Supporting Information

Visible-light promoted aerobic difunctionalization of alkenes with sulfonyl hydrazides for the synthesis of β-keto/hydroxyl sulfones

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List of contents

1. General Information

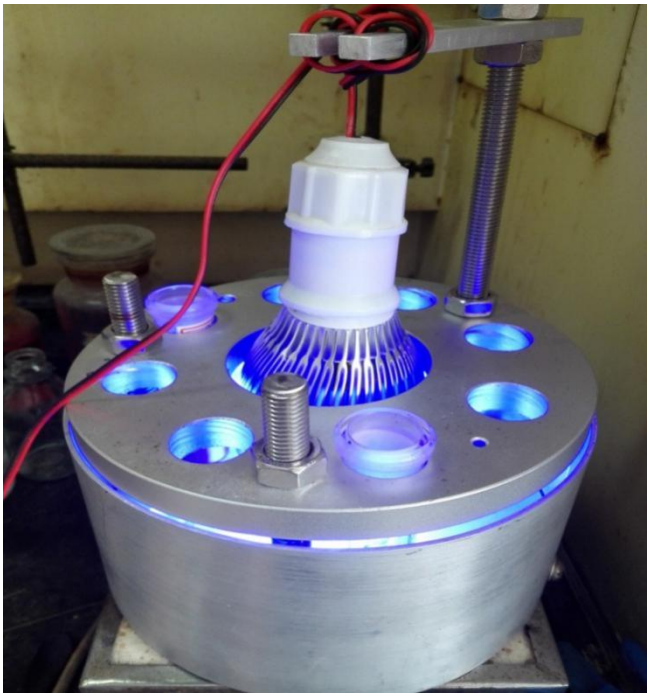
Column chromatography was generally performed on silica gel (200-300 mesh) and reactions were monitored by thin layer chromatography (TLC) using UV light to visualize the course of the reactions. The ^{1}H (400 MHz) and ^{13}C NMR (100 MHz) data were recorded on Bruker AVANCE II 400MHz spectrometer using $CDCl_3$ as solvent. The chemical shifts (δ) are reported in ppm and coupling constants (*J*) in Hz. ^{1}H NMR spectra was recorded with tetramethylsilane (δ=0.00 ppm)as internal reference; ^{13}C NMR spectra was recorded with $CDCl_3$ (δ=77.00 ppm) as internal reference.

2.General procedures for synthesis of 3aa-3as and 3ba-33be

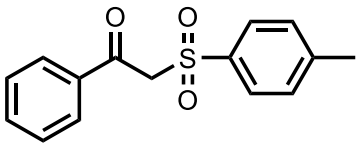
To a solution of sulfonhydrazide **2** (0.5 mmol) and alkene **1** (1.5 mmol) in EtOH (1.5 mL) was added Methylene Blue (0.01 mmol) and DABCO (1 mmol). The reaction mixture was stirred at 25°C under air atmosphere (open vial) and irradiated by blue LED (7 W). The reaction was monitored by thin layer chromatography (TLC). Removal of solvent followed by column chromatography afforded desired products.

Reaction Apparatus:

Photochemical reactions were carried out under visible light irradiation by blue led bulbs at room temperature.

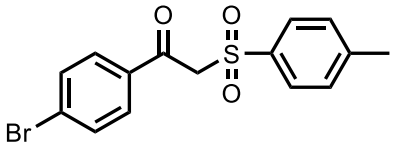


3.Compound characterizations



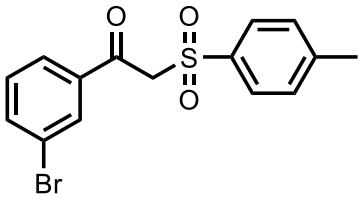
1-phenyl-2-tosylethan-1-one (3aa)[1].

Petroleum ether/ethyl acetate =10:1, white solid, 78% yield (106 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.97 (d, *J* = 7.7 Hz, 2H), 7.78 (d, *J* = 8.1 Hz, 2H), 7.64 (t, *J* = 7.3 Hz, 1H), 7.50 (t, *J* = 7.6 Hz, 2H), 7.35 (d, *J* = 8.0 Hz, 2H), 4.74 (s, 2H), 2.46 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 188.15, 145.36, 135.82, 134.31, 129.84, 129.34, 128.84, 128.62, 63.61, 21.70.



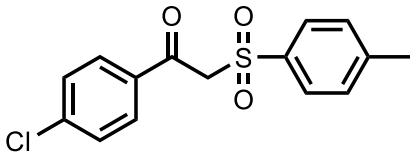
1-(4-bromophenyl)-2-tosylethan-1-one (3ba)[1].

Petroleum ether/ethyl acetate =10:1, white solid, 89% yield (155 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.02 (t, *J* = 1.8 Hz, 1H), 7.91 (ddd, *J* = 7.8, 1.6, 1.0 Hz, 1H), 7.80 – 7.71 (m, 3H), 7.38 (dd, *J* = 15.3, 7.8 Hz, 3H), 4.70 (s, 2H), 2.47 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 186.69, 144.92, 137.41, 132.04, 130.34, 128.55, 127.98, 123.18, 63.98.



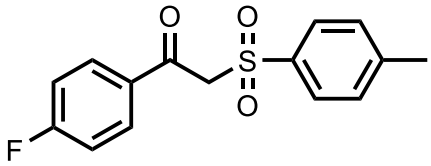
1-(3-bromophenyl)-2-tosylethan-1-one (3ca)[1].

Petroleum ether/ethyl acetate =10:1, white solid, 67% yield (118 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.02 (t, *J* = 1.6 Hz, 1H), 7.91 (d, *J* = 7.8 Hz, 1H), 7.76 (t, *J* = 6.9 Hz, 3H), 7.38 (dd, *J* = 15.3, 7.8 Hz, 3H), 4.70 (s, 2H), 2.47 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 186.98, 145.64, 137.41, 137.12, 135.54, 132.09, 130.40, 129.95, 128.60, 128.03, 123.18, 63.68, 21.75.



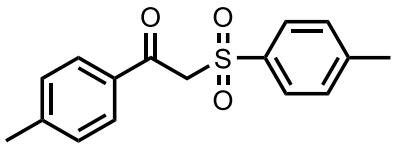
1-(4-chlorophenyl)-2-tosylethan-1-one (3da)[1].

Petroleum ether/ethyl acetate =10:1, white solid, 83% yield (130 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.91 (d, *J* = 6.8 Hz, 2H), 7.76 (d, *J* = 8.3 Hz, 2H), 7.47 (d, *J* = 8.6 Hz, 2H), 7.36 (d, *J* = 8.3 Hz, 2H), 4.70 (s, 2H), 2.46 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 186.90, 145.56, 141.08, 135.62, 134.11, 130.79, 129.91, 129.21, 128.58, 63.74, 21.72.



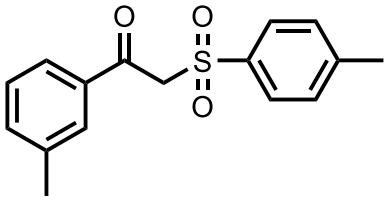
1-(4-fluorophenyl)-2-tosylethan-1-one (3ea)[1].

Petroleum ether/ethyl acetate =10:1, white solid, 72% yield (106 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.15 – 7.94 (m, 2H), 7.77 (d, *J* = 8.2 Hz, 2H), 7.36 (d, *J* = 8.0 Hz, 2H), 7.26 – 7.08 (m, 2H), 4.71 (s, 2H), 2.47 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 186.58, 167.76, 165.20, 145.52, 135.66, 132.51 – 132.12 (m), 129.90, 128.56, 116.21, 115.99, 63.75, 21.71.



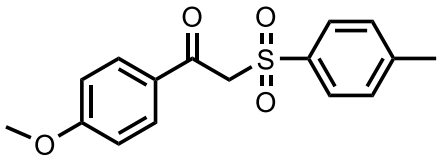
1-(p-tolyl)-2-tosylethan-1-one (3fa)[1].

Petroleum ether/ethyl acetate =20:1, white solid, 68% yield (98 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.87 (d, *J* = 8.3 Hz, 2H), 7.78 (d, *J* = 8.3 Hz, 2H), 7.35 (d, *J* = 8.0 Hz, 2H), 7.29 (d, *J* = 8.0 Hz, 2H), 4.71 (s, 2H), 2.46 (s, 3H), 2.44 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 187.67, 145.57, 145.30, 135.82, 133.39, 129.82, 129.54 (d, *J* = 3.7 Hz), 128.61, 63.58, 21.76 (d, *J* = 7.4 Hz).



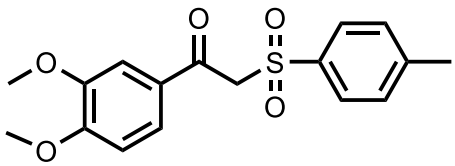
1-(m-tolyl)-2-tosylethan-1-one (3ga)[1].

Petroleum ether/ethyl acetate =20:1, white solid, 65% yield (93mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.79 (s, 1H), 7.77 (s, 2H), 7.75 (s, 1H), 7.73 (s, 1H), 7.44 (d, *J* = 7.6 Hz, 1H), 7.37 (dd, *J* = 15.3, 7.8 Hz, 3H), 4.72 (s, 2H), 2.46 (s, 3H), 2.42 (s, 3H).^{13}C NMR (101 MHz, $CDCl_3$) δ 188.30, 145.33, 138.74, 135.83, 135.15, 129.76 (d, *J* = 10.2 Hz), 128.67 (d, *J* = 5.5 Hz), 126.66, 63.58, 21.68, 21.31.



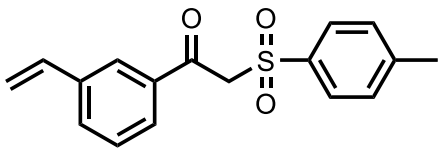
1-(4-methoxyphenyl)-2-tosylethan-1-one (3ha)[1].

Petroleum ether/ethyl acetate =5:1, white solid, 77% yield (117mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.95 (d, *J* = 8.9 Hz, 2H), 7.76 (d, *J* = 8.2 Hz, 2H), 7.34 (d, *J* = 8.1 Hz, 2H), 6.95 (d, *J* = 8.9 Hz, 2H), 4.68 (s, 2H), 3.96 (s, 3H), 2.45 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 186.36, 164.55, 145.26, 135.85, 131.93, 129.81, 128.92, 128.57, 114.07, 63.55, 55.64, 21.71.



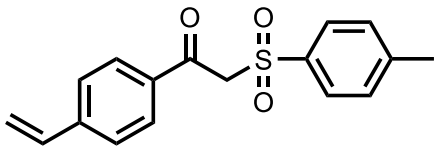
1-(3,4-dimethoxyphenyl)-2-tosylethan-1-one (3ia).

Petroleum ether/ethyl acetate =5:1, white solid, 82% yield (136mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.77 (d, *J* = 8.2 Hz, 2H), 7.62 (d, *J* = 10.3 Hz, 1H), 7.48 (s, 1H), 7.34 (d, *J* = 8.1 Hz, 2H), 6.91 (d, *J* = 8.5 Hz, 1H), 4.70 (s, 2H), 3.96 (s, 3H), 3.91 (s, 3H), 2.45 (s, 3H).^{13}C NMR (101 MHz, $CDCl_3$) δ 186.41, 154.48, 149.23, 145.27, 135.85, 129.81, 129.04, 128.57, 125.15, 110.67, 110.13, 63.48, 56.12 (d, *J* = 19.0 Hz), 21.71. MS (ESI, *m/z*) 335.1 ($M + H^+$), 357.1 ($M + Na^+$). Anal. calcd for $C_{17}H_{18}O_5S$: C, 61.06; H, 5.43. Found: C, 60.84; H, 5.56.



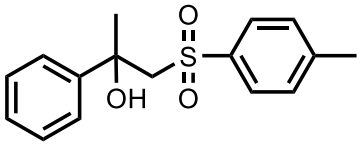
2-tosyl-1-(3-vinylphenyl)ethan-1-one (3ja).

Petroleum ether/ethyl acetate =20:1, white solid, 73% yield (109mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.93 (s, 1H), 7.85 (d, *J* = 7.8 Hz, 1H), 7.78 (d, *J* = 8.3 Hz, 2H), 7.67 (d, *J* = 7.7 Hz, 1H), 7.46 (t, *J* = 7.8 Hz, 1H), 7.35 (d, *J* = 8.1 Hz, 2H), 6.75 (dd, *J* = 17.6, 10.9 Hz, 1H), 5.84 (d, *J* = 17.6 Hz, 1H), 5.38 (d, *J* = 10.9 Hz, 1H), 4.75 (s, 2H), 2.46 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 188.12, 145.42, 138.36, 137.42, 136.08, 135.54, 131.74, 129.85, 129.04, 128.63, 126.96, 115.88, 63.69, 21.70. MS (ESI, *m/*z) 301.1 (M + H^+), 323.1 (M + Na^+). Anal. calcd for $C_{17}H_{16}O_3S$: C, 67.98; H, 5.37. Found: C, 67.74; H, 5.26.



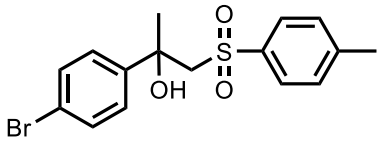
2-tosyl-1-(4-vinylphenyl)ethan-1-one (3ka).

Petroleum ether/ethyl acetate =40:1, white solid, 64% yield (96mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.93 (d, *J* = 8.4 Hz, 2H), 7.78 (d, *J* = 8.3 Hz, 2H), 7.51 (d, *J* = 8.3 Hz, 2H), 7.35 (d, *J* = 8.0 Hz, 2H), 6.78 (dd, *J* = 17.6, 10.9 Hz, 1H), 5.69 (dd, *J* = 189.7, 19.5 Hz, 2H), 4.72 (s, 2H), 2.46 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 187.46, 145.38, 143.33 (s), 135.77, 135.68, 134.89, 129.83 (d, *J* = 1.9 Hz), 128.61, 126.53, 117.76, 63.68, 21.71. MS (ESI, *m/*z) 301.1 (M + H^+), 323.1 (M + Na^+). Anal. calcd for $C_{17}H_{16}O_3S$: C, 67.98; H, 5.37. Found: C, 67.86; H, 5.24.



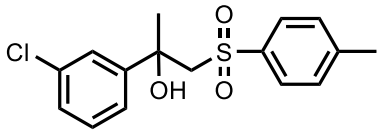
2-phenyl-1-tosylpropan-2-ol (3la)[2].

Petroleum ether/ethyl acetate =10:1, white solid, 72% yield (103mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.50 (d, *J* = 8.3 Hz, 2H), 7.33 – 7.29 (m, 2H), 7.24 – 7.14 (m, 5H), 4.66 (s, 1H), 3.67 (dd, *J* = 45.6, 14.6 Hz, 2H), 2.40 (s, 3H), 1.72 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 144.53, 137.39, 133.62, 129.71, 128.25, 127.56, 127.13, 124.65, 73.17, 66.69, 30.76, 21.57.



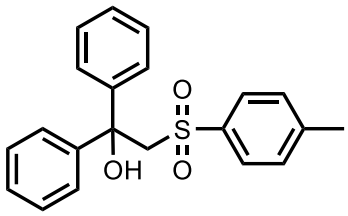
2-(4-bromophenyl)-1-tosylpropan-2-ol (3ma)[2].

Petroleum ether/ethyl acetate =10:1, white solid, 81% yield (183mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.45 (dd, *J* = 13.3, 5.4 Hz, 2H), 7.29 – 7.23 (m, 2H), 7.19 (d, *J* = 8.1 Hz, 2H), 7.15 – 7.08 (m, 2H), 4.72 (s, 1H), 3.66 (dd, *J* = 53.1, 14.7 Hz, 2H), 2.45 (d, *J* = 7.6 Hz, 3H), 1.64 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 144.81, 143.28, 136.84, 131.17, 129.75, 127.51, 126.61, 121.32, 72.80, 66.25, 31.02, 21.62.



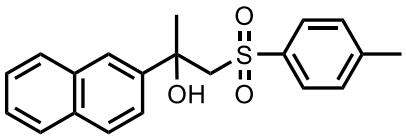
2-(3-chlorophenyl)-1-tosylpropan-2-ol (3na)[2].

Petroleum ether/ethyl acetate =10:1, white solid, 76% yield (161mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.02 (t, *J* = 1.6 Hz, 1H), 7.91 (d, *J* = 7.8 Hz, 1H), 7.76 (t, *J* = 6.9 Hz, 3H), 7.38 (dd, *J* = 15.3, 7.8 Hz, 3H), 4.70 (s, 2H), 2.47 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 186.98, 145.64, 137.41, 137.12, 135.54, 132.09, 130.40, 129.95, 128.60, 128.03, 123.18, 63.68, 21.75.



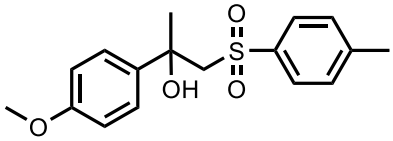
1,1-diphenyl-2-tosylethan-1-ol (3oa)[2].

Petroleum ether/ethyl acetate =10:1, white solid, 75% yield (132mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.44 (d, *J* = 8.3 Hz, 2H), 7.41 – 7.34 (m, 4H), 7.26 – 7.19 (m, 6H), 7.15 (d, *J* = 8.1 Hz, 2H), 5.41 (s, 1H), 4.21 (s, 2H), 2.41 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 144.51, 143.73, 137.42, 129.70, 128.28, 127.57 (d, *J* = 18.7 Hz), 125.87, 65.51, 21.61.



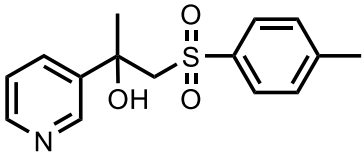
2-(naphthalen-2-yl)-1-tosylpropan-2-ol (3pa)[2].

Petroleum ether/ethyl acetate =10:1, white solid, 70% yield (119mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.04 – 7.93 (m, 1H), 7.87 (d, *J* = 7.3 Hz, 1H), 7.67 (dd, *J* = 8.7, 4.1 Hz, 2H), 7.49 – 7.40 (m, 1H), 7.39 – 7.32 (m, 2H), 7.16 (d, *J* = 8.2 Hz, 2H), 6.78 (d, *J* = 8.1 Hz, 2H), 4.87 (s, 1H), 4.13 (dd, *J* = 220.5, 15.0 Hz, 2H), 2.21 (s, 3H), 2.00 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 143.70, 139.04, 134.54, 129.37, 129.20, 128.82, 126.94, 125.72, 125.09, 124.77, 124.55, 124.38, 73.52, 65.00, 30.14, 21.35.



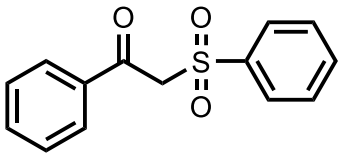
2-(4-methoxyphenyl)-1-tosylpropan-2-ol (3qa)[2].

Petroleum ether/ethyl acetate =5:1, white solid, 77% yield (123mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.49 (d, *J* = 7.1 Hz, 2H), 7.19 (dd, *J* = 8.6, 3.3 Hz, 4H), 6.71 (d, *J* = 8.8 Hz, 2H), 4.61 (s, 1H), 3.77 (s, 3H), 3.64 (dd, *J* = 49.7, 14.6 Hz, 2H), 2.40 (s, 3H), 1.69 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 158.70, 144.41, 136.64, 129.65, 127.57, 125.87, 113.50, 72.89, 66.85, 55.24, 30.70, 21.57.



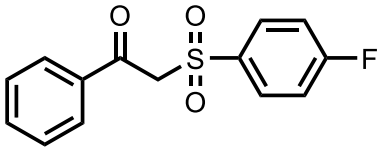
2-(pyridin-3-yl)-1-tosylpropan-2-ol (3ra)[3].

Petroleum ether/ethyl acetate =10:1, white solid, 63% yield (92mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.18 (d, *J* = 4.7 Hz, 1H), 7.66 (q, *J* = 8.4 Hz, 2H), 7.49 (d, *J* = 8.3 Hz, 2H), 7.17 (d, *J* = 8.1 Hz, 2H), 7.07 (ddd, *J* = 6.6, 4.8, 1.7 Hz, 1H), 3.90 (dd, *J* = 152.0, 14.5 Hz, 2H), 2.38 (s, 3H), 1.62 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 162.51, 147.95, 144.23, 137.45, 136.93, 129.55, 127.70, 122.13, 119.34, 74.04, 65.17, 30.11, 21.56.



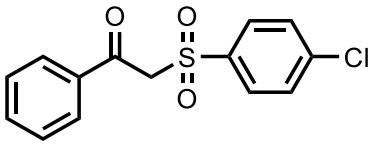
1-phenyl-2-(phenylsulfonyl)ethan-1-one (3ab)[4].

Petroleum ether/ethyl acetate =10:1, white solid, 75% yield (98mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 4.74 (s, 2H), 7.48(tt, *J* = 7.8, 1.6 Hz, 2H), 7.55 (tt, *J* = 7.8, 1.6 Hz, 2H), 7.62 (tt, *J* = 7.4, 1.2 Hz, 1H), 7.66 (tt, *J* =7.6, 1.2 Hz, 1H), 7.90 (m, 2H), 7.94 (m, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 188.1, 138.8, 135.8, 134.5, 134.4, 129.4, 129.3, 129.0, 128.7, 63.6.



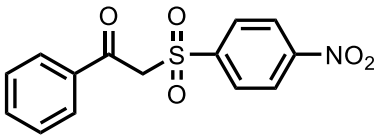
2-((4-fluorophenyl)sulfonyl)-1-phenylethan-1-one (3ac)[4].

Petroleum ether/ethyl acetate =10:1, white solid, 75% yield (104mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 4.75 (s, 2H),7.20-7.26 (m, 2H), 7.50 (t, *J* = 7.8 Hz, 2H), 7.64 (t, *J* = 7.4 Hz, 1H), 7.90-7.95 (m, 4H). ^{13}C NMR(100 MHz, $CDCl_3$) δ 188.1, 166.3 (d, *1JCF* = 245.4 Hz), 135.7, 134.8 (d, *4JCF* = 3.1 Hz), 134.7, 131.8 (d, *3JCF* = 9.7 Hz), 129.4, 129.1, 116.7 (d, *2JCF* = 22.6 Hz), 63.6.



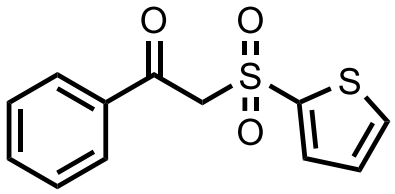
2-((4-chlorophenyl)sulfonyl)-1-phenylethan-1-one (3ad)[4].

Petroleum ether/ethyl acetate =10:1, white solid, 69% yield (101mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 4.75 (s, 2H),7.48-7.53 (m, 4H), 7.64 (t, *J* = 7.4 Hz, 1H), 7.83 (d, *J* = 8.8 Hz, 2H), 7.93 (d, *J* = 8.4 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 188.0, 141.3, 137.2, 135.7, 134.7, 130.3, 129.7, 129.4, 129.1, 63.5.



2-((4-nitrophenyl)sulfonyl)-1-phenylethan-1-one (3ae)[4].

Petroleum ether/ethyl acetate =10:1, white solid, 77% yield (117mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.45 – 8.35 (m, 1H), 8.14 (ddt, *J* = 11.3, 9.3, 2.4 Hz, 1H), 7.94 (dt, *J* = 7.1, 1.4 Hz, 1H), 7.72 – 7.63 (m, 0H), 7.52 (t, *J* = 7.8 Hz, 1H), 4.82 (s, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 187.60, 144.03, 135.33, 134.86, 130.34, 129.19, 129.09, 124.31, 63.00.

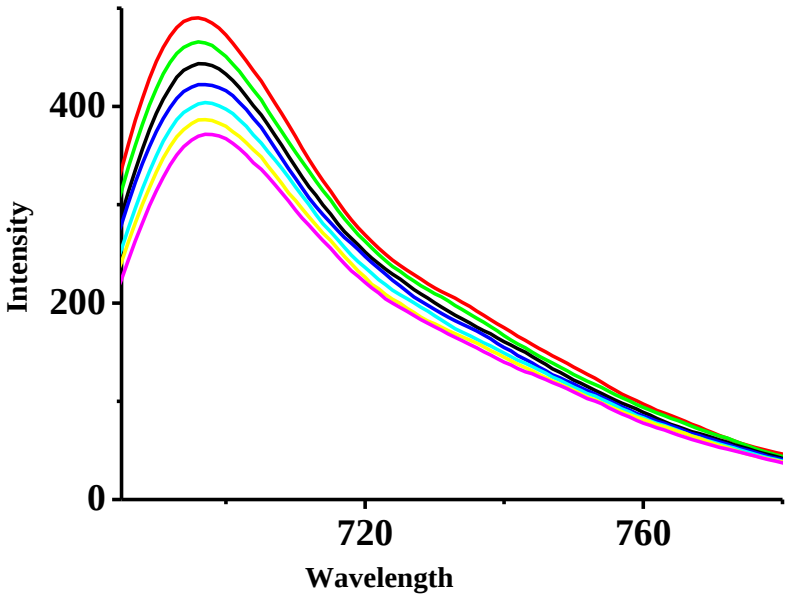


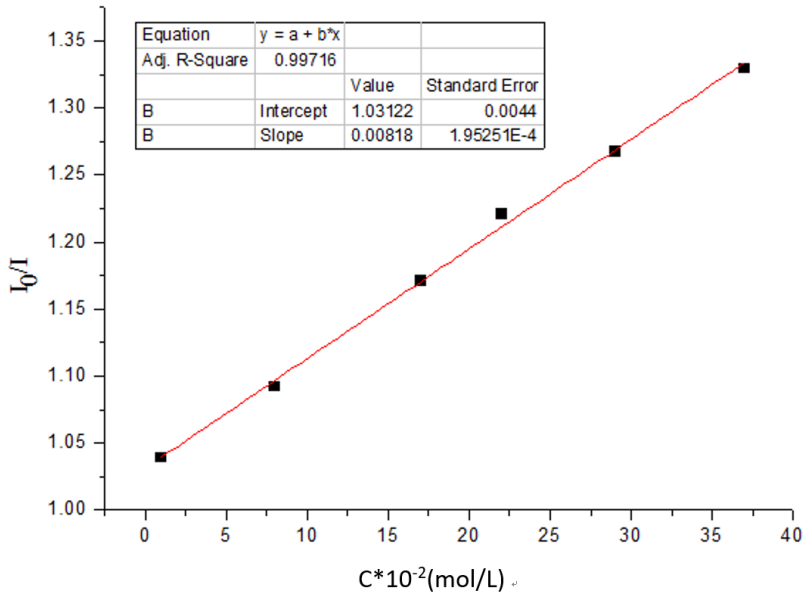
1-phenyl-2-(thiophen-2-ylsulfonyl)ethan-1-one (3af)[5].

Petroleum ether/ethyl acetate =5:1, white solid, 73% yield(102mg). ^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.95 (d, *J* = 7.4 Hz, 2 H), 7.74 (dd, *J* = 4.9, 1.3 Hz, 1 H), 7.69 (dd, *J* = 3.8, 1.2 Hz, 1 H), 7.63 (t, *J* = 7.4 Hz, 1 H), 7.49 (t, *J* = 7.4 Hz, 2 H), 7.13 (dd, *J* = 4.9, 3.9 Hz, 1 H), 4.83 (s, 2 H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ = 187.8, 139.4, 135.7, 135.5, 135.0, 134.5, 129.2, 128.9, 127.9, 64.4 ppm.

4. Luminescence quenching by compound 2a

A Varian Cary Eclipse fluorescence spectrometer was used to record the emission intensities. All the solutions were excited at 664 nm and the emission intensity at 685 nm was observed. EtOH was degassed with a stream of N_2 for 30 min. In a typical experiment, the emission spectrum of a 1×10^{-2} M solution of Methylene Blue in EtOH was collected. Then, appropriate amount of quencher **2a** was added to the measured solution in a quartz cuvette and the emission spectrum of the sample was collected. I_0 and I represent the intensities of the emission in the absence and presence of the quencher at 685 nm.





5.Reference

[1] L.-L. Xie, X.-M. Zhen, S.-P. Huang, X.-L. Su, M. Lin, Y. Li . *Green Chem,* **2017***, 19,* 3530–3534.

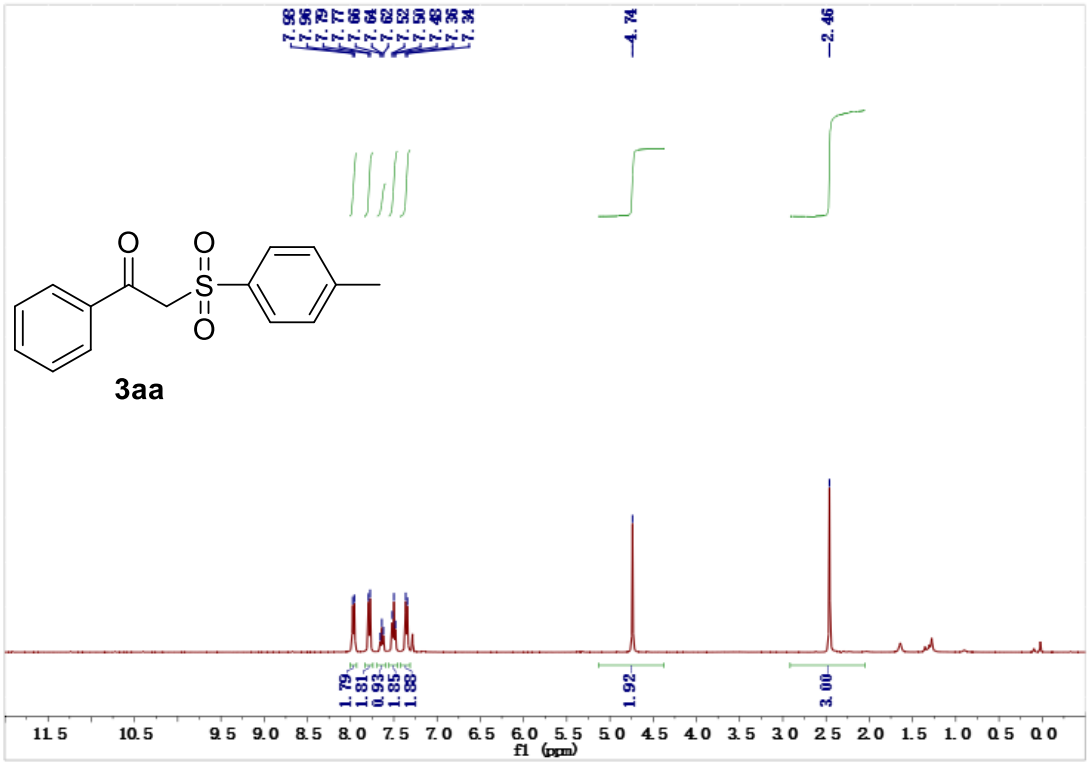
[2] C.-K. Chan, N.-C. Lo, P-Y. Chen, M.-Y. Chang. *Synthesis.* **2017**, *49.* 4469-4477.

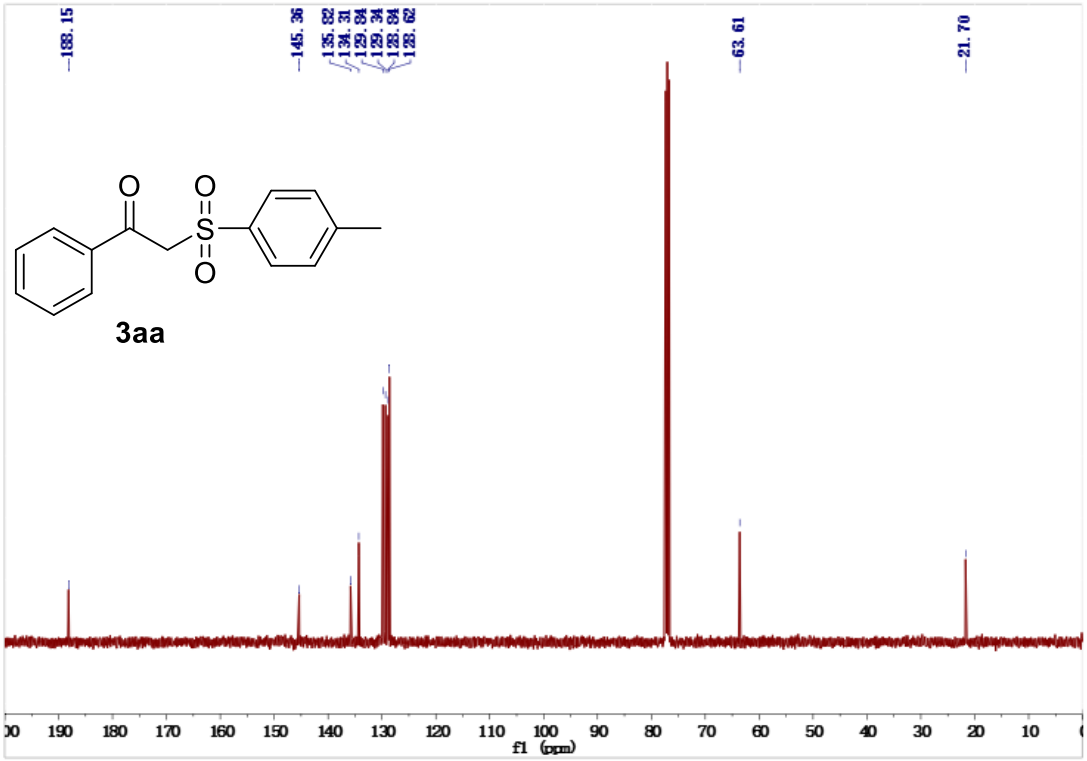
[3] T.-C. Tsuyoshi, I. Atsushi, I. Hiroyuki. *Org. Biomol. Chem*. **2011**, *9*, 3151 – 3153.

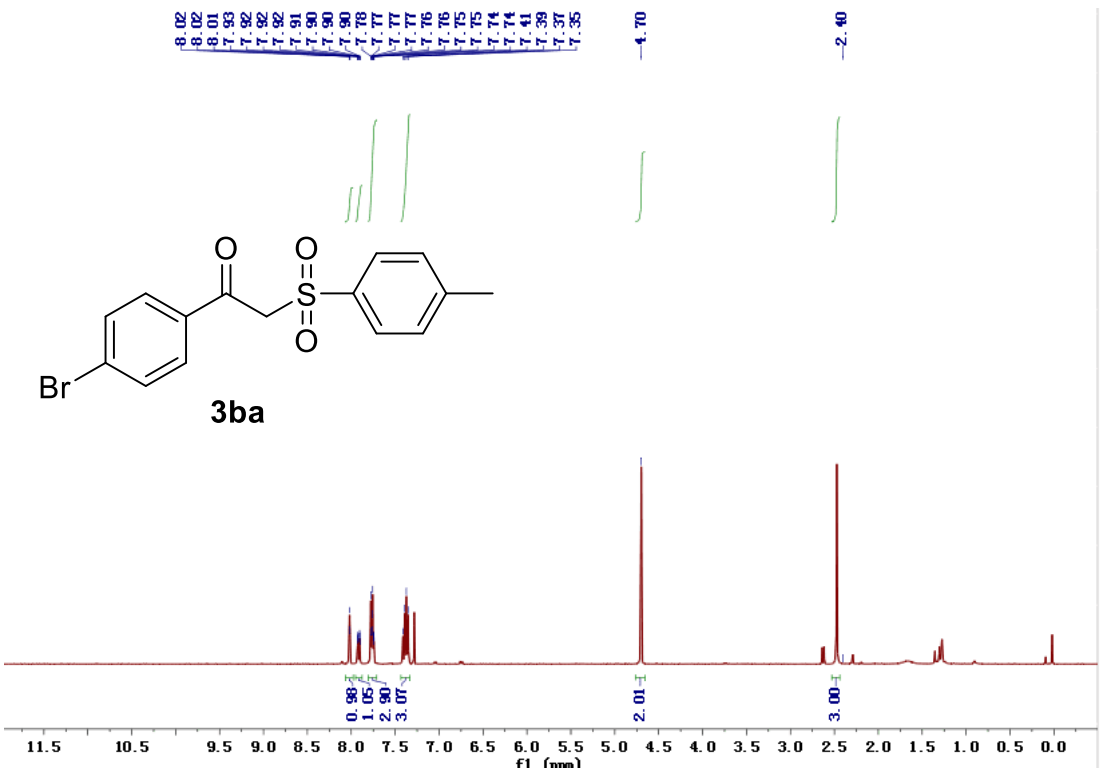
[4] Q.-Q. Lu, J. Zhang, G.-L. Zhao, Y. Qi, H.-M. Wang, A.-W. Lei. *J. Am. Chem. Soc*. **2013**, *135*, 11481−11484.

[5] H. Jiang, Y.-Z. Cheng, Y. Zhang, S.-Y. Yu. *Eur. J. Org. Chem*. **2013**, 5485–5492.

6. Spectroscopic Data for Products



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7.74
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1.05
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3.00
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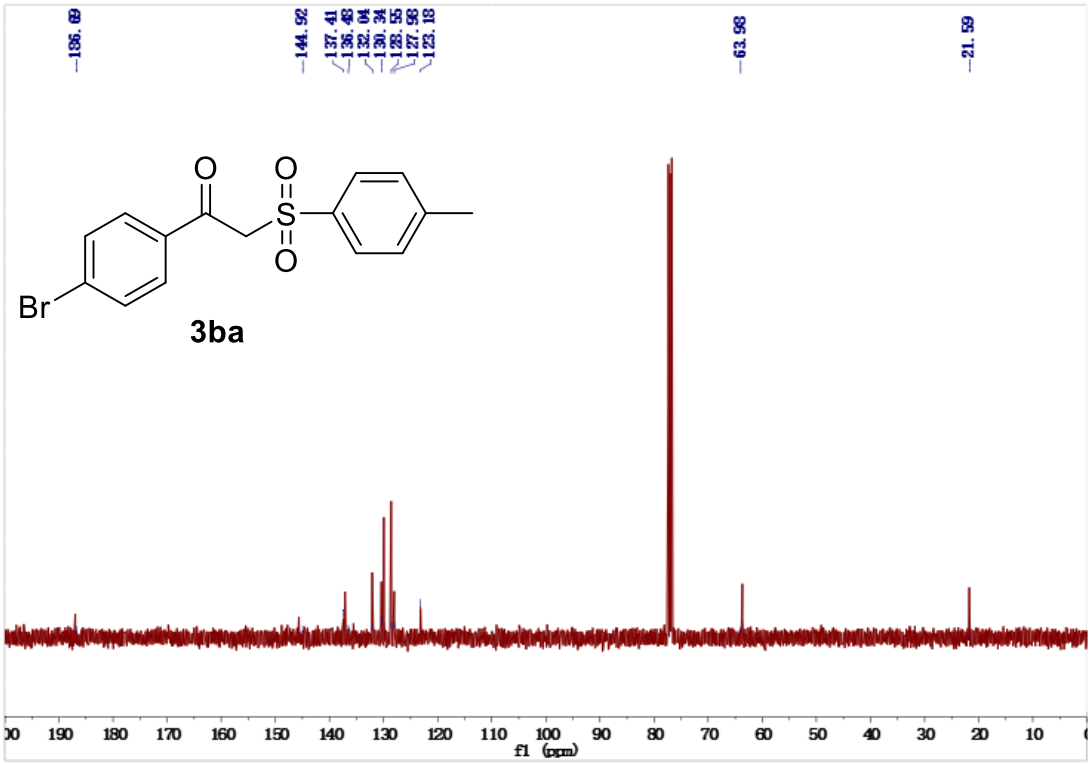
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O
Br
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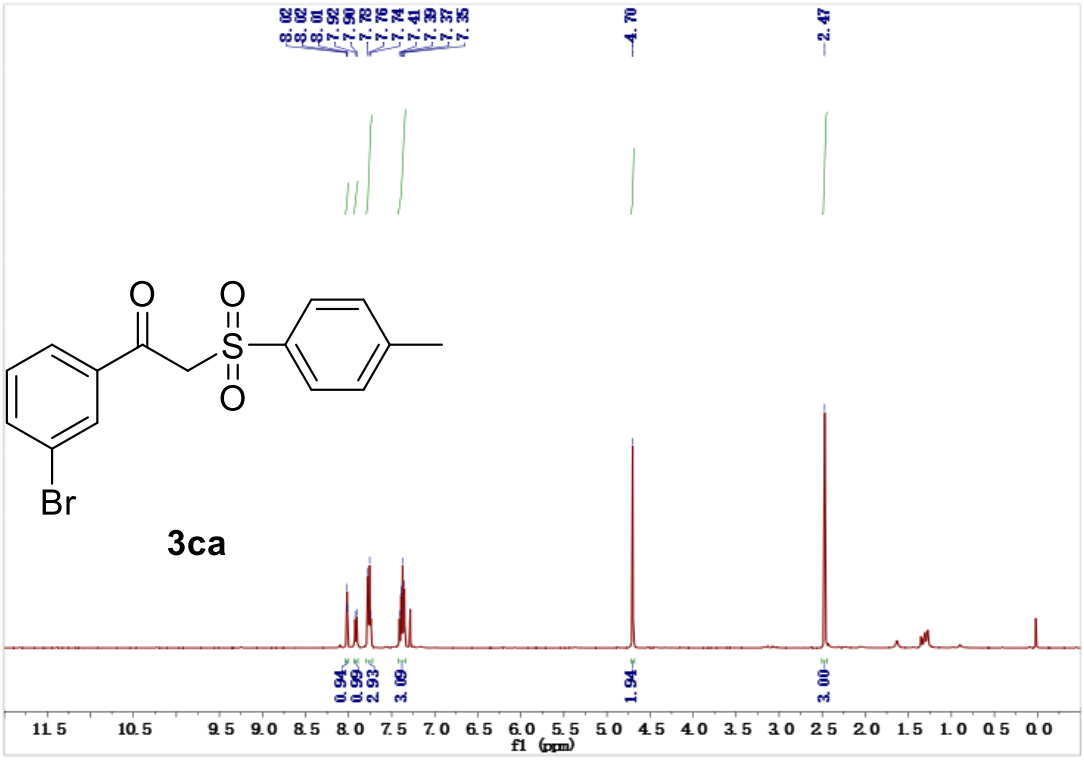
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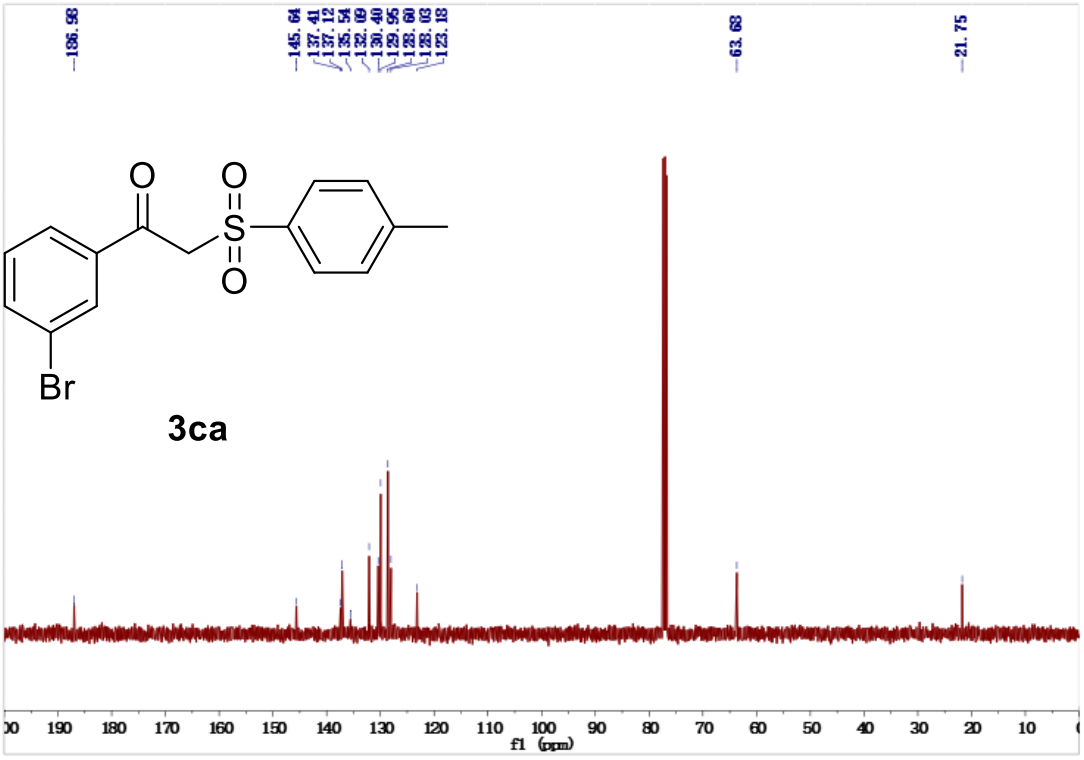
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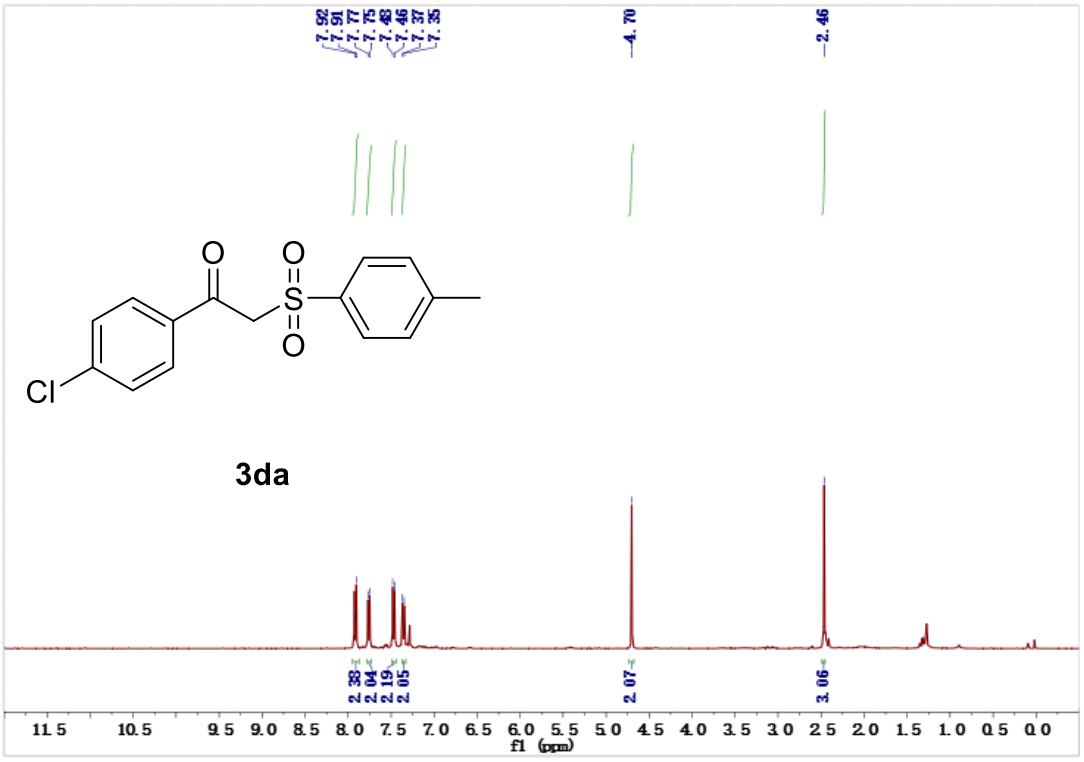
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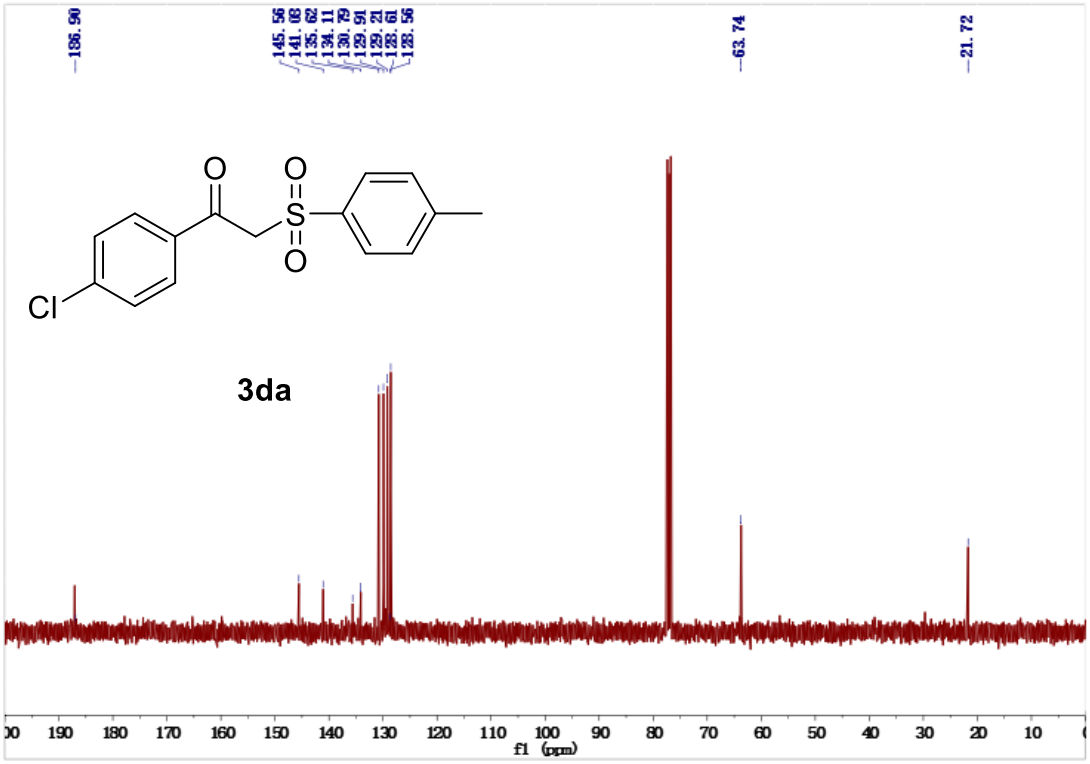
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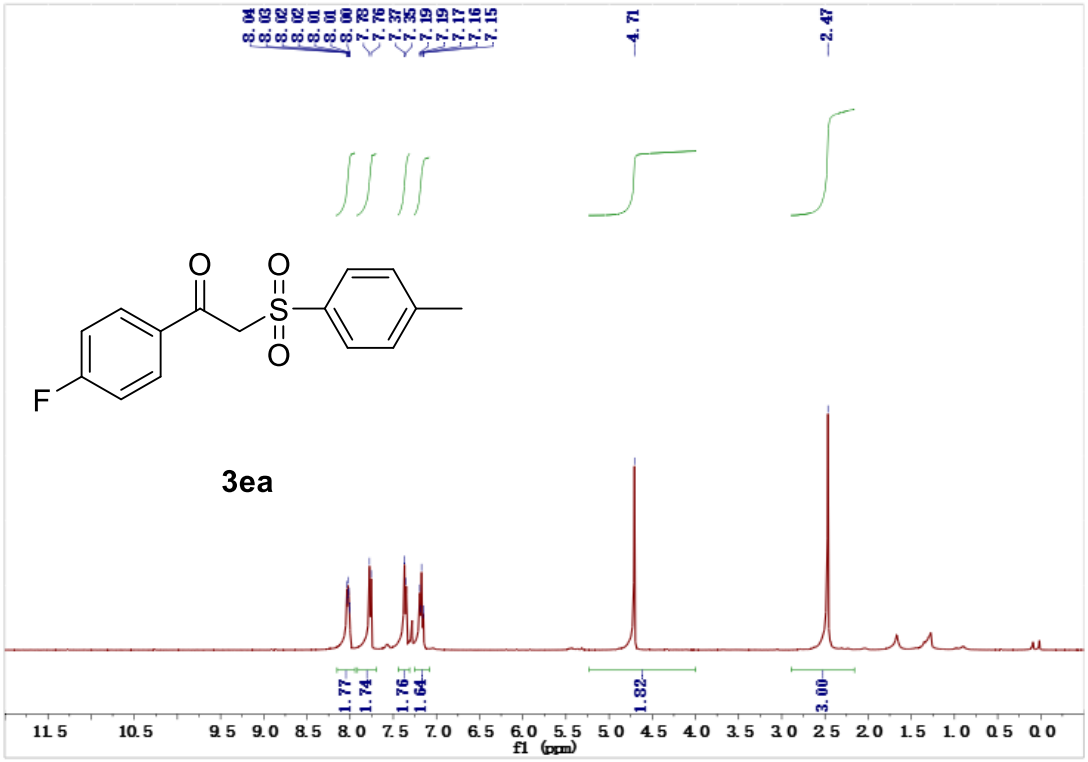
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S
O
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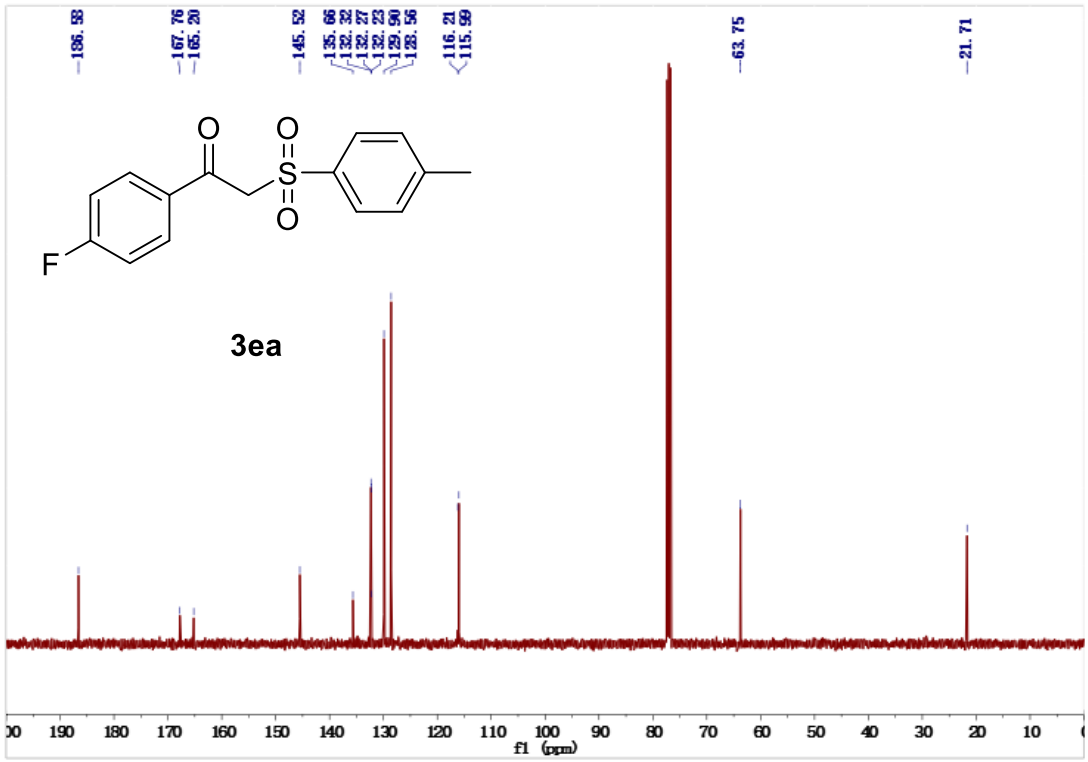
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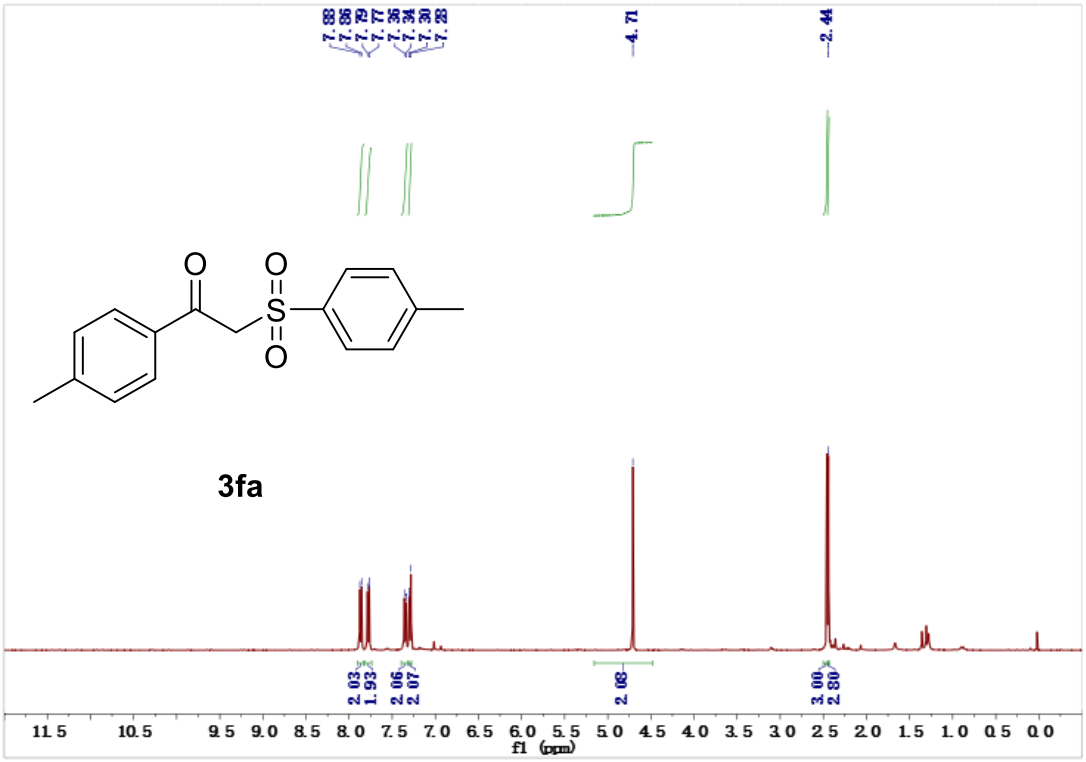
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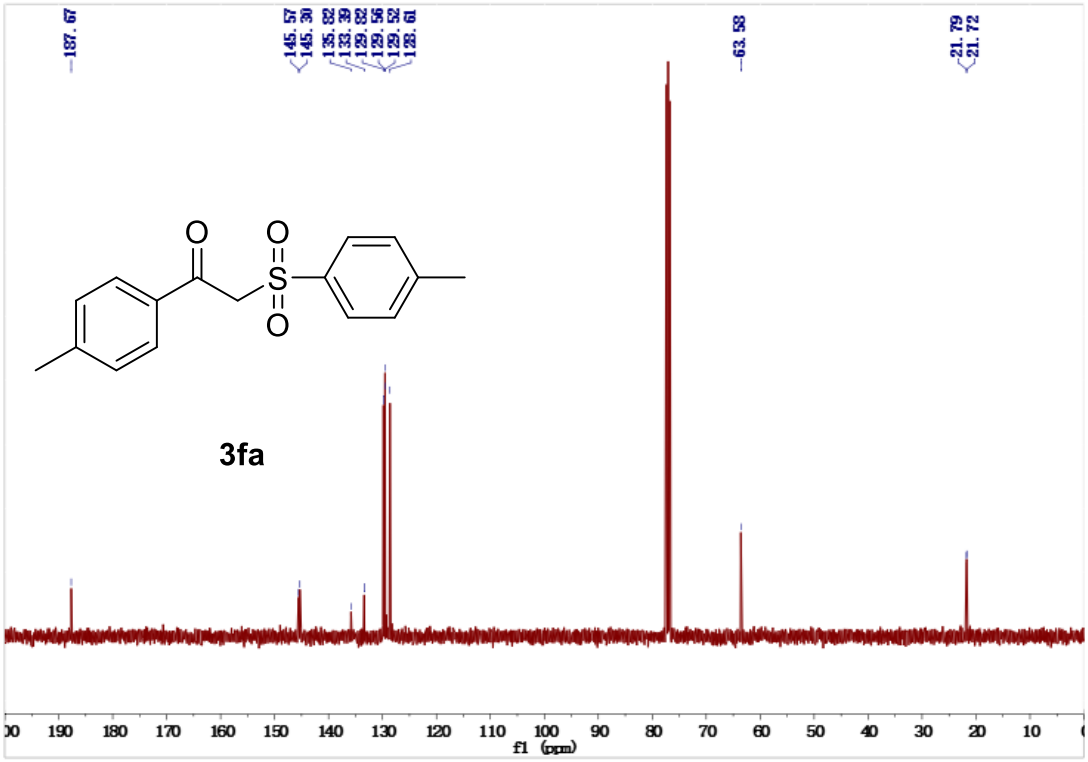
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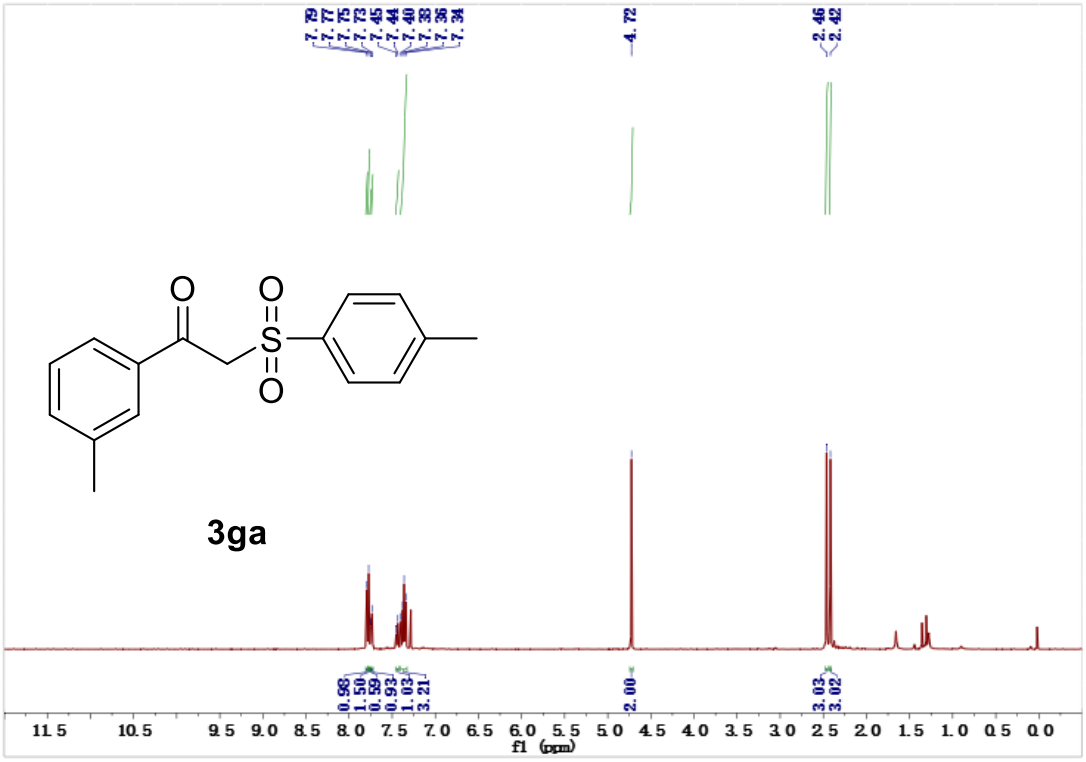
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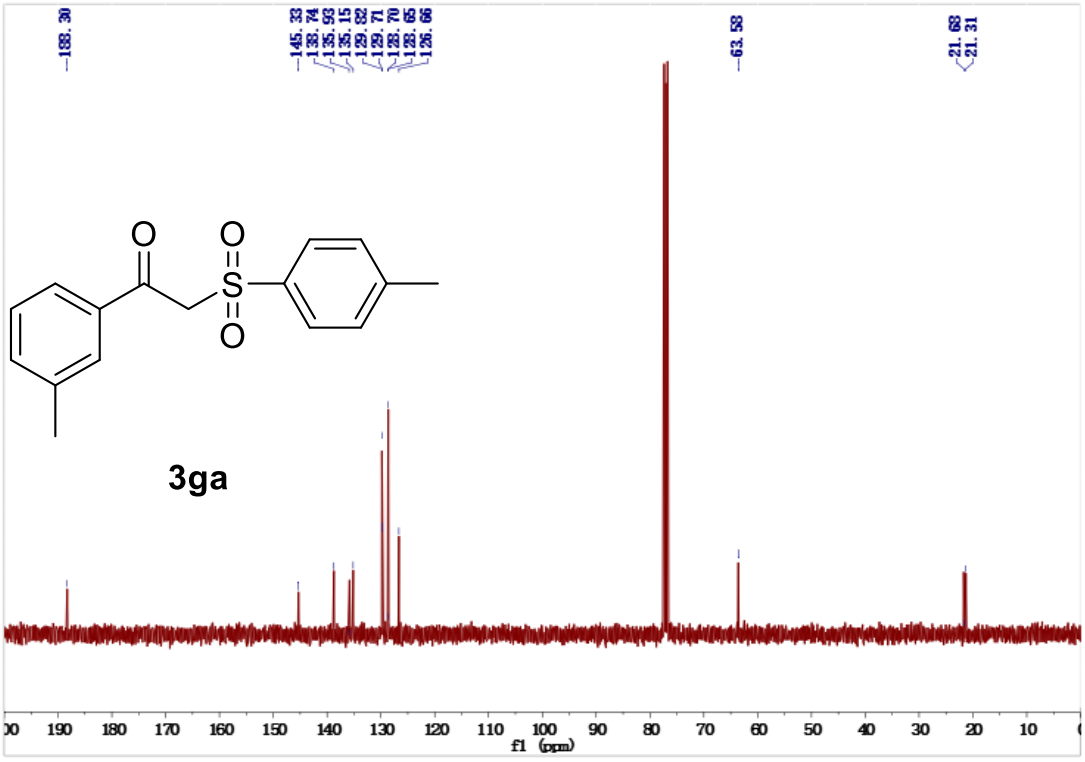
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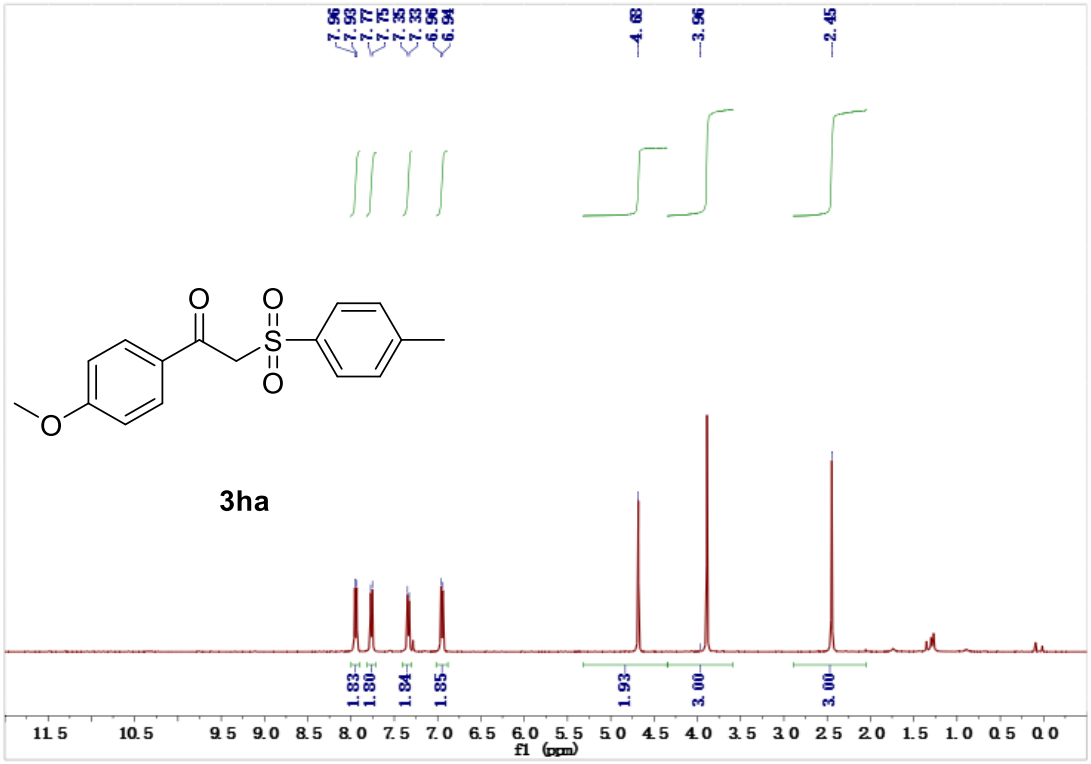
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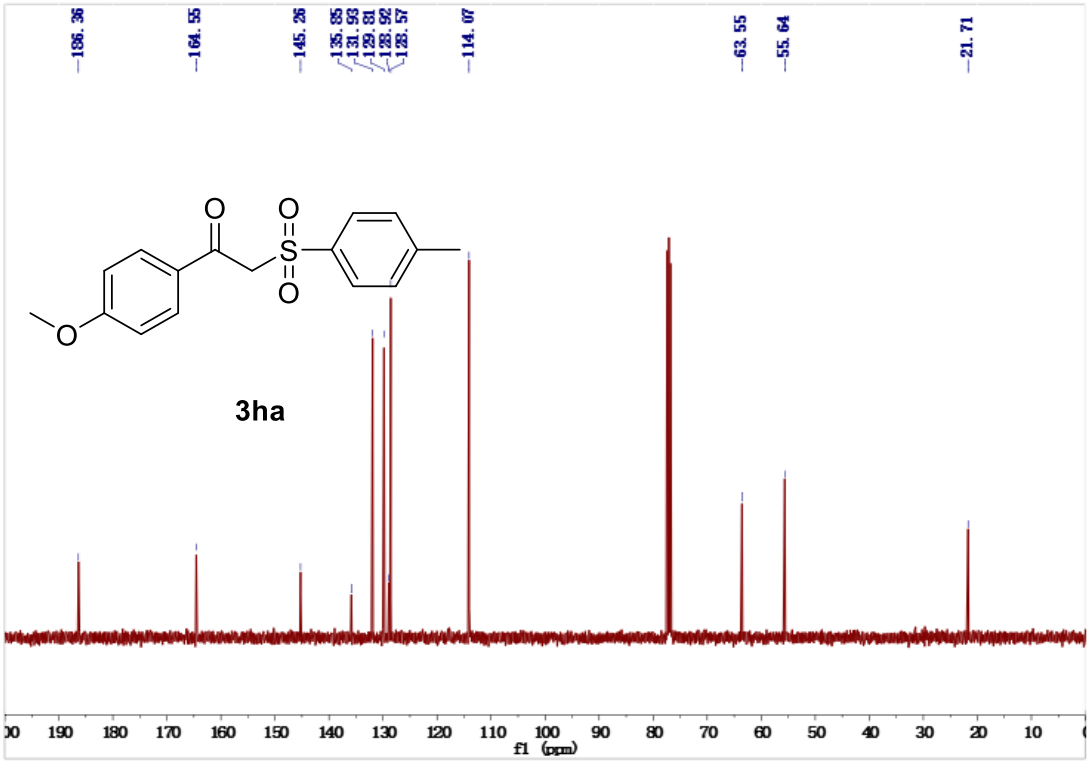
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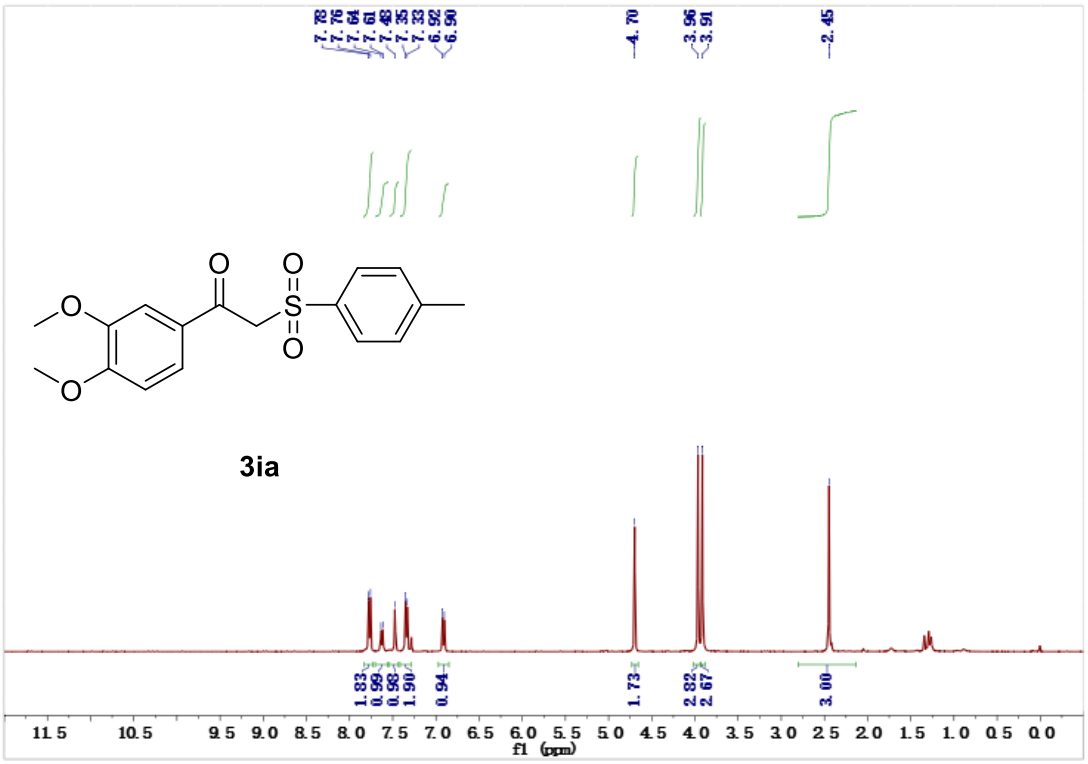
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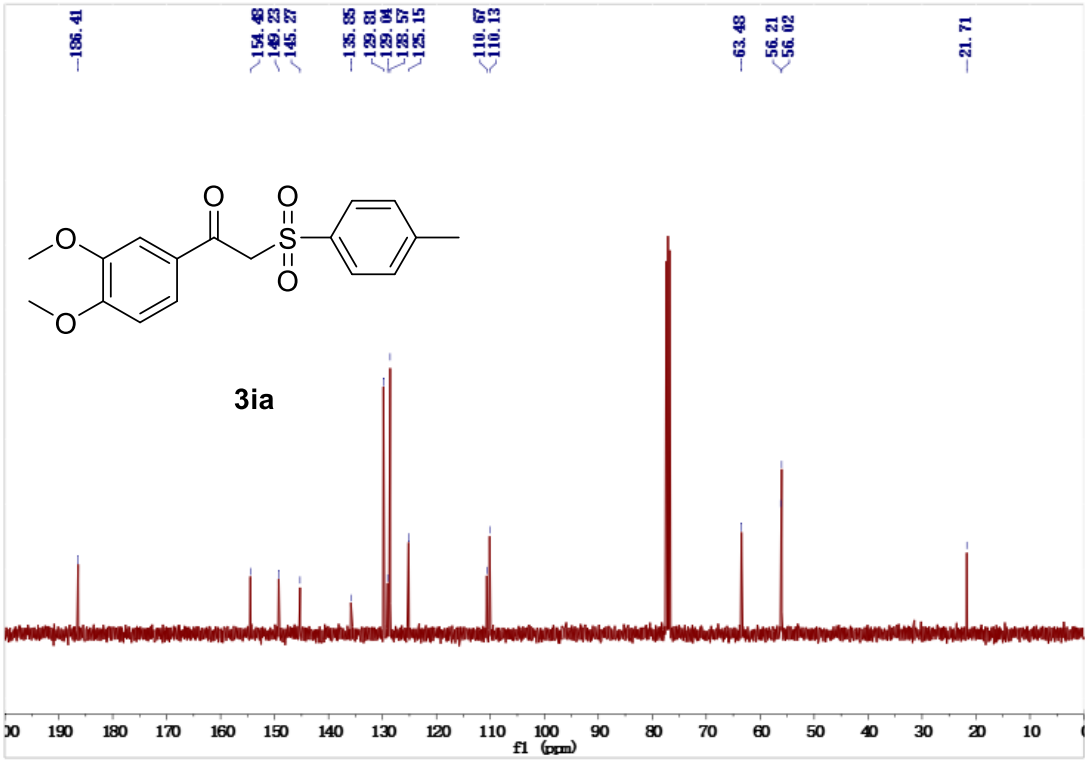
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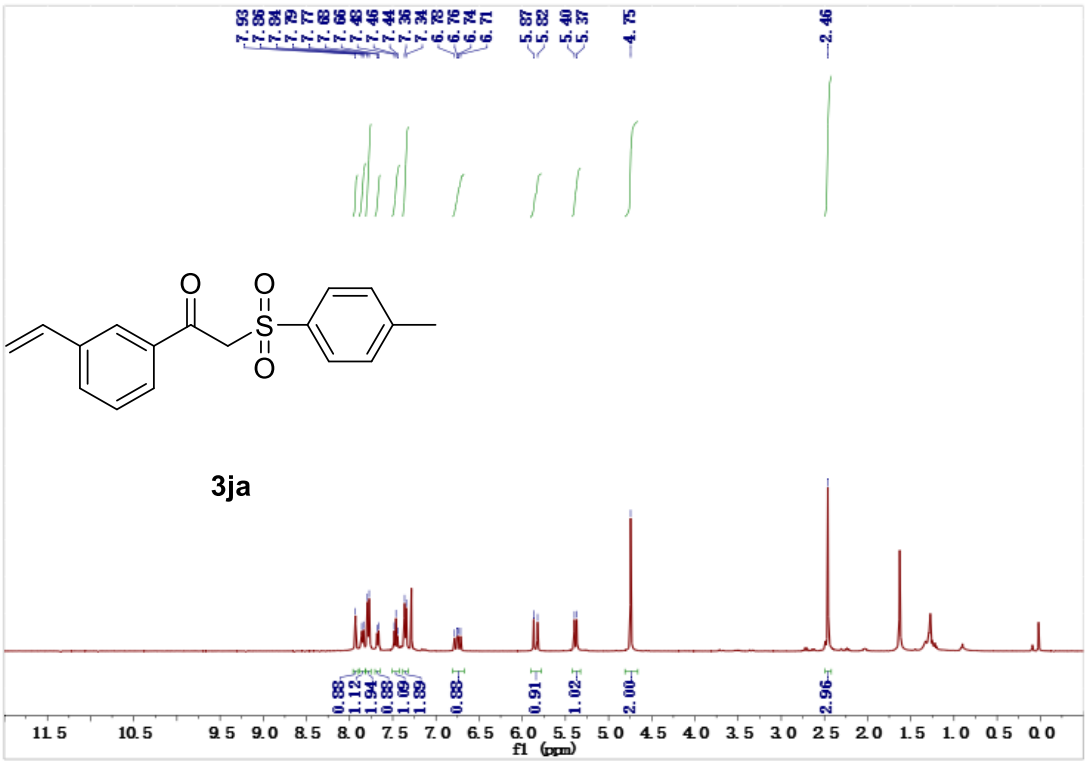
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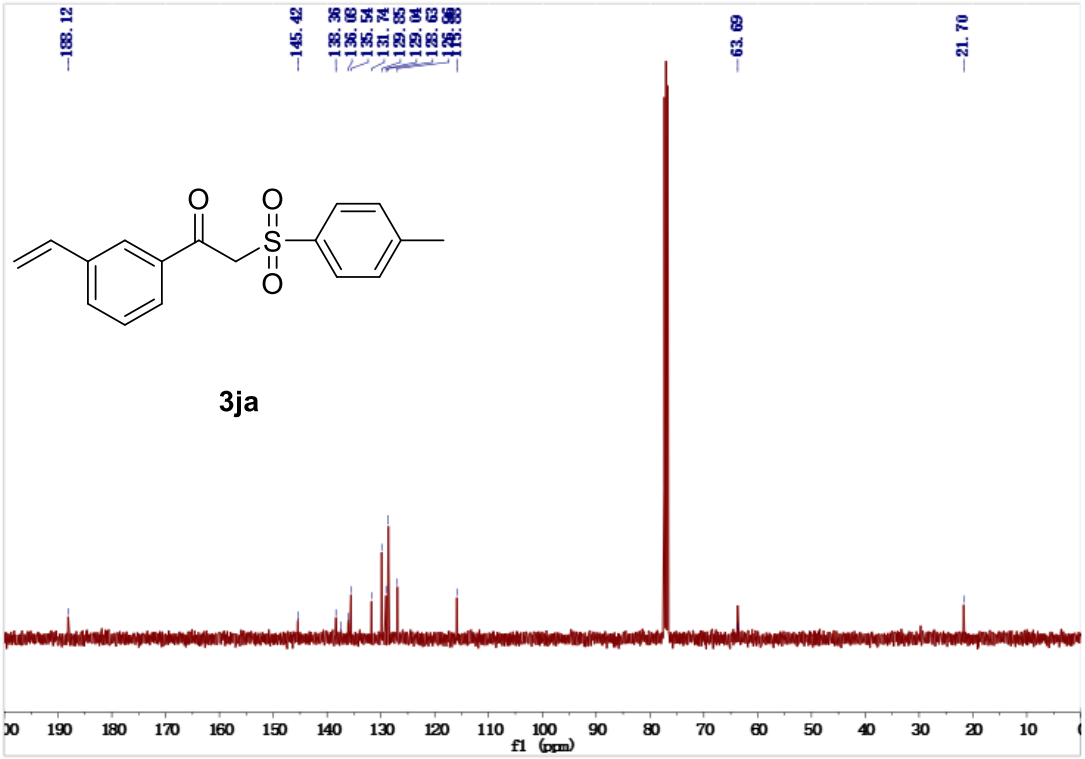
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80
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60
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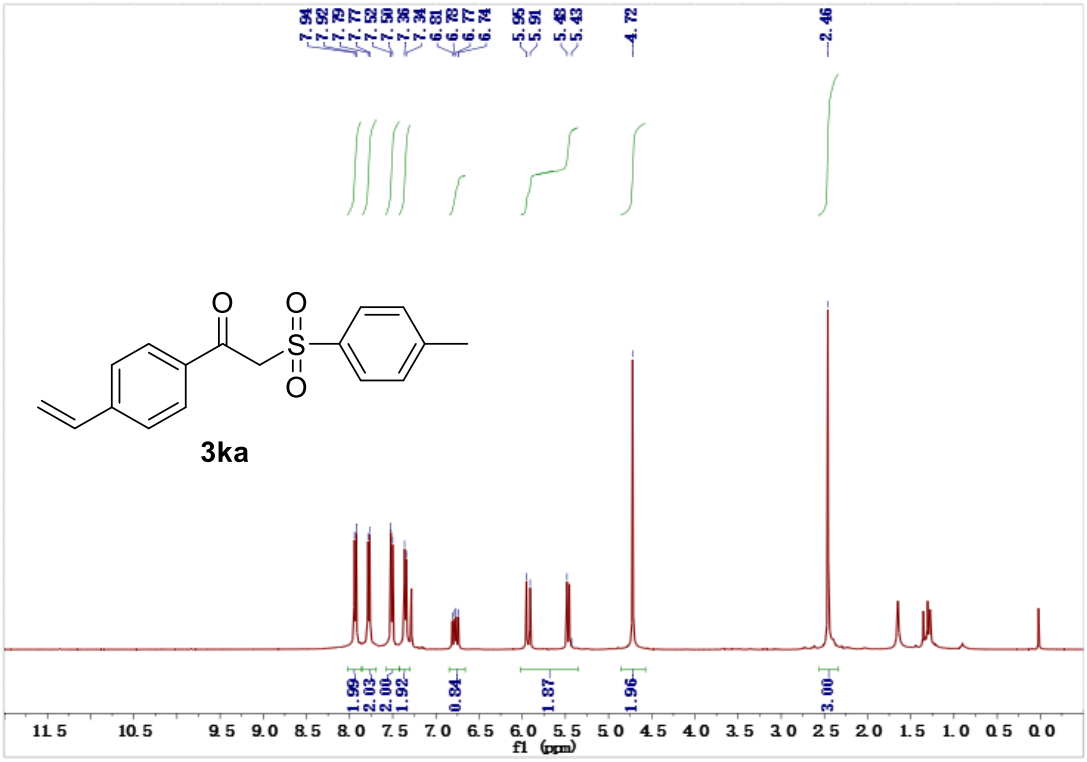
40
30
20
10
f1 (ppm)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7.92
7.79
7.77
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7.50
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7.34
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6.78
6.77
6.74
5.95
5.91
5.48
5.43
4.72
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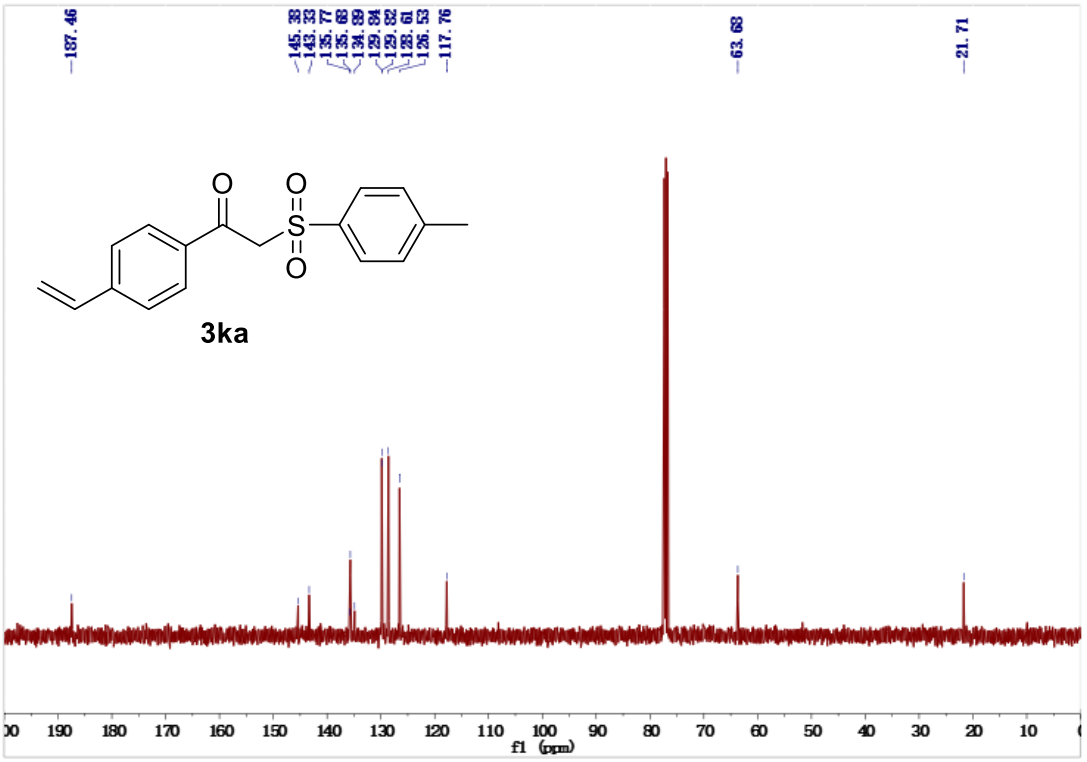
2.03
2.00
1.92
0.84
1.87
1.96
3.00
f1 (ppm)


187.46
145.33
143.33
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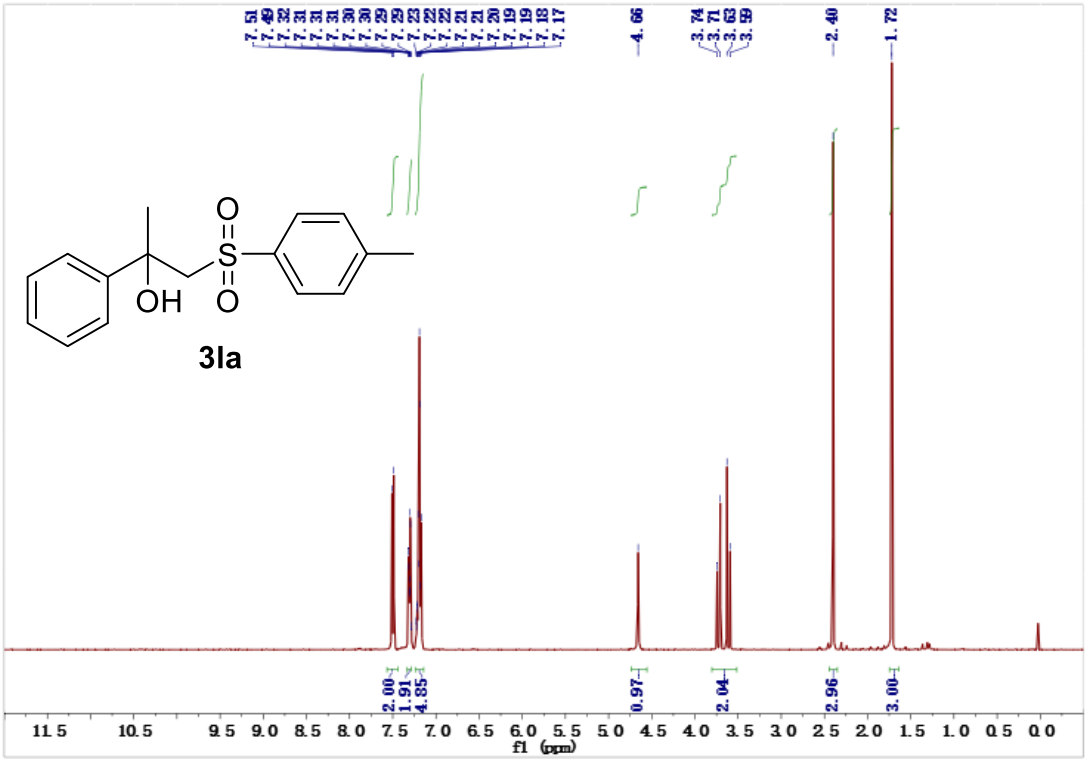
129.94
129.52
128.61
126.53
117.76
63.68
21.71
3ka
f1 (ppm)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7.23
7.22
7.22
7.21
7.21
7.20
7.19
7.19
7.18
7.17
4.66
3.74
3.71
3.63
3.59
2.40
1.72
OH
O
S
O
3la
2.00
1.91
4.85
0.97
2.04
2.96
3.00
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
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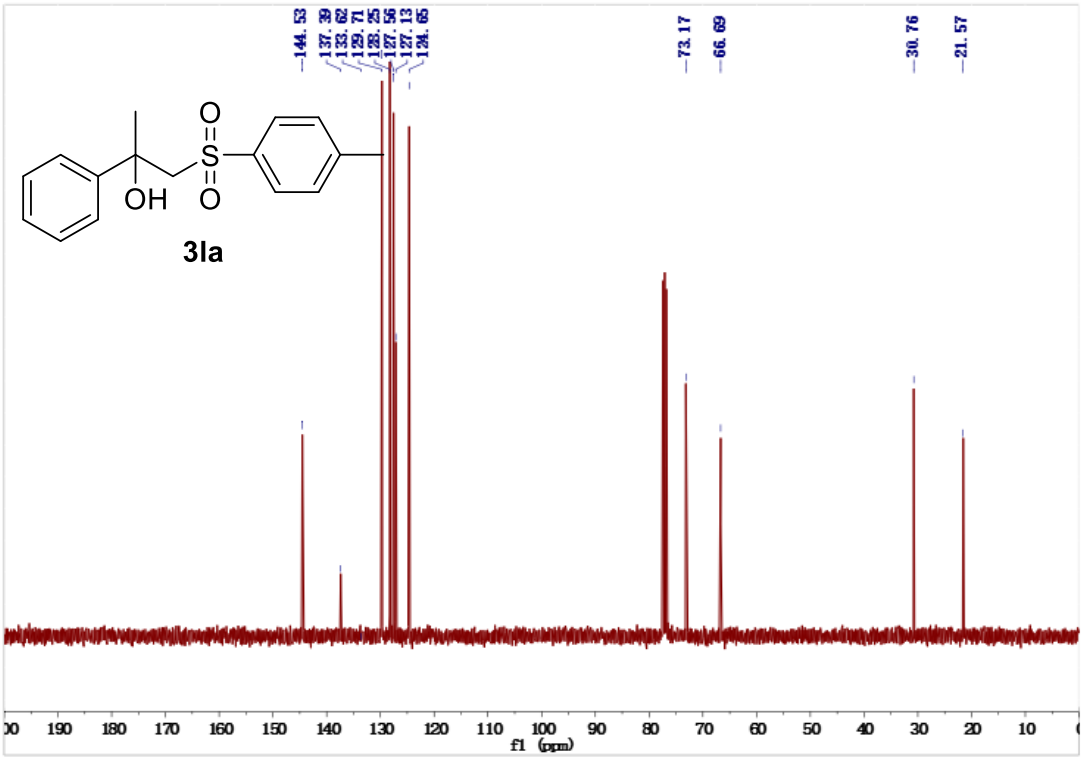
0.0
f1 (ppm)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127.13
124.65
73.17
66.69
30.76
21.57
OH
O
S
O
3la
190
180
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160
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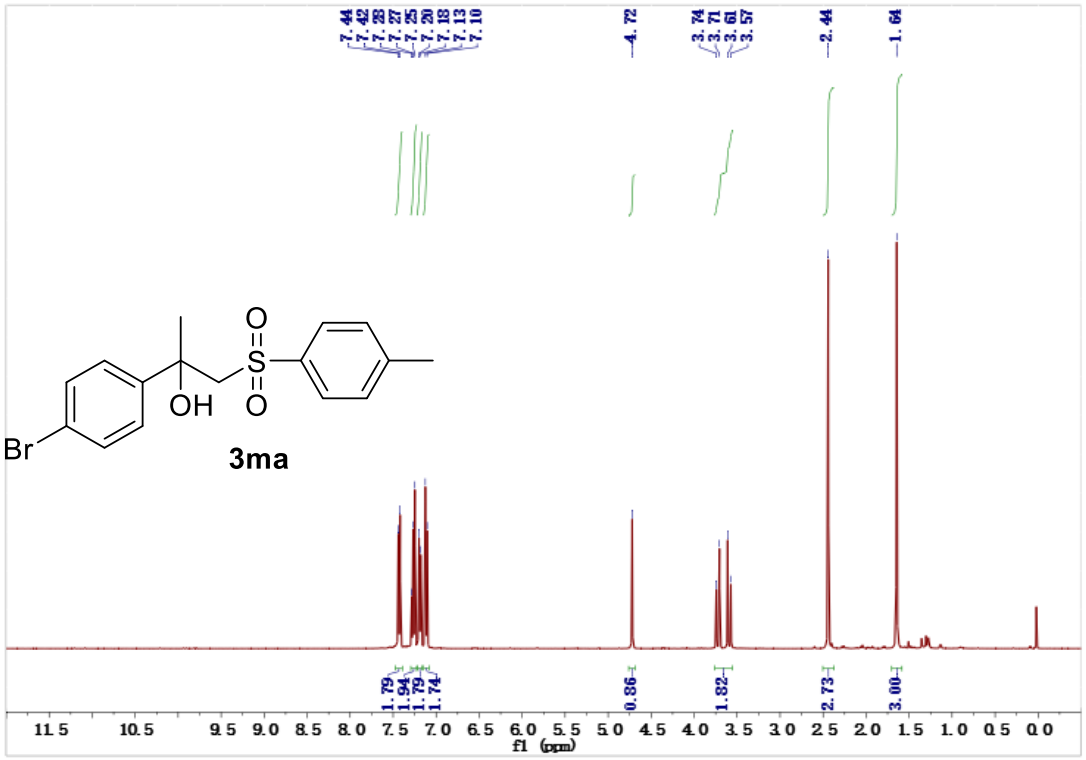
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)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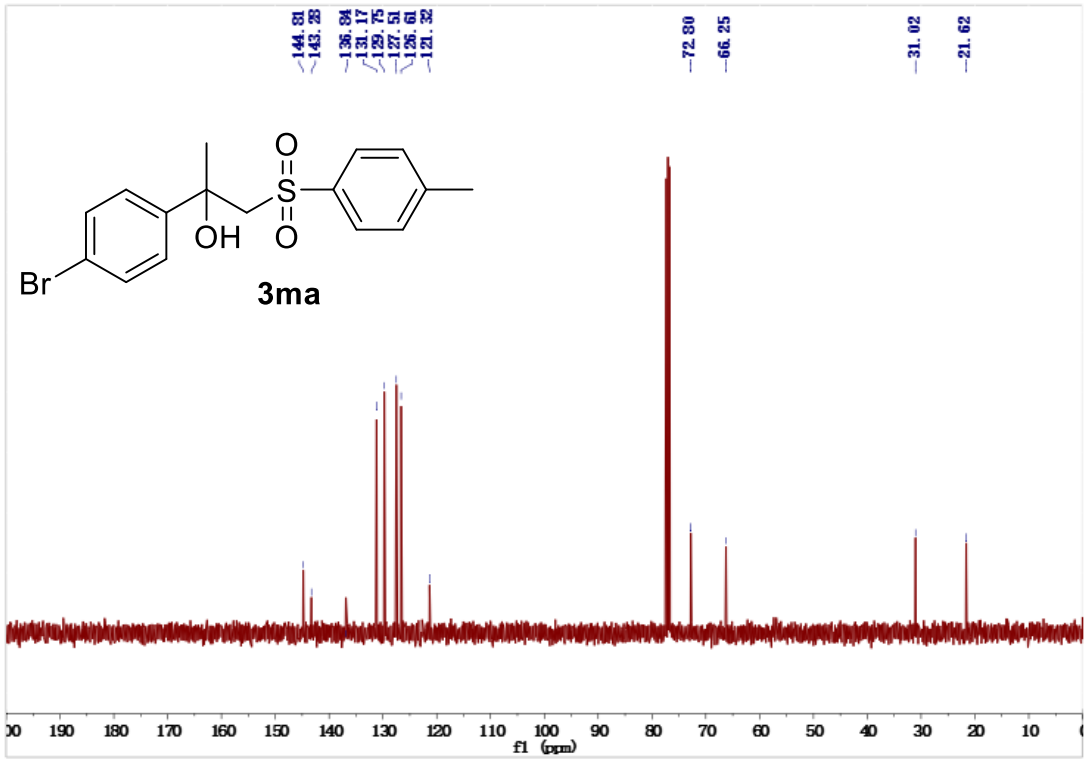
7.18
7.13
7.10
4.72
3.74
3.71
3.61
3.57
2.44
1.64
O
S
O
OH
Br
3ma
1.79
1.94
1.79
1.74
0.86
1.82
2.73
3.00
11.5 10.5 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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131.17
129.75
127.51
126.61
121.32
72.80
66.25
31.02
21.62
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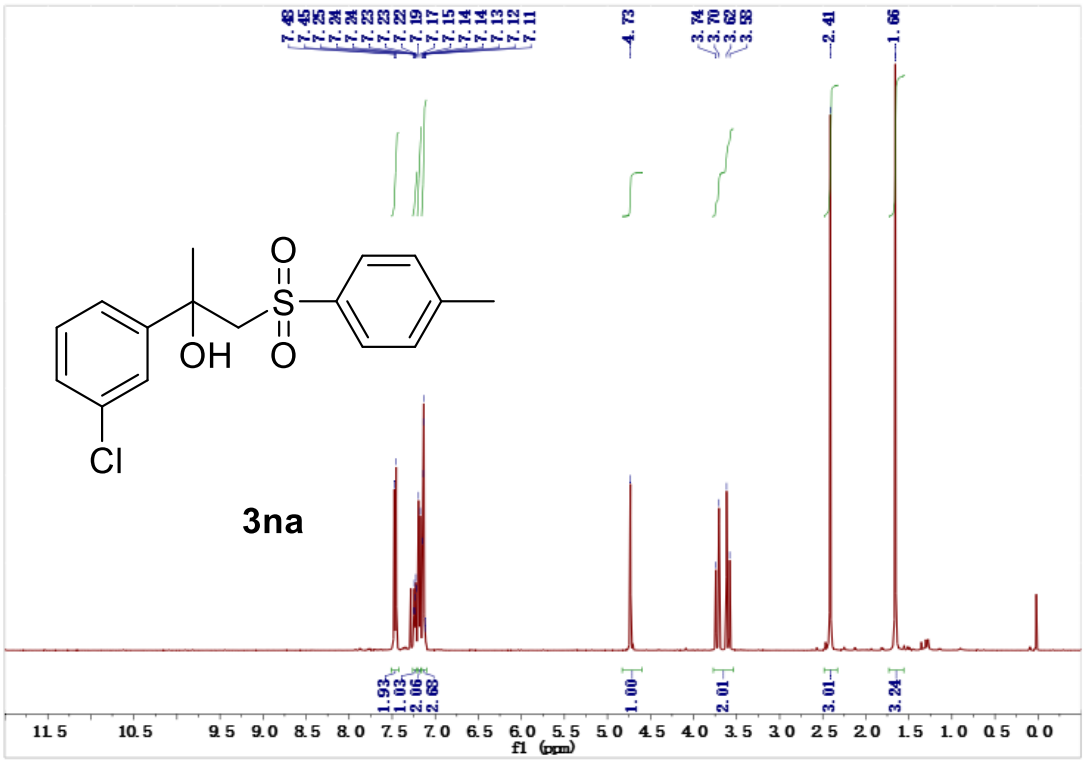
S
O
OH
Br
3ma
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
f1 (ppm)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7.17
7.15
7.14
7.14
7.13
7.12
7.11
4.73
3.74
3.70
3.62
3.53
2.41
1.66
O
S
O
OH
Cl
3na
1.93
1.03
2.06
2.68
1.00
2.01
3.01
3.24
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
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4.5
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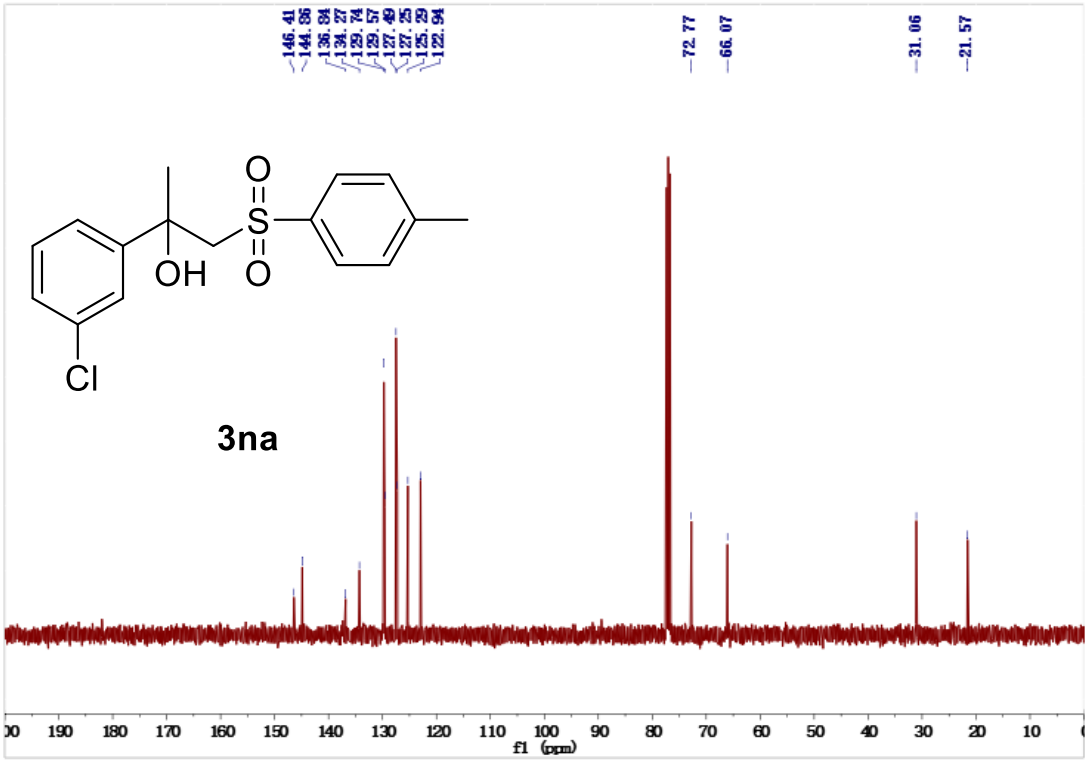
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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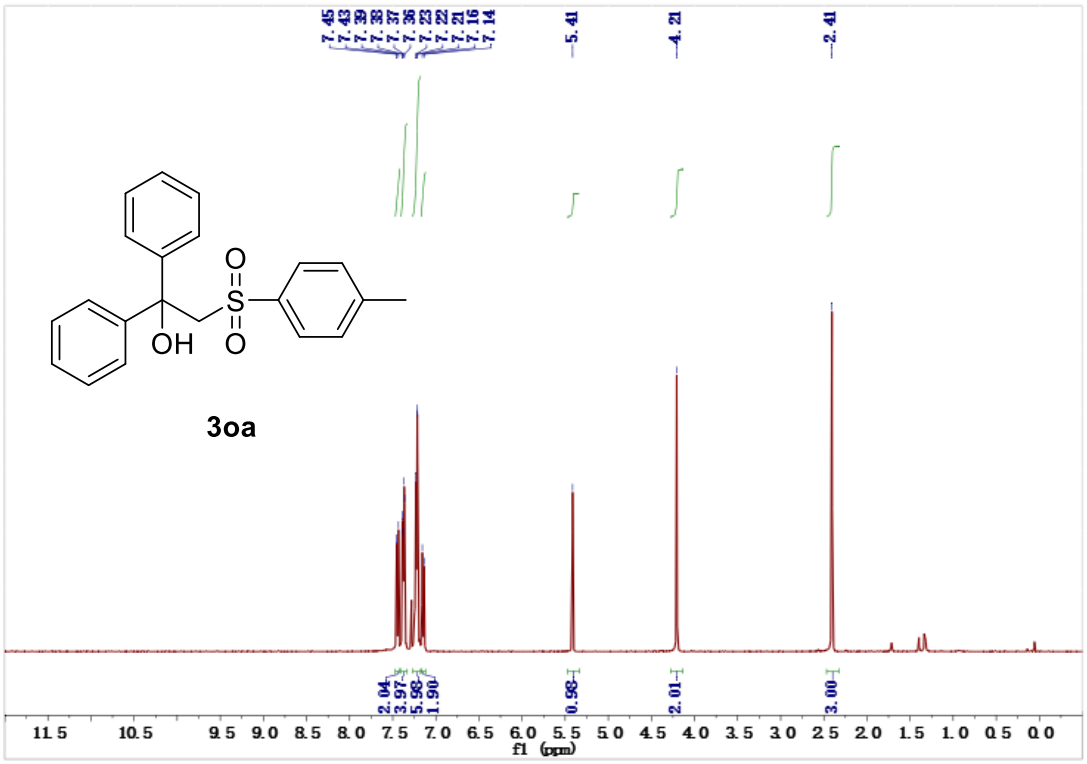
144.36
136.94
134.27
129.74
129.57
127.49
127.25
125.29
122.94
72.77
66.07
31.06
21.57
O
S
O
OH
Cl
3na
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)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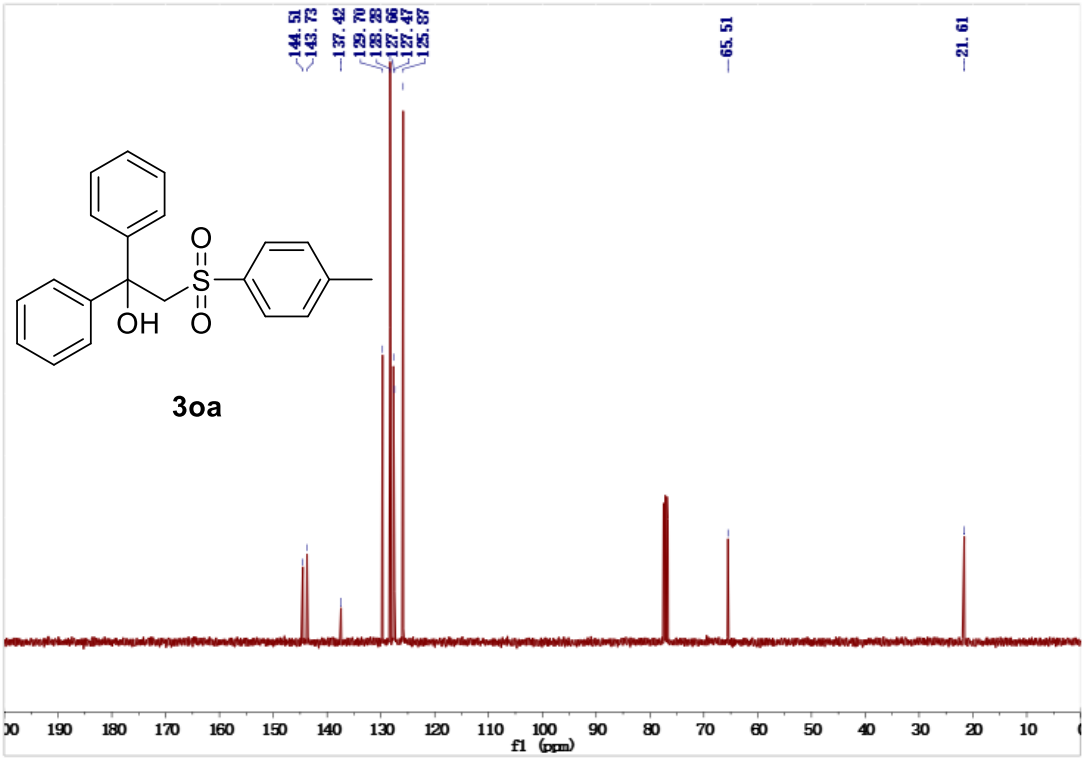
7.38
7.37
7.36
7.23
7.22
7.21
7.16
7.14
5.41
4.21
2.41
OH
O
S
O
3oa
2.04
3.97
5.98
1.90
0.98
2.01
3.00
f1 (ppm)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143.73
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127.66
127.47
125.87
65.51
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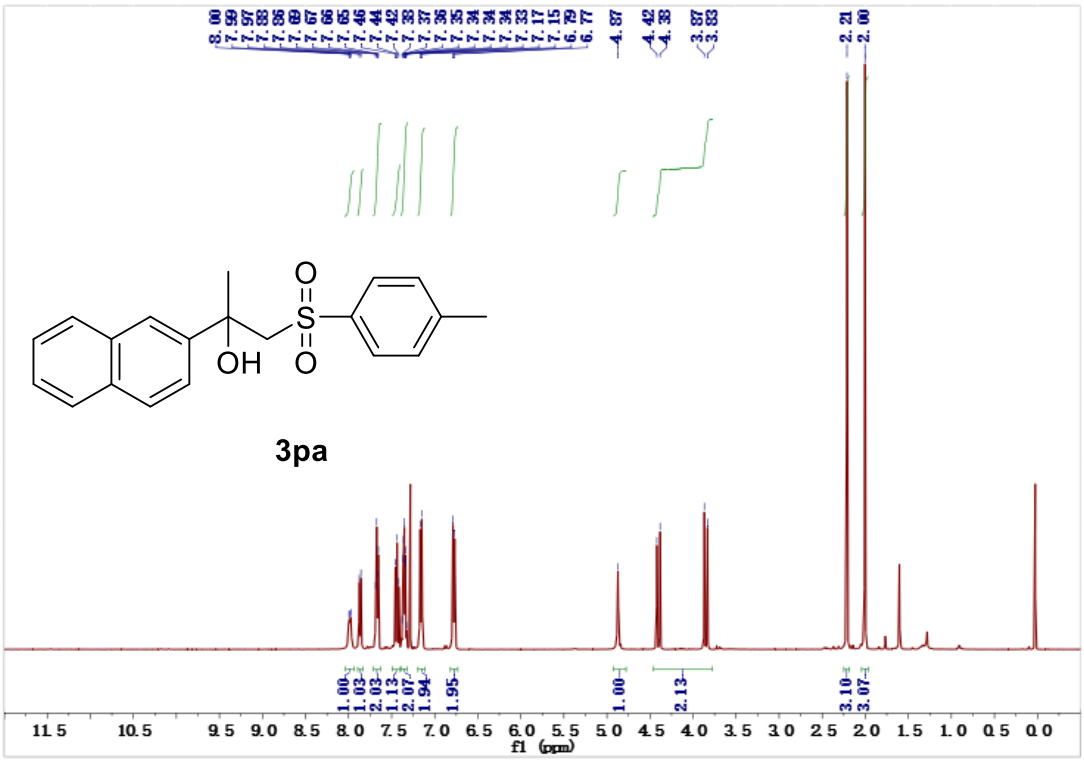
OH
O
S
O
3oa
f1 (ppm)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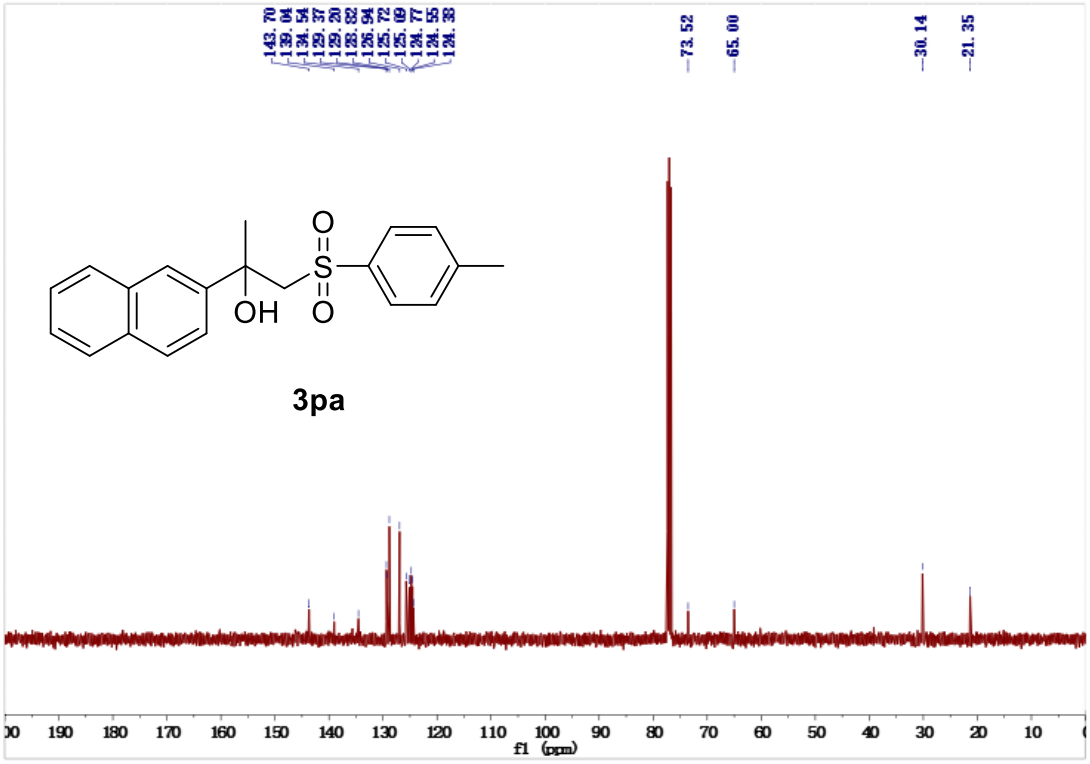
7.69
7.67
7.66
7.65
7.46
7.44
7.42
7.33
7.37
7.36
7.35
7.34
7.34
7.34
7.33
7.17
7.15
6.79
6.77
4.97
4.42
4.38
3.87
3.83
2.21
2.00
OH
3pa
1.00
1.03
2.03
1.13
2.07
1.94
1.95
1.00
2.13
3.10
3.07
f1 (ppm)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134.54
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129.20
128.82
126.94
125.72
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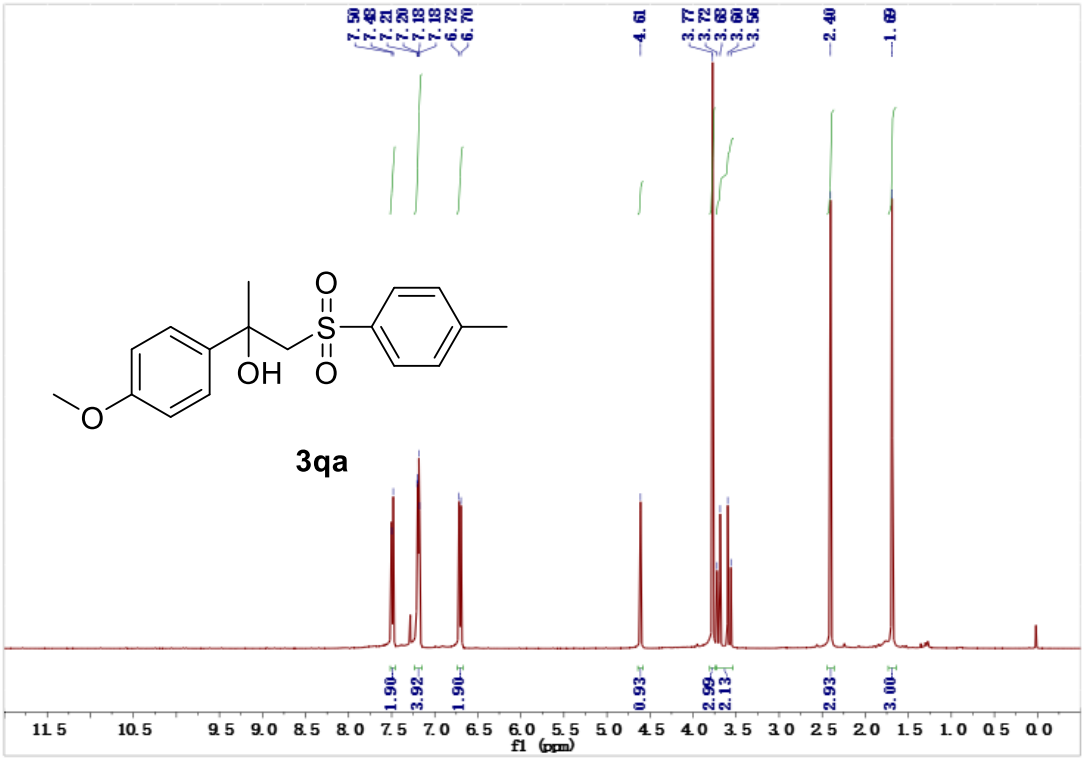
124.77
124.55
124.33
73.52
65.00
30.14
21.35
OH
3pa
f1 (ppm)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7.21
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7.13
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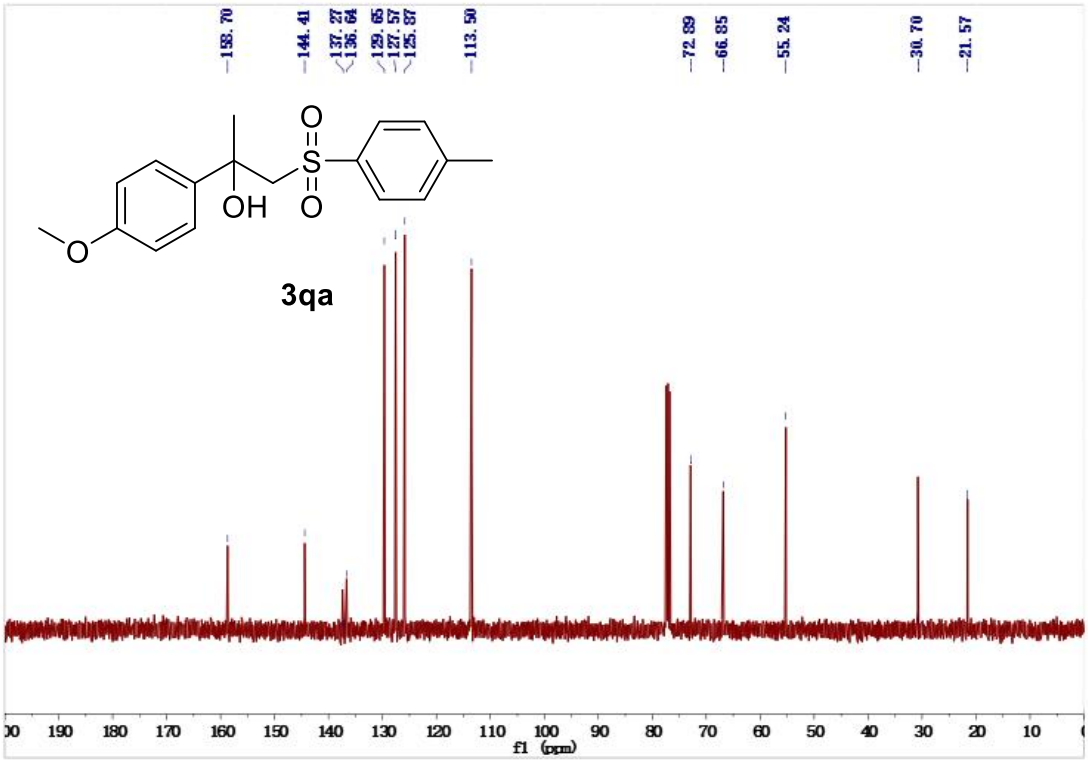
6.70
4.61
3.77
3.72
3.68
3.60
3.56
2.40
1.89
OH
O
S
O
O
3qa
1.90
3.92
1.90
0.93
2.99
2.13
2.93
3.00
11.5 10.5 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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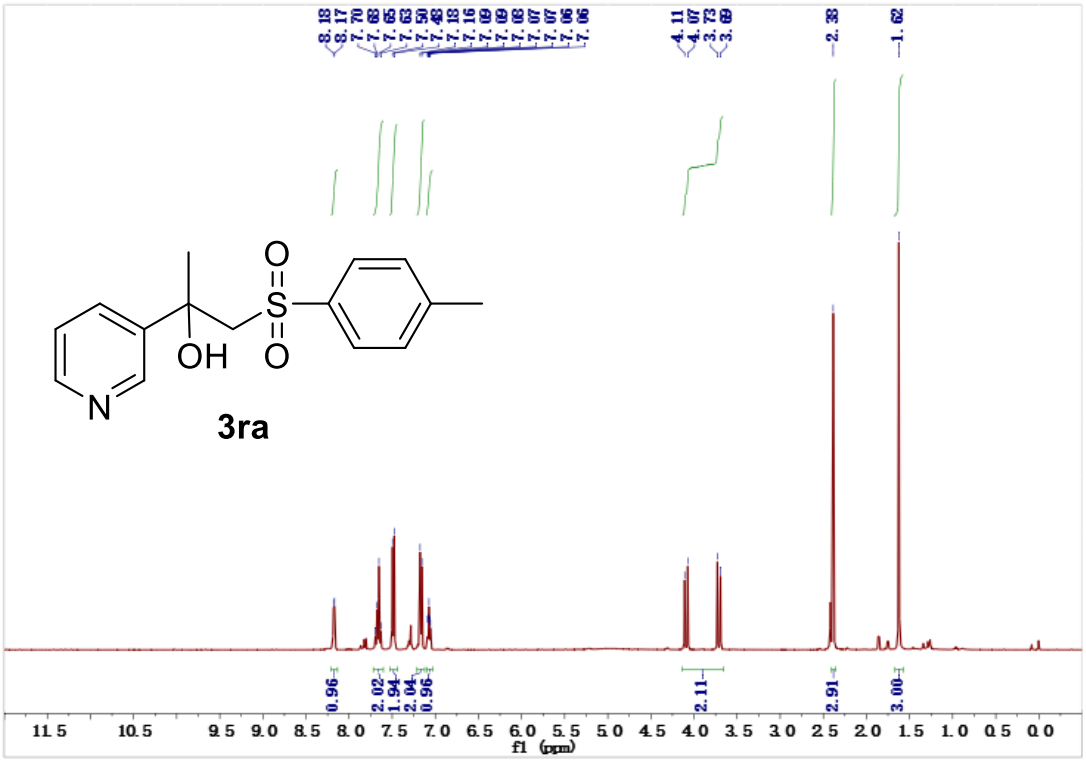
144.41
137.27
136.64
129.65
127.57
125.87
113.50
72.89
66.85
55.24
30.70
21.57
OH
O
S
O
O
3qa
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
f1 (ppm)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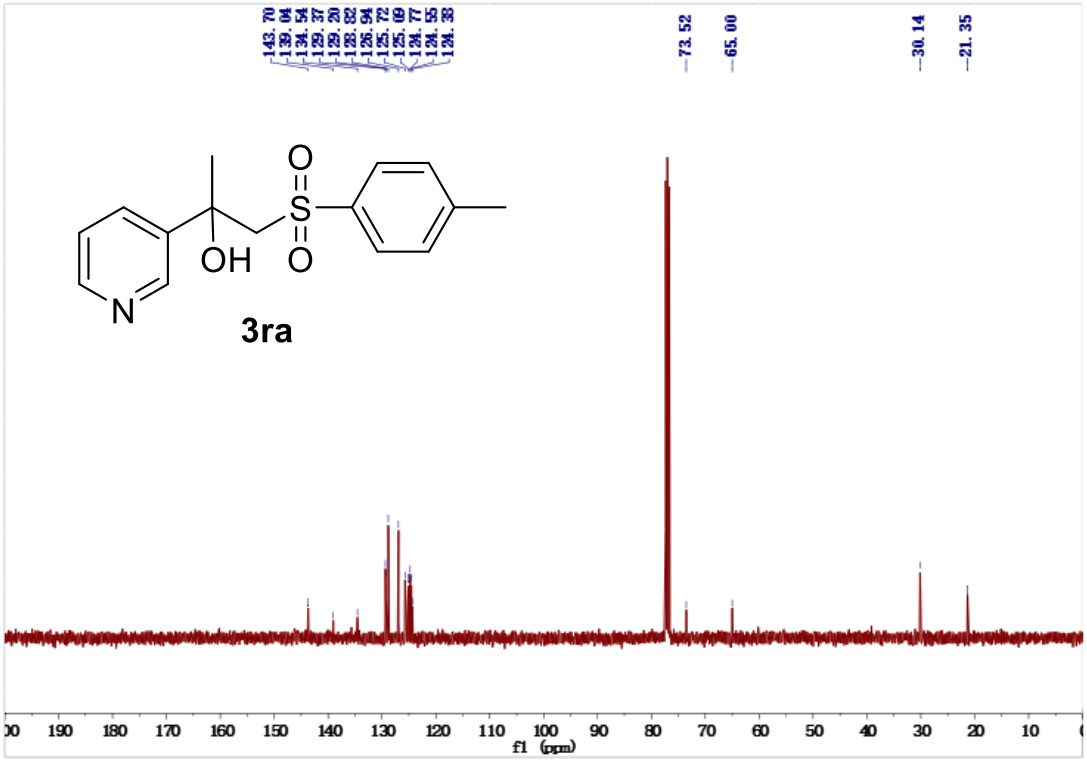
7.50
7.48
7.18
7.16
7.09
7.09
7.08
7.07
7.07
7.06
7.06
4.11
4.07
3.73
3.69
2.38
1.62
O
S
O
OH
N
3ra
0.96
2.02
1.94
2.04
0.96
2.11
2.91
3.00
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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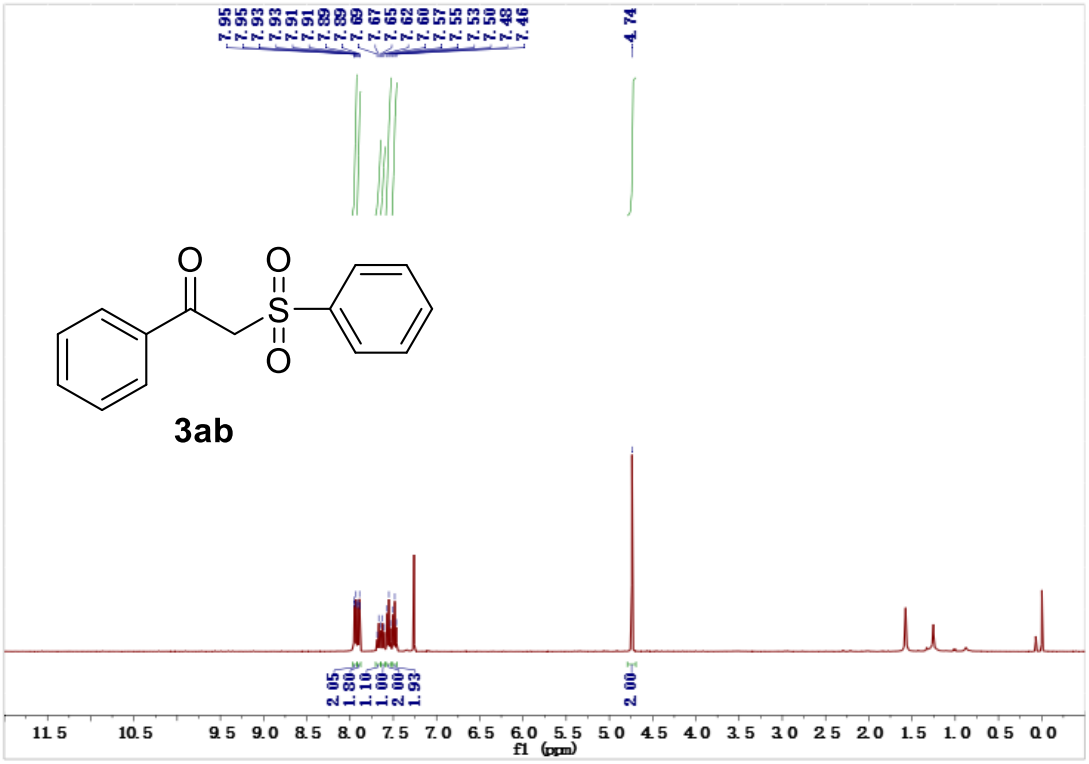
129.37
129.20
128.82
126.54
125.72
125.09
124.77
124.55
124.33
73.52
65.00
30.14
21.35
O
S
O
OH
N
3ra
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)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7.95
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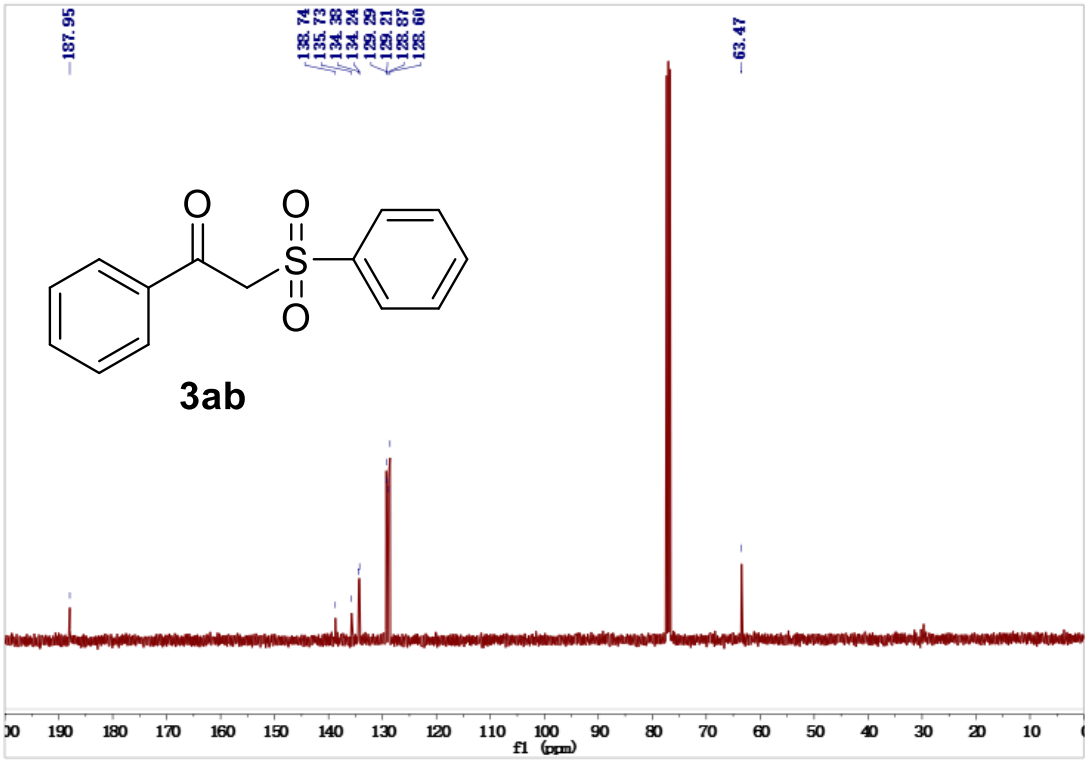
7.93
7.91
7.91
7.89
7.89
7.69
7.67
7.65
7.62
7.60
7.57
7.55
7.53
7.50
7.48
7.46
4.74
O
O
S
O
3ab
2.05
1.80
1.10
1.00
2.00
1.93
2.00
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


187.95
138.74
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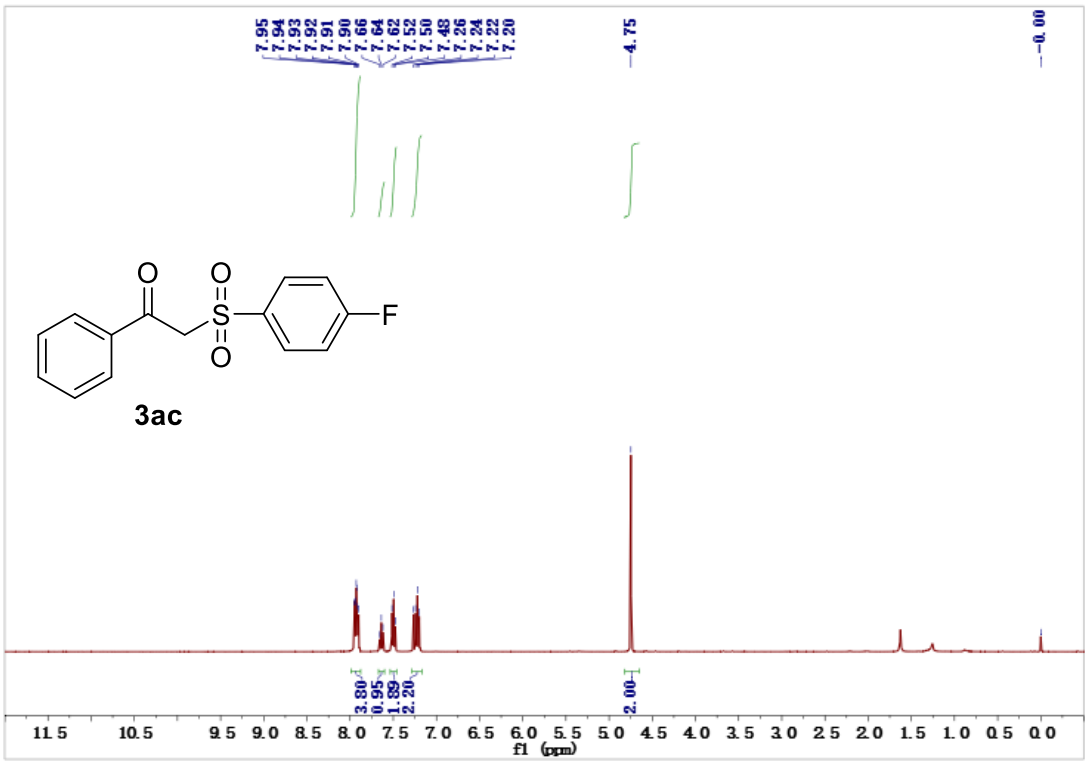
134.38
134.24
129.29
129.21
128.87
128.60
63.47
O
O
S
O
3ab
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)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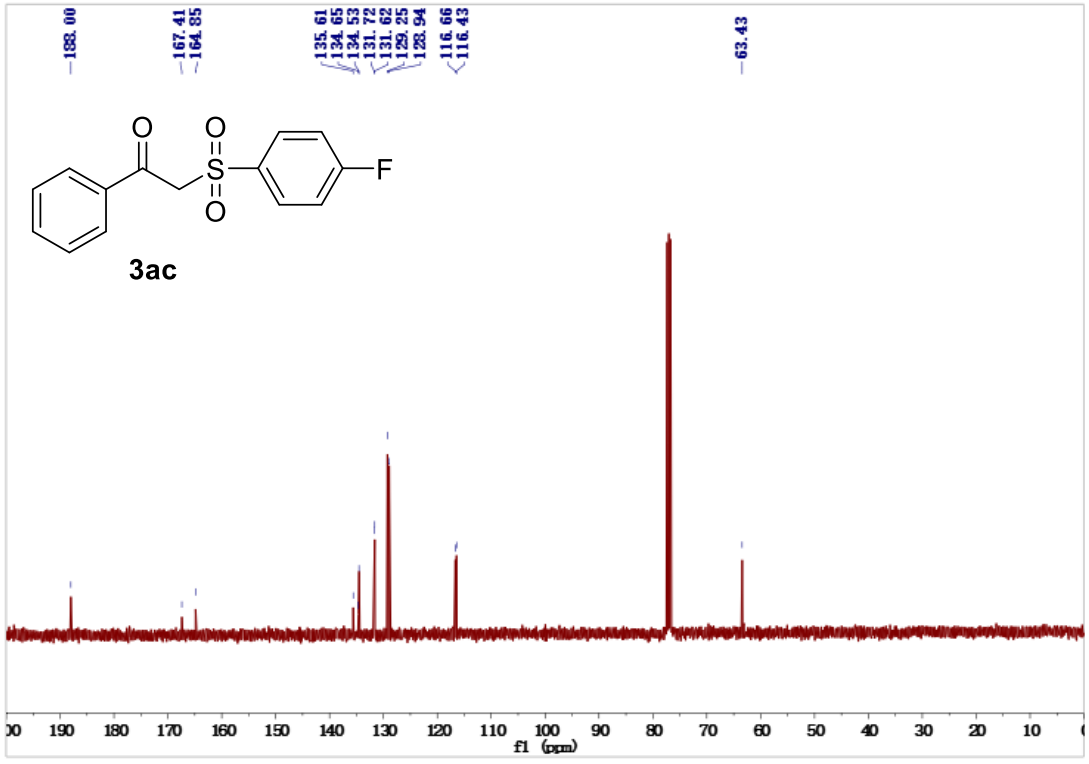
7.92
7.91
7.90
7.66
7.64
7.62
7.52
7.50
7.48
7.26
7.24
7.22
7.20
4.75
0.00
O
O
S
O
F
3ac
3.80
0.95
1.89
2.20
2.00
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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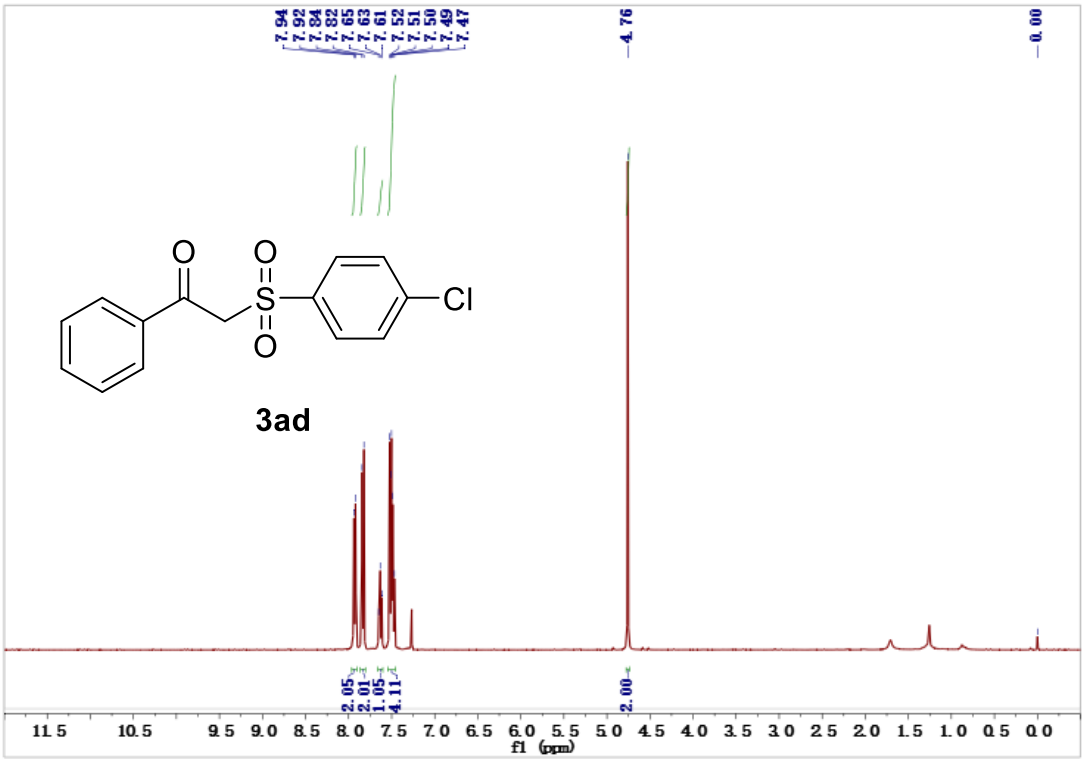
134.53
131.72
131.62
129.25
128.94
116.66
116.43
63.43
O
O
S
O
F
3ac
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)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7.50
7.49
7.47
4.76
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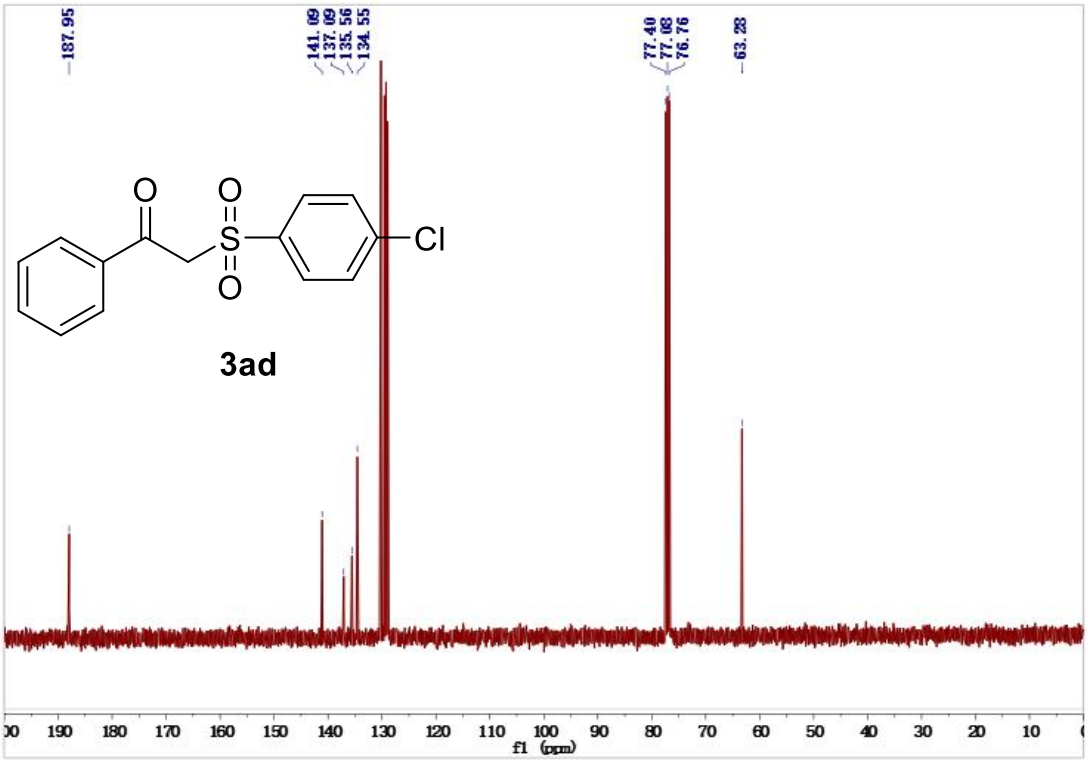
O
O
S
O
Cl
3ad
2.05
2.01
1.05
4.11
2.00
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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77.40
77.08
76.76
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O
O
S
O
Cl
3ad
190
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140
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120
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100
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80
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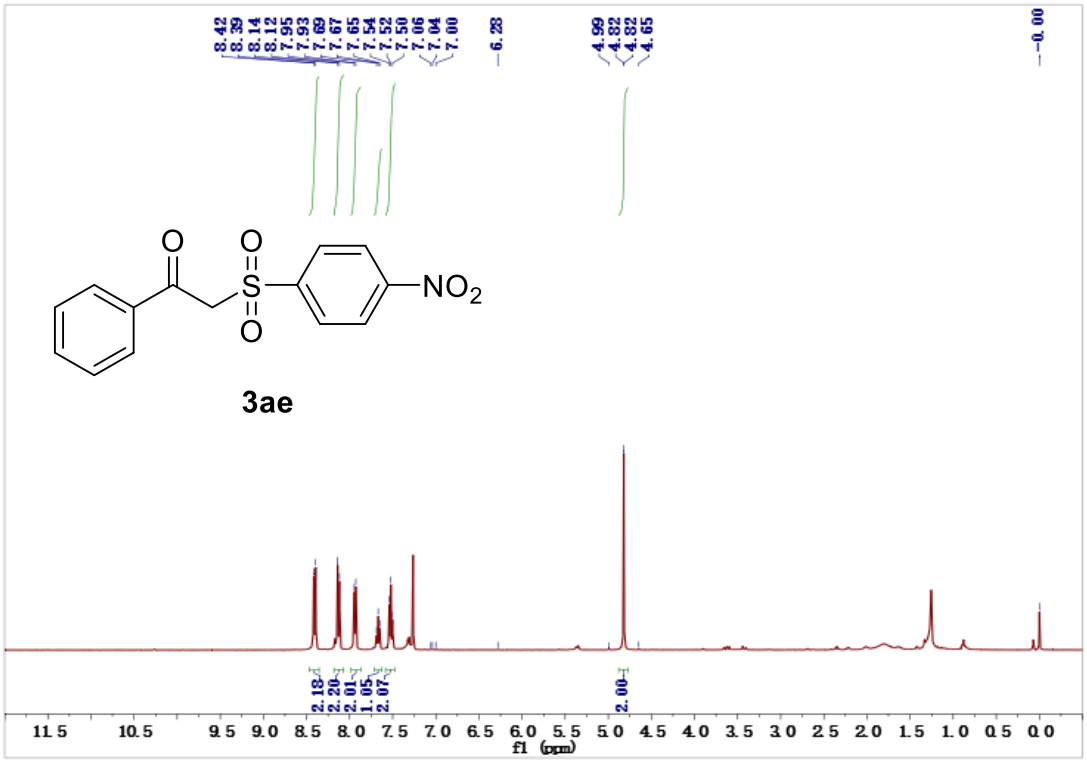
60
50
40
30
20
10
f1 (ppm)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7.54
7.52
7.50
7.06
7.04
7.00
6.28
4.99
4.82
4.82
4.65
0.00
O
O
S
O
NO2
2.18
2.20
2.01
1.05
2.07
2.00
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
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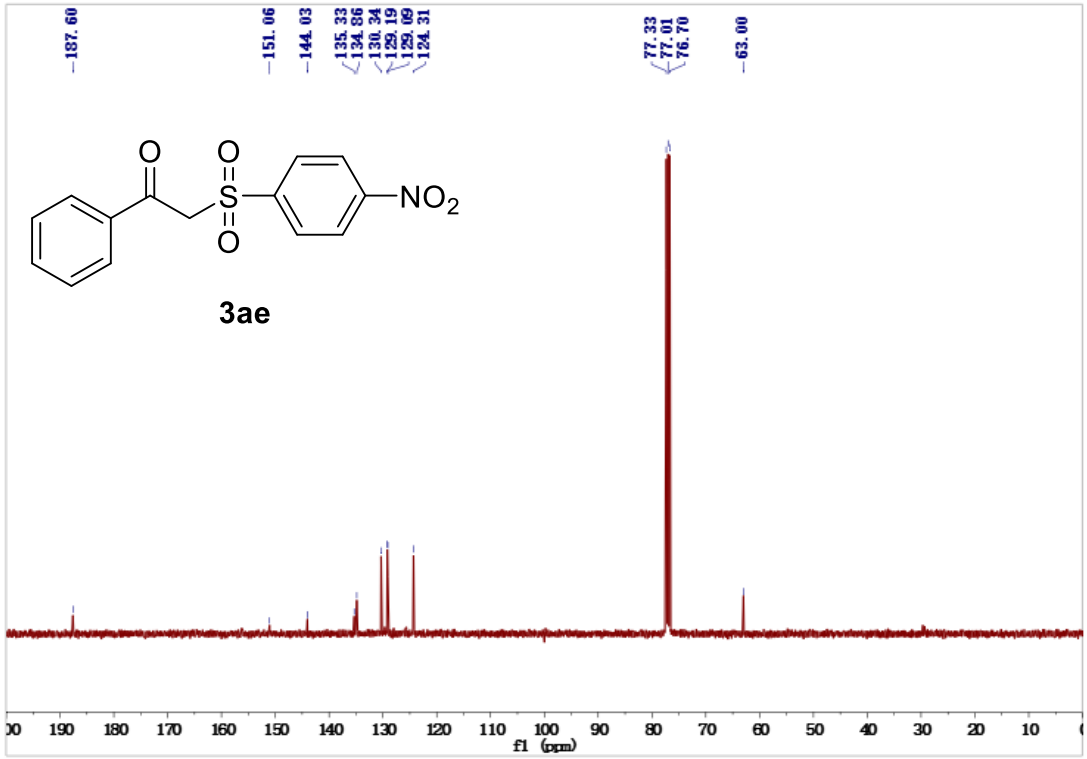
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

3ae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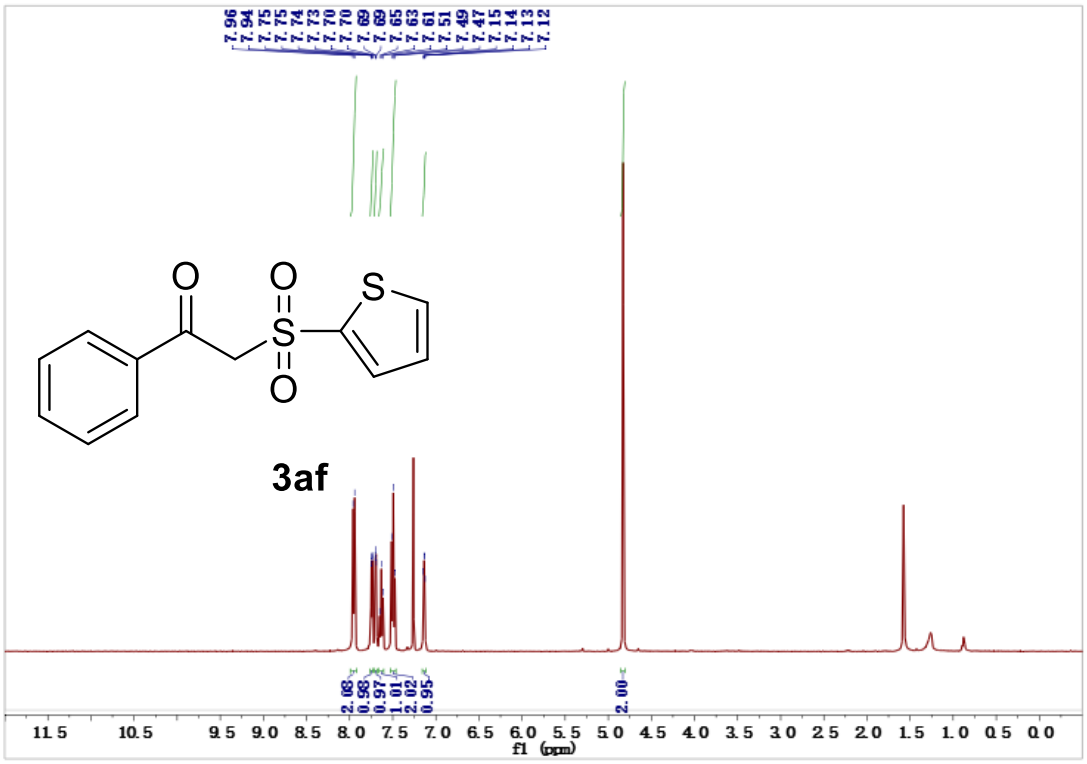
151.06
144.03
135.33
134.86
130.34
129.19
129.09
124.31
77.33
77.01
76.70
63.00
O
O
S
O
NO2
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

3ae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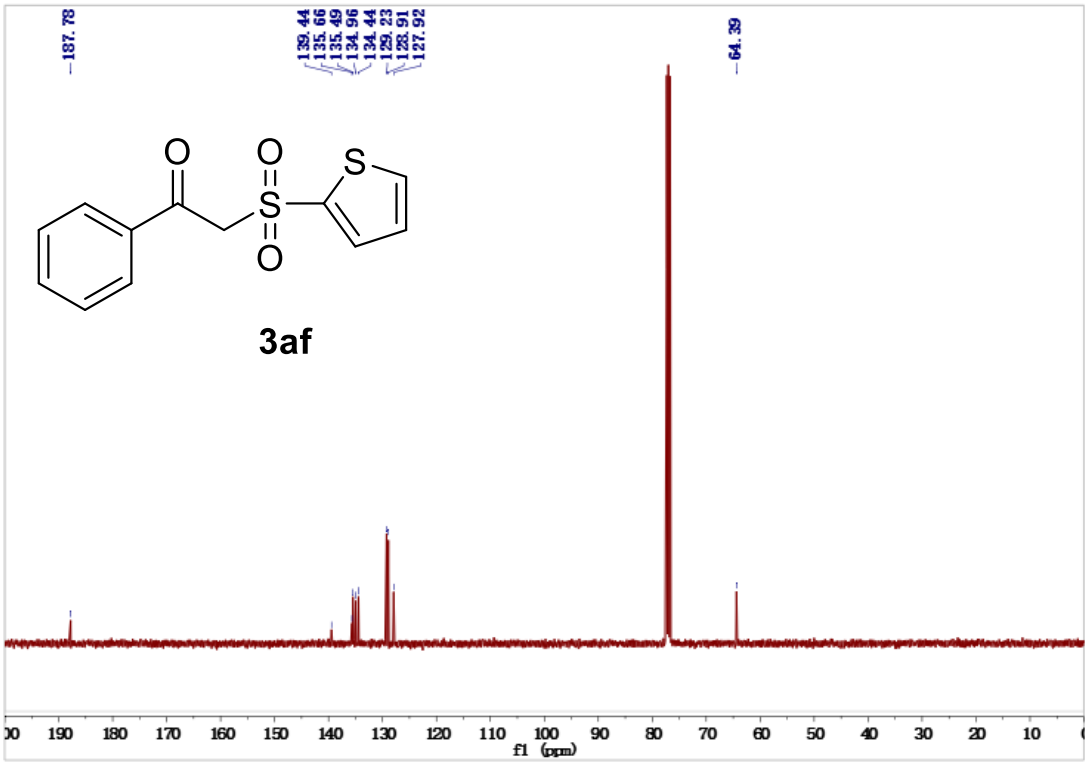
7.73
7.70
7.70
7.69
7.69
7.65
7.63
7.61
7.51
7.49
7.47
7.15
7.14
7.13
7.12
O
O
S
S
O
O
3af
2.08
0.98
0.97
1.01
2.02
0.95
2.00
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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135.66
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134.96
134.44
129.23
128.91
127.92
64.39
O
O
S
S
O
O
3af
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)