Electronic Supplementary Material (ESI) for ChemComm.

Supporting Information

Synthesis of dihydroquinolinones via iridium-catalyzed cascade C-H amidation and intramolecular aza-Michael addition

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1. General experimental details

General Information: All chemicals were used as received without further purification unless stated otherwise. NMR spectra were recorded at ambient temperature on a 400 MHz NMR spectrometer. Chemical shifts (δ) are given in ppm relative to TMS, the coupling constants *J* are given in Hz. HRMS were recorded on a TOF LC/MS equipped with electrospray ionization (ESI) probe operating in positive or negative ion mode.

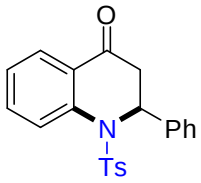
The synthesis of chalcones: According to the literature,[1] all chalcones were synthesized from commercially available aryl ketones and aldehydes and used without further purification.

Typical procedure for the synthesis of 3aa: Under N_2, the mixture of **1a** (0.2 mmol, 41.6 mg), **2a** (0.4 mmol, 78.8 mg), $[Cp^*IrCl_2]_2$ (5 mol%, 7.9 mg), $AgNTf_2$ (20 mol%, 15.5 mg), PivOH (0.2 mmol, 20.4 mg) and DCM (2 mL) were added into the tube and sealed. The mixture was stirred at 120 ^oC for 12 h. Then, the solvent was evaporated under reduced pressure and the residue was purified by flash column chromatography on silica gel (petroleum ether/ethyl acetate 5/1) gave a pale yellow solid (58.1 mg, 77%).

[1] L. C. C. Vieira, B. T. Matsuo, L. S. R. Martelli, M. Gall, M. W. Paixão and A. G. Corrêa, *Org. Biomol. Chem.*, 2017, **15**, 6098.

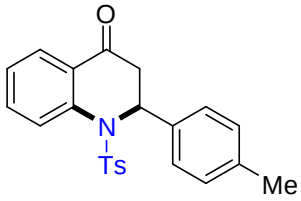
2. Characterization data of the products

2-phenyl-1-tosyl-2,3-dihydroquinolin-4(1H)-one (3aa)[2]



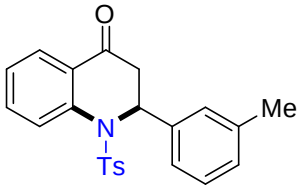
Flash column chromatography on silica gel (petroleum ether/ethyl acetate 5/1) gave a pale yellow solid (58.1 mg, 77%). R_f = 0.36 (Silica gel, petroleum/ethyl acetate = 5:1). ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.90 (d, *J* = 8.2 Hz, 1H), 7.86 (dd, *J* = 7.8, 1.6 Hz, 1H), 7.60 (d, *J* = 8.3 Hz, 2H), 7.56-7.51 (m, 1H), 7.31-7.18 (m, 8H), 5.95 (d, *J* = 5.6 Hz, 1H), 3.05-2.99 (m, 1H), 2.66-2.59 (m, 1H), 2.41 (s, 3H). ^{13}C NMR ($CDCl_3$, 100 MHz): δ 192.0, 144.6, 140.0, 137.6, 136.5, 135.0, 130.1, 128.6, 127.8, 127.1, 126.9, 126.8, 126.1, 125.8, 125.7, 57.7, 39.4, 21.6.

2-p-tolyl-1-tosyl-2,3-dihydroquinolin-4(1H)-one (3ba)[2]



Flash column chromatography on silica gel (petroleum ether/ethyl acetate 5/1) gave a pale yellow solid (58.6 mg, 75%). R_f = 0.34 (Silica gel, petroleum/ethyl acetate = 5:1). ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.90-7.85 (m, 2H), 7.60 (d, *J* = 8.3 Hz, 2H), 7.55-7.50 (m, 1H), 7.26 (d, *J* = 8.1 Hz, 2H), 7.21-7.17 (m, 3H), 7.03 (d, *J* = 8.1 Hz, 2H), 5.91 (d, *J* = 5.7 Hz, 1H), 3.02-2.97 (m, 1H), 2.63-2.57 (m, 1H), 2.41 (s, 3H), 2.24 (s, 3H). ^{13}C NMR ($CDCl_3$, 100 MHz): δ 192.4, 144.8, 140.2, 137.7, 136.8, 135.2, 134.8, 130.3, 129.4, 127.2, 127.1, 126.9, 126.3, 126.1, 125.9, 57.7, 39.6, 21.8, 21.1.

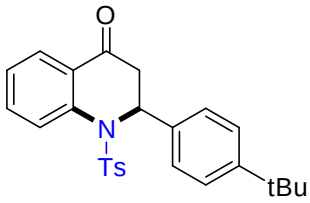
2-m-tolyl-1-tosyl-2,3-dihydroquinolin-4(1H)-one (3ca)[2]



Flash column chromatography on silica gel (petroleum ether/ethyl acetate 5/1) gave a white solid (61.8 mg, 79%). R_f = 0.32 (Silica gel, petroleum/ethyl acetate = 5:1). ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.91 (d, *J* = 8.3 Hz, 2H), 7.86 (dd, *J* = 7.8, 1.6 Hz, 1H), 7.60 (d, *J* = 8.3 Hz, 2H), 7.55-7.50 (m, 1H), 7.25 (d, *J* = 8.0 Hz, 2H), 7.21-7.17 (m, 1H), 7.12-7.05 (m, 3H), 6.98 (d, *J* = 7.1 Hz, 1H), 5.91 (d, *J* = 5.5 Hz, 1H), 3.04-2.99 (m, 1H), 2.64-2.58 (m, 1H), 2.40 (s, 3H), 2.25 (s, 3H). ^{13}C NMR ($CDCl_3$, 100 MHz): δ 192.3, 144.8, 140.3, 138.5, 137.8, 136.8, 135.2, 130.3, 128.8, 128.6, 127.9, 127.2, 127.1, 126.3, 126.1, 125.9, 124.0, 57.8, 39.6, 21.7, 21.6.

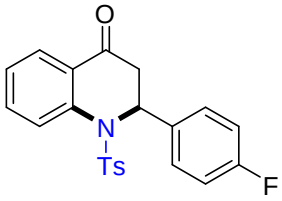
2-(4-*tert*-butylphenyl)-1-tosyl-2,3-dihydroquinolin-4(1*H*)-one (3da)

[2] X. Liu and Y. Lu, *Org. Lett.*, 2010, **12**, 5592.



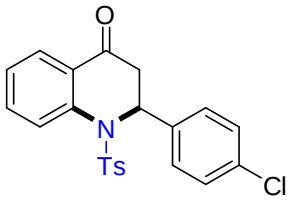
Flash column chromatography on silica gel (petroleum ether/ethyl acetate 5/1) gave a yellow liquid (73.6 mg, 85%). R_f = 0.37 (Silica gel, petroleum/ethyl acetate = 5:1). ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.93 (d, *J* = 8.2 Hz, 1H), 7.87 (dd, *J* = 7.8, 1.6 Hz, 1H), 7.61 (d, *J* = 8.3 Hz, 2H), 7.54-7.50 (m, 1H), 7.26-7.16 (m, 7H), 5.93 (d, *J* = 5.2 Hz, 1H), 3.04-2.99 (m, 1H), 2.67-2.61 (m, 1H), 2.39 (s, 3H), 1.23 (s, 9H). ^{13}C NMR ($CDCl_3$, 100 MHz): δ 192.3, 150.8, 144.7, 140.4, 136.8, 135.2, 134.8, 130.3, 127.3, 127.1, 126.7, 126.2, 126.0, 125.8, 125.7, 57.7, 39.8, 31.3, 21.8. HRMS (ESI) *m/z* calcd for $C_{26}H_{28}NO_3S$ $(M+H)^+$ 434.1784, found 434.1791.

2-(4-fluorophenyl)-1-tosyl-2,3-dihydroquinolin-4(1H)-one (3ea)



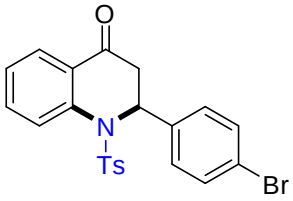
Flash column chromatography on silica gel (petroleum ether/ethyl acetate 5/1) gave a yellow liquid (57.8 mg, 73%). R_f = 0.32 (Silica gel, petroleum/ethyl acetate = 5:1). ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.91-7.85 (m, 2H), 7.60-7.52 (m, 3H), 7.29-7.18 (m, 5H), 6.91 (t, *J* = 8.6 Hz, 1H), 5.91 (d, *J* = 5.8 Hz, 1H), 2.99-2.95 (m, 1H), 2.64-2.58 (m, 1H), 2.41 (s, 3H). ^{13}C NMR ($CDCl_3$, 100 MHz): δ 192.0, 162.4 (d, $J_{C\text{-}F}$ = 246.4 Hz), 144.9, 140.0, 136.6, 135.3, 133.6 (d, $J_{C\text{-}F}$ = 3.4 Hz), 130.4, 128.9 (d, $J_{C\text{-}F}$ = 8.2 Hz), 127.3, 127.1, 126.3, 126.0, 125.9, 115.7 (d, $J_{C\text{-}F}$ = 21.5 Hz), 57.4, 39.6, 21.8. HRMS (ESI) *m/z* calcd for $C_{22}H_{19}FNO_3S$ $(M+H)^+$ 396.1064, found 396.1066.

2-(4-chlorophenyl)-1-tosyl-2,3-dihydroquinolin-4(1H)-one (3fa)[2]



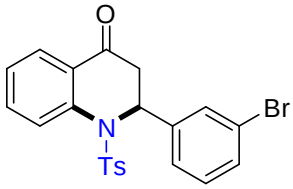
Flash column chromatography on silica gel (petroleum ether/ethyl acetate 5/1) gave a pale yellow solid (61.8 mg, 75%). R_f = 0.3 (Silica gel, petroleum/ethyl acetate = 5:1). ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.91-7.84 (m, 2H), 7.60-7.52 (m, 3H), 7.27-7.18 (m, 7H), 5.90 (d, *J* = 5.4 Hz, 1H), 2.99-2.95 (m, 1H), 2.64-2.58 (m, 1H), 2.40 (s, 3H). ^{13}C NMR ($CDCl_3$, 100 MHz): δ 191.9, 145.0, 139.9, 136.5, 136.4, 135.4, 134.0, 130.4, 128.9, 128.5, 127.3, 127.1, 126.3, 126.1, 125.9, 57.4, 39.4, 21.8.

2-(4-bromophenyl)-1-tosyl-2,3-dihydroquinolin-4(1H)-one (3ga)[2]



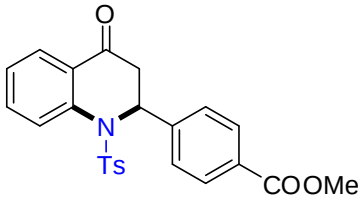
Flash column chromatography on silica gel (petroleum ether/ethyl acetate 5/1) gave a pale yellow solid (63.7 mg, 70%). R_f = 0.28 (Silica gel, petroleum/ethyl acetate = 5:1). ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.92 (d, *J* = 8.3 Hz, 1H), 7.86 (dd, *J* = 7.8, 1.6 Hz, 1H), 7.59-7.52 (m, 3H), 7.35 (d, *J* = 8.5 Hz, 2H), 7.27-7.17 (m, 5H), 5.90 (d, *J* = 5.5 Hz, 1H), 2.99-2.94 (m, 1H), 2.64-2.58 (m, 1H), 2.41 (s, 3H). ^{13}C NMR ($CDCl_3$, 100 MHz): δ 191.8, 145.0, 139.9, 136.9, 136.5, 135.4, 131.9, 130.4, 128.8, 127.3, 127.1, 126.3, 126.1, 125.9, 122.2, 57.4, 39.4, 21.8.

2-(3-bromophenyl)-1-tosyl-2,3-dihydroquinolin-4(1*H*)-one (3ha)



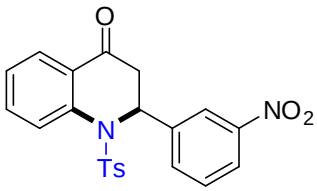
Flash column chromatography on silica gel (petroleum ether/ethyl acetate 5/1) gave a yellow solid (65.5 mg, 72%). m.p. 168-169 °C. R_f = 0.32 (Silica gel, petroleum/ethyl acetate = 5:1). ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.92 (d, *J* = 8.3 Hz, 1H), 7.86 (dd, *J* = 7.8, 1.6 Hz, 1H), 7.59-7.53 (m, 3H), 7.45 (s, 1H), 7.32-7.19 (m, 5H), 7.08 (t, *J* = 7.9 Hz, 1H), 5.90 (d, *J* = 5.6 Hz, 1H), 2.99-2.94 (m, 1H), 2.64-2.58 (m, 1H), 2.40 (s, 3H). ^{13}C NMR ($CDCl_3$, 100 MHz): δ 191.6, 145.1, 140.2, 139.9, 136.4, 135.4, 131.3, 130.4, 130.3, 127.4, 127.1, 126.3, 126.2, 125.9, 125.5, 123.1, 57.4, 39.4, 21.8. HRMS (ESI) *m/z* calcd for $C_{22}H_{19}BrNO_3S$ $(M+H)^+$ 456.0264, found 456.0268.

methyl 4-(4-oxo-1-tosyl-1,2,3,4-tetrahydroquinolin-2-yl)benzoate (3ia)



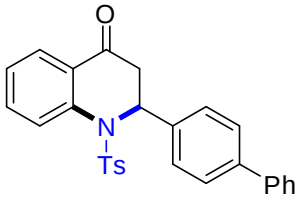
Flash column chromatography on silica gel (petroleum ether/ethyl acetate 3/1) gave a white solid (60.0 mg, 69%). m.p. 205-206 °C. R_f = 0.38 (Silica gel, petroleum/ethyl acetate = 3:1). ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.91-7.82 (m, 4H), 7.60-7.51 (m, 3H), 7.37 (d, *J* = 8.2 Hz, 2H), 7.25 (d, *J* = 8.0 Hz, 2H), 7.18 (t, *J* = 7.8 Hz, 1H), 5.97 (d, *J* = 5.5 Hz, 1H), 3.84 (s, 3H), 3.05-3.01 (m, 1H), 2.68-2.62 (m, 1H), 2.39 (s, 3H). ^{13}C NMR ($CDCl_3$, 100 MHz): δ 191.7, 166.6, 145.0, 142.9, 140.1, 136.5, 135.4, 130.4, 130.0, 129.8, 127.4, 127.1, 126.2, 126.1, 125.9, 100.1, 57.8, 52.3, 39.5, 21.8. HRMS (ESI) *m/z* calcd for $C_{24}H_{22}NO_5S$ $(M+H)^+$ 436.1213, found 436.1209.

2-(3-nitrophenyl)-1-tosyl-2,3-dihydroquinolin-4(1H)-one (3ja)



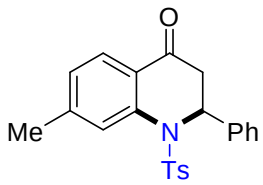
Flash column chromatography on silica gel (petroleum ether/ethyl acetate 3/1) gave a yellow solid (54.9 mg, 65%). m.p. 150-152 ^{o}C. R_f = 0.37 (Silica gel, petroleum/ethyl acetate = 3:1). ^{1}H NMR ($CDCl_3$, 400 MHz): δ 8.13 (s, 1H), 8.04 (d, *J* = 8.1 Hz, 1H), 7.96 (d, *J* = 8.3 Hz, 1H), 7.85 (d, *J* = 7.8 Hz, 1H), 7.67-7.56 (m, 4H), 7.43 (t, *J* = 8.0 Hz, 1H), 7.28 (d, *J* = 8.2 Hz, 1H), 7.22 (t, *J* = 7.6 Hz, 1H), 6.01 (d, *J* = 5.5 Hz, 1H), 3.08-3.03 (m, 1H), 2.74-2.68 (m, 1H), 2.41 (s, 3H). ^{13}C NMR ($CDCl_3$, 100 MHz): δ 191.1, 148.6, 145.3, 140.3, 139.8, 136.2, 135.7, 132.9, 130.5, 129.9, 127.5, 127.2, 126.4, 126.2, 125.8, 123.2, 122.0, 57.4, 39.5, 21.8. HRMS (ESI) *m/z* calcd for $C_{22}H_{19}N_2O_5S$ $(M+H)^+$ 423.1009, found 423.1015.

2-(biphenyl-4-yl)-1-tosyl-2,3-dihydroquinolin-4(1H)-one (3ka)



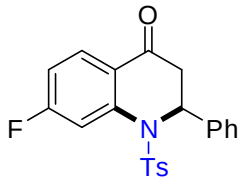
Flash column chromatography on silica gel (petroleum ether/ethyl acetate 3/1) gave a yellow liquid (63.4 mg, 70%). R_f = 0.51 (Silica gel, petroleum/ethyl acetate = 3:1). ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.96 (d, *J* = 8.1 Hz, 1H), 7.90 (dd, *J* = 7.8, 1.6 Hz, 1H), 7.63 (d, *J* = 8.3 Hz, 2H), 7.58-7.19 (m, 14H), 6.00 (d, *J* = 5.4 Hz, 1H), 3.09-3.04 (m, 1H), 2.70-2.64 (m, 1H), 2.42 (s, 3H). ^{13}C NMR ($CDCl_3$, 100 MHz): δ 192.2, 144.9, 140.8, 140.3, 136.8, 136.7, 135.3, 130.4, 128.9, 127.6, 127.5, 127.4, 127.3, 127.2, 127.1, 126.3, 126.0, 125.9, 57.8, 39.7, 21.8. HRMS (ESI) *m/z* calcd for $C_{28}H_{24}NO_3S$ $(M+H)^+$ 454.1471, found 454.1475.

7-methyl-2-phenyl-1-tosyl-2,3-dihydroquinolin-4(1H)-one (3la)



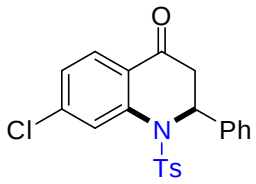
Flash column chromatography on silica gel (petroleum ether/ethyl acetate 5/1) gave a brown liquid (57.9 mg, 74%). R_f = 0.29 (Silica gel, petroleum/ethyl acetate = 5:1). ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.75 (d, *J* = 8.0 Hz, 1H), 7.71 (s, 1H), 7.60 (d, *J* = 8.3 Hz, 2H), 7.32-7.17 (m, 7H), 7.00 (d, *J* = 8.0 Hz, 1H), 5.91 (d, *J* = 5.6 Hz, 1H), 2.99-2.94 (m, 1H), 2.59-2.53 (m, 1H), 2.41 (s, 3H), 2.39 (s, 3H). ^{13}C NMR ($CDCl_3$, 100 MHz): δ 192.0, 146.6, 144.8, 140.1, 138.0, 136.8, 130.3, 128.7, 127.9, 127.2, 127.13, 127.11, 126.7, 123.9, 57.9, 39.3, 22.3, 21.8. HRMS (ESI) *m/z* calcd for $C_{23}H_{22}NO_3S$ $(M+H)^+$ 392.1315, found 392.1312.

7-fluoro-2-phenyl-1-tosyl-2,3-dihydroquinolin-4(1H)-one (3ma)



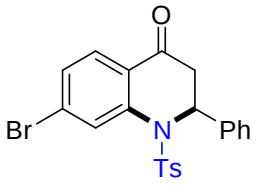
Flash column chromatography on silica gel (petroleum ether/ethyl acetate 5/1) gave a brown liquid (52.1 mg, 66%). R_f = 0.29 (Silica gel, petroleum/ethyl acetate = 5:1). ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.91-7.87 (m, 1H), 7.69-7.64 (m, 3H), 7.31-7.21 (m, 7H), 6.89-6.85 (m, 1H), 5.98 (d, *J* = 5.3 Hz, 1H), 3.06-3.01 (m, 1H), 2.65-2.59 (m, 1H), 2.43 (s, 3H). ^{13}C NMR ($CDCl_3$, 100 MHz): δ 190.8, 166.4 (d, $J_{C\text{-}F}$ = 265.3 Hz), 145.2, 142.4 (d, $J_{C\text{-}F}$ = 12.4 Hz), 137.5, 136.5, 130.5, 130.0 (d, $J_{C\text{-}F}$ = 10.8 Hz), 128.9, 128.2, 127.1, 126.9, 122.4 (d, $J_{C\text{-}F}$ = 2.6 Hz), 113.5 (d, $J_{C\text{-}F}$ = 22.1 Hz), 112.8 (d, $J_{C\text{-}F}$ = 26.4 Hz), 58.1, 39.5, 21.8. HRMS (ESI) *m/z* calcd for $C_{22}H_{19}FNO_3S$ $(M+H)^+$ 396.1064, found 396.1065.

7-chloro-2-phenyl-1-tosyl-2,3-dihydroquinolin-4(1H)-one (3na)



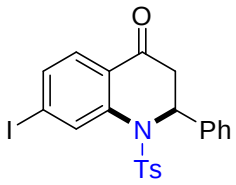
Flash column chromatography on silica gel (petroleum ether/ethyl acetate 5/1) gave a brown liquid (55.9 mg, 68%). R_f = 0.32 (Silica gel, petroleum/ethyl acetate = 5:1). ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.95 (d, *J* = 1.9 Hz, 1H), 7.79 (d, *J* = 8.4 Hz, 1H), 7.65 (d, *J* = 8.3 Hz, 2H), 7.30-7.20 (m, 7H), 7.15-7.12 (m, 1H), 5.93 (d, *J* = 5.2 Hz, 1H), 3.06-3.01 (m, 1H), 2.63-2.57 (m, 1H), 2.42 (s, 3H). ^{13}C NMR ($CDCl_3$, 100 MHz): δ 191.2, 145.2, 141.4, 141.1, 137.4, 136.4, 130.5, 128.9, 128.6, 128.2, 127.2, 127.0, 126.3, 125.8, 124.2, 57.9, 39.5, 21.8. HRMS (ESI) *m/z* calcd for $C_{22}H_{19}ClNO_3S$ $(M+H)^+$ 412.0769, found 412.0773.

7-bromo-2-phenyl-1-tosyl-2,3-dihydroquinolin-4(1H)-one (3oa)



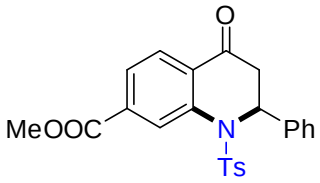
Flash column chromatography on silica gel (petroleum ether/ethyl acetate 5/1) gave a yellow liquid (63.7 mg, 70%). R_f = 0.3 (Silica gel, petroleum/ethyl acetate = 5:1). ^{1}H NMR ($CDCl_3$, 400 MHz): δ 8.12 (d, *J* = 1.7 Hz, 1H), 7.70 (d, *J* = 8.4 Hz, 1H), 7.64 (d, *J* = 8.2 Hz, 2H), 7.31-7.18 (m, 8H), 5.94 (d, *J* = 5.4 Hz, 1H), 3.06-3.01 (m, 1H), 2.62-2.56 (m, 1H), 2.42 (s, 3H). ^{13}C NMR ($CDCl_3$, 100 MHz): δ 191.4, 145.2, 141.1, 137.4, 136.4, 130.5, 130.1, 129.2, 128.9, 128.7, 128.5, 128.2, 127.2, 127.0, 124.5, 57.9, 39.5, 21.8. HRMS (ESI) *m/z* calcd for $C_{22}H_{19}BrNO_3S$ $(M+H)^+$ 456.0264, found 456.0268.

7-iodo-2-phenyl-1-tosyl-2,3-dihydroquinolin-4(1H)-one (3pa)



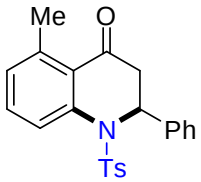
Flash column chromatography on silica gel (petroleum ether/ethyl acetate 5/1) gave a white solid. (55.3 mg, 55%). m.p. 194-196 ^{o}C. R_f = 0.29 (Silica gel, petroleum/ethyl acetate = 5:1). ^{1}H NMR ($CDCl_3$, 400 MHz): δ 8.31 (s, 1H), 7.64 (d, *J* = 8.3 Hz, 1H), 7.53 (d, *J* = 1.4 Hz, 2H), 7.30-7.21 (m, 7H), 5.93 (d, *J* = 5.7 Hz, 1H), 3.05-3.00 (m, 1H), 2.61-2.55 (m, 1H), 2.42 (s, 3H). ^{13}C NMR ($CDCl_3$, 100 MHz): δ 191.7, 145.2, 140.6, 137.3, 136.4, 135.2, 134.7, 130.5, 128.9, 128.24, 128.23, 127.2, 127.0, 125.1, 103.1, 57.9, 39.5, 21.8. HRMS (ESI) *m/z* calcd for $C_{22}H_{19}INO_3S$ $(M+H)^+$ 504.0125, found 504.0117.

<u>methyl 4-oxo-2-phenyl-1-tosyl-1,2,3,4-tetrahydroquinoline-7-carboxylate</u> (3qa)



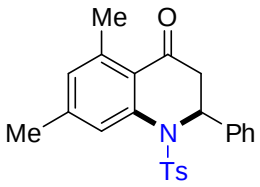
Flash column chromatography on silica gel (petroleum ether/ethyl acetate 3/1) gave a yellow solid. (56.5 mg, 65%). m.p. 146-148 ^{o}C. R_f = 0.49 (Silica gel, petroleum/ethyl acetate = 3:1). ^{1}H NMR ($CDCl_3$, 400 MHz): δ 8.54 (d, *J* = 1.3 Hz, 1H), 7.91 (d, *J* = 8.1 Hz, 1H), 7.83-7.80 (m, 1H), 7.63 (d, *J* = 8.3 Hz, 1H), 7.29-7.17 (m, 7H), 5.97 (d, *J* = 5.3 Hz, 1H), 3.95 (s, 3H), 3.10-3.05 (m, 1H), 2.70-2.64 (m, 1H), 2.42 (s, 3H). ^{13}C NMR ($CDCl_3$, 100 MHz): δ 191.8, 165.8, 145.1, 140.3, 137.4, 136.5, 135.8, 130.4, 128.9, 128.5, 128.2, 127.4, 127.3, 127.0, 126.4, 57.8, 52.8, 39.8, 21.8. HRMS (ESI) *m/z* calcd for $C_{24}H_{22}NO_5S$ $(M+H)^+$ 436.1213, found 436.1210.

<u>5-methyl-2-phenyl-1-tosyl-2,3-dihydroquinolin-4(1H)-one</u> (3ra)



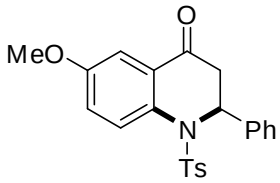
Flash column chromatography on silica gel (petroleum ether/ethyl acetate 5/1) gave a yellow liquid (41.4 mg, 53%). R_f = 0.37 (Silica gel, petroleum/ethyl acetate = 5:1). ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.70 (d, *J* = 8.2 Hz, 1H), 7.58 (d, *J* = 8.3 Hz, 2H), 7.38-7.16 (m, 9H), 7.00 (d, *J* = 7.6 Hz, 1H), 5.87 (d, *J* = 6.1 Hz, 1H), 3.03-2.98 (m, 1H), 2.73-2.67 (m, 1H), 2.53 (s, 3H), 2.42 (s, 3H). ^{13}C NMR ($CDCl_3$, 100 MHz): δ 193.9, 144.7, 141.9, 141.1, 138.2, 136.8, 133.6, 130.3, 130.2, 128.7, 127.8, 127.2, 127.0, 125.4, 57.1, 41.4, 23.4, 21.8. HRMS (ESI) *m/z* calcd for $C_{23}H_{22}NO_3S$ $(M+H)^+$ 392.1315, found 392.1312.

<u>5,7-dimethyl-2-phenyl-1-tosyl-2,3-dihydroquinolin-4(1H)-one</u> (3sa)



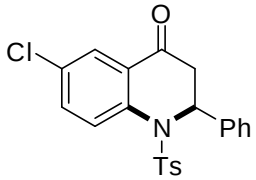
Flash column chromatography on silica gel (petroleum ether/ethyl acetate 5/1) gave a yellow liquid (39.7 mg, 49%). R_f = 0.36 (Silica gel, petroleum/ethyl acetate = 5:1). ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.58 (d, *J* = 8.3 Hz, 2H), 7.51 (s, 1H), 7.30-7.18 (m, 7H), 6.82 (s, 1H), 5.87 (d, *J* = 6.1 Hz, 1H), 2.97-2.92 (m, 1H), 2.66-2.60 (m, 1H), 2.49 (s, 3H), 2.42 (s, 3H, 2.33(s, 3H). ^{13}C NMR ($CDCl_3$, 100 MHz): δ 193.5, 144.7, 144.6, 141.8, 141.0, 138.3, 136.8, 131.4, 130.2, 128.7, 127.8, 127.2, 127.1, 125.8, 123.1, 57.1, 41.0, 23.4, 21.9, 21.8. HRMS (ESI) *m/z* calcd for $C_{24}H_{24}NO_3S$ $(M+H)^+$ 406.1471, found 406.1474.

6-methoxy-2-phenyl-1-tosyl-2,3-dihydroquinolin-4(1H)-one (3ta)



Flash column chromatography on silica gel (petroleum ether/ethyl acetate 3/1) gave a brown liquid (46.7 mg, 46%). R_f = 0.42 (Silica gel, petroleum/ethyl acetate = 3:1).^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.80 (d, *J* = 9.0 Hz, 1H), 7.56 (d, *J* = 8.3 Hz, 1H), 7.31-7.19 (m, 8H), 7.10 (dd, *J* = 9.0, 3.2 Hz, 1H), 5.89 (d, *J* = 5.7 Hz, 1H), 3.78 (s, 3H), 2.99-2.94 (m, 1H), 2.58-2.52 (m, 1H), 2.42 (s, 3H). ^{13}C NMR ($CDCl_3$, 100 MHz): δ 192.3, 157.6, 144.7, 137.9, 136.6, 133.5, 130.3, 128.7, 128.5, 127.9, 127.1, 127.0, 123.0, 109.1, 57.8, 55.7, 39.1, 21.8. HRMS (ESI) *m/z* calcd for $C_{23}H_{22}NO_4S$ $(M+H)^+$ 408.1264, found 408.1268.

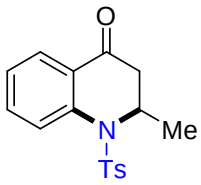
6-chloro-2-phenyl-1-tosyl-2,3-dihydroquinolin-4(1H)-one (3ua)



Flash column chromatography on silica gel (petroleum ether/ethyl acetate 5/1) gave a yellow liquid (33.7 mg, 41%). R_f = 0.37 (Silica gel, petroleum/ethyl acetate = 5:1). ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.87 (d, *J* = 8.8 Hz, 1H), 7.81 (d, *J* = 2.6 Hz, 1H), 7.61 (d, *J* = 8.2 Hz, 2H), 7.47 (dd, *J* = 8.8, 2.6 Hz, 1H), 7.30-7.19 (m, 7H), 5.93 (d, *J* = 5.3 Hz, 1H), 3.05-3.00 (m, 1H), 2.60-2.54 (m, 1H), 2.43 (s, 3H). ^{13}C NMR ($CDCl_3$, 100 MHz): δ 191.1, 145.1, 137.9, 137.4, 136.5, 135.0, 132.0, 130.5, 128.9, 128.2, 127.8, 127.1, 127.0, 126.9, 126.8, 57.8, 39.2, 21.8. HRMS (ESI) *m/z* calcd for $C_{22}H_{19}ClNO_3S$ $(M+H)^+$ 412.0769, found 412.0771.

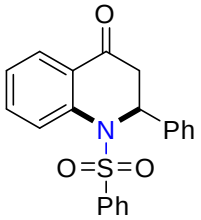
2-methyl-1-tosyl-2,3-dihydroquinolin-4(1H)-one (3va)[3]

[3] T. Yang, T. Zhang, S. Yang, S. Chen and X. Li, *Org. Biomol. Chem.*, 2014, **12**, 4290.



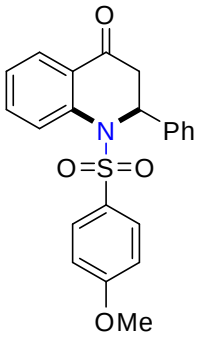
Flash column chromatography on silica gel (petroleum ether/ethyl acetate 5/1) gave a yellow liquid (32.8 mg, 52%). R_f = 0.38 (Silica gel, petroleum/ethyl acetate = 5:1). ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.95-7.89 (m, 2H), 7.61 (t, *J* = 7.5 Hz, 1H), 7.52 (d, *J* = 8.0 Hz, 2H), 7.31-7.27 (m, 1H), 7.22 (t, *J* = 8.0 Hz, 2H), 4.93-4.89 (m, 1H), 2.42-2.36 (m, 4H), 2.27-2.22 (m, 1H), 1.29 (t, *J* = 6.9 Hz, 2H). ^{13}C NMR ($CDCl_3$, 100 MHz): δ 192.6, 144.6, 139.8, 136.7, 135.1, 130.2, 127.3, 127.0, 126.5, 125.8, 125.6, 52.0, 42.1, 21.7, 19.8.

2-phenyl-1-(phenylsulfonyl)-2,3-dihydroquinolin-4(1H)-one (3ab)[4]



Flash column chromatography on silica gel (petroleum ether/ethyl acetate 3/1) gave a yellow liquid (49.4 mg, 68%). R_f = 0.58 (Silica gel, petroleum/ethyl acetate = 3:1). ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.92-7.85 (m, 2H), 7.74-7.72 (m, 2H), 7.60 (t, *J* = 7.4 Hz, 1H), 7.56-7.52 (m, 1H), 7.47 (t, *J* = 7.8 Hz, 2H), 7.31-7.17 (m, 6H), 5.97 (d, *J* = 5.5 Hz, 1H), 3.05-3.00 (m, 1H), 2.63-2.57 (m, 1H). ^{13}C NMR ($CDCl_3$, 100 MHz): δ 192.0, 140.1, 139.6, 137.7, 135.2, 133.8, 129.7, 128.8, 128.0, 127.3, 127.1, 127.0, 126.2, 126.1, 126.0, 57.9, 39.6.

1-(4-methoxyphenylsulfonyl)-2-phenyl-2,3-dihydroquinolin-4(1H)-one (3ac)[5]

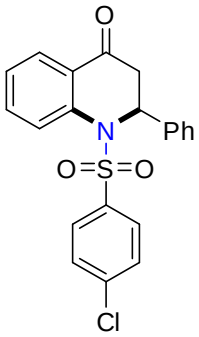


Flash column chromatography on silica gel (petroleum ether/ethyl acetate 3/1) gave a yellow liquid (51.9 mg, 66%). R_f = 0.45 (Silica gel, petroleum/ethyl acetate = 3:1). ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.91-7.85 (m, 2H), 7.66-7.52 (m, 2H), 7.52 (t, *J* = 7.4 Hz, 1H), 7.31-7.29 (m, 2H), 7.25-7.16 (m, 4H), 6.91 (d, *J* = 8.8 Hz, 1H), 5.94 (d, *J* = 5.5 Hz, 1H), 3.84 (s, 3H), 3.06-3.01 (m,

[4] John. A. Donnelly and D. F. Farrell, *J. Org. Chem.*, 1990, **55**, 1757.
[5] S. Cheng, L. Zhao and S. Yu, *Adv. Synth. Catal.*, 2014, **356**, 982.

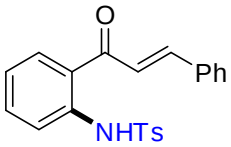
1H), 2.70-2.64 (m, 1H). ^{13}C NMR ($CDCl_3$, 100 MHz): δ 192.2, 163.7, 140.3, 137.8, 135.2, 131.1, 129.3, 128.8, 127.9, 127.2, 127.1, 126.3, 126.1, 125.8, 114.8, 57.8, 55.8, 39.7.

1-(4-chlorophenylsulfonyl)-2-phenyl-2,3-dihydroquinolin-4(1H)-one (3ad)



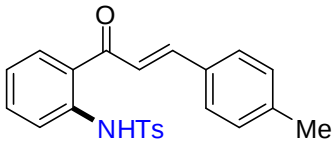
Flash column chromatography on silica gel (petroleum ether/ethyl acetate 5/1) gave a yellow liquid (55.7 mg, 70%). R_f = 0.39 (Silica gel, petroleum/ethyl acetate = 5:1). ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.89-7.87 (m, 2H), 7.67-7.65 (m, 2H), 7.55-7.52 (m, 1H), 7.47 (d, *J* = 8.4 Hz, 2H), 7.29-7.17 (m, 6H), 5.98 (d, *J* = 5.4 Hz, 1H), 3.11-3.06 (m, 1H), 2.72-2.66 (m, 1H). ^{13}C NMR ($CDCl_3$, 100 MHz): δ 191.7, 140.4, 139.8, 138.1, 137.5, 135.3, 130.0, 128.8, 128.5, 128.1, 127.5, 127.0, 126.2, 126.1, 126.0, 58.1, 39.9. HRMS (ESI) *m/z* calcd for $C_{21}H_{17}ClNO_3S$ $(M+H)^+$ 398.0612, found 398.0615.

(E)-N-(2-cinnamoylphenyl)-4-methylbenzenesulfonamide (4a)[6]



Flash column chromatography on silica gel (petroleum ether/ethyl acetate 3/1) gave a yellow solid (57.3 mg, 76%). R_f = 0.49 (Silica gel, petroleum/ethyl acetate = 3:1). ^{1}H NMR ($CDCl_3$, 400 MHz): δ 11.1 (s, 1H), 7.86-7.83 (m, 1H), 7.76-7.74 (m, 1H), 7.70-7.59 (m, 5H), 7.52-7.42 (m, 4H), 7.33 (d, *J* = 15.6 Hz, 1H), 7.17-7.13 (m, 3H), 2.22 (s, 3H). ^{13}C NMR ($CDCl_3$, 100 MHz): δ 193.0, 146.1, 143.9, 139.9, 136.4, 134.5, 134.4, 131.2, 130.7, 129.8, 129.2, 128.7, 127.4, 125.2, 123.4, 122.3, 121.2, 21.5.

(E)-4-methyl-N-(2-(3-p-tolylacryloyl)phenyl)benzenesulfonamide (4b)[7]

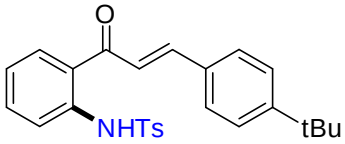


Flash column chromatography on silica gel (petroleum ether/ethyl acetate 5/1) gave a yellow solid (56.3 mg, 72%). R_f = 0.33 (Silica gel, petroleum/ethyl acetate = 5:1). ^{1}H NMR ($CDCl_3$, 400 MHz): δ 11.1 (s, 1H), 7.83 (d, *J* = 7.9 Hz, 1H), 7.74 (d, *J* = 7.6 Hz, 1H), 7.68 (d, *J* = 8.3 Hz, 2H),

[6] J. Kim and S. Chang, *Angew. Chem. Int. Ed.*, 2014, **53**, 2203.
[7] Z. Wang, X. Xu, Z. Gu, W. Feng, H. Qian, Z. Li, X. Sun and O. Kwon, *Chem. Commun.*, 2016, **52**, 2811.

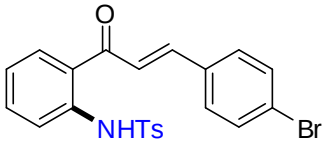
7.63 (d, *J* = 15.5 Hz, 1H), 7.51-7.46 (m, 3H), 7.16-7.12 (m, 3H), 2.40 (s, 3H), 2.22 (s, 3H). ^{13}C NMR ($CDCl_3$, 100 MHz): δ 193.1, 146.3, 143.9, 141.9, 139.8, 136.4, 134.3, 131.8, 130.7, 129.9, 129.7, 128.8, 127.4, 125.4, 123.4, 121.2, 121.1, 21.7, 21.5.

(E)-N-(2-(3-(4-tert-butylphenyl)acryloyl)phenyl)-4-methylbenzenesulfonamide (4c)



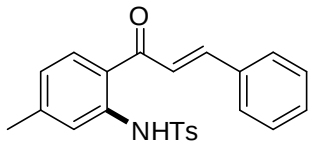
Flash column chromatography on silica gel (petroleum ether/ethyl acetate 5/1) gave a yellow solid (58.9 mg, 68%). m.p. 142-143 ^{o}C. R_f = 0.42 (Silica gel, petroleum/ethyl acetate = 5:1). ^{1}H NMR ($CDCl_3$, 400 MHz): δ 11.1 (s, 1H), 7.84 (d, *J* = 7.9 Hz, 1H), 7.75 (d, *J* = 8.3 Hz, 1H), 7.69 (d, *J* = 8.3 Hz, 2H), 7.65 (d, *J* = 15.6 Hz, 1H), 7.56-7.45 (m, 5H), 7.55 (d, *J* = 15.6 Hz, 1H), 7.17-7.13 (m, 3H), 2.22 (s, 3H), 1.36 (s, 9H). ^{13}C NMR ($CDCl_3$, 100 MHz): δ 193.1, 155.0, 146.2, 143.9, 139.8, 136.5, 134.3, 131.8, 130.7, 129.7, 128.7, 127.4, 126.2, 125.4, 123.4, 121.4, 121.1, 35.2, 31.3, 21.5. HRMS (ESI) *m/z* calcd for $C_{26}H_{28}NO_3S$ $(M+H)^+$ 434.1784, found 434.1789.

(E)-N-(2-(3-(4-bromophenyl)acryloyl)phenyl)-4-methylbenzenesulfonamide (4d)[7]



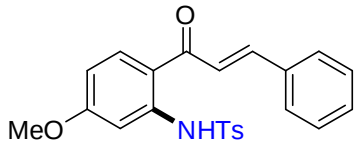
Flash column chromatography on silica gel (petroleum ether/ethyl acetate 5/1) gave a yellow solid (60.1 mg, 66%). R_f = 0.33 (Silica gel, petroleum/ethyl acetate = 5:1). ^{1}H NMR ($CDCl_3$, 400 MHz): δ 11.1 (s, 1H), 7.85 (d, *J* = 8.0 Hz, 1H), 7.74-7.69 (m, 3H), 7.61-7.55 (m, 3H), 7.49-7.46 (m, 3H), 7.35 (d, *J* = 15.6 Hz, 1H), 7.18-7.12 (m, 3H), 2.25 (s, 3H). ^{13}C NMR ($CDCl_3$, 100 MHz): δ 192.7, 144.6, 144.0, 140.1, 136.5, 134.6, 133.5, 132.5, 130.8, 130.1, 129.8, 127.4, 125.5, 124.7, 123.3, 122.7, 120.7, 21.6.

(E)-N-(2-cinnamoyl-5-methylphenyl)-4-methylbenzenesulfonamide (4e)



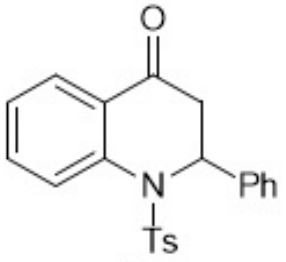
Flash column chromatography on silica gel (petroleum ether/ethyl acetate 5/1) gave a yellow liquid (50.0 mg,64%). R_f = 0.34 (Silica gel, petroleum/ethyl acetate = 5:1). ^{1}H NMR ($CDCl_3$, 400 MHz): δ 11.3 (s, 1H), 7.77-7.57 (m, 7H), 7.44 (s, 3H), 7.36 (d, *J* = 15.5 Hz, 1H), 7.18 (d, *J* = 7.8 Hz, 2H), 6.95 (d, *J* = 7.8 Hz, 1H), 2.38 (s, 3H), 2.25 (s, 3H). ^{13}C NMR ($CDCl_3$, 100 MHz): δ 192.6, 145.9, 145.6, 143.9, 140.3, 136.5, 134.6, 131.1, 130.8, 129.7, 129.2, 128.7, 127.4, 124.2, 122.4, 122.2, 121.2, 22.2, 21.5. HRMS (ESI) *m/z* calcd for $C_{23}H_{22}NO_3S$ $(M+H)^+$ 392.1315, found 392.1316.

(E)-N-(2-cinnamoyl-5-methoxyphenyl)-4-methylbenzenesulfonamide (4f)



Flash column chromatography on silica gel (petroleum ether/ethyl acetate 3/1) gave a yellow liquid (50.5 mg, 62%). R_f = 0.41 (Silica gel, petroleum/ethyl acetate = 3:1). ^{1}H NMR ($CDCl_3$, 400 MHz): δ 12.0 (s, 1H), 7.86 (d, *J* = 9.0 Hz, 1H), 7.77 (d, *J* = 8.3 Hz, 2H), 7.72 (d, *J* = 15.5 Hz, 1H), 7.63-7.60 (m, 2H), 7.45-7.42 (m, 4H), 7.26-7.21 (m, 3H), 3.85 (s, 3H), 2.32 (s, 3H). ^{13}C NMR ($CDCl_3$, 100 MHz): δ 191.3, 164.4, 145.0, 144.0, 143.4, 136.6, 134.8, 133.0, 130.9, 129.8, 129.2, 128.6, 127.5, 121.9, 117.0, 109.4, 103.9, 55.8, 21.6. HRMS (ESI) *m/z* calcd for $C_{23}H_{22}NO_4S$ $(M+H)^+$ 408.1264, found 408.1266.

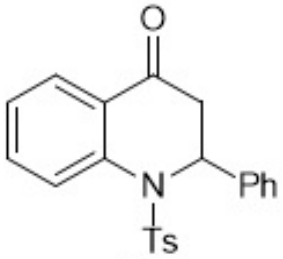
3. Copies of ^{1}H NMR and ^{13}C NMR spectra of the products


O
N
Ph
Ts

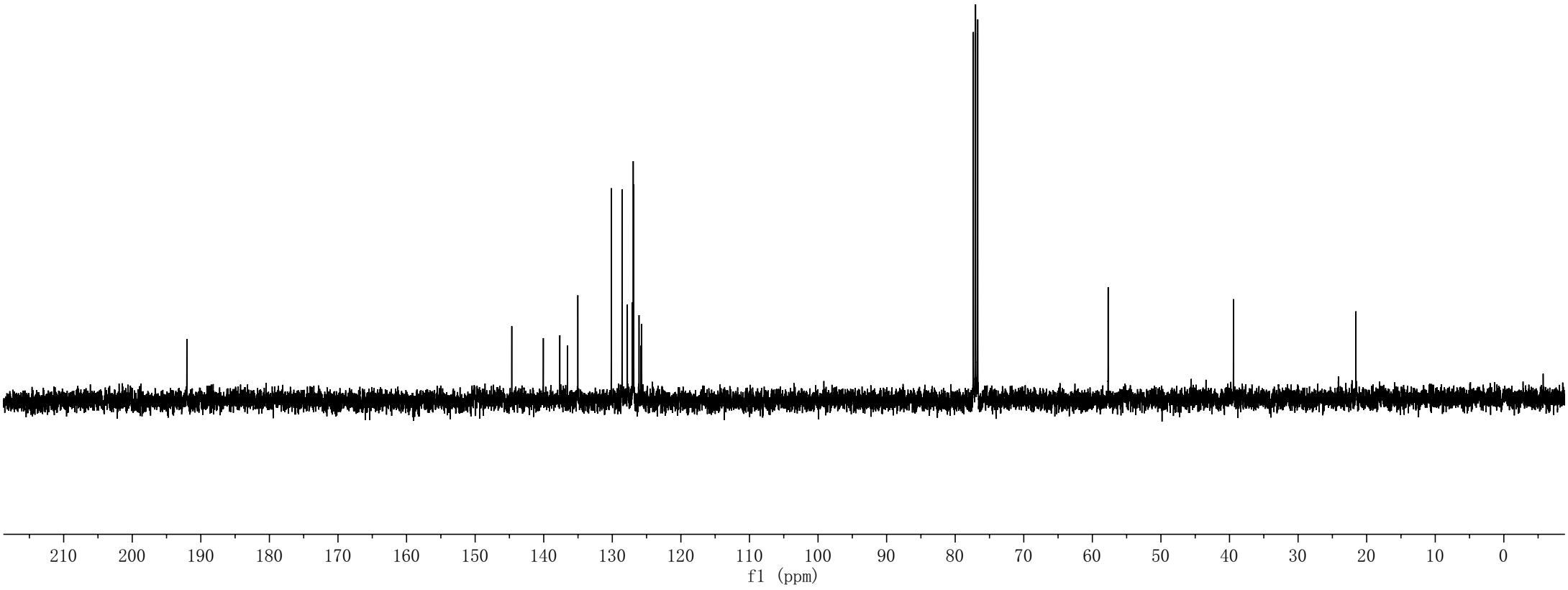
3aa

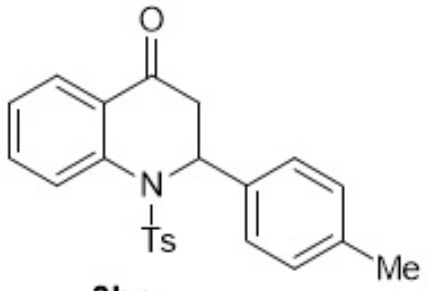
7.9191
7.8985
7.8737
7.8697
7.8542
7.8501
7.6128
7.5920
7.5566
7.5525
7.5350
7.5175
7.5134
7.3156
7.2969
7.2722
7.2389
7.2191
7.1966
7.1778
5.9589
5.9449
3.0463
3.0421
3.0015
2.9974
2.6587
2.6435
2.6139
2.5987
2.4144
0.98
0.98
2.04
1.05
8.25
0.99
1.02
1.01
3.11
11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

192.037
144.655
140.054
137.651
136.541
135.024
130.140
128.571
127.804
127.065
126.946
126.874
126.100
125.848
125.717
77.348
77.030
76.711
57.698
39.426
21.568



3aa




O
N
Ts
Me

3ba

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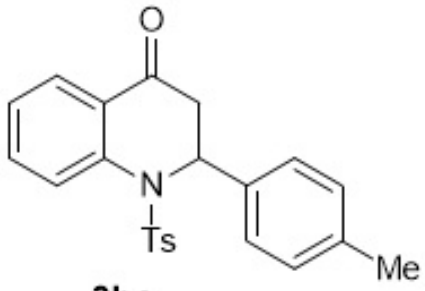
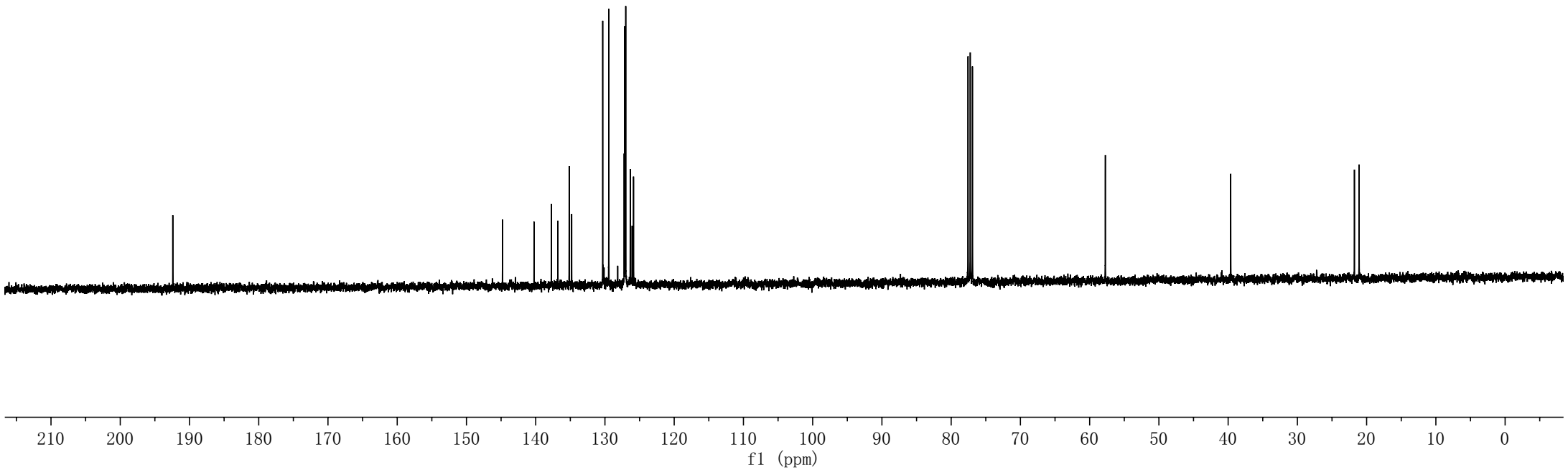
7.8724
7.8683
7.8529
7.8488
7.6077
7.5869
7.5488
7.5446
7.5270
7.5097
7.5055
7.2776
7.2669
7.2466
7.2085
7.1924
7.1731
7.0426
7.0224
5.9187
5.9045
3.0205
3.0163
2.9758
2.9716
2.6344
2.6192
2.5896
2.5745
2.4109
2.2385
1.97
2.00
1.03
2.24
3.00
2.00
0.96
0.98
1.00
3.07
3.01
11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

192.4121
144.7972
140.2419
137.7438
136.7985
135.1677
134.8025
130.3208
129.4475
127.2232
127.1331
126.9979
126.3429
126.0753
125.8716
77.5611
77.2430
76.9251
57.7351
39.6255
21.7627
21.0845



3ba



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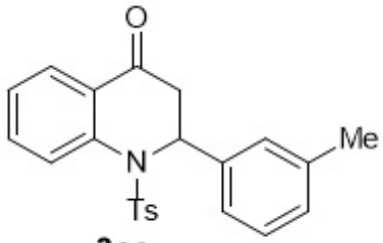
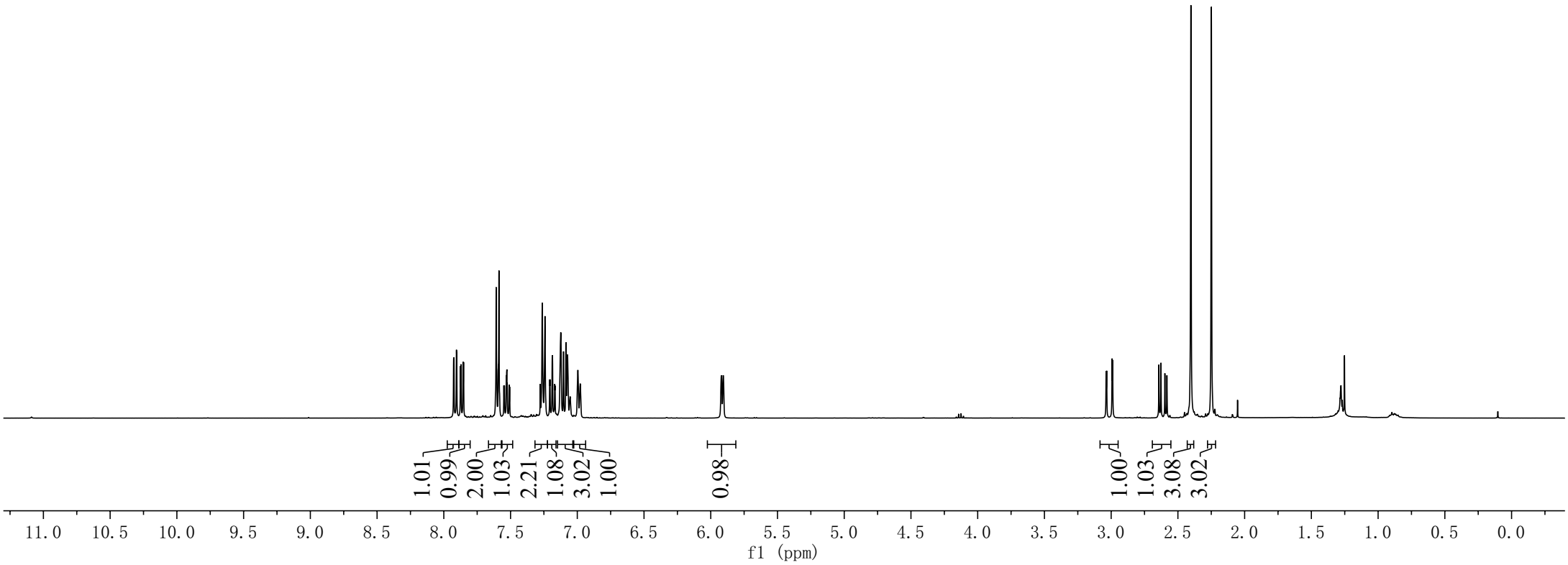
7.9052
7.8754
7.8713
7.8559
7.8518
7.6077
7.5869
7.5500
7.5457
7.5109
7.5066
7.2775
7.2623
7.2422
7.2067
7.2043
7.1689
7.1665
7.1236
7.1032
7.0731
7.0534
6.9954
6.9777
5.9202
5.9065

3.0378
3.0335
2.9930
2.9888
2.6422
2.6270
2.5974
2.5822
2.4027
2.2494



3ca



192.3302
144.8107
140.2840
138.4745
137.7749
136.7732
135.1816
130.3193
128.7990
128.5888
127.9006
127.2496
127.1339
126.3400
126.0795
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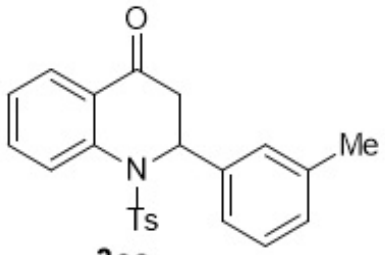
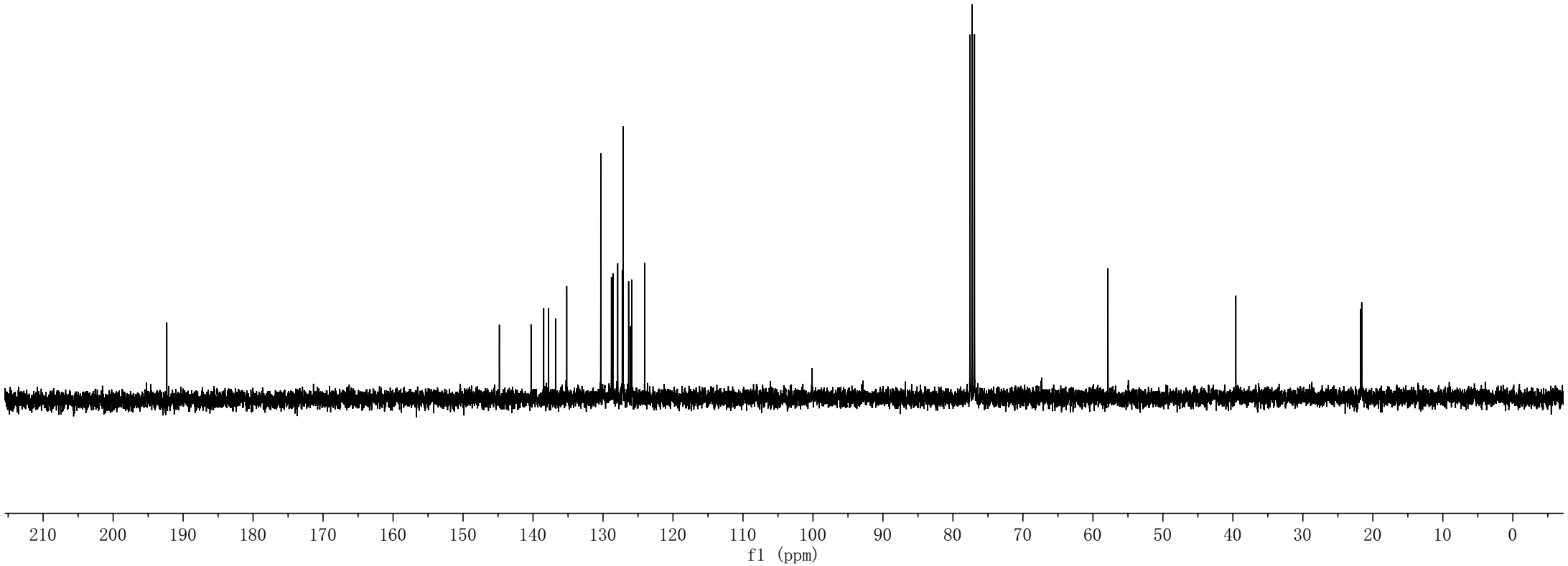
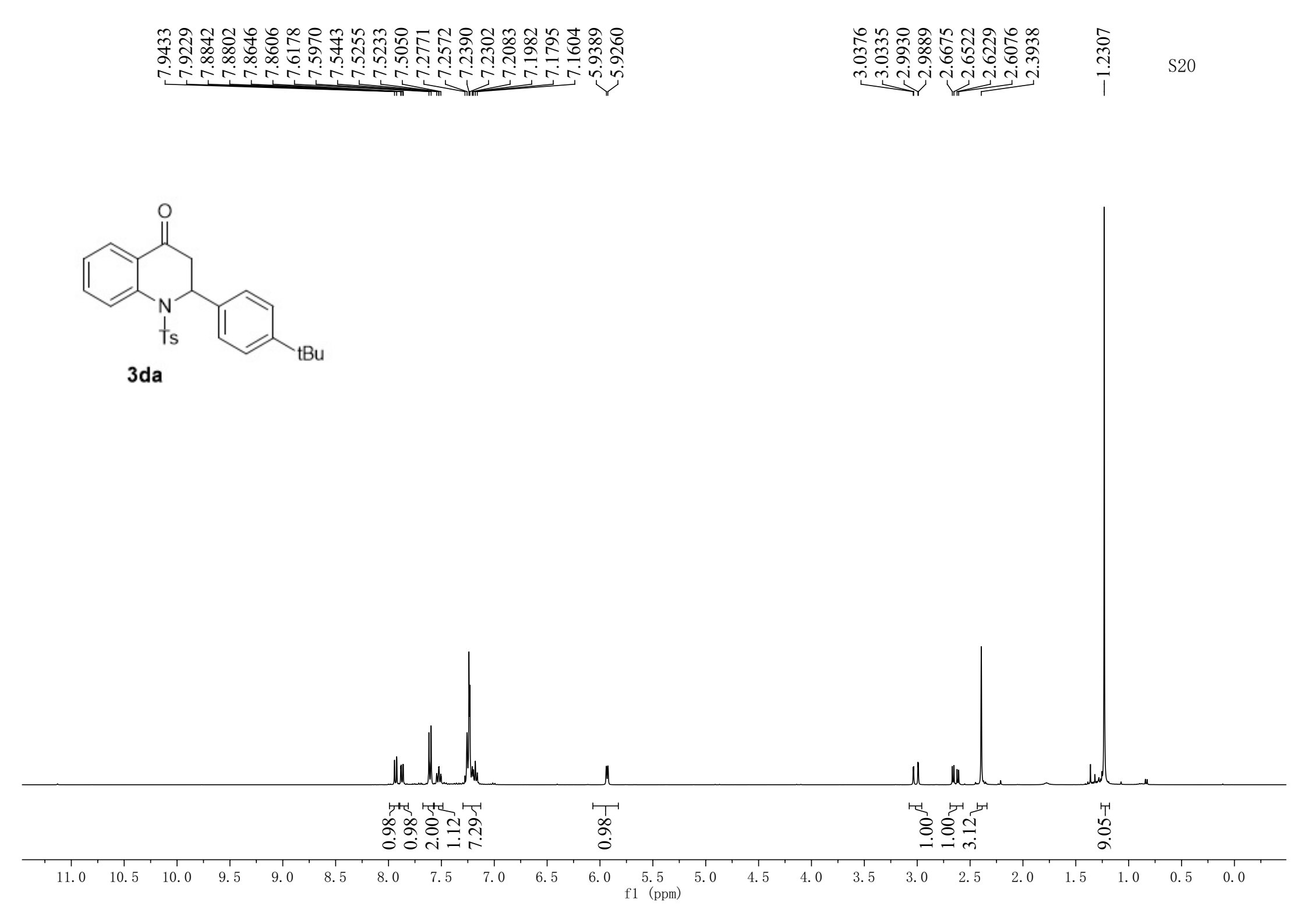
124.0514
77.5604
77.2422
76.9242
57.8505
39.5803
21.7599
21.5937



3ca

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7.8842
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7.6178
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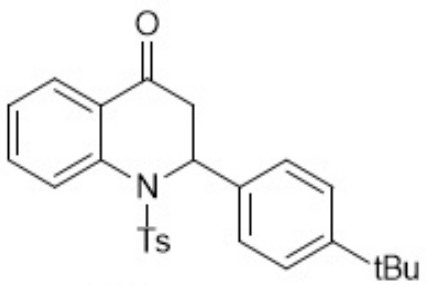
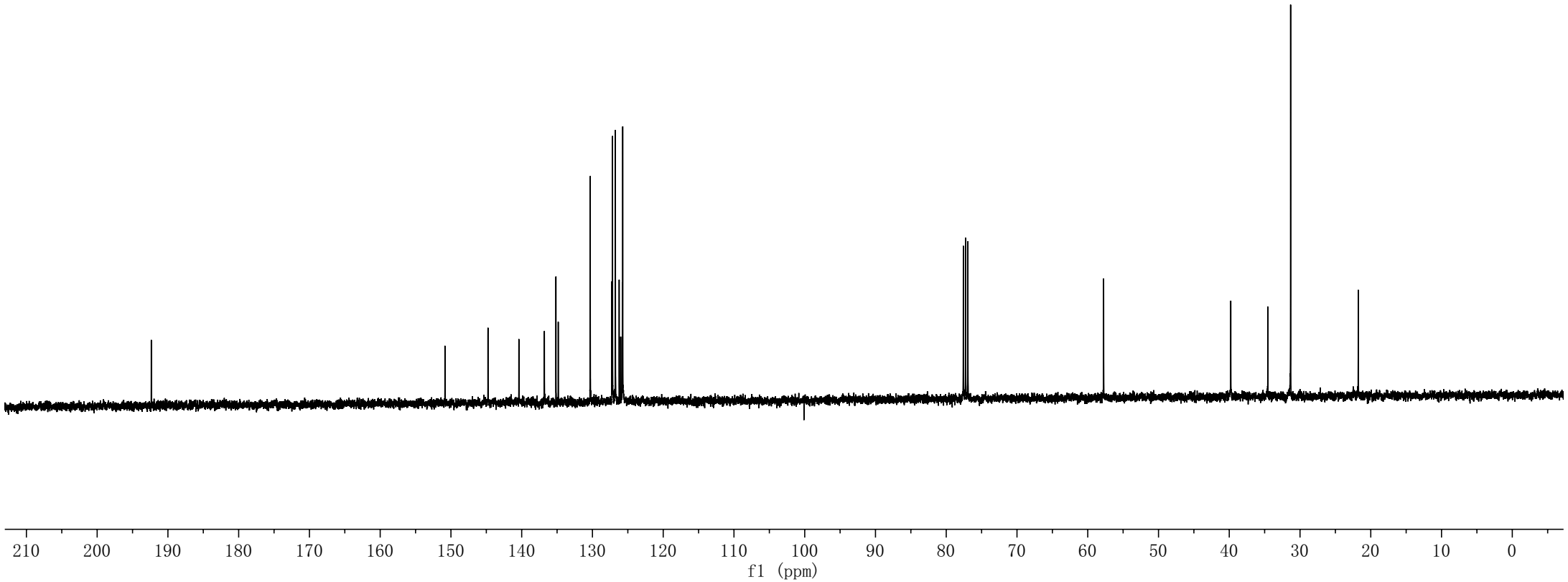
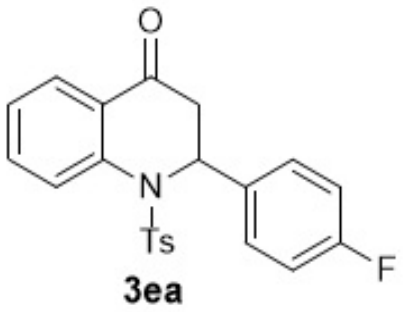
7.5443
7.5255
7.5233
7.5050
7.2771
7.2572
7.2390
7.2302
7.2083
7.1982
7.1795
7.1604
5.9389
5.9260
3.0376
3.0335
2.9930
2.9889
2.6675
2.6522
2.6229
2.6076
2.3938
1.2307
O
N
Ts
tBu
3da
0.98
0.98
2.00
1.12
7.29
0.98
1.00
1.00
3.12
9.05
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

192.3500
150.8478
144.7663
140.3985
136.7931
135.1615
134.8336
130.3110
127.2755
127.1594
126.7564
126.2232
126.0039
125.7734
125.7205
77.5795
77.2623
76.9435
57.7542
39.7829
34.5492
31.3281
21.7663

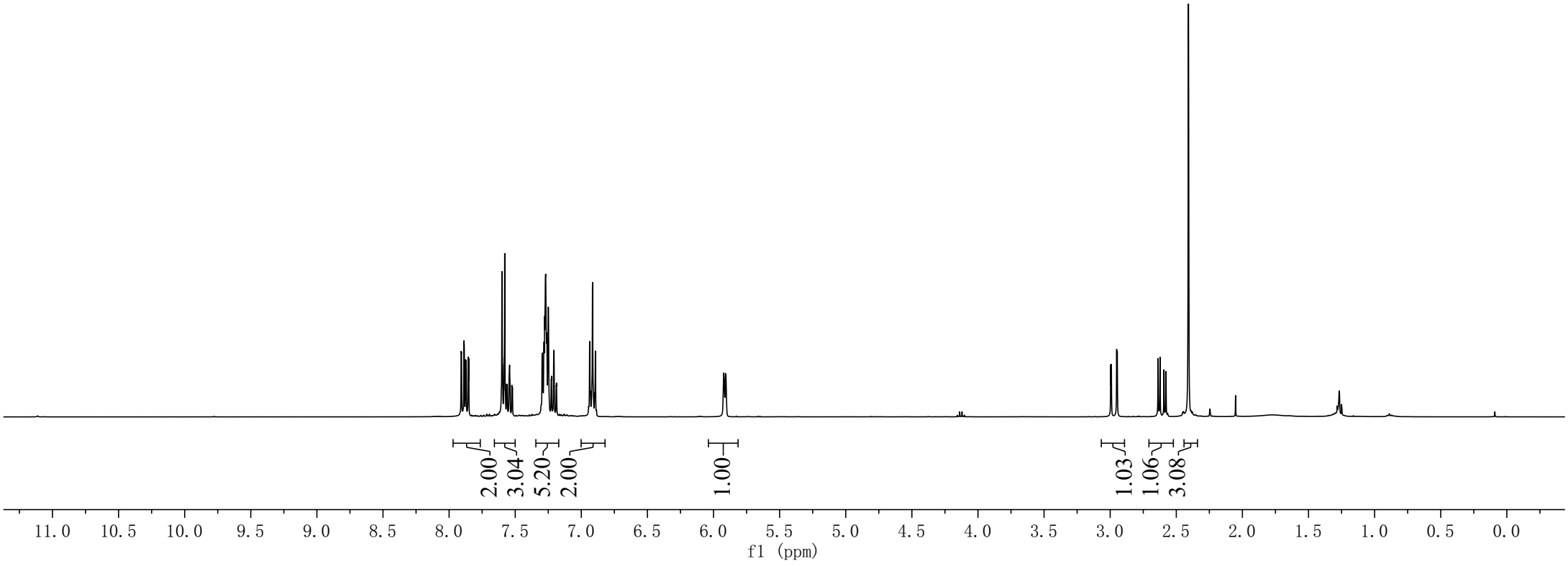


3da




O
N
Ts
F

3ea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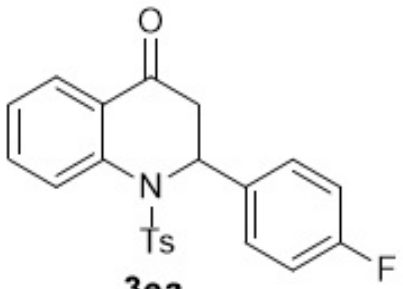
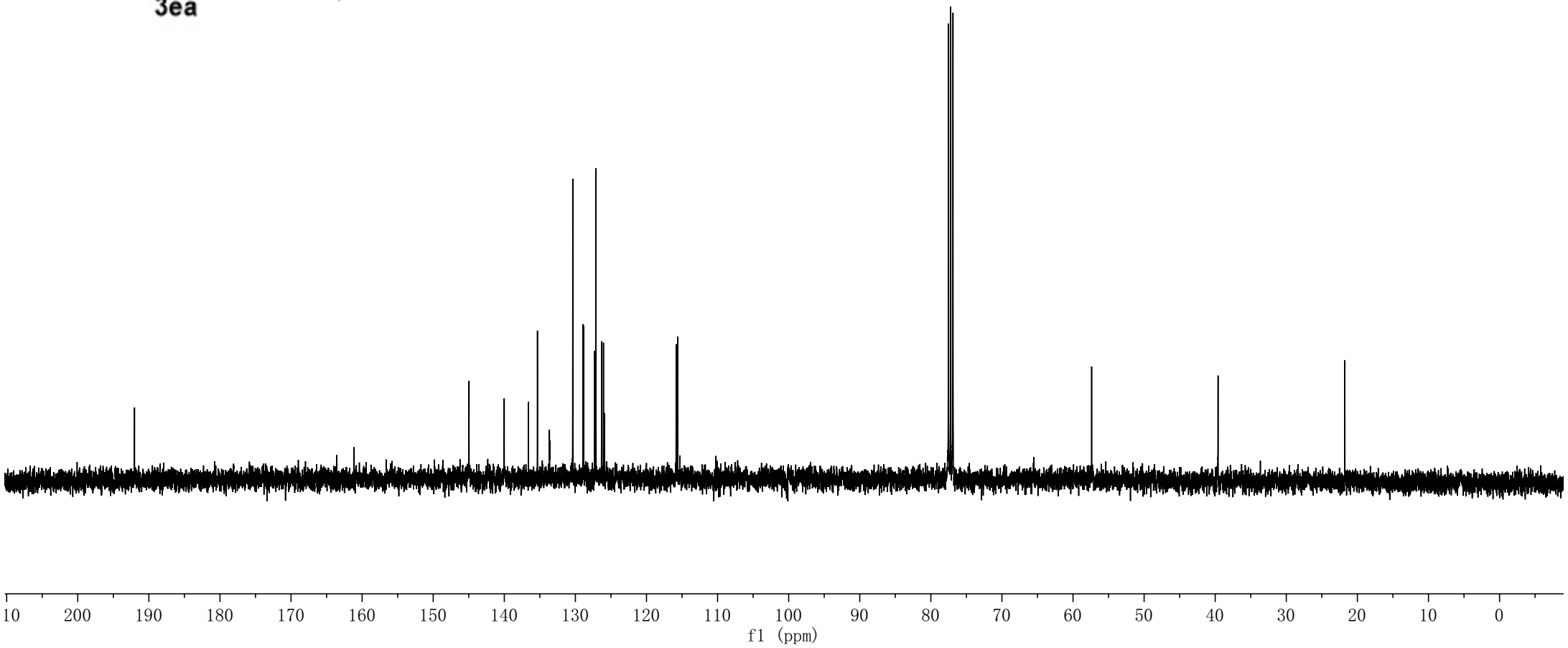
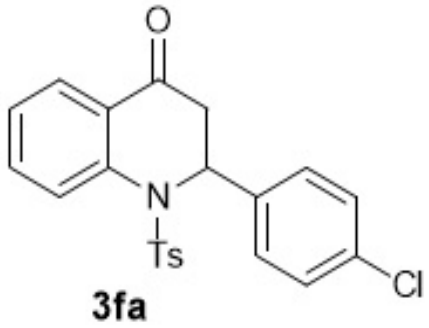
7.8752
7.8711
7.8556
7.8515
7.6001
7.5793
7.5645
7.5423
7.5212
7.2952
7.2697
7.2494
7.2257
7.2076
7.1879
6.9368
6.9152
6.8936
5.9221
5.9076
2.9956
2.9913
2.9508
2.9465
2.6379
2.6228
2.5931
2.5779
2.4081
2.00
3.04
5.20
2.00
1.00
1.03
1.06
3.08
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

192.0194
163.6154
161.1515
144.9617
136.6017
135.3365
130.3721
128.9161
128.8345
127.2864
127.1152
126.3124
126.0493
115.8264
115.6112
77.5223
77.2048
76.8865
57.3802
39.5969
21.7656



3ea




O
N
Ts
Cl

3fa

7.9097
7.8890
7.8653
7.8614
7.8458
7.8418
7.5974
7.5767
7.5641
7.5614
7.5449
7.5431
7.5248
7.5223
7.2775
7.2662
7.2512
7.2460
7.2305
7.2240
7.2037
7.1826
5.9127
5.8991
2.9953
2.9910
2.9504
2.9462
2.6396
2.6245
2.5947
2.5797
2.4020
1.98
3.01
7.09
0.98
1.00
1.02
3.00
11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

191.8876
145.0162
139.9883
136.5286
136.4209
135.3893
134.0130
130.3939
128.9666
128.4992
127.3356
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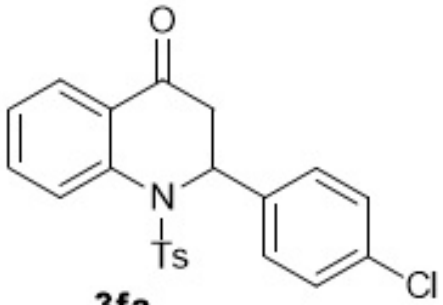
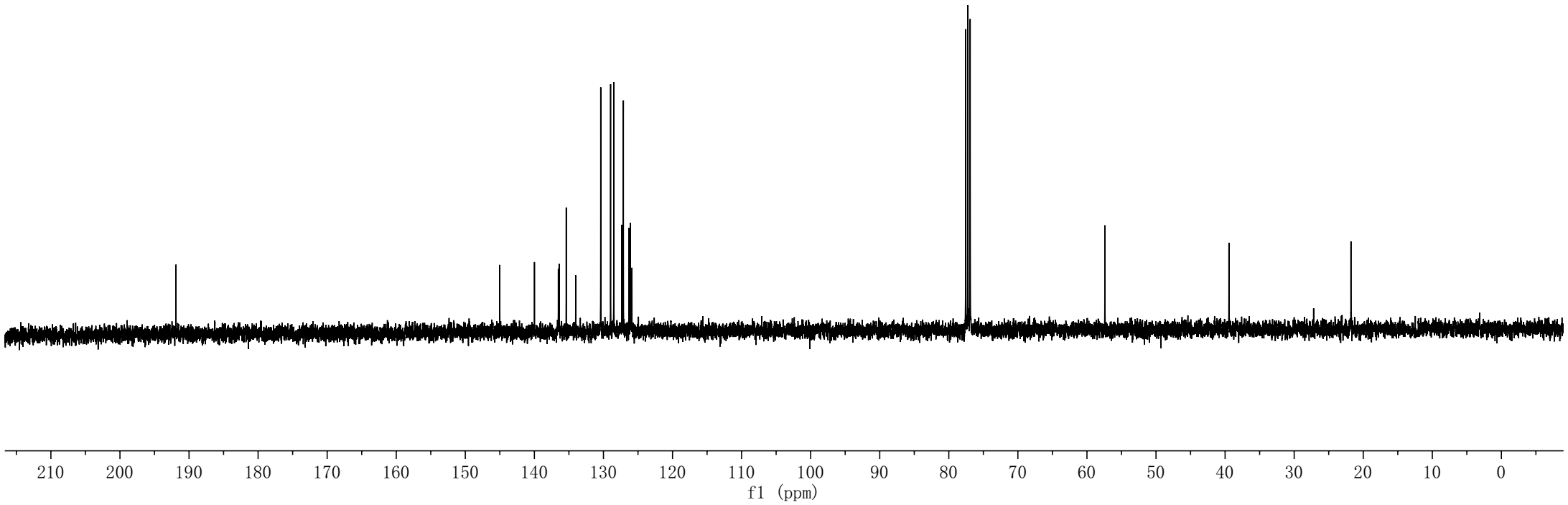
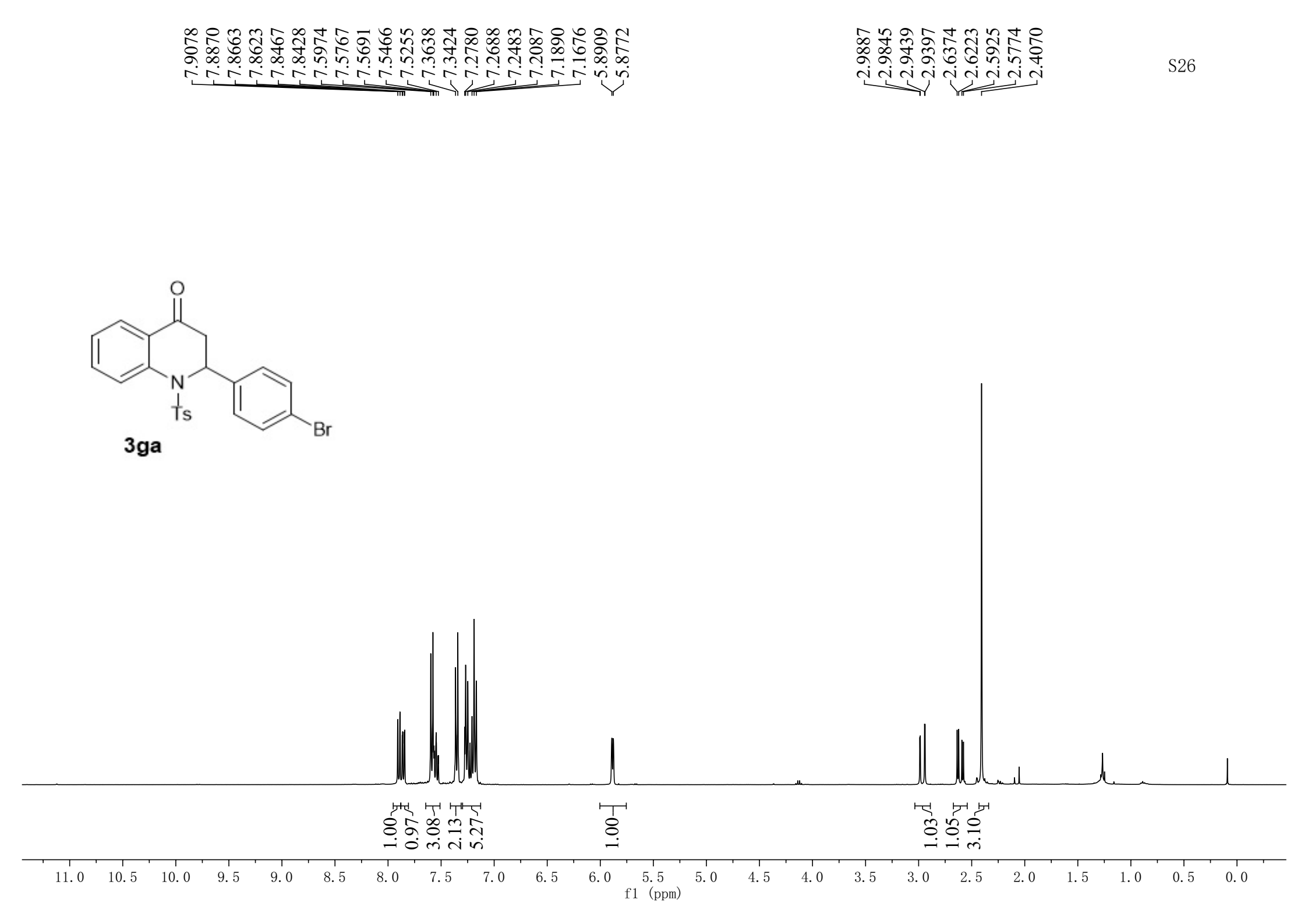
77.2263
76.9076
57.4051
39.4439
21.7796



3fa

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7.8428
7.5974
7.5767
7.5691
7.5466
7.5255
7.3638
7.3424
7.2780
7.2688
7.2483
7.2087
7.1890
7.1676
5.8909
5.8772
2.9887
2.9845
2.9439
2.9397
2.6374
2.6223
2.5925
2.5774
2.4070
O
N
Ts
Br
3ga
1.00
0.97
3.08
2.13
5.27
1.00
1.03
1.05
3.10
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

191.8297
145.0190
139.9819
136.9639
136.5255
135.3939
131.9245
130.3937
128.8230
127.3465
127.1205
126.2787
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125.8819
122.2157
77.5340
77.2162
76.8986
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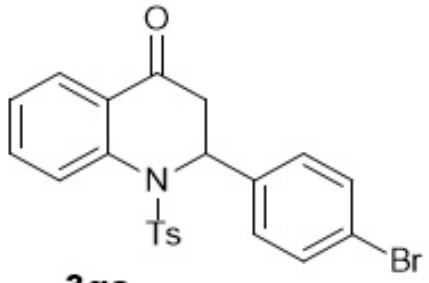
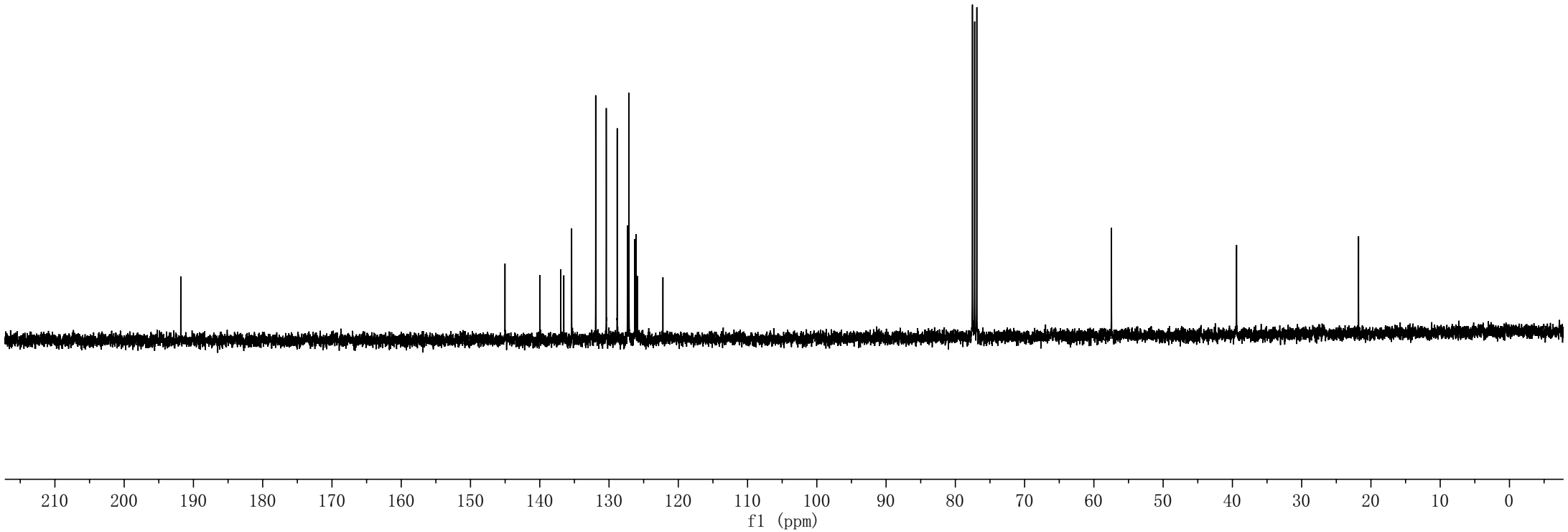
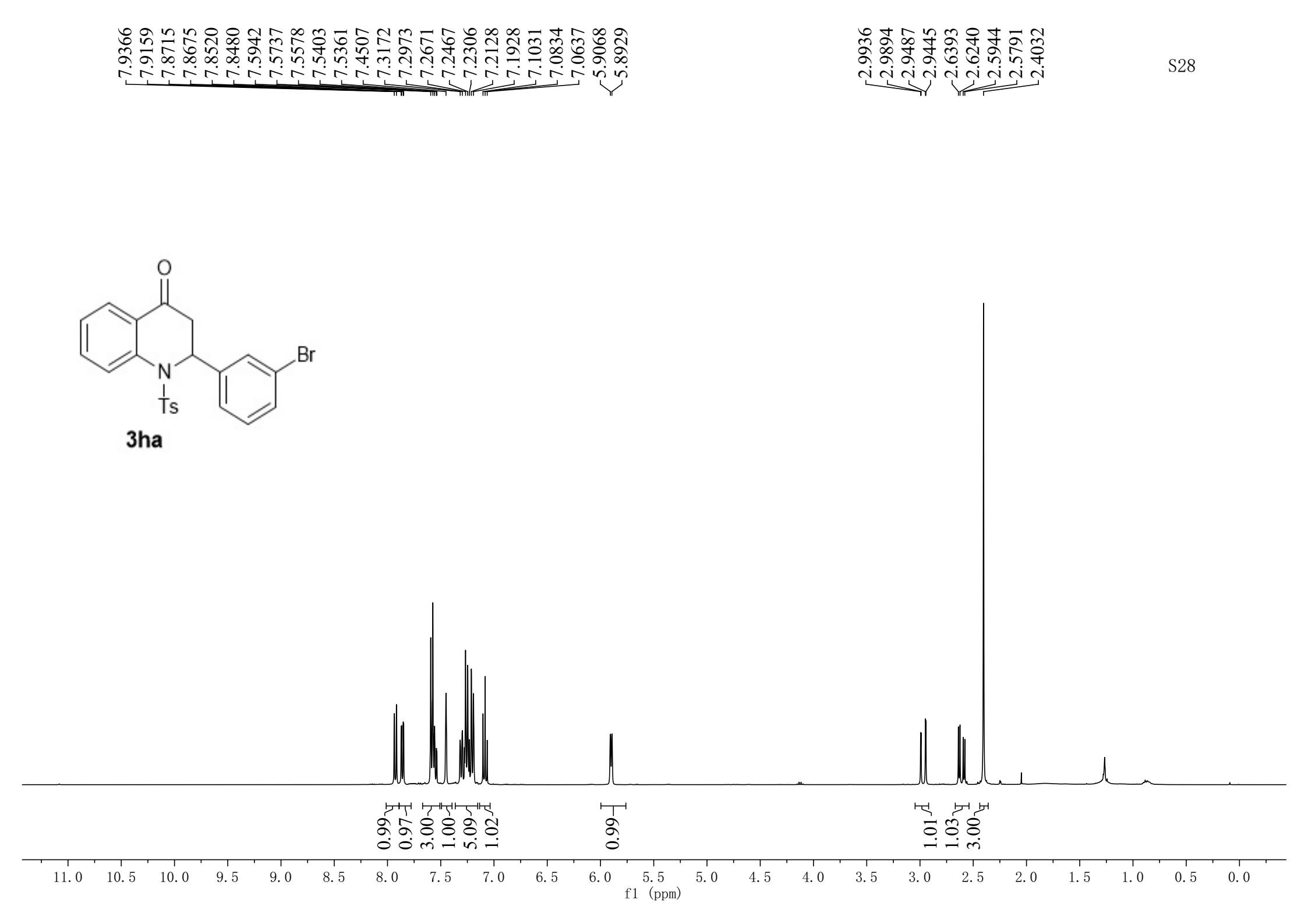
39.4008
21.7866



3ga

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7.8520
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7.5942
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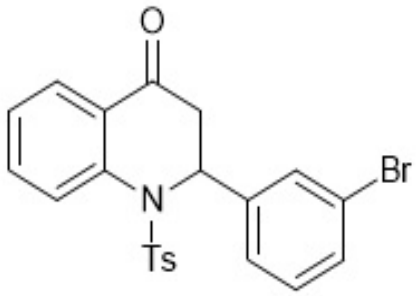
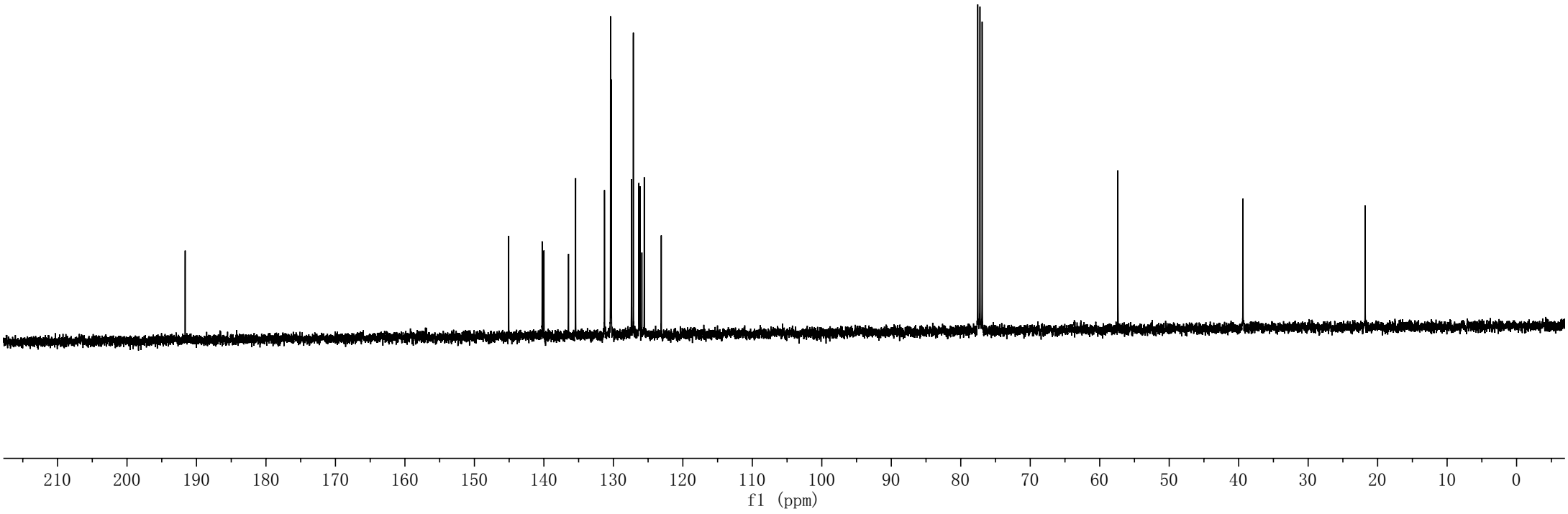
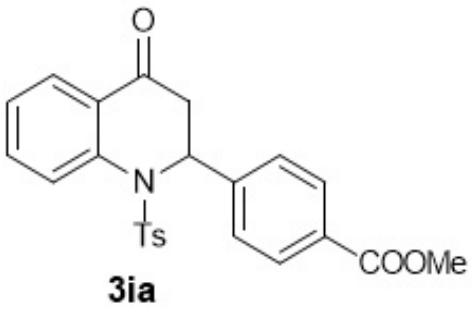
7.5578
7.5403
7.5361
7.4507
7.3172
7.2973
7.2671
7.2467
7.2306
7.2128
7.1928
7.1031
7.0834
7.0637
5.9068
5.8929
2.9936
2.9894
2.9487
2.9445
2.6393
2.6240
2.5944
2.5791
2.4032
O
N
Ts
Br
3ha
0.99
0.97
3.00
1.00
5.09
1.02
0.99
1.01
1.03
3.00
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

191.6267
145.0638
140.2482
139.9878
136.4562
135.4334
131.2748
130.4103
130.3000
127.3923
127.1248
126.3274
126.1729
125.8957
125.5558
123.1044
77.5546
77.2363
76.9192
57.3834
39.3831
21.7971



3ha




O
N
Ts
COOMe

3ia

7.9130
7.8917
7.8706
7.8391
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7.6023
7.5816
7.5477
7.5302
7.5086
7.3817
7.3613
7.2774
7.2623
7.2422
7.2030
7.1835
7.1640
5.9815
5.9678
3.8389
3.0563
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3.0114
3.0075
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2.6706
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4.06
3.07
2.08
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1.06
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3.01
1.03
1.02
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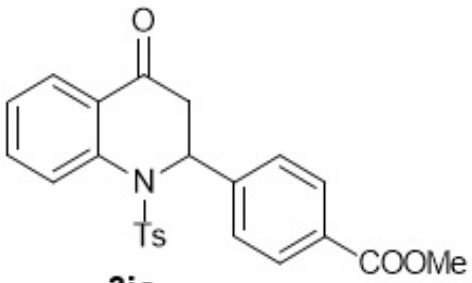
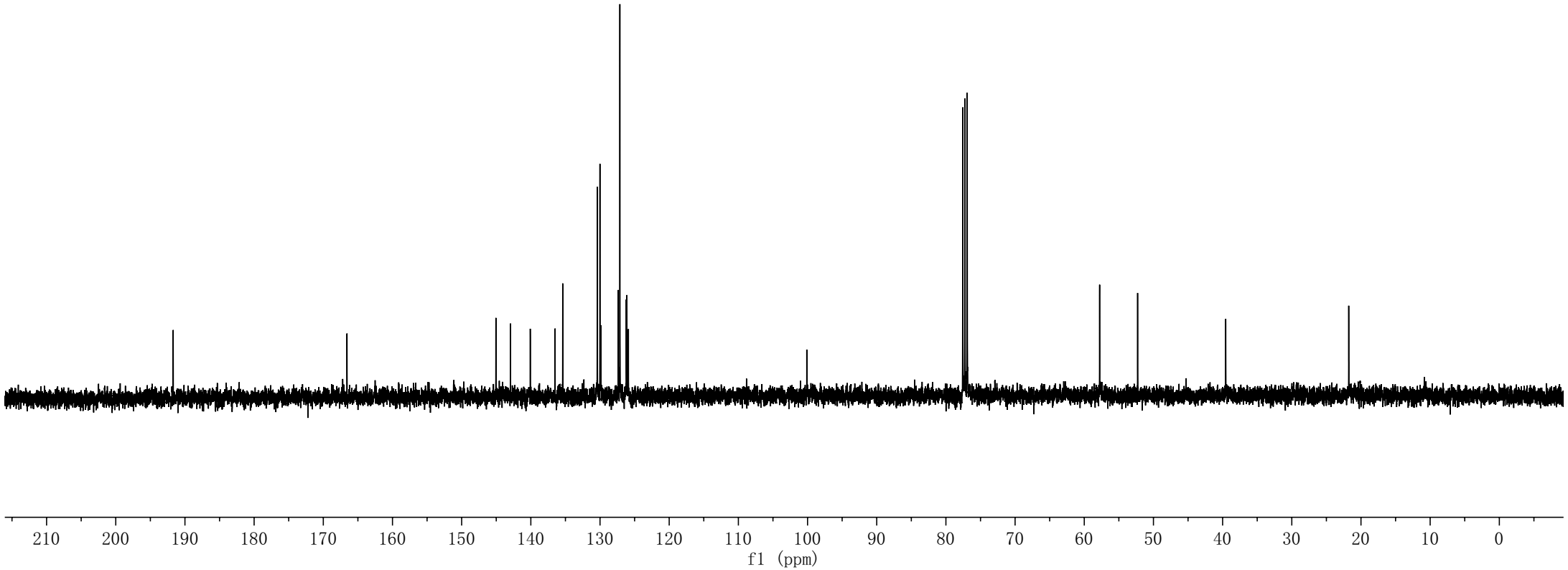
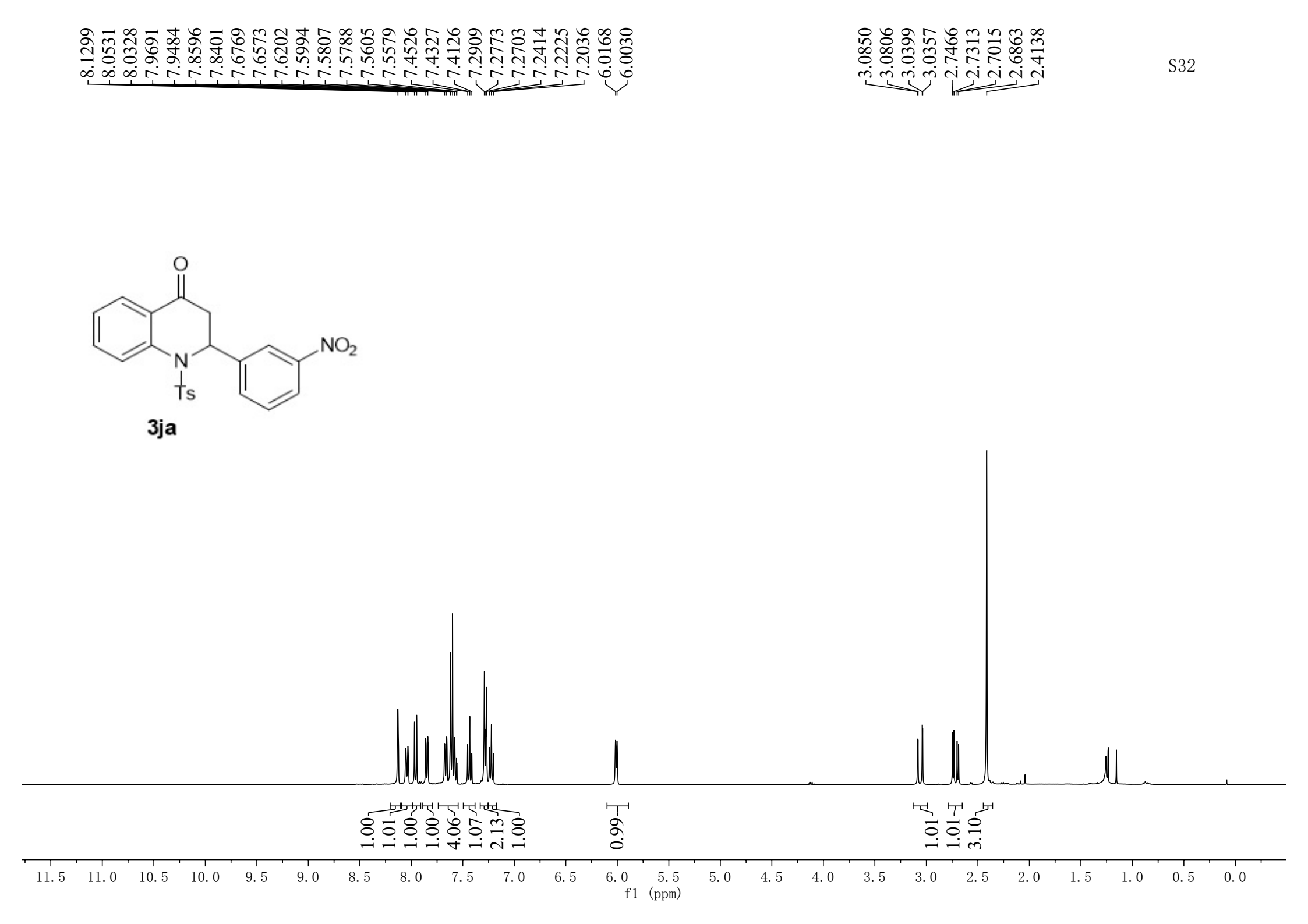
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

191.6980
166.5751
145.0492
142.9422
140.0809
136.4997
135.3894
130.3984
130.0101
129.8645
127.3616
127.1298
126.2020
126.1136
125.8962
100.1104
77.5587
77.2408
76.9228
57.7795
52.2868
39.5496
21.7691



3ia

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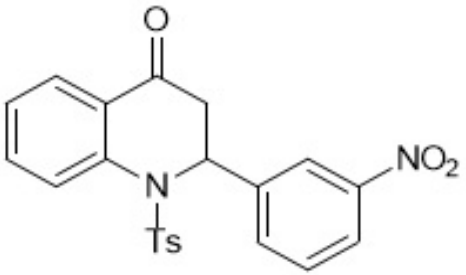
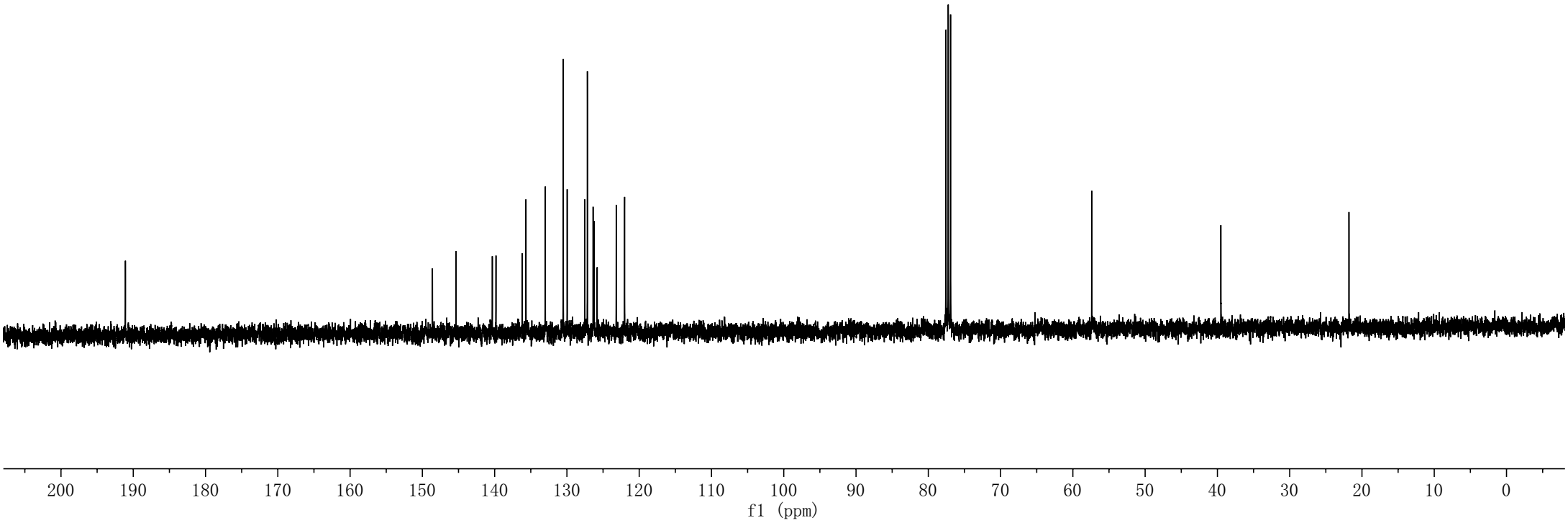
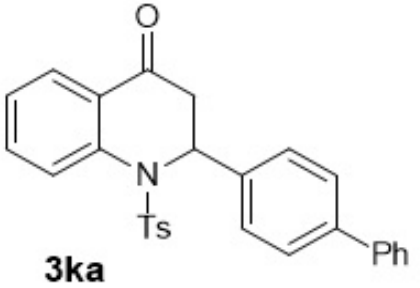
8.0328
7.9691
7.9484
7.8596
7.8401
7.6769
7.6573
7.6202
7.5994
7.5807
7.5788
7.5605
7.5579
7.4526
7.4327
7.4126
7.2909
7.2773
7.2703
7.2414
7.2225
7.2036
6.0168
6.0030
3.0850
3.0806
3.0399
3.0357
2.7466
2.7313
2.7015
2.6863
2.4138
O
N
Ts
NO2
3ja
1.00
1.01
1.00
1.00
4.06
1.07
2.13
1.00
0.99
1.01
1.01
3.10
11.5
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

191.0840
148.6053
145.3355
140.3205
139.8149
136.1934
135.6637
132.9907
130.5093
129.9639
127.5291
127.1700
126.3768
126.2436
125.8105
123.1773
122.0210
77.5586
77.2401
76.9221
57.3919
39.5214
21.7981

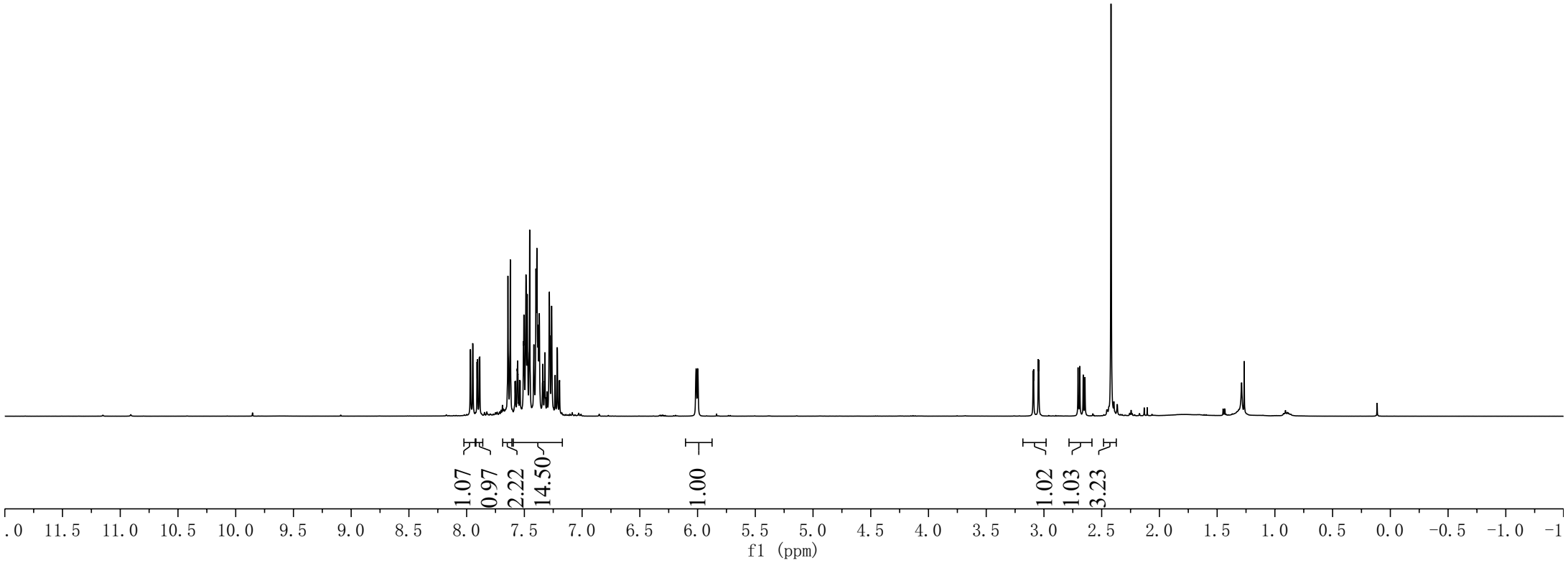


3ja




O
N
Ts
Ph

3ka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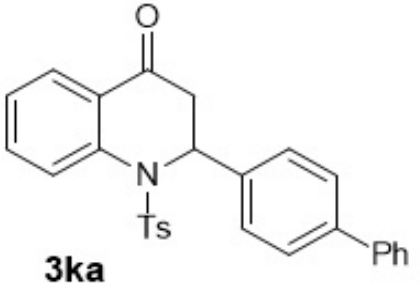
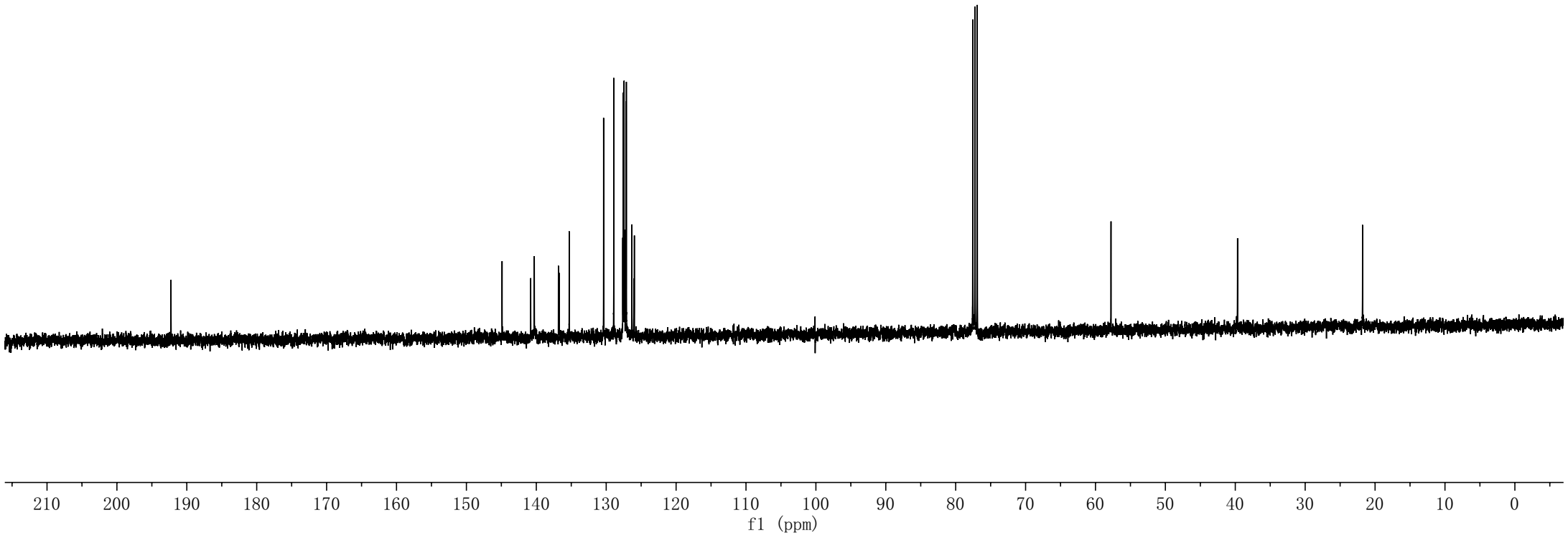
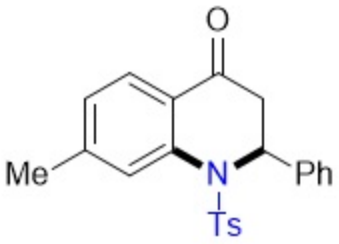
7.9098
7.9058
7.8903
7.8863
7.6422
7.6215
7.5804
7.5370
7.5078
7.4860
7.4540
7.4177
7.3913
7.3706
7.3402
7.2840
7.2330
7.1952
6.0124
5.9989
3.0937
3.0896
3.0490
3.0449
2.7047
2.6895
2.6599
2.6448
2.4190
1.07
0.97
2.22
14.50
1.00
1.02
1.03
3.23
f1 (ppm)

192.2630
144.8957
140.8002
140.2856
136.8337
136.7440
135.2925
130.3706
128.9153
127.6340
127.5430
127.4411
127.3348
127.1694
127.1121
126.3258
126.0433
125.9709
77.5509
77.2334
76.9150
57.7793
39.6771
21.7915



3ka

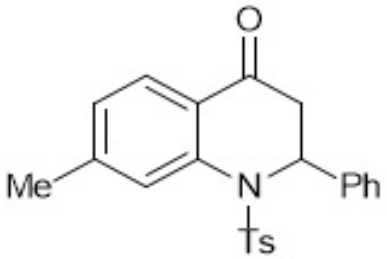



O
Me
N
Ts
Ph

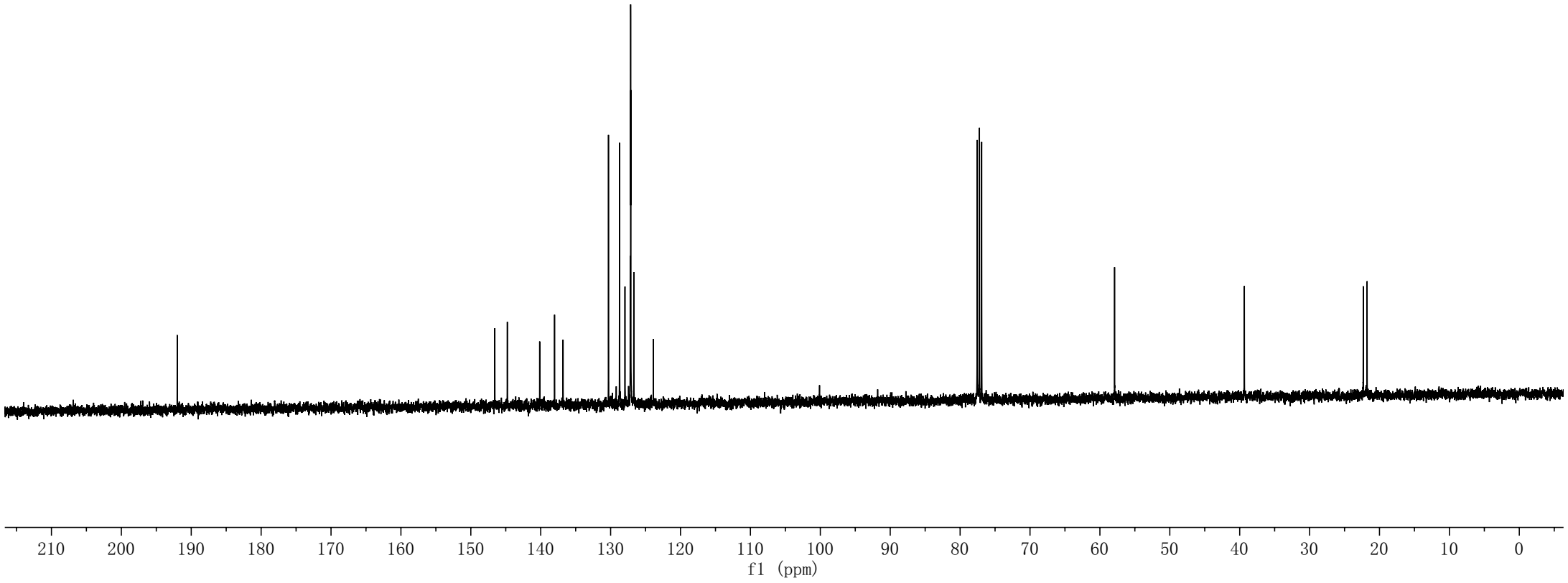
3la

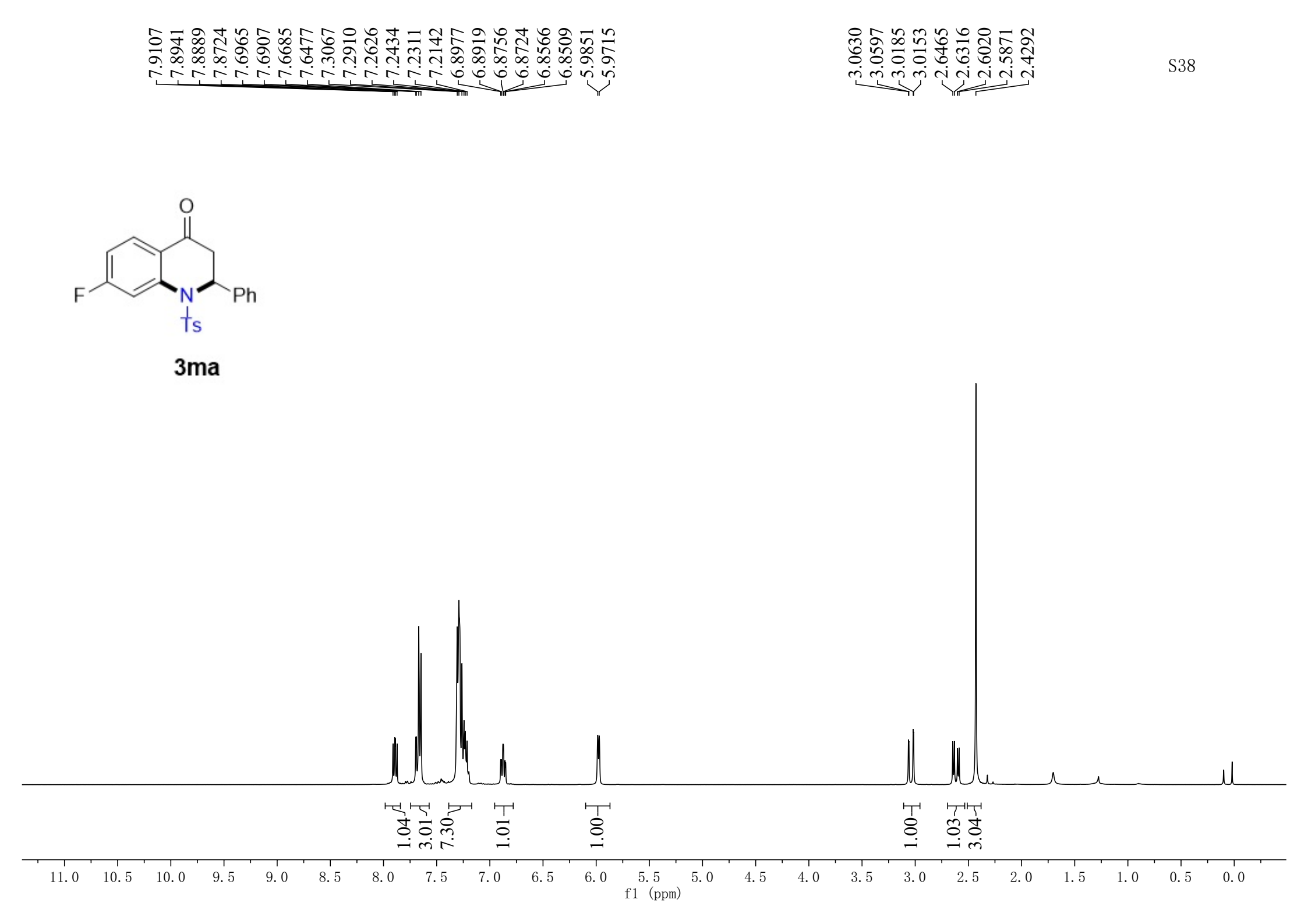
7.7682
7.7483
7.7087
7.6127
7.5926
7.3230
7.3043
7.2710
7.2509
7.2426
7.2229
7.1871
7.1710
7.0141
6.9943
5.9233
5.9092
2.9904
2.9457
2.5939
2.5788
2.5491
2.5340
2.4114
2.3928
2.07
2.02
7.16
1.02
0.96
1.00
1.02
6.00
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0
f1 (ppm)

192.0040
146.5639
144.7789
140.1493
138.0203
136.8014
130.3065
128.7299
127.9483
127.1945
127.1327
127.1093
126.6836
123.8973
77.5530
77.2349
76.9169
57.9012
39.3330
22.3238
21.7716



3la

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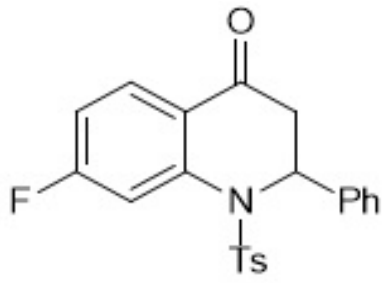
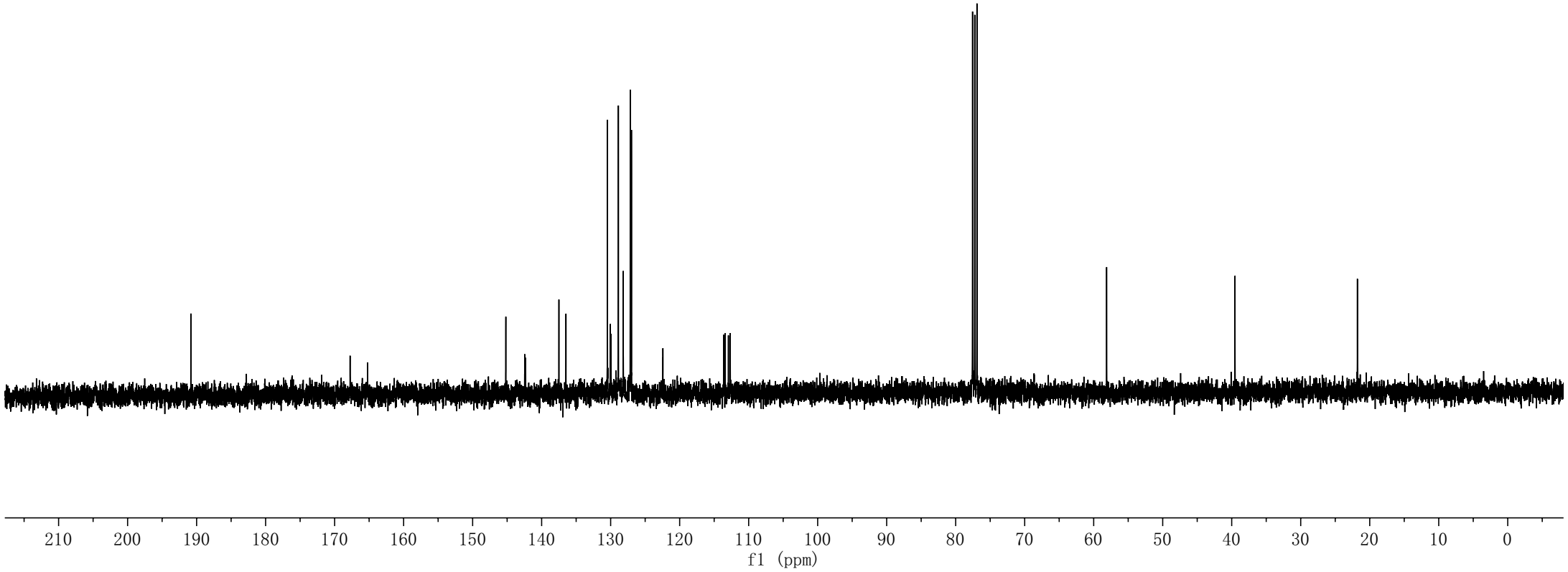
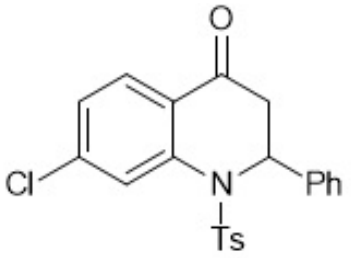
7.8889
7.8724
7.6965
7.6907
7.6685
7.6477
7.3067
7.2910
7.2626
7.2434
7.2311
7.2142
6.8977
6.8919
6.8756
6.8724
6.8566
6.8509
5.9851
5.9715
3.0630
3.0597
3.0185
3.0153
2.6465
2.6316
2.6020
2.5871
2.4292
O
F
N
Ts
Ph
3ma
1.04
3.01
7.30
1.01
1.00
1.00
1.03
3.04
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

190.8226
167.7581
165.1054
145.1888
137.4957
136.4735
130.4666
130.0456
129.9371
128.8774
128.1770
127.1588
126.9807
122.4249
122.4282
113.6282
113.4071
112.9353
112.6715
77.5548
77.2366
76.9192
58.1263
39.5301
21.7857



3ma

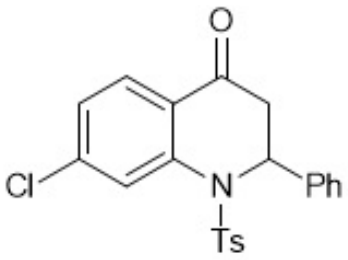



O
Cl
N
Ph
Ts

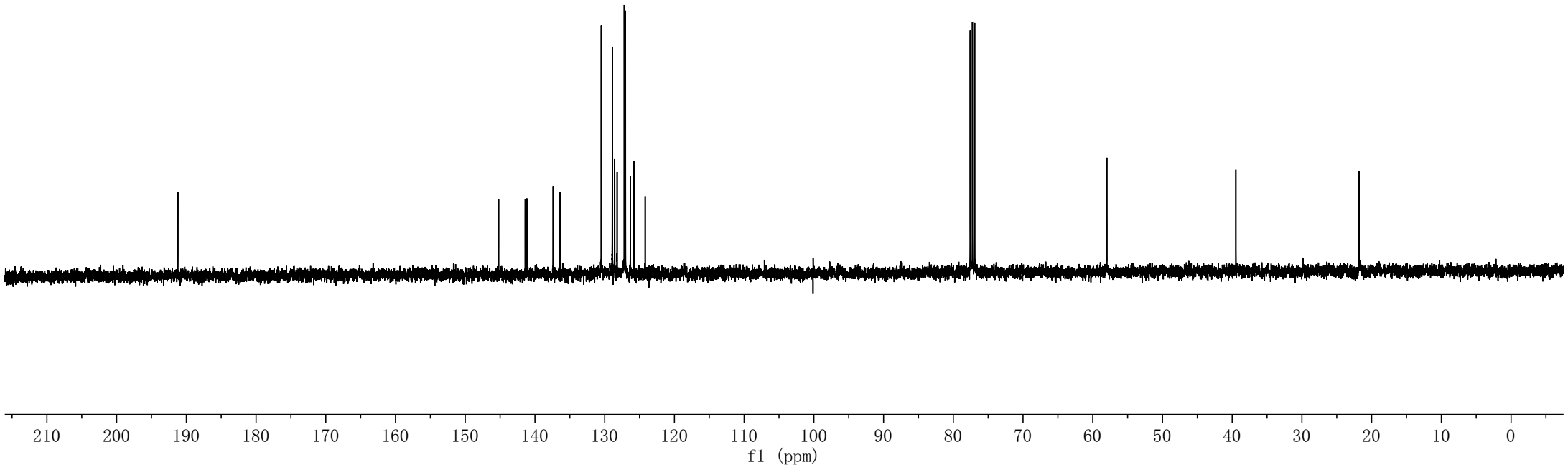
3na

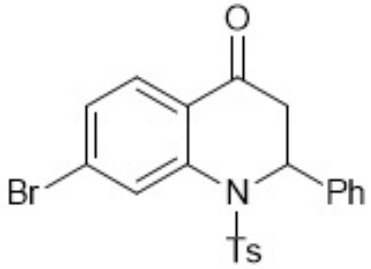
7.9595
7.9547
7.8038
7.7827
7.6585
7.6377
7.3002
7.2785
7.2512
7.2319
7.2190
7.2098
7.2021
7.1509
7.1463
7.1269
7.1253
5.9569
5.9440
3.0594
3.0551
3.0147
3.0105
2.6333
2.6183
2.5886
2.5737
2.4176
0.92
1.01
2.01
7.19
0.98
0.98
1.00
1.02
3.05
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

191.2250
145.2119
141.3974
141.1546
137.3931
136.4298
130.4907
128.9039
128.5629
128.2184
127.1931
127.0203
126.3164
125.8174
124.1976
77.5723
77.2545
76.9361
57.9833
39.4710
21.8076

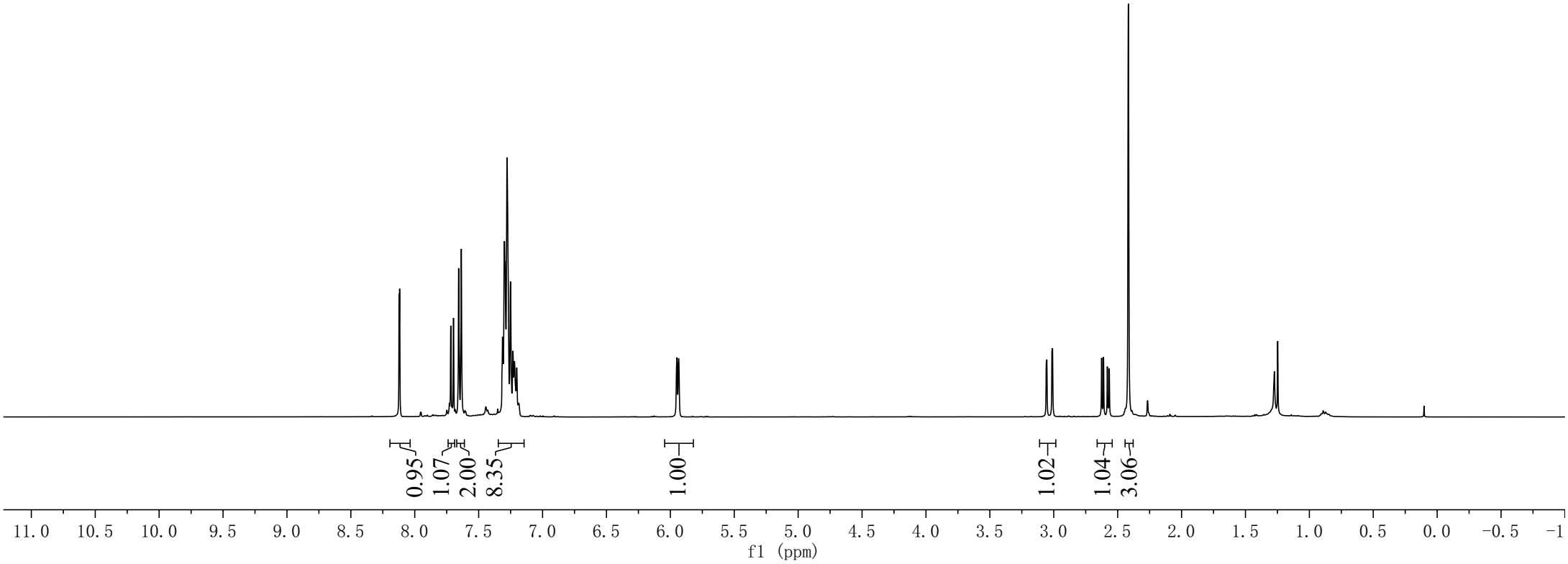


3na




O
Br
N
Ph
Ts

3oa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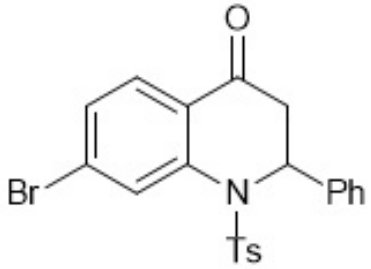
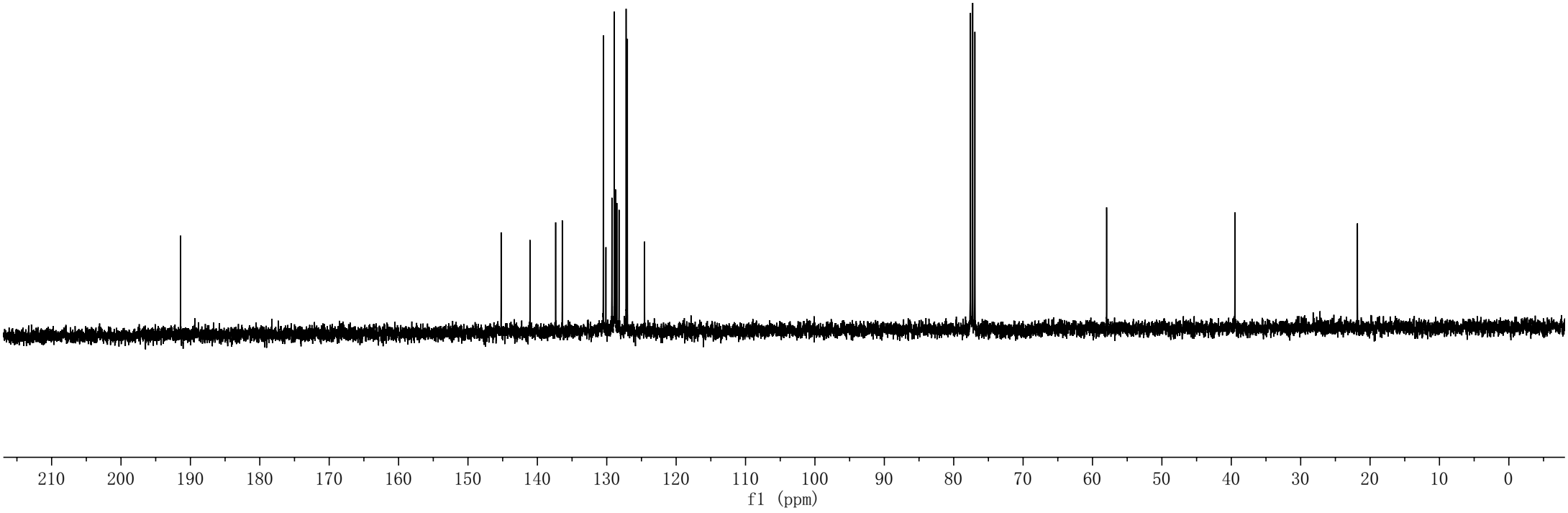
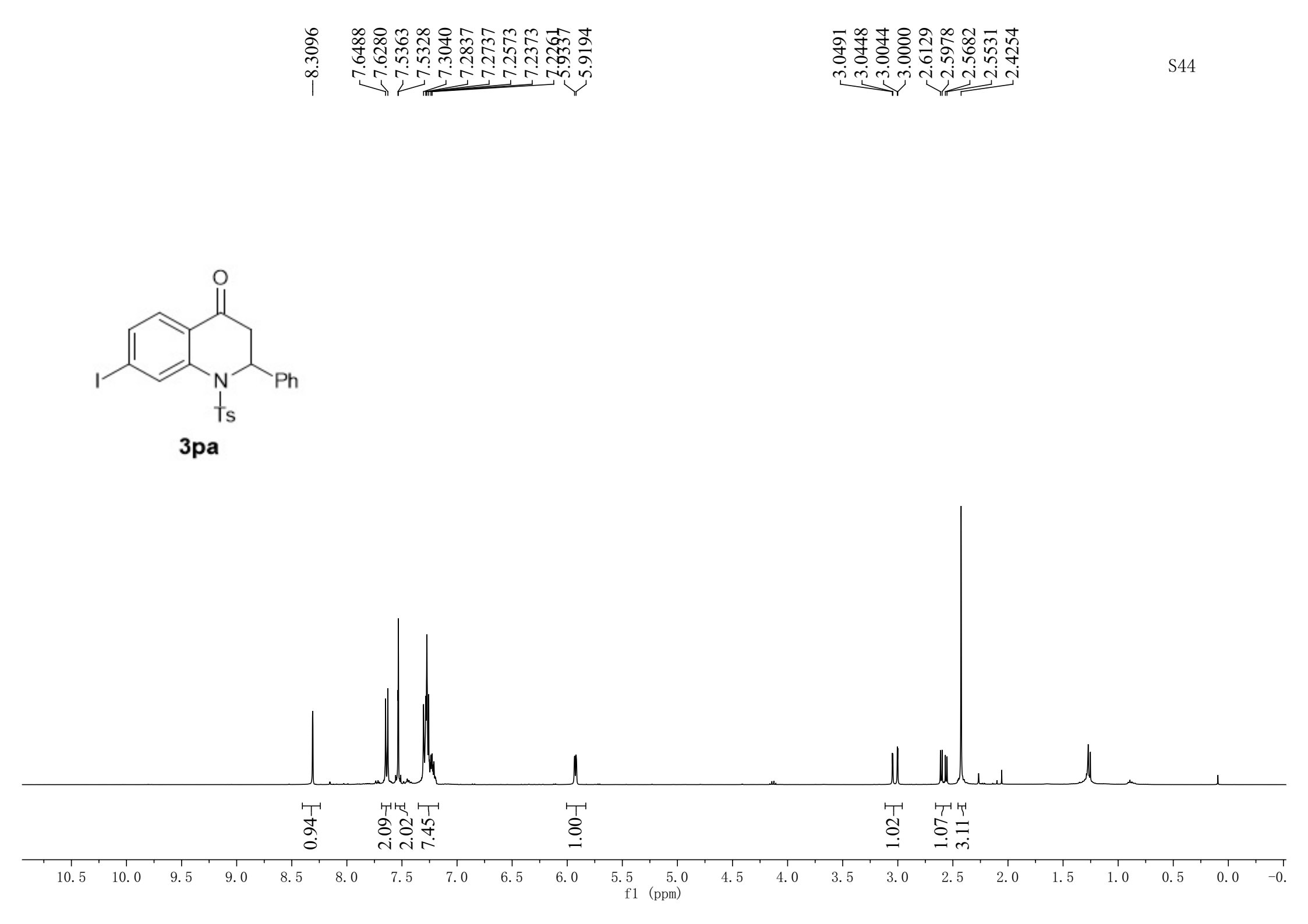
8.1182
7.7177
7.6968
7.6563
7.6357
7.3133
7.2988
7.2978
7.2931
7.2775
7.2507
7.2320
7.2197
7.2020
7.1909
7.1864
5.9487
5.9352
3.0584
3.0545
3.0137
3.0098
2.6256
2.6106
2.5809
2.5659
2.4163
0.95
1.07
2.00
8.35
1.00
1.02
1.04
3.06
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1
f1 (ppm)

191.4228
145.2216
141.0612
137.3642
136.4083
130.4966
130.1201
129.2562
128.9145
128.7343
128.5465
128.2314
127.2085
127.0282
124.5529
77.5830
77.2647
76.9471
57.9639
39.4774
21.8195



3oa

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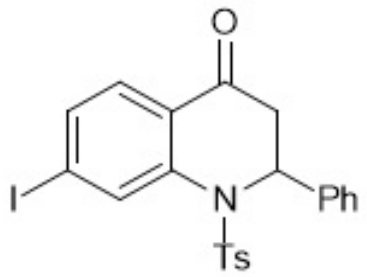
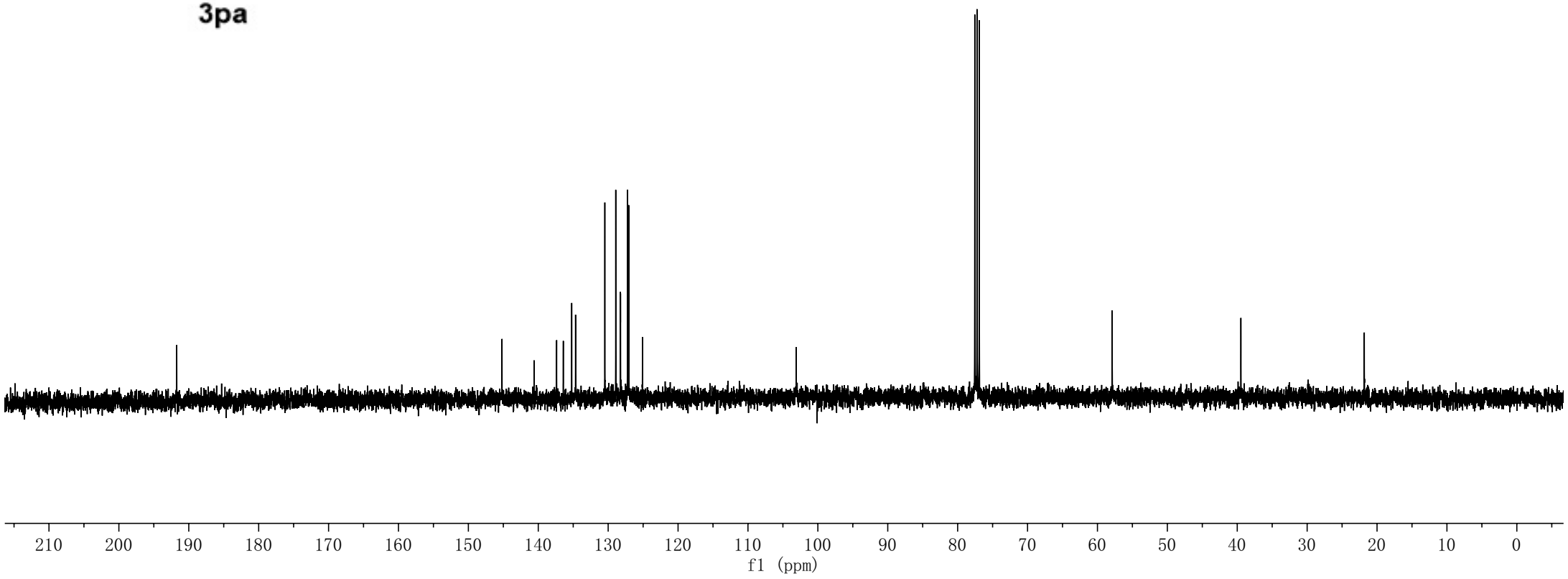
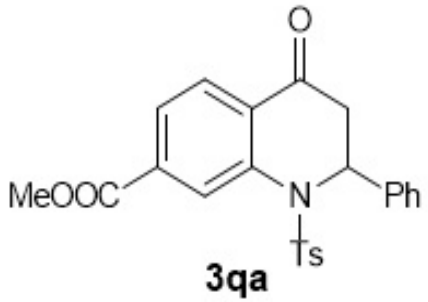
7.6488
7.6280
7.5363
7.5328
7.3040
7.2837
7.2737
7.2573
7.2373
7.2261
5.9337
5.9194
3.0491
3.0448
3.0044
3.0000
2.6129
2.5978
2.5682
2.5531
2.4254
O
I
N
Ph
Ts
3pa
0.94
2.09
2.02
7.45
1.00
1.02
1.07
3.11
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.
f1 (ppm)

191.7194
145.1858
140.5907
137.3727
136.4181
135.2127
134.6642
130.4751
128.9140
128.2443
128.2291
127.2303
127.0472
125.0945
103.1015
77.5472
77.2290
76.9119
57.8909
39.4778
21.8254



3pa

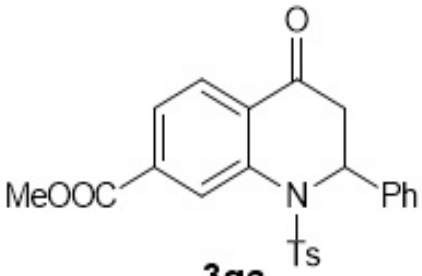



O
MeOOC
N
Ph
Ts

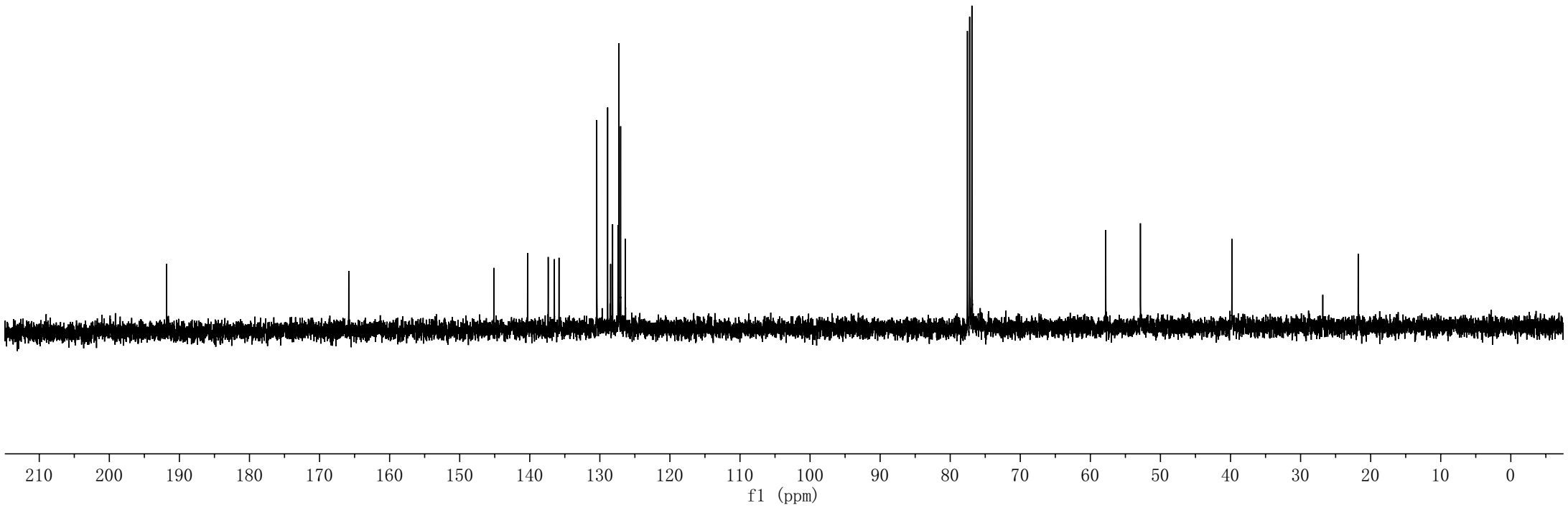
3qa

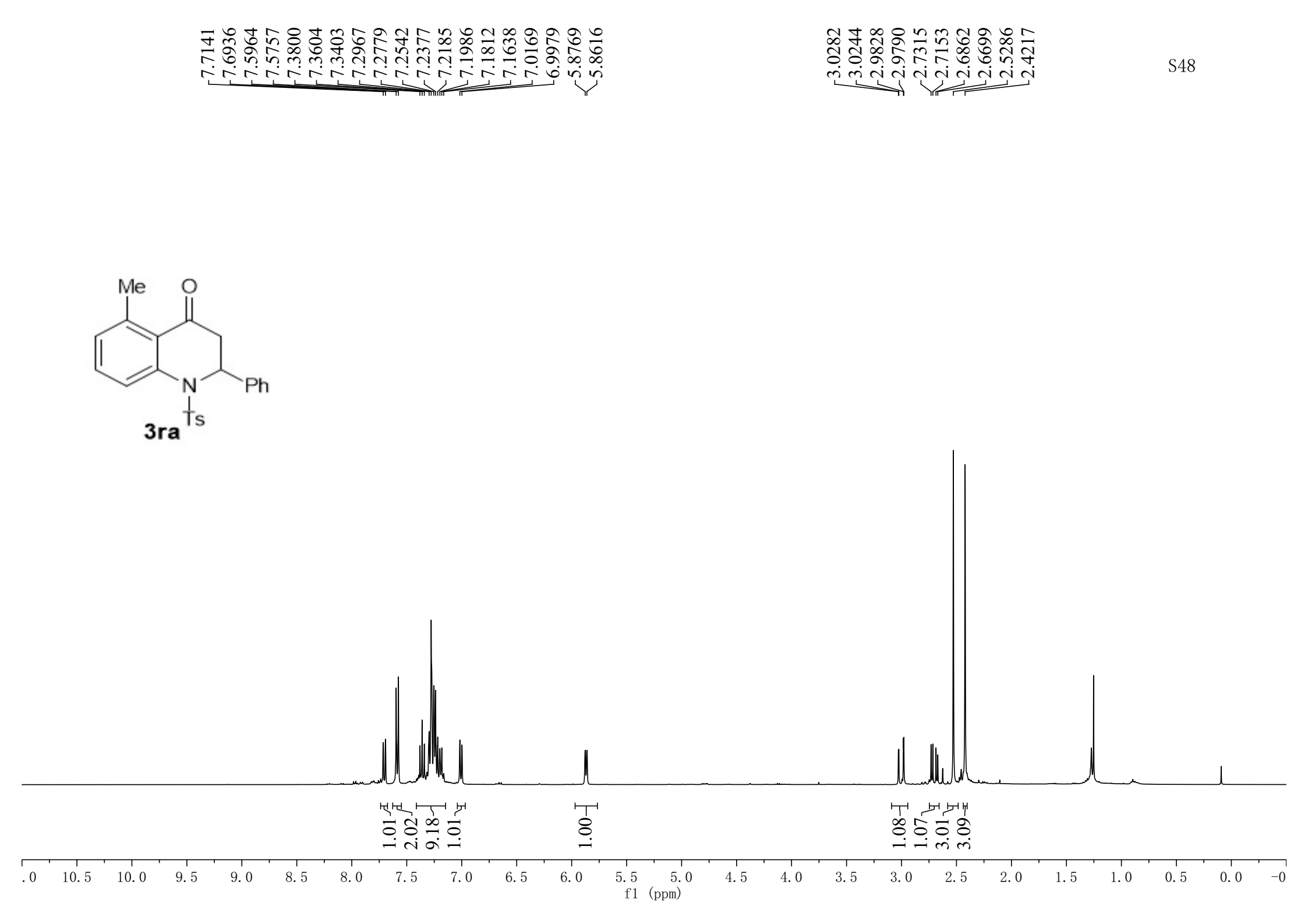
8.5451
8.5419
7.9278
7.9075
7.8314
7.8278
7.8111
7.8075
7.6429
7.6222
7.2913
7.2831
7.2702
7.2665
7.2503
7.2444
7.2336
7.2030
7.1862
5.9786
5.9654
3.9513
3.1041
3.0999
3.0593
3.0551
2.7023
2.6872
2.6574
2.6424
2.4215
0.91
1.02
1.00
2.00
7.21
1.00
3.15
1.01
1.02
3.07
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
−1
−2
−3
f1 (ppm)

191.8270
165.8309
145.1236
140.3166
137.3688
136.4890
135.8268
130.4372
128.8861
128.4647
128.1780
127.4120
127.2796
127.0362
126.3739
77.5447
77.2268
76.9083
57.8074
52.8562
39.8007
21.7809



3qa

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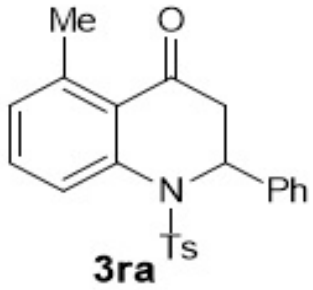
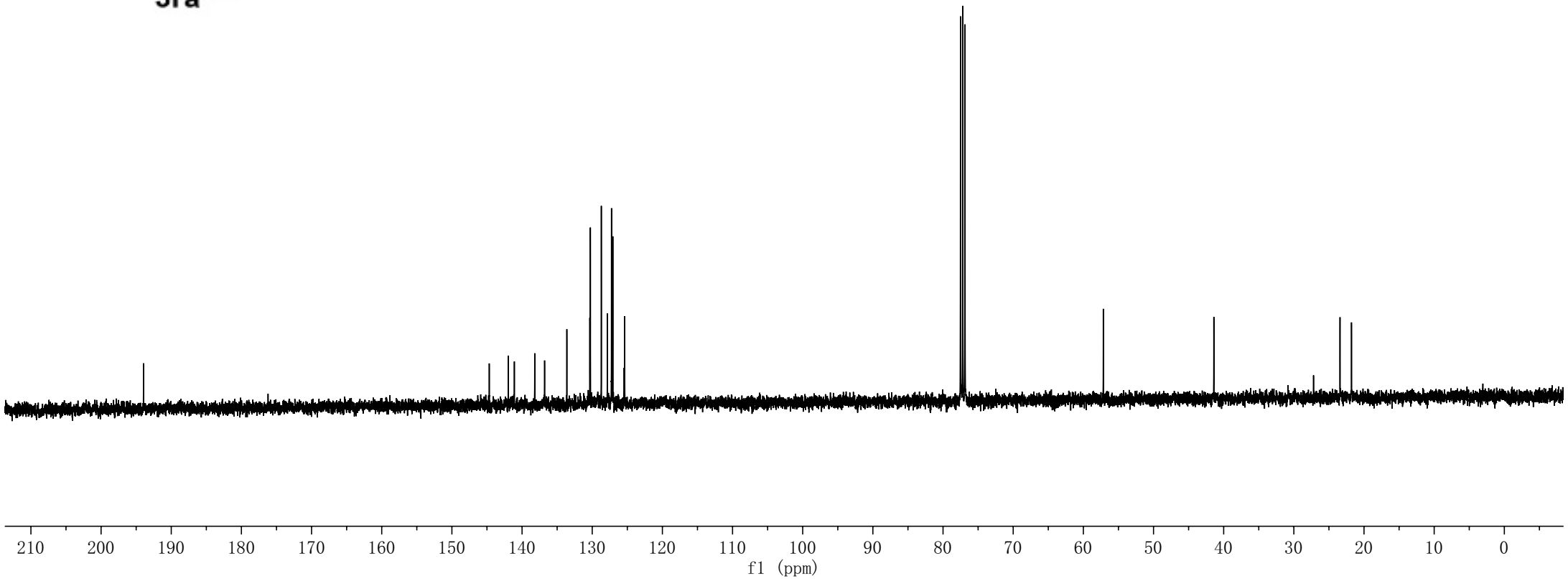
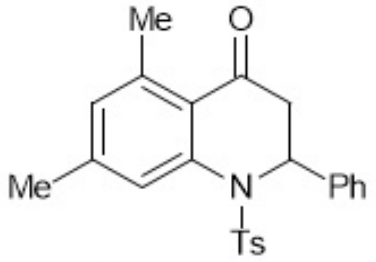
7.3800
7.3604
7.3403
7.2967
7.2779
7.2542
7.2377
7.2185
7.1986
7.1812
7.1638
7.0169
6.9979
5.8769
5.8616
3.0282
3.0244
2.9828
2.9790
2.7315
2.7153
2.6862
2.6699
2.5286
2.4217
Me
O
N
Ph
Ts
3ra
1.01
2.02
9.18
1.01
1.00
1.08
1.07
3.01
3.09
f1 (ppm)

193.9442
144.6732
141.9578
141.0961
138.1939
136.7862
133.6150
130.3413
130.2617
128.7026
127.8418
127.2532
127.0600
125.3768
77.5101
77.1919
76.8749
57.1569
41.4022
23.4203
21.7836

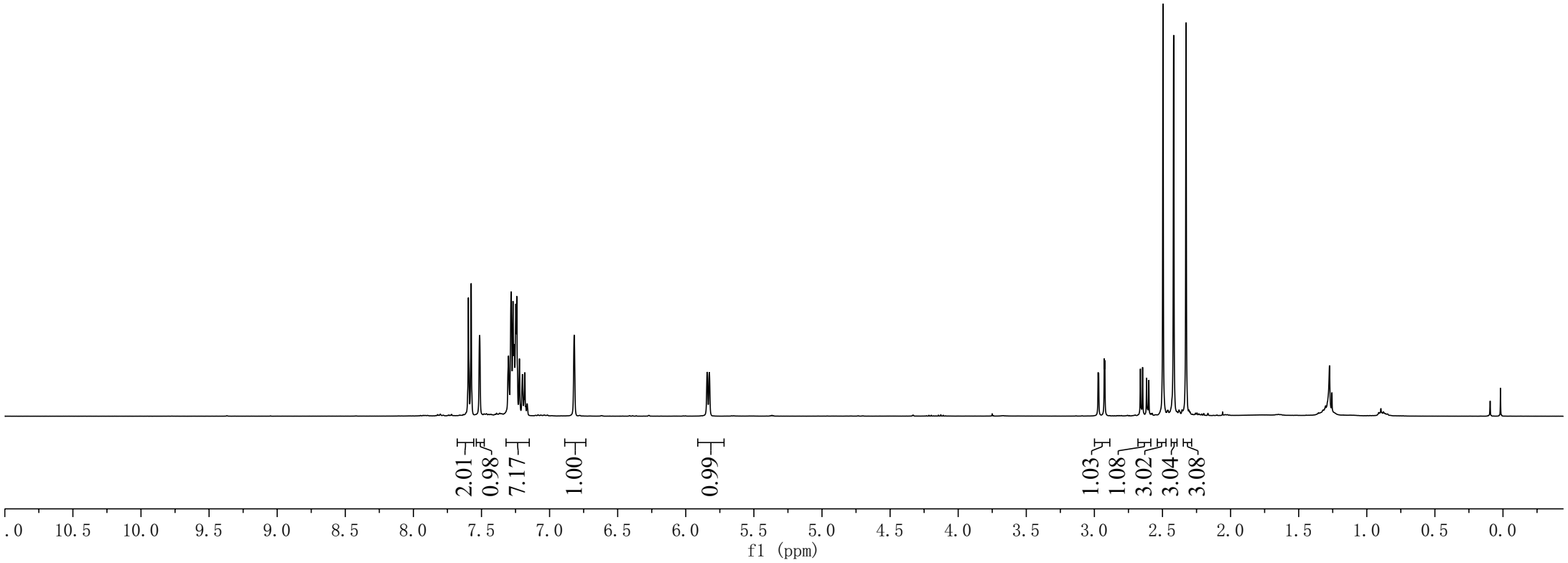


3ra

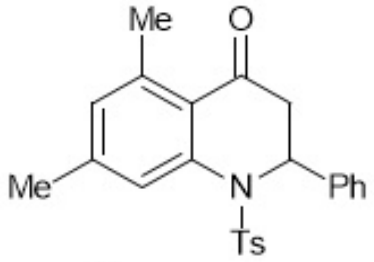



Me
O
Me
N
Ph
Ts

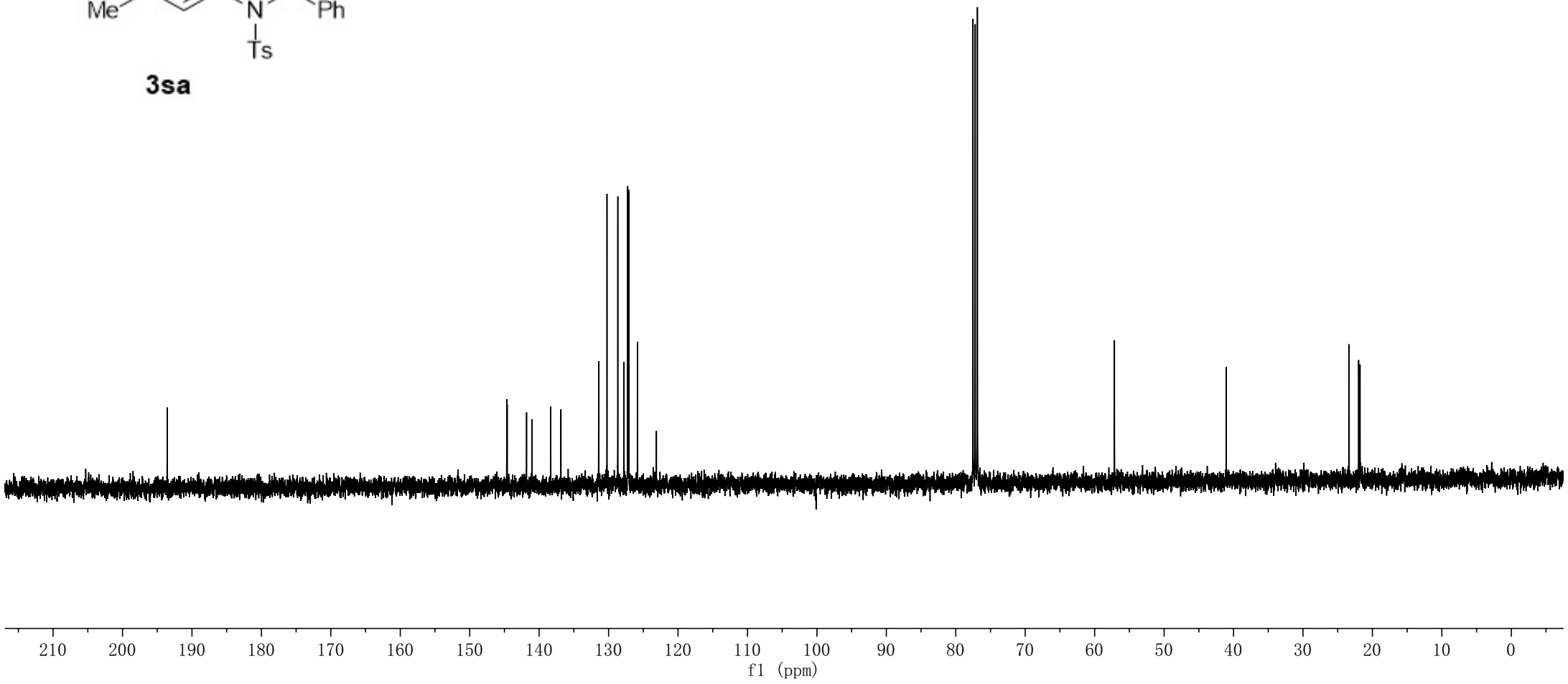
3sa

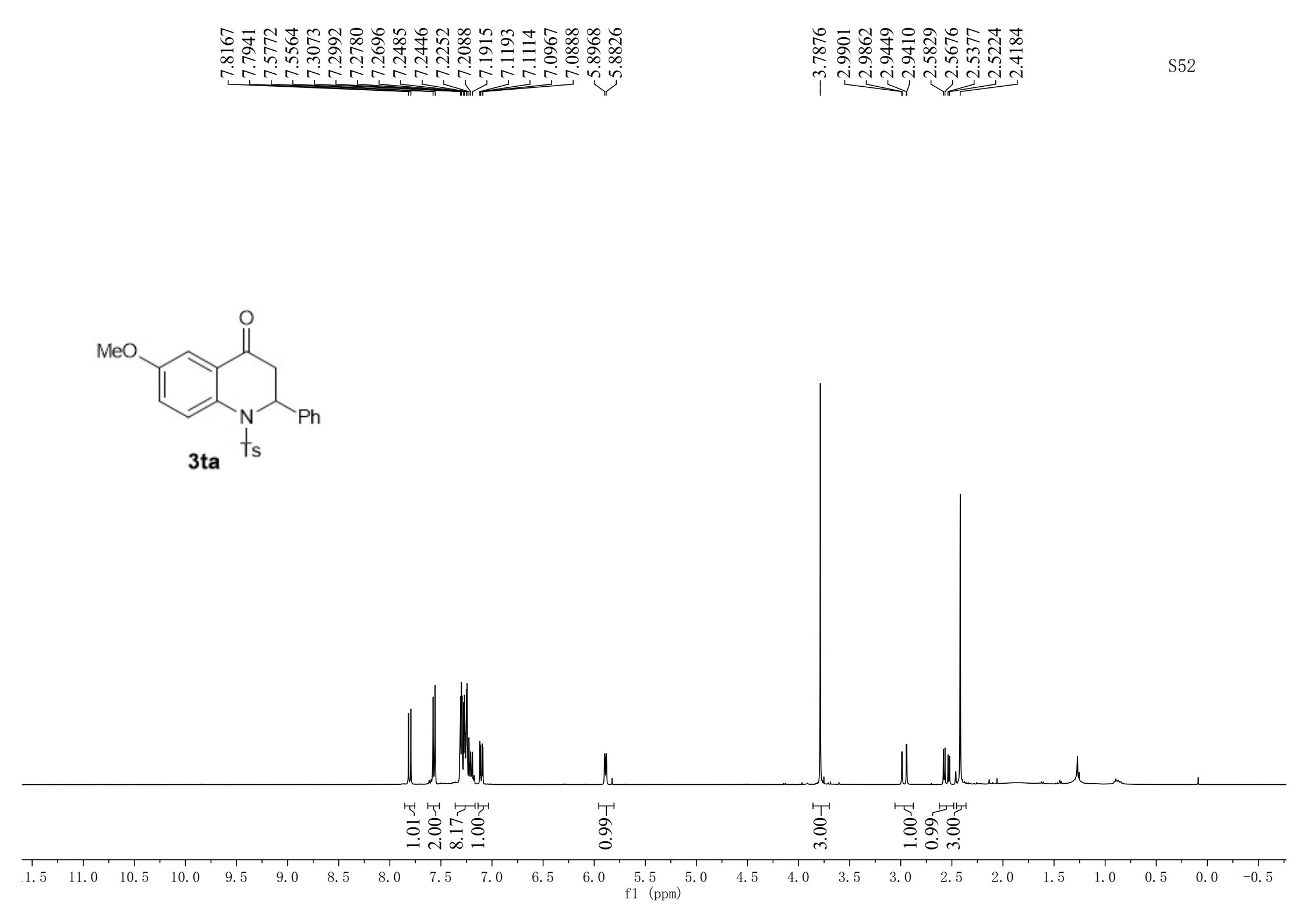

7.5962
7.5755
7.5137
7.3017
7.2825
7.2686
7.2578
7.2478
7.2407
7.2212
7.1995
7.1820
6.8192
5.8426
5.8273
2.9723
2.9687
2.9270
2.9235
2.6620
2.6458
2.6166
2.6005
2.4961
2.4180
2.3270
2.01
0.98
7.17
1.00
0.99
1.03
1.08
3.02
3.04
3.08
f1 (ppm)

193.5649
144.6644
144.5997
141.8114
141.0193
138.3281
136.8615
131.4281
130.2265
128.6686
127.7890
127.2470
127.1003
125.8459
123.1124
77.5196
77.2017
76.8843
57.1498
41.0515
23.3892
21.9807
21.7801

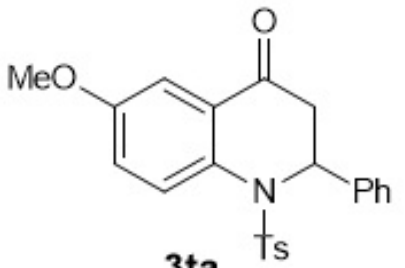


3sa

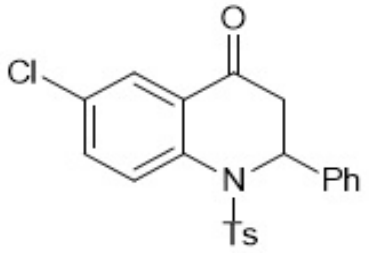



7.8167
7.7941
7.5772
7.5564
7.3073
7.2992
7.2780
7.2696
7.2485
7.2446
7.2252
7.2088
7.1915
7.1193
7.1114
7.0967
7.0888
5.8968
5.8826
3.7876
2.9901
2.9862
2.9449
2.9410
2.5829
2.5676
2.5377
2.5224
2.4184
MeO
O
N
Ph
Ts
3ta
1.01
2.00
8.17
1.00
0.99
3.00
1.00
0.99
3.00
f1 (ppm)

192.3494
157.5887
144.7329
137.9723
136.6341
133.4624
130.3113
128.7312
128.5324
127.9739
127.1358
127.0905
123.0135
109.0707
77.5122
77.1947
76.8768
57.8494
55.6850
39.0909
21.7779



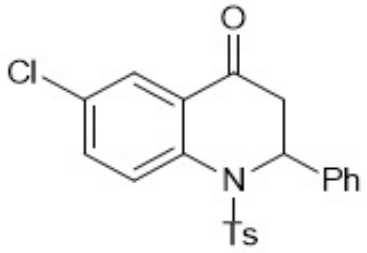
3ta


O
Cl
N
Ph
Ts

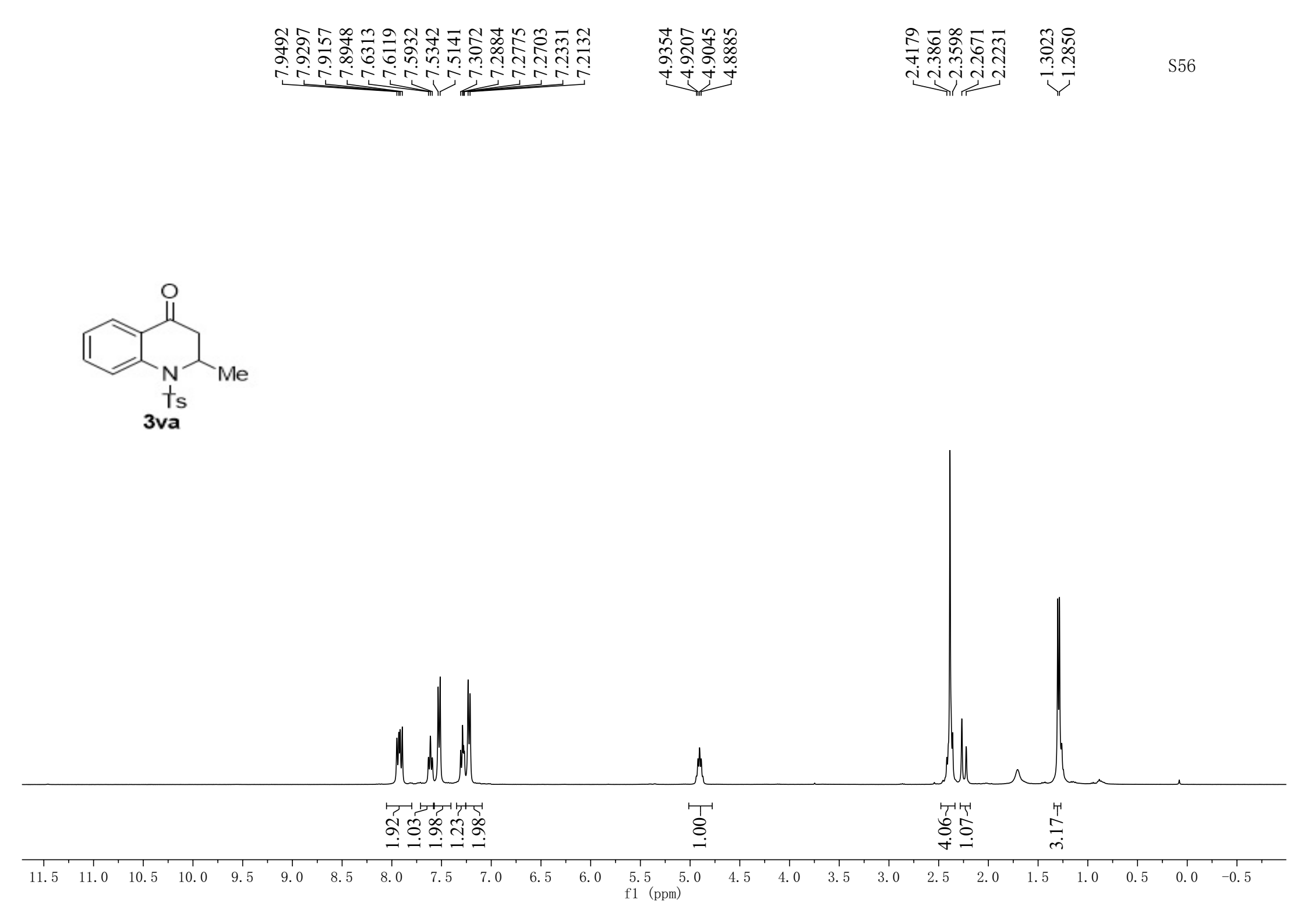
3ua

7.8892
7.8671
7.8153
7.8088
7.6212
7.6006
7.4894
7.4829
7.4673
7.4607
7.3033
7.2776
7.2576
7.2377
7.2122
7.1960
5.9389
5.9256
3.0538
3.0499
3.0088
3.0050
2.5994
2.5843
2.5545
2.5394
2.4340
1.07
1.01
2.04
1.07
7.34
0.97
1.00
1.12
3.19
f1 (ppm)

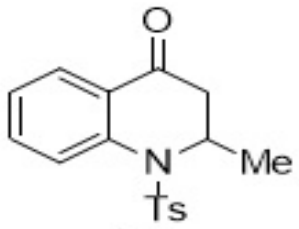
191.1444
145.1446
137.9694
137.3748
136.4748
135.0163
132.0039
130.4799
128.8872
128.2219
127.8633
127.1265
127.0207
126.9249
126.8982
77.5016
77.1838
76.8659
57.8055
39.2654
21.8006



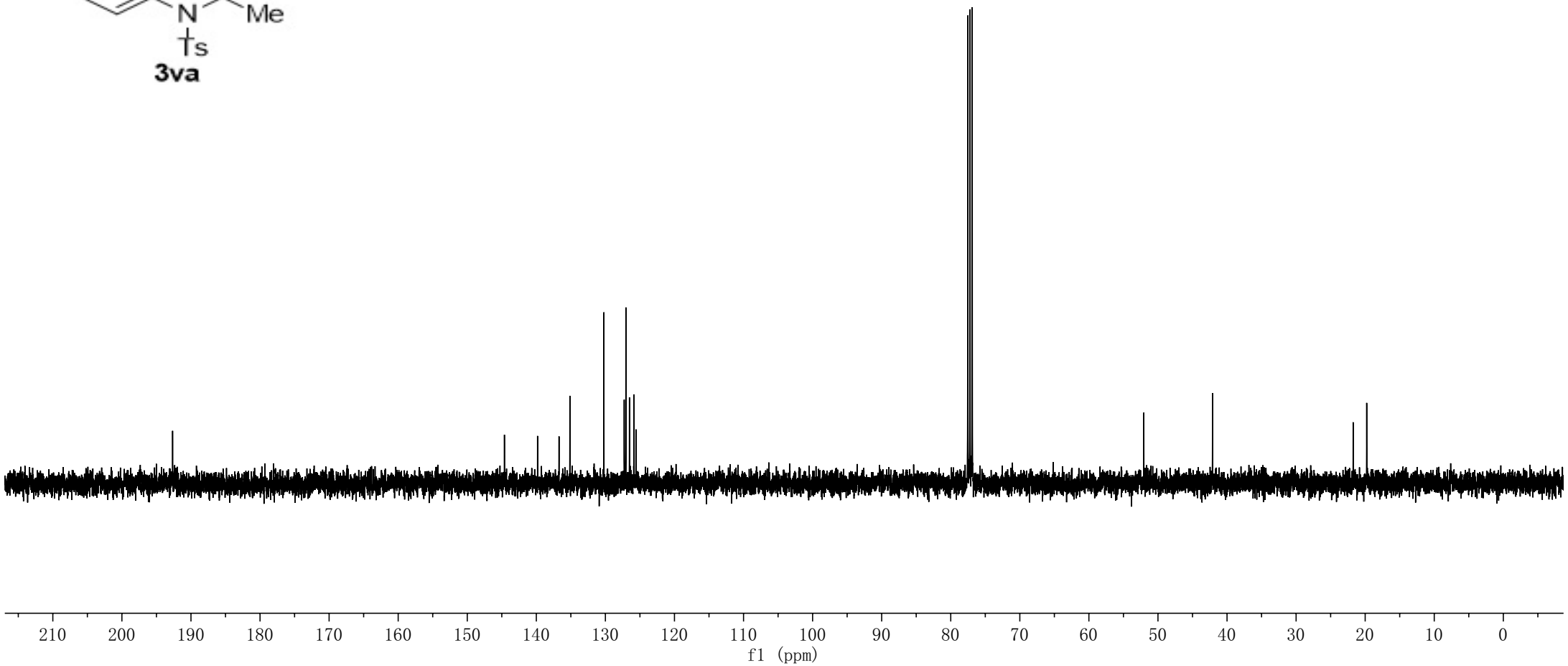
3ua


7.9492
7.9297
7.9157
7.8948
7.6313
7.6119
7.5932
7.5342
7.5141
7.3072
7.2884
7.2775
7.2703
7.2331
7.2132
4.9354
4.9207
4.9045
4.8885
2.4179
2.3861
2.3598
2.2671
2.2231
1.3023
1.2850
O
N
Me
Ts
3va
1.92
1.03
1.98
1.23
1.98
1.00
4.06
1.07
3.17
11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

192.6586
144.6163
139.8205
136.7118
135.1377
130.2209
127.2747
127.0317
126.5174
125.8468
125.5617
77.5276
77.2107
76.8926
52.0495
42.0980
21.7389
19.7775

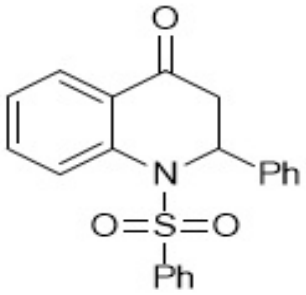


3va

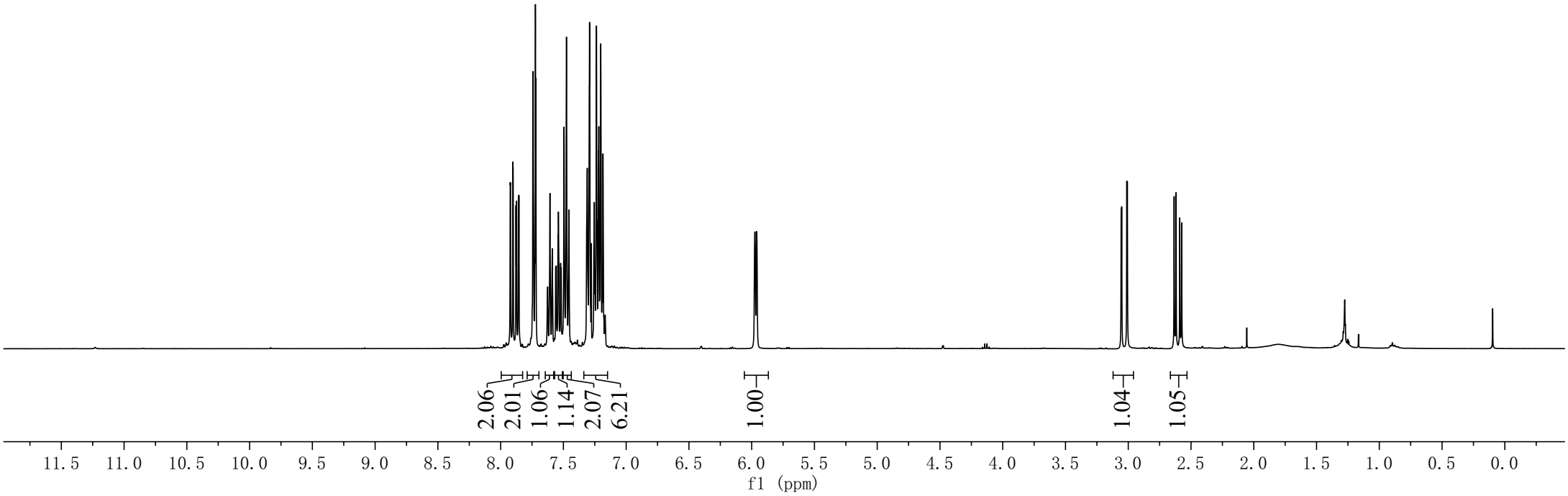


7.9218
7.9010
7.8737
7.8542
7.7433
7.7409
7.7229
7.7195
7.6255
7.6071
7.5881
7.5612
7.5397
7.5179
7.4952
7.4755
7.4560
7.3099
7.2916
7.2364
7.2025
7.1847
7.1673
5.9743
5.9605

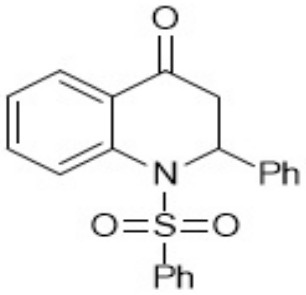
3.0564
3.0521
3.0116
3.0073
2.6344
2.6192
2.5896
2.5743



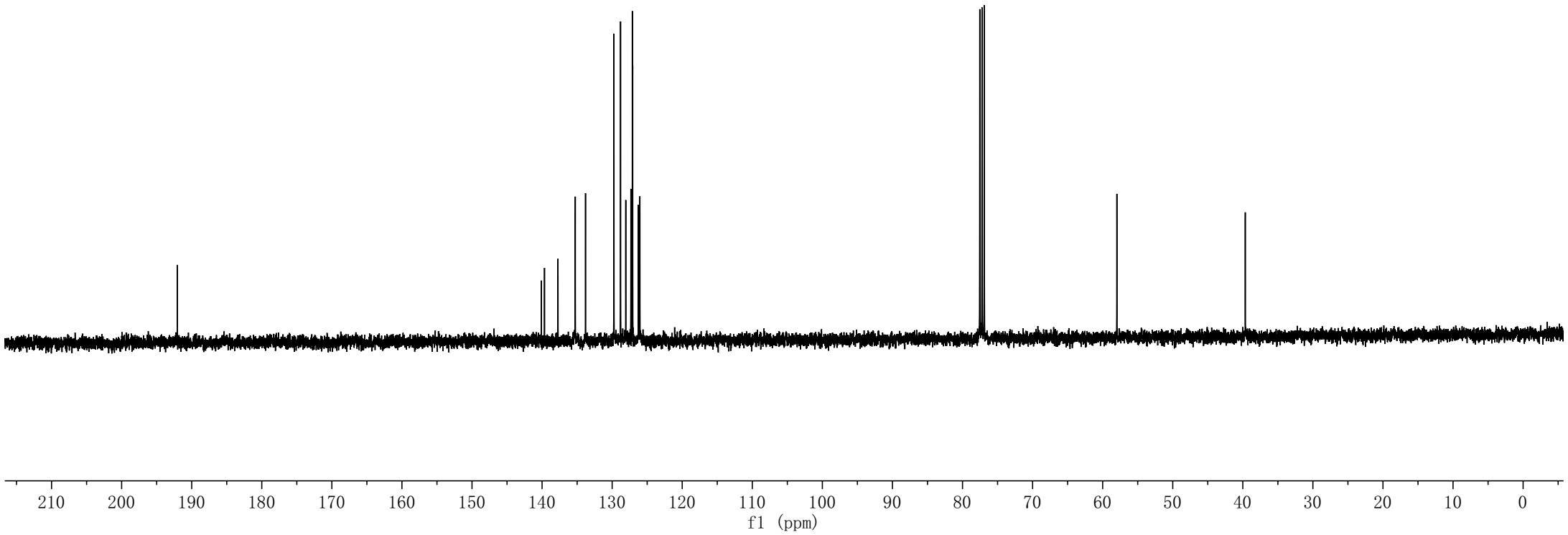
3ab

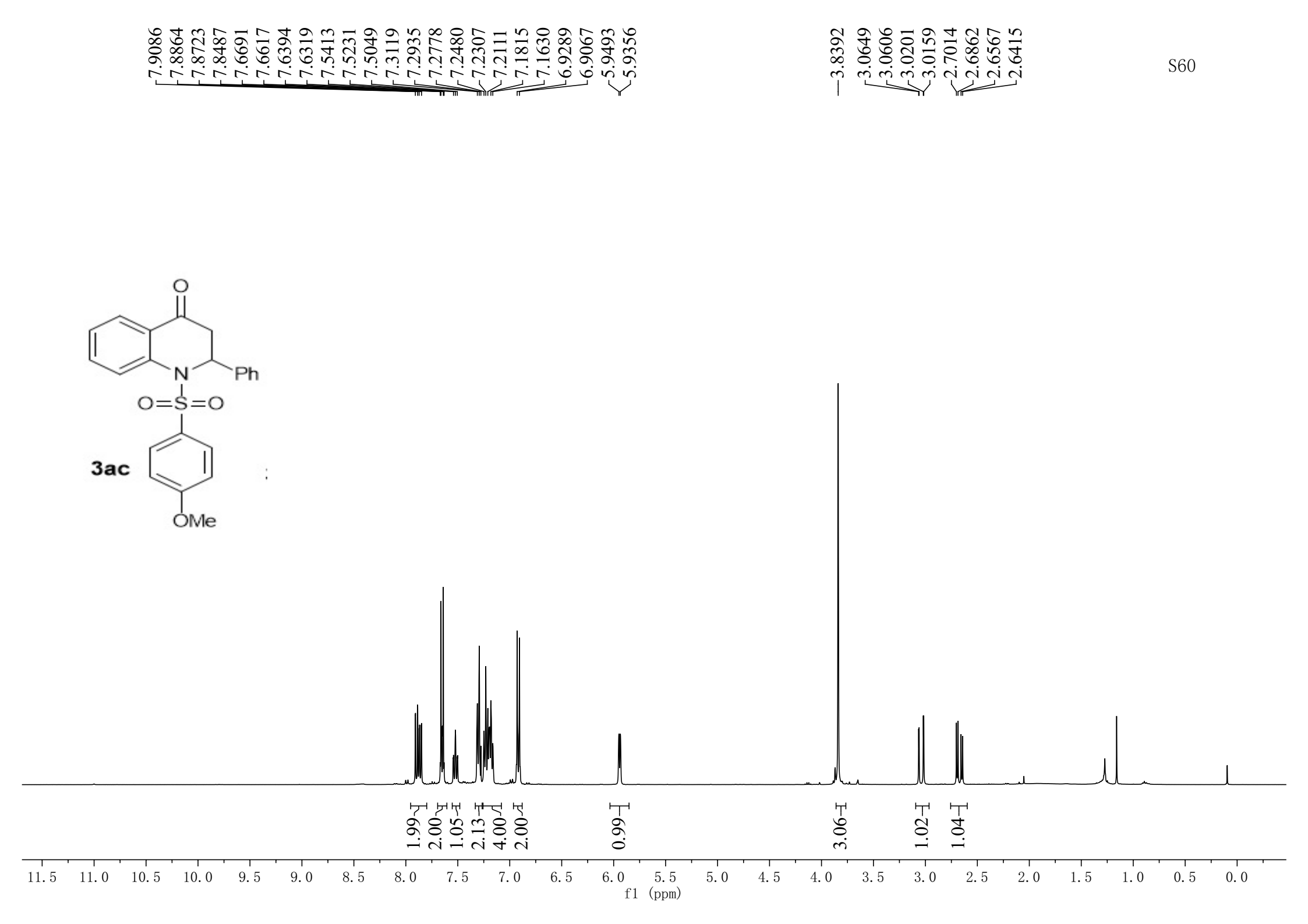


192.0533
140.1110
139.6543
137.7277
135.2589
133.8000
129.7397
128.7983
128.0560
127.3248
127.1207
127.0663
126.2455
126.0839
126.0415
77.5351
77.2176
76.8997
57.9726
39.6493

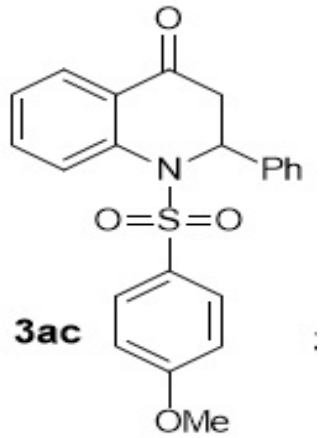


3ab

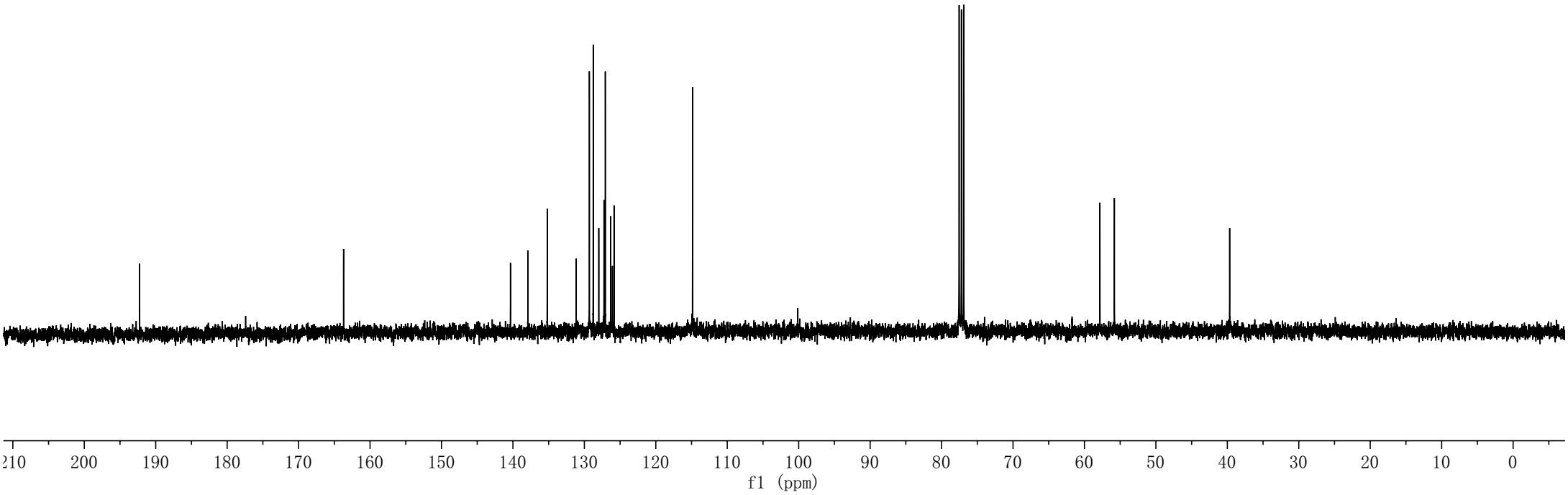


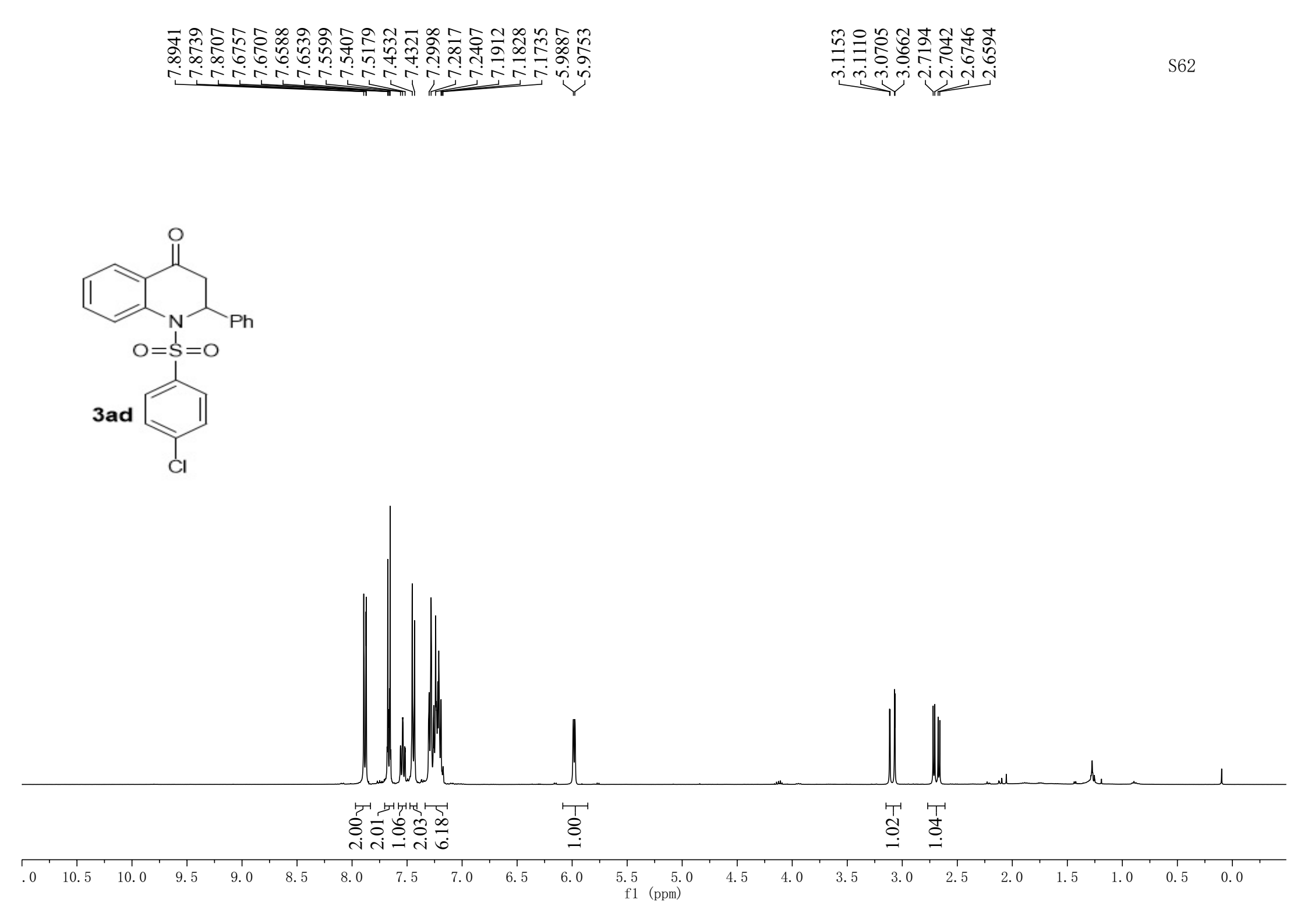

7.9086
7.8864
7.8723
7.8487
7.6691
7.6617
7.6394
7.6319
7.5413
7.5231
7.5049
7.3119
7.2935
7.2778
7.2480
7.2307
7.2111
7.1815
7.1630
6.9289
6.9067
5.9493
5.9356
3.8392
3.0649
3.0606
3.0201
3.0159
2.7014
2.6862
2.6567
2.6415
O
N
Ph
O=S=O
3ac
OMe
1.99
2.00
1.05
2.13
4.00
2.00
0.99
3.06
1.02
1.04
11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

192.2529
163.7049
140.3442
137.8979
135.1934
131.1453
129.2988
128.7617
127.9792
127.2529
127.0682
126.3194
126.0750
125.8448
114.8536
77.5411
77.2226
76.9053
57.8349
55.8101
39.6752

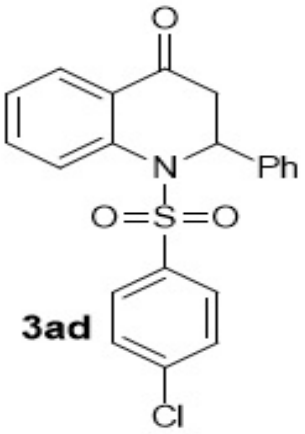


3ac

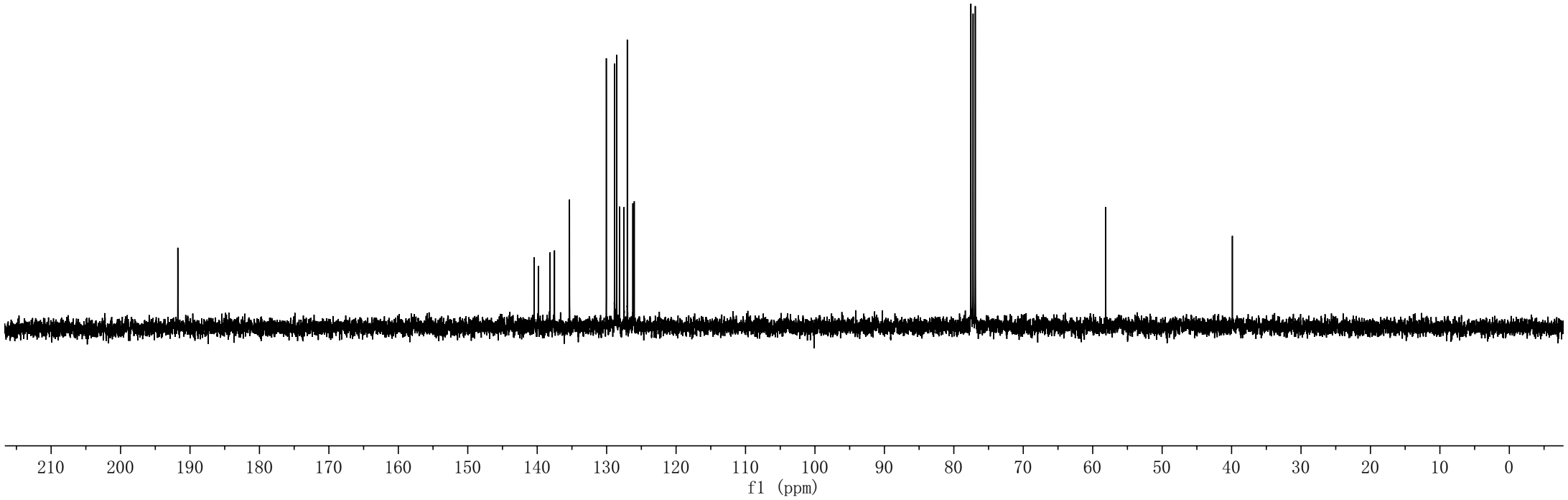


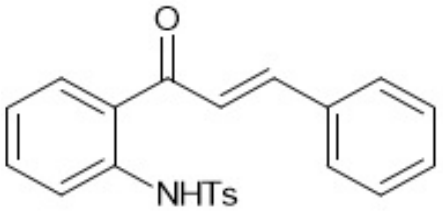

7.8941
7.8739
7.8707
7.6757
7.6707
7.6588
7.6539
7.5599
7.5407
7.5179
7.4532
7.4321
7.2998
7.2817
7.2407
7.1912
7.1828
7.1735
5.9887
5.9753
3.1153
3.1110
3.0705
3.0662
2.7194
2.7042
2.6746
2.6594
O
N
Ph
O=S=O
3ad
Cl
2.00
2.01
1.06
2.03
6.18
1.00
1.02
1.04
f1 (ppm)

191.7545
140.4502
139.8386
138.1503
137.5097
135.3498
130.0425
128.8612
128.5560
128.1559
127.5045
127.0272
126.2259
126.0942
126.0217
77.5406
77.2224
76.9056
58.1304
39.8904



3ad

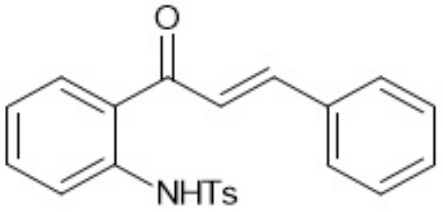



O
NHTs

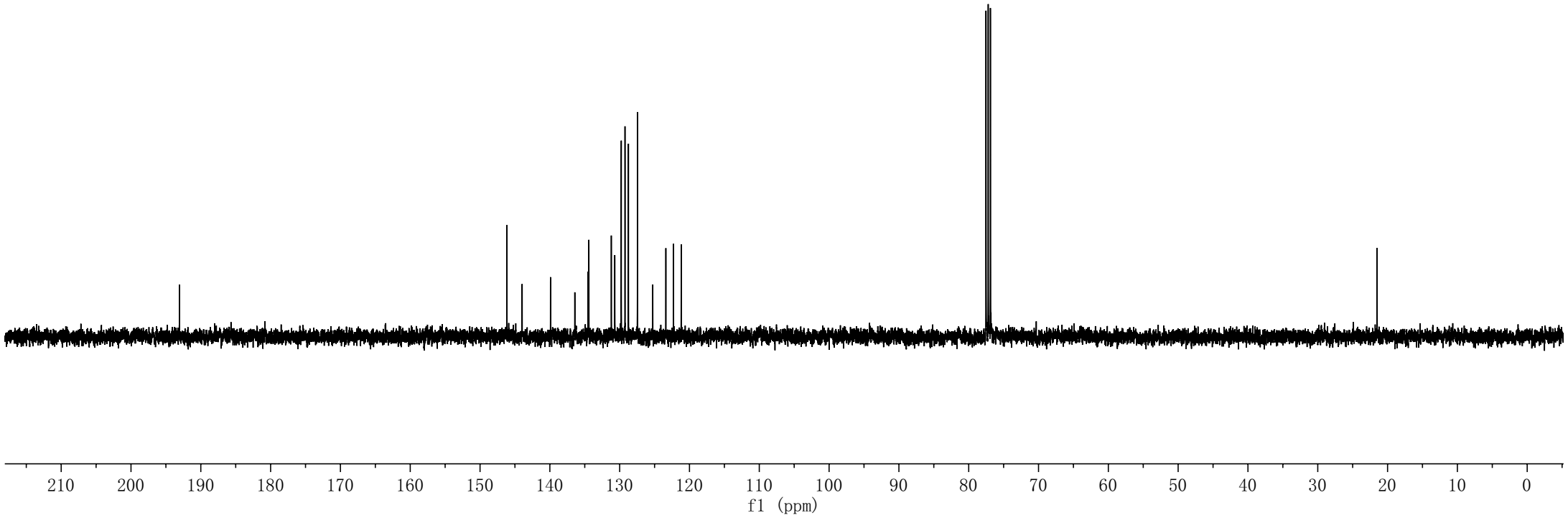
4a

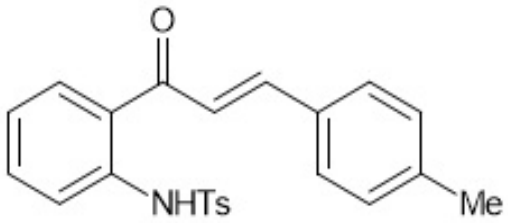
11.0816
7.8594
7.8561
7.8396
7.8362
7.7653
7.7635
7.7445
7.7427
7.7009
7.6801
7.6646
7.6256
7.6134
7.6037
7.5946
7.5161
7.4947
7.4734
7.4608
7.4516
7.4350
7.4261
7.3560
7.3170
7.2775
7.1743
7.1546
7.1387
7.1361
2.2224
0.96
1.02
1.00
5.00
4.14
1.16
3.03
3.00
12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

193.0454
146.1492
143.9684
139.9039
136.4225
134.5214
134.4091
131.1959
130.6981
129.7704
129.2336
128.7434
127.4489
125.2562
123.3807
122.2915
121.1782
77.5247
77.2064
76.8894
21.5014



4a

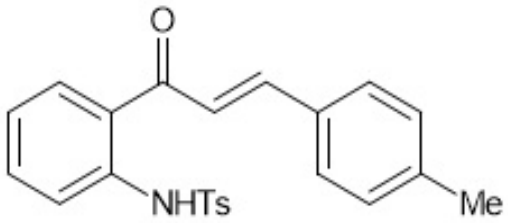



O
NHTs
Me

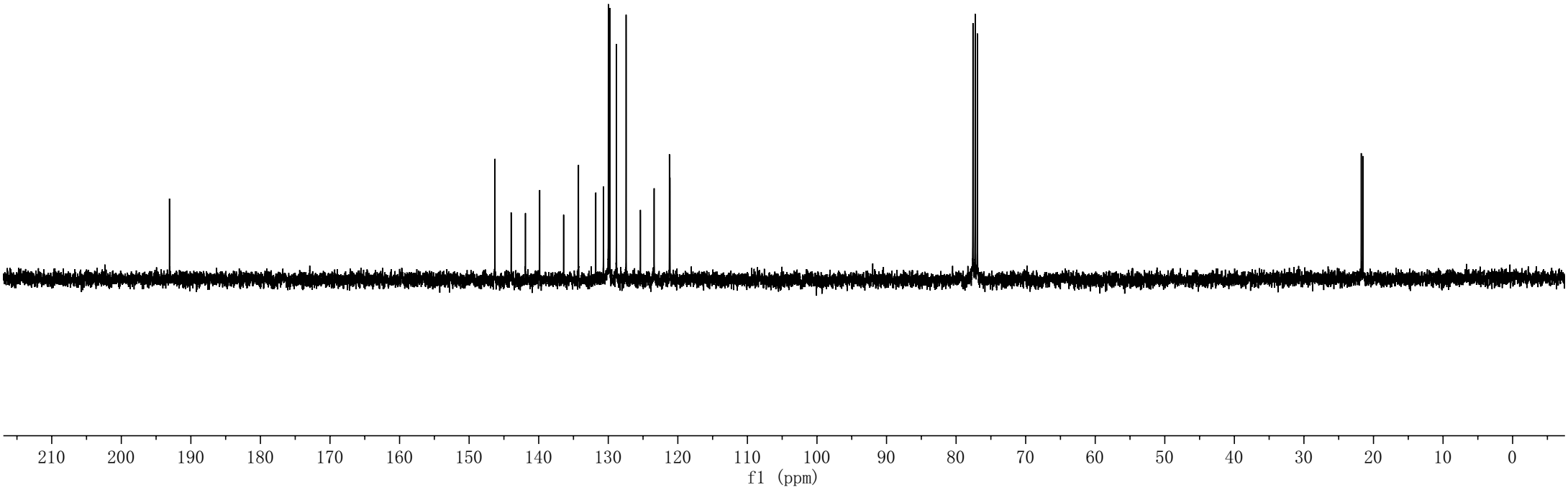
4b

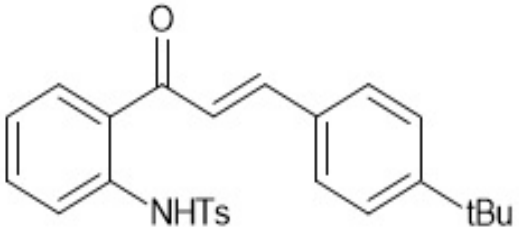
11.1137
7.8486
7.8287
7.7579
7.7389
7.6941
7.6733
7.6460
7.6072
7.5101
7.4899
7.4809
7.4595
7.3072
7.2774
7.2683
7.2498
7.2299
7.1647
7.1451
7.1287
7.1262
2.4049
2.2205
0.94
1.00
1.01
1.98
1.01
3.01
3.17
2.98
3.09
3.00
12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

193.0743
146.2893
143.9592
141.9095
139.8566
136.4164
134.2821
131.7947
130.6850
129.9870
129.7688
128.8241
127.4330
125.3764
123.4064
121.2067
121.1344
77.5771
77.2586
76.9410
21.7566
21.5225



4b

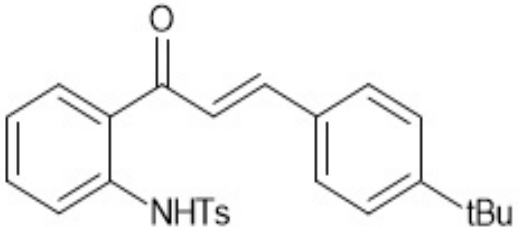



O
NHTs
tBu

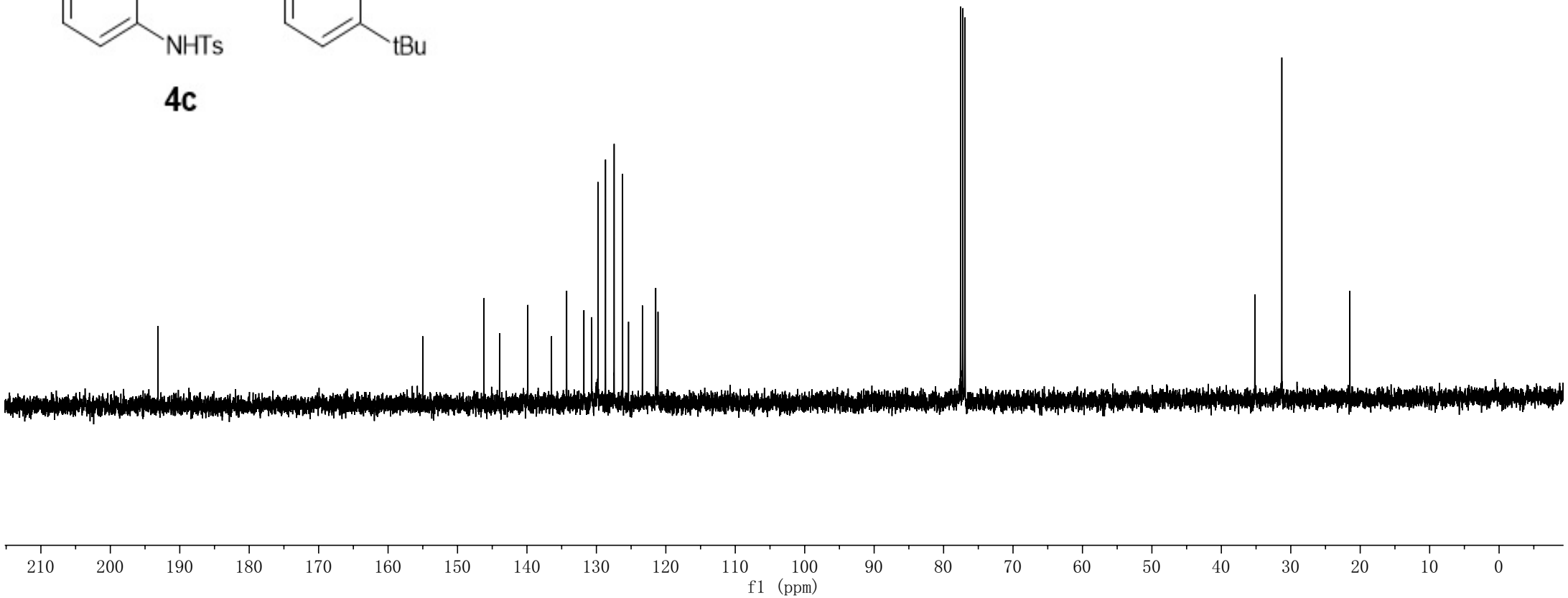
4c

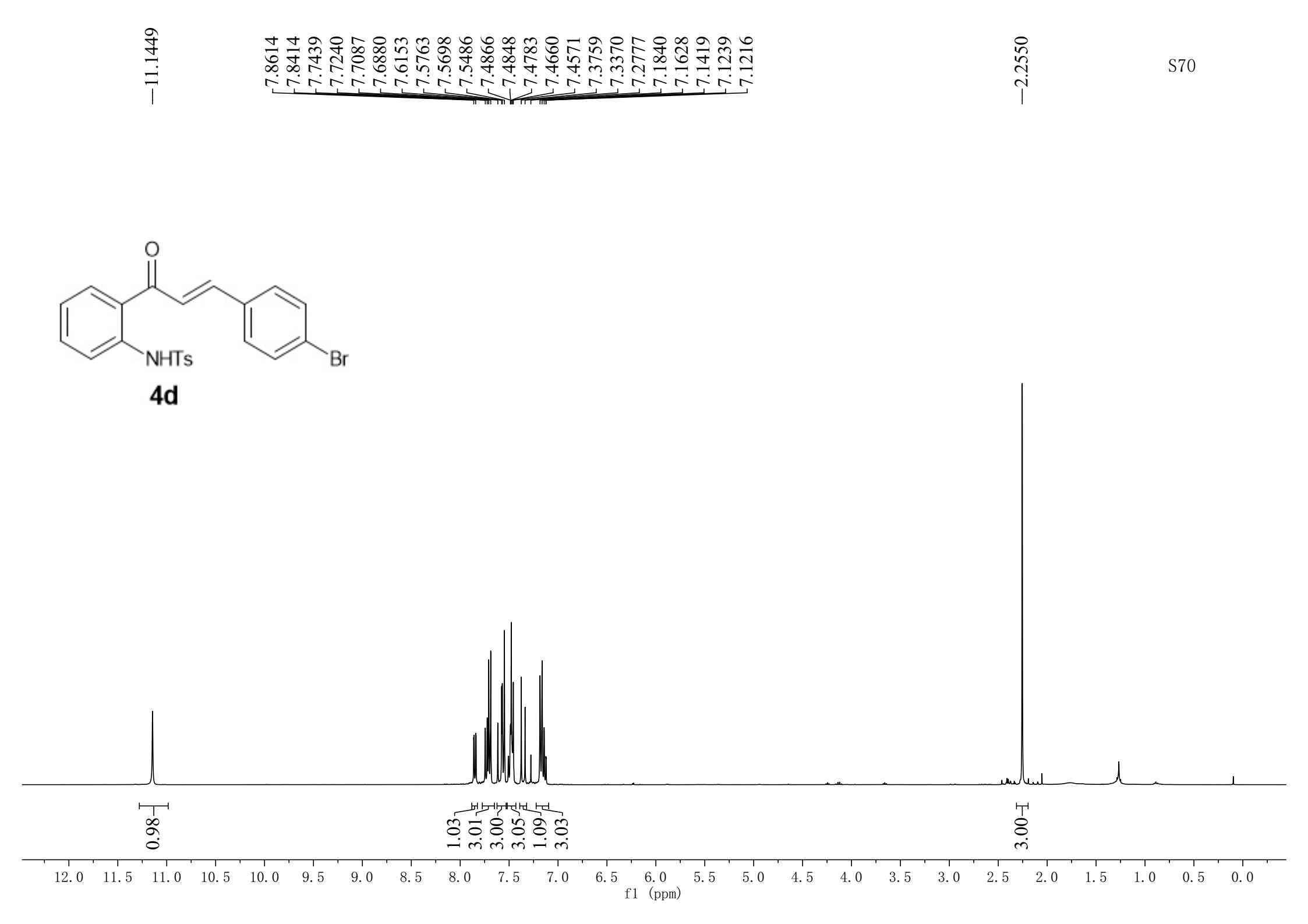
11.1059
7.8548
7.8349
7.7687
7.7479
7.7040
7.6832
7.6662
7.6273
7.5643
7.5434
7.5112
7.4762
7.4719
7.4594
7.4551
7.3265
7.2876
7.2778
7.1724
7.1528
7.1368
7.1340
2.2227
1.3625
0.97
1.04
1.08
2.01
1.02
5.03
1.17
3.01
3.00
9.03
12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

193.1221
155.0090
146.1959
143.9451
139.8727
136.4620
134.2808
131.7943
130.6695
129.7658
128.6877
127.4433
126.2233
125.3725
123.3742
121.4566
121.1265
77.5472
77.2293
76.9120
35.1766
31.2855
21.4862

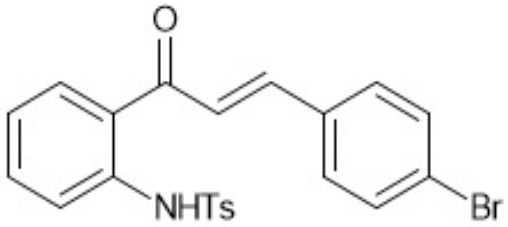


4c

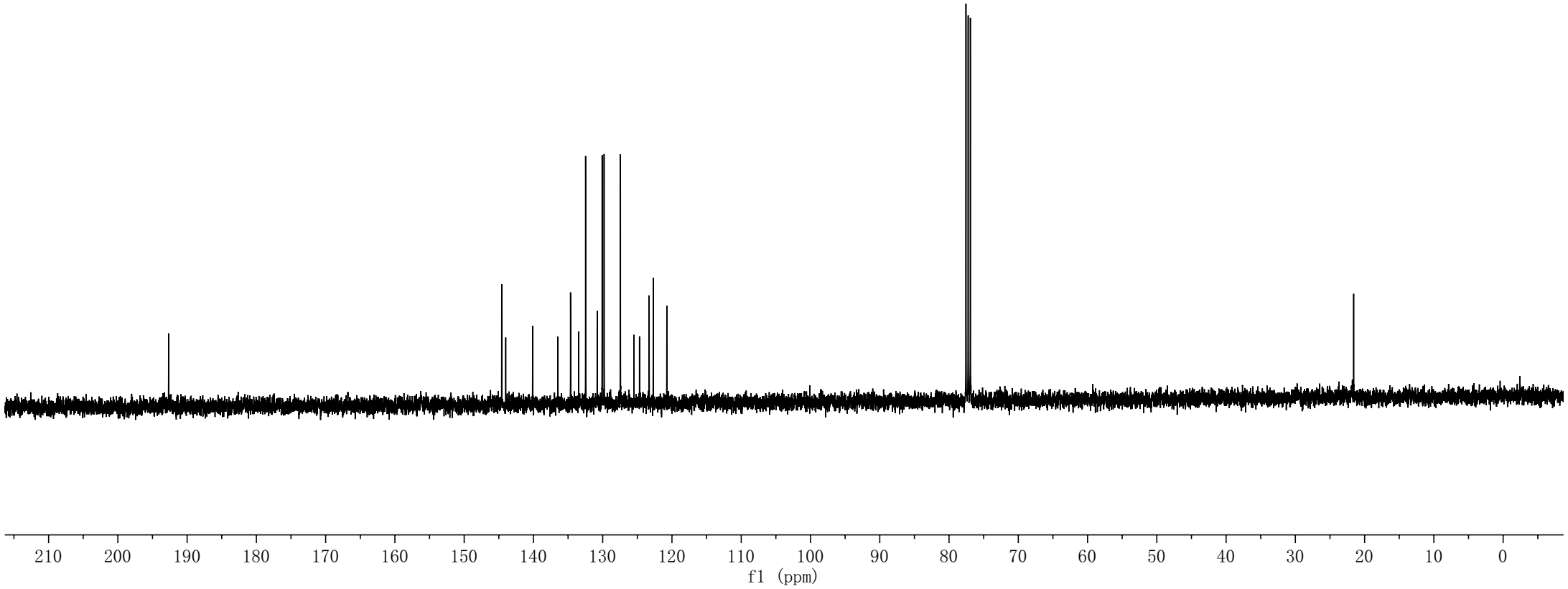


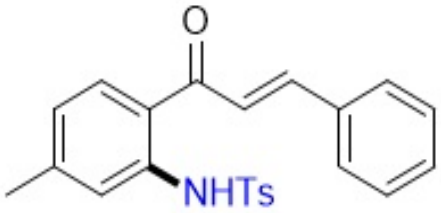

11.1449
7.8614
7.8414
7.7439
7.7240
7.7087
7.6880
7.6153
7.5763
7.5698
7.5486
7.4866
7.4848
7.4783
7.4660
7.4571
7.3759
7.3370
7.2777
7.1840
7.1628
7.1419
7.1239
7.1216
2.2550
O
NHTs
Br
4d
0.98
1.03
3.01
3.00
3.05
1.09
3.03
3.00
12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

192.6699
144.5816
144.0009
140.1157
136.4655
134.6436
133.4695
132.4697
130.7955
130.0817
129.7967
127.4401
125.4870
124.6880
123.2929
122.7032
120.7422
77.5554
77.2373
76.9198
21.5819



4d

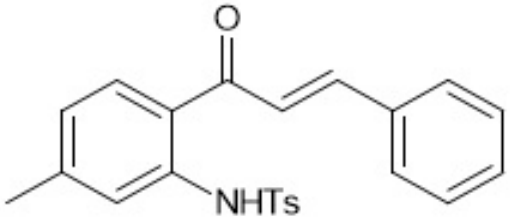



O
NHTs

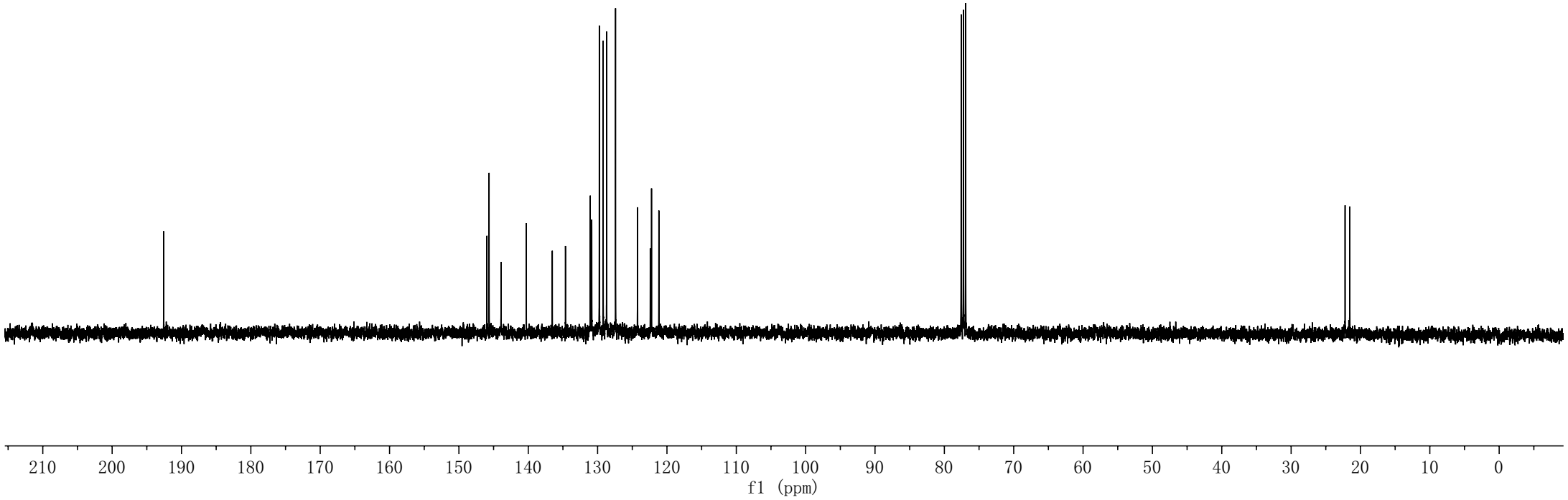
4e

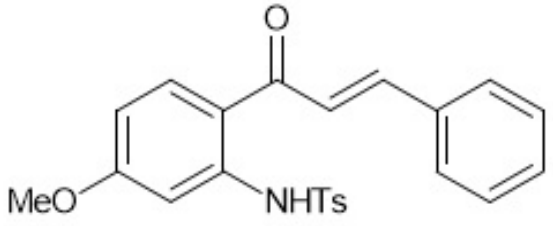
11.3282
7.7684
7.7482
7.7213
7.7014
7.6770
7.6378
7.6075
7.5692
7.4433
7.3838
7.3451
7.2814
7.1919
7.1723
6.9589
6.9393
2.3838
2.2525
0.92
7.08
2.95
1.16
2.06
1.00
3.02
3.00
12.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

192.5715
145.9536
145.6466
143.9152
140.2801
136.5321
134.6344
131.0593
130.8444
129.7540
129.2037
128.7008
127.4139
124.2414
122.4040
122.2222
121.1639
77.5719
77.2542
76.9361
22.2185
21.5428



4e

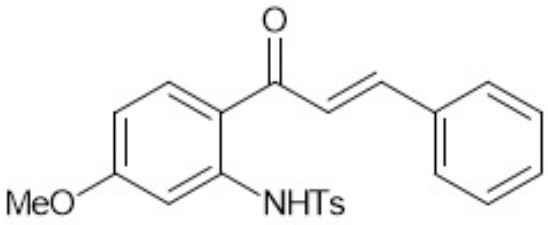



O
MeO
NHTs

4f

12.0139
7.8708
7.8483
7.7848
7.7640
7.7460
7.7072
7.6198
7.6117
7.6052
7.4555
7.4377
7.4298
7.4218
7.4170
7.2591
7.2530
7.2291
7.2088
6.6223
6.6160
6.6000
6.5937
3.8495
2.3170
1.00
1.04
1.99
0.97
2.07
4.13
3.29
0.99
3.04
3.03
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
−1
f1 (ppm)

191.3121
164.4548
145.0488
144.0434
143.3921
136.6445
134.8057
133.0411
130.8845
129.8251
129.1690
128.6390
127.4770
121.9882
117.0301
109.4363
103.8805
77.5396
77.2215
76.9038
55.8030
21.6315



4f