Supporting Information

Access to Indenones by Rhodium(III)-Catalyzed C-H Annulation of Arylnitrones with Internal Alkynes

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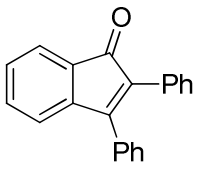
I. General

All chemicals were obtained from commercial sources and were used as received unless otherwise noted. All reactions were carried out using Schlenk techniques or in an argon-filled glovebox. NMR Spectra were recorded on a Bruker 400 MHz or 500 MHz NMR spectrometer in the solvents indicated. The chemical shift is given in dimensionless δ values and is frequency referenced relative to TMS in ^{1}H and ^{13}C NMR spectroscopy. HRMS data were obtained on a Thermo Scientific LTQ Orbirap Discovery (Bremen, Germany). Column chromatography was performed on silica gel (300-400 mesh) using 1,2-dichloroethane (DCE)/petroleum ether (PE).

N-tert-butyl-α-phenylnitrone (PBN), phenylethynyltrimethylsilane, ethyl phenylpropiolate and diphenylacetylene were obtained from commercial sources. Other *N-tert*-butyl-α-arylnitrones [1] and diarylacetylenes [2] were prepared according to literature reports and the NMR data agree with those in the literature reports.

II. General procedures for the synthesis of indenones

N-tert-butyl-α-arylnitrones (0.36 mmol), diarylacetylenes (0.25 mmol), $[Cp^*Rh(MeCN)_3](SbF_6)_2$ (6 mol%), PivOH (1.0 equiv) and DCE (2 mL) were charged into the sealed tube. The reaction mixture was stirred at 80 °C for 15 h. After cooled to room temperature, the solvent was removed under reduced pressure and the residue was purified by silica gel chromatography using DCE/PE to afford compounds **3**.

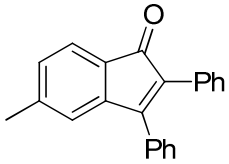


2,3-Diphenyl-1*H*-inden-1-one **(3aa)**

3aa was obtained according to the general procedure in 70% yield.

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.58 (d, J = 7.0 Hz, 1H), 7.42 – 7.34 (m, 6H), 7.30 – 7.23 (m, 6H), 7.14 (d, J = 7.2 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 196.7, 155.5, 145.4, 133.6, 132.9, 132.6, 130.9, 130.1, 129.4, 129.1, 128.9, 128.7, 128.2, 127.9, 123.1, 121.4. One carbon is not visible due to overlapping peaks. The NMR data

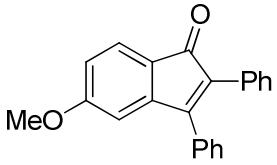
agree with those in a literature report. [3]



2,3-Diphenyl-5-methyl-1*H*-inden-1-one **(3ba)**

3ba was obtained according to the general procedure in 63% yield.

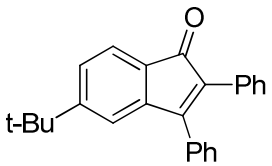
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.46 (d, *J* = 7.3 Hz, 1H), 7.43 – 7.34 (m, 5H), 7.28 – 7.20 (m, 5H), 7.06 (d, *J* = 7.3 Hz, 1H), 6.93 (s, 1H), 2.33 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 196.3, 155.1, 145.9, 144.6, 133.0, 132.9, 131.0, 130.1, 129.3, 129.1, 128.9, 128.7, 128.5, 128.2, 127.8, 123.2, 122.7, 22.2. The NMR data agree with those in a literature report. [3]



2,3-Diphenyl-5-methoxy-1*H*-inden-1-one **(3ca)**

3ca was obtained according to the general procedure in 49% yield.

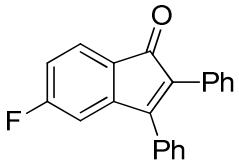
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.54 (d, *J* = 7.9 Hz, 1H), 7.43 – 7.33 (m, 5H), 7.29 – 7.19 (m, 5H), 6.70 – 6.63 (m, 2H), 3.82 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 195.3, 164.6, 153.3, 148.1, 134.0, 132.8, 131.0, 130.2, 129.3, 129.0, 128.7, 128.2, 127.9, 125.1, 123.6, 110.6, 110.5, 55.9. The NMR data agree with those in a literature report. [3]



5-(*tert*-Butyl)-2,3-diphenyl-1*H*-inden-1-one **(3da)**

3da was obtained according to the general procedure in 70% yield.

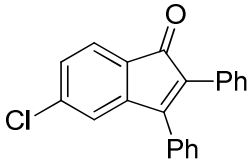
^{1}H NMR (500 MHz, $CDCl_3$) δ 7.52 (d, *J* = 7.5 Hz, 1H), 7.44 – 7.40 (m, 3H), 7.39 – 7.36 (m, 2H), 7.29 (dd, *J* = 7.6, 1.6 Hz, 1H), 7.26 – 7.22 (m, 5H), 7.17 (d, *J* = 1.3 Hz, 1H), 1.30 (s, 9H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 196.4, 157.8, 155.4, 145.5, 133.1, 133.0, 131.1, 130.14 129.4, 129.0, 128.7, 128.6, 128.2, 127.8, 125.4, 123.1, 119.2, 35.7, 31.3. The NMR data agree with those in a literature report. [3]



2,3-Diphenyl-5-fluoro-1*H*-inden-1-one **(3ea)**

3ea was obtained according to the general procedure in 73% yield.

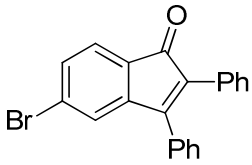
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.55 (dd, *J* = 7.9, 5.2 Hz, 1H), 7.44 – 7.38 (m, 3H), 7.37 – 7.32 (m, 2H), 7.28 – 7.22 (m, 5H), 6.91 (ddd, *J* = 9.0, 8.0, 2.2 Hz, 1H), 6.85 (dd, *J* = 8.5, 2.1 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 194.9, 166.6 (d, J_{C-F} = 252.6 Hz), 153.2 (d, J_{C-F} = 2.3 Hz), 148.8 (d, J_{C-F} = 9.3 Hz), 133.9, 132.4, 130.6, 130.1, 129.7, 129.1, 128.6, 128.3, 128.2, 126.7, 124.9 (d, J_{C-F} = 9.7 Hz), 114.6 (d, J_{C-F} = 22.9 Hz), 110.3 (d, J_{C-F} = 25.7 Hz). The NMR data agree with those in a literature report. [3]



5-Chloro-2,3-diphenyl-1*H*-inden-1-one **(3fa)**

3fa was obtained according to the general procedure in 83% yield.

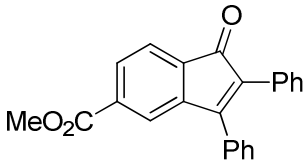
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.49 (d, *J* = 7.6 Hz, 1H), 7.44 – 7.38 (m, 3H), 7.37 – 7.32 (m, 2H), 7.27 – 7.22 (m, 6H), 7.10 (d, *J* = 1.6 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 195.1, 154.2, 147.4, 139.9, 133.7, 132.3, 130.5, 130.1, 129.7, 129.2, 129.0, 128.7, 128.5, 128.3, 128.2, 124.0, 122.1. The NMR data agree with those in a literature report. [3]



5-Bromo-2,3-diphenyl-1*H*-inden-1-one **(3ga)**

3ga was obtained according to the general procedure in 85% yield.

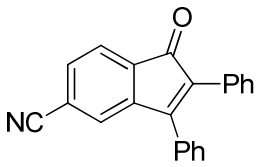
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.46 – 7.40 (m, 5H), 7.37 – 7.32 (m, 2H), 7.25 (s, 6H). ^{13}C NMR (125MHz, $CDCl_3$) δ 195.4, 154.3, 147.4, 133.5, 132.3, 131.8, 130.4, 130.1, 129.7, 129.5, 129.2, 128.5, 128.5, 128.3, 128.2, 124.8, 124.2. The NMR data agree with those in a literature report. [3]



Methyl 1-oxo-2,3-diphenyl-1*H*-indene-5-carboxylate **(3ha)**

3ha was obtained according to the general procedure in 79% yield.

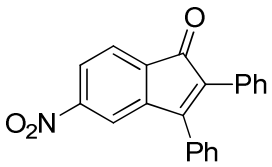
^{1}H NMR (500 MHz, $CDCl_3$) δ 8.02 (dd, *J* = 7.4, 1.2 Hz, 1H), 7.77 (d, *J* = 0.7 Hz, 1H), 7.63 (d, *J* = 7.4 Hz, 1H), 7.46 – 7.42 (m, 3H), 7.41 – 7.37 (m, 2H), 7.28 – 7.24 (m, 5H), 3.90 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 195.7, 166.3, 155.4, 145.5, 134.8, 134.4, 133.4, 132.3, 131.4, 130.43, 130.1, 129.8, 129.1, 128.6, 128.3, 128.2, 122.7, 121.7, 52.6. The NMR data agree with those in a literature report. [3]



5-Cyano-2,3-diphenyl-1*H*-inden-1-one **(3ia)**

3ia was obtained according to the general procedure in 51% yield.

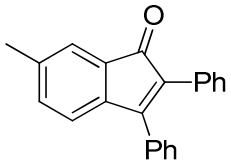
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.68 – 7.62 (m, 2H), 7.48 – 7.43 (m, 3H), 7.40 – 7.34 (m, 3H), 7.30 – 7.24 (m, 5H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 194.7, 154.6, 146.2, 134.1, 134.0, 133.9, 131.8, 130.2, 130.1, 129.9, 129.3, 128.6, 128.5, 128.4, 123.8, 123.1, 118.3, 116.8. HRMS: $[M + H]^+$ calculated for $C_{22}H_{14}NO$: 308.10699, found 308.10663. The NMR data agree with those in a literature report. [4]



2,3-Diphenyl-5-nitro-1*H*-inden-1-one **(3ja)**

3ja was obtained according to the general procedure in 68% yield.

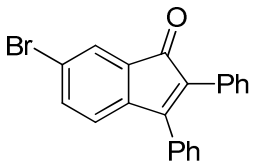
^{1}H NMR (500 MHz, $CDCl_3$) δ 8.22 (dd, *J* = 7.8, 1.9 Hz, 1H), 7.95 (d, *J* = 1.8 Hz, 1H), 7.72 (d, *J* = 7.8 Hz, 1H), 7.50 – 7.45 (m, 3H), 7.43 – 7.37 (m, 2H), 7.31 – 7.26 (m, 5H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 194.3, 154.3, 151.6, 147.0, 135.3, 134.6, 131.7, 130.3, 130.1, 129.9, 129.4, 128.7, 128.5, 128.5, 125.4, 123.2, 115.9. HRMS: $[M + H]^+$ calculated for $C_{21}H_{14}NO_3$: 328.09682, found 328.09689. The NMR data agree with those in a literature report. [5]



6-Methyl-2,3-diphenyl-1*H*-inden-1-one **3ka**

3ka was obtained according to the general procedure in 66% yield.

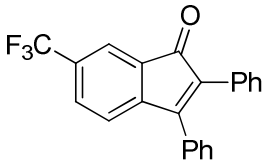
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.43 – 7.33 (m, 6H), 7.27 – 7.20 (m, 5H), 7.14 (dd, *J* = 7.4, 0.6 Hz, 1H), 7.01 (d, *J* = 7.4 Hz, 1H), 2.36 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 196.9, 155.8, 142.6, 139.4, 133.5, 133.1, 132.0, 131.3, 131.1, 130.1, 129.4, 128.9, 128.7, 128.2, 127.7, 124.2, 121.3, 21.5. The NMR data agree with those in a literature report. [3]



6-Bromo-2,3-diphenyl-1*H*-inden-1-one **3la**

3la was obtained according to the general procedure in 73% yield.

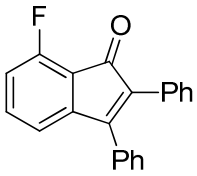
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.65 (d, *J* = 1.8 Hz, 1H), 7.47 (dd, *J* = 7.8, 1.8 Hz, 1H), 7.42 – 7.37 (m, 3H), 7.36 – 7.31 (m, 2H), 7.24 (s, 5H), 7.00 (d, *J* = 7.8 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 195.2, 155.3, 143.9, 135.8, 132.6, 132.5, 132.4, 130.5, 130.1, 129.7, 129.1, 128.6, 128.3, 128.1, 126.4, 123.0, 122.7. The NMR data agree with those in a literature report. [3]



2,3-Diphenyl-6-trifluoromethyl-1*H*-inden-1-one **3ma**

3ma was obtained according to the general procedure in 68% yield.

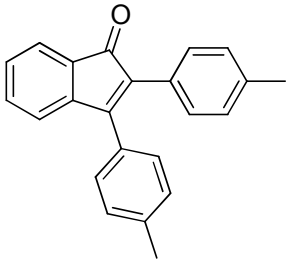
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.81 (s, 1H), 7.66 (d, *J* = 7.6 Hz, 1H), 7.46 – 7.41 (m, 3H), 7.39 – 7.35 (m, 2H), 7.29 – 7.24 (m, 6H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 194.9, 154.5, 148.7, 134.4, 132.2, 131.4, 131.3 (q, $J_{C\text{-}F}$ = 32.7 Hz), 130.9 (q, $J_{C\text{-}F}$ = 3.9 Hz), 130.21, 130.15, 129.9, 129.2, 128.6, 128.5, 128.4, 123.9 (q, $J_{C\text{-}F}$ = 270.5 Hz), 121.3, 119.9 (q, $J_{C\text{-}F}$= 3.5 Hz). HRMS: $[M + H]^+$ calculated for $C_{21}H_{14}F_3O$: 351.09913, found 351.09879.



2,3-Diphenyl-7-fluoro-1*H*-inden-1-one **3na**

3na was obtained according to the general procedure in 52% yield.

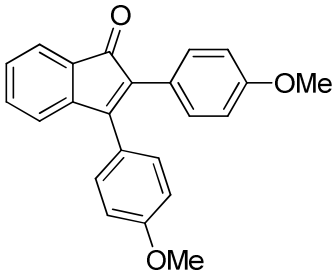
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.43 – 7.37 (m, 3H), 7.37 – 7.31 (m, 3H), 7.24 (s, 5H), 6.93 (dd, J = 11.6, 5.1 Hz, 2H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 192.73, 158.0 (d, $J_{C\text{-}F}$ = 262.3 Hz), 154.6 (d, $J_{C\text{-}F}$ = 4.5 Hz), 147.5, 136.0 (d, $J_{C\text{-}F}$ = 8.2 Hz), 133.1, 132.6, 130.4, 130.2, 129.6, 129.0, 128.7, 128.2, 128.1, 118.4 (d, $J_{C\text{-}F}$ = 21.4 Hz), 117.9 (d, $J_{C\text{-}F}$ = 1.7 Hz), 115.8 (d, $J_{C\text{-}F}$ = 12.4 Hz). HRMS: $[M + H]^+$ calculated for $C_{21}H_{14}FO$: 301.10232, found 301.10263.



2,3-Di-*p*-tolyl-1*H*-inden-1-one **3ab**

3ab was obtained according to the general procedure in 61% yield.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.55 (d, J = 7.0 Hz, 1H), 7.34 (t, J = 7.4 Hz, 1H), 7.31 – 7.24 (m, 3H), 7.24 – 7.12 (m, 5H), 7.07 (d, J = 8.0 Hz, 2H), 2.39 (s, 3H), 2.31 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 197.0, 155.0, 145.6, 139.5, 137.7, 133.5, 132.2, 131.1, 130.1, 130.0, 129.6, 129.0, 128.9, 128.7, 128.1, 123.0, 121.3, 21.7, 21.5. The NMR data agree with those in a literature report. [3]

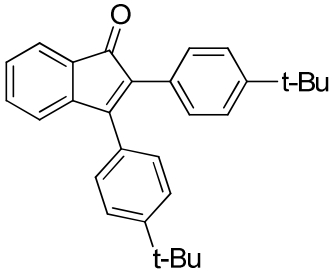


2,3-Bis(4-methoxyphenyl)-1*H*-inden-1-one **3ac**

3ac was obtained according to the general procedure in 42% yield.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.54 (d, J = 7.1 Hz, 1H), 7.38 – 7.31 (m, 3H), 7.28 –

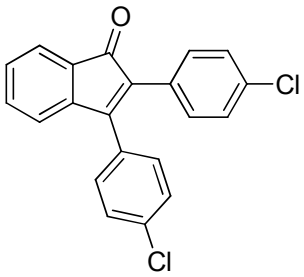
7.21 (m, 3H), 7.15 (d, *J* = 7.2 Hz, 1H), 6.93 (d, *J* = 8.8 Hz, 2H), 6.81 (d, *J* = 8.8 Hz, 2H), 3.85 (s, 3H), 3.79 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 197.1, 160.5, 159.2, 154.0, 145.6, 133.4, 131.43, 131.38, 131.2, 130.3, 128.8, 125.3, 123.6, 122.9, 121.1, 114.4, 113.8, 55.5, 55.3. The NMR data agree with those in a literature report. [3]



2,3-Bis(4-*tert*-butylphenyl)-1*H*-inden-1-one **3ad**

3ad was obtained according to the general procedure in 47% yield.

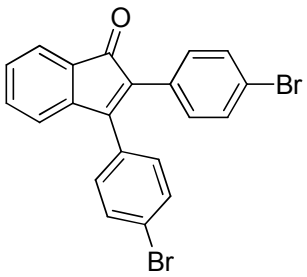
^{1}H NMR (500 MHz, $CDCl_3$) δ 7.56 (d, *J* = 6.9 Hz, 1H), 7.46 – 7.39 (m, 2H), 7.39 – 7.31 (m, 3H), 7.30 – 7.21 (m, 5H), 7.16 (d, *J* = 7.3 Hz, 1H), 1.36 (s, 9H), 1.30 (s, 9H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 197.2, 154.9, 152.6, 150.7, 145.8, 133.5, 132.0, 131.1, 130.1, 129.8, 128.8, 128.5, 128.1, 125.8, 125.2, 122.9, 121.5, 35.1, 34.8, 31.5. HRMS: $[M + H]^+$ calculated for $C_{29}H_{31}O$: 395.23694, found 395.23696.



2,3-Bis(4-chlorophenyl)-1*H*-inden-1-one **3ae**

3ae was obtained according to the general procedure in 79% yield.

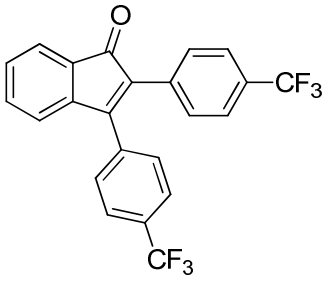
^{1}H NMR (500 MHz, $CDCl_3$) δ 7.57 (d, *J* = 7.1 Hz, 1H), 7.42 – 7.35 (m, 3H), 7.33 – 7.27 (m, 3H), 7.26 – 7.22 (m, 2H), 7.20 – 7.16 (m, 2H), 7.10 (d, *J* = 7.3 Hz, 1H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 195.9, 154.4, 144.8, 135.7, 134.2, 133.8, 131.7, 131.4, 131.0, 130.6, 130.0, 129.5, 129.0, 128.7, 123.4, 121.3. One carbon is not visible due to overlapping peaks. The NMR data agree with those in a literature report. [3]



2,3-Bis(4-bromophenyl)-1*H*-inden-1-one **3af**

3af was obtained according to the general procedure in 65% yield.

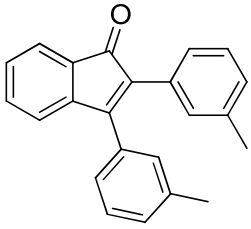
^{1}H NMR (500 MHz, $CDCl_3$) δ 7.60 – 7.53 (m, 3H), 7.42 – 7.35 (m, 3H), 7.32 – 7.27 (m, 1H), 7.26 – 7.21 (m, 2H), 7.14 – 7.08 (m, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 195.8, 154.5, 144.69, 133.83, 132.46, 131.64, 131.61, 131.43, 130.59, 130.20, 129.52, 129.45, 123.97, 123.45, 122.53, 121.34. One carbon is not visible due to overlapping peaks. The NMR data agree with those in a literature report. [3]



2,3-Bis(4-trifluoromethylphenyl)-1*H*-inden-1-one **3ag**

3ag was obtained according to the general procedure in 74% yield.

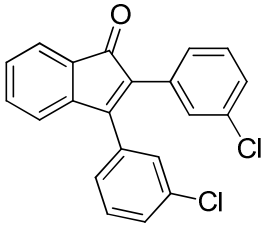
^{1}H NMR (500 MHz, $CDCl_3$) δ 7.72 (d, J = 8.1 Hz, 2H), 7.65 – 7.60 (m, 1H), 7.56 – 7.48 (m, 4H), 7.42 (td, J = 7.6, 1.2 Hz, 1H), 7.38 – 7.32 (m, 3H), 7.14 – 7.09 (m, 1H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 195.5, 155.2, 144.5, 136.1, 134.1, 134.0, 132.1, 131.7 (q, $J_{C\text{-}F}$ = 32.6 Hz), 130.41, 130.36 (q, $J_{C\text{-}F}$ = 11.4 Hz), 130.0, 129.7, 129.0, 126.3 (q, $J_{C\text{-}F}$= 3.7 Hz), 125.4 (q, $J_{C\text{-}F}$ = 3.7 Hz), 124.2 (q, $J_{C\text{-}F}$ = 270.5 Hz), 124.9 (q, $J_{C\text{-}F}$ = 270.8 Hz) , 123.8, 121.6. The NMR data agree with those in a literature report. [3]



2,3-Bis(3-methylphenyl)-1*H*-inden-1-one **3ah**

3ah was obtained according to the general procedure in 73% yield.

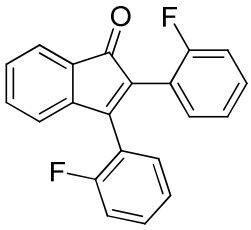
^{1}H NMR (500 MHz, $CDCl_3$) δ 7.56 (ddd, *J* = 7.1, 1.1, 0.6 Hz, 1H), 7.35 (td, *J* = 7.6, 1.2 Hz, 1H), 7.30 – 7.25 (m, 2H), 7.22 – 7.19 (m, 2H), 7.16 – 7.10 (m, 4H), 7.05 (d, *J* = 7.6 Hz, 1H), 7.00 (d, *J* = 7.6 Hz, 1H), 2.34 (s, 3H), 2.27 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 196.9, 155.6, 145.6, 138.5, 137.7, 133.5, 132.9, 132.5, 131.0, 130.9, 130.8, 130.2, 129.0, 128.8, 128.7, 128.0, 127.2, 125.8, 123.0, 121.4, 21.64, 21.63. One carbon is not visible due to overlapping peaks. The NMR data agree with those in a literature report. [3]



2,3-Bis(3-chlorophenyl)-1*H*-inden-1-one **3ai**

3ai was obtained according to the general procedure in 82% yield.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.59 (d, *J* = 7.0 Hz, 1H), 7.43 – 7.28 (m, 6H), 7.26 – 7.15 (m, 3H), 7.13 – 7.05 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 195.6, 154.7, 144.6, 135.1, 134.3, 133.9, 132.2, 131.7, 130.5, 130.5, 130.0, 129.9, 129.7, 129.6, 128.3, 128.2, 126.9, 123.5, 121.5. Two carbon are not visible due to overlapping peaks. The NMR data agree with those in a literature report. [3]

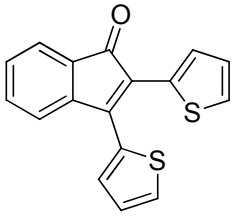


2,3-Bis(2-fluorophenyl)-1*H*-inden-1-one **3aj**

3aj was obtained according to the general procedure in 77% yield.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.59 (d, *J* = 7.0 Hz, 1H), 7.42 – 7.34 (m, 2H), 7.32 – 7.21 (m, 4H), 7.17 – 7.04 (m, 4H), 6.97 (t, *J* = 9.1 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 195.1, 160.3 (d, $J_{C\text{-}F}$ = 248.3 Hz), 159.6 (d, $J_{C\text{-}F}$ = 249.4 Hz), 153.0, 144.7, 133.9, 131.8 (d, $J_{C\text{-}F}$ = 3.3 Hz), 131.5(d, $J_{C\text{-}F}$ = 8.1 Hz), 130.7, 130.5, 130.2 (d, $J_{C\text{-}F}$ = 8.1 Hz), 129.9 (d, $J_{C\text{-}F}$ = 3.1 Hz), 129.4, 124.5 (d, $J_{C\text{-}F}$ = 3.5 Hz), 124.0 (d, $J_{C\text{-}F}$ = 3.6 Hz), 123.3, 121.8 (d, $J_{C\text{-}F}$ = 2.4 Hz), 121.0 (d, $J_{C\text{-}F}$ = 16.9 Hz), 119.1 (d, $J_{C\text{-}F}$ = 15.7

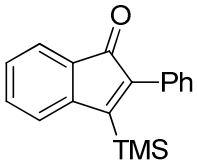
Hz), 116.5 (d, J_{C-F} = 21.3 Hz), 116.37 (d, J_{C-F} = 21.8 Hz). HRMS: $[M + H]^+$ calculated for $C_{21}H_{13}F_2O$: 319.09290, found 319.09329.



2,3-Bis(thiophen-2-yl)-1*H*-inden-1-one **3ak**

3ak was obtained according to the general procedure in 71% yield.

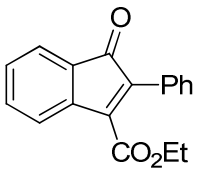
^{1}H NMR (500 MHz, $CDCl_3$) δ 7.58 (dd, *J* = 5.1, 1.1 Hz, 1H), 7.54 (d, *J* = 7.0 Hz, 1H), 7.48 (dd, *J* = 3.7, 1.1 Hz, 1H), 7.40 – 7.32 (m, 3H), 7.27 – 7.22 (m, 2H), 7.20 (dd, *J* = 5.0, 3.6 Hz, 1H), 7.02 (dd, *J* = 5.1, 3.7 Hz, 1H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 195.2, 146.2, 145.8, 134.1, 133.3, 132.2, 130.3, 129.5, 129.3, 129.1, 129.0, 128.1, 127.9, 127.5, 127.2, 123.2, 121.5. HRMS: $[M + H]^+$ calculated for $C_{17}H_{11}OS_2$: 295.02458, found 295.02491.



2-Phenyl-3-(trimethylsilyl)-1*H*-inden-1-one **3al**

3al was obtained according to the general procedure in 62% yield.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.49 (d, *J* = 7.0 Hz, 1H), 7.41 – 7.34 (m, 4H), 7.27 -7.18 (m, 4H), 0.16 (s, 9H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 197.9, 157.0, 148.9, 148.1, 134.2, 133.5, 130.2, 129.9, 128.5, 128.2, 128.0, 123.34, 123.33, 0.2. HRMS: $[M + H]^+$ calculated for $C_{18}H_{19}OSi$: 279.119967, found 279.12006. The NMR data agree with those in a literature report. [6]



Ethyl 1-oxo-2-phenyl-1*H*-indene-3-carboxylate **3am**

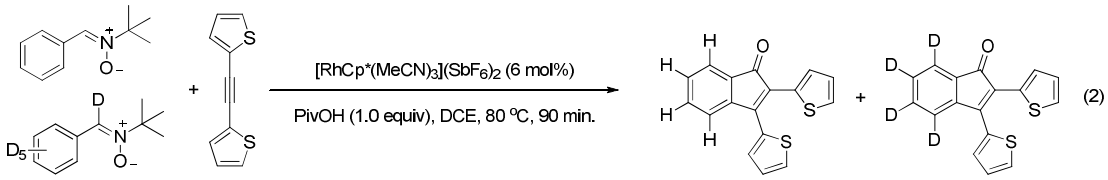
3am was obtained according to the general procedure in 46% yield.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.60 – 7.50 (m, 2H), 7.49 – 7.35 (m, 6H), 7.32 – 7.23

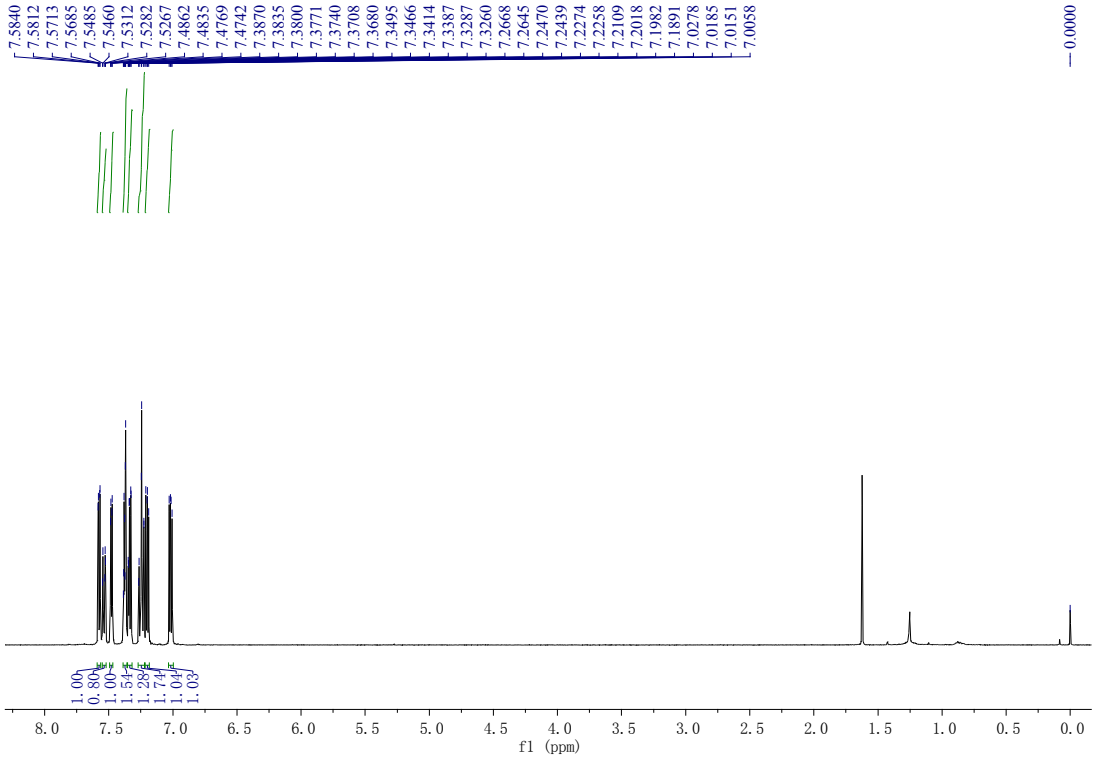
(m, 1H), 4.31 (q, J = 7.1 Hz, 2H), 1.22 (t, J = 7.1 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 196.1, 164.7, 143.0, 142.7, 138.7, 134.7, 129.92, 129.86, 129.5, 129.3, 129.2, 128.1, 123.9, 122.8, 61.6, 14.0. HRMS: $[M + H]^+$ calculated for $C_{18}H_{15}O_3$: 279.10157, found 279.10177.

III. Mechanic Studies

1. KIE mesurement

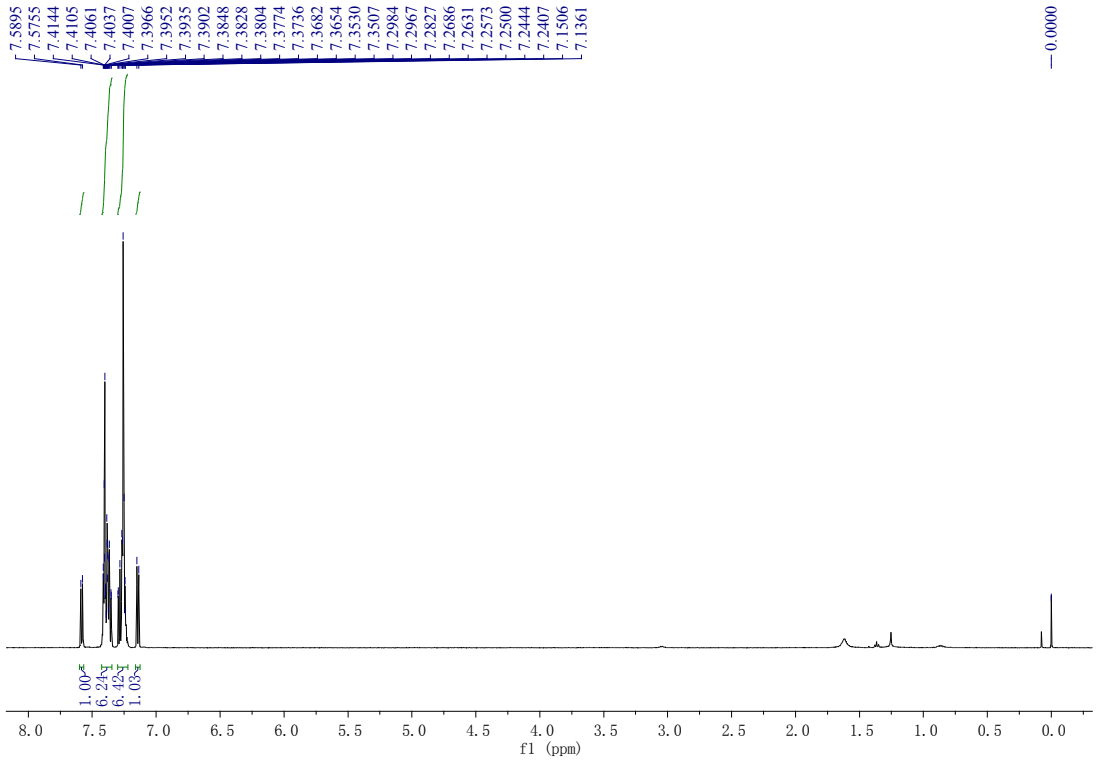


An equimolar mixture of PBN and PBN-d_5 (0.5 mmol in total, 90.0 mg), di(2-thienyl)acetylene (0.25 mmol, 47.6 mg), $[Cp^*Rh(MeCN)_3](SbF_6)_2$ (6 mol%, 12.5 mg), PivOH (1.0 equiv, 25.5 mg) and DCE (2 mL) were charged into a pressure tube under argon. The reaction mixture was stirred at 80 °C for 1.5 h. After cooled to room temperature, the solvent was removed under reduced pressure and the residue was purified by silica gel chromatography using PE/DCE to afford the mixed product. KIE value (k_H/k_D = 4.0) was determined on the basis of ^{1}H NMR analysis.



2. ^{18}O Labeled Experiment

PBN (0.24 mmol, 42.5 mg), diphenylacetylene (0.2 mmol, 35.6 mg), $[Cp^*Rh(MeCN)_3](SbF_6)_2$ (6 mol%, 10.0 mg), PivOH (1.0 equiv, 20.4 mg), water-^{18}O (6 equiv, 24.0 mg) and DCE (2 mL) were charged into a pressure tube under argon. The reaction mixture was stirred at 80 °C for 12 h. After cooled to room temperature, the solvent was removed under reduced pressure and the residue was purified by silica gel chromatography using PE/DCE to afford the mixture products of 2,3-Diphenyl-1*H*-inden-1-one (**3aa**) and ^{18}O-labeled 2,3-Diphenyl-1*H*-inden-1-one (**3aa-^{18}O**) (**3aa/3aa-^{18}O** = 22/100). HRMS: $[M + H]^+$ calculated for $C_{21}H_{15}{}^{18}O$: 285.11599, found 285.11615.



IV. References

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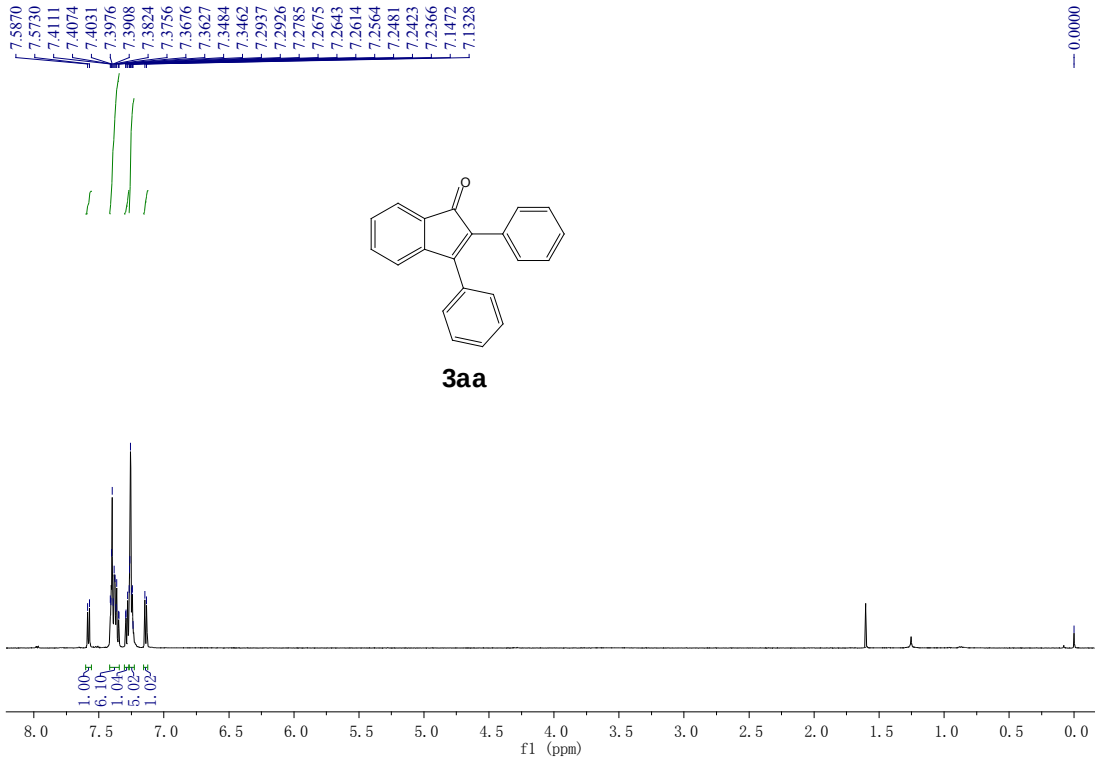
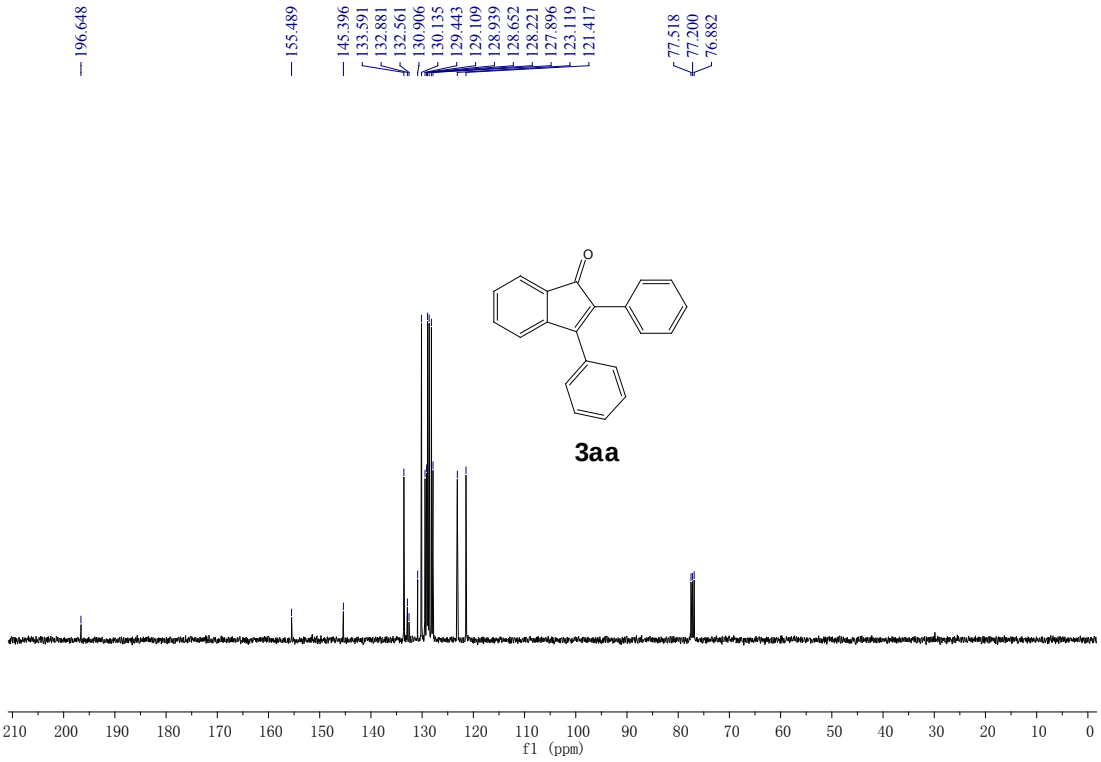
V. NMR Spectra



3aa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127.896
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77.200
76.882
O
3aa
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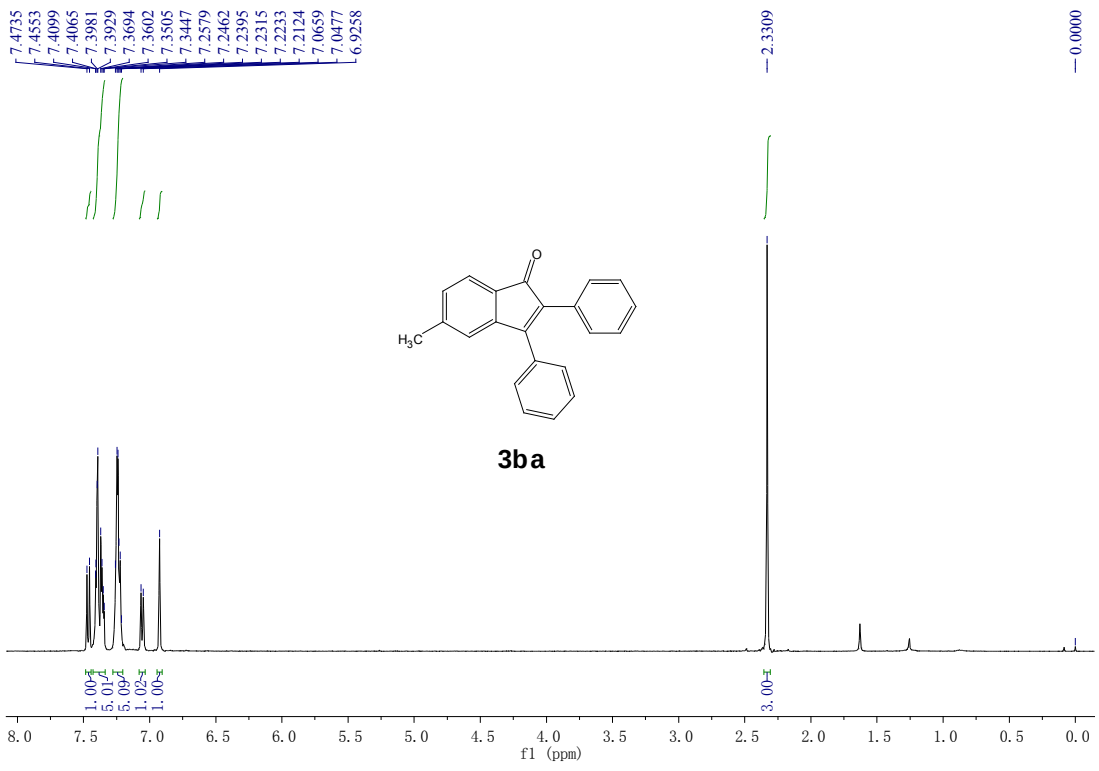
f1 (ppm)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7.4553
7.4099
7.4065
7.3981
7.3929
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7.3505
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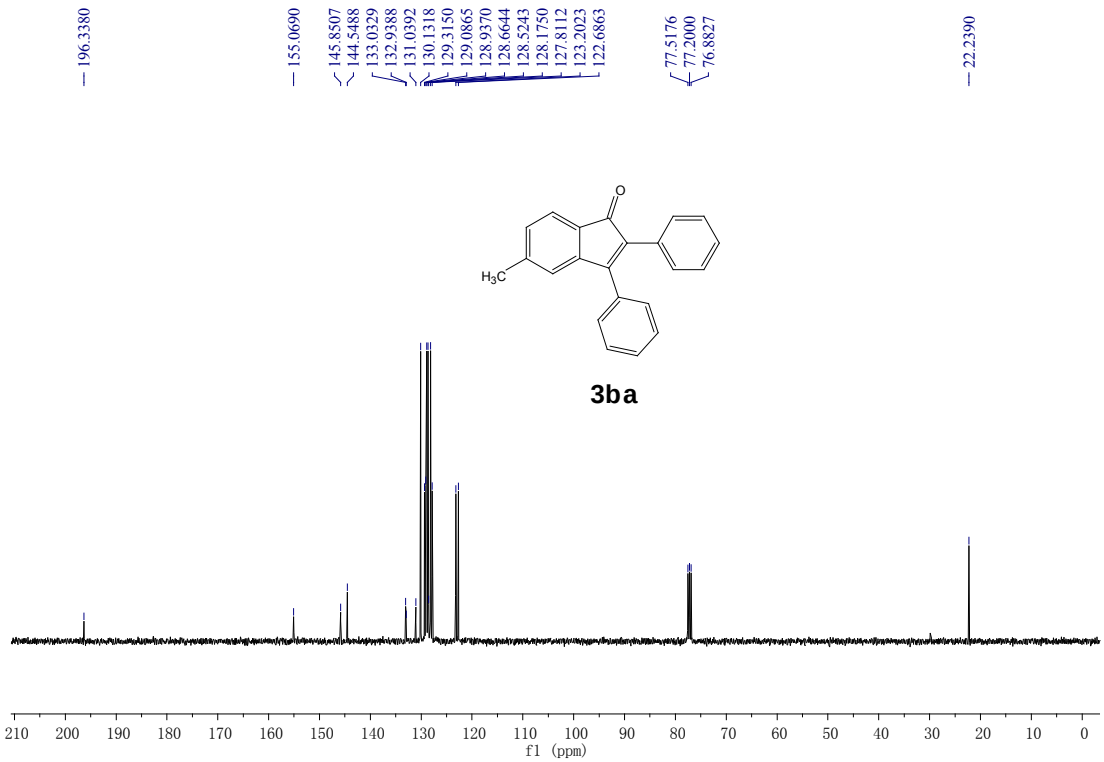
7.2579
7.2462
7.2395
7.2315
7.2233
7.2124
7.0659
7.0477
6.9258
2.3309
0.0000
O
H3C
3ba
1.00
5.01
5.09
1.02
1.00
3.00
8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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131.0392
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128.9370
128.6644
128.5243
128.1750
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122.6863
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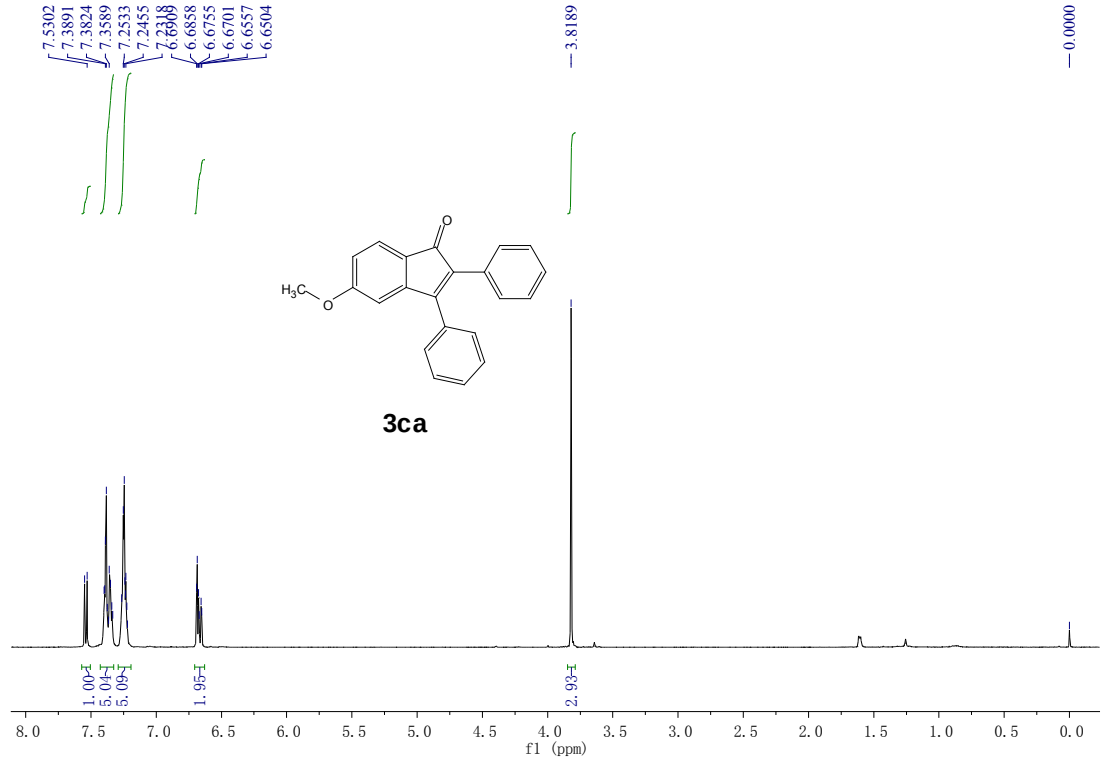
22.2390
O
H3C
3ba
f1 (ppm)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7.3824
7.3589
7.2533
7.2455
7.2318
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6.6858
6.6755
6.6701
6.6557
6.6504
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H3C
O
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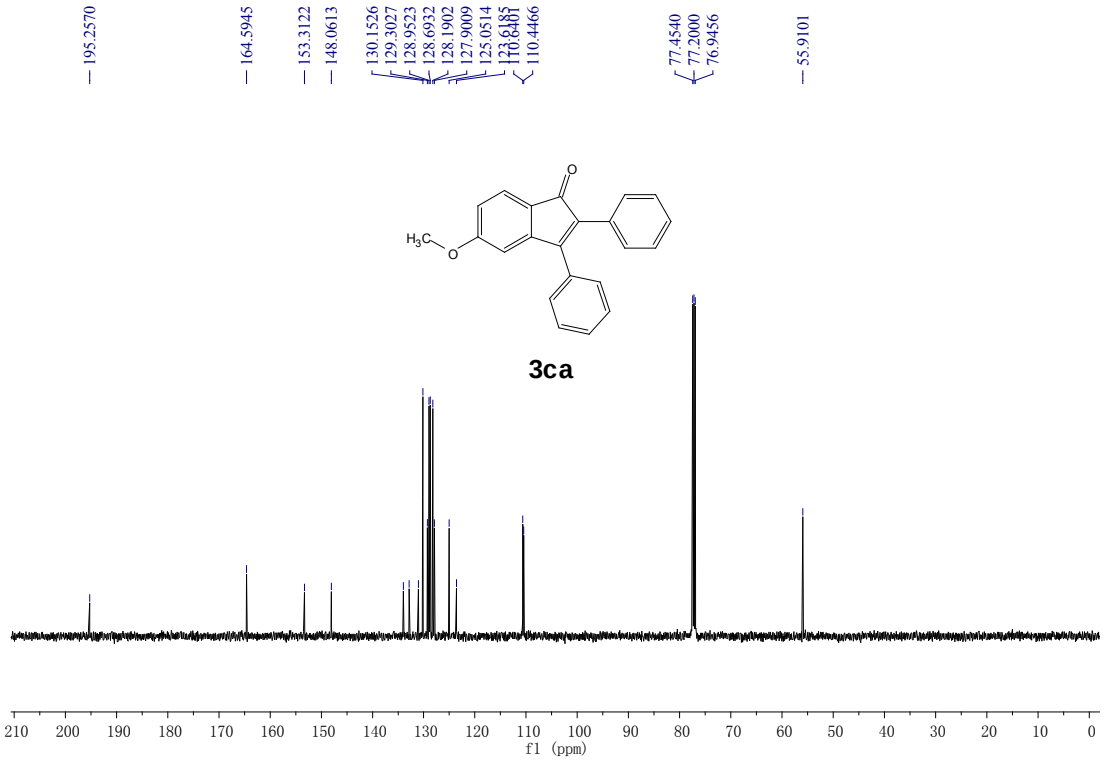
5.09
1.95
2.93
f1 (ppm)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128.1902
127.9009
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77.2000
76.9456
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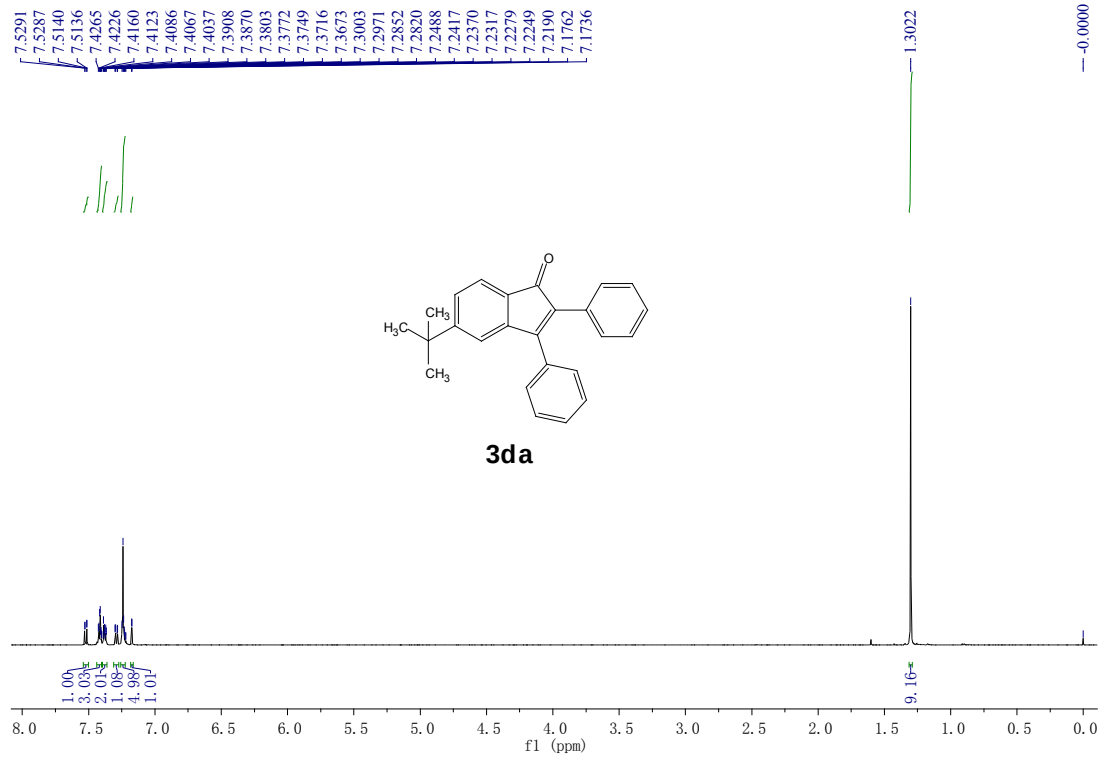
O
H3C
O
3ca
f1 (ppm)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7.4086
7.4067
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7.2820
7.2488
7.2417
7.2370
7.2317
7.2279
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7.2190
7.1762
7.1736
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H3C
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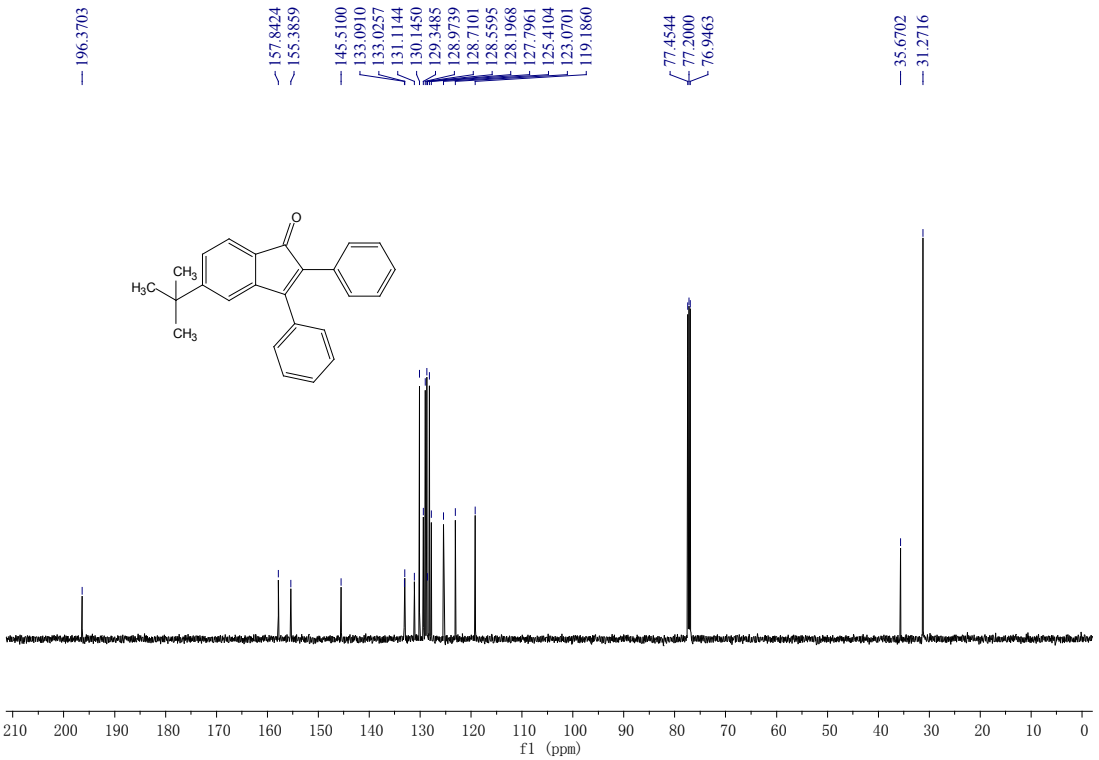
2.01
1.08
4.98
1.01
9.16
f1 (ppm)

3da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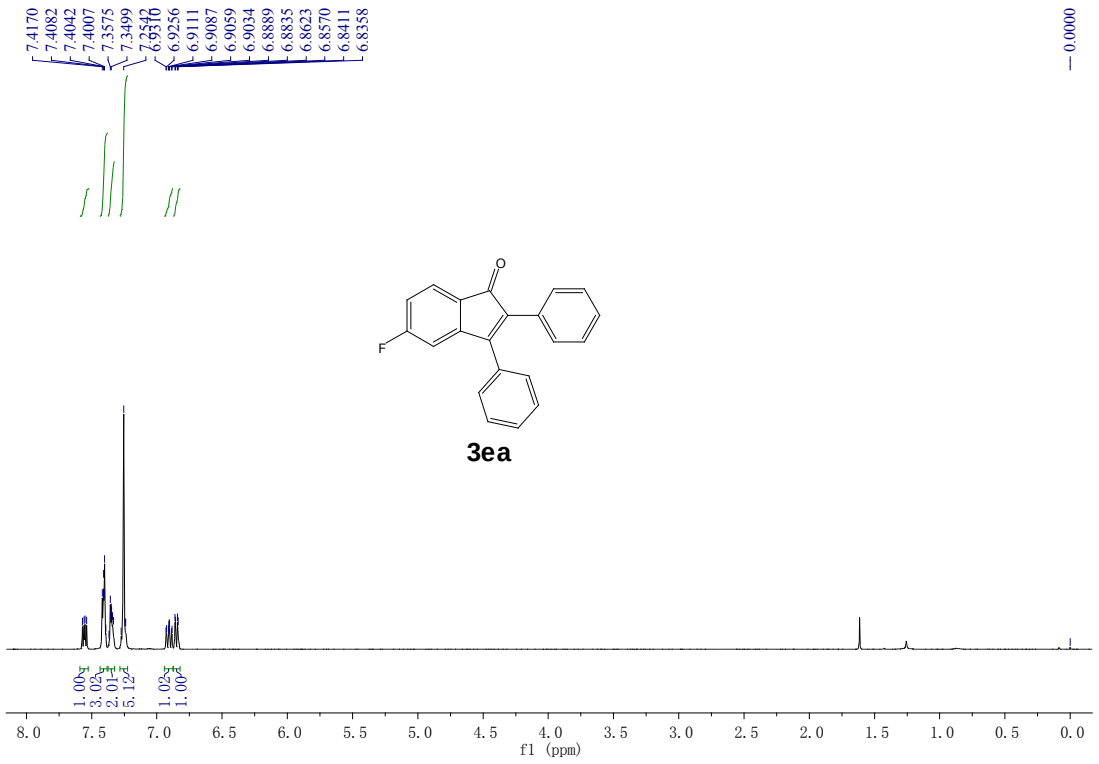
f1 (ppm)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6.9034
6.8889
6.8835
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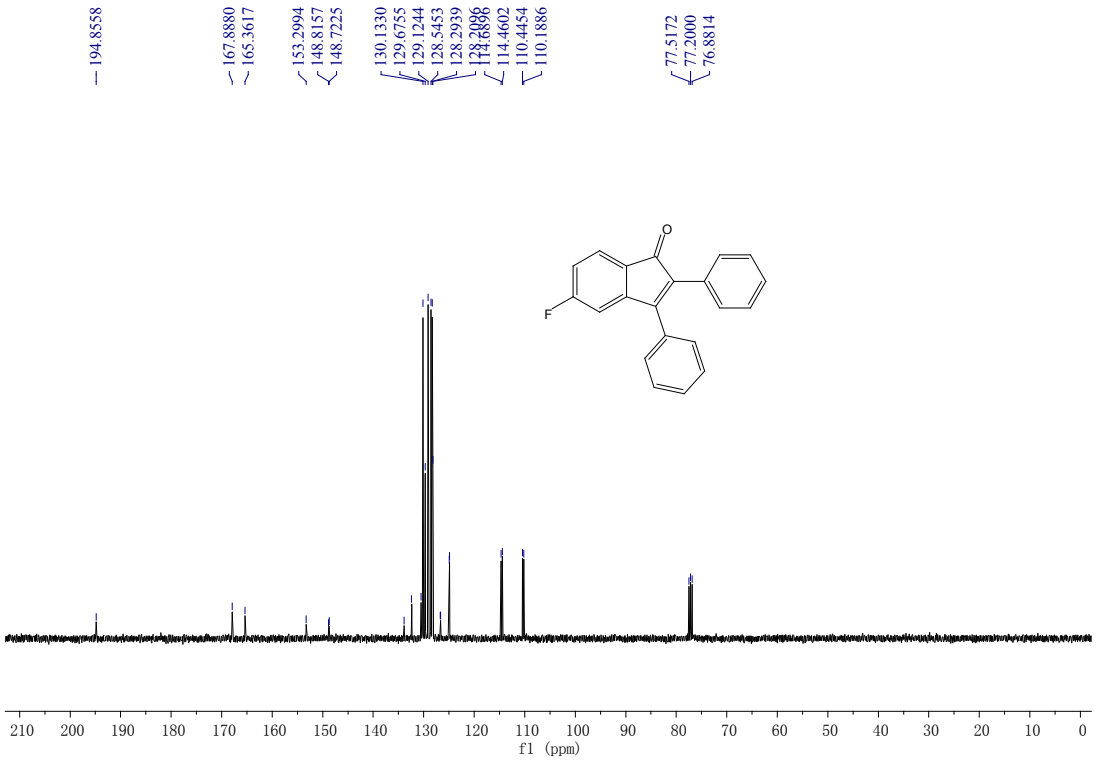
6.8570
6.8411
6.8358
0.0000
O
F
1.00
3.02
2.01
5.12
1.02
1.00
8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

3ea

3ea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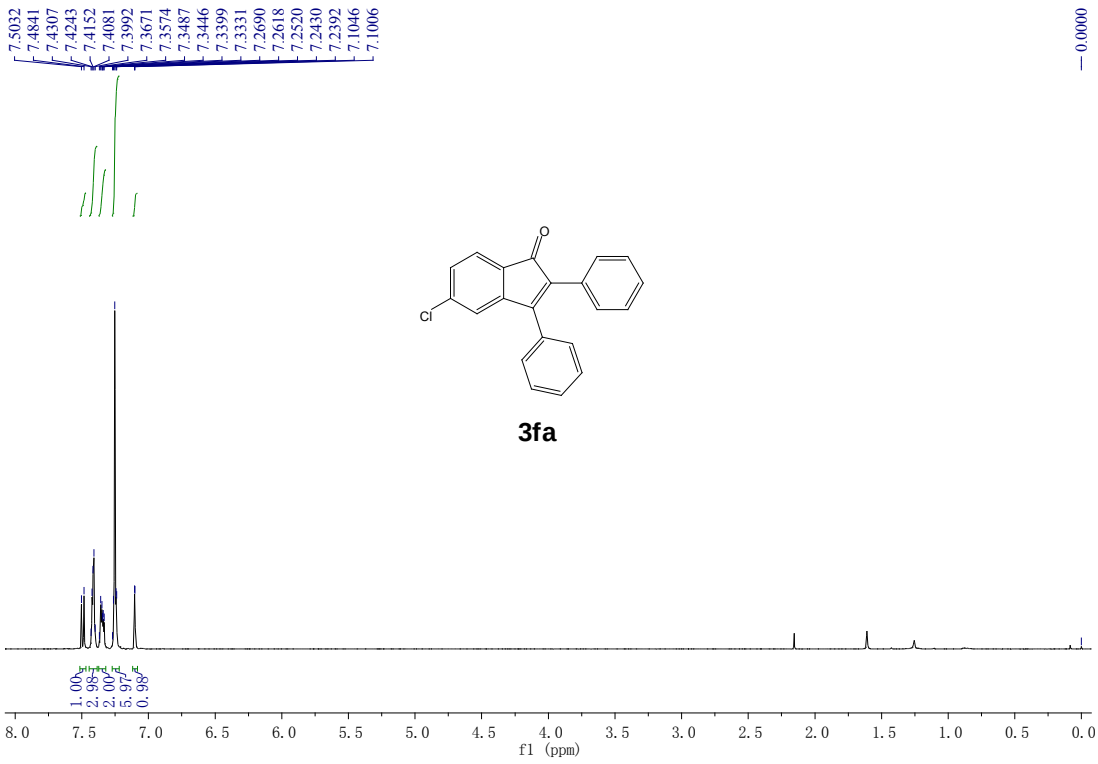
F
f1 (ppm)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7.3574
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7.3446
7.3399
7.3331
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7.2618
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7.2430
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5.97
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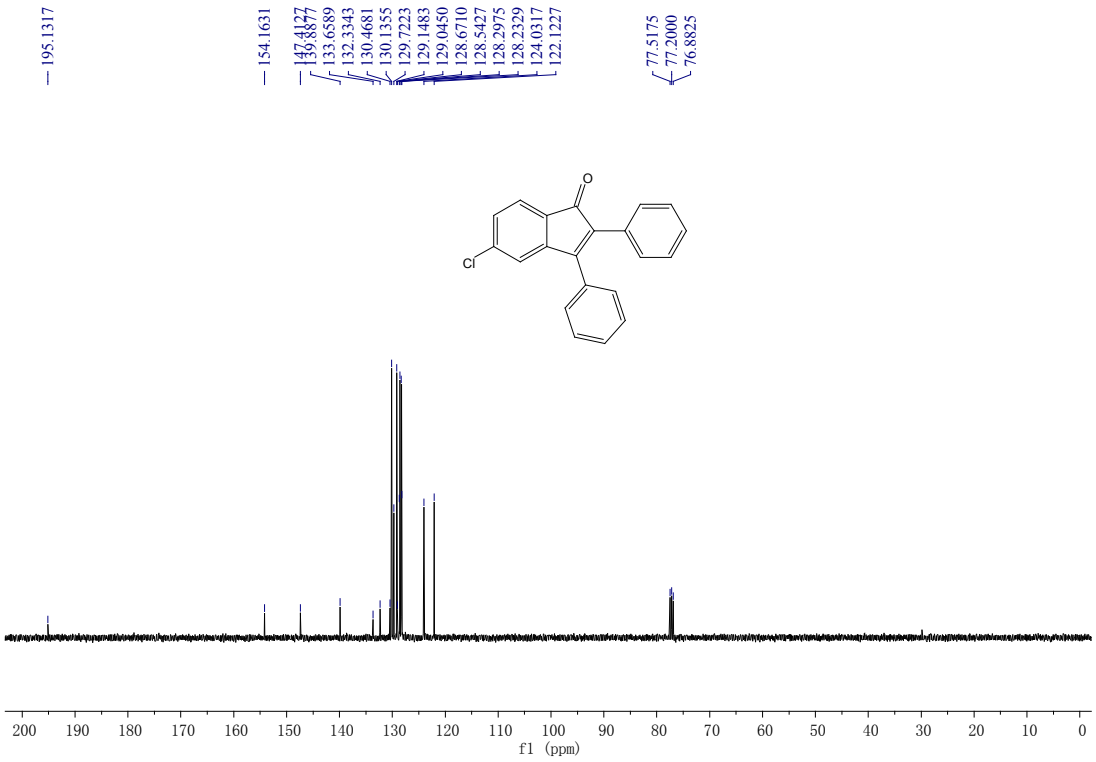
f1 (ppm)

3fa

3fa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128.5427
128.2975
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Cl
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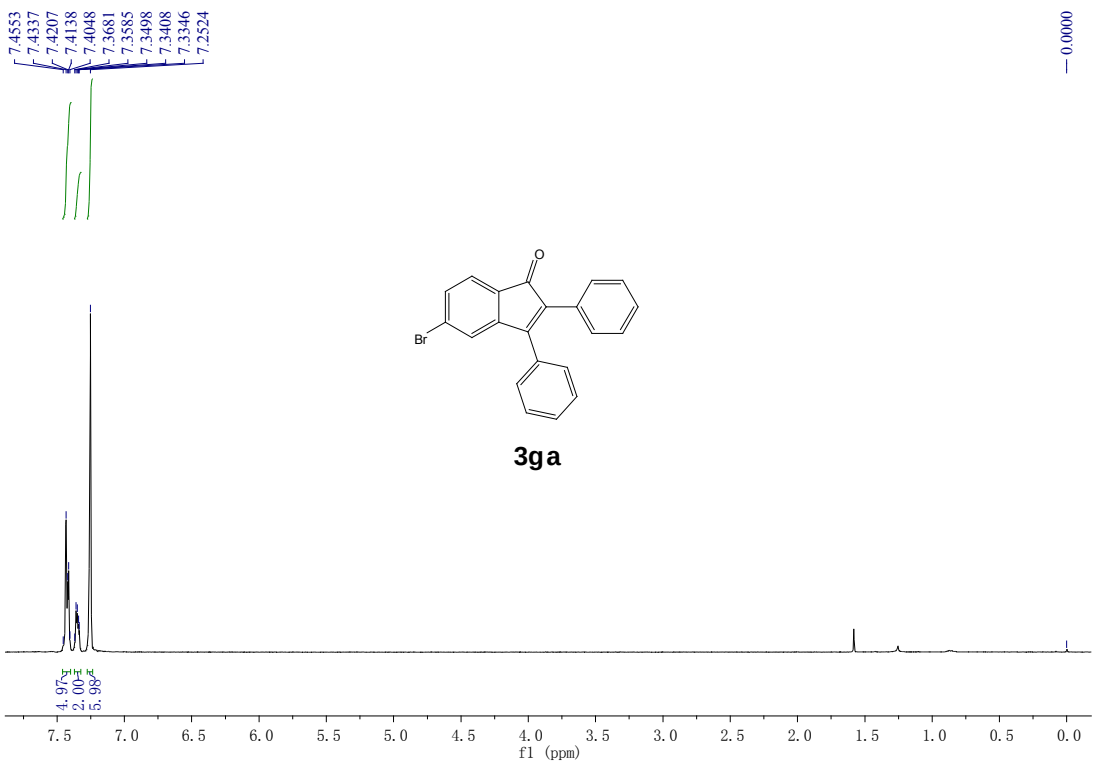
f1 (ppm)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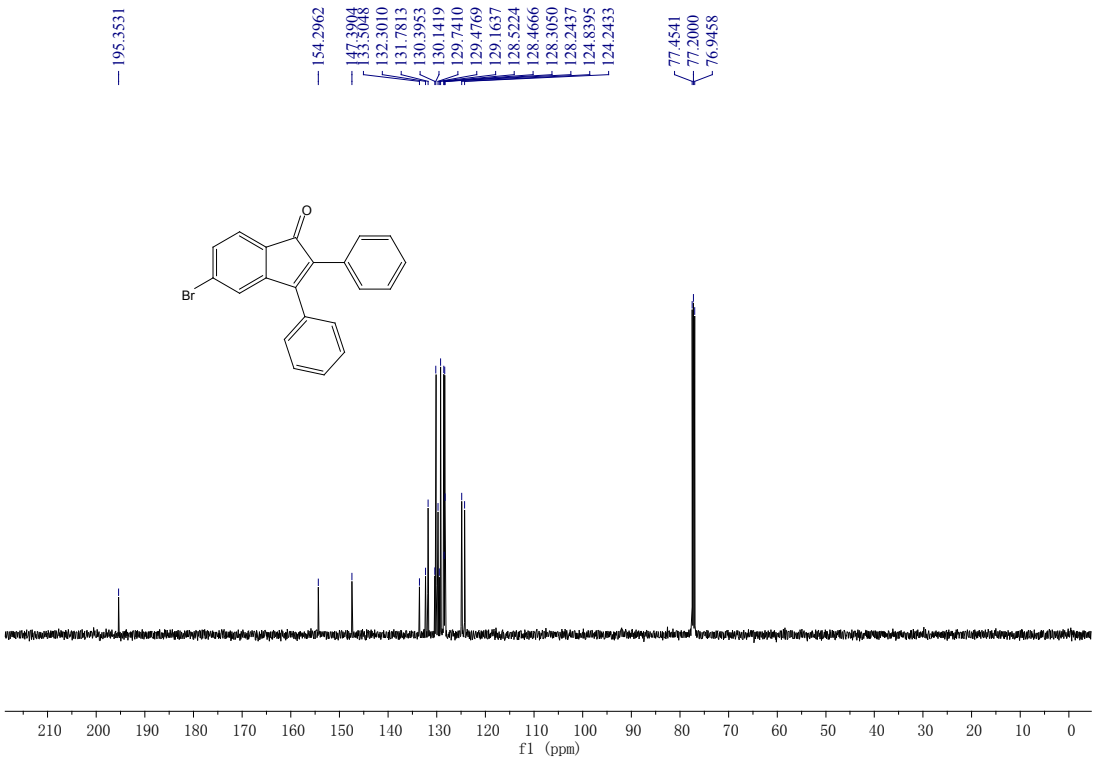
0.0000
O
Br
4.97
2.00
5.98
7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

3ga

3ga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128.3050
128.2437
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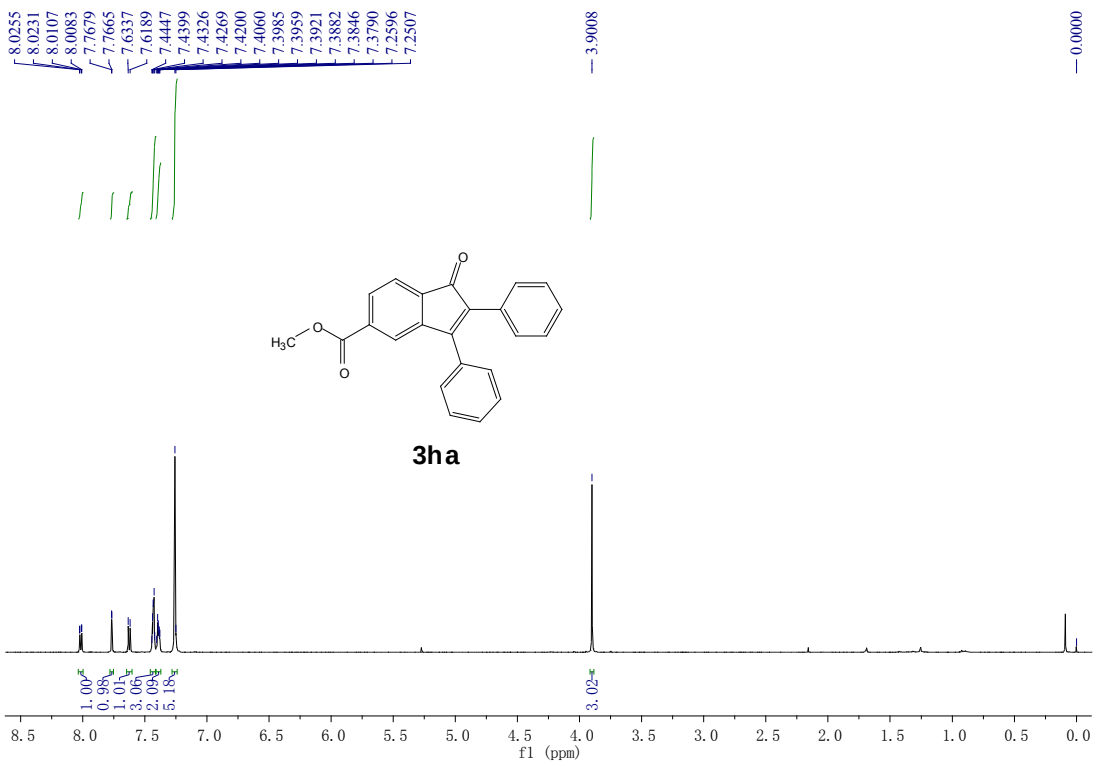
124.2433
77.4541
77.2000
76.9458
O
Br
f1 (ppm)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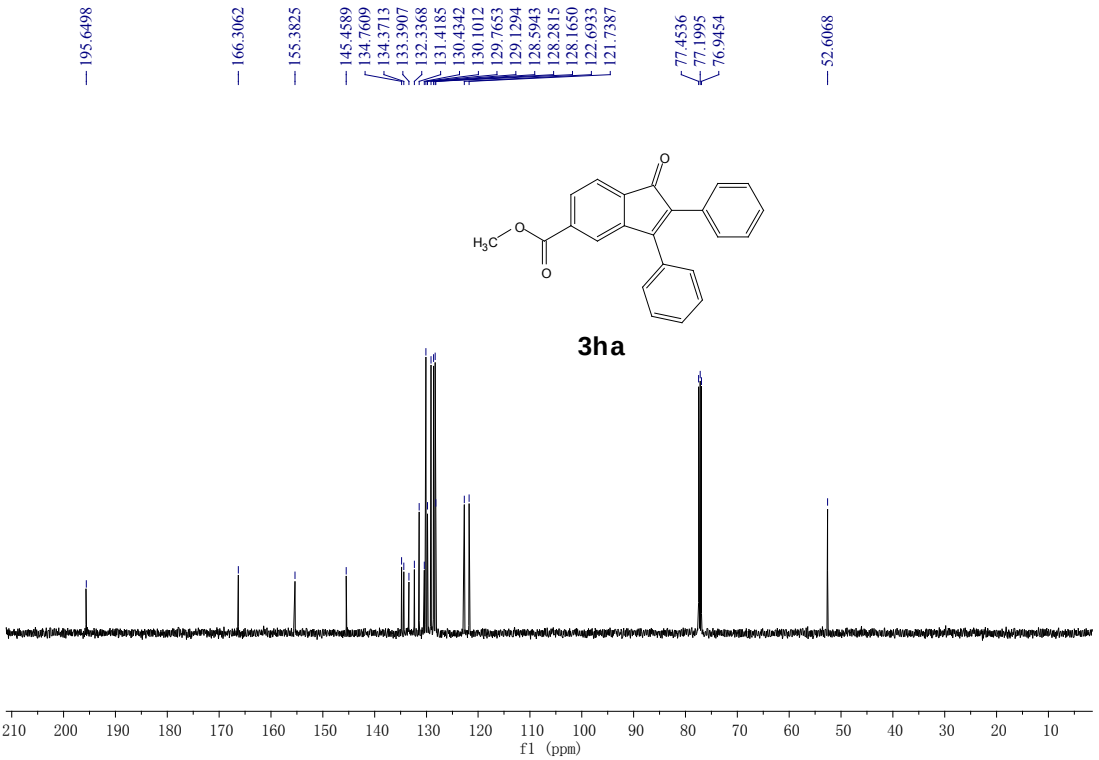
8.0231
8.0107
8.0083
7.7679
7.7665
7.6337
7.6189
7.4447
7.4399
7.4326
7.4269
7.4200
7.4060
7.3985
7.3959
7.3921
7.3882
7.3846
7.3790
7.2596
7.2507
3.9008
0.0000
O
H3C
O
O
1.00
0.98
1.01
3.06
2.09
5.18
3.02
f1 (ppm)

3ha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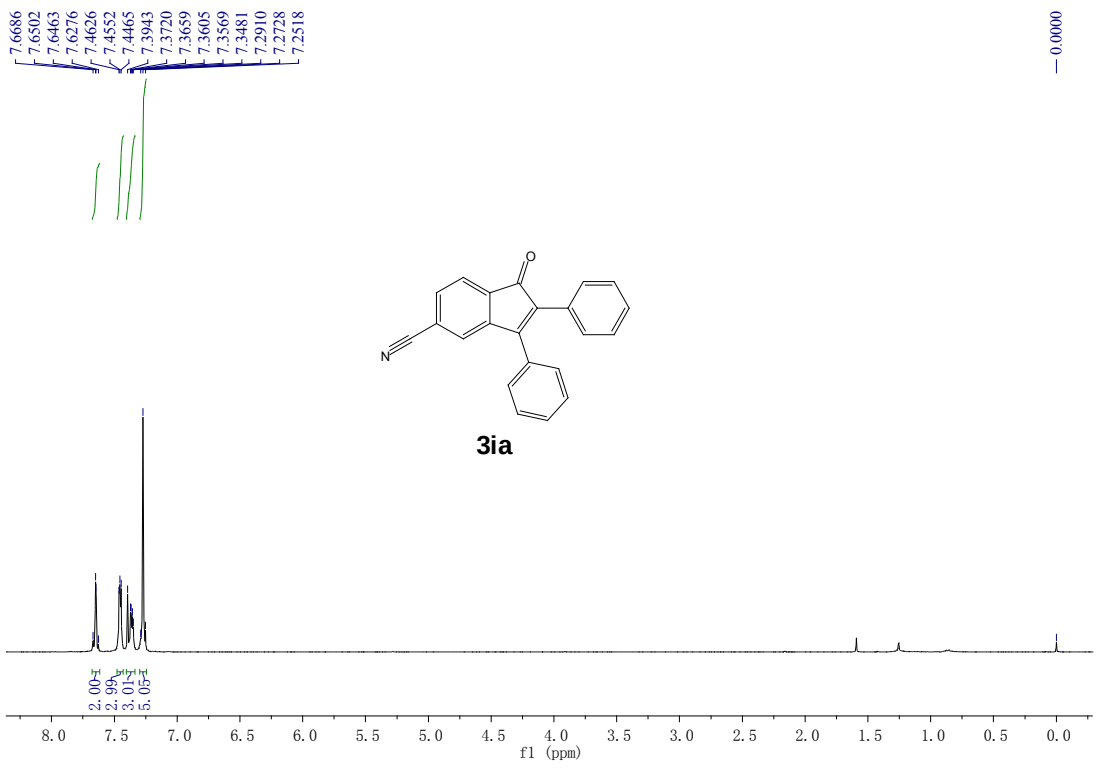
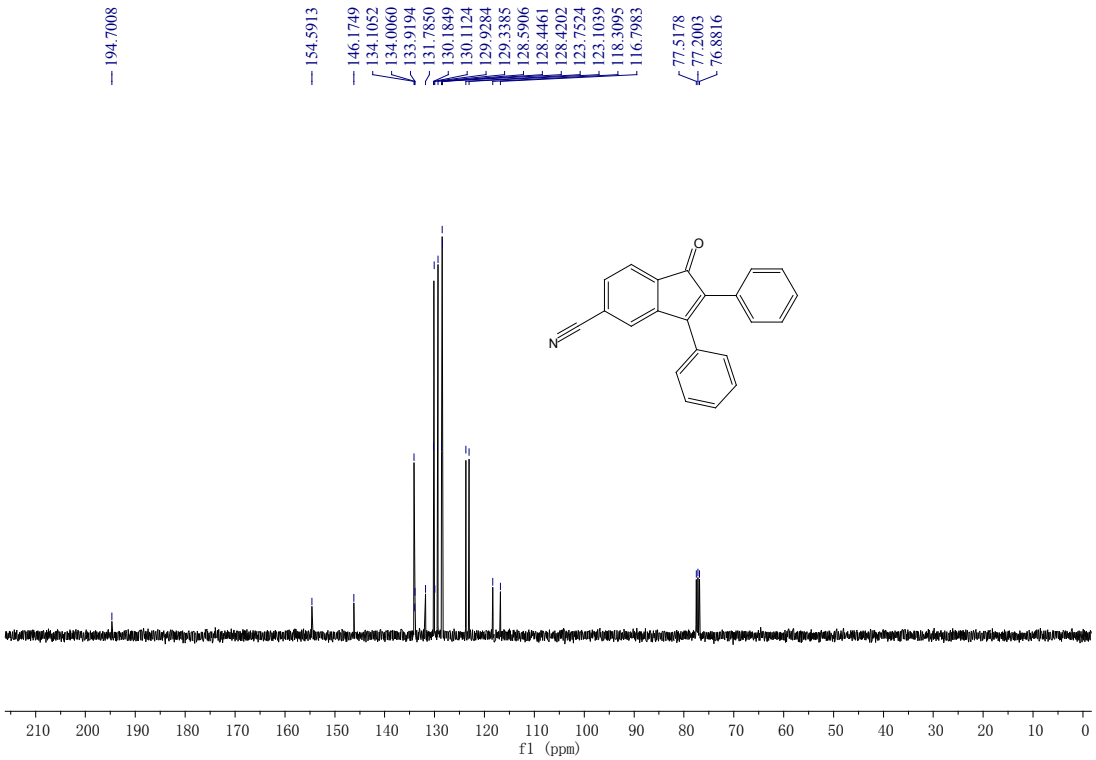
166.3062
155.3825
145.4589
134.7609
134.3713
133.3907
132.3368
131.4185
130.4342
130.1012
129.7653
129.1294
128.5943
128.2815
128.1650
122.6933
121.7387
77.4536
77.1995
76.9454
52.6068
O
O
O
H3C
3ha
f1 (ppm)


7.6686
7.6502
7.6463
7.6276
7.4626
7.4552
7.4465
7.3943
7.3720
7.3659
7.3605
7.3569
7.3481
7.2910
7.2728
7.2518
0.0000
O
N
3ia
2.00
2.99
3.01
5.05
f1 (ppm)

3ia


194.7008
154.5913
146.1749
134.1052
134.0060
133.9194
131.7850
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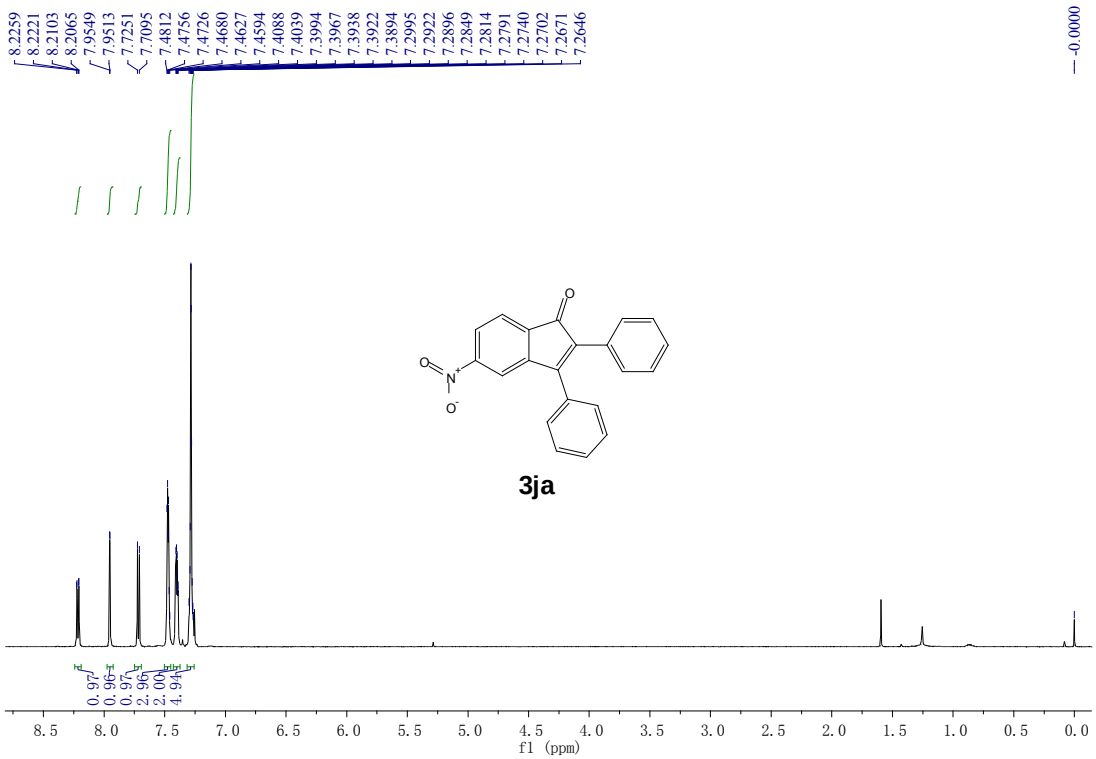
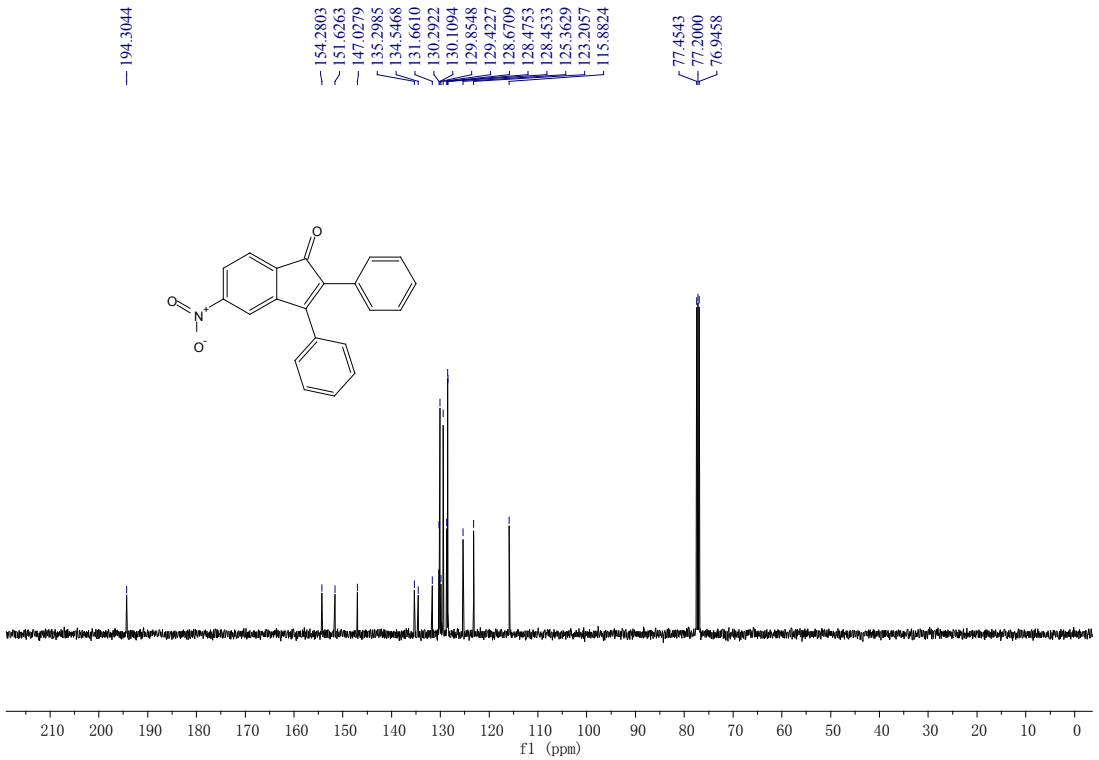
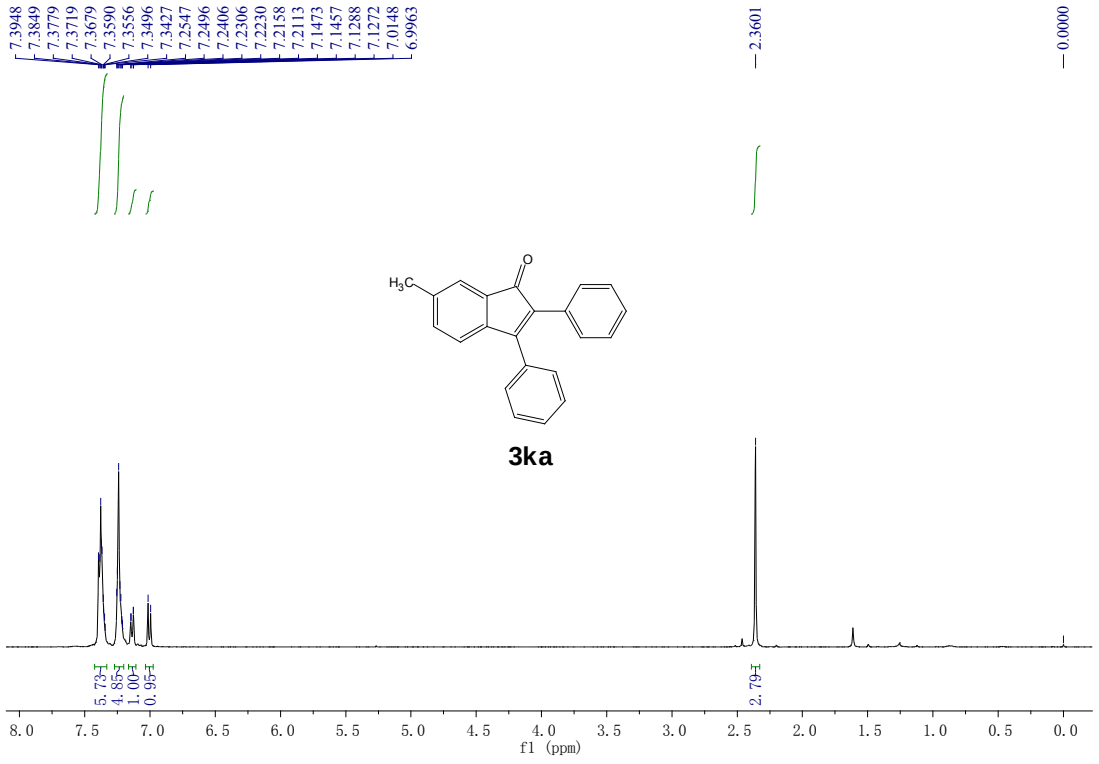
130.1124
129.9284
129.3385
128.5906
128.4461
128.4202
123.7524
123.1039
118.3095
116.7983
77.5178
77.2003
76.8816
O
N
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


8.2259
8.2221
8.2103
8.2065
7.9549
7.9513
7.7251
7.7095
7.4812
7.4756
7.4726
7.4680
7.4627
7.4594
7.4088
7.4039
7.3994
7.3967
7.3938
7.3922
7.3894
7.2995
7.2922
7.2896
7.2849
7.2814
7.2791
7.2740
7.2702
7.2671
7.2646
-0.0000
O
N
O
0.97
0.96
0.97
2.96
2.00
4.94
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

3ja

3ja


194.3044
154.2803
151.6263
147.0279
135.2985
134.5468
131.6610
130.2922
130.1094
129.8548
129.4227
128.6709
128.4753
128.4533
125.3629
123.2057
115.8824
77.4543
77.2000
76.9458
O
O
N+
O-
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


7.3948
7.3849
7.3779
7.3719
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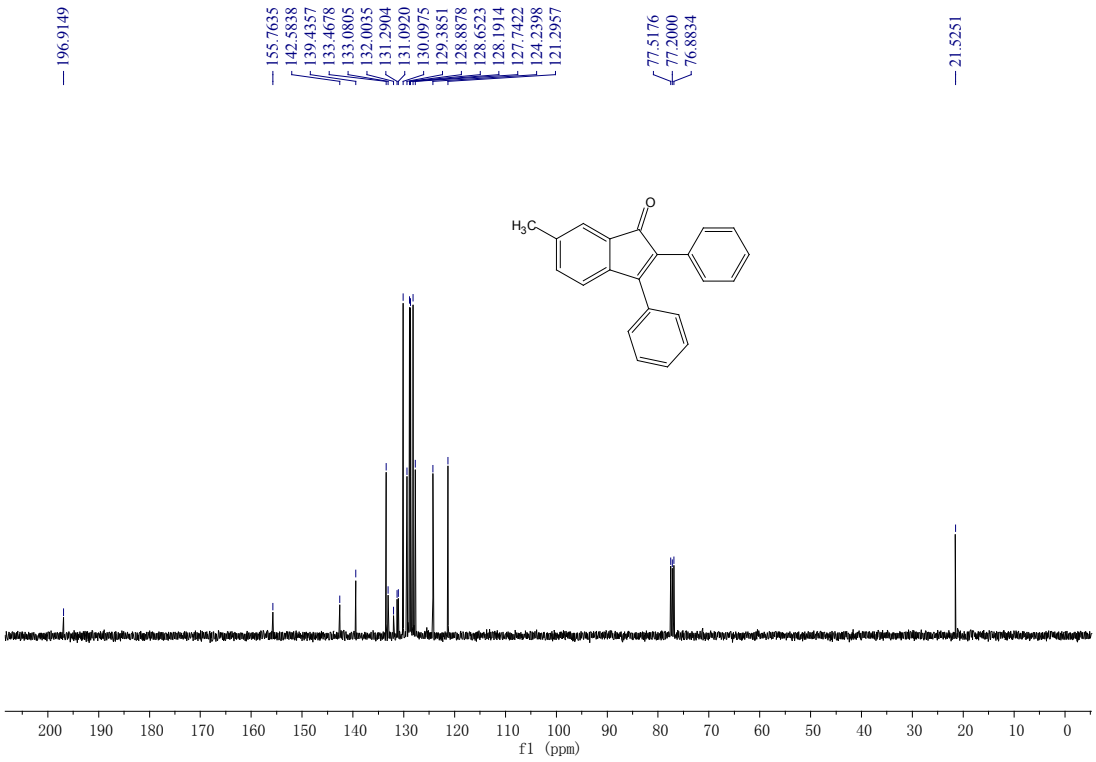
7.3590
7.3556
7.3496
7.3427
7.2547
7.2496
7.2406
7.2306
7.2230
7.2158
7.2113
7.1473
7.1457
7.1288
7.1272
7.0148
6.9963
2.3601
0.0000
H3C
O
5.73
4.85
1.00
0.95
2.79
8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

3ka

3ka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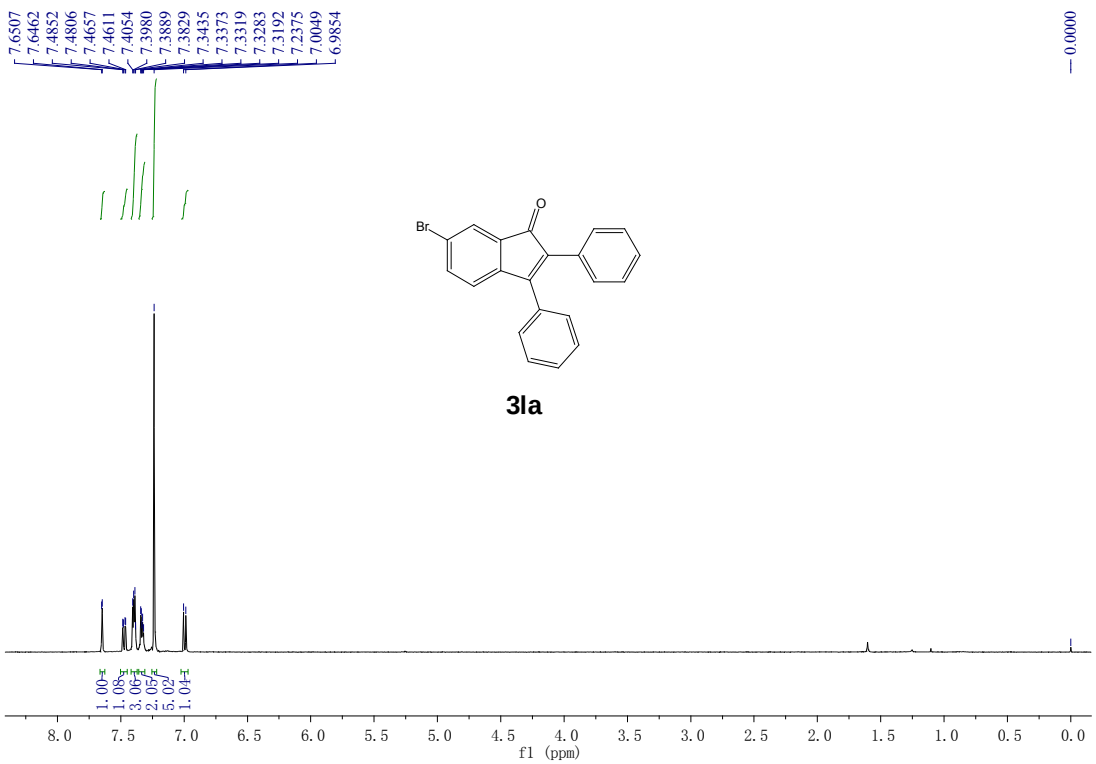
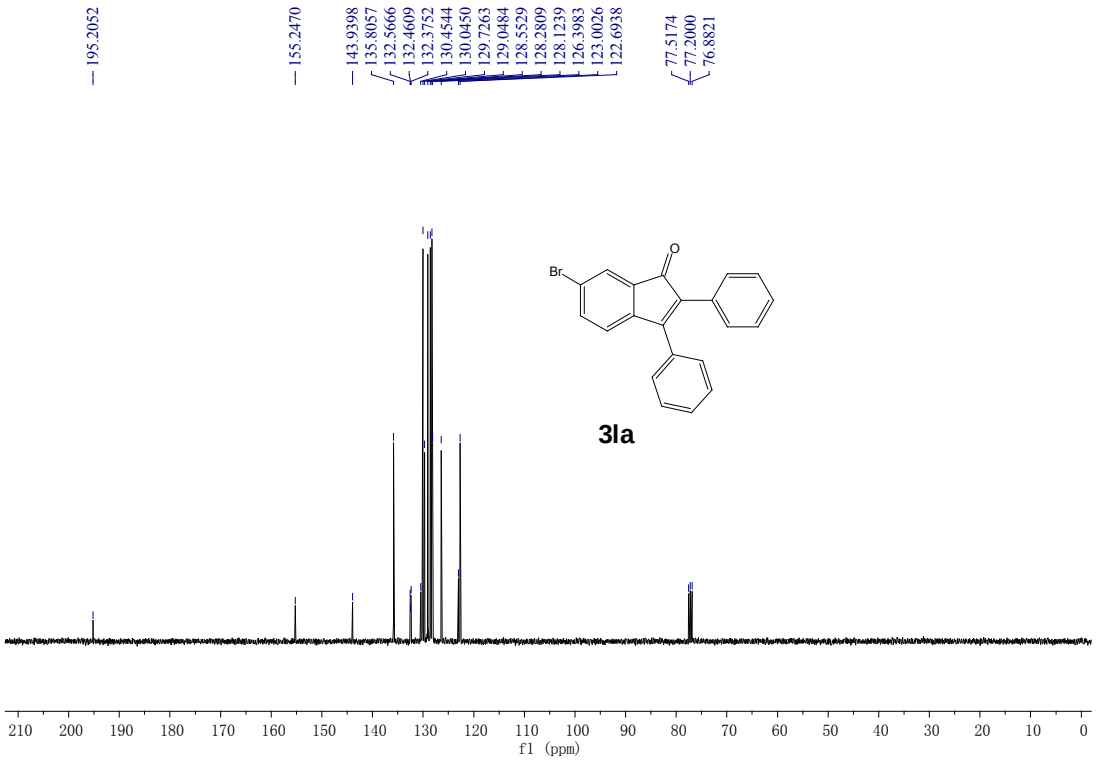
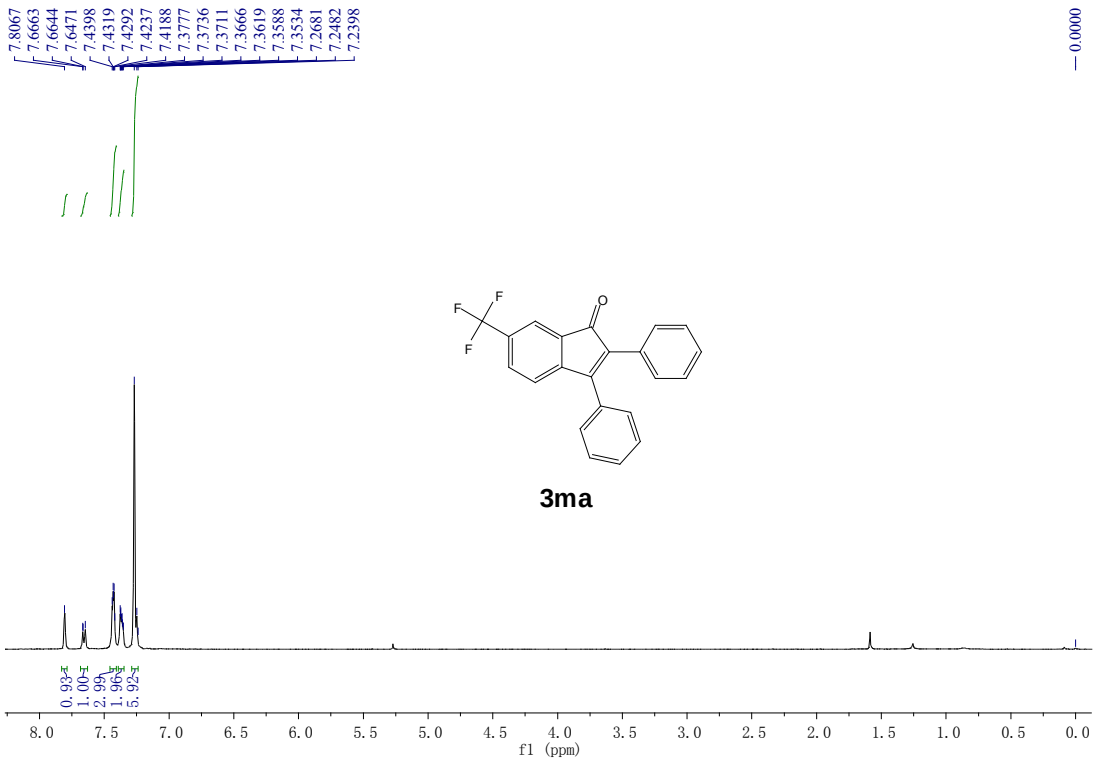
155.7635
142.5838
139.4357
133.4678
133.0805
132.0035
131.2904
131.0920
130.0975
129.3851
128.8878
128.6523
128.1914
127.7422
124.2398
121.2957
77.5176
77.2000
76.8834
21.5251
H3C
O
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


7.6507
7.6462
7.4852
7.4806
7.4657
7.4611
7.4054
7.3980
7.3889
7.3829
7.3435
7.3373
7.3319
7.3283
7.3192
7.2375
7.0049
6.9854
0.0000
Br
O
1.00
1.08
3.06
2.05
5.02
1.04
8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

3la

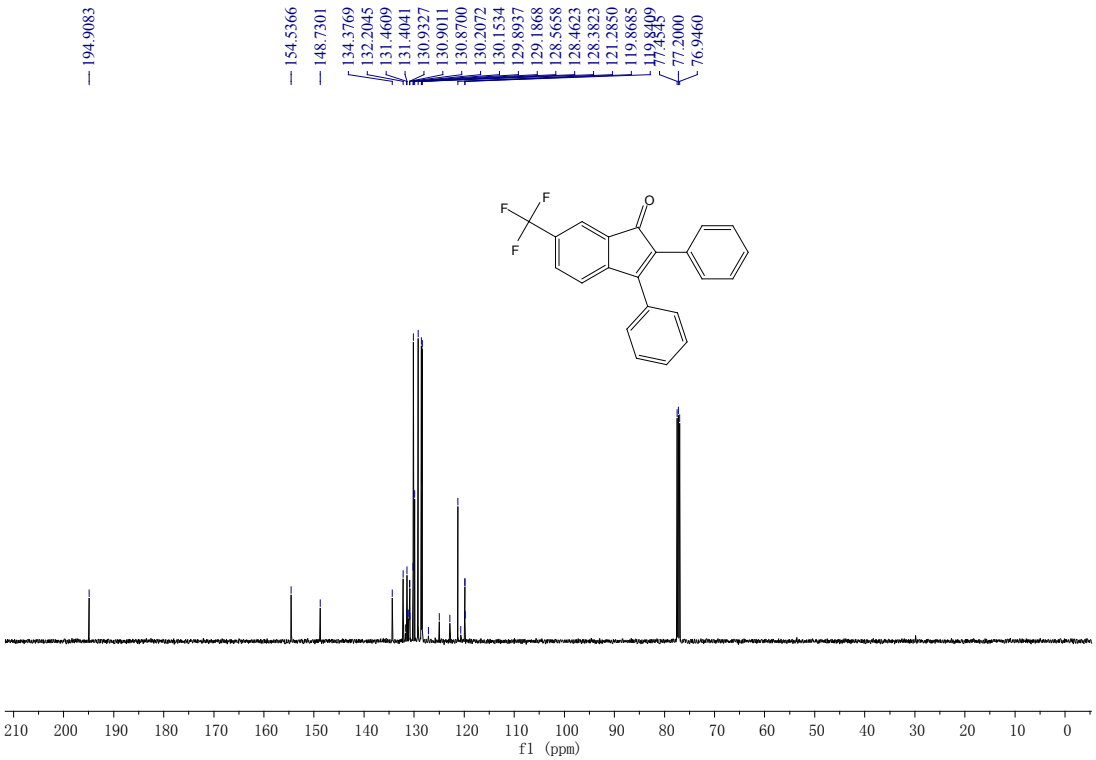

195.2052
155.2470
143.9398
135.8057
132.5666
132.4609
132.3752
130.4544
130.0450
129.7263
129.0484
128.5529
128.2809
128.1239
126.3983
123.0026
122.6938
77.5174
77.2000
76.8821
Br
O
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

3la


7.8067
7.6663
7.6644
7.6471
7.4398
7.4319
7.4292
7.4237
7.4188
7.3777
7.3736
7.3711
7.3666
7.3619
7.3588
7.3534
7.2681
7.2482
7.2398
0.0000
F
F
F
O
0.93
1.00
2.99
1.96
5.92
8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

3ma

3ma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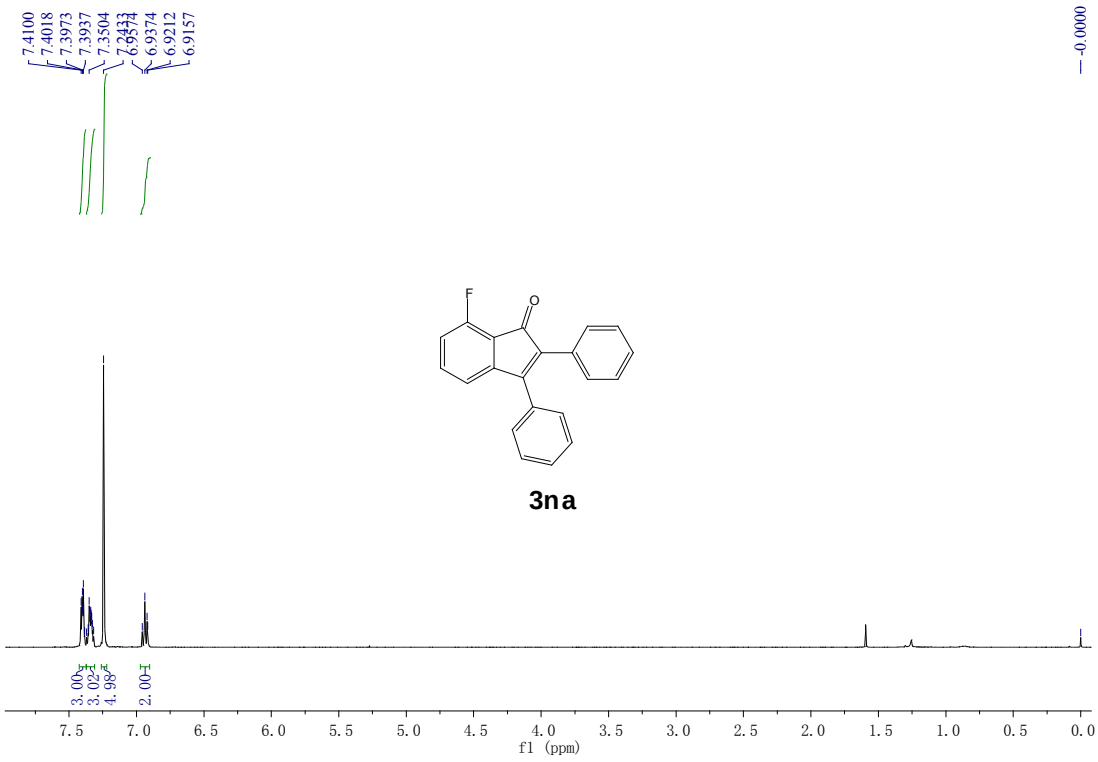
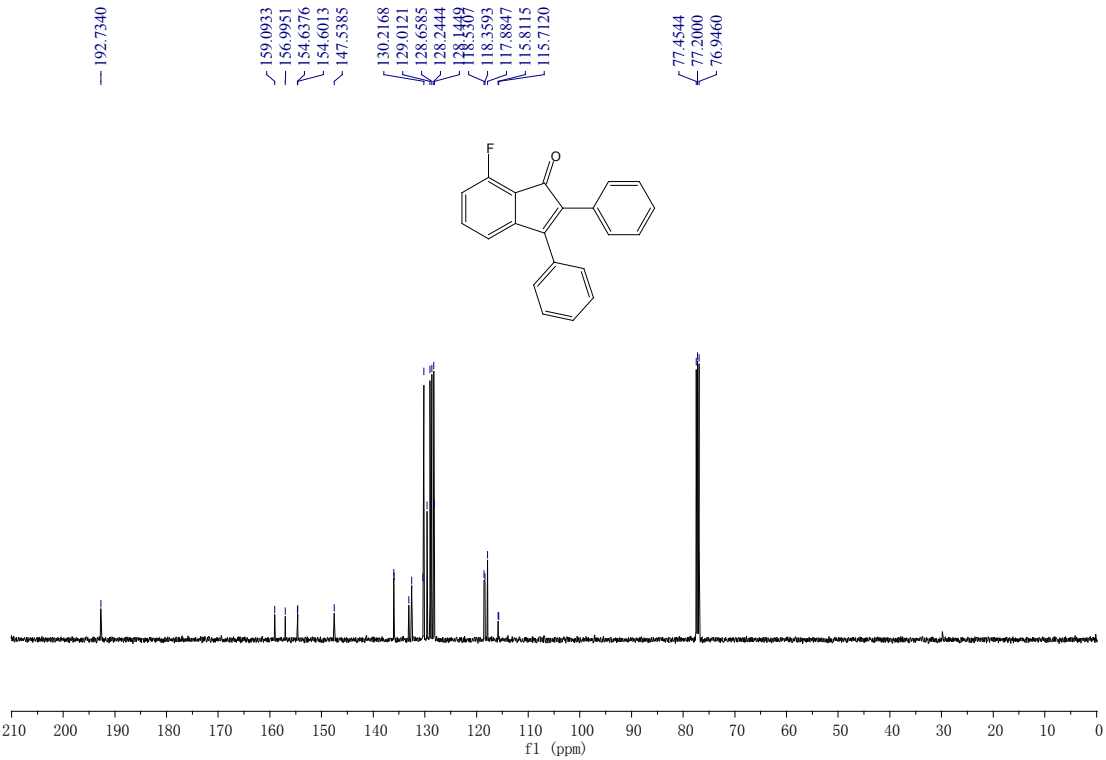
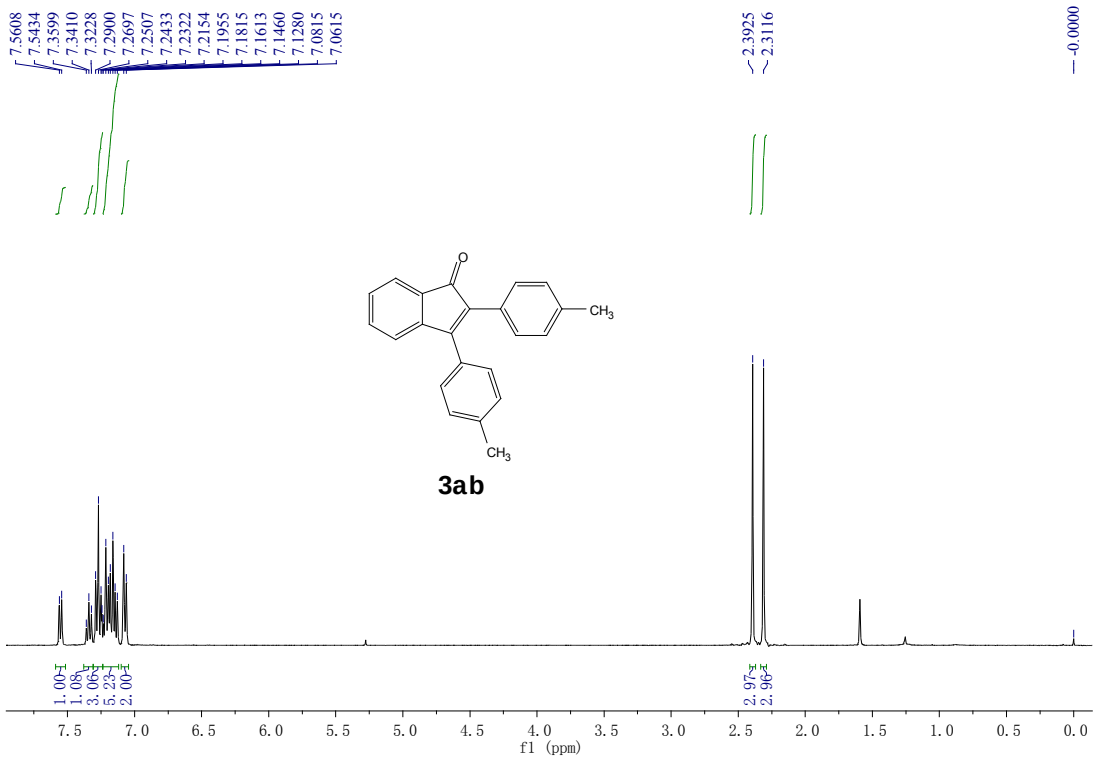
131.4609
131.4041
130.9327
130.9011
130.8700
130.2072
130.1534
129.8937
129.1868
128.5658
128.4623
128.3823
121.2850
119.8685
119.8409
77.2000
76.9460
F
F
F
O
f1 (ppm)


7.4100
7.4018
7.3973
7.3937
7.3504
6.9374
6.9212
6.9157
-0.0000
F
O
3.00
3.02
4.98
2.00
f1 (ppm)

3na

3na


192.7340
159.0933
156.9951
154.6376
154.6013
147.5385
130.2168
129.0121
128.6585
128.2444
118.3593
117.8847
115.8115
115.7120
77.4544
77.2000
76.9460
F
O
f1 (ppm)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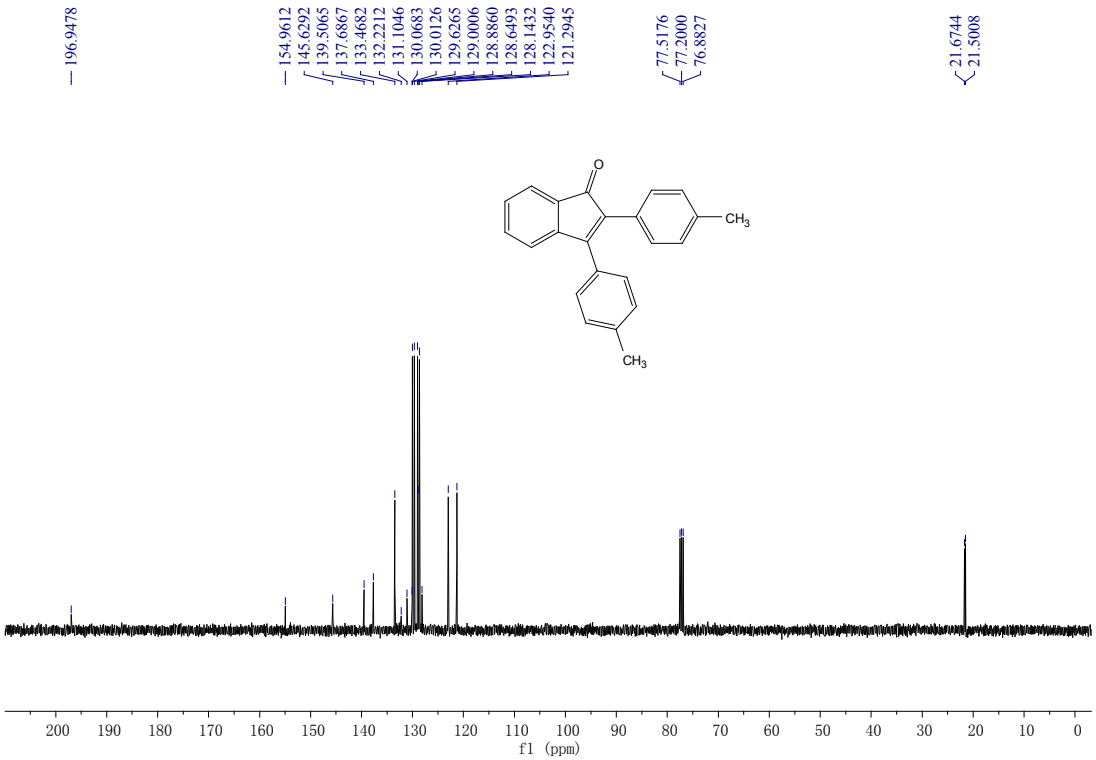
7.3410
7.3228
7.2900
7.2697
7.2507
7.2433
7.2322
7.2154
7.1955
7.1815
7.1613
7.1460
7.1280
7.0815
7.0615
2.3925
2.3116
-0.0000
O
CH3
CH3
1.00
1.08
3.06
5.23
2.00
2.97
2.98
f1 (ppm)

3ab

3ab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137.6867
133.4682
132.2212
131.1046
130.0683
130.0126
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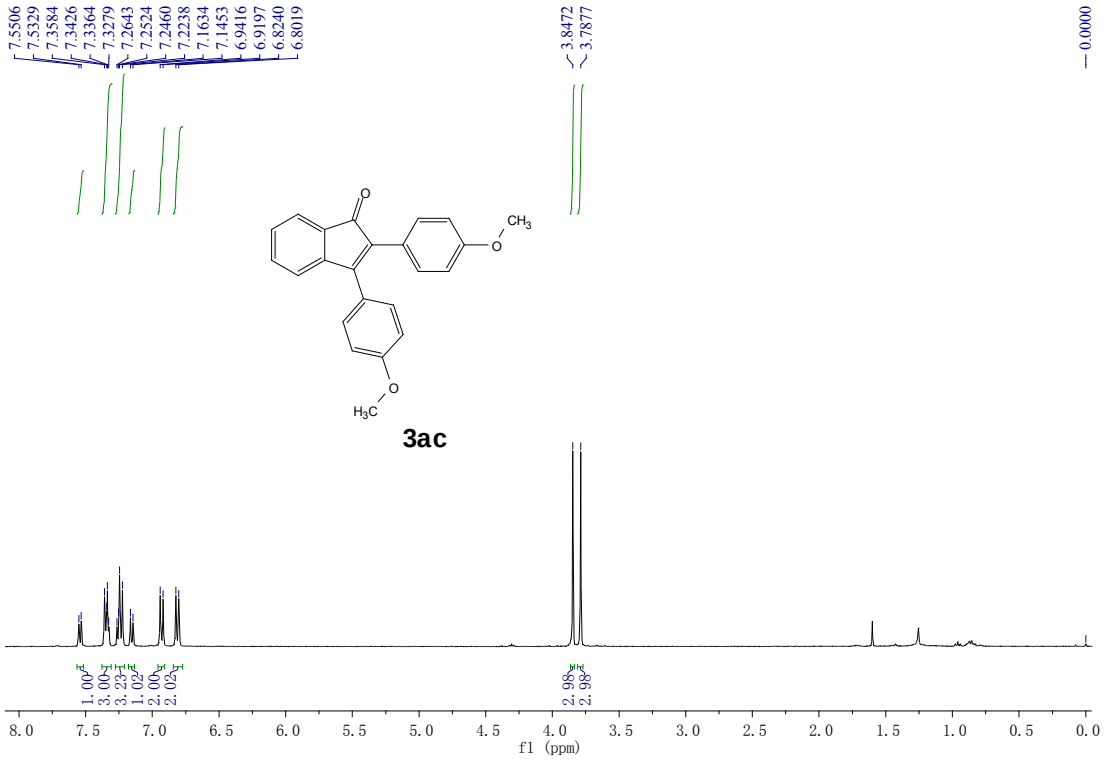
129.0006
128.8860
128.6493
128.1432
122.9540
121.2945
77.5176
77.2000
76.8827
21.6744
21.5008
O
CH3
CH3
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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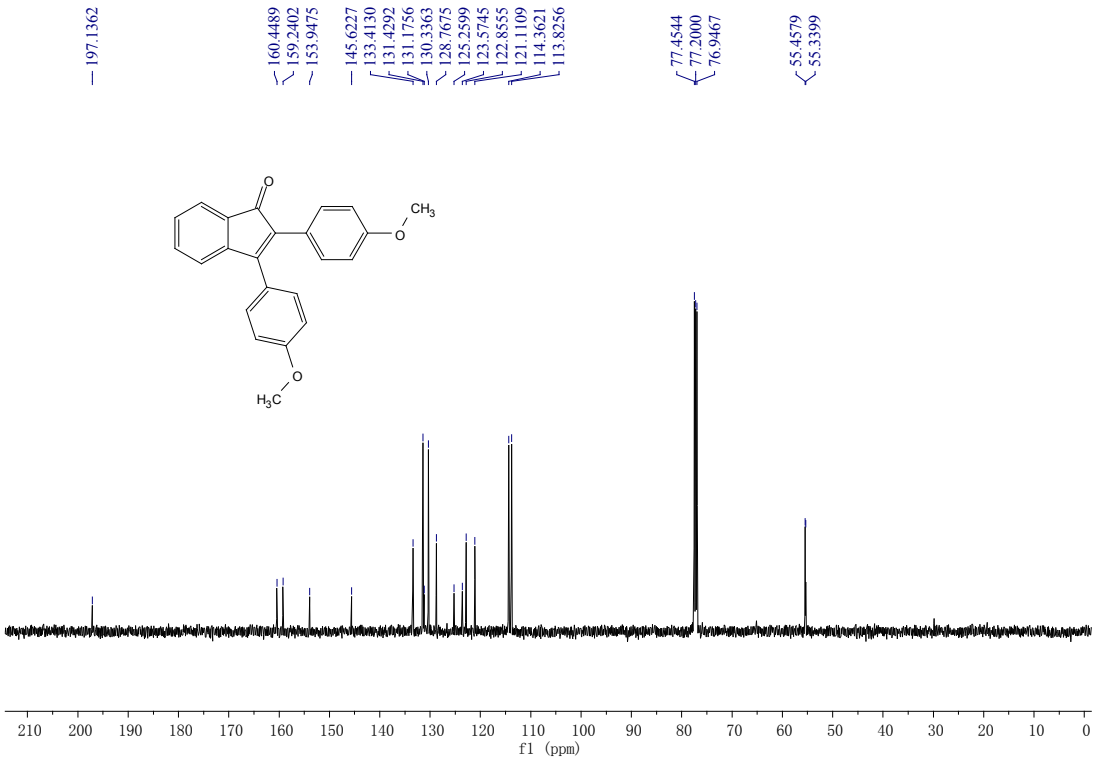
7.3426
7.3364
7.3279
7.2643
7.2524
7.2460
7.2238
7.1634
7.1453
6.9416
6.9197
6.8240
6.8019
3.8472
3.7877
0.0000
O
CH3
O
O
H3C
1.00
3.00
3.23
1.02
2.00
2.02
2.98
2.98
8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

3ac

3ac


197.1362
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159.2402
153.9475
145.6227
133.4130
131.4292
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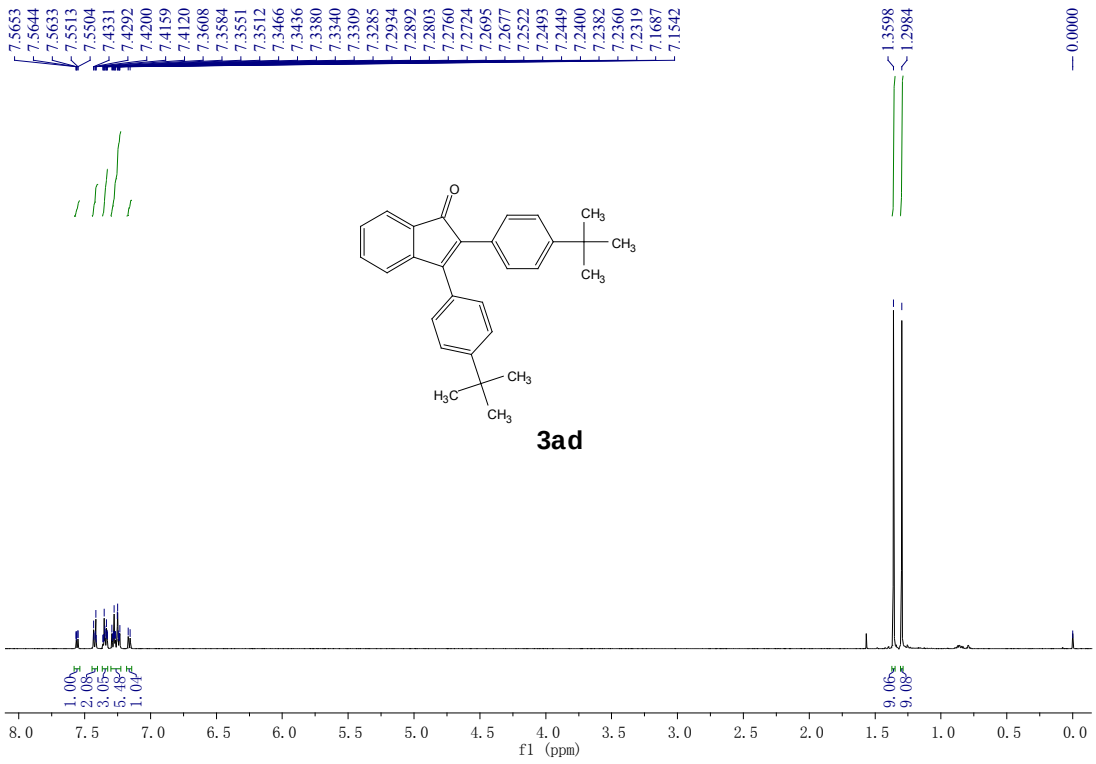
130.3363
128.7675
125.2599
123.5745
122.8555
121.1109
114.3621
113.8256
77.4544
77.2000
76.9467
55.4579
55.3399
O
CH3
O
O
H3C
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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7.4292
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7.4159
7.4120
7.3608
7.3584
7.3551
7.3512
7.3466
7.3436
7.3380
7.3340
7.3309
7.3285
7.2934
7.2892
7.2803
7.2760
7.2724
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7.2677
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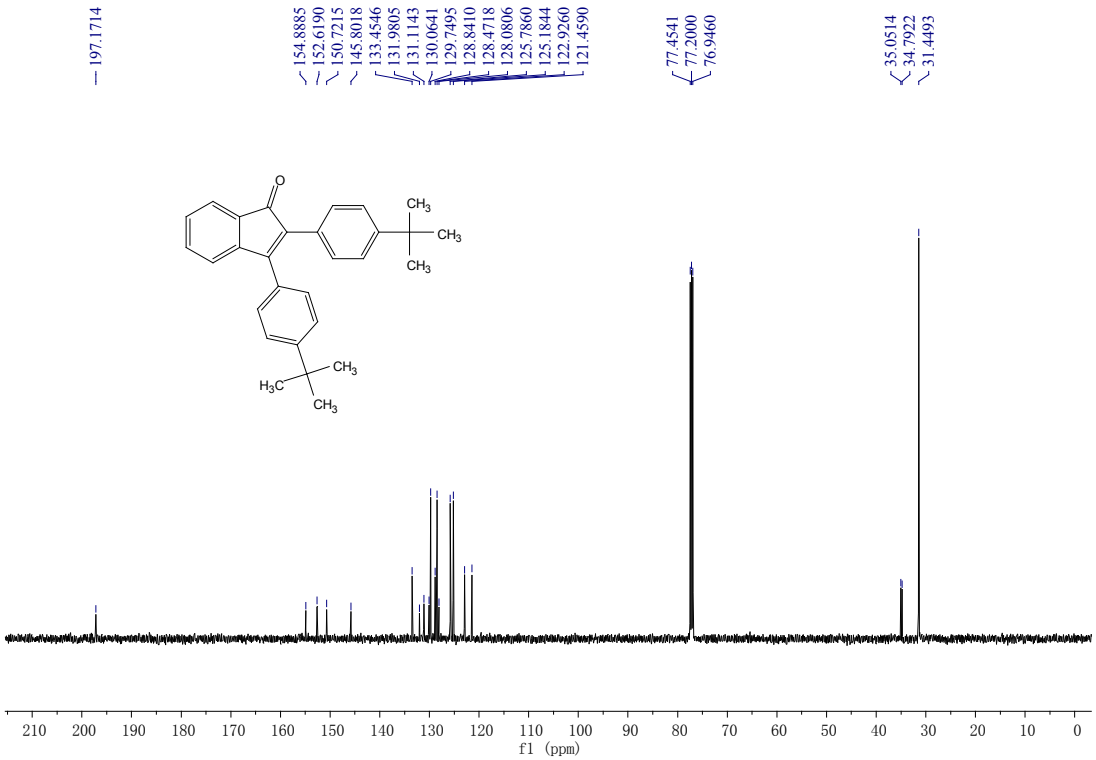
7.2493
7.2449
7.2400
7.2382
7.2360
7.2319
7.1687
7.1542
1.3598
1.2984
0.0000
O
CH3
CH3
CH3
CH3
H3C
CH3
1.00
2.08
3.05
6.48
1.04
9.06
9.08
8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

3ad

3ad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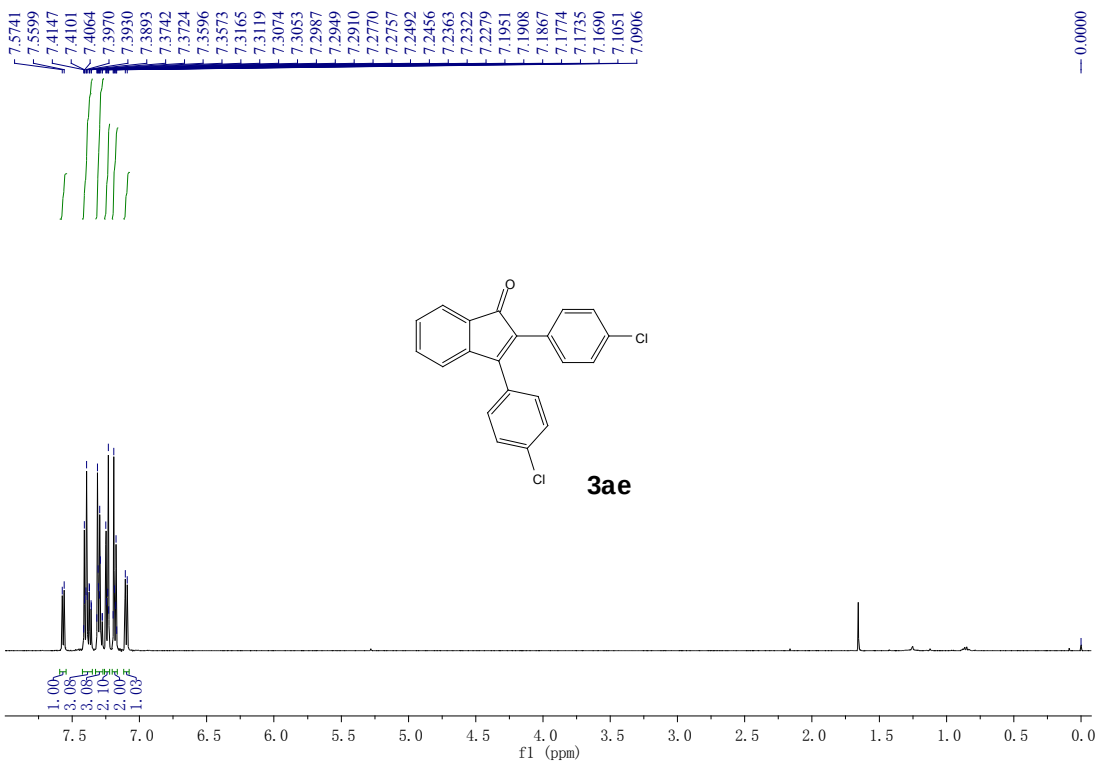
128.8410
128.4718
128.0806
125.7860
125.1844
122.9260
121.4590
77.4541
77.2000
76.9460
35.0514
34.7922
31.4493
O
CH3
CH3
CH3
CH3
H3C
CH3
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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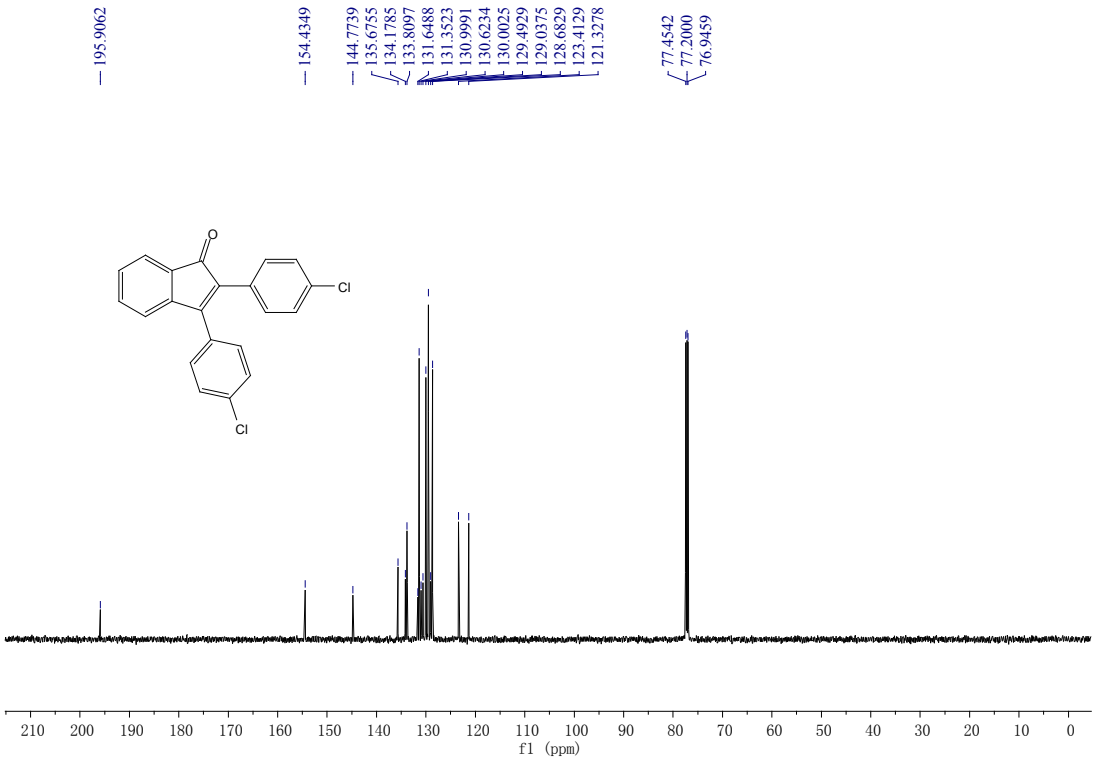
7.3596
7.3573
7.3165
7.3119
7.3074
7.3053
7.2987
7.2949
7.2910
7.2770
7.2757
7.2492
7.2456
7.2363
7.2322
7.2279
7.1951
7.1908
7.1867
7.1774
7.1735
7.1690
7.1051
7.0906
0.0000
O
Cl
Cl
1.00
3.08
3.08
2.10
2.02
1.03
7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

3ae

3ae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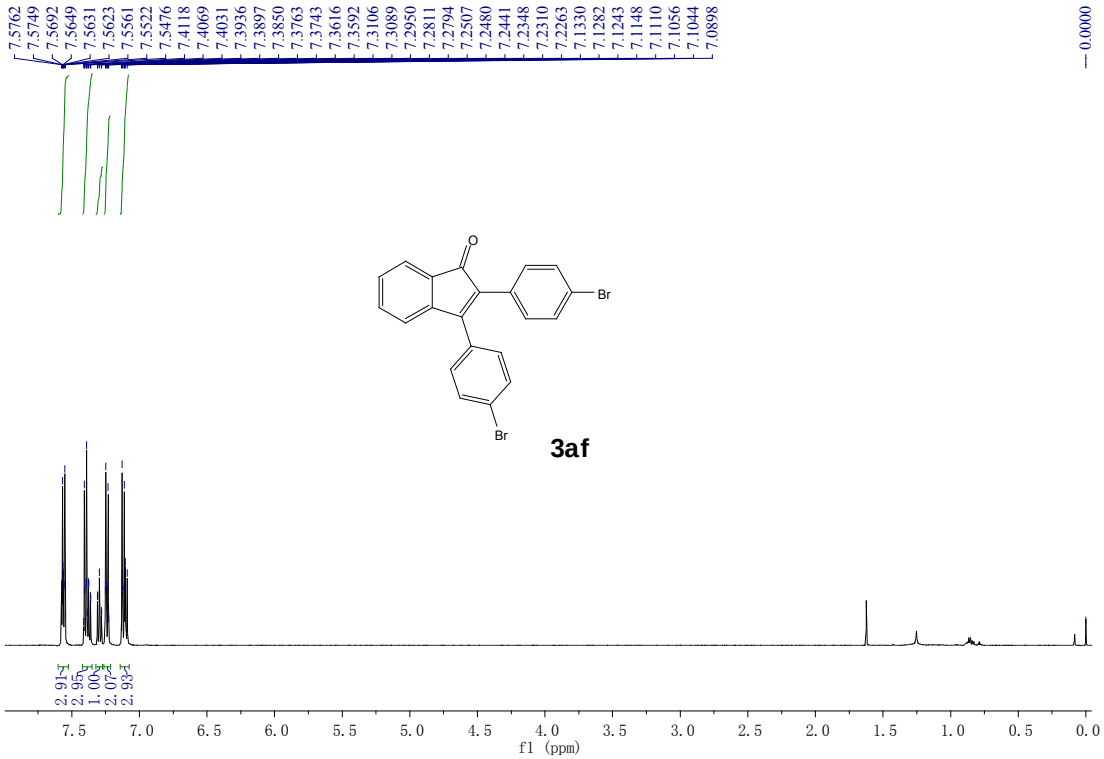
130.0025
129.4929
129.0375
128.6829
123.4129
121.3278
77.4542
77.2000
76.9459
O
Cl
Cl
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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7.5561
7.5522
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7.4031
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7.3897
7.3850
7.3763
7.3743
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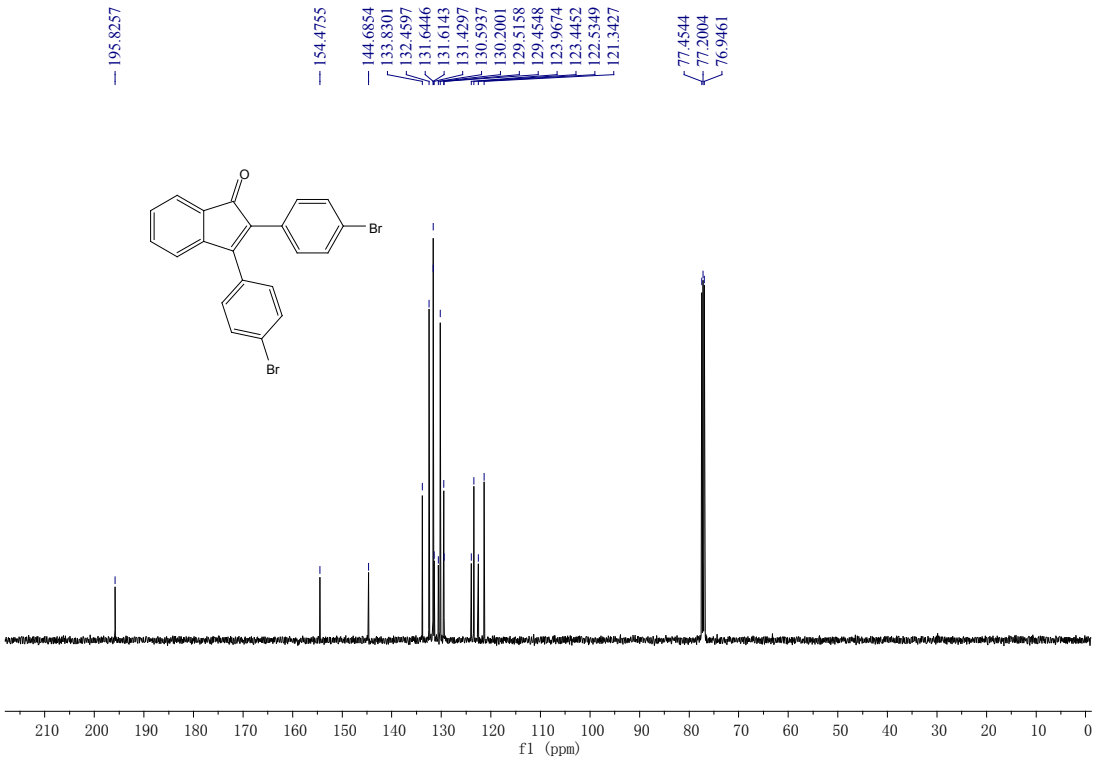
7.3592
7.3106
7.3089
7.2950
7.2811
7.2794
7.2507
7.2480
7.2441
7.2348
7.2310
7.2263
7.1330
7.1282
7.1243
7.1148
7.1110
7.1056
7.1044
7.0898
0.0000
O
Br
Br
2.91
2.95
1.00
2.07
2.93
7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

3af

3af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129.5158
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122.5349
121.3427
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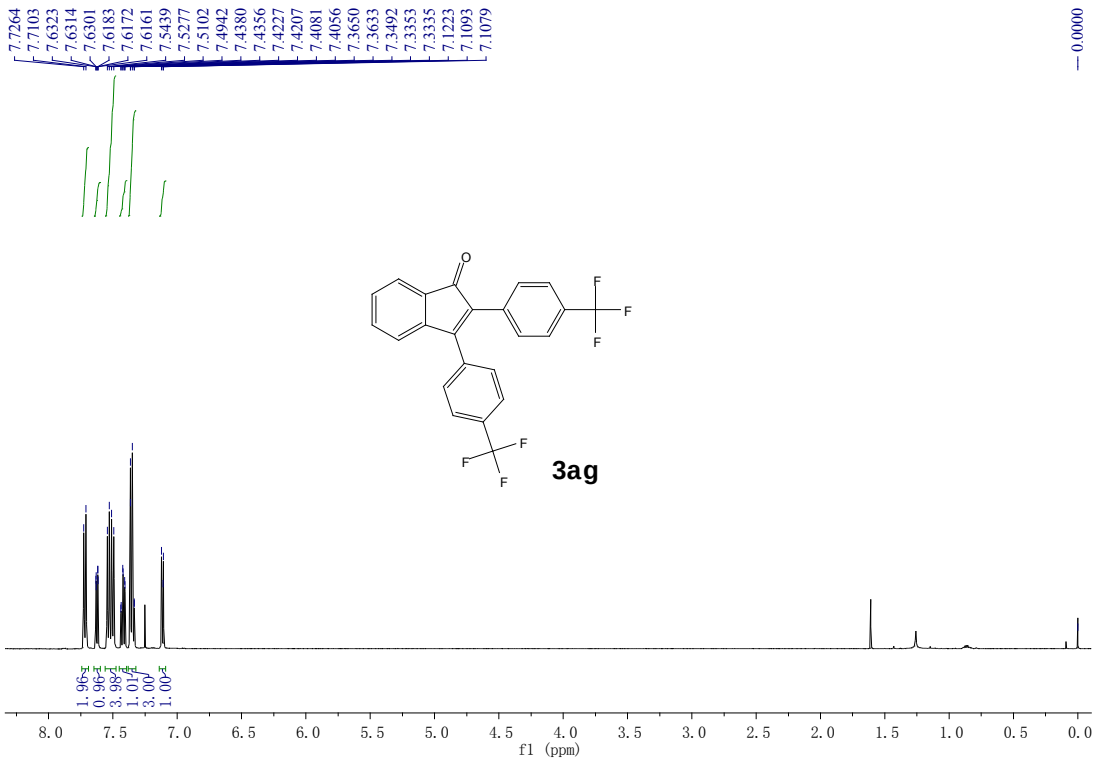
76.9461
O
Br
Br
f1 (ppm)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7.6301
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7.6172
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7.5439
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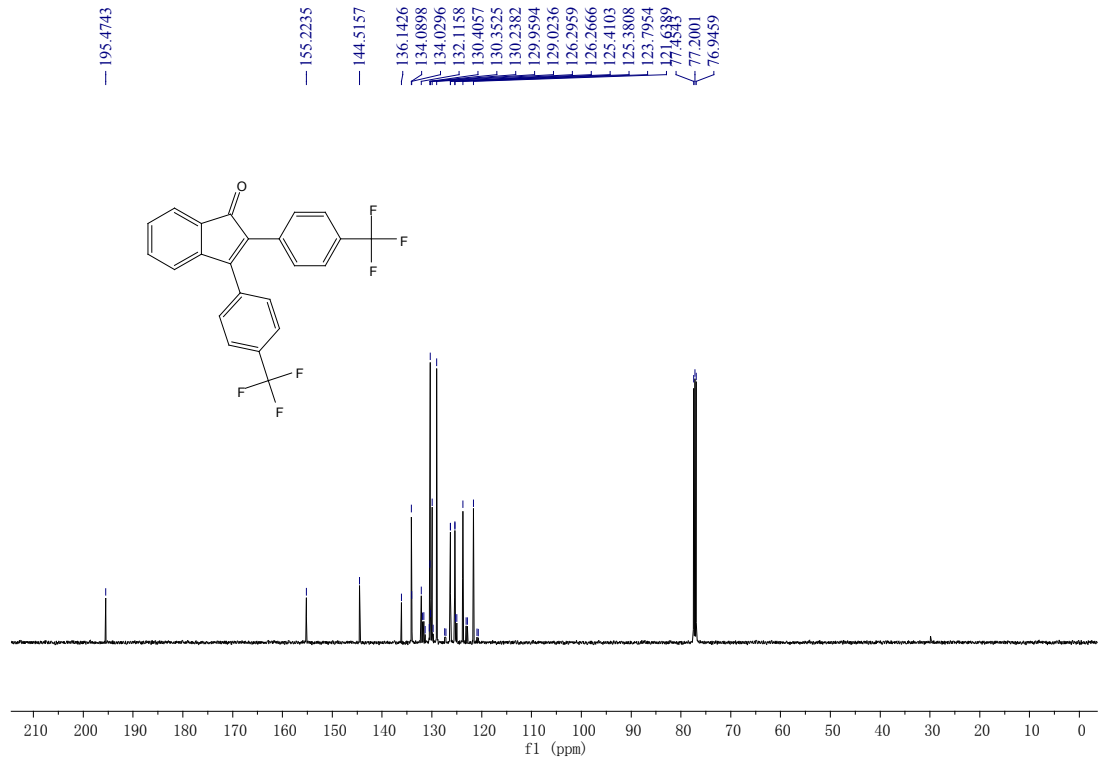
7.4942
7.4380
7.4356
7.4227
7.4207
7.4081
7.4056
7.3650
7.3633
7.3492
7.3353
7.3335
7.1223
7.1093
7.1079
0.0000
O
F
F
F
F
F
F
3ag
1.96
0.96
3.98
1.01
3.00
1.00
f1 (ppm)

3ag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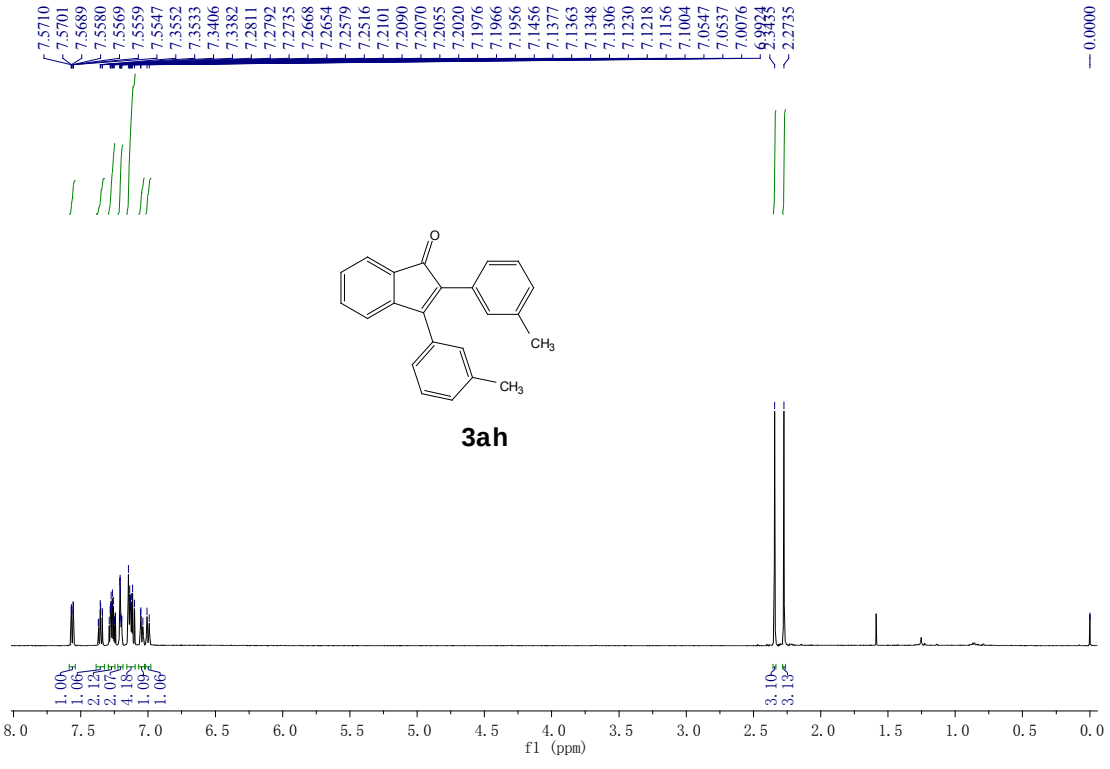
129.9594
129.0236
126.2959
126.2666
125.4103
125.3808
123.7954
121.6389
77.4543
77.2001
76.9459
O
F
F
F
F
F
F
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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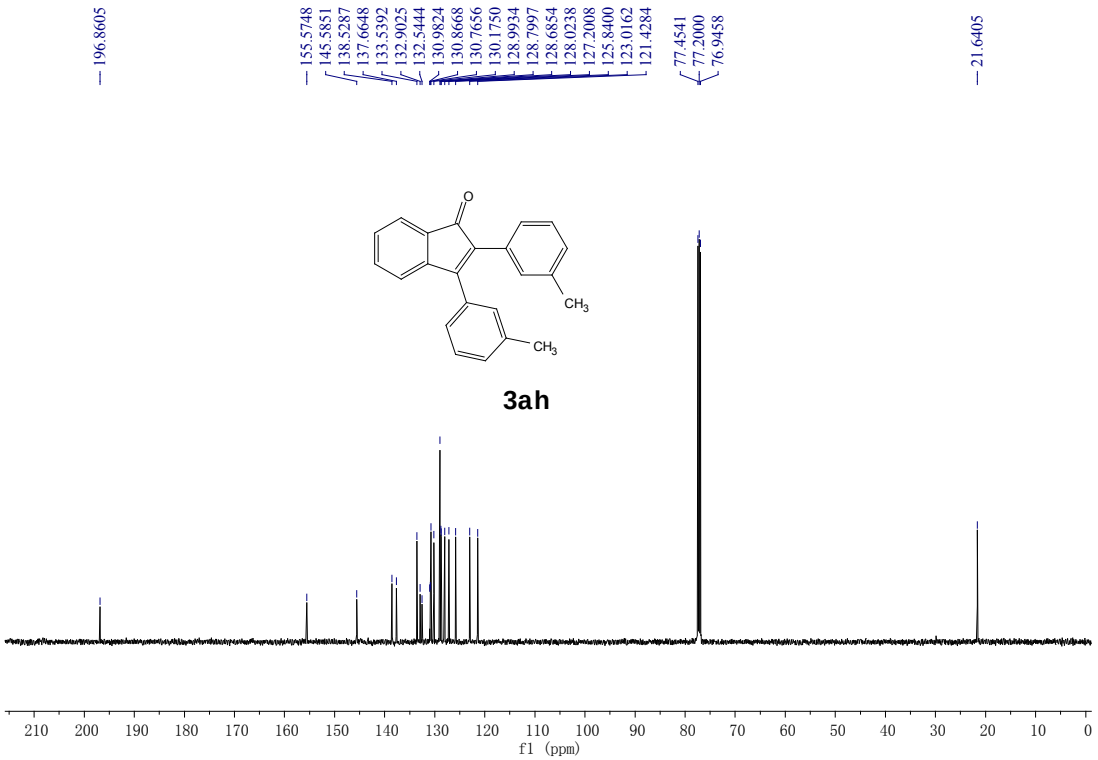
7.3382
7.2811
7.2792
7.2735
7.2668
7.2654
7.2579
7.2516
7.2101
7.2090
7.2070
7.2055
7.2020
7.1976
7.1966
7.1956
7.1456
7.1377
7.1363
7.1348
7.1306
7.1230
7.1218
7.1156
7.1004
7.0547
7.0537
7.0076
6.9924
2.3435
2.2735
0.0000
O
CH3
CH3
1.00
1.06
2.12
2.01
4.18
1.09
1.06
3.10
3.13
8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

3ah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130.7656
130.1750
128.9934
128.7997
128.6854
128.0238
127.2008
125.8400
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77.4541
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O
CH3
CH3
3ah
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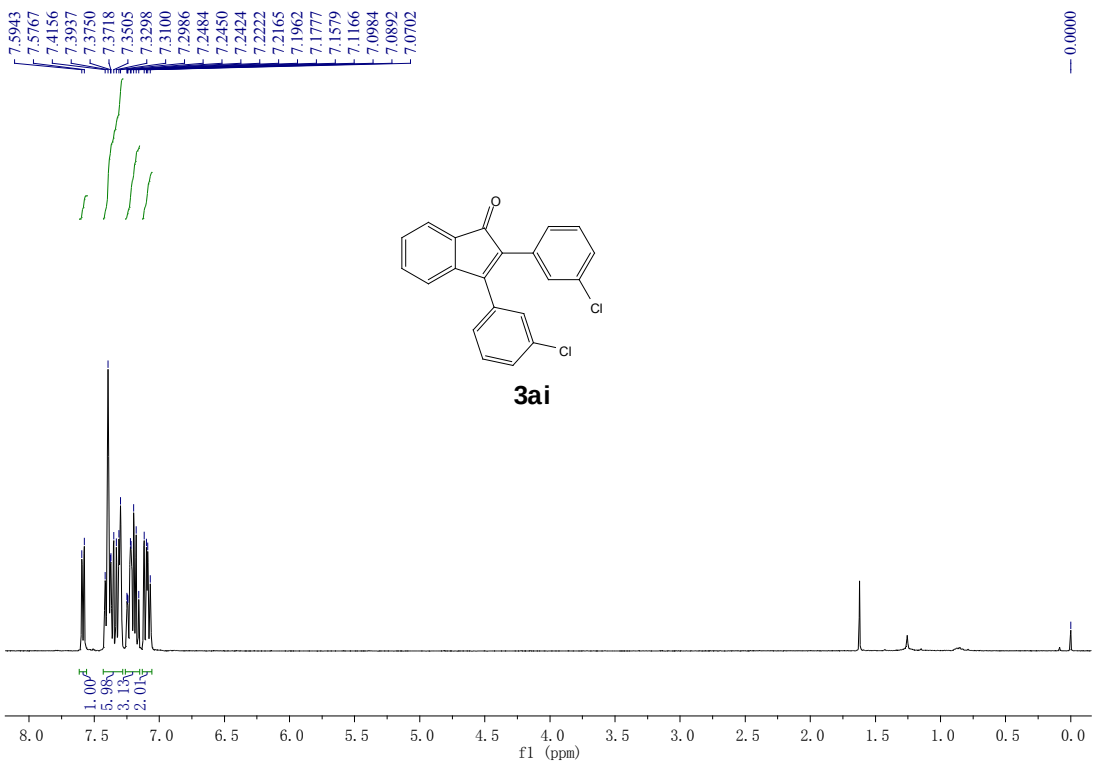
f1 (ppm)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7.3937
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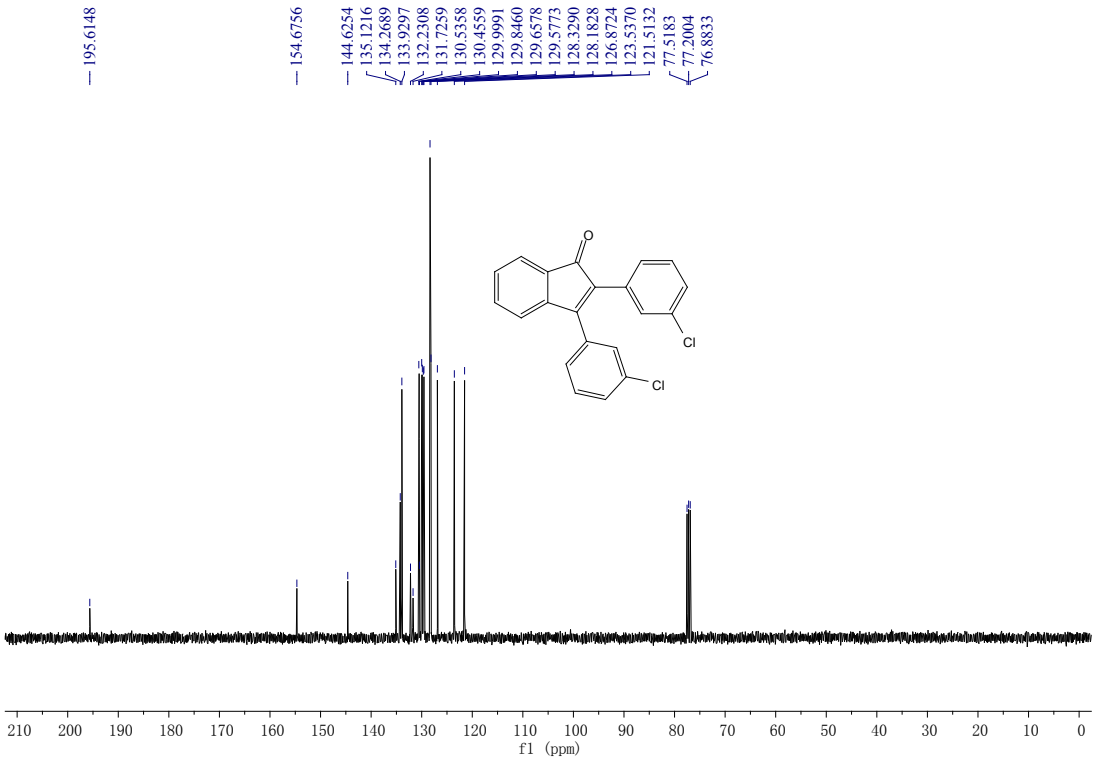
7.2484
7.2450
7.2424
7.2222
7.2165
7.1962
7.1777
7.1579
7.1166
7.0984
7.0892
7.0702
0.0000
O
Cl
Cl
3ai
1.00
5.98
3.15
2.01
8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

3ai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129.8460
129.6578
129.5773
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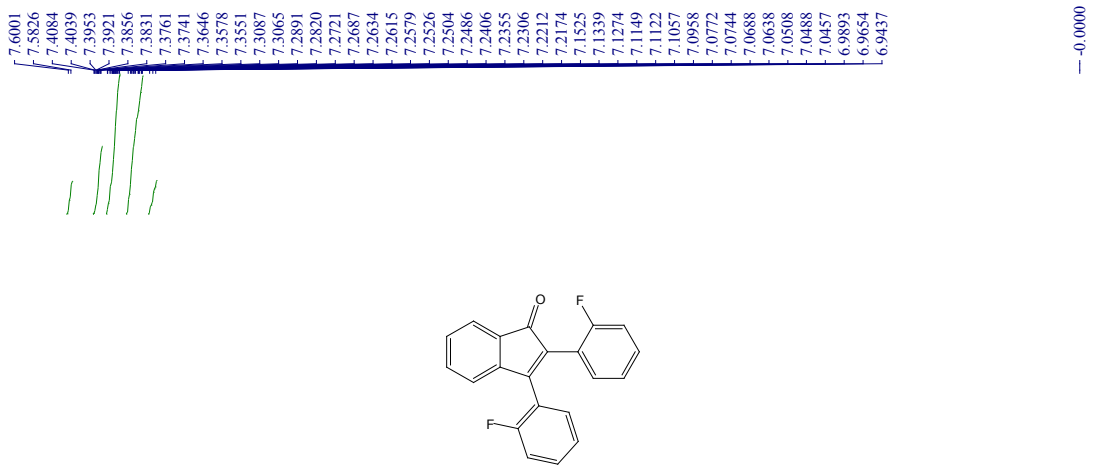
123.5370
121.5132
77.5183
77.2004
76.8833
O
Cl
Cl
f1 (ppm)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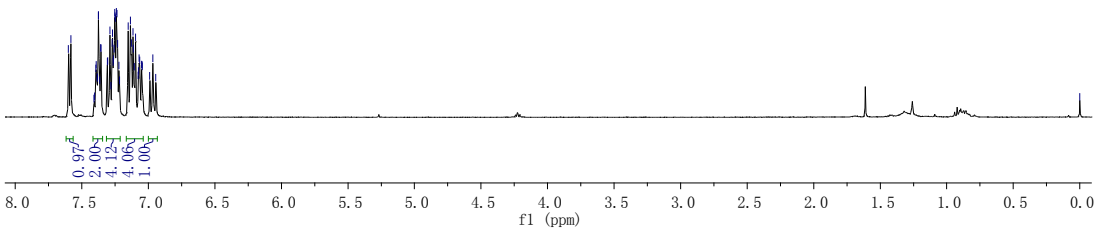
7.3761
7.3741
7.3646
7.3578
7.3551
7.3087
7.3065
7.2891
7.2820
7.2721
7.2687
7.2634
7.2615
7.2579
7.2526
7.2504
7.2486
7.2406
7.2355
7.2306
7.2212
7.2174
7.1525
7.1339
7.1274
7.1149
7.1122
7.1057
7.0958
7.0772
7.0744
7.0688
7.0638
7.0508
7.0488
7.0457
6.9893
6.9654
6.9437
-0.0000
O
F
F

3aj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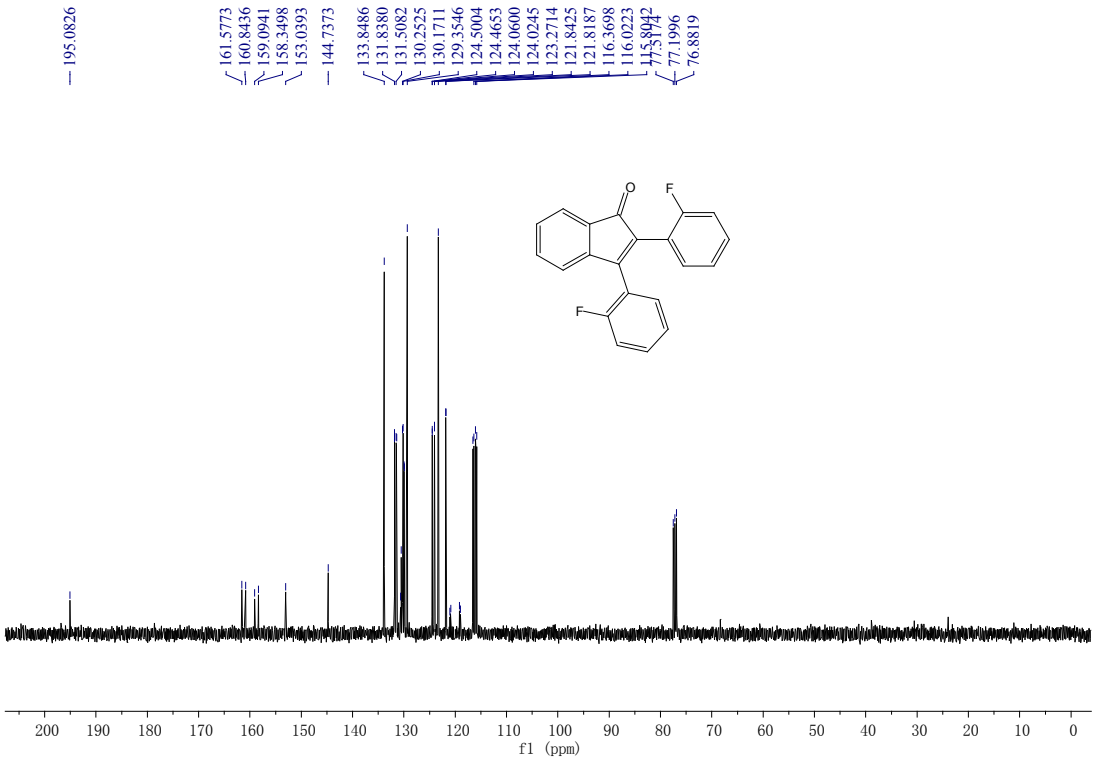
2.00
4.12
4.06
1.00
f1 (ppm)

3aj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158.3498
153.0393
144.7373
133.8486
131.8380
131.5082
130.2525
130.1711
129.3546
124.5004
124.4653
124.0600
124.0245
123.2714
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121.8187
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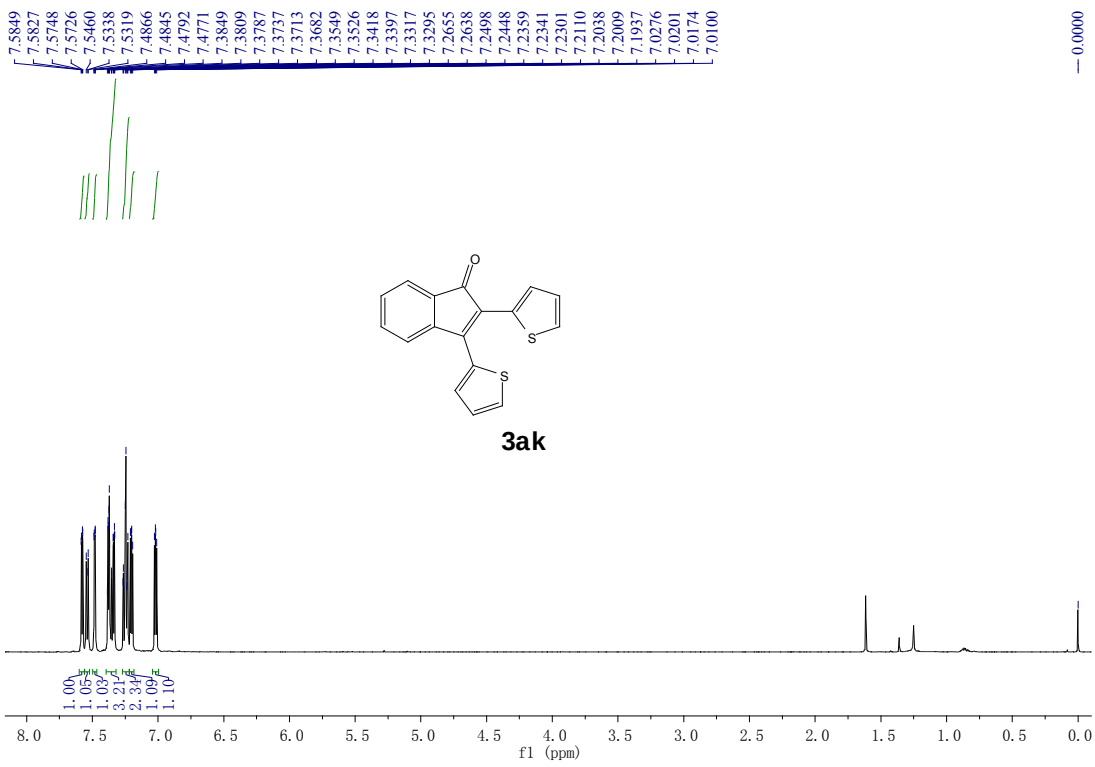
116.0223
115.8042
77.3174
77.1996
76.8819
O
F
F
f1 (ppm)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7.4845
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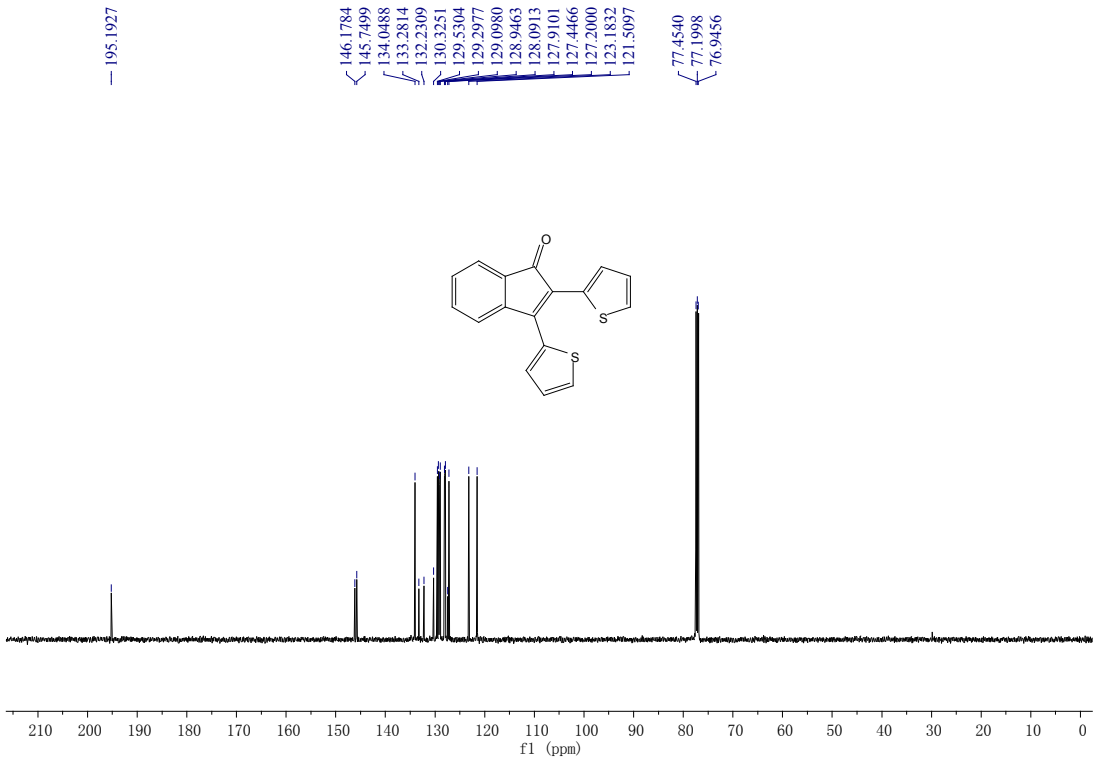
7.4771
7.3849
7.3809
7.3787
7.3737
7.3713
7.3682
7.3549
7.3526
7.3418
7.3397
7.3317
7.3295
7.2655
7.2638
7.2498
7.2448
7.2359
7.2341
7.2301
7.2110
7.2038
7.2009
7.1937
7.0276
7.0201
7.0174
7.0100
0.0000
1.00
1.05
1.03
3.21
2.34
1.09
1.10
f1 (ppm)

O
S
S

3ak

3ak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133.2814
132.2309
130.3251
129.5304
129.2977
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128.9463
128.0913
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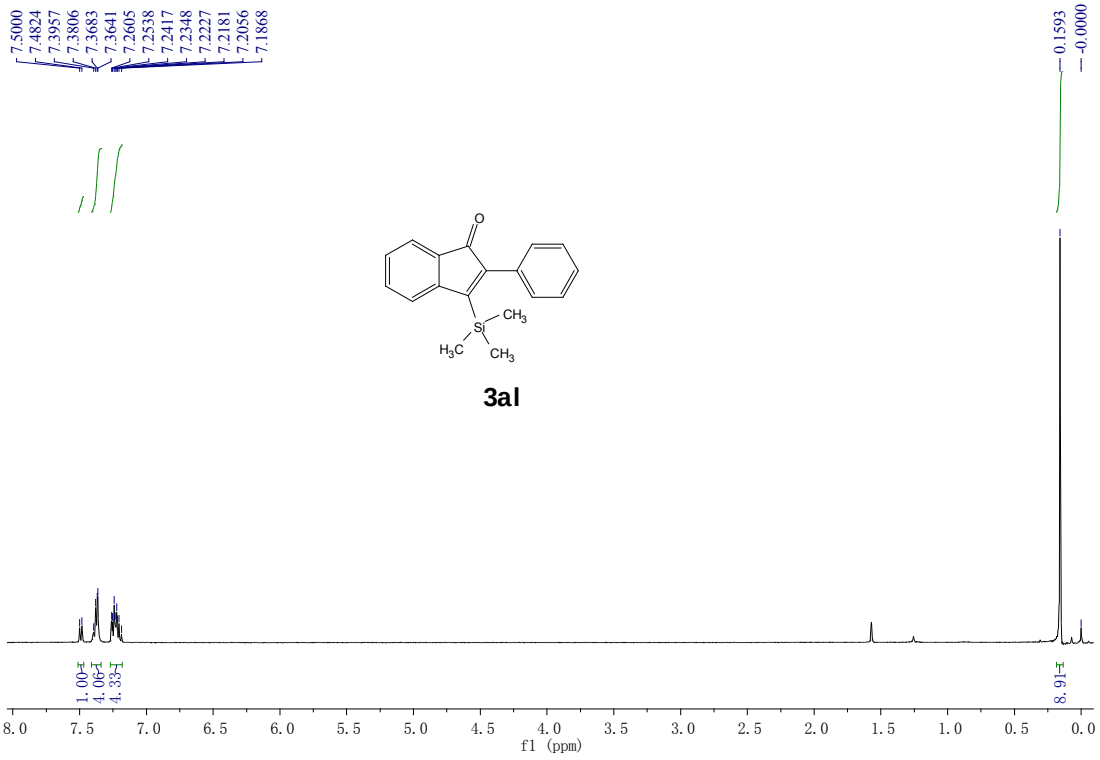
127.2000
123.1832
121.5097
77.4540
77.1998
76.9456
O
S
S
f1 (ppm)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7.3957
7.3806
7.3683
7.3641
7.2605
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7.2417
7.2348
7.2227
7.2181
7.2056
7.1868
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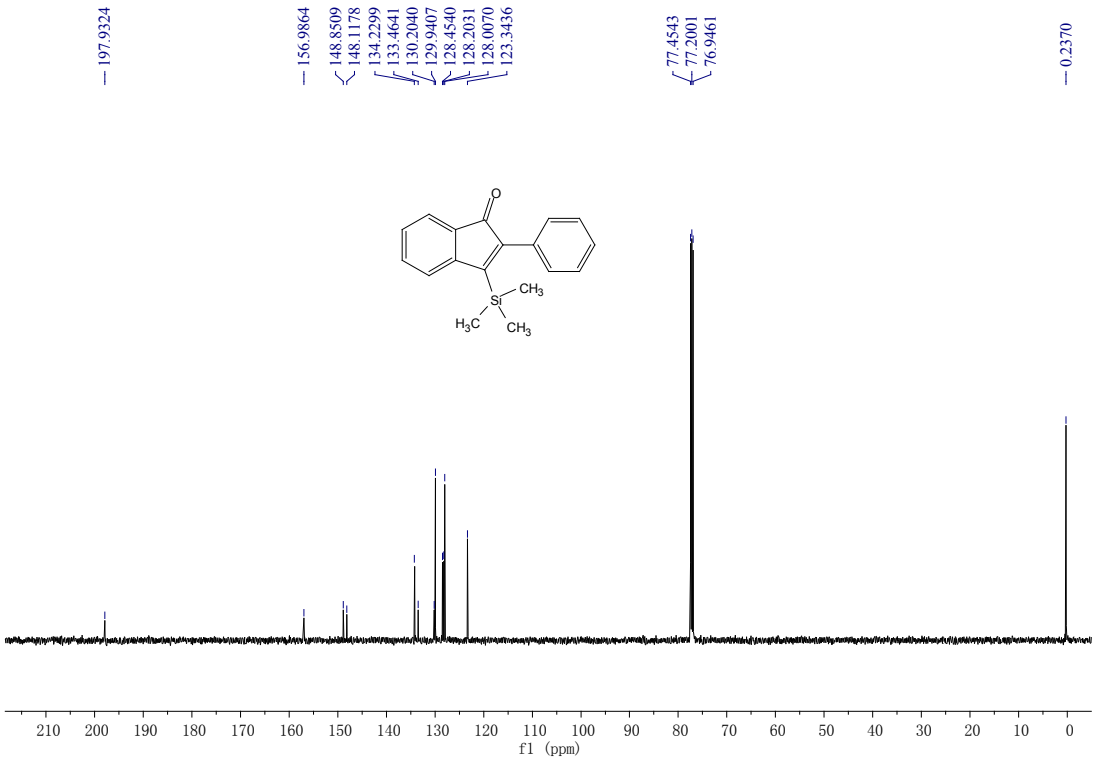
O
CH3
Si
H3C
CH3
1.00
4.06
4.33
8.91
f1 (ppm)

3al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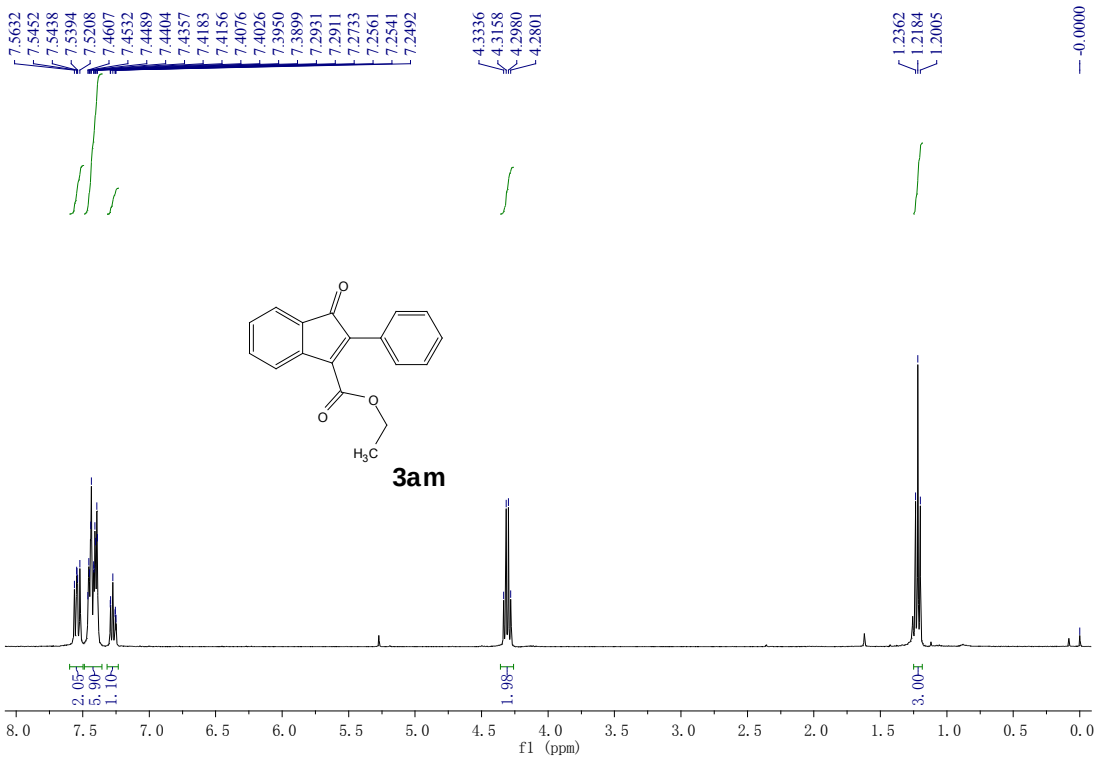
148.1178
134.2299
133.4641
130.2040
129.9407
128.4540
128.2031
128.0070
123.3436
77.4543
77.2001
76.9461
0.2370
O
Si
CH3
H3C
CH3
f1 (ppm)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7.5438
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7.5208
7.4607
7.4532
7.4489
7.4404
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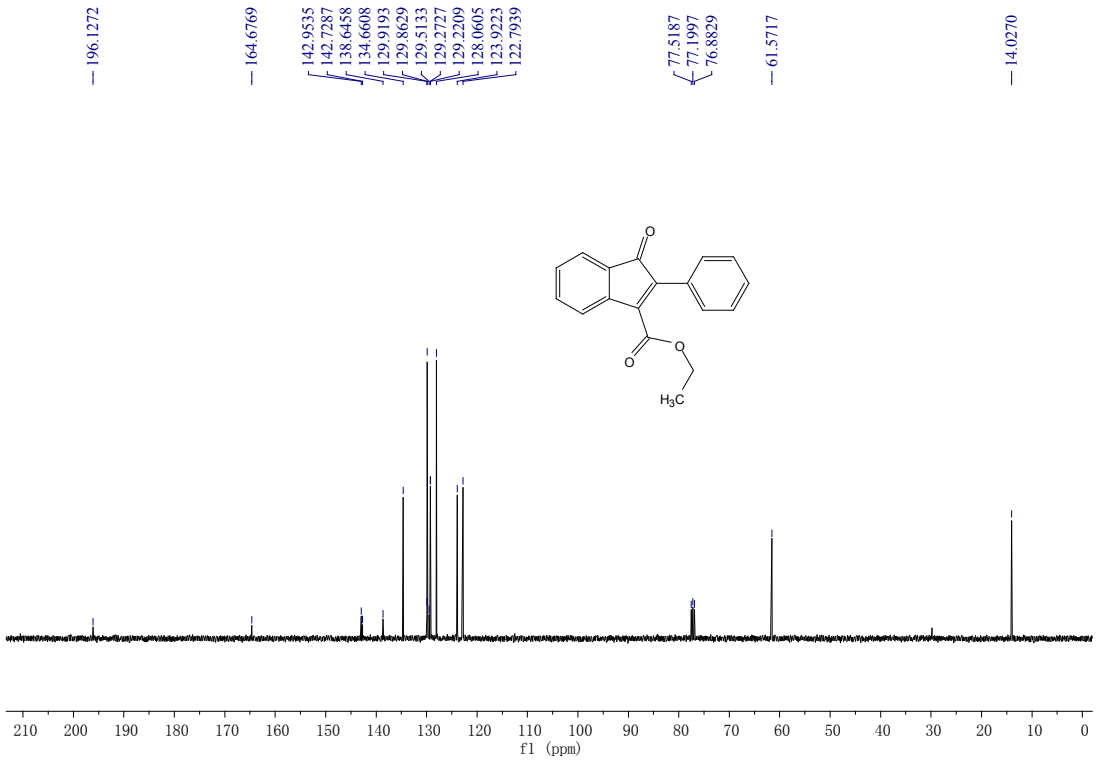
7.4183
7.4156
7.4076
7.4026
7.3950
7.3899
7.2931
7.2911
7.2733
7.2561
7.2541
7.2492
4.3336
4.3158
4.2980
4.2801
1.2362
1.2184
1.2005
-0.0000
O
O
O
H3C
2.05
5.90
1.10
1.98
3.00
f1 (ppm)

3am

3am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129.2209
128.0605
123.9223
122.7939
77.5187
77.1997
76.8829
61.5717
14.0270
O
O
O
H3C
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)