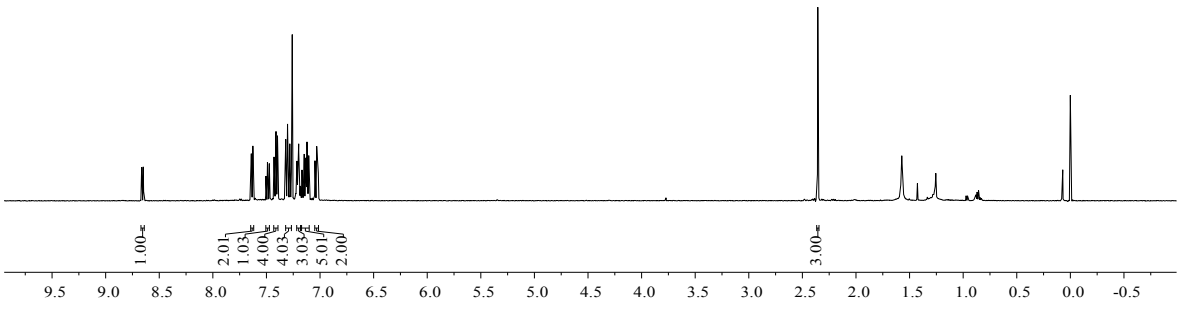
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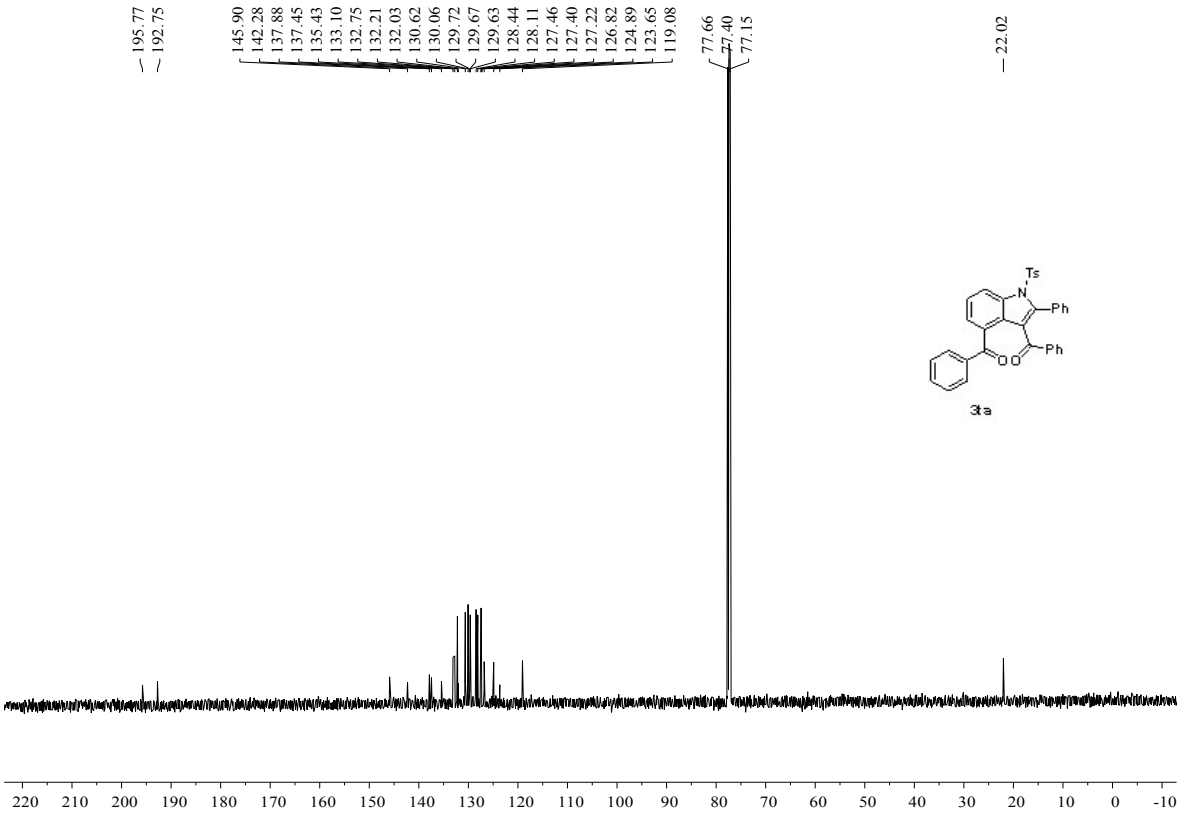
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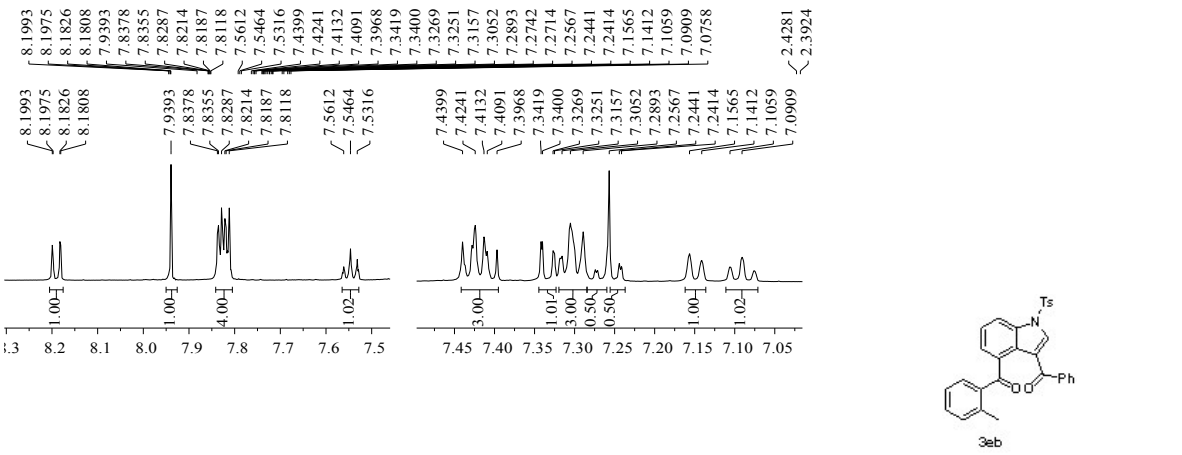
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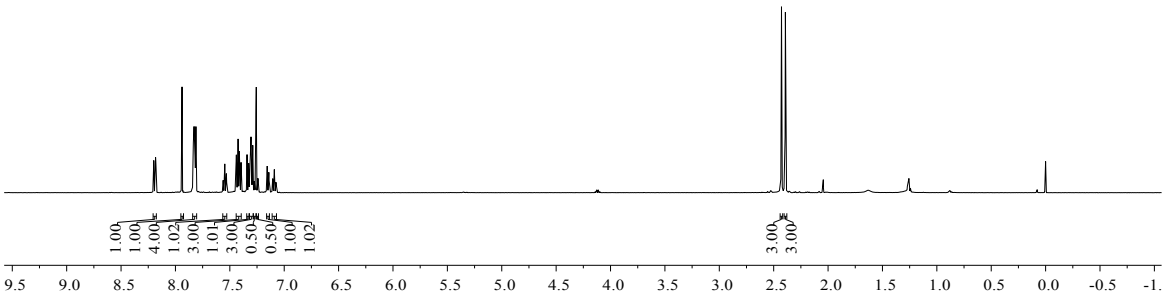
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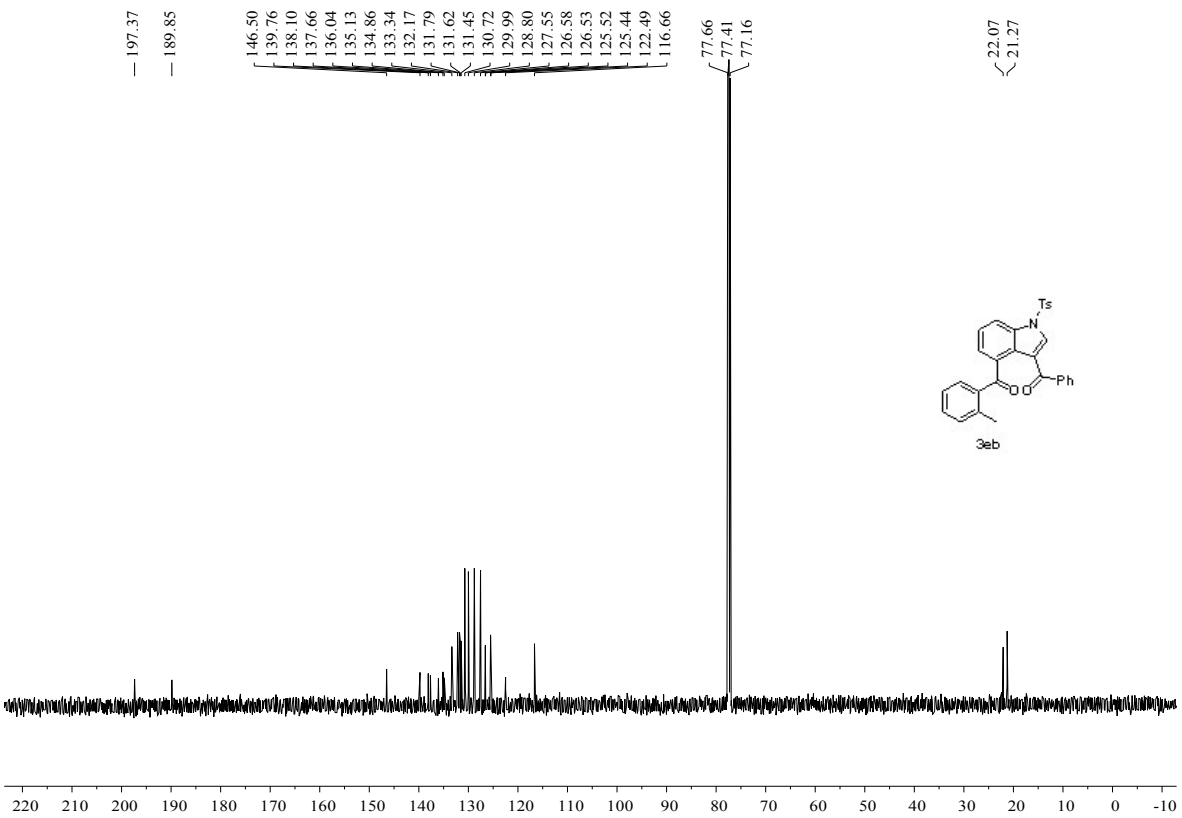
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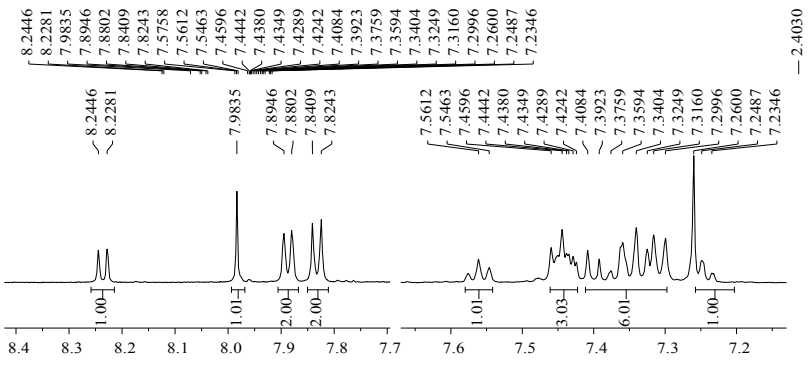
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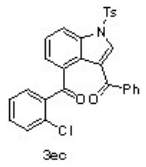
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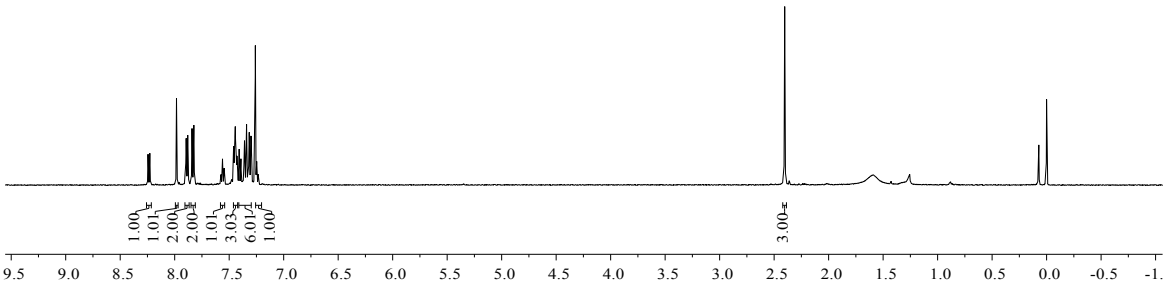
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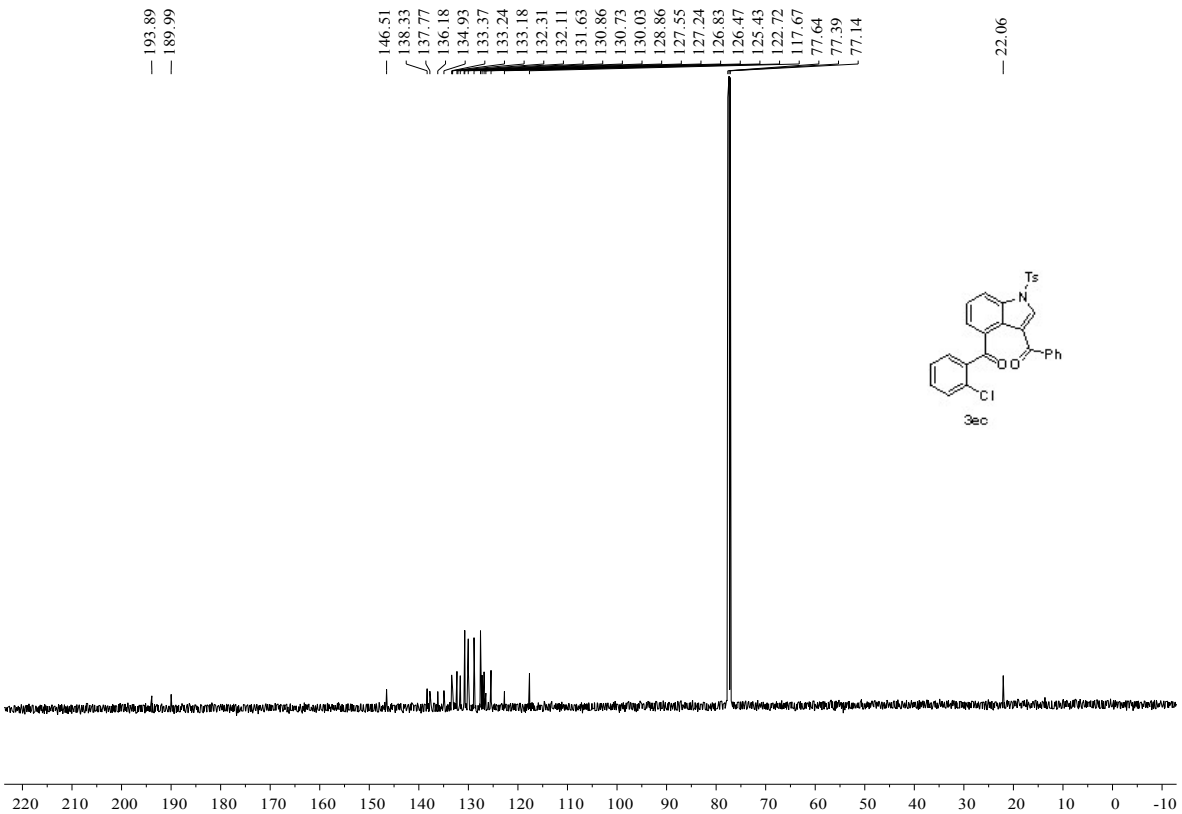
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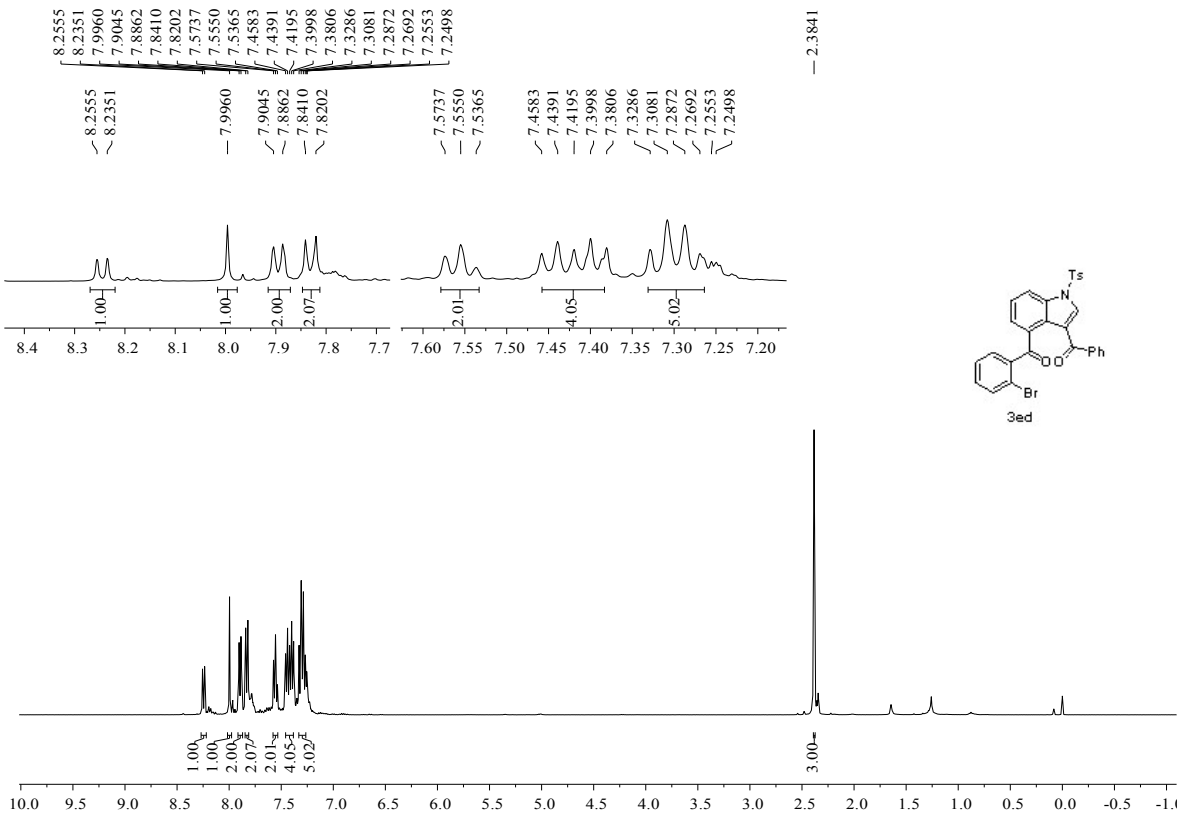
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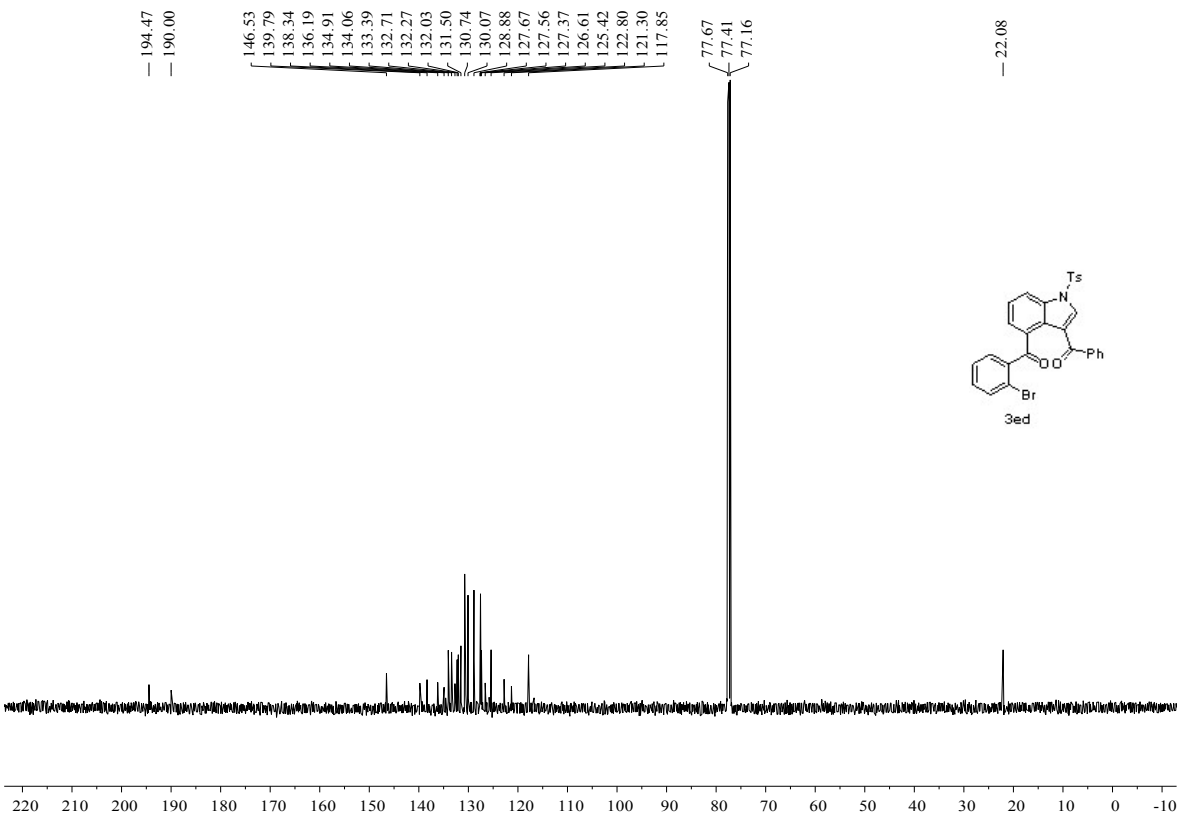
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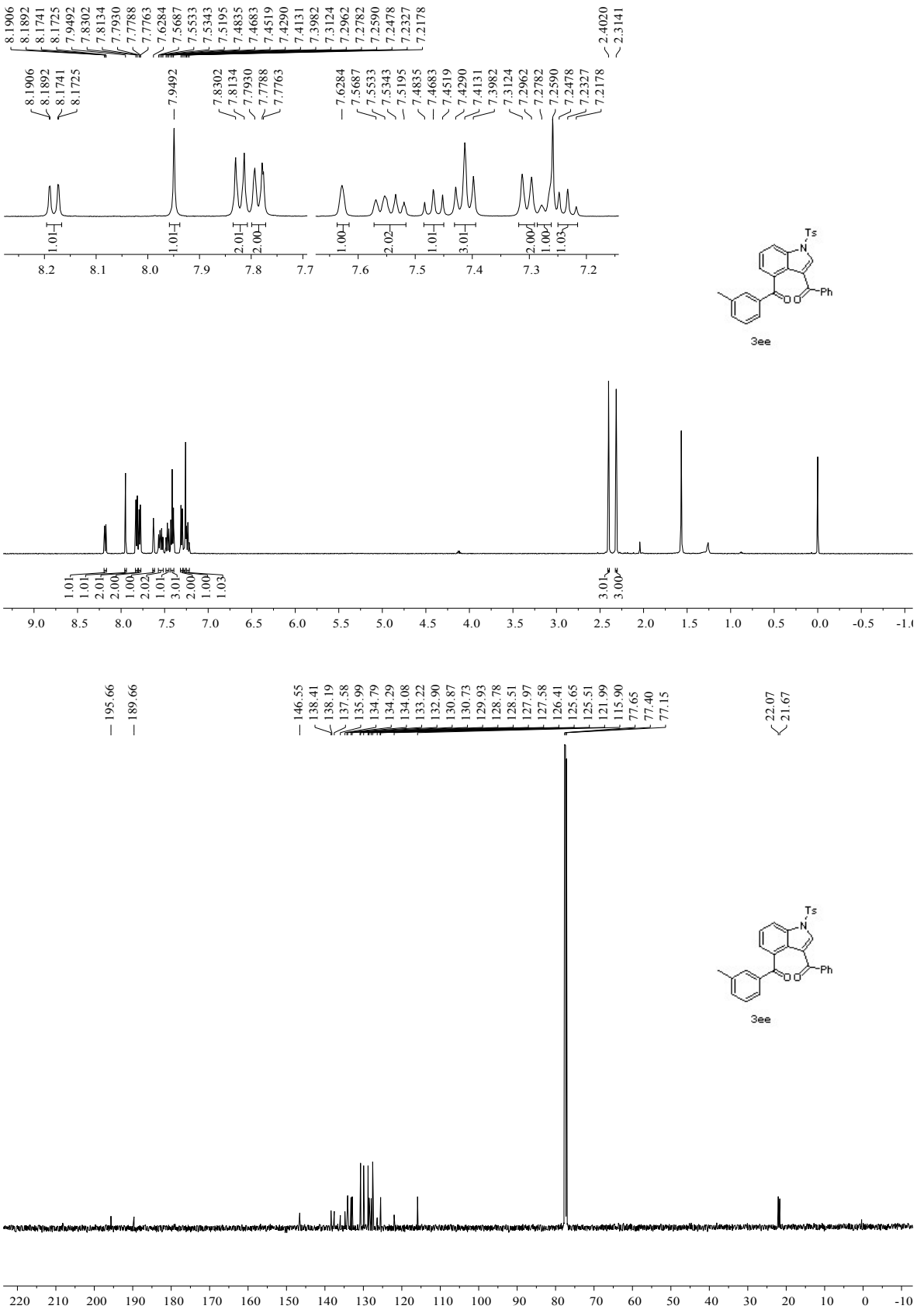
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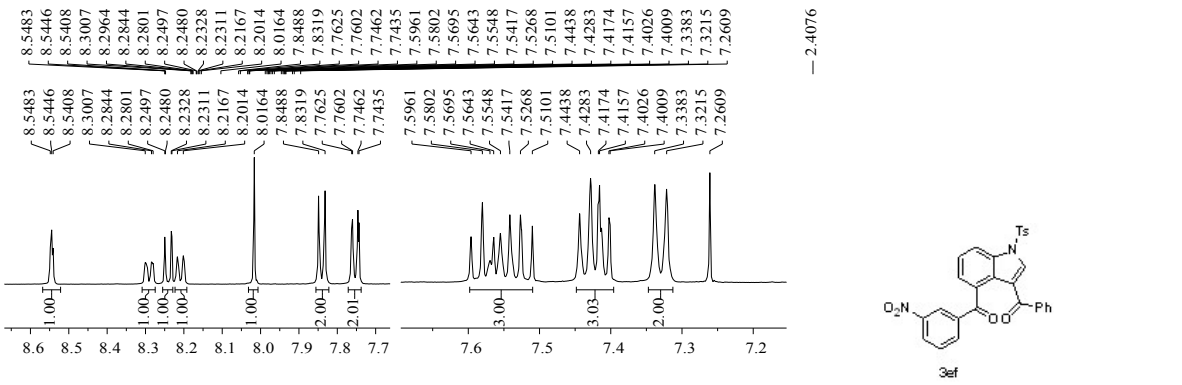
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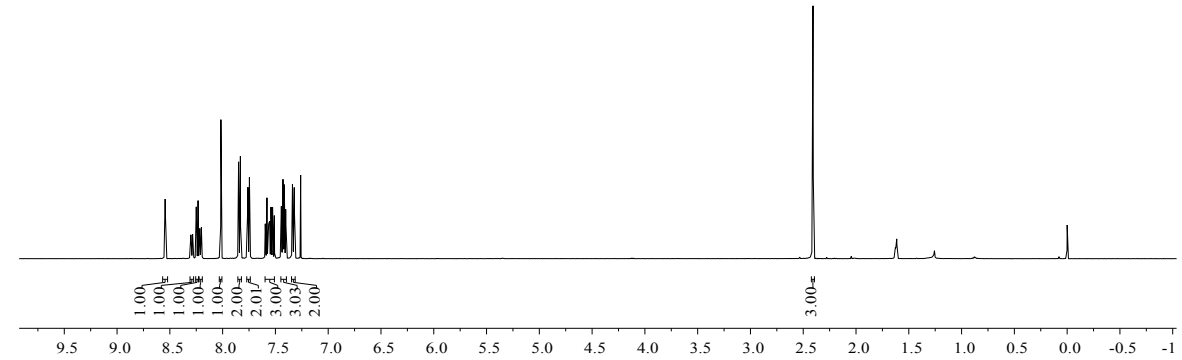
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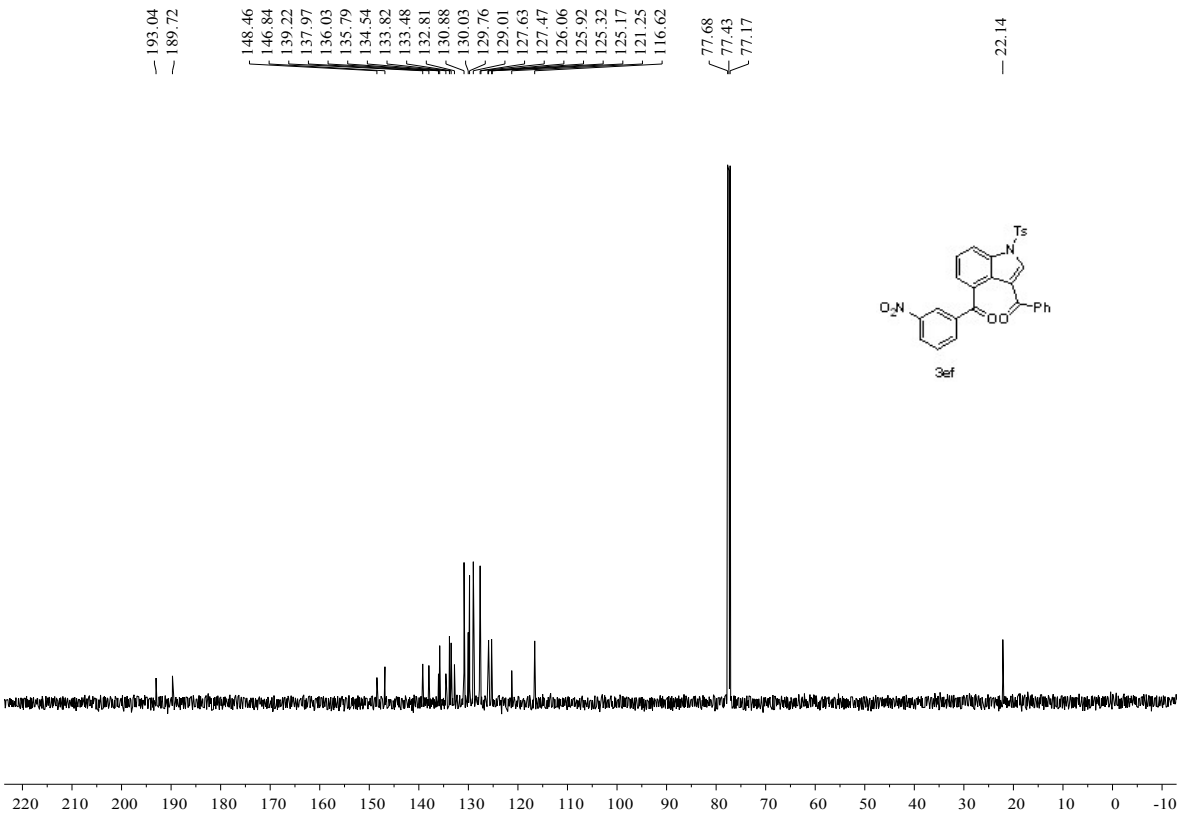
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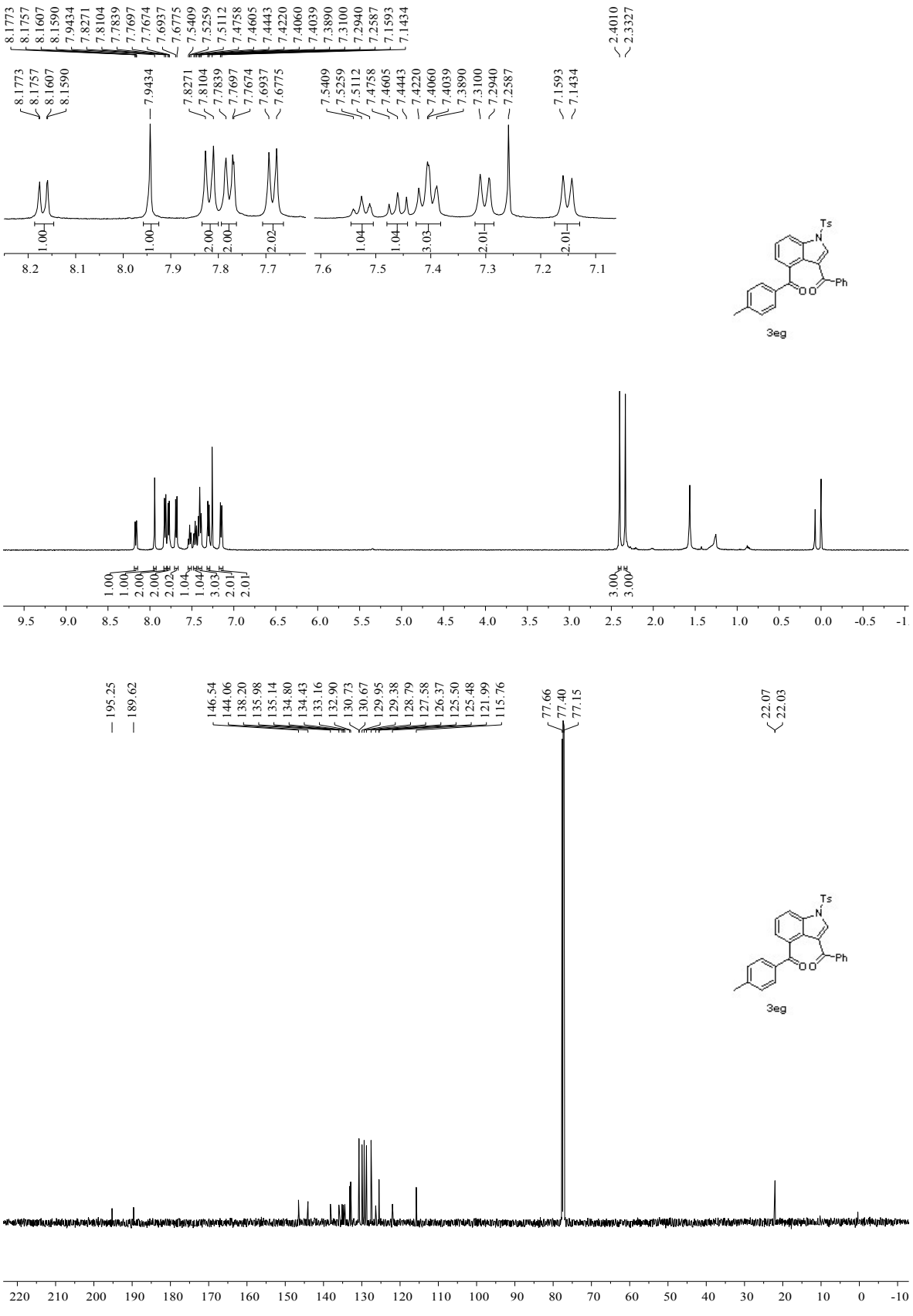
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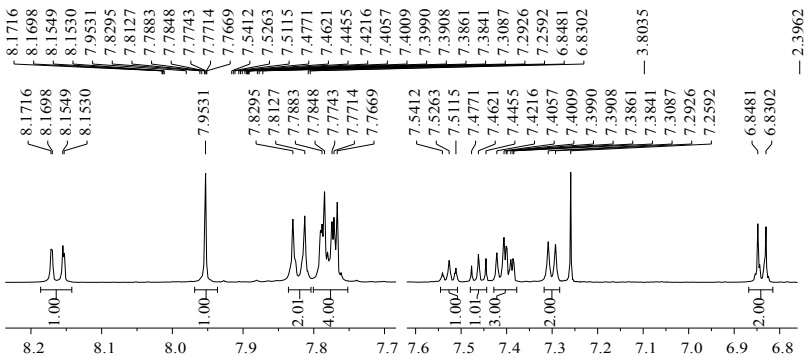
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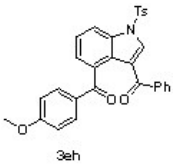
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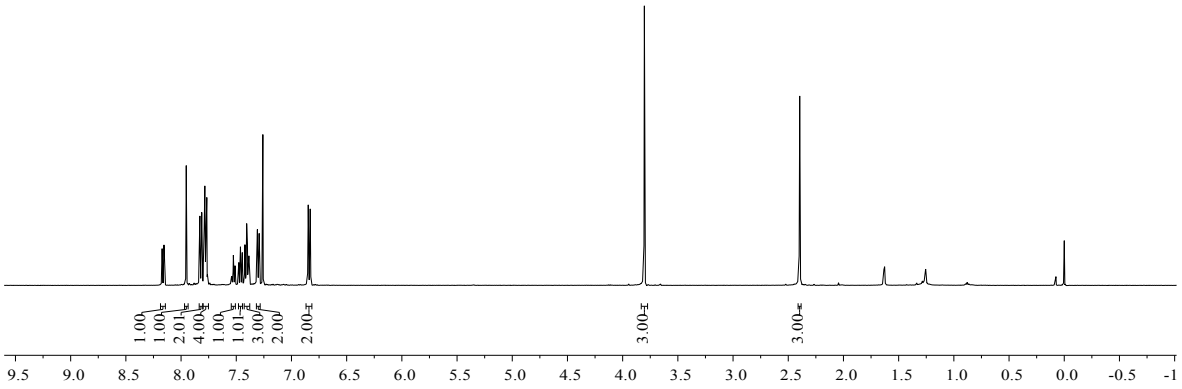

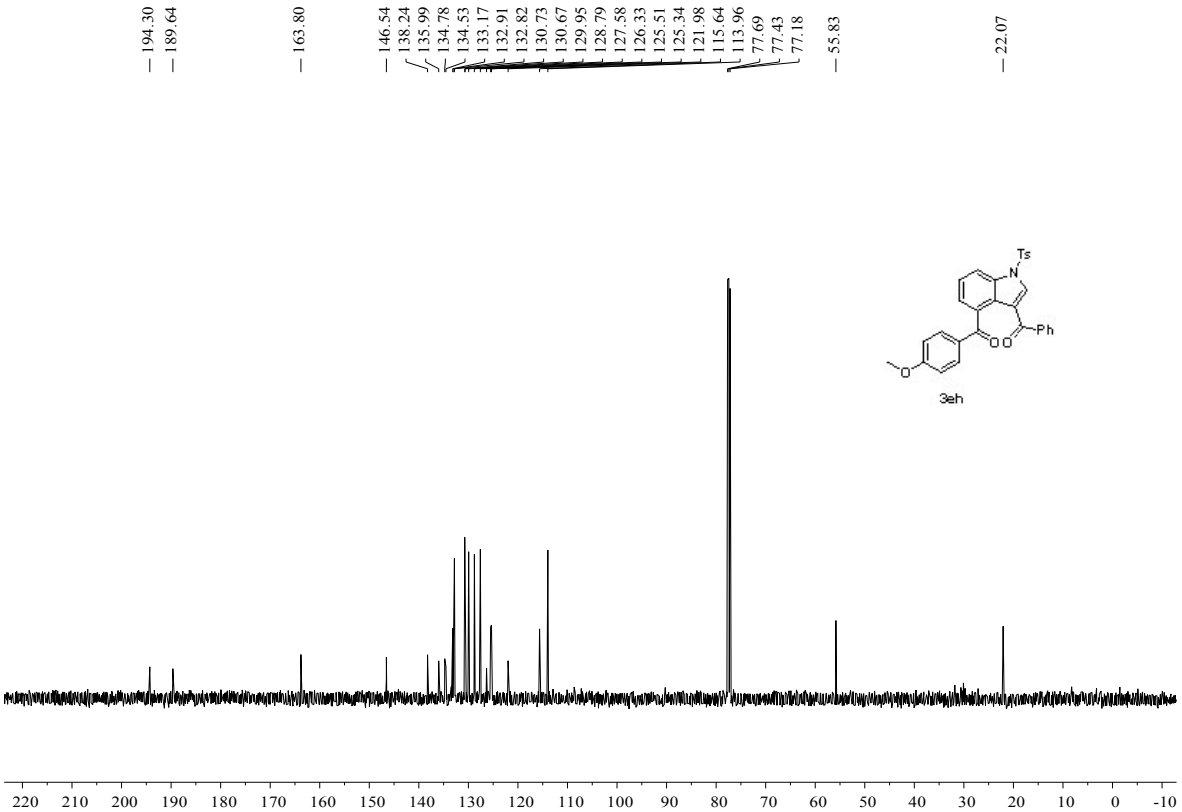
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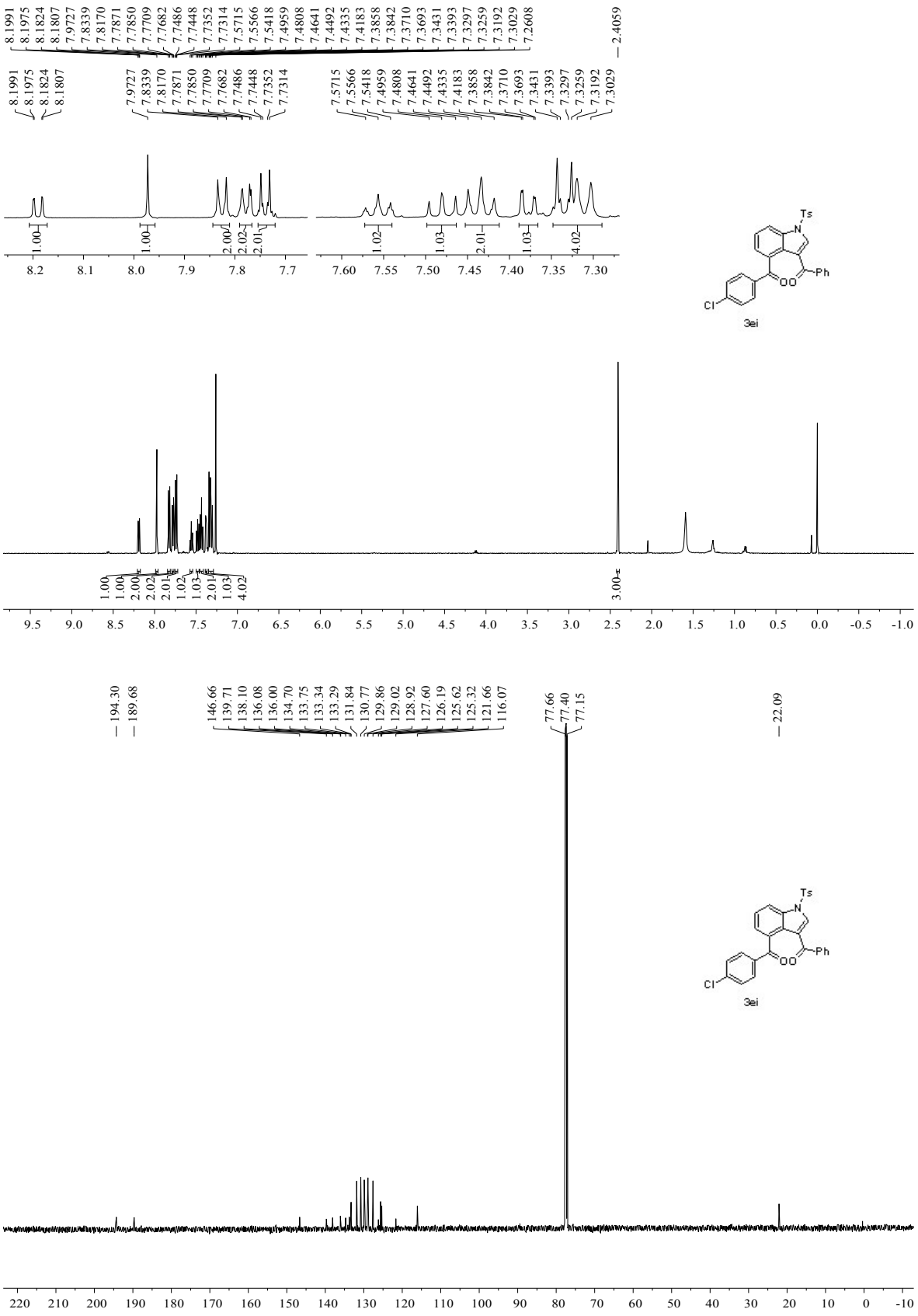
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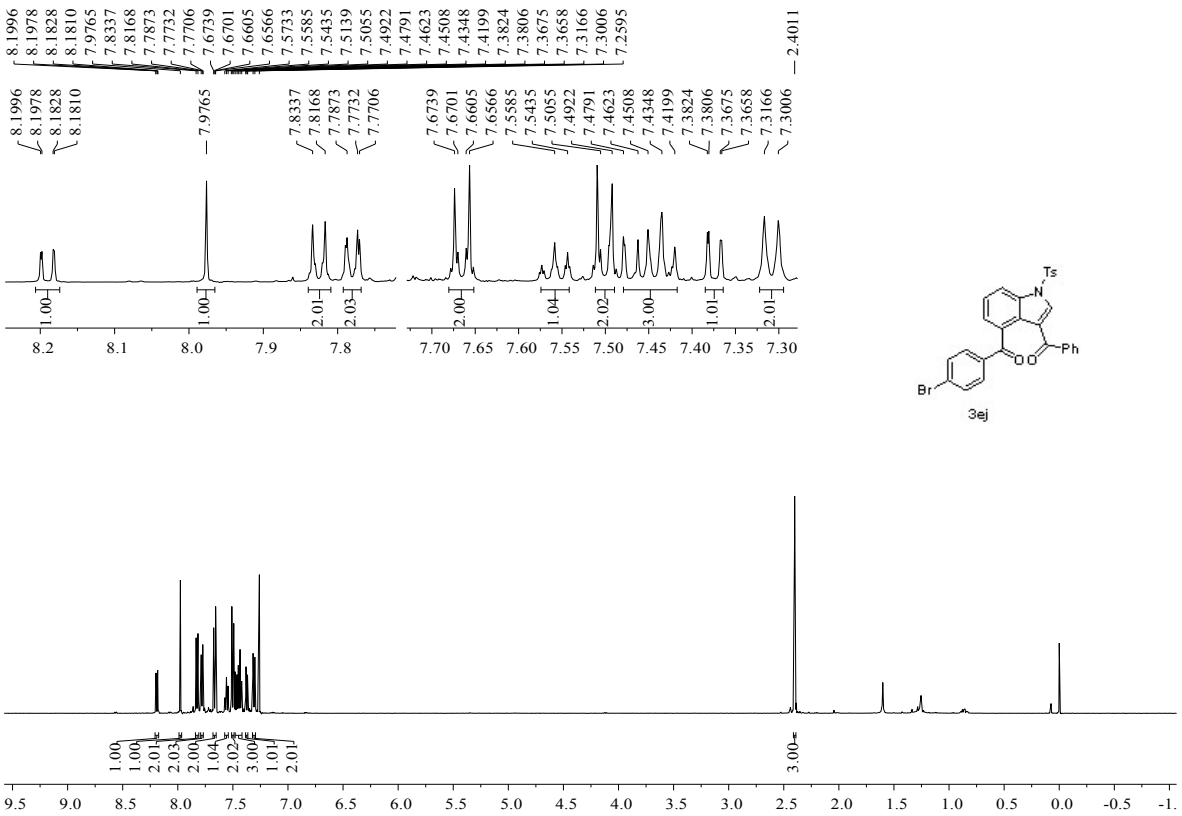
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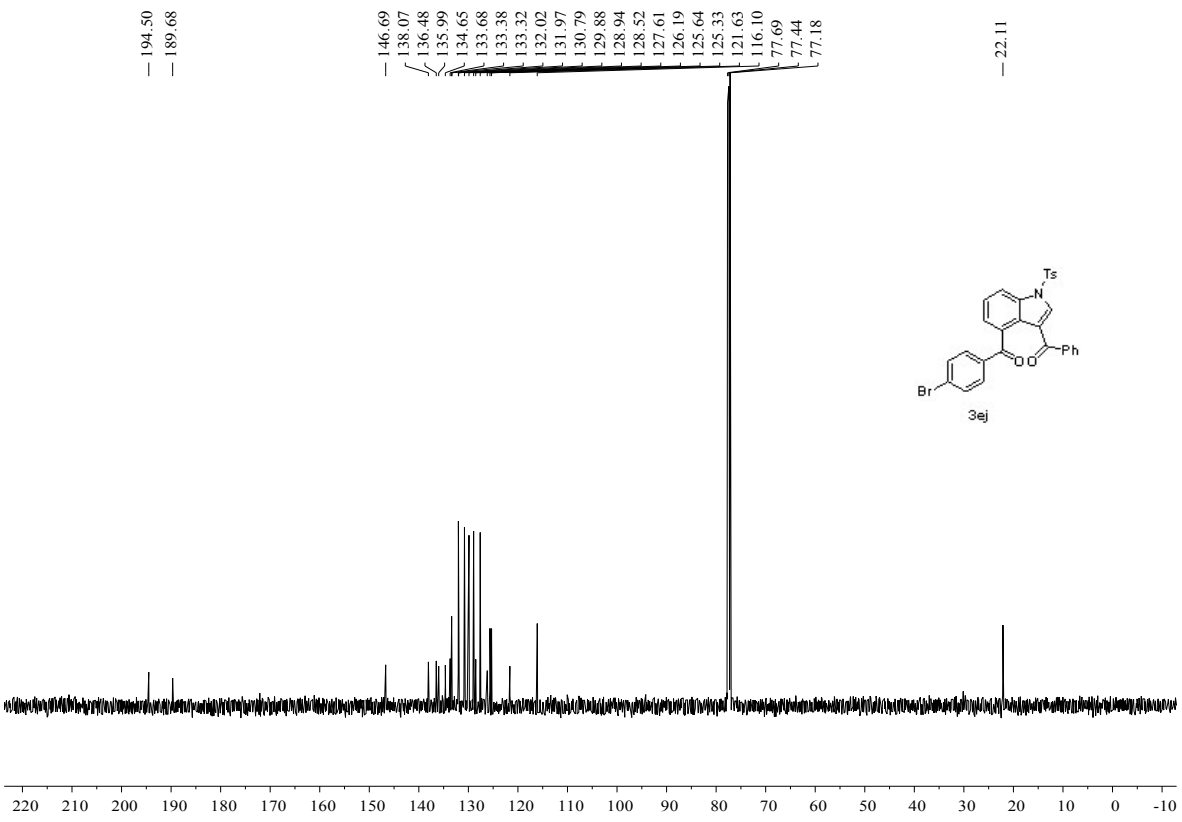
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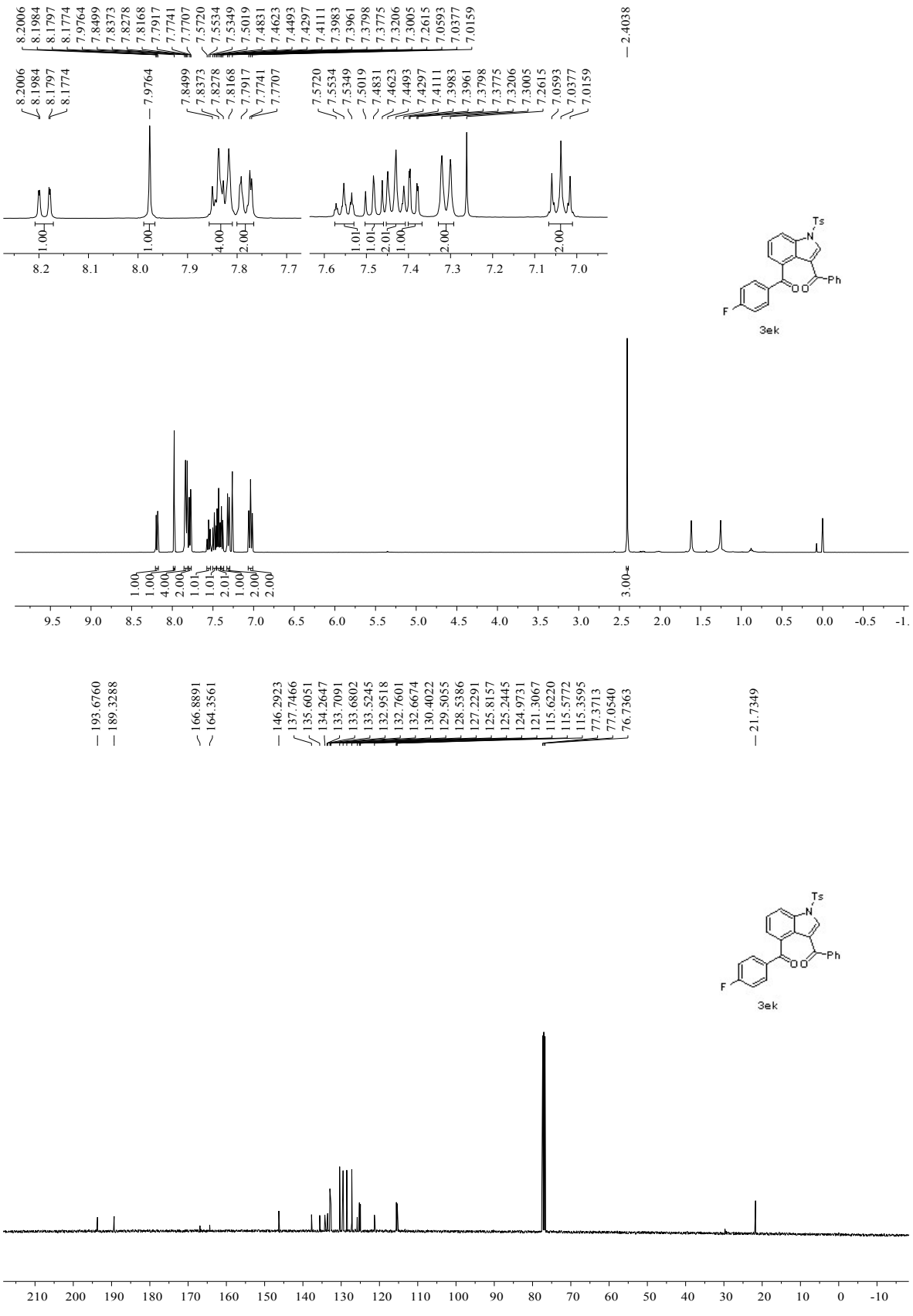
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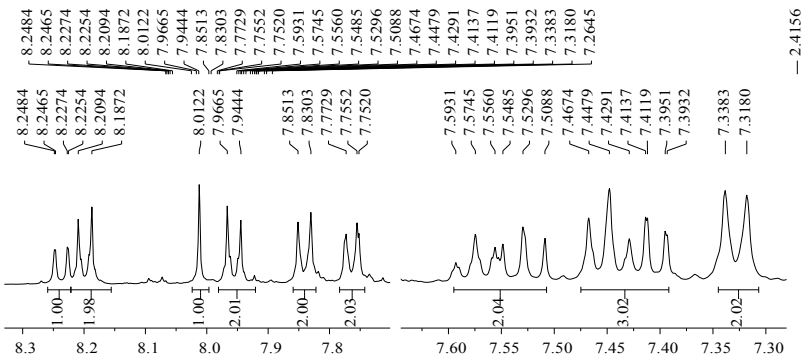
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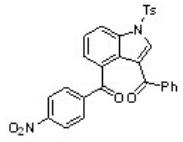
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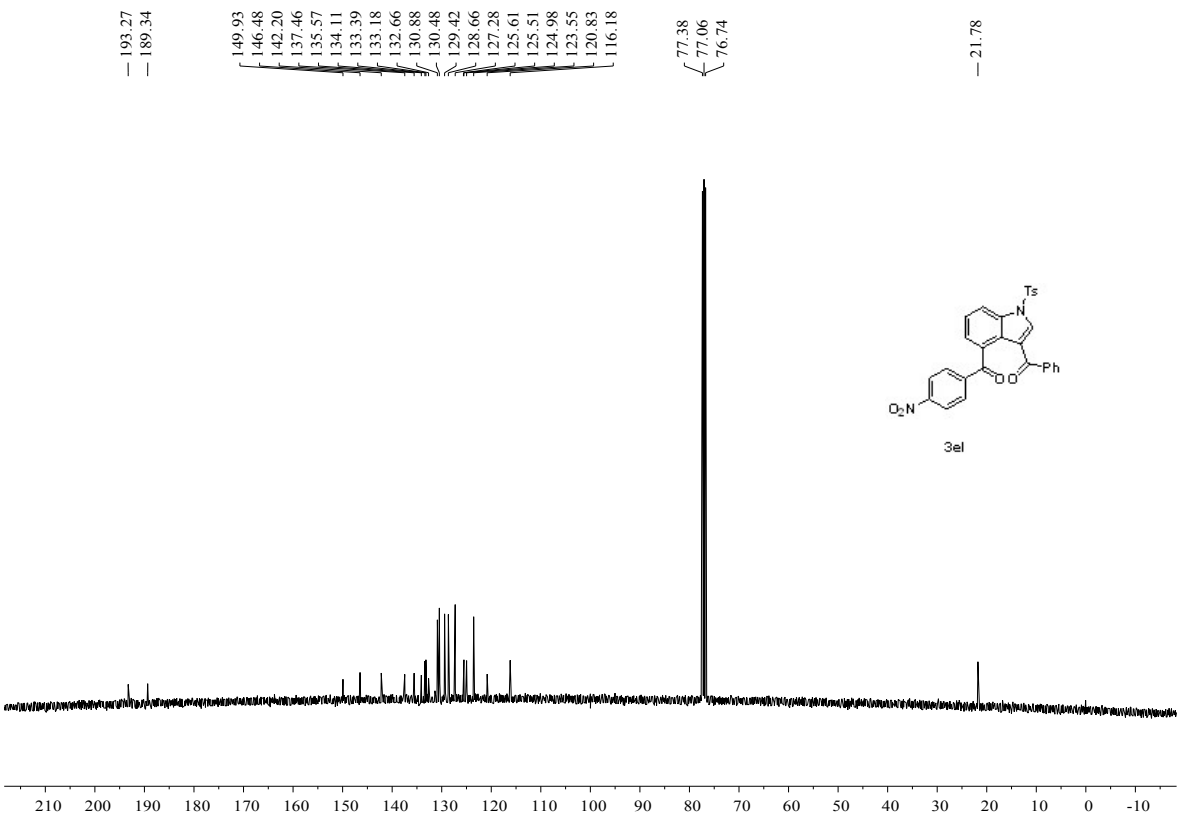
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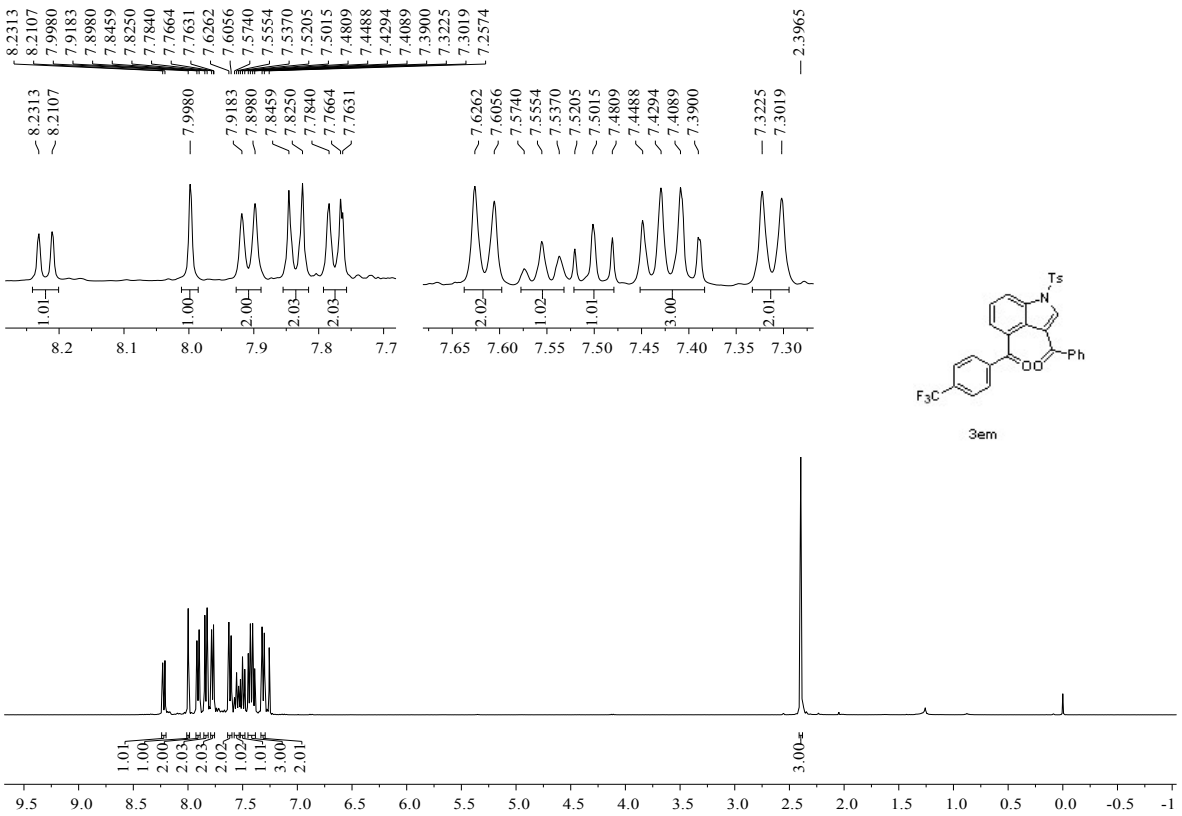
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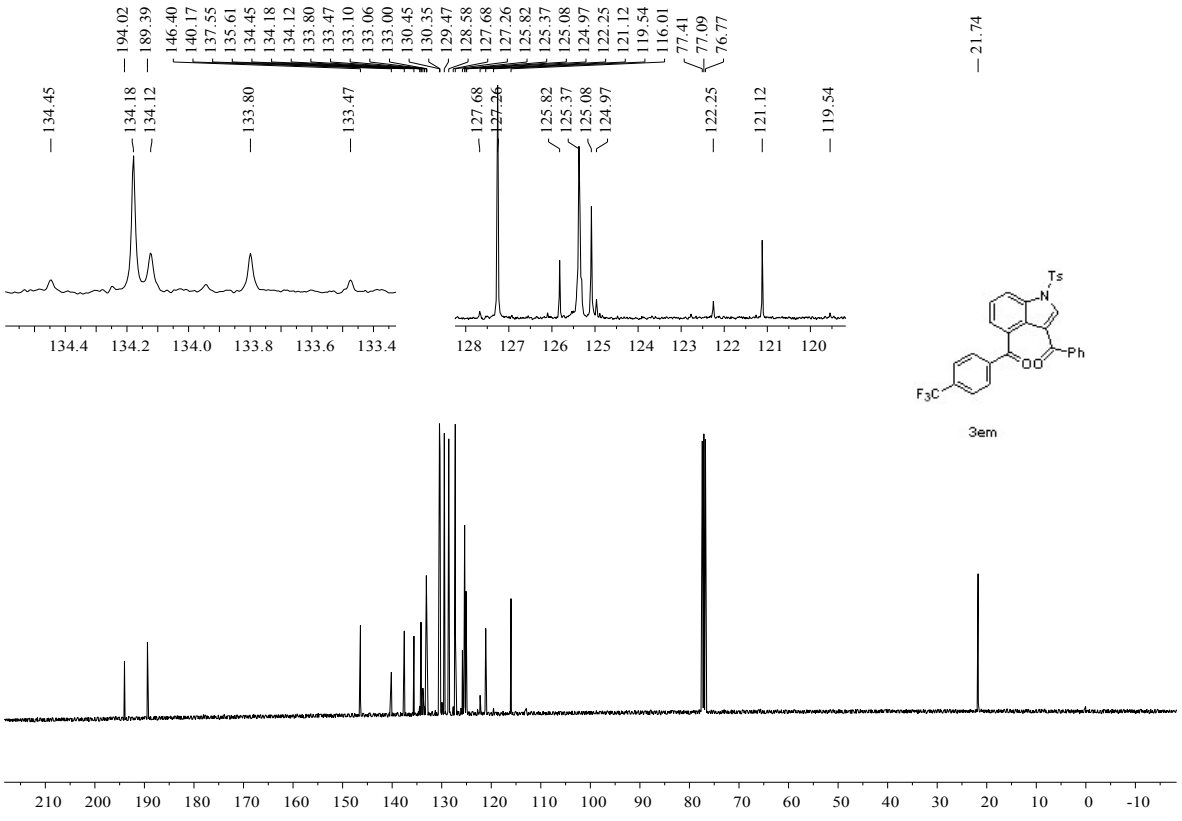
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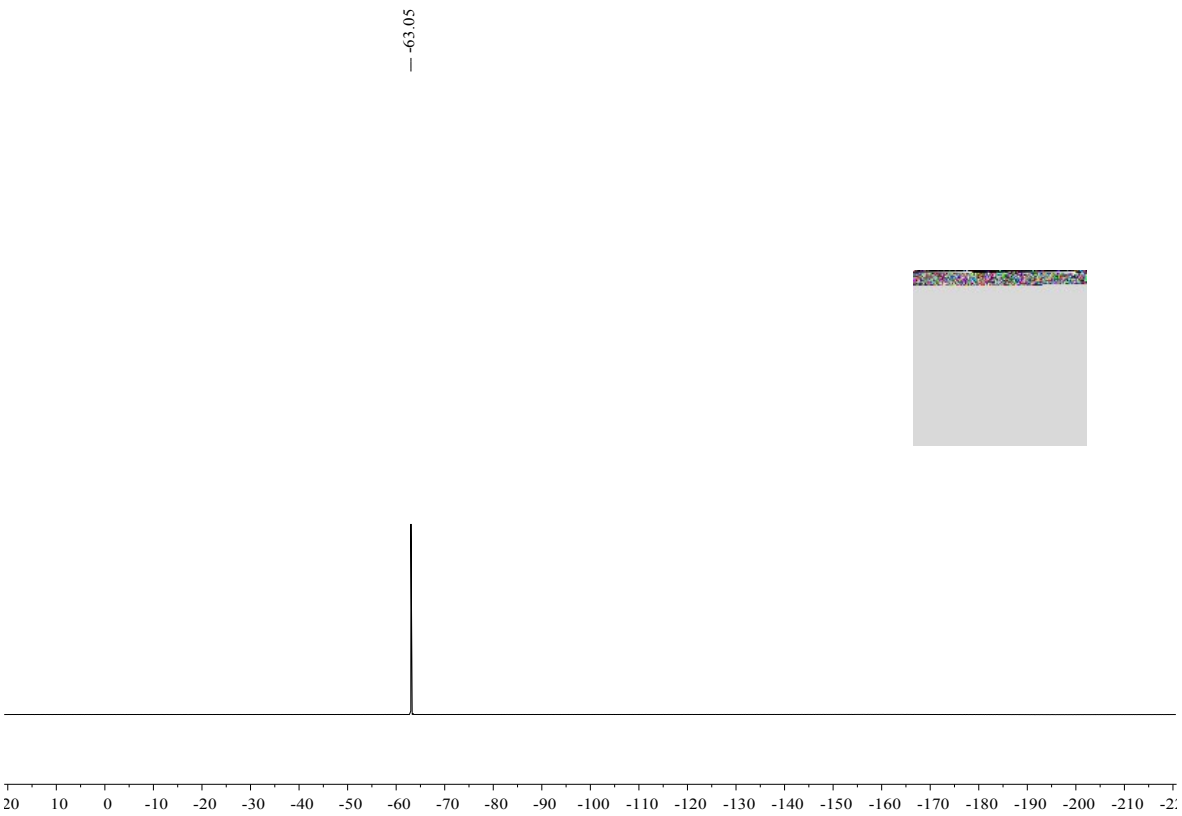
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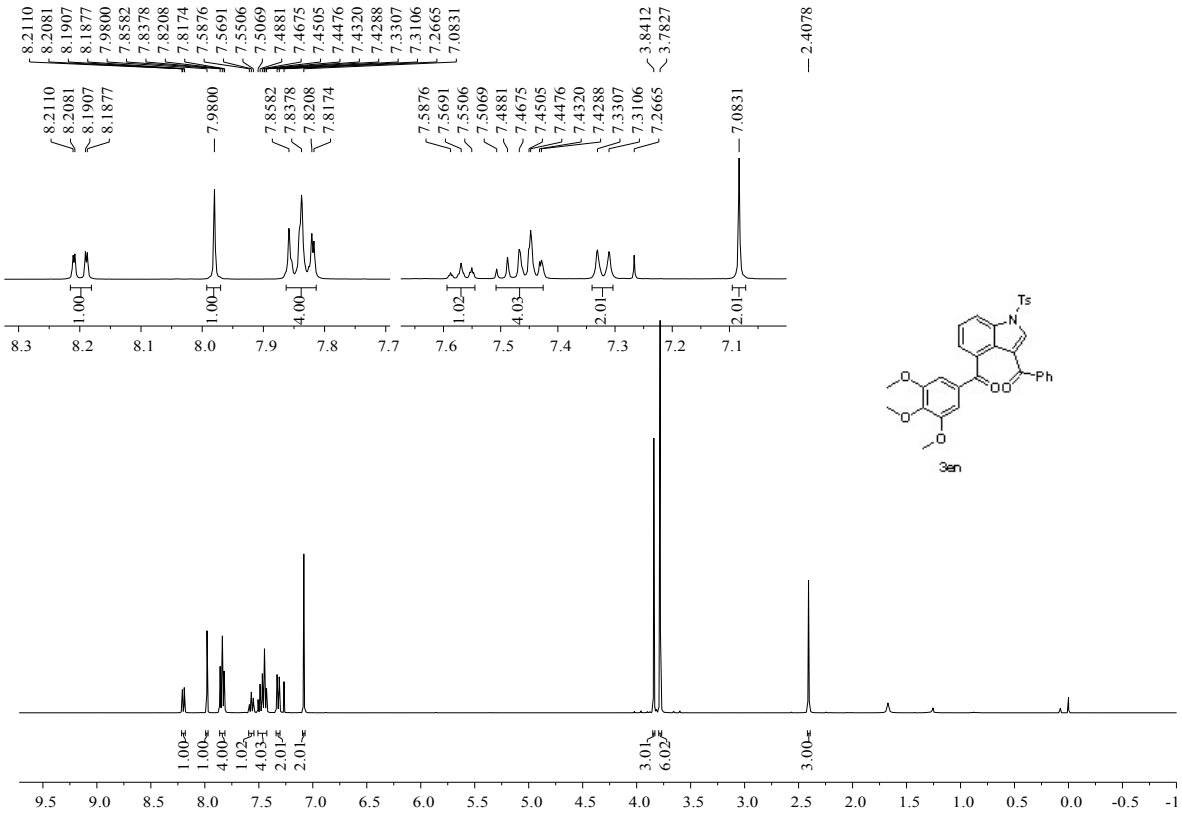
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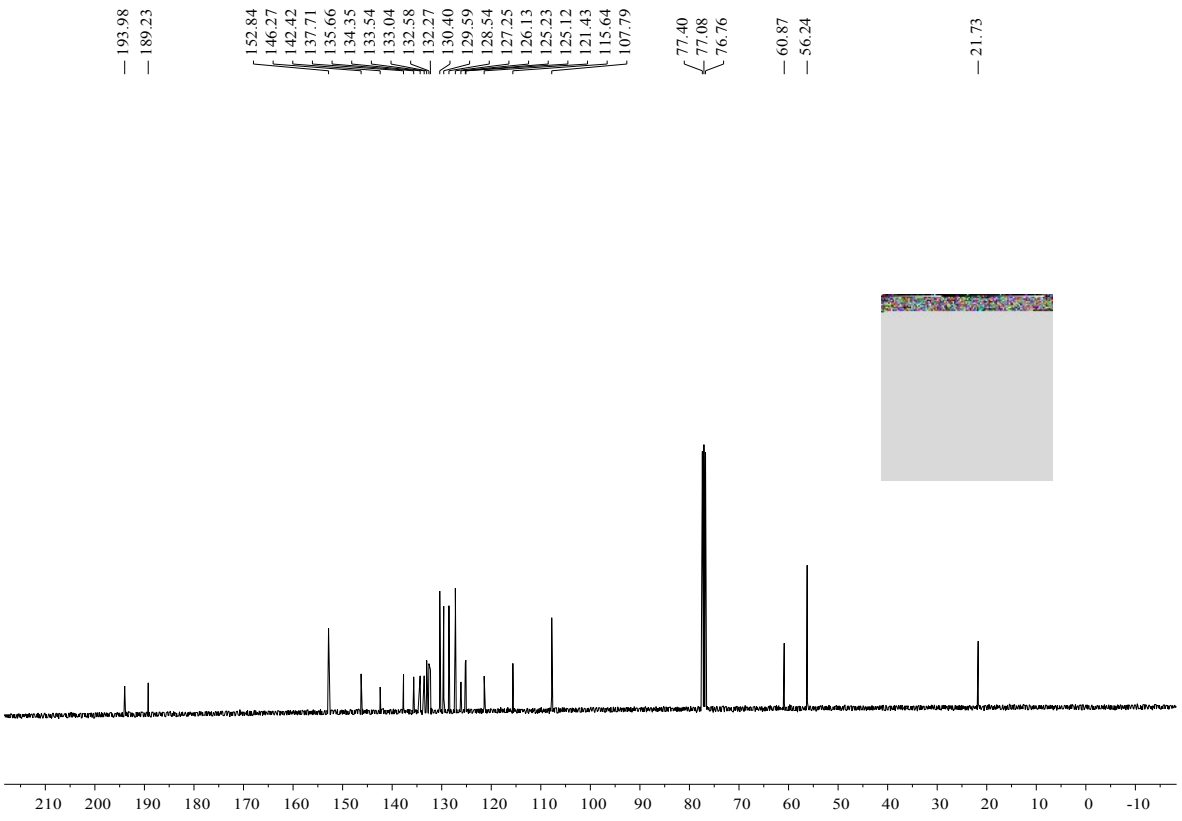
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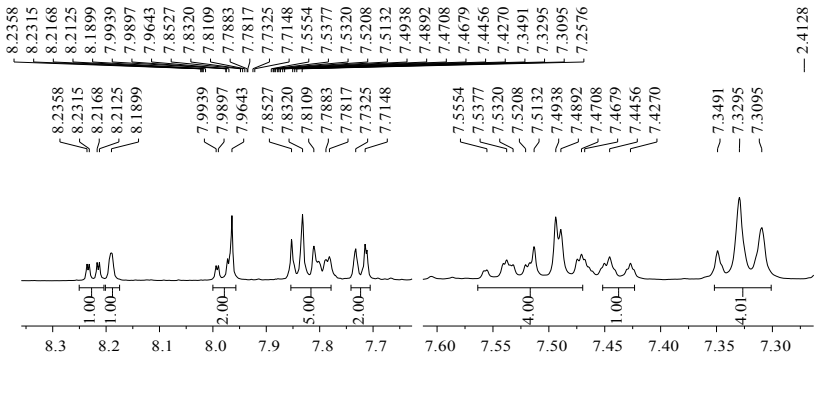
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7.5377
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7.3295
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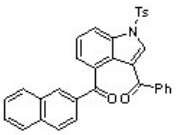
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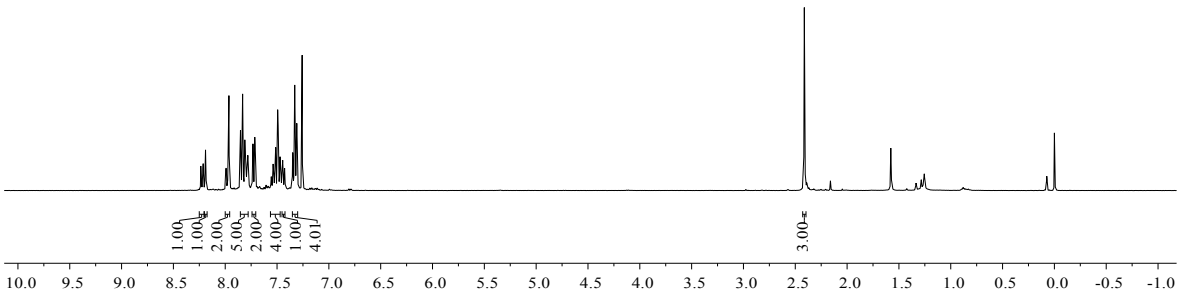
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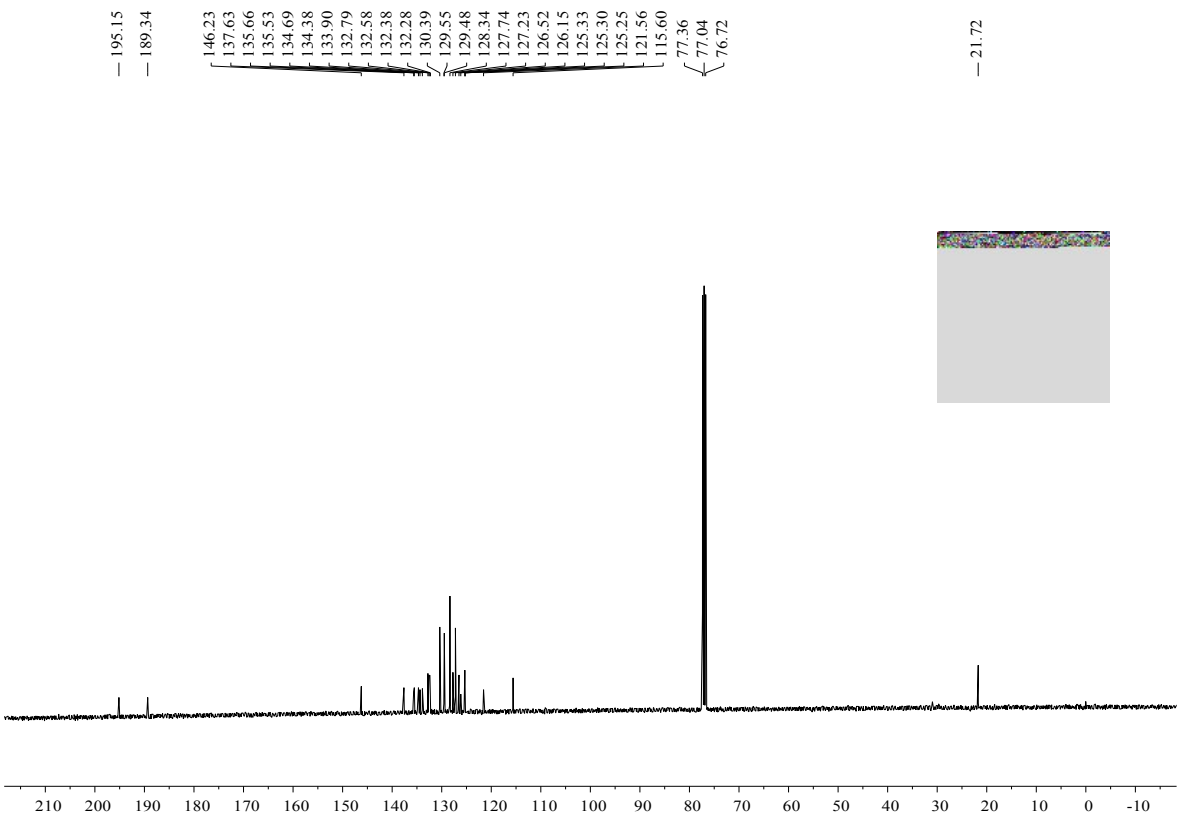
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76.72
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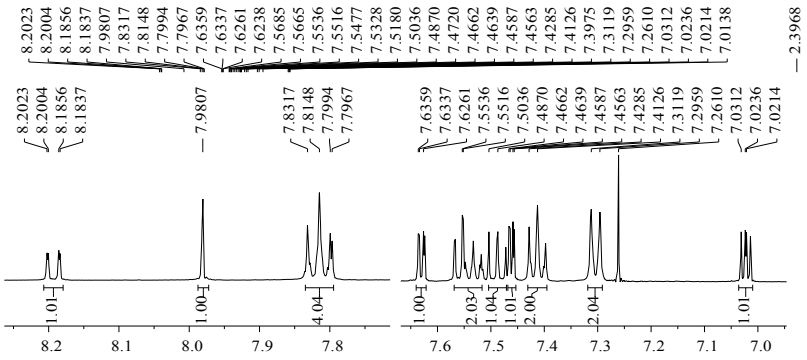
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2.03
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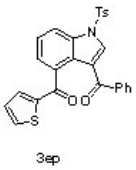
Ts
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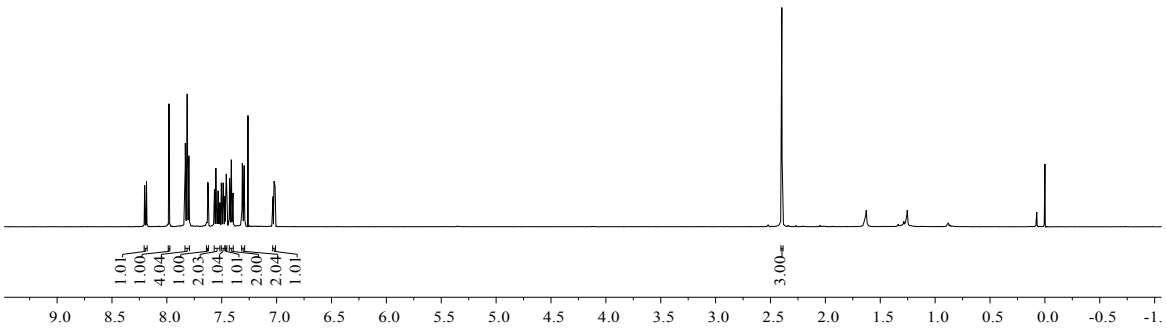
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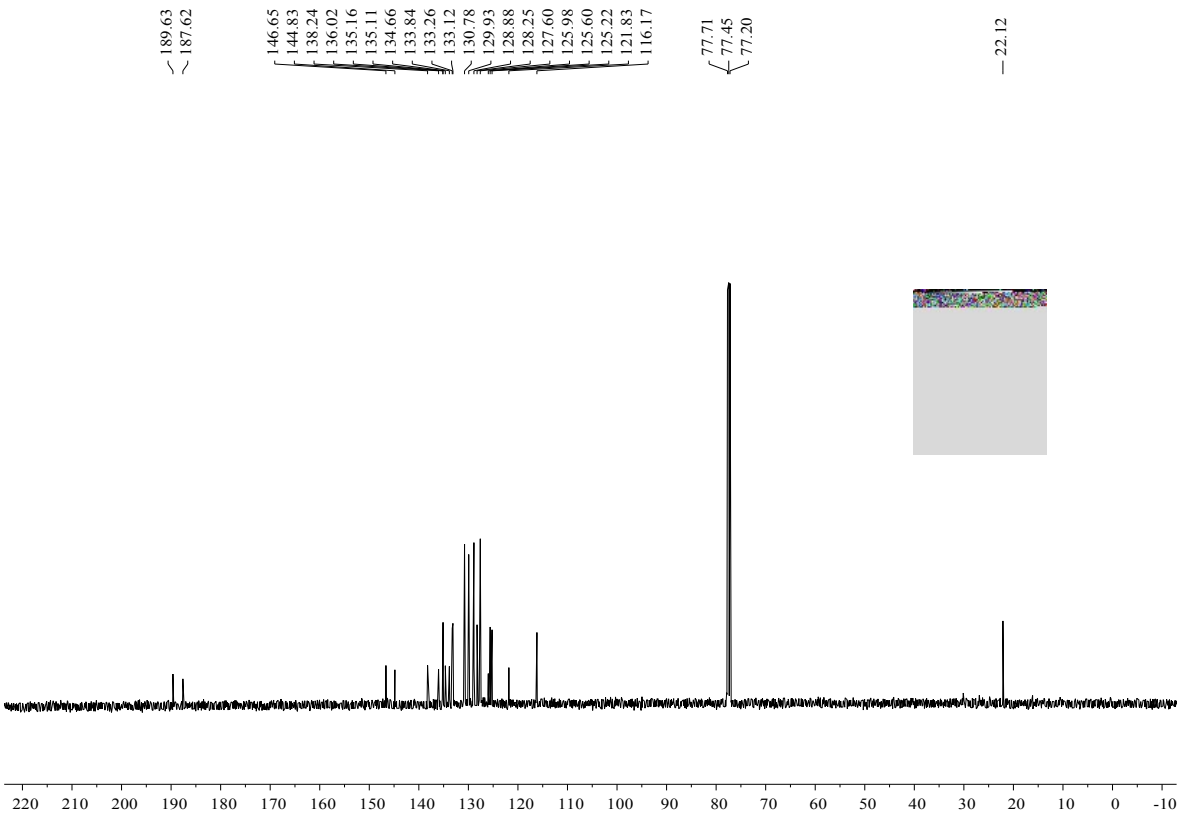
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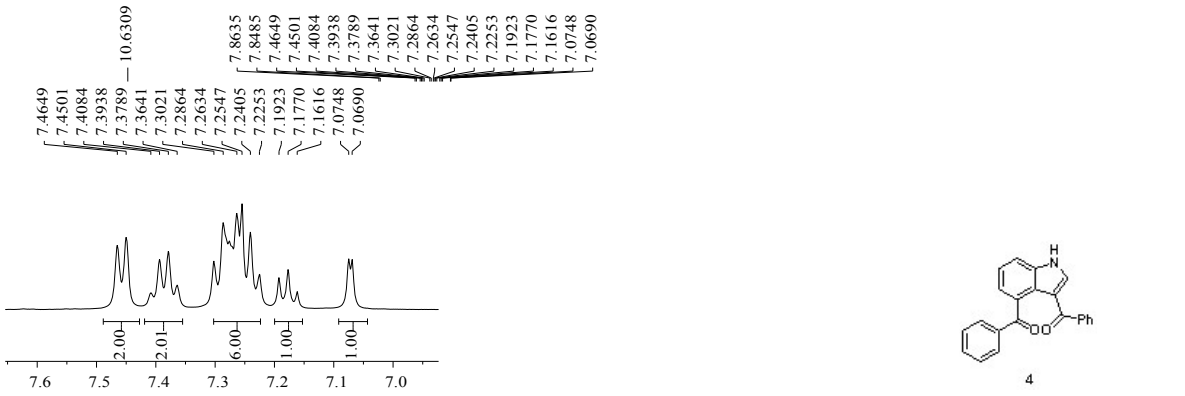
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6.00
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H
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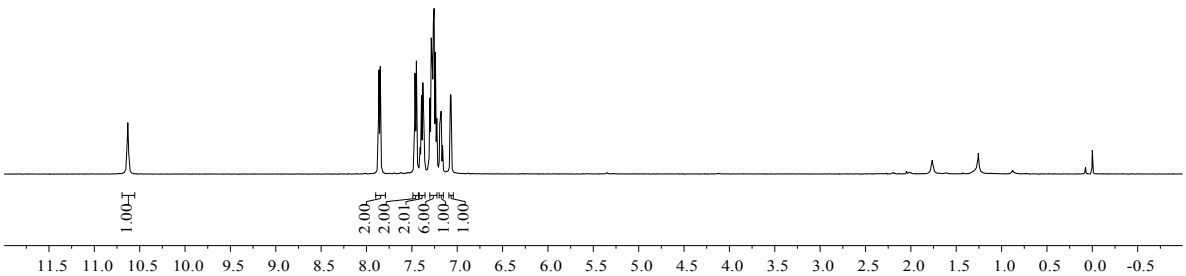
Ph

4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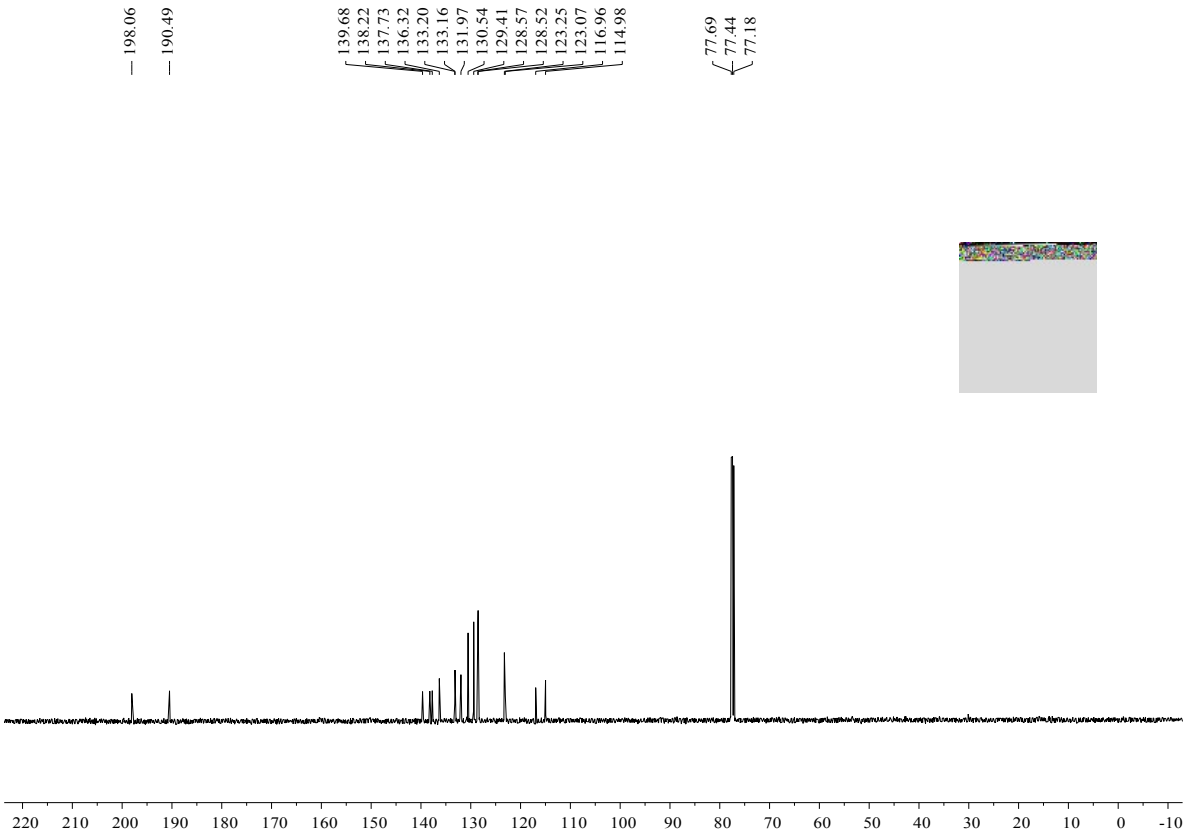
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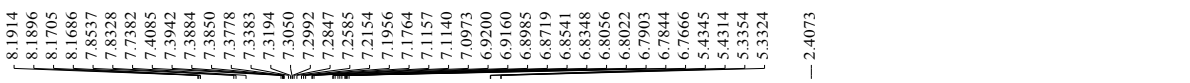
77.18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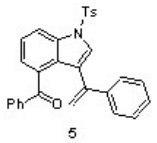
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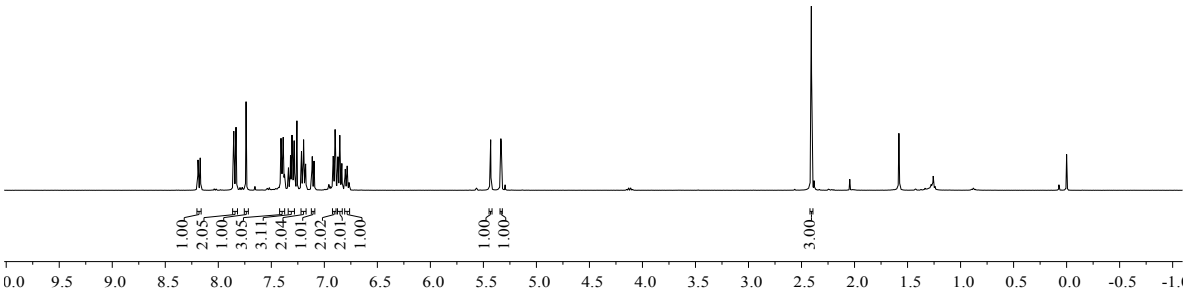
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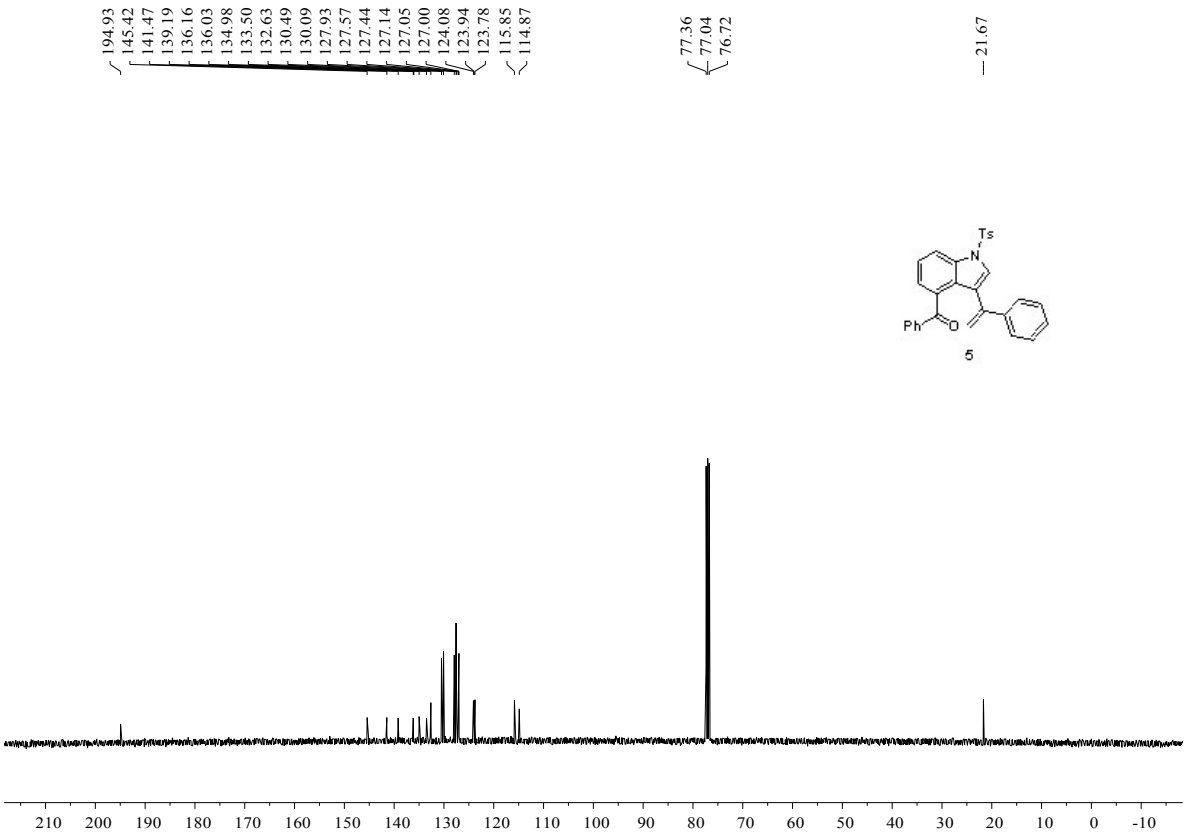
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114.87
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Ph
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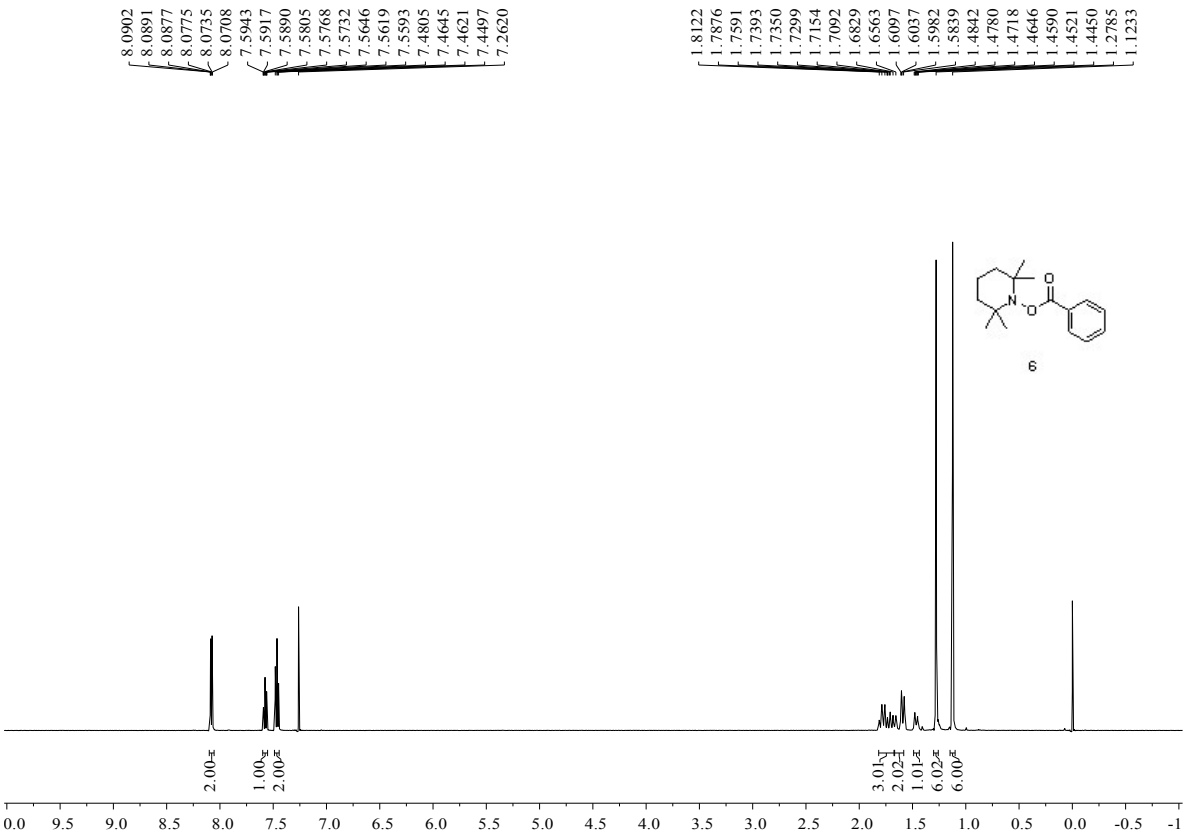
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1.2785
1.1233
O
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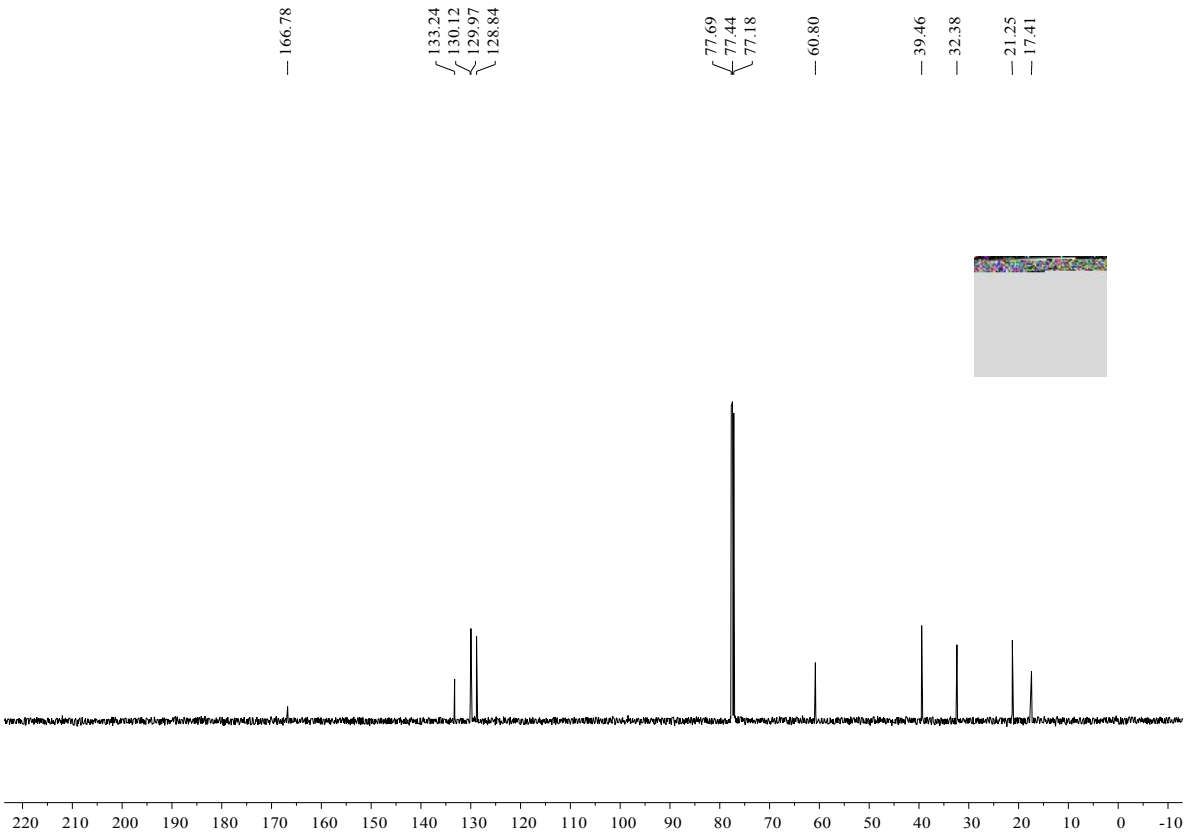
O
6
2.00
1.00
2.00
3.01
2.02
1.01
6.02
6.00
0.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1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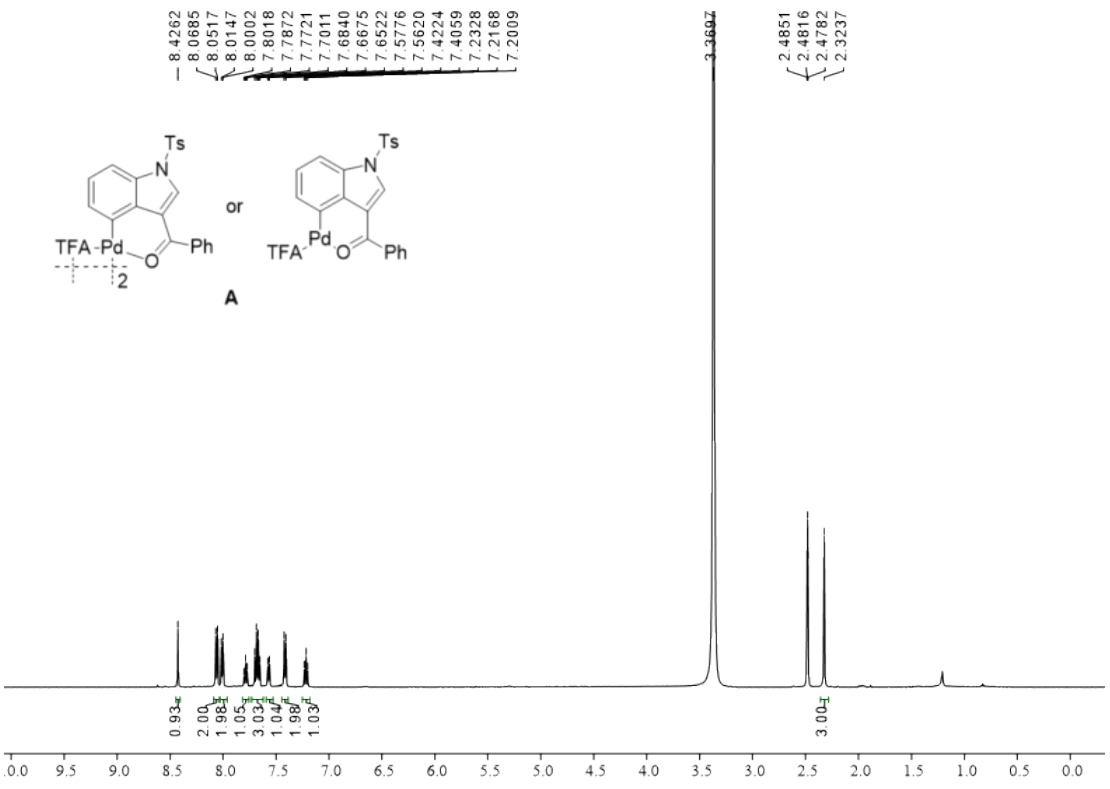
17.41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7.2009
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2.3237
Ts
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TFA
Pd
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Ph
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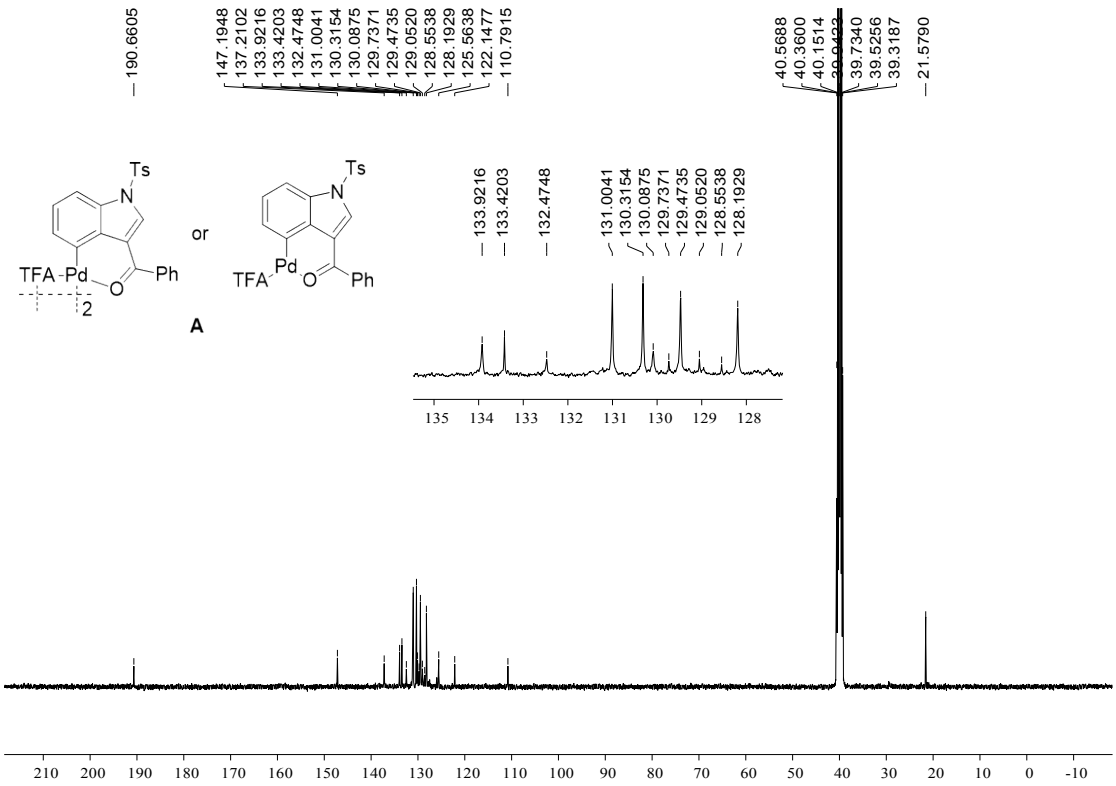
or
A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TFA-Pd
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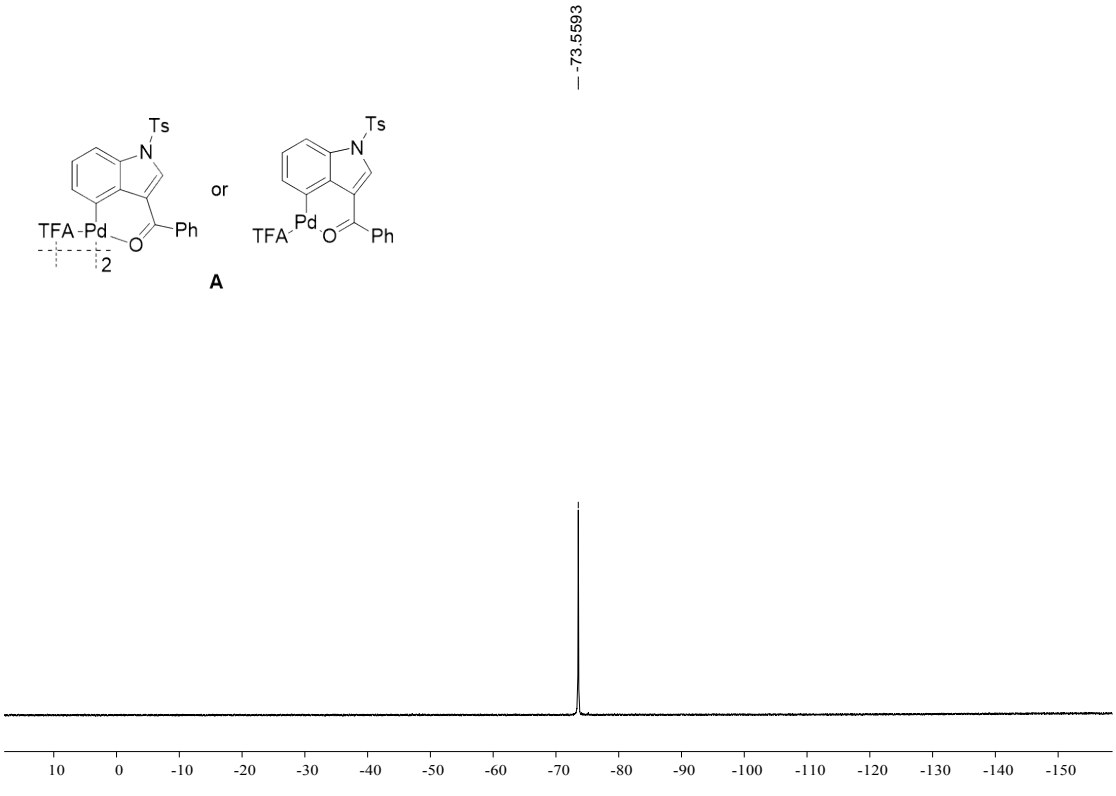
Ph
2
or
A
135 134 133 132 131 130 129 128
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10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TFA-Pd
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or
A
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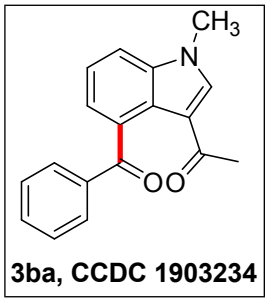
Crystal Structures of 3ba and 3ek



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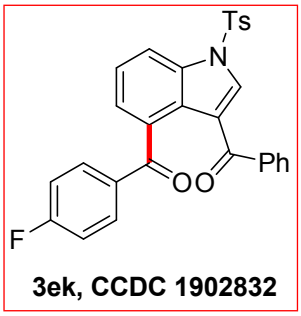

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