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# A metal-free reaction of sulfur dioxide, cyclopropanols and electron-deficient olefins

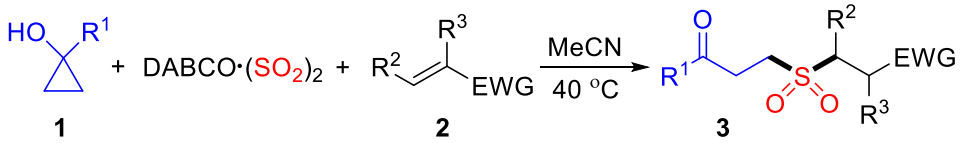
Chun Zhang, Jiapian Huang, Shengqing Ye,* Jie Tang,* and Jie Wu*

# Supporting Information

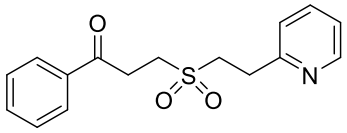
**General experimental methods:**

Unless otherwise stated, all commercial reagents were used as received. All solvents were dried and distilled according to standard procedures. Flash column chromatography was performed using silica gel (60-Å pore size, 32-63 μm, standard grade). Analytical thin-layer chromatography was performed using glass plates pre-coated with 0.25 mm 230-400 mesh silica gel impregnated with a fluorescent indicator (254 nm). Thin layer chromatography plates were visualized by exposure to ultraviolet light. Organic solutions were concentrated on rotary evaporators at ~20 Torr at 25-35 °C. Nuclear magnetic resonance (NMR) spectra are recorded in parts per million from internal tetramethylsilane on the δ scale. $^{1}H$、$^{19}F$ NMR and $^{13}C$ NMR spectra were recorded in $CDCl_3$ or DMSO-$d_6$ on a Bruker DRX-400 spectrometer operating at 400 MHz、376MHz and 100 MHz, respectively. All chemical shift values were quoted in ppm and coupling constants quoted in Hz. High resolution mass spectrometry (HRMS) spectra were obtained on a micrOTOF II Instrument.

*General experimental procedure for the reaction of cyclopropanol **1**, (DABCO)·$(SO_2)_2$, and alkenes **2**.*

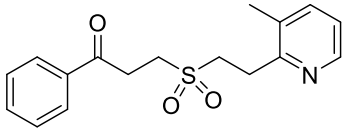



Alkene **2** (0.3 mmol) was added to a mixture of cyclopropanol **1** (0.6 mmol), DABCO·$(SO_2)_2$ (0.6 mmol) in MeCN (3.0 mL) under $N_2$ atmosphere. The mixture was stirred at 40 °C for 24 h. After completion of reaction as indicated by TLC, the solvent was evaporated and the residue was purified directly by flash column chromatography ($CH_2Cl_2$/MeOH (v/v): 30/1 to 50/1) to give the corresponding product **3**.



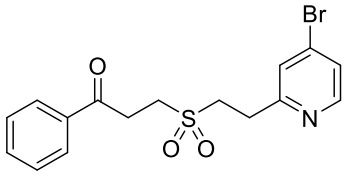
1-phenyl-3-((2-(pyridin-2-yl)ethyl)sulfonyl)propan-1-one (**3aa**)

$^1$H NMR (400 MHz, $CDCl_3$) δ 8.49 (d, *J* = 4.4 Hz, 1H), 7.99 – 7.90 (m, 2H), 7.65 – 7.54 (m, 2H), 7.51 – 7.41 (m, 2H), 7.23 (d, *J* = 7.8 Hz, 1H), 7.13 (dd, *J* = 7.3, 5.0 Hz, 1H), 3.63 – 3.49 (m, 4H), 3.41 – 3.30 (m, 4H); $^{13}$C NMR (100 MHz, $CDCl_3$) δ 195.7, 157.1, 149.6, 136.9, 135.8, 133.9, 128.9, 128.2, 123.5, 122.2, 52.4, 47.8, 30.9, 30.1; HRMS (ESI) calcd for $C_{16}H_{18}NO_3S^+$ ($M+H^+$): 304.1002, found: 304.1007.



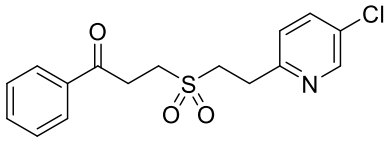
3-((2-(3-methylpyridin-2-yl)ethyl)sulfonyl)-1-phenylpropan-1-one (**3ab**)

$^1$H NMR (400 MHz, $CDCl_3$) δ 8.31 (d, *J* = 4.7Hz, 1H), 8.00 – 7.92 (m, 2H), 7.64 – 7.55 (m, 1H), 7.51 – 7.40 (m,3H), 7.07 (dd, *J* = 7.6, 4.8 Hz, 1H), 3.67 (dd, *J* = 9.6, 5.9 Hz, 2H), 3.58 (dd, *J* = 8.6, 6.6 Hz, 2H), 3.43 (dd, *J* = 8.2, 6.6 Hz, 2H), 3.36 – 3.29 (m, 2H), 2.32 (s, 3H); $^3$C NMR (100 MHz, $CDCl_3$) δ 195.8, 155.2, 146.6, 137.9, 135.8, 133.9, 131.6, 128.9, 128.2, 122.2, 51.3, 48.0, 31.0, 26.7, 18.7; HRMS(ESI) calcd for $C_{17}H_{20}NO_3S^+$ ($M+H^+$): 318.1158, found: 318.1166.



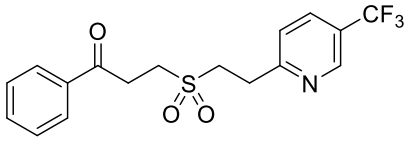
3-((2-(4-bromopyridin-2-yl)ethyl)sulfonyl)-1-phenylpropan-1-one (**3ac**)

$^1$H NMR (400 MHz, $CDCl_3$) δ 8.32 (d, *J* = 5.3 Hz, 1H), 8.01 – 7.94 (m, 2H), 7.60 (t, *J* = 7.4 Hz, 1H), 7.52 – 7.43 (m, 3H), 7.34 (dd, *J* = 5.3, 1.7 Hz, 1H), 3.62 – 3.54 (m, 4H), 3.44 (t, *J* = 7.2 Hz, 2H), 3.38 – 3.30 (m, 2H); $^{13}$C NMR (100 MHz, $CDCl_3$) δ 195.7, 158.7, 150.3, 135.8, 134.0, 133.6, 129.0, 128.3, 126.9, 125.7, 52.1, 48.0, 31.0, 29.8; HRMS(ESI) calcd for $C_{16}H_{16}NO_3NaSBr^+$ ($M+Na^+$): 403.9926, found: 403.9931.



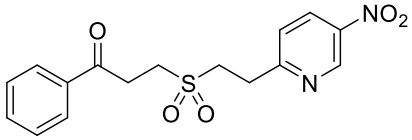
3-((2-(5-chloropyridin-2-yl)ethyl)sulfonyl)-1-phenylpropan-1-one (**3ad**)

$^1$H NMR (400 MHz, $CDCl_3$) δ 8.47 (d, *J* = 2.4 Hz, 1H), 8.03 – 7.91 (m, 2H), 7.67 – 7.57 (m, 2H), 7.49 (t, *J* = 7.7 Hz, 2H), 7.21 (d, *J* = 8.3 Hz, 1H), 3.62 – 3.53 (m, 4H), 3.44 (t, *J* = 7.2 Hz, 2H), 3.35 (dd, *J* = 8.8, 6.7 Hz, 2H); $^{13}$C NMR (100 MHz, $CDCl_3$) δ 195.8, 155.3, 148.5, 136.7, 135.8, 134.1, 130.7, 129.0, 128.3, 124.3, 52.3, 48.0, 30.9, 29.5; HRMS(ESI) calcd for $C_{16}H_{16}NO_3NaSCl^+$ ($M+Na^+$): 360.0432, found: 360.0440.



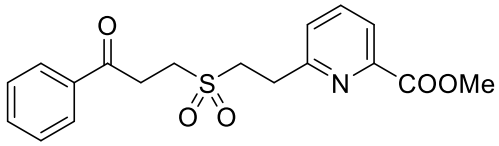
1-phenyl-3-((2-(5-(trifluoromethyl)pyridin-2-yl)ethyl)sulfonyl)propan-1-one (**3ae**)

$^1$H NMR (400 MHz, $CDCl_3$) δ 8.77 (s, 1H), 8.01 – 7.94 (m, 2H), 7.88 (dd, *J* = 8.1, 2.1 Hz, 1H), 7.61 (t, *J* = 7.4 Hz, 1H), 7.49 (t, *J* = 7.7 Hz, 2H), 7.39 (d, *J* = 8.1 Hz, 1H), 3.67 – 3.54 (m, 4H), 3.52 – 3.41 (m, 4H); $^{19}$F NMR (376 MHz, $CDCl_3$) δ -62.34; $^{13}$C NMR (100 MHz, CDCl3) δ 195.7, 161.2, 146.5 (q, *J* = 4.0 Hz), 135.8, 134.1, 134.0 (q, *J* = 3.5Hz) 129.0, 128.3, 125.3 (q, *J* = 33.1 Hz), 123.6(q, *J* = 272.2Hz), 123.3, 52.0, 48.0, 31.0, 30.0; HRMS(ESI) calcd for $C_{17}H_{16}NO_3F_3NaS^+$ ($M+Na^+$): 394.0695, found: 394.0698.



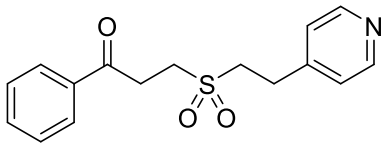
3-((2-(5-nitropyridin-2-yl)ethyl)sulfonyl)-1-phenylpropan-1-one (**3af**)

$^1$H NMR (400 MHz, $CDCl_3$) δ 9.34 (d, *J* = 2.6 Hz, 1H), 8.44 (dd, *J* = 8.5, 2.7 Hz, 1H), 8.05 – 7.89 (m, 2H), 7.62 (dd, *J* = 10.6, 4.3 Hz, 1H), 7.56 – 7.41 (m, 3H), 3.66 (dd, *J* = 8.4, 6.8 Hz, 2H), 3.63 – 3.56 (m, 2H), 3.55 – 3.47 (m, 4H); $^{13}$C NMR (100 MHz, $CDCl_3$) δ 195.7, 163.9, 145.0, 143.3, 135.7, 134.2, 131.9, 129.0, 128.3, 123.8, 51.8, 48.1, 31.0, 30.0; HRMS(ESI) calcd for $C_{16}H_{16}N_2O_5NaS^+$ ($M+Na^+$): 371.0672, found: 371.0687.



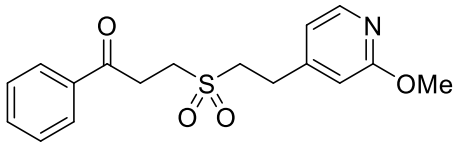
methyl 6-(2-((3-oxo-3-phenylpropyl)sulfonyl)ethyl)picolinate (**3ag**)

$^1$H NMR (400 MHz, $CDCl_3$) δ 8.03 – 7.93 (m, 3H), 7.81 (t, *J* = 7.8 Hz, 1H), 7.61 (t, *J* = 7.4 Hz, 1H), 7.52 – 7.43 (m, 3H), 3.91 (s, 3H), 3.68 (t, *J* = 7.5 Hz, 2H), 3.61 – 3.54 (m, 2H), 3.48 (t, *J* = 7.5 Hz, 2H), 3.44 – 3.38 (m, 2H); $^{13}$C NMR (100 MHz, $CDCl_3$) δ 195.7, 165.5, 157.7, 147.9, 137.9, 135.9, 133.9, 128.9, 128.2, 127.0, 123.8, 52.9, 52.1, 48.2, 31.1, 30.3; HRMS(ESI) calcd for $C_{18}H_{19}NO_5NaS^+$ ($M+Na^+$): 384.0876, found: 384.0880.



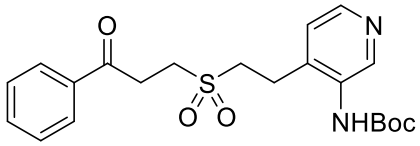
1-phenyl-3-((2-(pyridin-4-yl)ethyl)sulfonyl)propan-1-one (**3ah**)

$^1$H NMR (400 MHz, $CDCl_3$) δ 8.55 (d, *J* = 5.8 Hz, 2H), 8.02 – 7.92 (m, 2H), 7.61 (t, *J* = 7.4 Hz, 1H), 7.49 (t, *J* = 7.7 Hz, 2H), 7.19 (d, *J* = 5.8 Hz, 2H), 3.60 (dd, *J* = 10.5, 3.7 Hz, 2H), 3.48 (dd, *J* = 10.5, 3.6 Hz, 2H), 3.36 – 3.28 (m, 2H), 3.20 (dd, *J* = 10.8, 5.3 Hz, 2H); $^{13}$C NMR (100 MHz, $CDCl_3$) δ 195.9, 150.3, 146.7, 135.7, 134.1, 129.0, 128.2, 123.8, 53.9, 47.8, 31.1, 27.4; HRMS(ESI) calcd for $C_{16}H_{18}NO_3S^+$ ($M+H^+$): 304.1002, found: 304.1004.



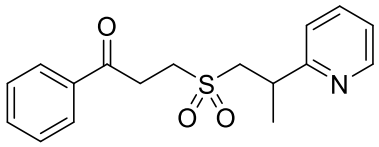
3-((2-(2-methoxypyridin-4-yl)ethyl)sulfonyl)-1-phenylpropan-1-one (**3ai**)

$^1$H NMR (400 MHz, $CDCl_3$) δ 8.10 (d, *J* = 5.3 Hz, 1H), 8.02 – 7.93 (m, 2H), 7.61 (t, *J* = 7.4 Hz, 1H), 7.49 (t, *J* = 7.7 Hz, 2H), 6.76 (dd, *J* = 5.3, 1.2 Hz, 1H), 6.62 (d, *J* = 0.5 Hz, 1H), 3.91 (s, 3H), 3.59 (dd, *J* = 10.6, 3.8 Hz, 2H), 3.48 (t, *J* = 7.1 Hz, 2H), 3.33 – 3.25 (m, 2H), 3.14 (dd, *J* = 10.4, 6.1 Hz, 2H); $^{13}$C NMR (100 MHz, $CDCl_3$) δ 195.8, 164.8, 149.3, 147.5, 135.7, 134.1, 129.0, 128.3, 117.1, 110.6, 53.9, 53.6, 47.8, 31.0, 27.3; HRMS(ESI) calcd for $C_{17}H_{20}NO_4S^+$ ($M+H^+$): 334.1008, found: 334.1114.



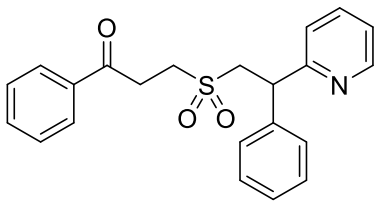
tert-butyl (4-(2-((3-oxo-3-phenylpropyl)sulfonyl)ethyl)pyridin-3-yl)carbamate (**3aj**)

$^1$H NMR (400 MHz, $CDCl_3$) δ 8.74 (s, 1H), 8.35 (d, *J* = 4.3 Hz, 1H), 8.01 – 7.94 (m, 2H), 7.61 (t, *J* = 7.4 Hz, 1H), 7.48 (t, *J* = 7.7 Hz, 2H), 7.17 (d, *J* = 4.9 Hz, 1H), 7.00 (s, 1H), 3.59 (t, *J* = 7.0 Hz, 2H), 3.46 (t, *J* = 6.8 Hz, 2H), 3.36 (dd, *J* = 9.8, 6.2 Hz, 2H), 3.19 (dd, *J* = 9.8, 6.2 Hz, 2H), 1.49 (s, 9H); $^{13}$C NMR (100 MHz, $CDCl_3$) δ 196.0, 153.9, 146.9, 146.6, 139.76, 135.6, 134.2, 132.9, 129.0, 128.3, 124.0, 81.4, 53.0, 47.8, 31.3, 28.4, 23.5; HRMS(ESI) calcd for $C_{21}H_{27}N_2O_5S^+$ ($M+H^+$): 419.1635, found: 419.1648.



1-phenyl-3-((2-(pyridin-2-yl)propyl)sulfonyl)propan-1-one (**3ak**)

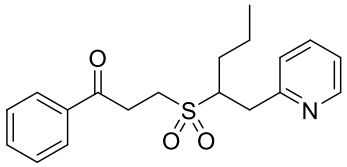
$^1$H NMR (400 MHz, $CDCl_3$) δ 8.56 – 8.47 (d, J = 4.7Hz, 1H), 7.98 – 7.89 (m, 2H), 7.66 (td, *J* = 7.7, 1.8 Hz, 1H), 7.60 (t, *J* = 7.4 Hz, 1H), 7.48 (t, *J* = 7.7 Hz, 2H), 7.28 (s, 1H), 7.17 (ddd, *J* = 7.5, 4.9, 0.9 Hz, 1H), 4.00 (dd, *J* = 14.3, 8.1 Hz, 1H), 3.76 – 3.57 (m, 1H), 3.54 – 3.36 (m, 2H), 3.25 (dd, *J* = 14.3, 5.0 Hz, 1H), 3.15 – 3.00 (m, 2H), 1.47 (d, *J* = 7.0 Hz, 3H); $^{13}$C NMR (100 MHz, $CDCl_3$) δ 195.6, 162.0, 149.6, 137.2, 135.8, 133.9, 128.9, 128.2, 122.9, 122.4, 58.5, 48.6, 36.6, 30.9, 22.3; HRMS(ESI) calcd for $C_{17}H_{20}NO_3S^+$ ($M+H^+$): 318.1158, found: 318.1166.



1-phenyl-3-((2-phenyl-2-(pyridin-2-yl)ethyl)sulfonyl)propan-1-one (**3al**)

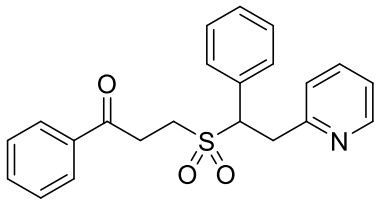
$^1$H NMR (400 MHz, $CDCl_3$) δ 8.54 (d, *J* = 4.2 Hz, 1H), 7.95 – 7.85 (m, 2H), 7.63 – 7.53 (m, 2H), 7.46 (t, *J* = 7.7 Hz, 2H), 7.38 (d, *J* = 7.3 Hz, 2H), 7.30 (t, *J* = 7.5 Hz, 2H), 7.23 (q, *J* = 7.0 Hz, 2H), 7.17 – 7.10 (m, 1H), 4.79 (dd, *J* = 8.1, 5.3 Hz, 1H), 4.56 (dd, *J* = 14.6, 8.2 Hz, 1H), 3.64 (dd, *J* = 14.6, 5.3 Hz, 1H), 3.51 – 3.31 (m, 2H), 3.08 – 2.90 (m, 2H); $^{13}$C NMR (100 MHz, $CDCl_3$) δ 195.6, 159.5, 149.2, 141.3, 137.1, 135.8, 133.8, 129.1,

128.8, 128.1, 128.0, 127.6, 124.0, 122.5, 58.0, 48.8, 47.6, 30.9; HRMS(ESI) calcd for $C_{22}H_{22}NO_3S^+$ ($M+H^+$): 380.1315, found: 380.1324.



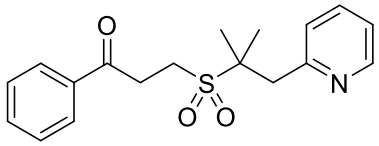
1-phenyl-3-((1-(pyridin-2-yl)pentan-2-yl)sulfonyl)propan-1-one (**3am**)

$^1$H NMR (400 MHz, $CDCl_3$) δ 8.50 (d, *J* = 4.1 Hz, 1H), 7.99 – 7.91 (m, 2H), 7.67 – 7.54 (m, 2H), 7.47 (t, *J* = 7.7 Hz, 2H), 7.24 (d, *J* = 7.8 Hz, 1H), 7.15 (dd, *J* = 7.1, 5.1 Hz, 1H), 3.89 – 3.70 (m, 1H), 3.60 – 3.38 (m, 3H), 3.25 (t, *J* = 7.7 Hz, 2H), 3.10 (dd, *J* = 15.1, 7.0 Hz, 1H), 2.16 – 1.90 (m, 1H), 1.81 – 1.59 (m, 1H), 1.55 – 1.33 (m, 2H), 0.87 (t, *J* = 7.3 Hz, 3H); $^{13}$C NMR (100 MHz, $CDCl_3$) δ 196.0, 157.4, 149.6, 136.9, 135.9, 133.8, 128.9, 128.2, 124.1, 122.2, 61.7, 46.2, 36.8, 30.5, 29.9, 20.2, 14.0; HRMS(ESI) calcd for $C_{19}H_{24}NO_3S^+$ ($M+H^+$): 346.1471, found: 346.1486.



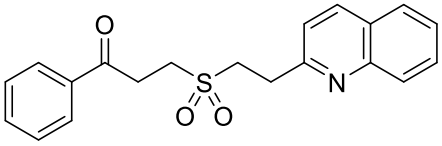
1-phenyl-3-((1-phenyl-2-(pyridin-2-yl)ethyl)sulfonyl)propan-1-one (**3an**)

$^1$H NMR (400 MHz, $CDCl_3$) δ 8.50 – 8.44 (d, J = 4.7 Hz, 1H), 7.93 – 7.84 (m, 2H), 7.57 (t, *J* = 7.4 Hz, 1H), 7.50 – 7.40 (m, 5H), 7.35 – 7.27 (m, 3H), 7.05 (dd, *J* = 7.2, 5.1 Hz, 1H), 6.99 (d, *J* = 7.8 Hz, 1H), 4.98 (dd, *J* = 10.3, 4.5 Hz, 1H), 3.97 (dd, *J* = 14.3, 4.5 Hz, 1H), 3.54 – 3.40 (m, 2H), 3.39 – 3.24 (m, 2H), 3.21 – 3.08 (m, 1H); $^{13}$C NMR (100 MHz, $CDCl_3$) δ 195.8, 156.5, 149.5, 136.6, 135.8, 133.8, 132.4, 129.8, 129.2, 129.03, 128.9, 128.2, 124.2, 121.9, 68.4, 46.0, 36.2, 30.6; HRMS(ESI) calcd for $C_{22}H_{22}NO_3S^+$ ($M+H^+$): 380.1315, found: 380.1321.



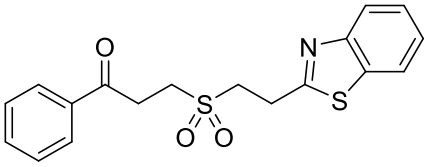
3-((2-methyl-1-(pyridin-2-yl)propan-2-yl)sulfonyl)-1-phenylpropan-1-one (**3ao**)

$^1$H NMR (400 MHz, $CDCl_3$) δ 8.60 – 8.54 (d, J = 4.8Hz, 1H), 8.04 – 7.95 (m, 2H), 7.67 – 7.56 (m, 2H), 7.48 (t, *J* = 7.7 Hz, 2H), 7.25 – 7.17 (m, 2H), 3.61 (dd, *J* = 8.7, 6.5 Hz, 2H), 3.48 – 3.41 (m, 2H), 3.28 (s, 2H), 1.44 (s, 6H); $^{13}$C NMR (100 MHz, $CDCl_3$) δ 196.3, 156.1, 149.5, 136.5, 136.0, 133.9, 128.9, 128.3, 125.7, 122.2, 63.1, 42.4, 41.1, 29.8, 20.6; HRMS(ESI) calcd for $C_{18}H_{22}NO_3S^+$ ($M+H^+$): 332.1315, found: 332.1317.



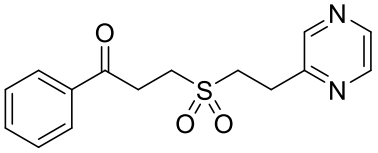
1-phenyl-3-((2-(quinolin-2-yl)ethyl)sulfonyl)propan-1-one (**3ap**)

$^1$H NMR (400 MHz, $CDCl_3$) δ 8.11 (d, *J* = 8.4 Hz, 1H), 7.99 – 7.92 (m, 3H), 7.79 (d, *J* = 8.1 Hz, 1H), 7.66 (td, 1H), 7.59 (t, *J* = 7.4 Hz, 1H), 7.54 – 7.43 (m, 3H), 7.34 (d, *J* = 8.4 Hz, 1H), 3.83 – 3.75 (m, 2H), 3.63 – 3.53 (m, 4H), 3.52 – 3.45 (m, 2H); $^{13}$C NMR (100 MHz, $CDCl_3$) δ 195.8, 157.4, 147.8, 137.0, 135.9, 133.9, 129.9, 128.9, 128.2, 127.8, 127.2, 126.5, 121.5, 52.0, 48.0, 31.0, 30.8; HRMS(ESI) calcd for $C_{20}H_{20}NO_3S^+$ ($M+H^+$): 354.1158, found: 354.1159.



3-((2-(benzo[d]thiazol-2-yl)ethyl)sulfonyl)-1-phenylpropan-1-one (**3aq**)

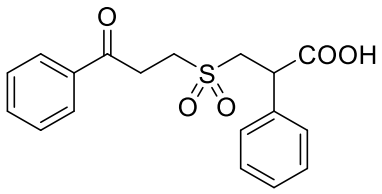
$^1$H NMR (400 MHz, $CDCl_3$) δ 8.00 – 7.95 (m, 2H), 7.93 (d, *J* = 8.1 Hz, 1H), 7.85 (dd, *J* = 7.9, 0.5 Hz, 1H), 7.61 (t, *J* = 7.4 Hz, 1H), 7.52 – 7.42 (m, 3H), 7.41 – 7.35 (m, 1H), 3.78 – 3.65 (m, 4H), 3.64 – 3.58 (m, 2H), 3.53 (dd, *J* = 11.0, 4.5 Hz, 2H); $^{13}$C NMR (100 MHz, $CDCl_3$) δ 195.6, 166.5, 153.0, 135.8, 135.3, 134.1, 129.0, 128.3, 126.4, 125.5, 122.9, 121.8, 51.9, 48.2, 31.1, 26.7; HRMS(ESI) calcd for $C_{18}H_{17}NO_3NaS^+$ ($M+Na^+$): 382.0542, found: 382.0547.



1-phenyl-3-((2-(pyrazin-2-yl)ethyl)sulfonyl)propan-1-one (**3ar**)

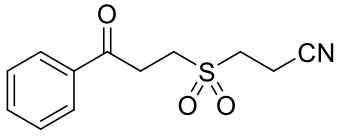
$^1$H NMR (400 MHz, $CDCl_3$) δ 8.58 (s, 1H), 8.54 – 8.44 (m, 2H), 8.02 – 7.94 (m, 2H), 7.62 (t, *J* = 7.4 Hz, 1H), 7.50 (t, *J* = 7.7 Hz, 2H), 3.64 – 3.56 (m, 4H), 3.53 – 3.46 (m, 2H),

3.46 – 3.39 (m, 2H); $^{13}$C NMR (100 MHz, $CDCl_3$) δ 195.8, 153.1, 145.0, 144.3, 143.4, 135.9, 134.1, 129.0, 128.3, 51.9, 48.1, 31.0, 27.4; HRMS(ESI) calcd for $C_{15}H_{16}N_2O_3NaS^+$ (M+$Na^+$): 327.0774, found: 327.0785.



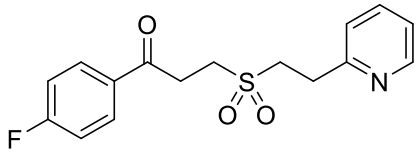

3-((3-oxo-3-phenylpropyl)sulfonyl)-2-phenylpropanoic acid (**3as**)

$^1$H NMR (400 MHz, DMSO) δ 8.05 – 7.92 (m, 2H), 7.66 (t, *J* = 7.4 Hz, 1H), 7.54 (t, *J* = 7.7 Hz, 2H), 7.33 (d, *J* = 7.1 Hz, 2H), 7.28 (t, *J* = 7.4 Hz, 2H), 7.22 (t, *J* = 7.1 Hz, 1H), 4.07 – 3.86 (m, 2H), 3.54 – 3.21 (m, 5H); $^{13}$C NMR (100 MHz, DMSO) δ 196.3, 172.7, 139.3, 136.0, 133.6, 128.8, 128.4, 128.1, 128.0, 126.9, 55.7, 47.9, 46.8, 31.2; HRMS(ESI) calcd for $C_{18}H_{18}O_5NaS^+$ (M+$Na^+$): 369.0767, found: 369.0774.



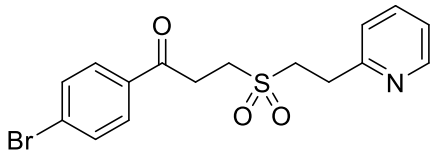

3-((3-oxo-3-phenylpropyl)sulfonyl)propanenitrile (**3at**)

$^1$H NMR (400 MHz, DMSO) δ 8.05 – 7.99 (m, 2H), 7.68 (t, *J* = 7.4 Hz, 1H), 7.56 (t, *J* = 7.7 Hz, 2H), 3.63 (t, *J* = 7.2 Hz, 2H), 3.56 (s, 4H), 3.02 (t, *J* = 7.2 Hz, 2H); $^{13}$C NMR (100 MHz, DMSO) δ 196.2, 135.9, 133.7, 128.8, 128.2, 118.4, 47.2, 46.8, 31.1, 10.8; HRMS(ESI) calcd for $C_{12}H_{13}NO_3NaS^+$ (M+$Na^+$): 274.0508, found: 274.0514.



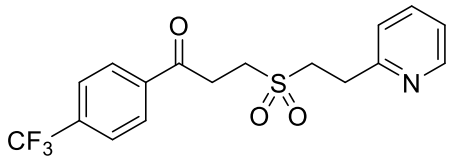

1-(4-fluorophenyl)-3-((2-(pyridin-2-yl)ethyl)sulfonyl)propan-1-one (**3ba**)

$^1$H NMR (400 MHz, $CDCl_3$) δ 8.50 (d, *J* = 4.3 Hz, 1H), 8.03 – 7.93 (m, 2H), 7.63 (td, *J* = 7.7, 1.7 Hz, 1H), 7.24 (d, *J* = 7.8 Hz, 1H), 7.20 – 7.10 (m, 3H), 3.64 – 3.56 (m, 2H), 3.55 – 3.49 (m, 2H), 3.42 – 3.31 (m, 4H); $^{19}$F NMR (376 MHz, $CDCl_3$) δ -103.69 (dq, J = 8.3, 5.4 Hz); $^{13}$C NMR (100 MHz, $CDCl_3$) δ 194.2, 166.2 (d, *J* = 256.0 Hz), 157.1, 149.6, 136.9, 132.3 (d, *J* = 3.0 Hz), 130.9 (d, *J* = 9.5 Hz), 123.5, 122.2, 116.1 (d, *J* = 22.0 Hz), 52.5, 47.8, 30.8, 30.2; HRMS(ESI) calcd for $C_{16}H_{17}NO_3SF^+$ (M+$H^+$): 322.0908, found: 322.0918.



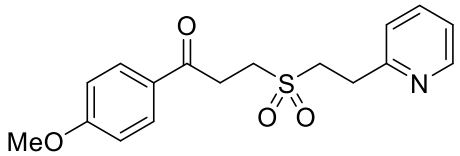
1-(4-bromophenyl)-3-((2-(pyridin-2-yl)ethyl)sulfonyl)propan-1-one (**3ca**)

$^1$H NMR (400 MHz, $CDCl_3$) δ 8.51 (d, *J* = 4.2 Hz, 1H), 7.86 – 7.80 (m, 2H), 7.69 – 7.59 (m, 3H), 7.24 (s, 1H), 7.18 (dd, *J* = 7.5, 4.9 Hz, 1H), 3.64 – 3.58 (m, 2H), 3.55 – 3.49 (m, 2H), 3.41 – 3.33 (m, 4H); $^{13}$C NMR (100 MHz, $CDCl_3$) δ 194.8, 157.0, 149.6, 137.0, 134.6, 132.3, 129.7, 129.3, 123.6, 122.3, 52.5, 47.8, 30.9, 30.2; HRMS(ESI) calcd for $C_{16}H_{17}NO_3SBr^+$ (M+H$^+$): 382.0107, found: 382.0116.



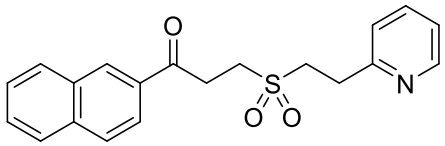
3-((2-(pyridin-2-yl)ethyl)sulfonyl)-1-(4-(trifluoromethyl)phenyl)propan-1-one (**3da**)

$^1$H NMR (400 MHz, DMSO) δ 8.50 (d, *J* = 4.2 Hz, 1H), 8.21 (d, *J* = 8.1 Hz, 2H), 7.92 (d, *J* = 8.2 Hz, 2H), 7.74 (td, *J* = 7.7, 1.7 Hz, 1H), 7.39 (d, *J* = 7.8 Hz, 1H), 7.26 (dd, *J* = 6.9, 5.3 Hz, 1H), 3.69 – 3.57 (m, 4H), 3.52 (t, *J* = 6.8 Hz, 2H), 3.21 (dd, *J* = 9.4, 6.6 Hz, 2H); $^{19}$F NMR (376 MHz, DMSO) δ -61.60; $^{13}$C NMR (100 MHz, DMSO) δ 195.9, 157.6, 149.0, 139.1, 136.8, 132.8 (q, *J* = 31.9 Hz), 128.9, 125.7 (q, *J* = 3.6 Hz), 123.7 (q, *J* = 272.6 Hz), 123.3, 121.9, 50.9, 47.1, 31.6, 29.2; HRMS(ESI) calcd for $C_{17}H_{17}NO_3F_3S^+$ (M+H$^+$): 372.0876, found: 372.0883.



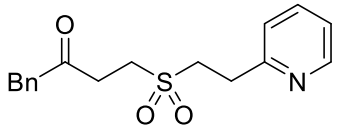
1-(4-methoxyphenyl)-3-((2-(pyridin-2-yl)ethyl)sulfonyl)propan-1-one (**3ea**)

$^1$H NMR (400 MHz, $CDCl_3$) δ 8.49 (s, 1H), 7.93 (d, *J* = 8.2 Hz, 2H), 7.62 (t, *J* = 7.6 Hz, 1H), 7.29 – 7.20 (m, 1H), 7.15 (s, 1H), 6.93 (d, *J* = 8.2 Hz, 2H), 3.86 (s, 3H), 3.58 (t, *J* = 7.6 Hz, 2H), 3.49 (t, *J* = 6.9 Hz, 2H), 3.42 – 3.30 (m, 4H); $^{13}$C NMR (100 MHz, $CDCl_3$) δ 194.1, 164.1, 157.2, 149.6, 136.9, 130.5, 128.9, 123.5, 122.2, 114.0, 55.6, 52.4, 48.0, 30.5, 30.2; HRMS(ESI) calcd for $C_{17}H_{20}NO_4S^+$ (M+H$^+$): 334.1108, found: 334.1118.



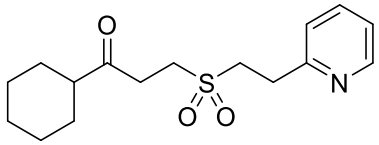
1-(naphthalen-2-yl)-3-((2-(pyridin-2-yl)ethyl)sulfonyl)propan-1-one (**3fa**)

$^1$H NMR (400 MHz, $CDCl_3$) δ 8.52 (d, *J* = 6.9 Hz, 2H), 8.04 – 7.95 (m, 2H), 7.94 – 7.86 (m, 2H), 7.68 – 7.54 (m, 3H), 7.25 (s, 1H), 7.17 (dd, *J* = 6.9, 5.3 Hz, 1H), 3.74 – 3.68 (m, 2H), 3.68 – 3.62 (m, 2H), 3.49 – 3.43 (m, 2H), 3.43 – 3.36 (m, 2H); $^{13}$C NMR (100 MHz, $CDCl_3$) δ 195.6, 157.1, 149.6, 136.9, 135.9, 133.2, 132.5, 130.2, 129.7, 129.0, 128.8, 127.9, 127.1, 123.54, 123.51, 122.2, 52.5, 48.0, 30.9, 30.2; HRMS(ESI) calcd for $C_{20}H_{20}NO_3S^+$ ($M+H^+$): 354.1158, found: 354.1160.



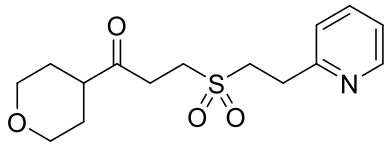
1-phenyl-4-((2-(pyridin-2-yl)ethyl)sulfonyl)butan-2-one (**3ga**)

$^1$H NMR (400 MHz, $CDCl_3$) δ 8.50 (s, 1H), 7.63 (t, *J* = 7.6 Hz, 1H), 7.39 – 7.26 (m, 3H), 7.25 – 7.13 (m, 4H), 3.76 (s, 2H), 3.52 (t, *J* = 7.6 Hz, 2H), 3.31 (t, *J* = 7.6 Hz, 2H), 3.19 (t, *J* = 7.1 Hz, 2H), 3.02 (t, *J* = 7.1 Hz, 2H); $^{13}$C NMR (100 MHz, $CDCl_3$) δ 204.1, 157.0, 149.6, 136.9, 133.3, 129.5, 129.0, 127.5, 123.5, 122.2, 52.4, 50.1, 47.6, 33.8, 30.1; HRMS(ESI) calcd for $C_{17}H_{20}NO_3S^+$ ($M+H^+$): 318.1158, found: 318.1170.



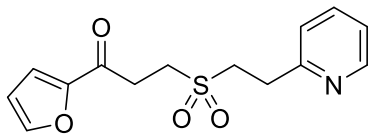
1-cyclohexyl-3-((2-(pyridin-2-yl)ethyl)sulfonyl)propan-1-one (**3ha**)

$^1$H NMR (400 MHz, $CDCl_3$) δ 8.47 (d, *J* = 4.4 Hz, 1H), 7.59 (td, *J* = 7.7, 1.7 Hz, 1H), 7.19 (d, *J* = 7.8 Hz, 1H), 7.13 (dd, *J* = 7.2, 5.1 Hz, 1H), 3.49 (t, *J* = 9.0, 6.5 Hz, 2H), 3.28 (t, *J* = 9.0, 6.5 Hz, 2H), 3.16 (t, *J* = 7.4 Hz, 2H), 2.96 (t, *J* = 7.4 Hz, 2H), 2.40 – 2.24 (m, 1H), 1.91 – 1.52 (m, 5H), 1.39 – 1.07 (m, 5H); $^{13}$C NMR (100 MHz, $CDCl_3$) δ 209.6, 157.0, 149.5, 136.8, 123.4, 122.1, 52.3, 50.7, 47.5, 32.3, 30.1, 28.4, 25.7, 25.5; HRMS(ESI) calcd for $C_{16}H_{24}NO_3S^+$ ($M+H^+$): 310.1471, found: 310.1478.



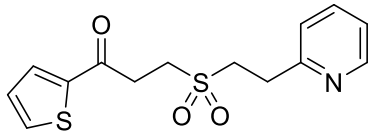
3-((2-(pyridin-2-yl)ethyl)sulfonyl)-1-(tetrahydro-2H-pyran-4-yl)propan-1-one (**3ia**)

$^1$H NMR (400 MHz, $CDCl_3$) δ 8.48 (s, 1H), 7.60 (s, 1H), 7.24 – 7.07 (m, 2H), 3.95 (d, *J* = 9.0 Hz, 2H), 3.51 (s, 2H), 3.38 (t, *J* = 11.1 Hz, 2H), 3.29 (d, *J* = 5.0 Hz, 2H), 3.19 (d, *J* = 6.9 Hz, 2H), 2.97 (s, 2H), 2.57 (d, *J* = 11.0 Hz, 1H), 1.86 – 1.53 (m, 4H); $^{13}$C NMR (100 MHz, $CDCl_3$) δ 207.6, 157.0, 149.5, 136.9, 123.5, 122.2, 67.1, 52.4, 47.5, 47.4, 32.1, 30.1, 28.0; HRMS(ESI) calcd for $C_{15}H_{22}NO_4S^+$ ($M+H^+$): 312.1264, found: 312.1270.



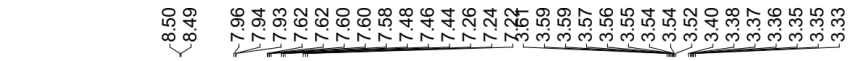
1-(furan-2-yl)-3-((2-(pyridin-2-yl)ethyl)sulfonyl)propan-1-one (**3ja**)

$^1$H NMR (400 MHz, $CDCl_3$) δ 8.54 (d, *J* = 4.3 Hz, 1H), 7.71 – 7.62 (m, 2H), 7.31 – 7.27 (m, 2H), 7.20 (dd, *J* = 7.0, 5.4 Hz, 1H), 6.60 (dd, *J* = 3.6, 1.7 Hz, 1H), 3.65 – 3.59 (m, 2H), 3.48 – 3.42 (m, 2H), 3.42 – 3.35 (m, 4H); $^{13}$C NMR (100 MHz, $CDCl_3$) δ 184.7, 157.1, 151.8, 149.6, 147., 136.9, 123.5, 122.2, 118.1, 112.7, 52.4, 47.4, 30.7, 30.2; HRMS(ESI) calcd for $C_{14}H_{16}NO_4S^+$ ($M+H^+$): 294.0795, found: 294.0800.



3-((2-(pyridin-2-yl)ethyl)sulfonyl)-1-(thiophen-2-yl)propan-1-one (**3ka**)

$^1$H NMR (400 MHz, $CDCl_3$) δ 8.52 (s, 1H), 8.13 (s, 1H), 7.64 (t, *J* = 6.5 Hz, 1H), 7.54 (s, 1H), 7.35 (s, 1H), 7.25 (d, *J* = 7.6 Hz, 1H), 7.17 (s, 1H), 3.60 (t, *J* = 7.3 Hz, 2H), 3.46 (d, *J* = 7.0 Hz, 2H), 3.42 – 3.32 (m, 4H); $^{13}$C NMR (100 MHz, $CDCl_3$) δ 189.9, 157.1, 149.6, 141.0, 136.9, 132.9, 126.9, 126.8, 123.5, 122.2, 52.4, 47.7, 31.8, 30.2; HRMS(ESI) calcd for $C_{14}H_{16}NO_3S_2^+$ ($M+H^+$): 310.0566, found: 310.0565.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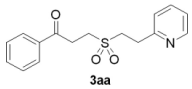
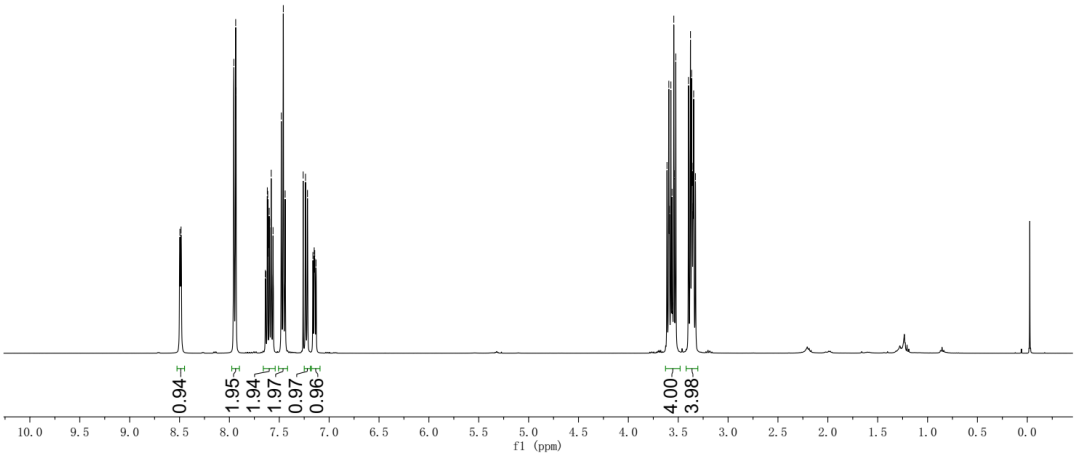
3.33


3aa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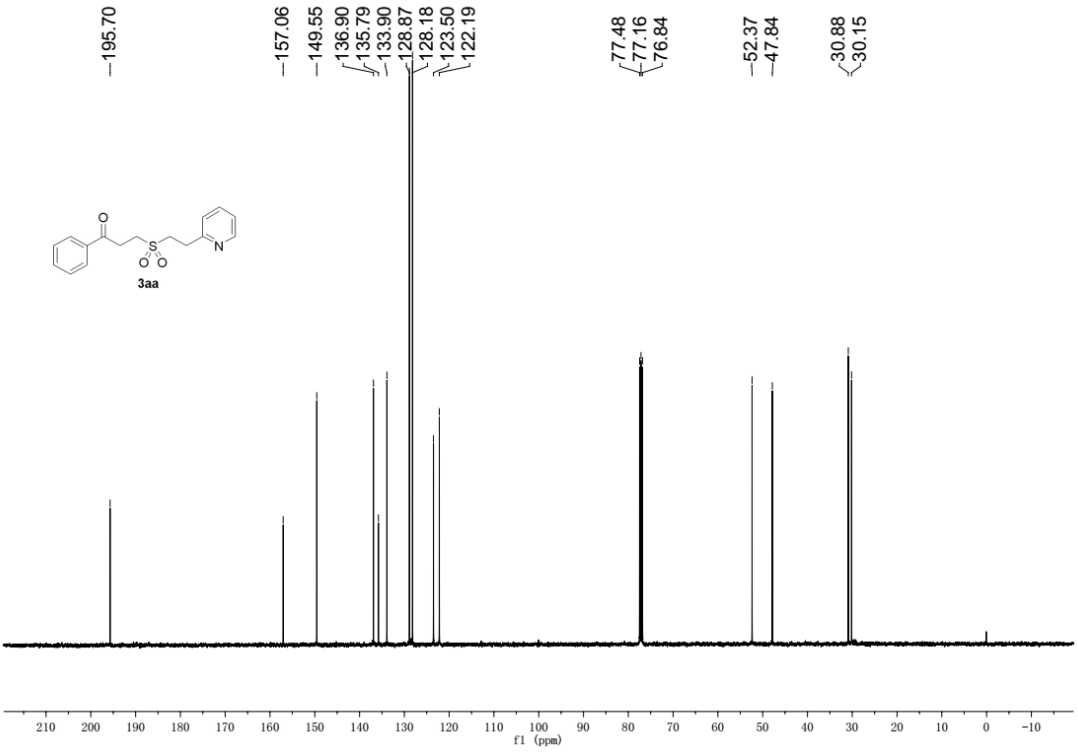
1.95
1.94
1.97
0.97
0.96
4.00
3.98
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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122.19
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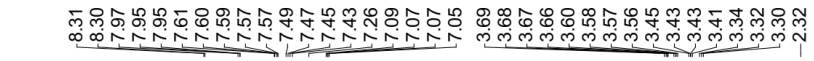
f1 (ppm)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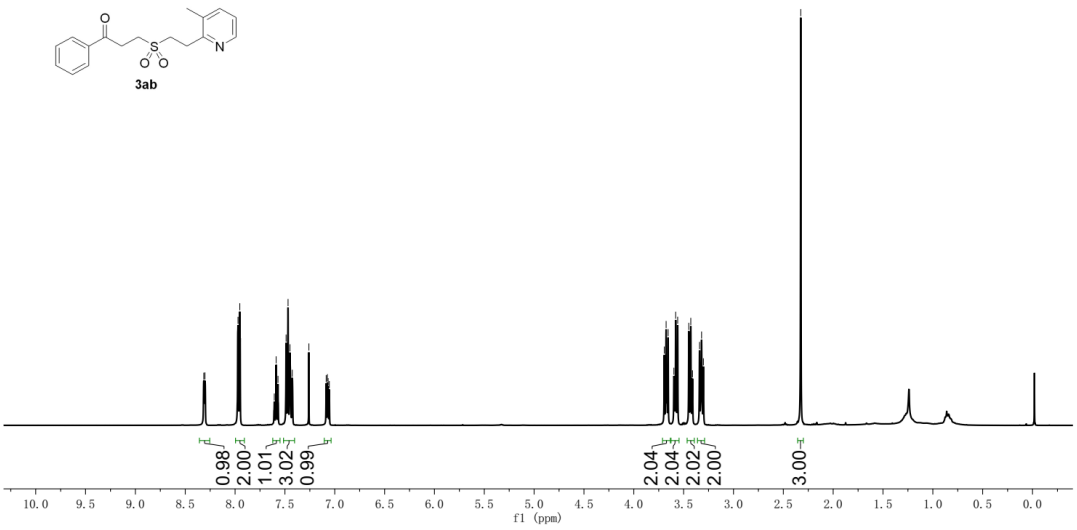
2.32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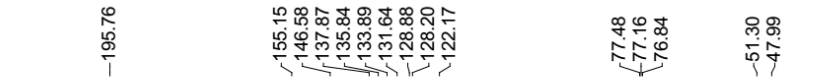
1.01
3.02
0.99
2.04
2.04
2.02
2.00
3.00
f1 (ppm)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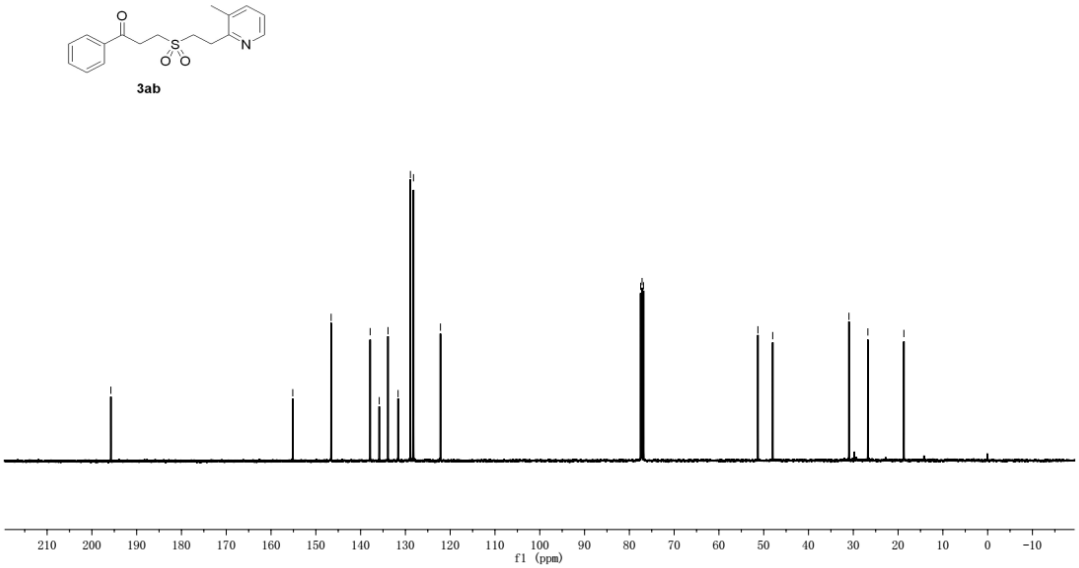
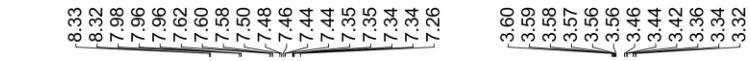
155.15
146.58
137.87
135.84
133.89
131.64
128.88
128.20
122.17
77.48
77.16
76.84
51.30
47.99
30.97
26.74
18.71


3ab
f1 (ppm)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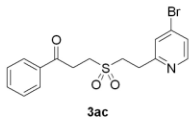
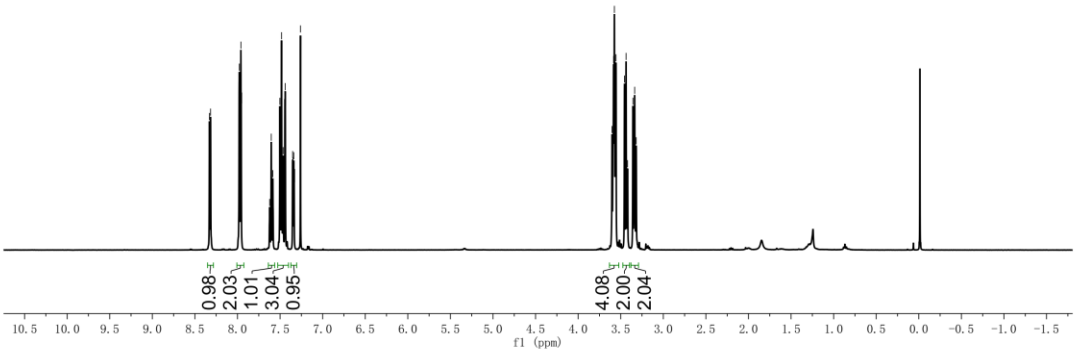
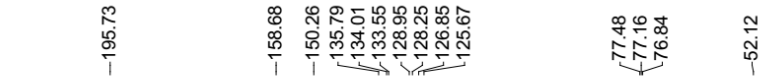
8.32
7.98
7.96
7.96
7.62
7.60
7.58
7.50
7.48
7.46
7.44
7.44
7.35
7.35
7.34
7.34
7.26
3.60
3.59
3.58
3.57
3.56
3.56
3.46
3.44
3.42
3.36
3.34
3.32


Br
O
S
O
O
N

3ac


0.98
2.03
1.01
3.04
0.95
4.08
2.00
2.04
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 -1.0 -1.5
f1 (ppm)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135.79
134.01
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128.25
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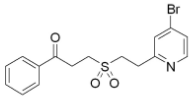
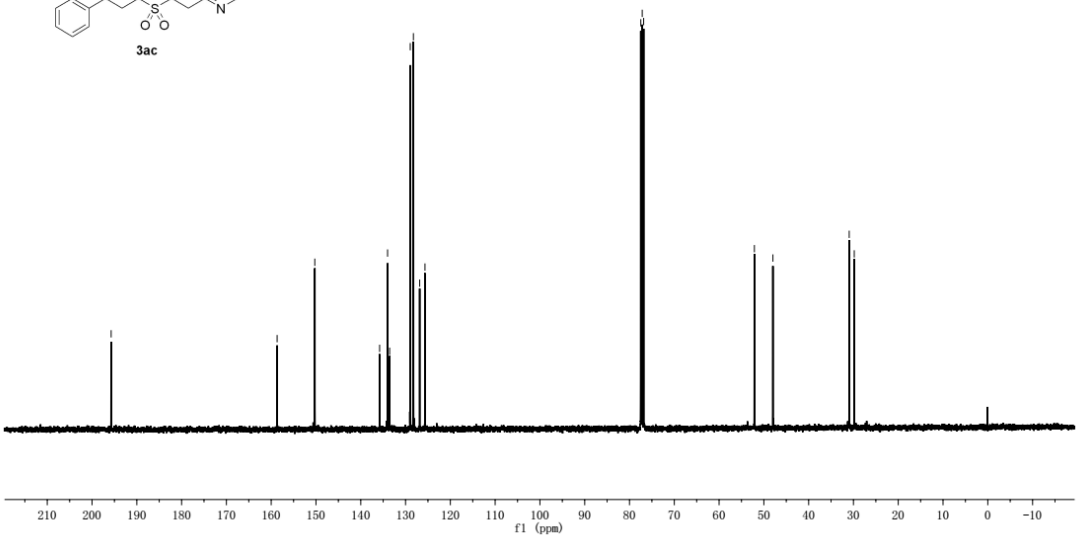
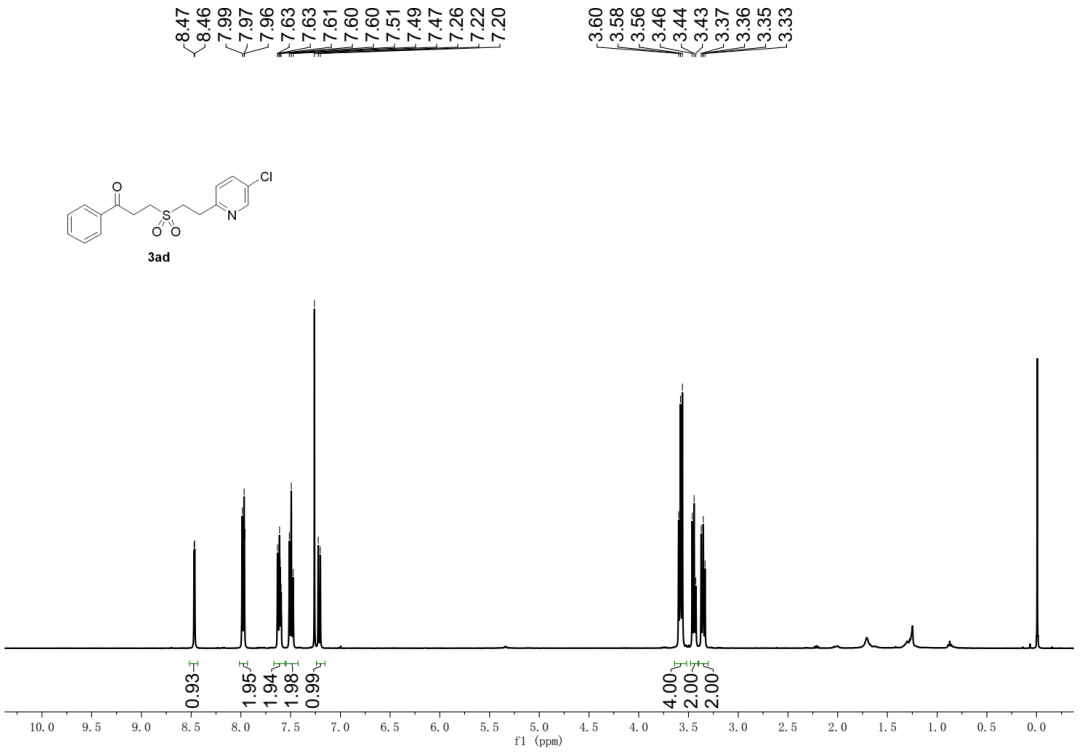
125.67
77.48
77.16
76.84
52.12
47.98
30.95
29.82


Br
O
S
O
O
N

3ac


210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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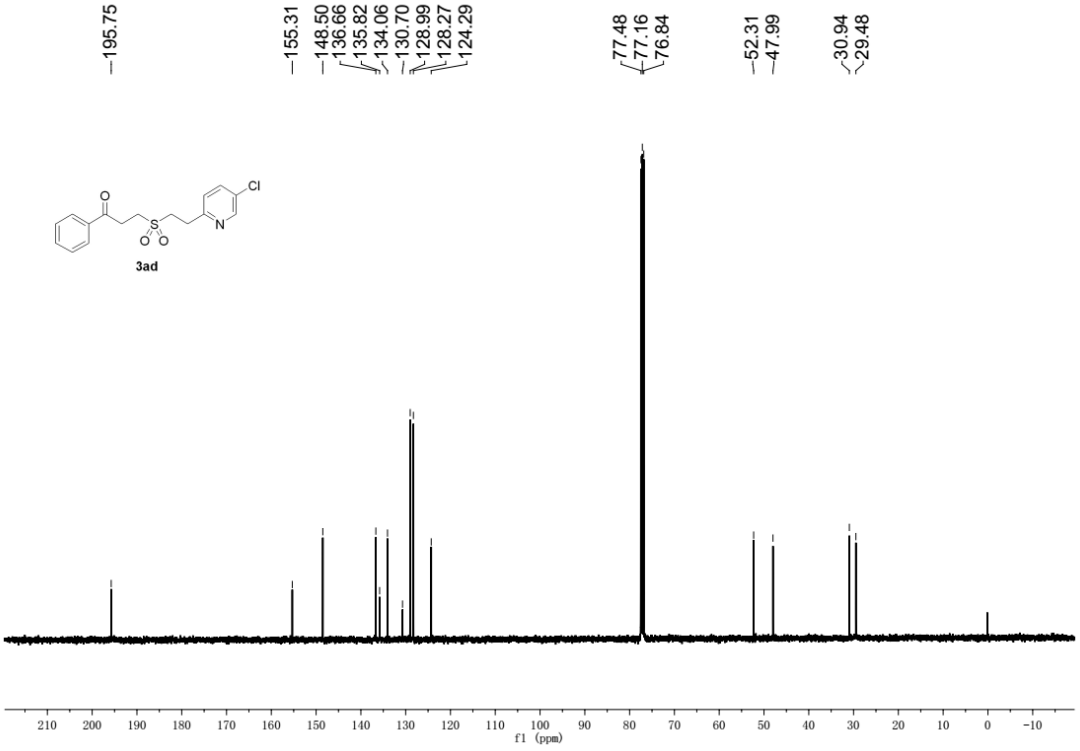
7.97
7.96
7.63
7.63
7.61
7.60
7.60
7.51
7.49
7.47
7.26
7.22
7.20
3.60
3.58
3.56
3.46
3.44
3.43
3.37
3.36
3.35
3.33
3ad
0.93
1.95
1.94
1.98
0.99
4.00
2.00
2.00
f1 (ppm)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134.06
130.70
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124.29
77.48
77.16
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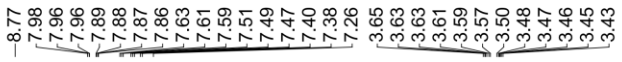
47.99
30.94
29.48
3ad
f1 (ppm)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7.87
7.86
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7.61
7.59
7.51
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7.47
7.40
7.38
7.26
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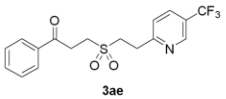
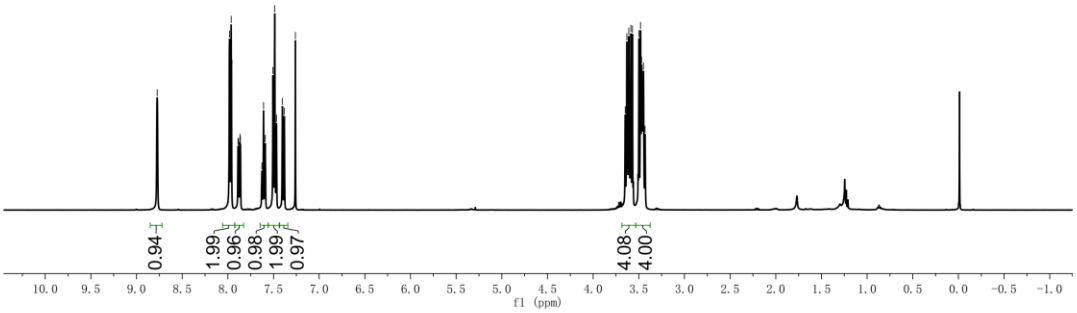
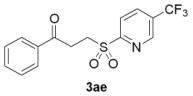
3.50
3.48
3.47
3.46
3.45
3.43


O
CF3
S
O
O
N

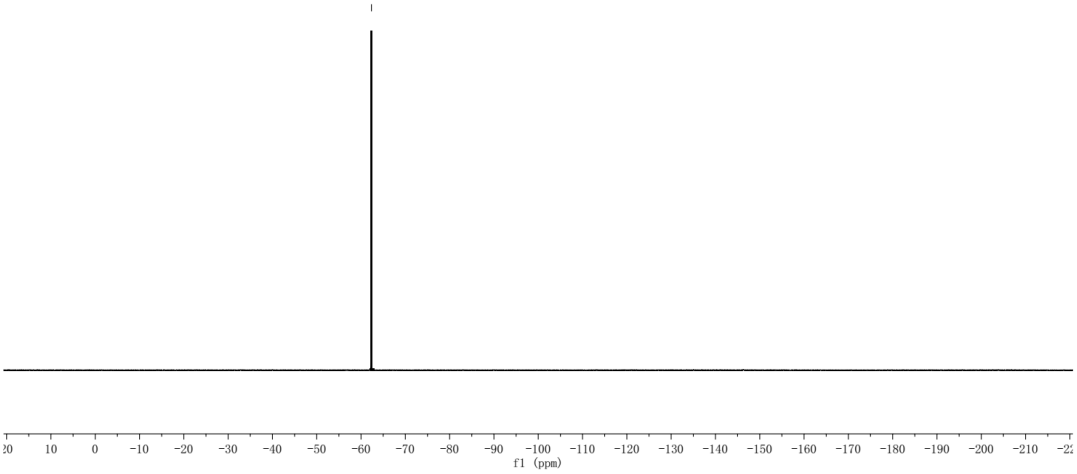
3ae

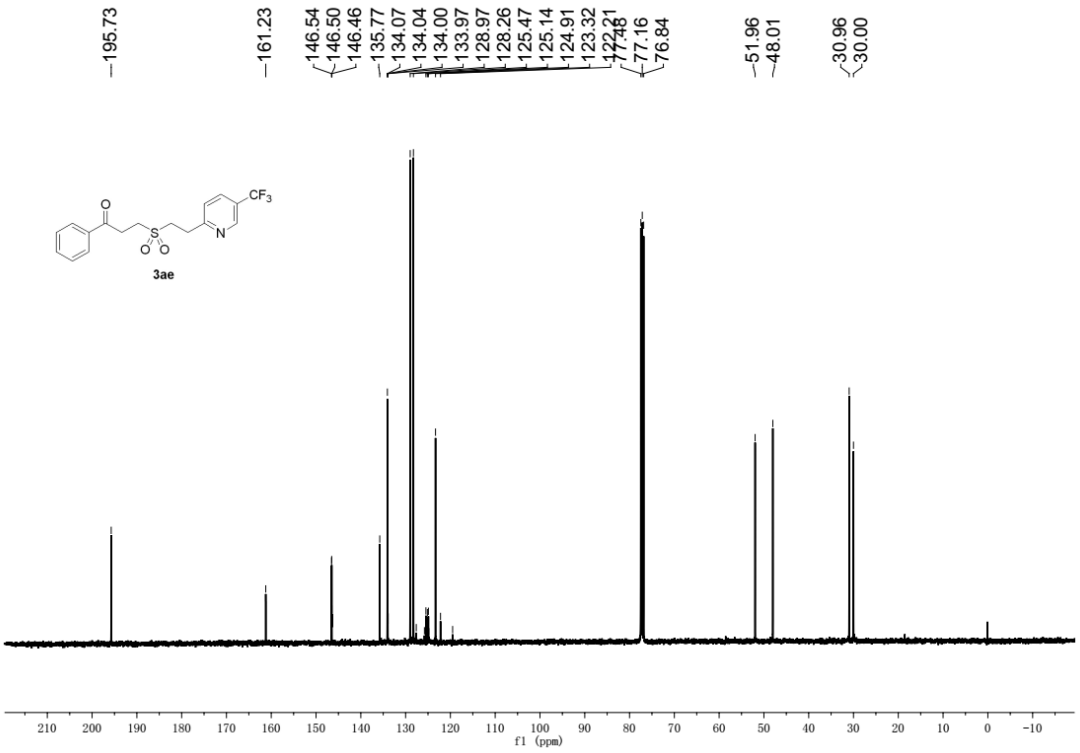

0.94
1.99
0.96
0.98
1.99
0.97
4.08
4.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)


-62.34


O
CF3
S
O
O
N

3ae


20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)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161.23
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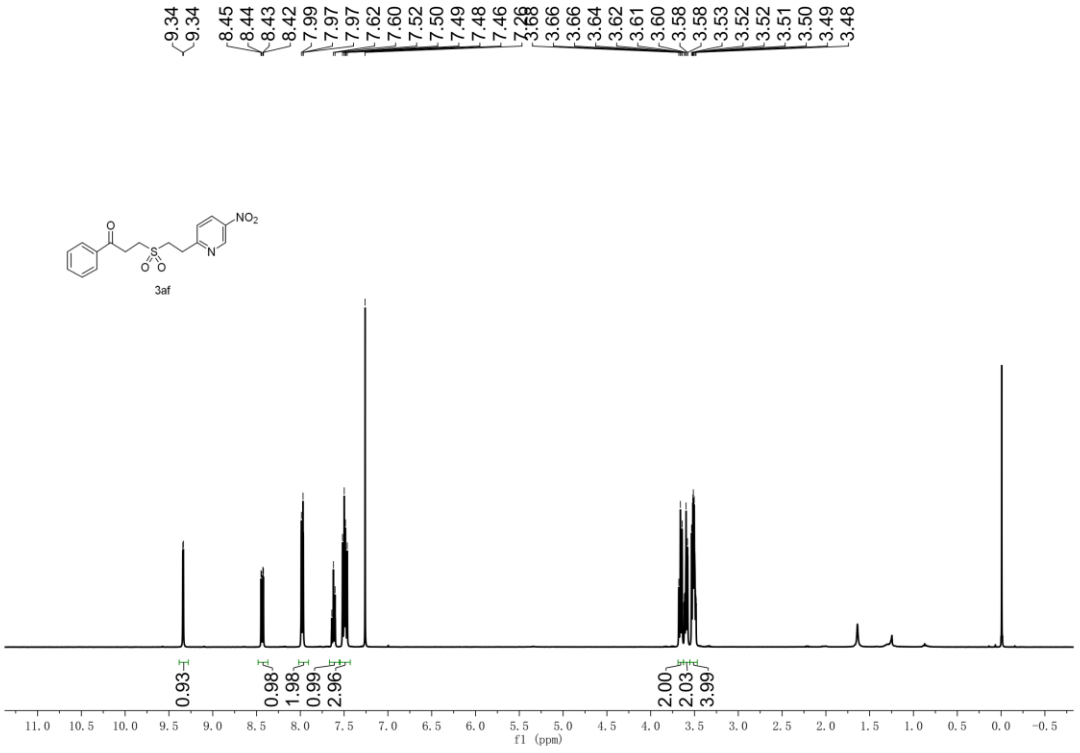
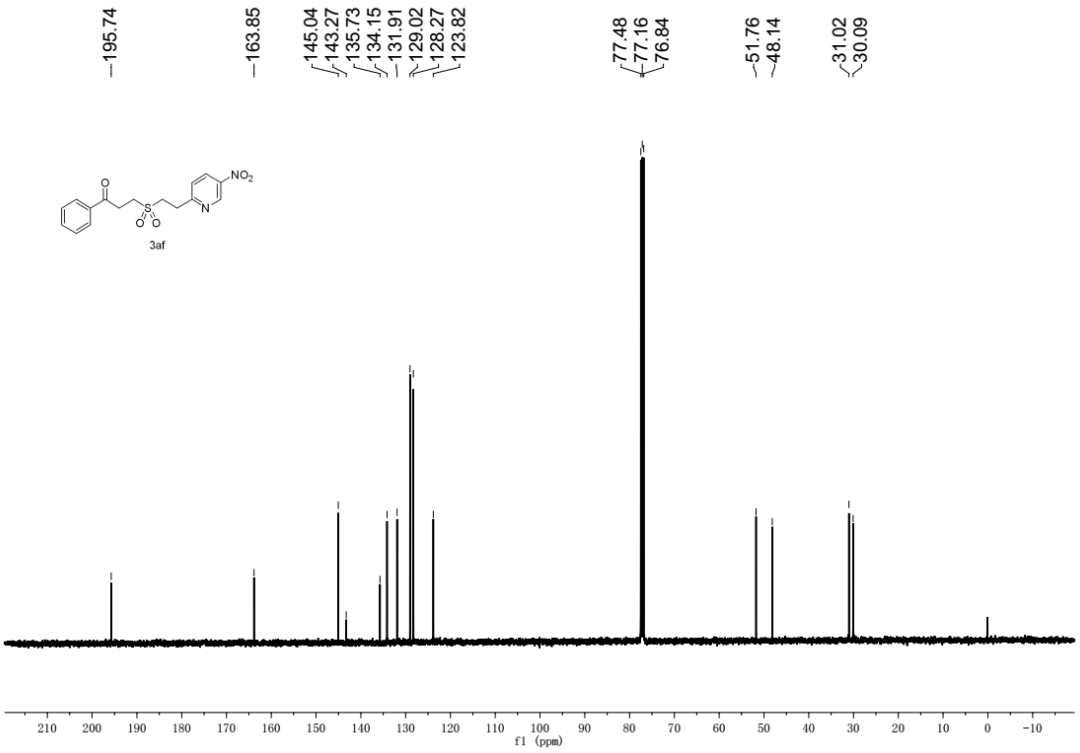
146.50
146.46
135.77
134.07
134.04
134.00
133.97
128.97
128.26
125.47
125.14
124.91
123.32
122.21
77.48
77.16
76.84
51.96
48.01
30.96
30.00
CF3
O
S
O
O
N
3ae
f1 (ppm)


9.34
9.34
8.45
8.44
8.43
8.42
7.99
7.97
7.97
7.62
7.60
7.52
7.50
7.49
7.48
7.46
3.66
3.66
3.64
3.62
3.61
3.60
3.58
3.58
3.53
3.52
3.52
3.51
3.50
3.49
3.48
NO2
O
S
O
O
N
3af
0.93
0.98
1.98
0.99
2.96
2.00
2.03
3.99
f1 (ppm)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163.85
145.04
143.27
135.73
134.15
131.91
129.02
128.27
123.82
77.48
77.16
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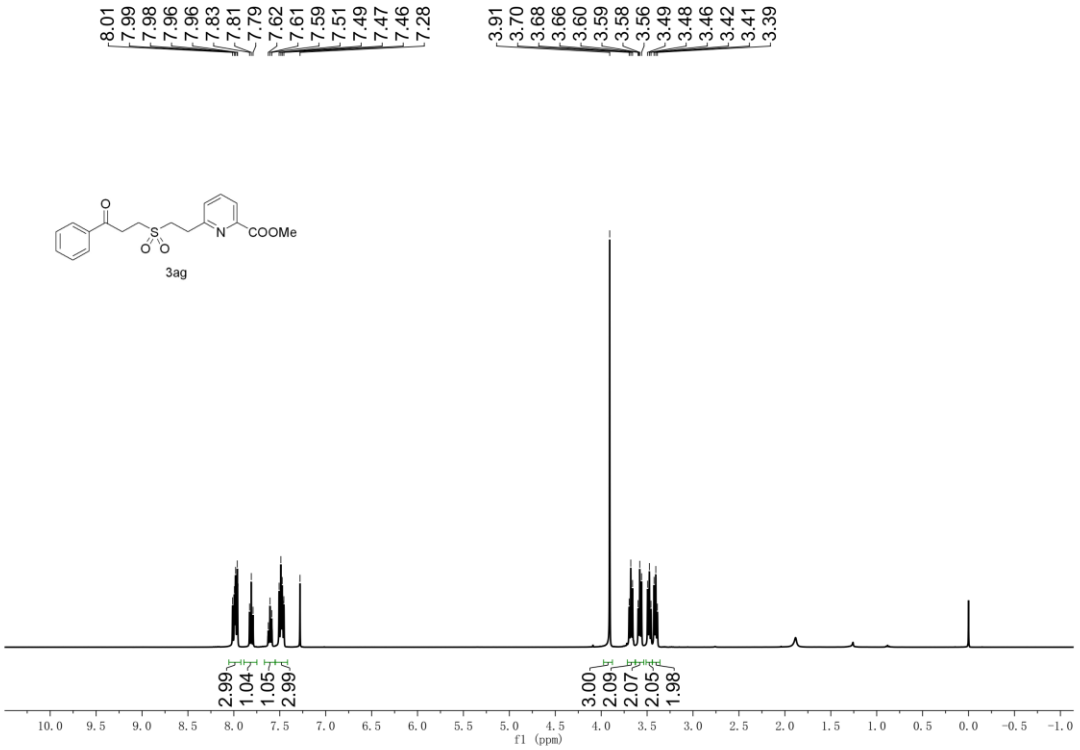
48.14
31.02
30.09
3af
f1 (ppm)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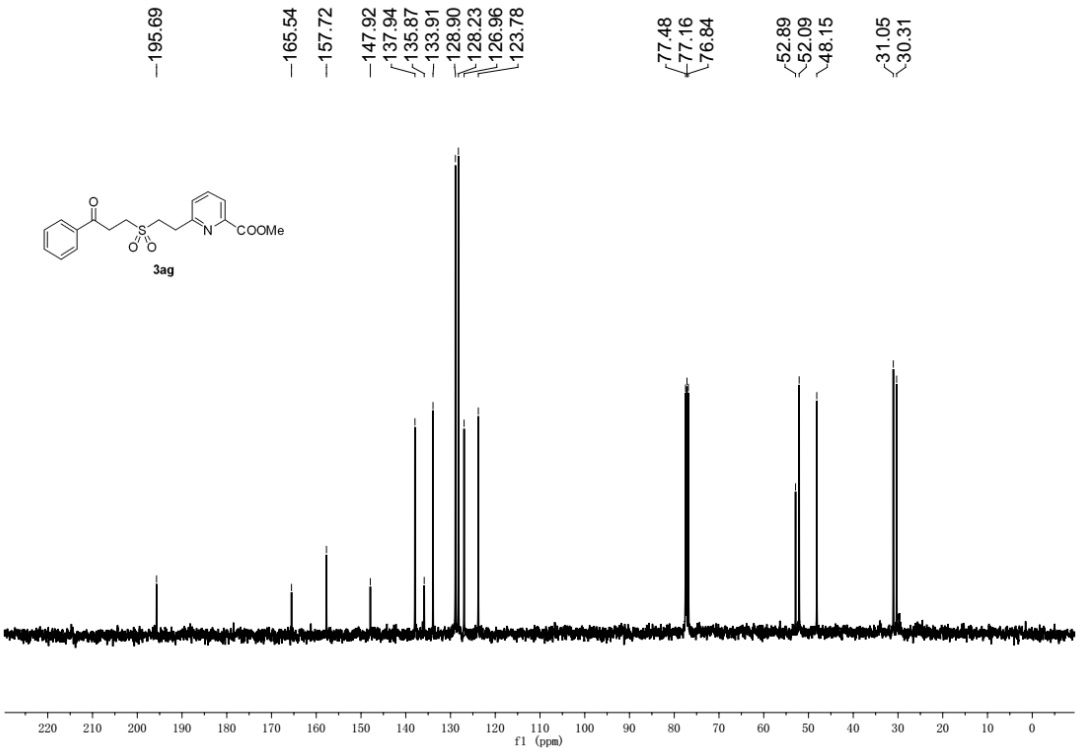
7.96
7.83
7.81
7.79
7.62
7.61
7.59
7.51
7.49
7.47
7.46
7.28
3.91
3.70
3.68
3.66
3.60
3.59
3.58
3.56
3.49
3.48
3.46
3.42
3.41
3.39
COOMe
3ag
2.99
1.04
1.05
2.99
3.00
2.09
2.07
2.05
1.98
f1 (ppm)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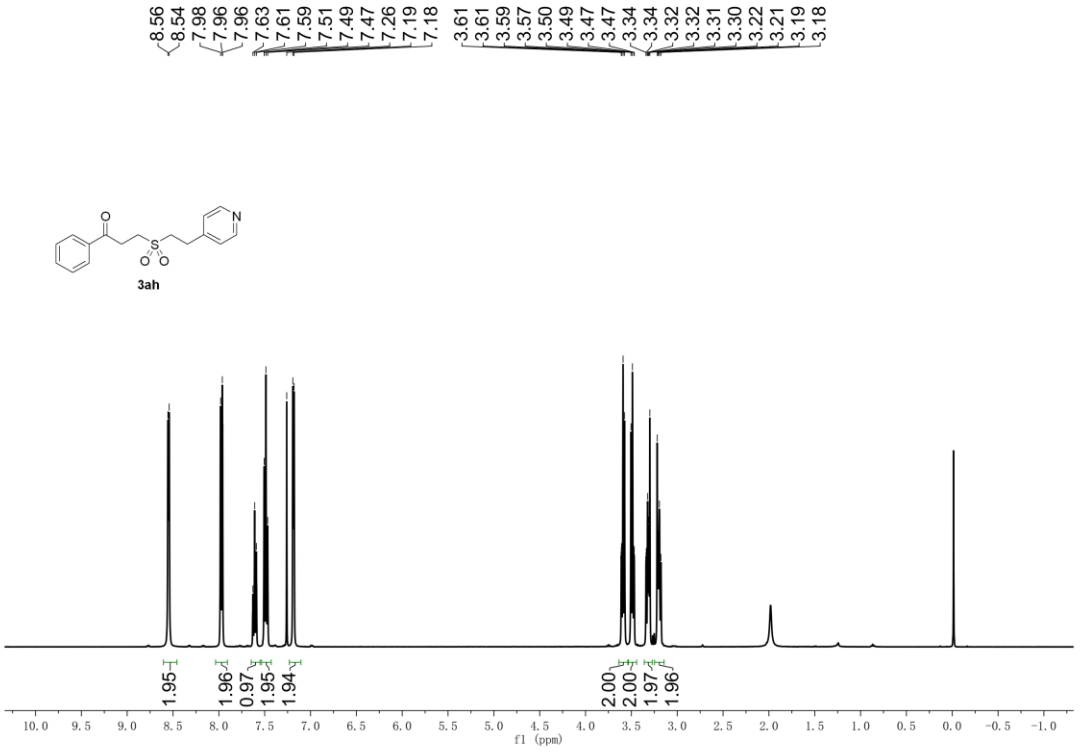
137.94
135.87
133.91
128.90
128.23
126.96
123.78
77.48
77.16
76.84
52.89
52.09
48.15
31.05
30.31
COOMe
3ag
f1 (ppm)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7.61
7.59
7.51
7.49
7.47
7.26
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7.18
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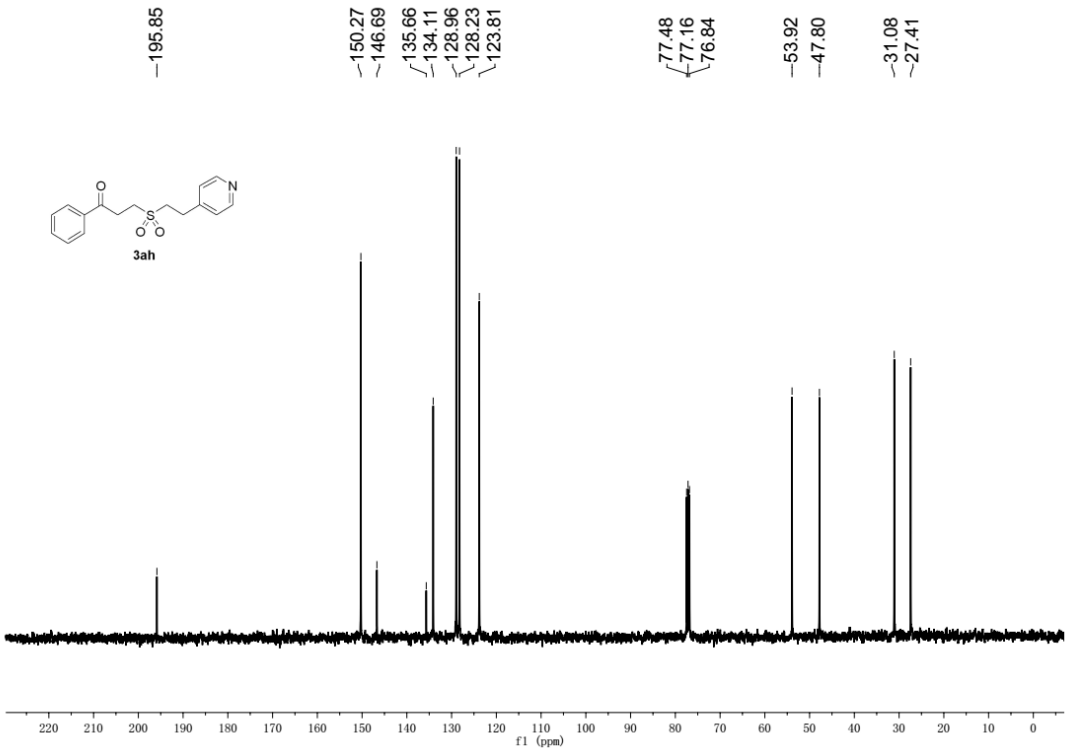
3.61
3.59
3.57
3.50
3.49
3.47
3.47
3.34
3.34
3.32
3.32
3.31
3.30
3.22
3.21
3.19
3.18
3ah
1.95
1.96
0.97
1.95
1.94
2.00
2.00
1.97
1.96
f1 (ppm)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77.16
76.84
53.92
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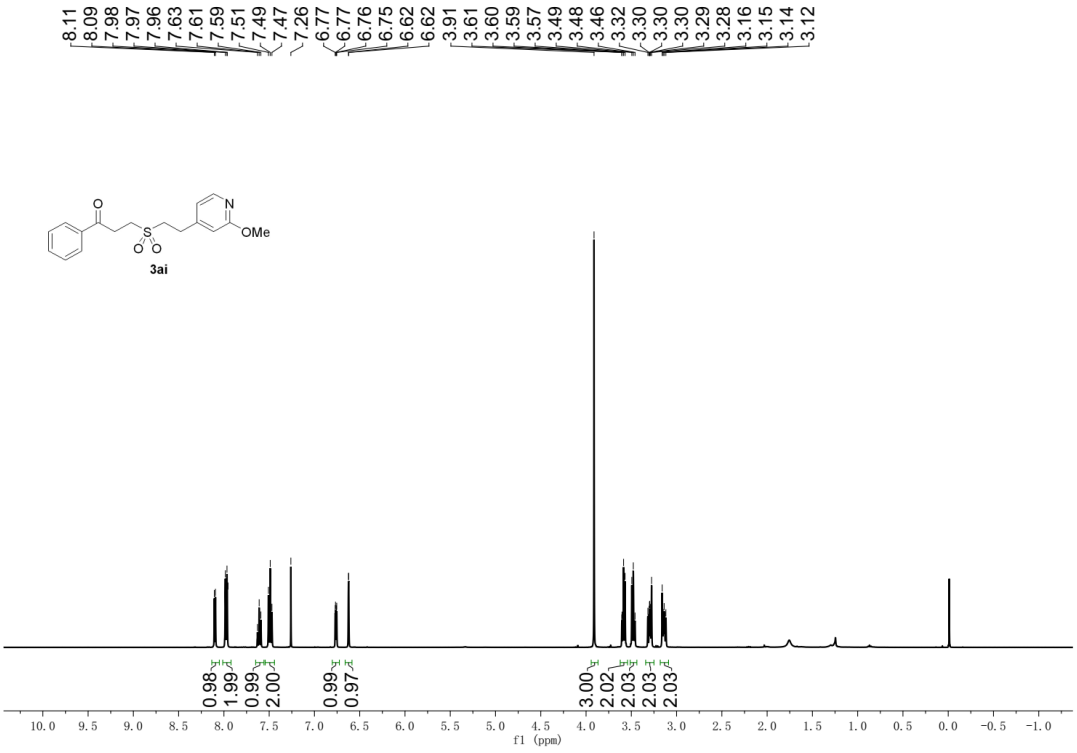
31.08
27.41
3ah
f1 (ppm)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7.63
7.61
7.59
7.51
7.49
7.47
7.26
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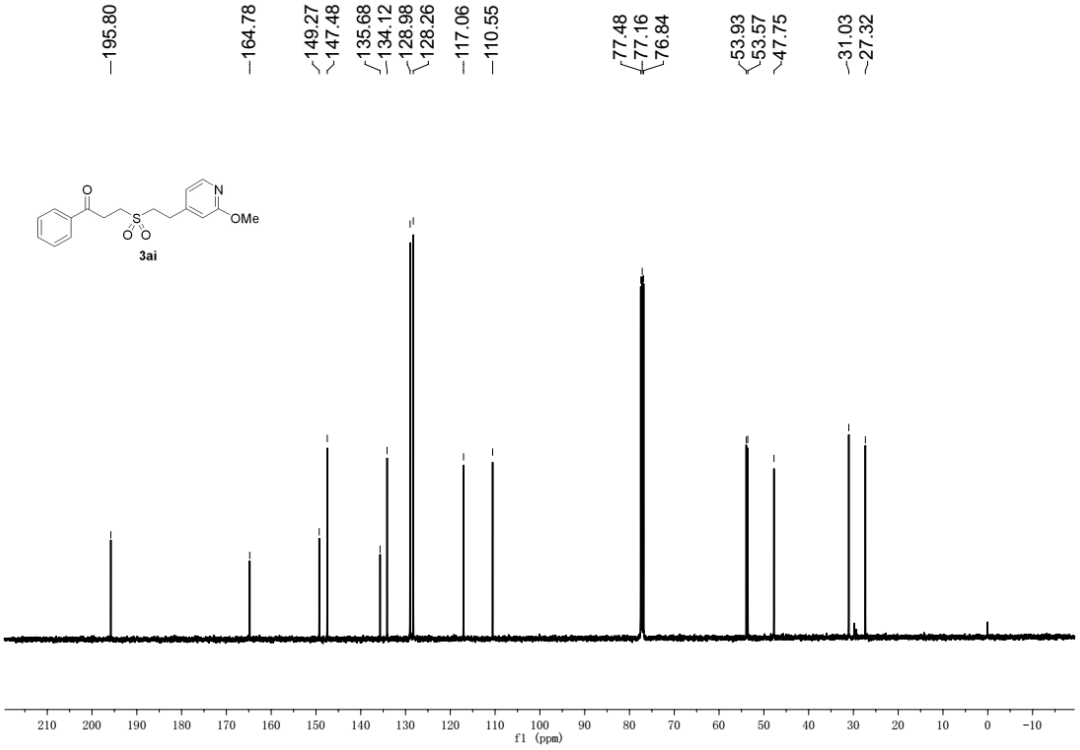
6.77
6.76
6.75
6.62
6.62
3.91
3.61
3.60
3.59
3.57
3.49
3.48
3.46
3.32
3.30
3.30
3.30
3.29
3.28
3.16
3.15
3.14
3.12
OMe
3ai
0.98
1.99
0.99
2.00
0.99
0.97
3.00
2.02
2.03
2.03
2.03
f1 (ppm)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147.48
135.68
134.12
128.98
128.26
117.06
110.55
77.48
77.16
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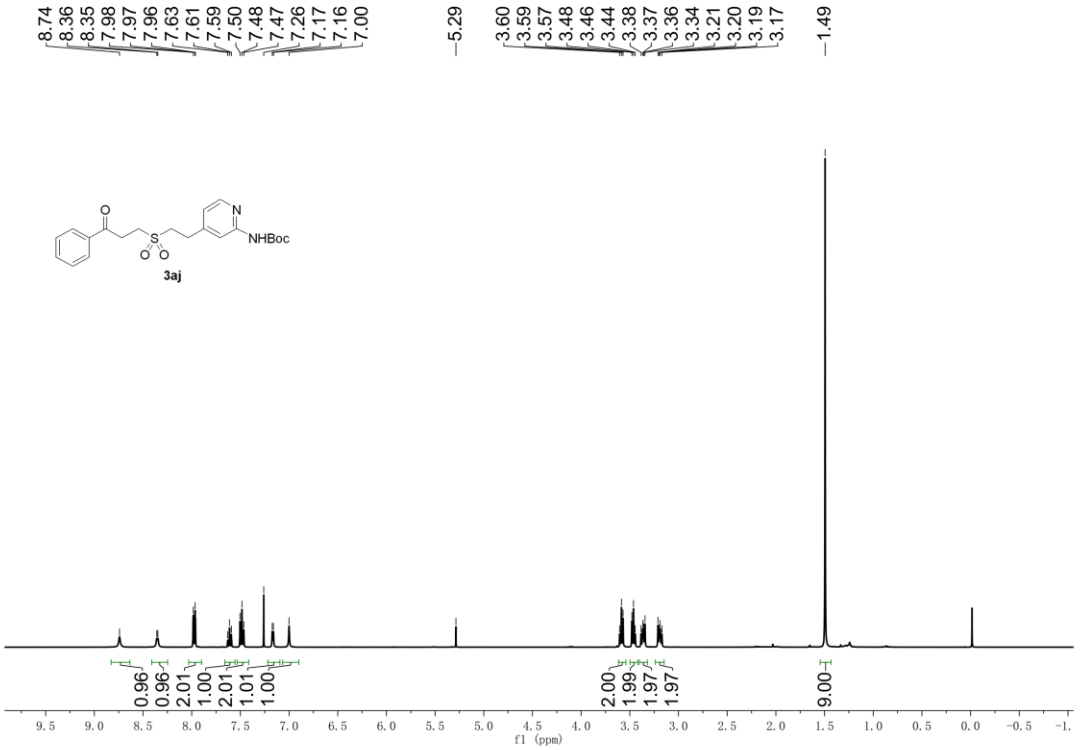
O
N
OMe
S
O O
3ai
f1 (ppm)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7.96
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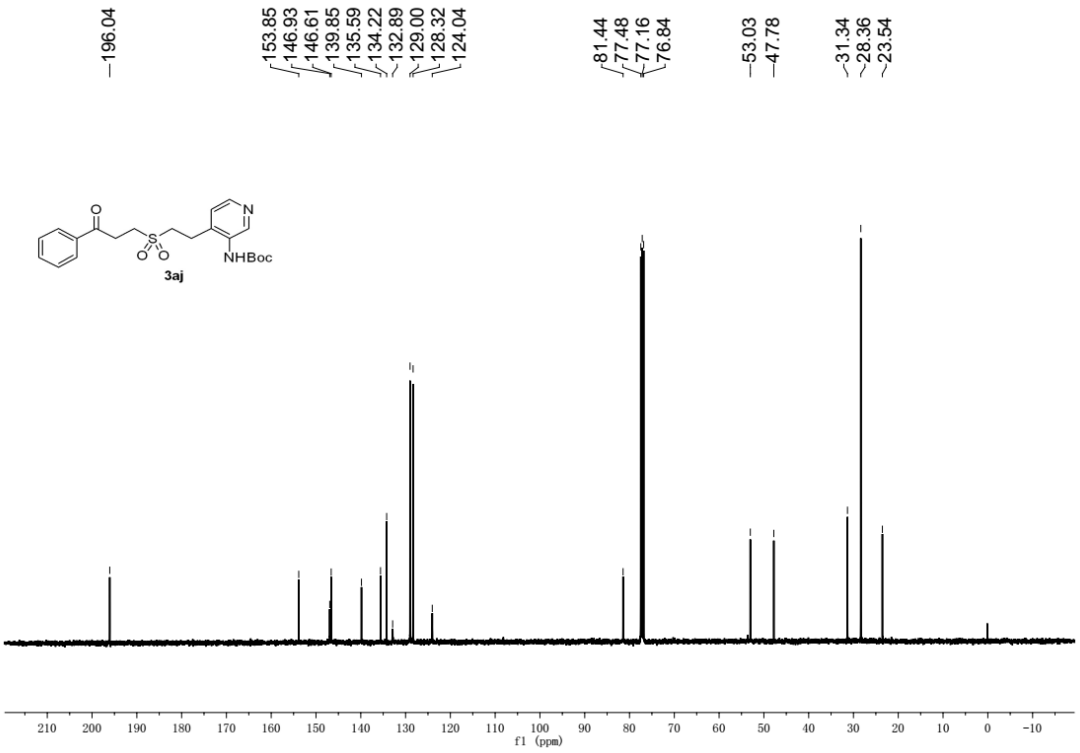
7.61
7.59
7.50
7.48
7.47
7.26
7.17
7.16
7.00
5.29
3.60
3.59
3.57
3.48
3.46
3.44
3.38
3.37
3.36
3.34
3.21
3.20
3.19
3.17
1.49
O
N
NHBoc
S
O O
3aj
0.96
0.96
2.01
1.00
2.01
1.01
1.00
2.00
1.99
1.97
1.97
9.00
f1 (ppm)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139.85
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134.22
132.89
129.00
128.32
124.04
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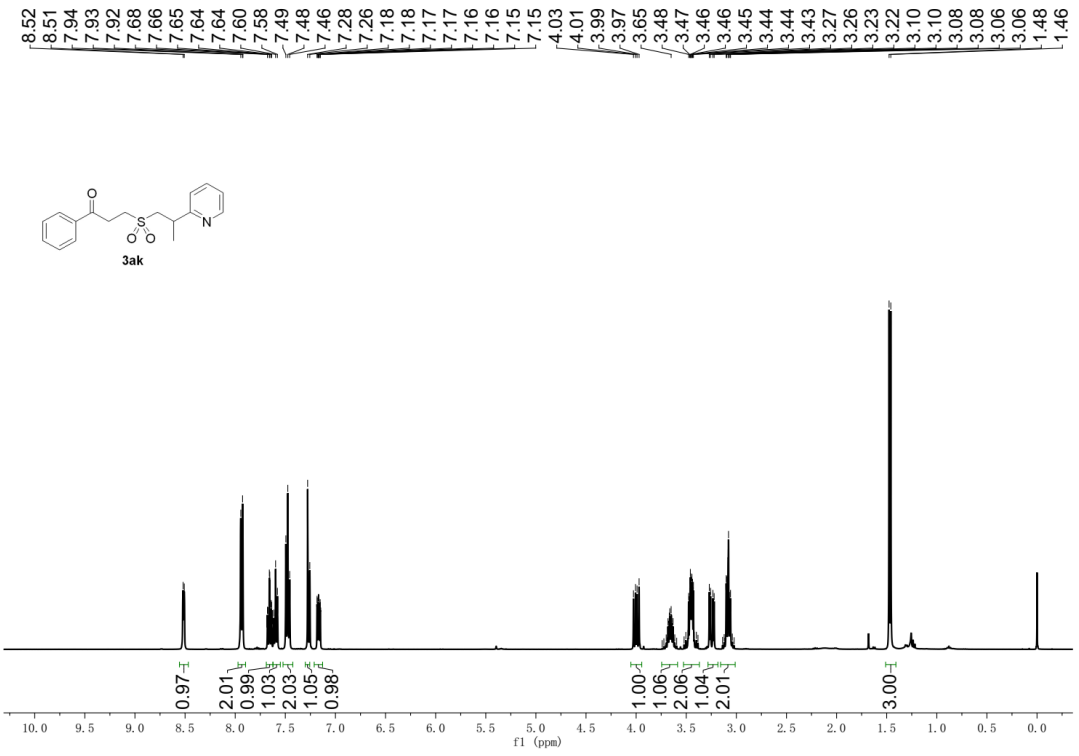
76.84
53.03
47.78
31.34
28.36
23.54
NHBoc
3aj
f1 (ppm)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7.60
7.58
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7.48
7.46
7.28
7.26
7.18
7.18
7.17
7.17
7.16
7.16
7.15
7.15
4.03
4.01
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3.65
3.48
3.47
3.46
3.46
3.45
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3.27
3.26
3.23
3.22
3.10
3.10
3.08
3.08
3.06
3.06
1.48
1.46
3ak
0.97
2.01
0.99
1.03
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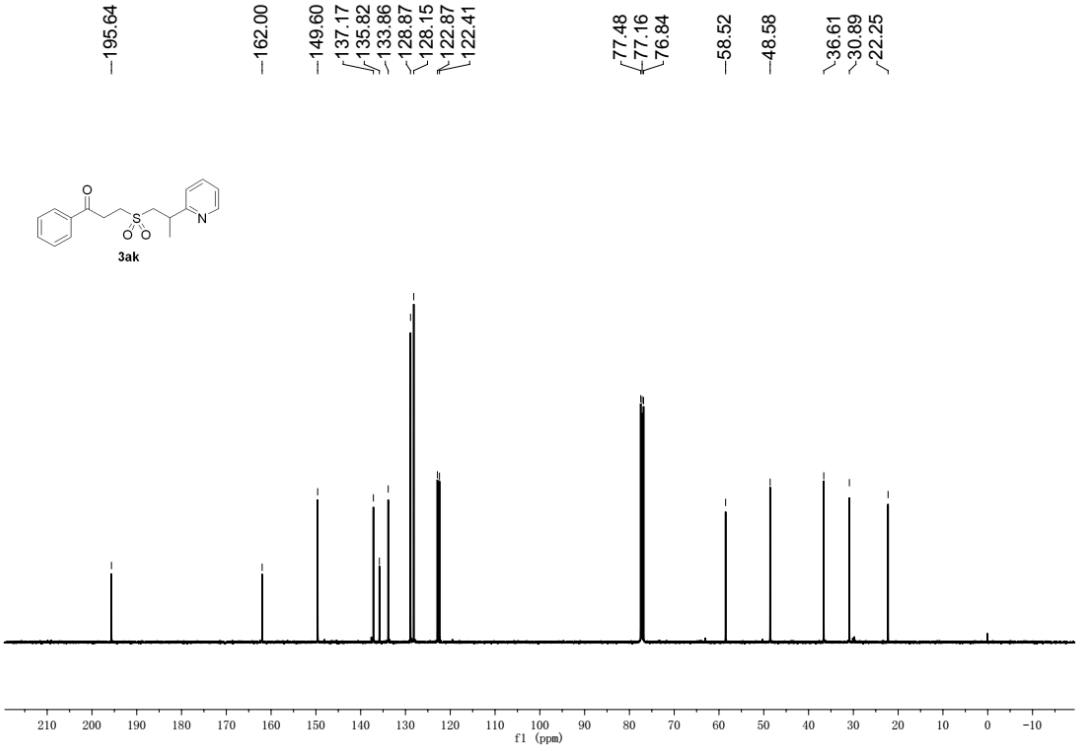
1.05
0.98
1.00
1.06
2.06
1.04
2.01
3.00
f1 (ppm)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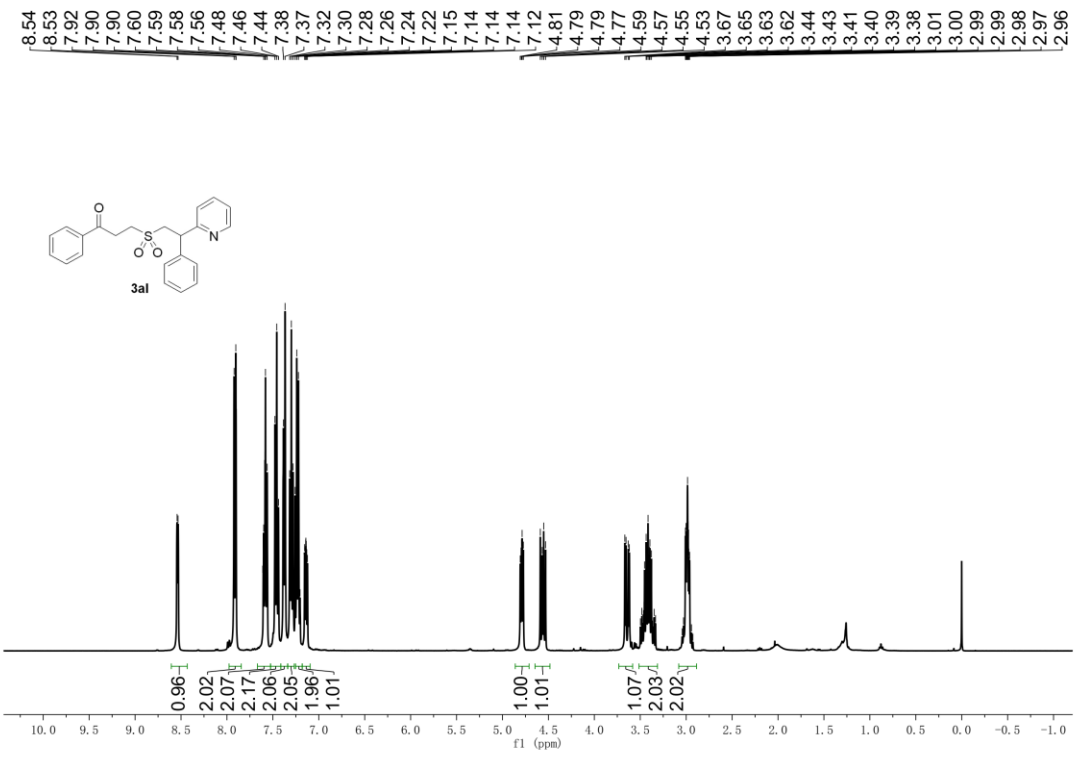
36.61
30.89
22.25
3ak
f1 (ppm)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7.38
7.37
7.32
7.30
7.28
7.26
7.24
7.22
7.15
7.14
7.14
7.14
7.12
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4.77
4.59
4.57
4.55
4.53
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3.65
3.63
3.62
3.44
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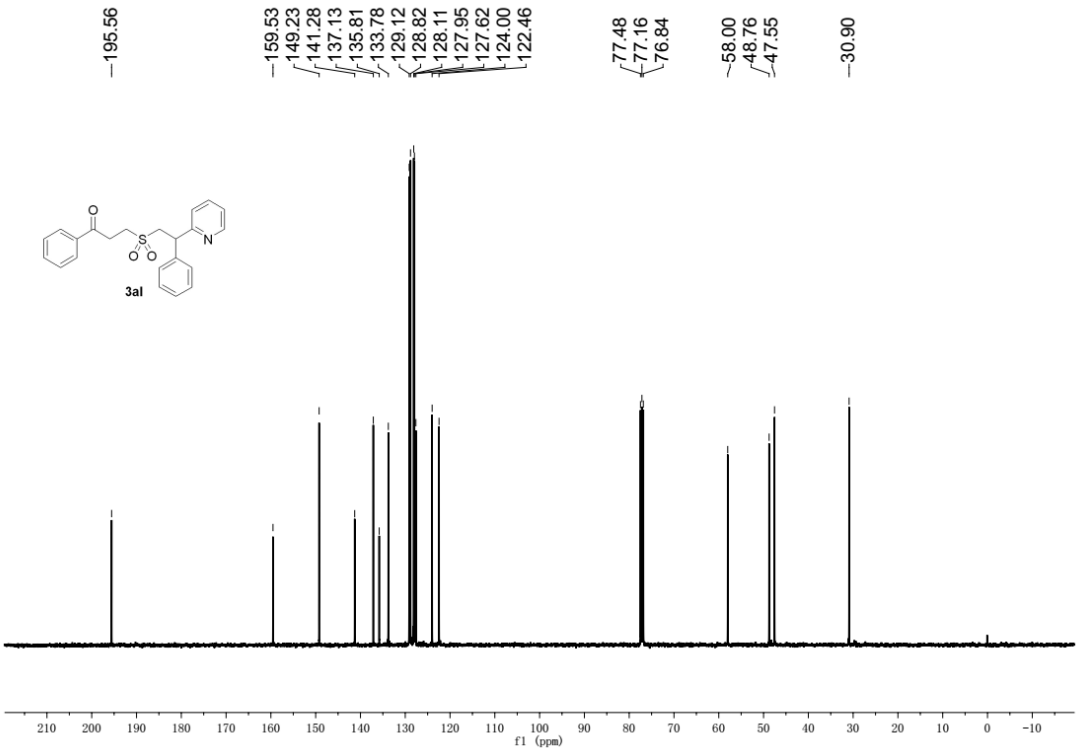
3.41
3.40
3.39
3.38
3.01
3.00
2.99
2.99
2.98
2.97
2.96
3al
0.96
2.02
2.07
2.17
2.06
2.05
1.96
1.01
1.00
1.01
1.07
2.03
2.02
f1 (ppm)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137.13
135.81
133.78
129.12
128.82
128.11
127.95
127.62
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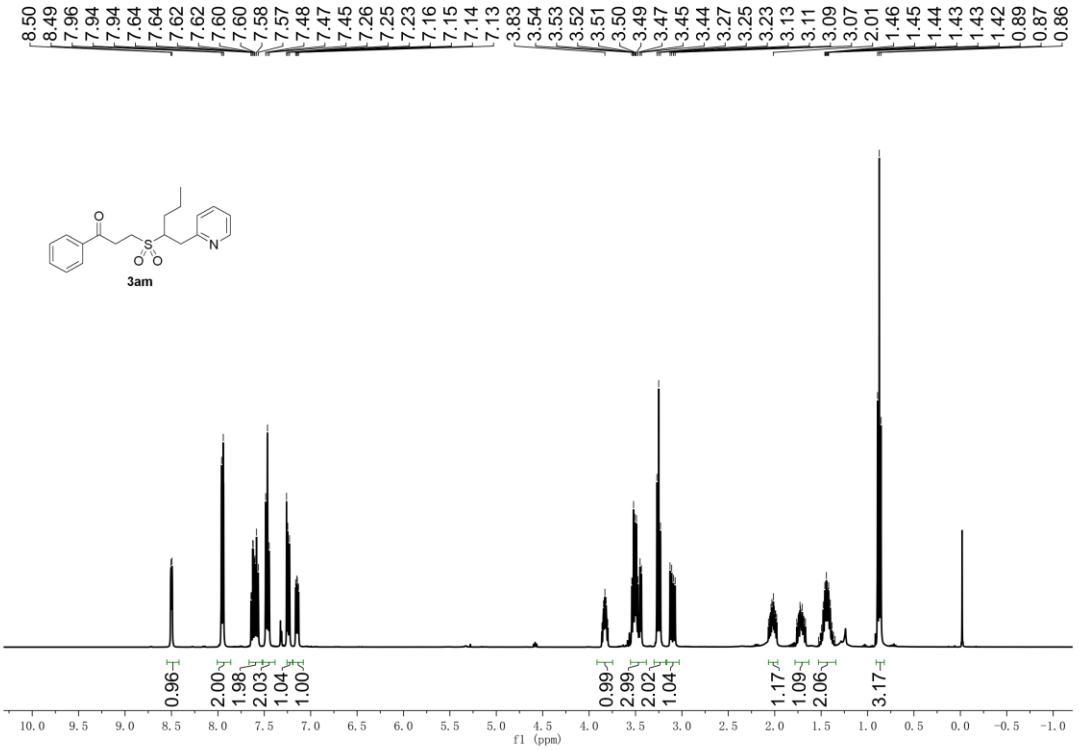
48.76
47.55
30.90
3al
f1 (ppm)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7.64
7.64
7.62
7.62
7.60
7.60
7.58
7.57
7.48
7.47
7.45
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7.25
7.23
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3.54
3.53
3.52
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3.50
3.49
3.47
3.45
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3.23
3.13
3.11
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3.07
2.01
1.46
1.45
1.44
1.43
1.43
1.42
0.89
0.87
0.86
3am
0.96
2.00
1.98
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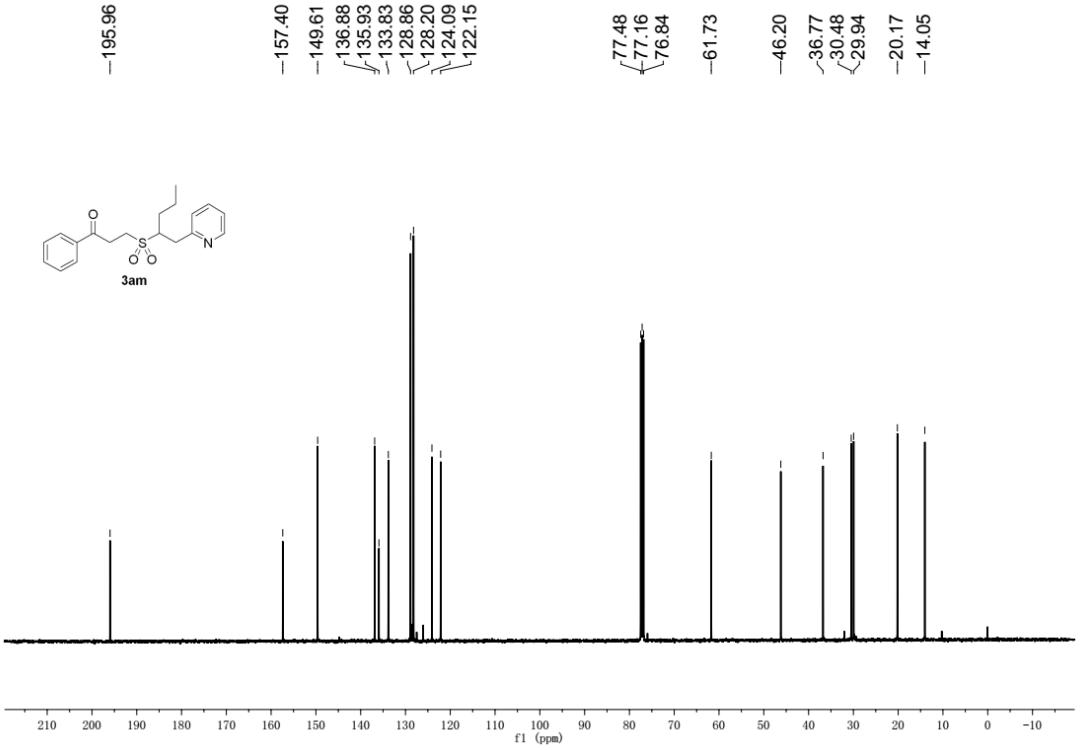
2.02
1.04
1.17
1.09
2.06
3.17
f1 (ppm)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29.94
20.17
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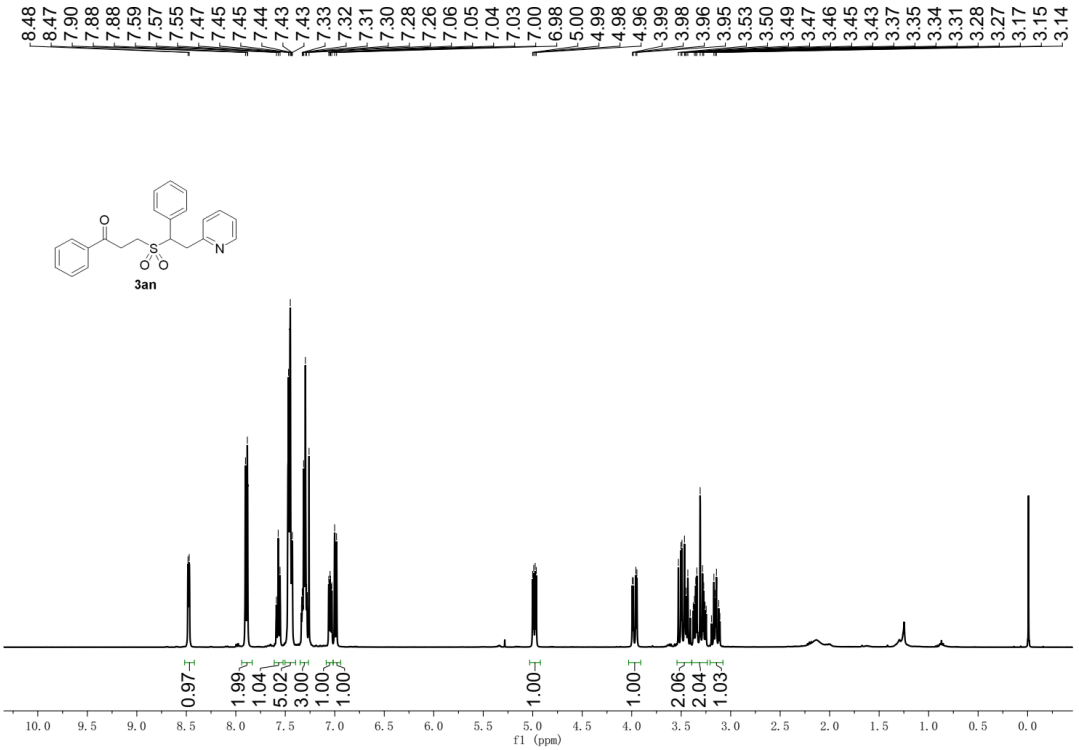
3am
f1 (ppm)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7.43
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7.32
7.31
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7.28
7.26
7.06
7.05
7.04
7.03
7.00
6.98
5.00
4.99
4.98
4.96
3.99
3.98
3.96
3.95
3.53
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3.49
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3.46
3.45
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3.34
3.31
3.28
3.27
3.17
3.15
3.14
3an
0.97
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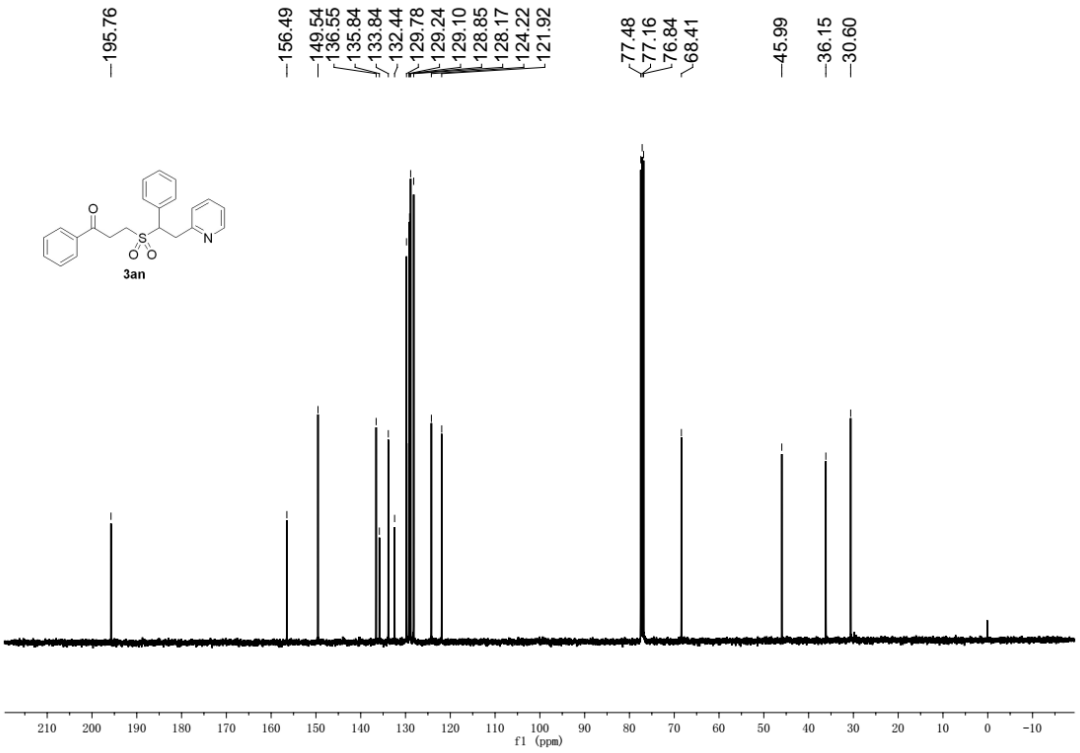
1.00
1.00
1.00
2.06
2.04
1.03
f1 (ppm)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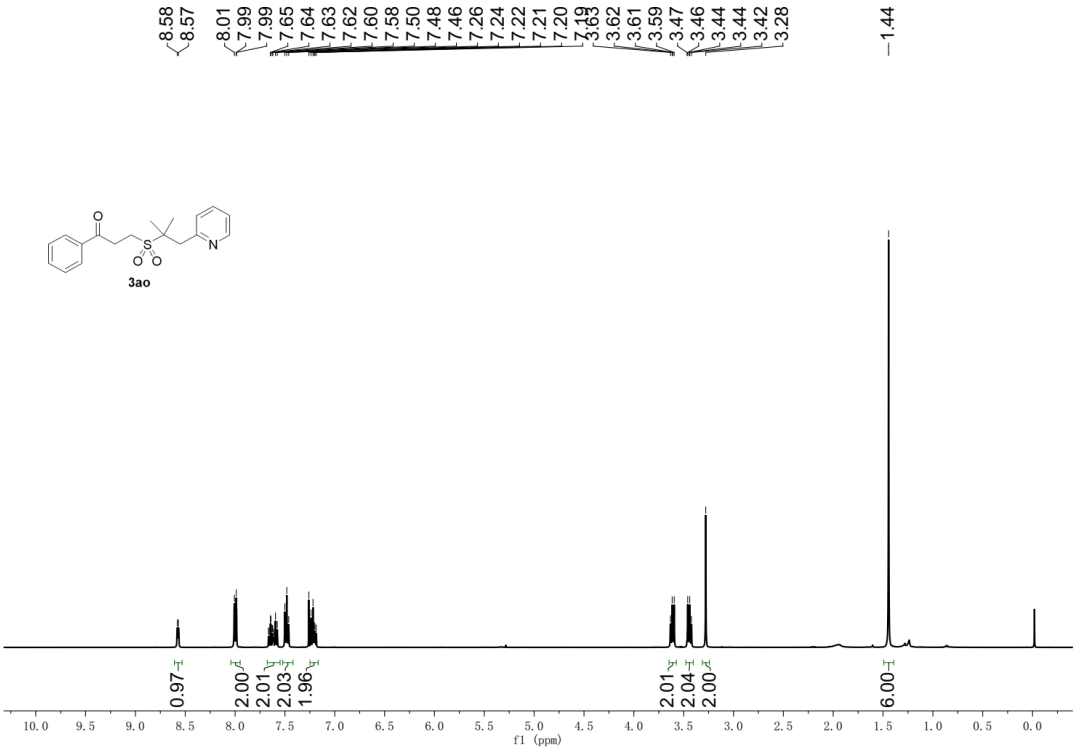
3an
f1 (ppm)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7.48
7.46
7.26
7.24
7.22
7.21
7.20
7.19
3.63
3.62
3.61
3.59
3.47
3.46
3.44
3.44
3.42
3.28
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2.03
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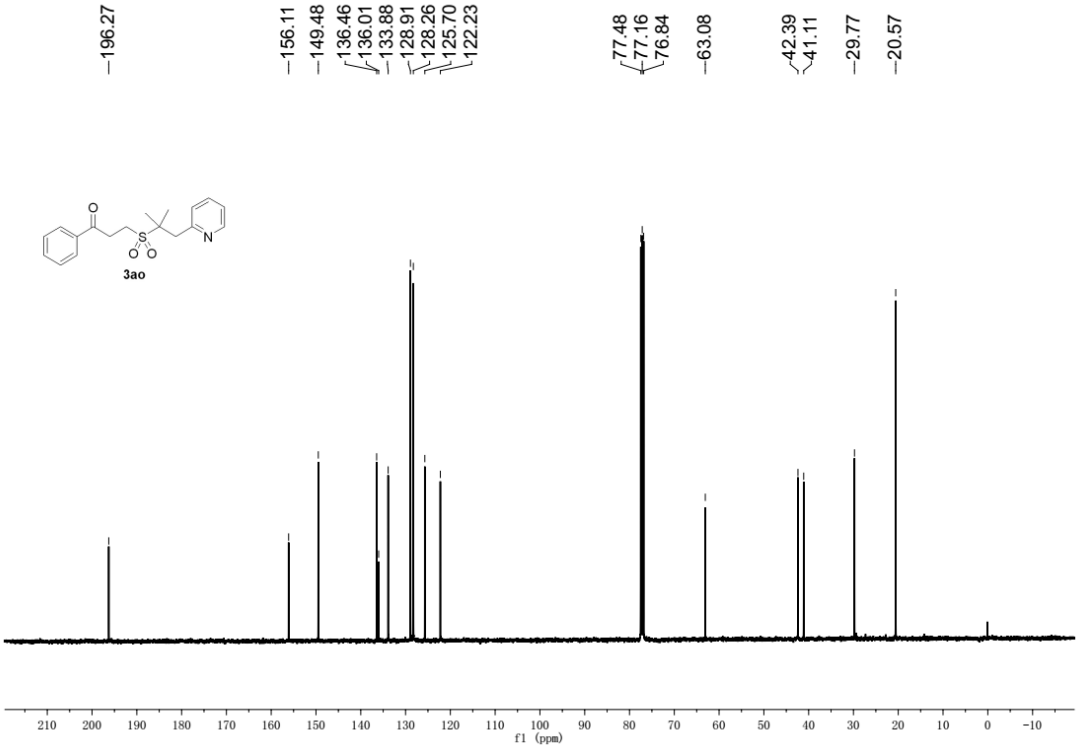
2.01
2.04
2.00
6.00
f1 (ppm)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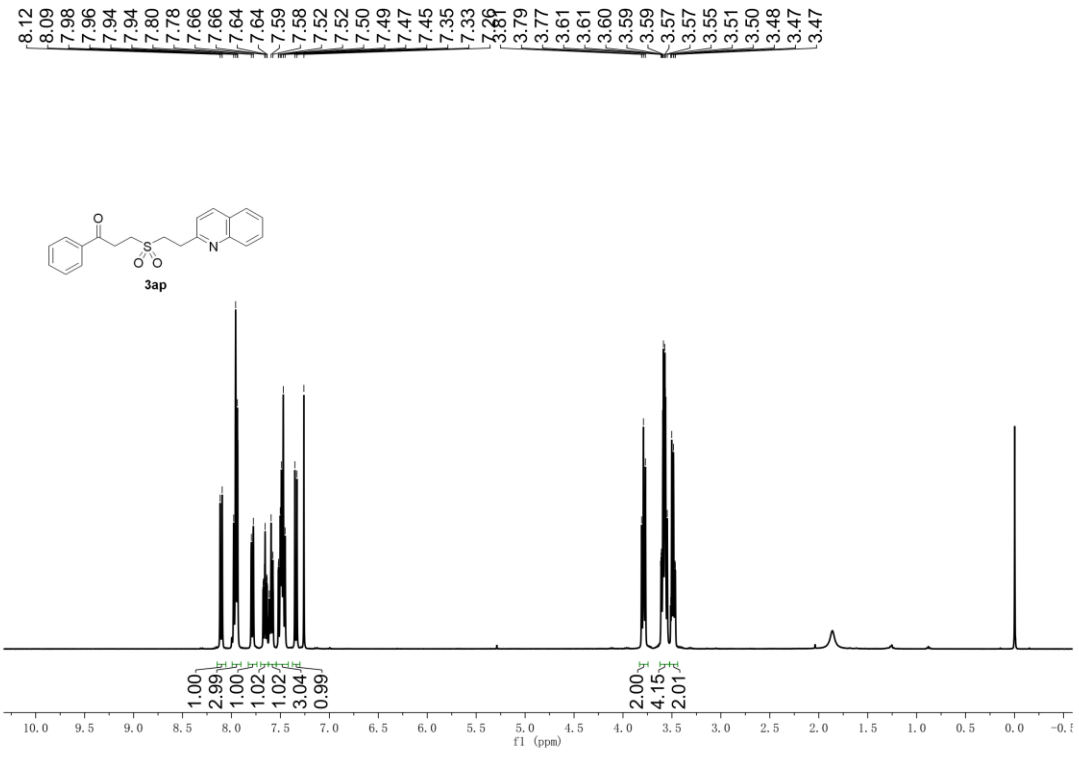
63.08
42.39
41.11
29.77
20.57
3ao
f1 (ppm)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7.58
7.52
7.52
7.50
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7.47
7.45
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3.61
3.61
3.60
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3.59
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3.57
3.55
3.51
3.50
3.48
3.47
3.47
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1.02
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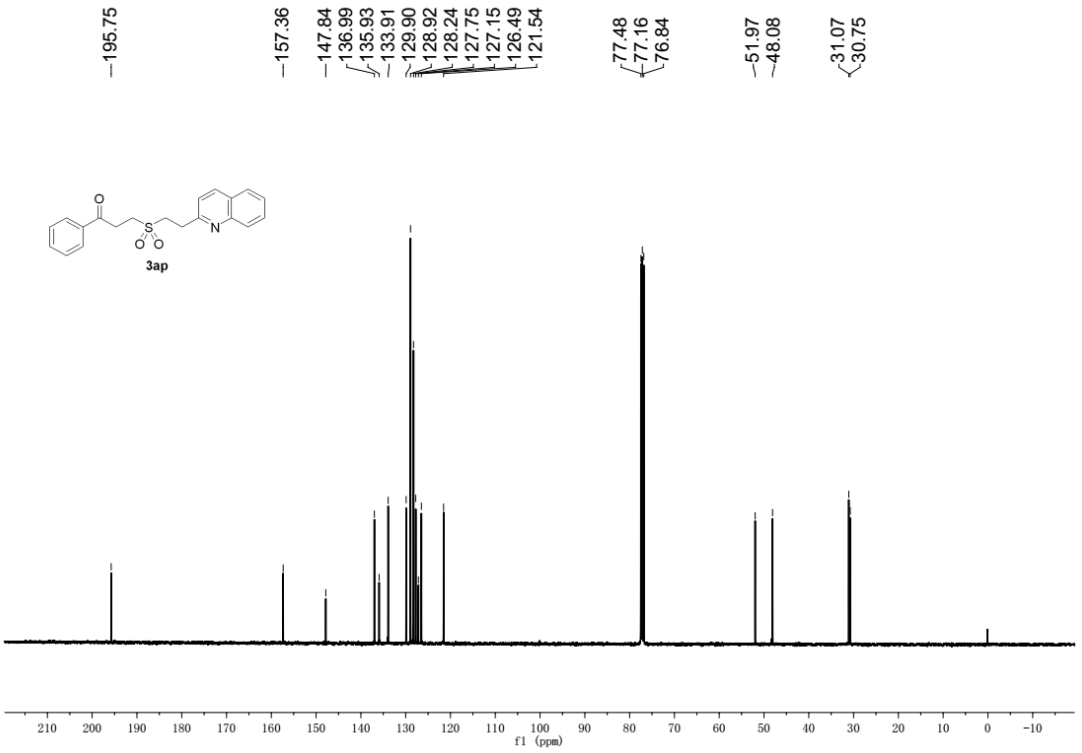
2.01
f1 (ppm)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76.84
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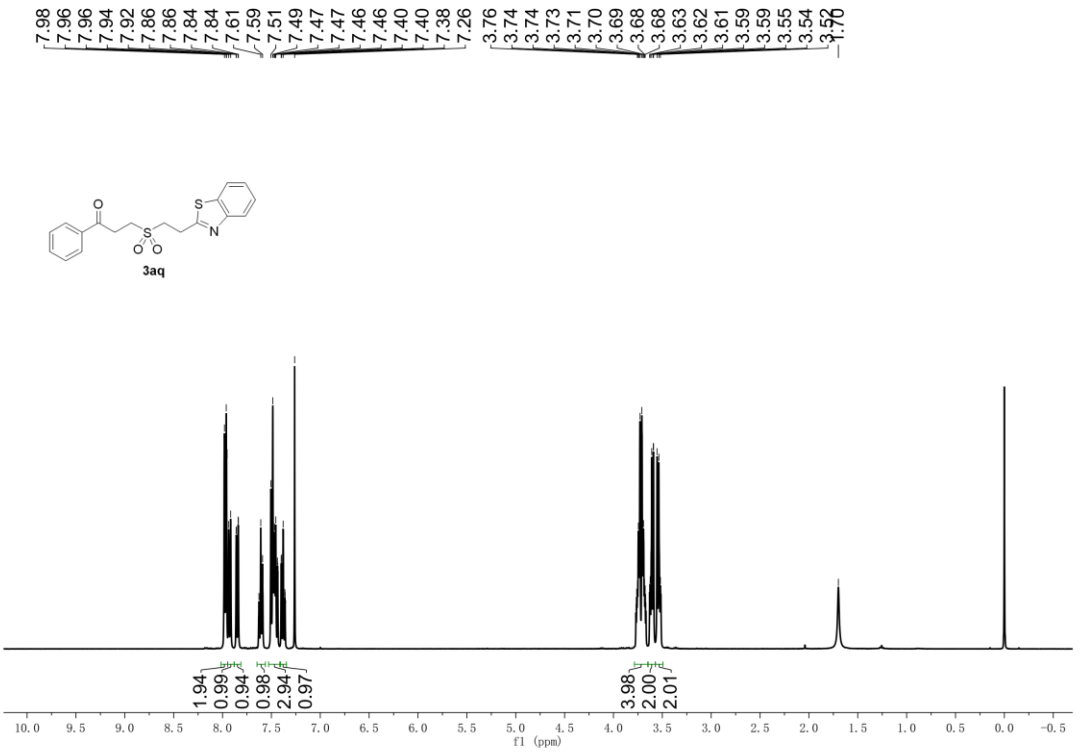
48.08
31.07
30.75
3ap
f1 (ppm)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7.86
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7.47
7.47
7.46
7.46
7.40
7.40
7.38
7.26
3.76
3.74
3.74
3.73
3.71
3.70
3.69
3.68
3.68
3.63
3.62
3.61
3.59
3.59
3.55
3.54
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0.94
0.98
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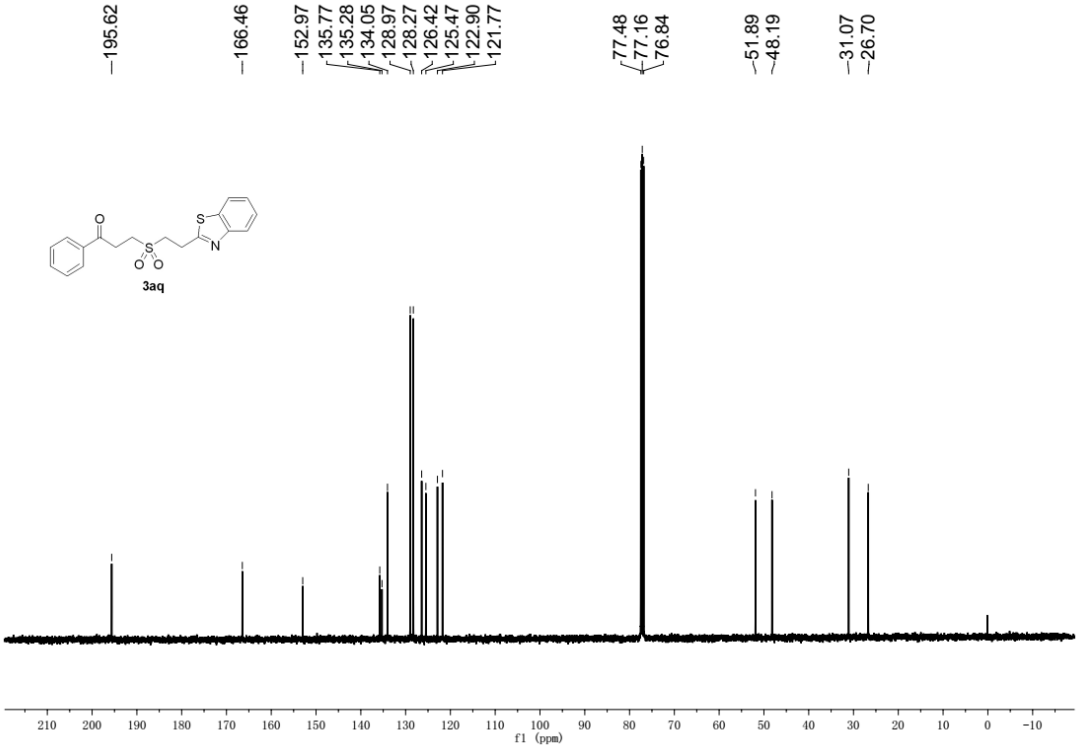
0.97
3.98
2.00
2.01
f1 (ppm)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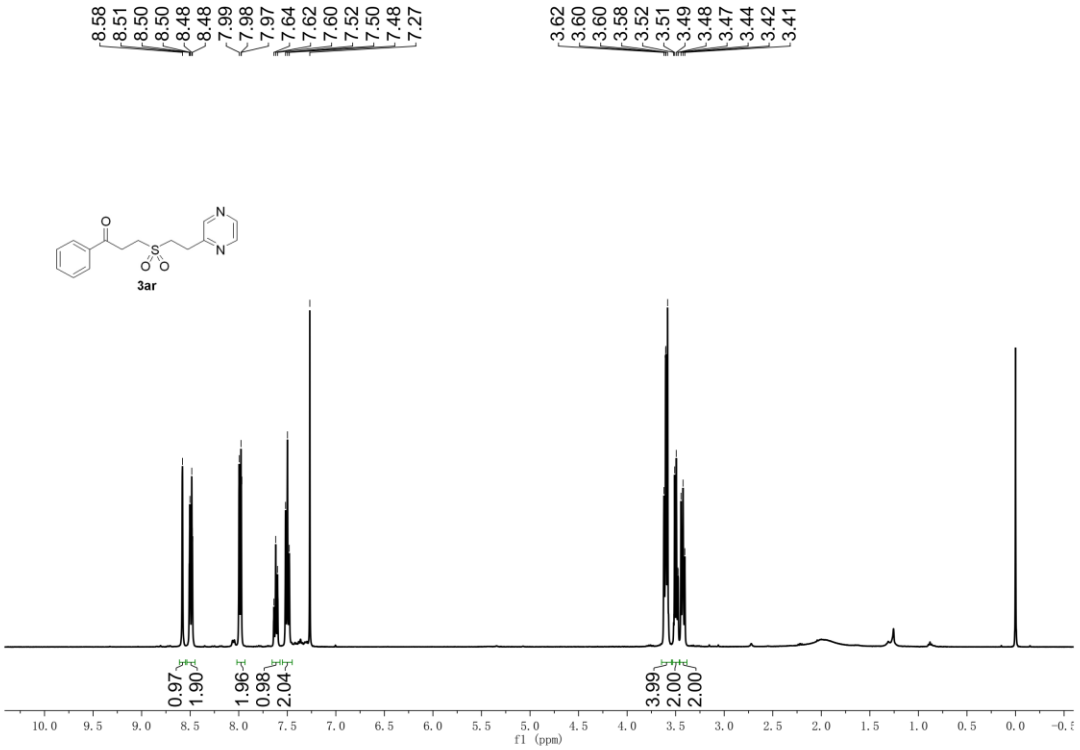
76.84
51.89
48.19
31.07
26.70
3aq
f1 (ppm)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7.62
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3.60
3.60
3.58
3.52
3.51
3.49
3.48
3.47
3.44
3.42
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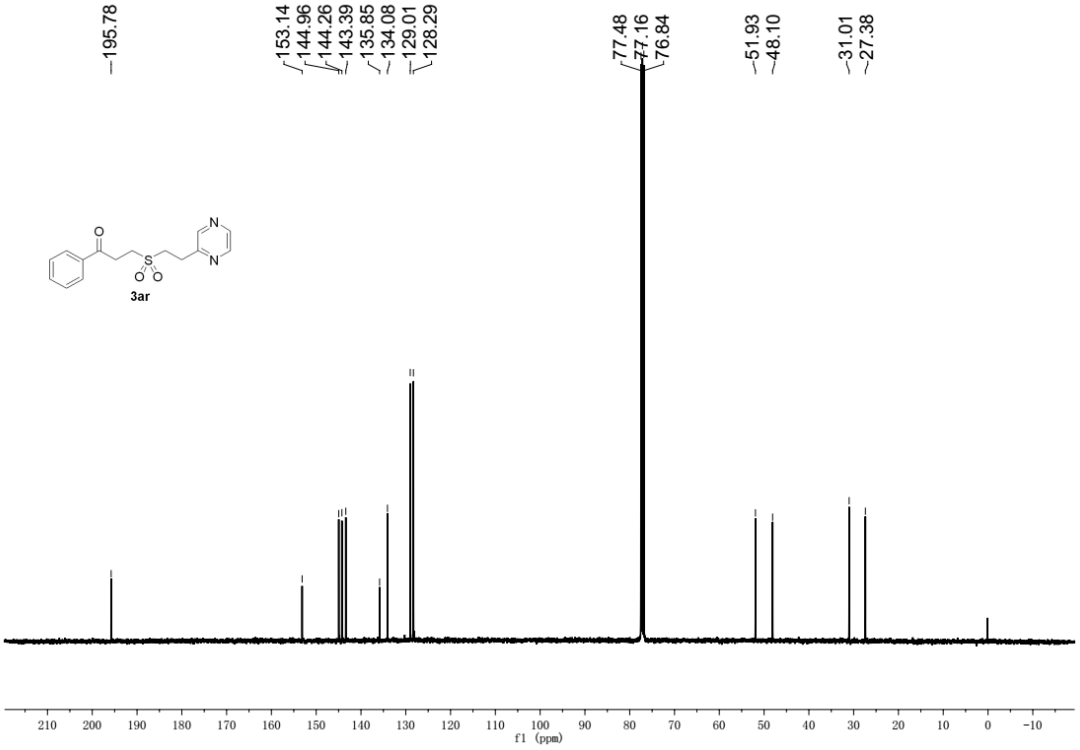
1.96
0.98
2.04
3.99
2.00
2.00
f1 (ppm)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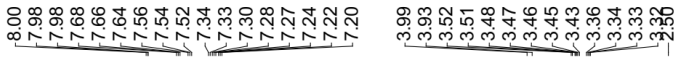
48.10
31.01
27.38
3ar
f1 (ppm)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7.33
7.30
7.28
7.27
7.24
7.22
7.20
3.99
3.93
3.52
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3.47
3.46
3.45
3.43
3.36
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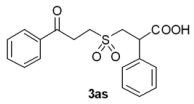
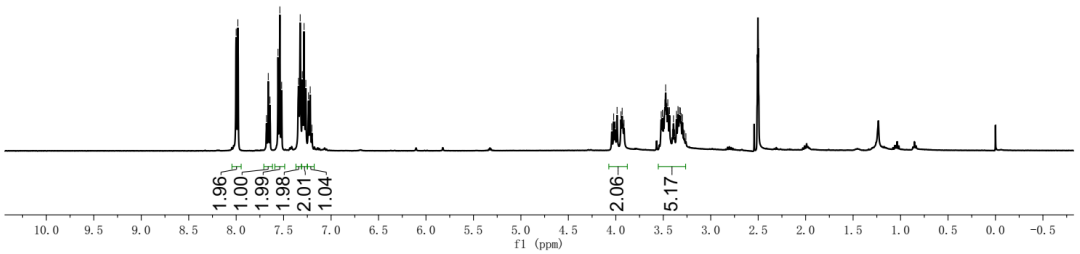
3.33
3.32
2.50


COOH
3as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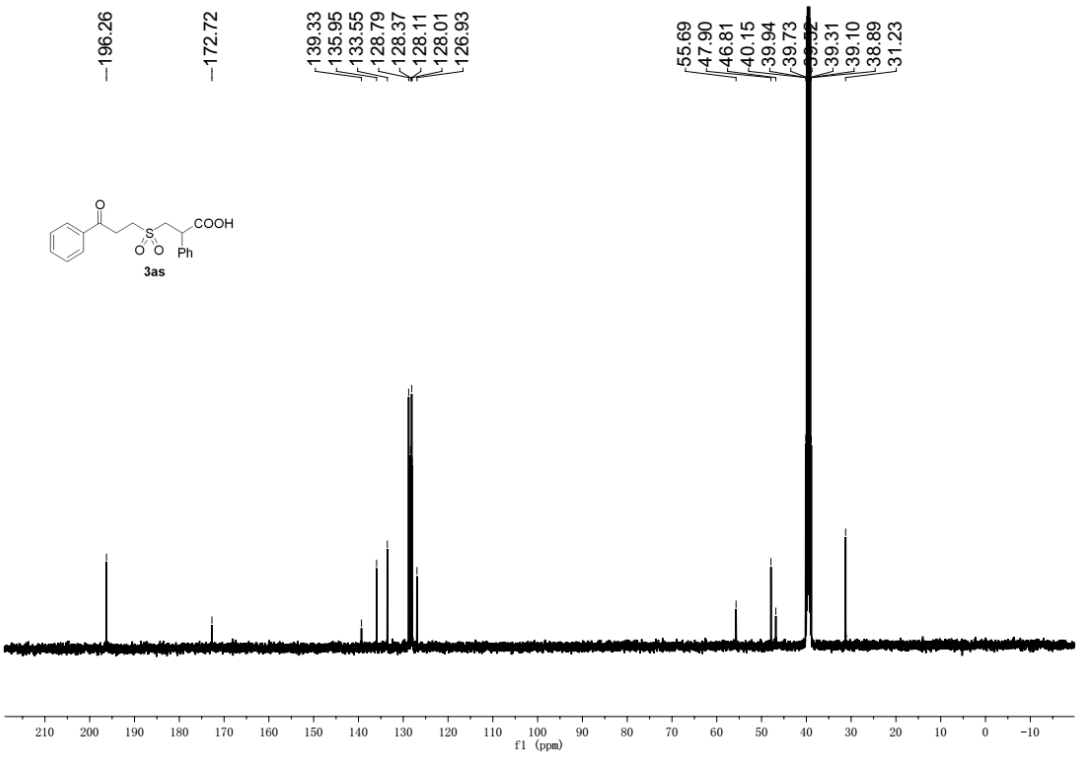
1.00
1.99
1.98
2.01
1.04
2.06
5.17
f1 (ppm)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128.11
128.01
126.93
55.69
47.90
46.81
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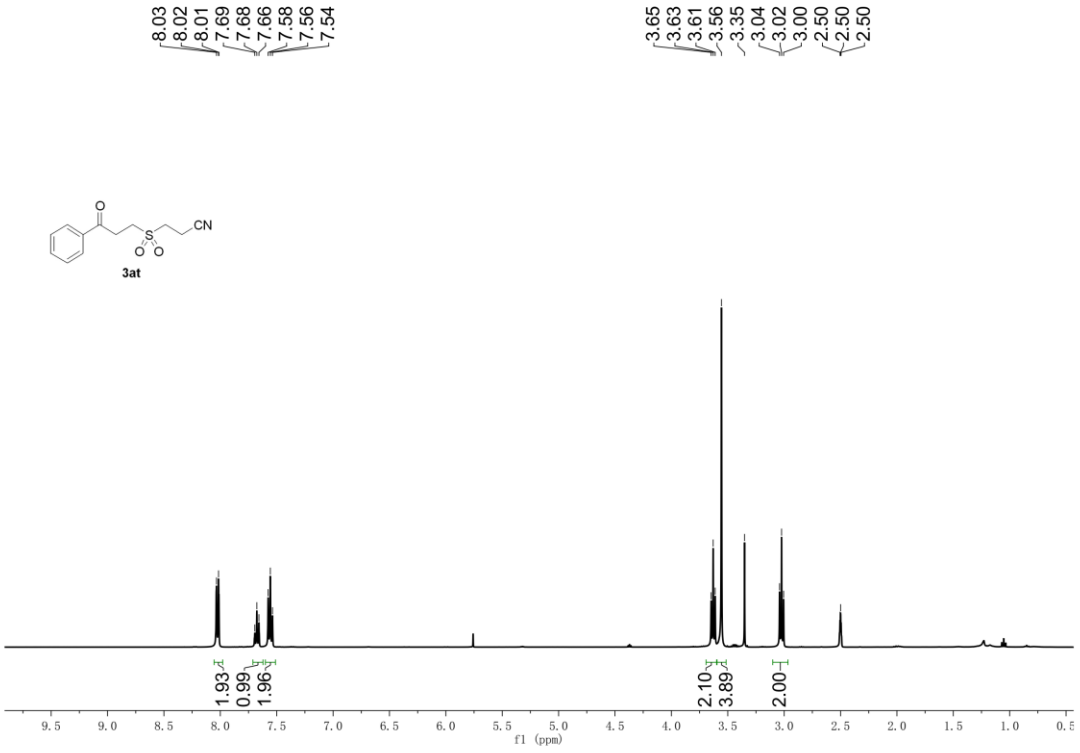
39.73
39.52
39.31
39.10
38.89
31.23
COOH
Ph
3as
f1 (ppm)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8.02
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3.63
3.61
3.56
3.35
3.04
3.02
3.00
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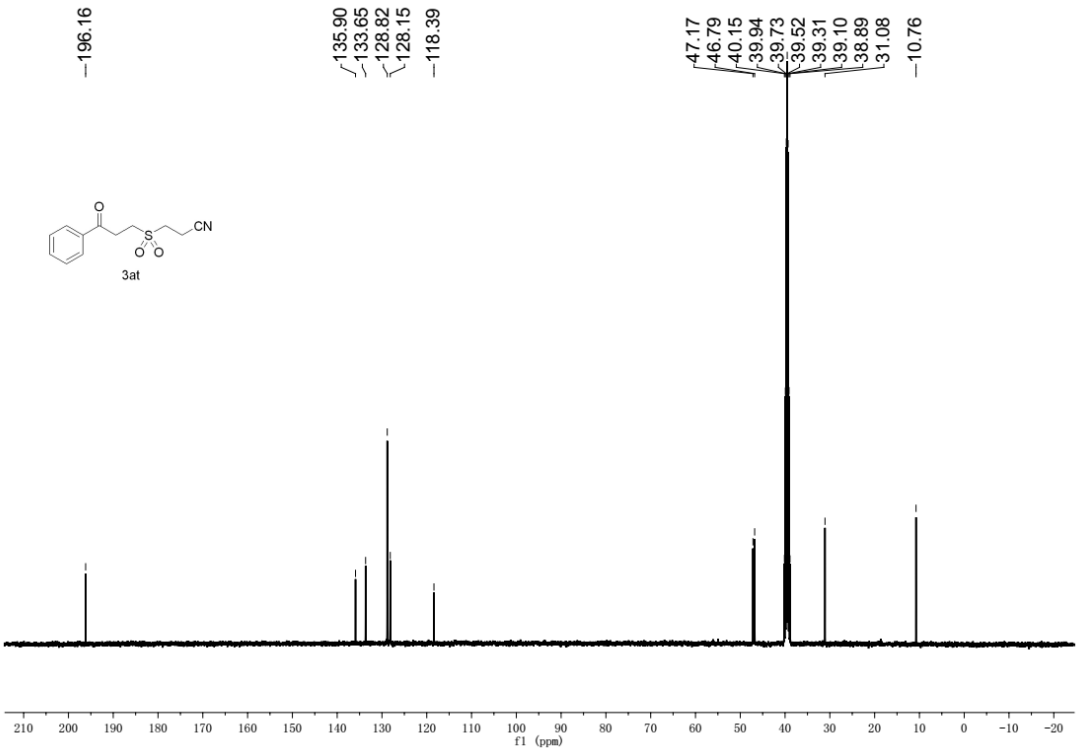
2.50
CN
3at
1.93
0.99
1.96
2.10
3.89
2.00
f1 (ppm)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128.15
118.39
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39.94
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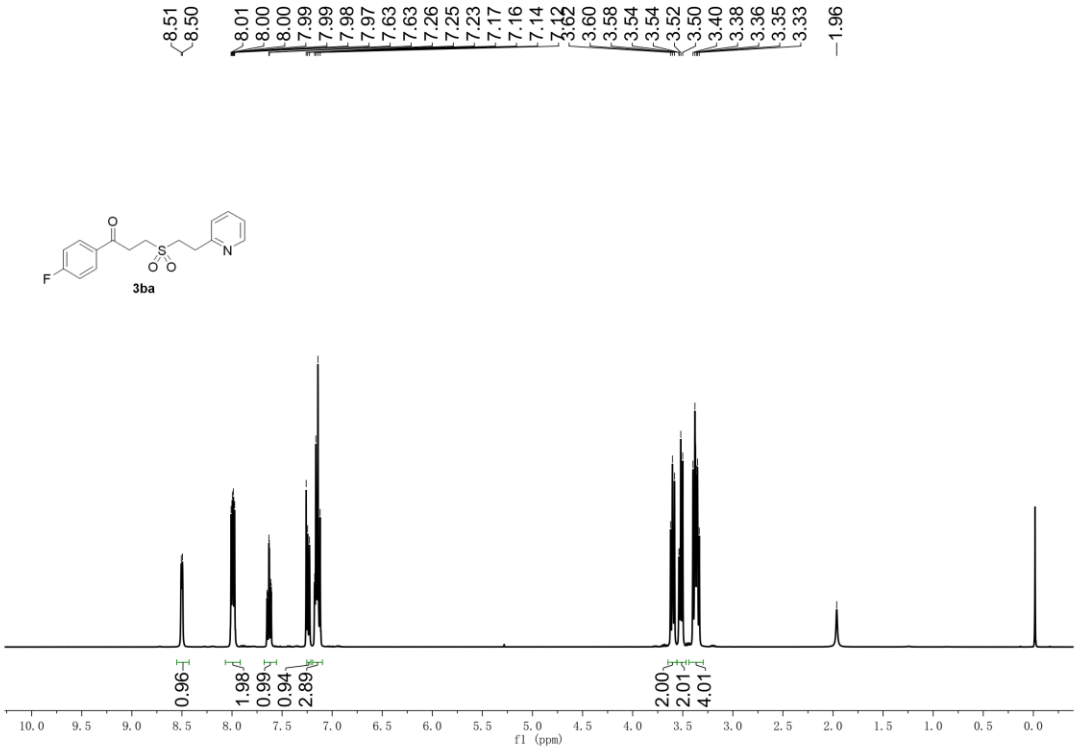
39.10
38.89
31.08
10.76
O
S
O
O
CN
3at
f1 (ppm)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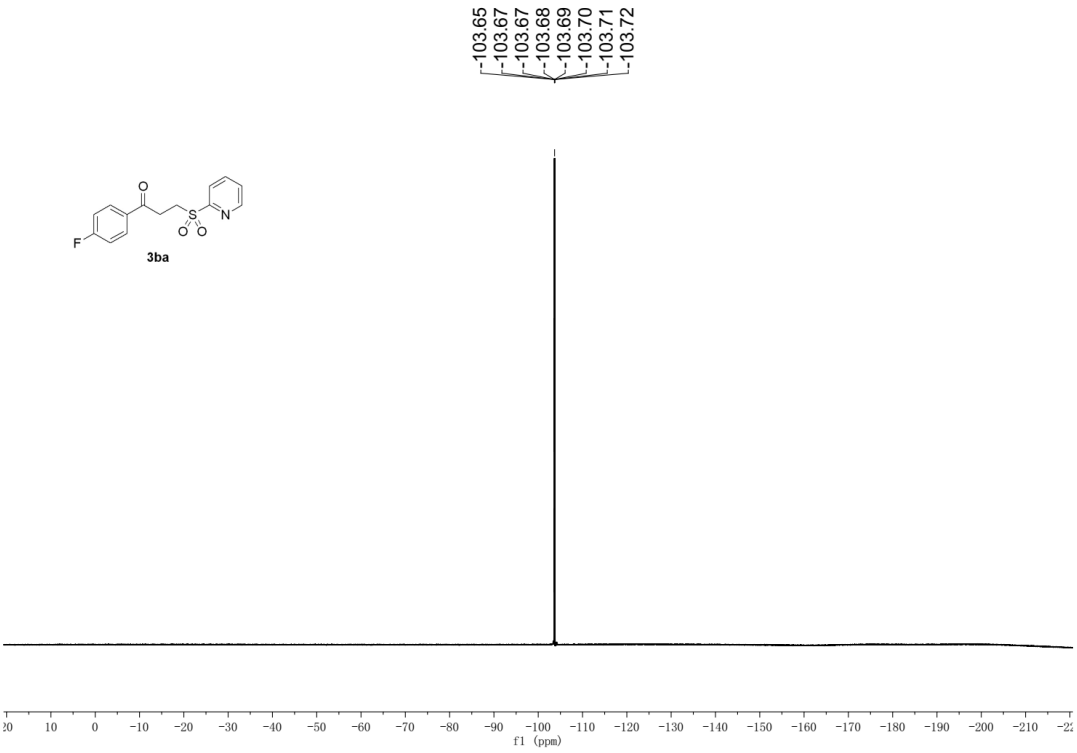
7.63
7.26
7.25
7.23
7.17
7.16
7.14
3.60
3.58
3.54
3.54
3.52
3.50
3.40
3.38
3.36
3.35
3.33
1.96
O
S
O
O
N
F
3ba
0.96
1.98
0.99
0.94
2.89
2.00
2.01
4.01
f1 (ppm)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-103.67
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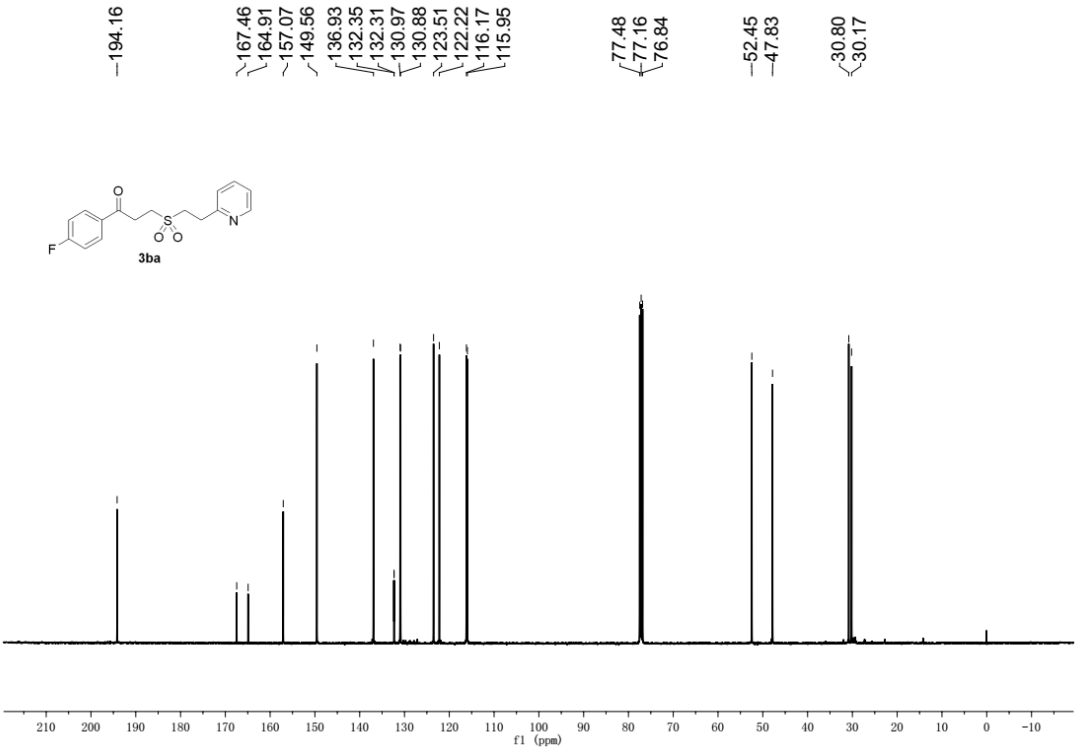
-103.69
-103.70
-103.71
-103.72
3ba
f1 (ppm)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132.31
130.97
130.88
123.51
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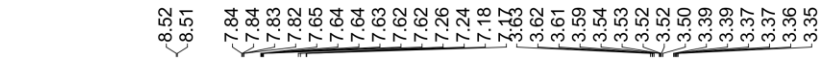
47.83
30.80
30.17
3ba
f1 (ppm)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7.63
7.62
7.62
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7.24
7.18
3.63
3.62
3.61
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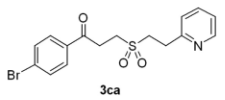
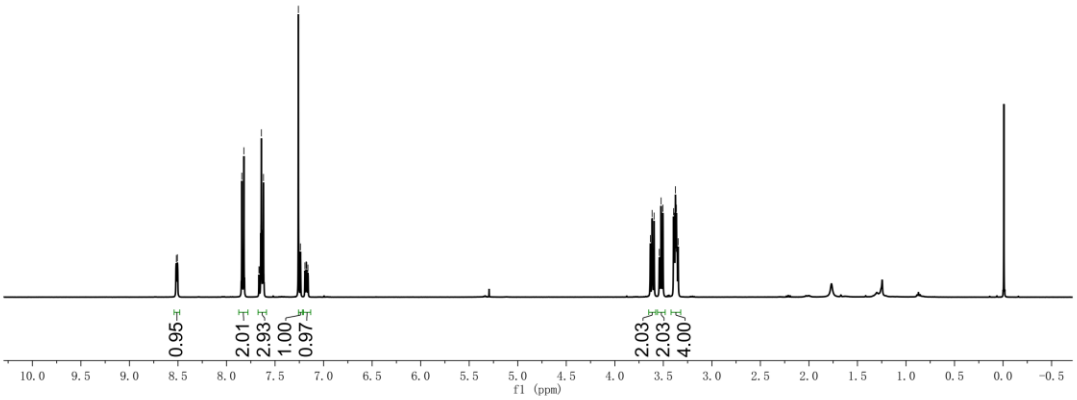
3.52
3.52
3.50
3.39
3.39
3.37
3.37
3.36
3.35


O
S
O
O
N
Br

3ca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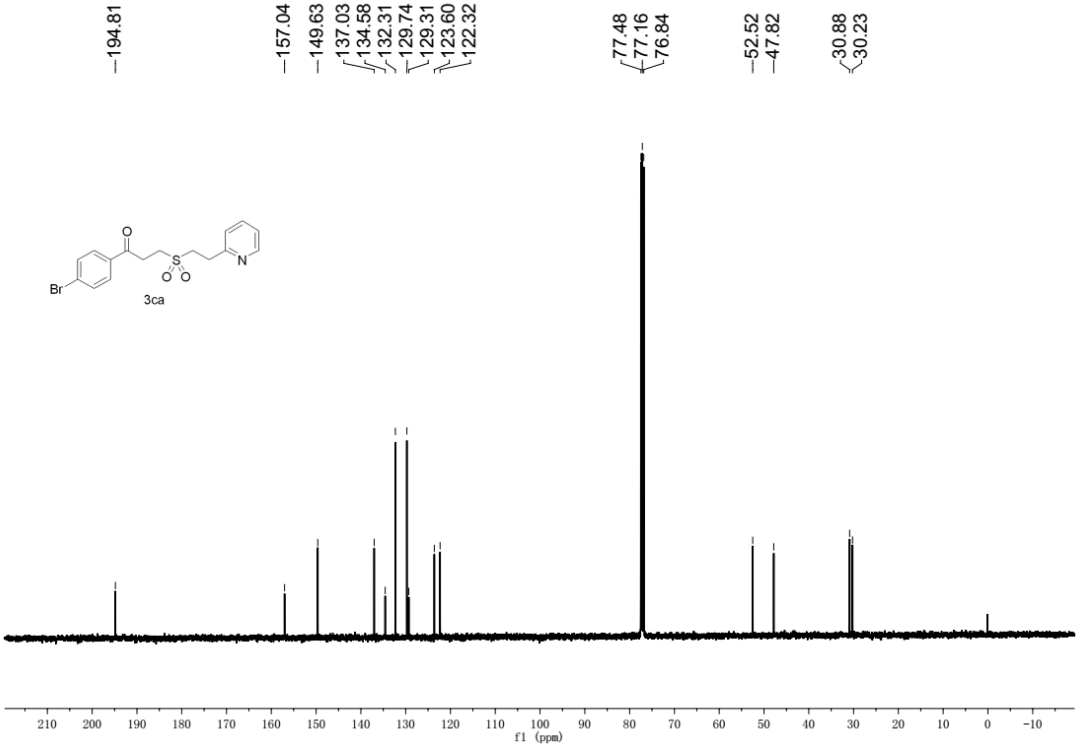
2.01
2.93
1.00
0.97
2.03
2.03
4.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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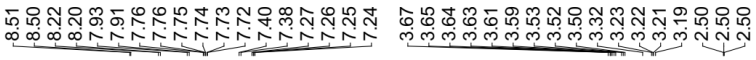
129.31
123.60
122.32
77.48
77.16
76.84
52.52
47.82
30.88
30.23
O
S
O
O
N
Br
3ca
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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7.76
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7.74
7.73
7.72
7.40
7.38
7.27
7.26
7.25
7.24
3.67
3.65
3.64
3.63
3.61
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3.50
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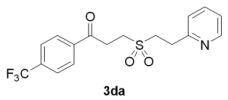
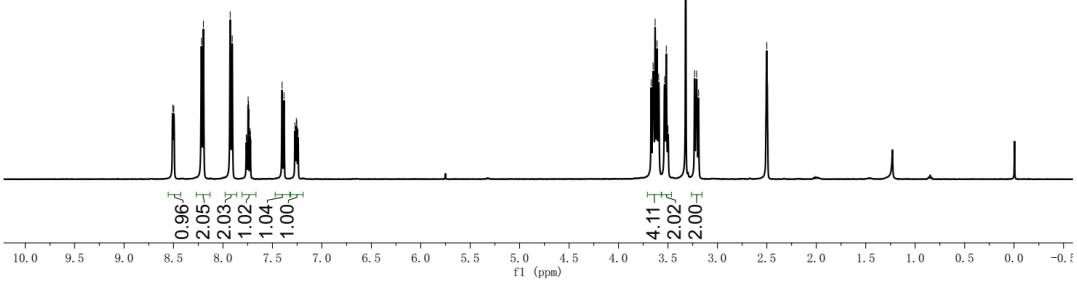
3.22
3.21
3.19
2.50
2.50
2.50


O
S
O
O
N
F3C

3da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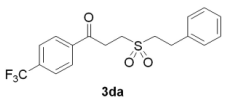
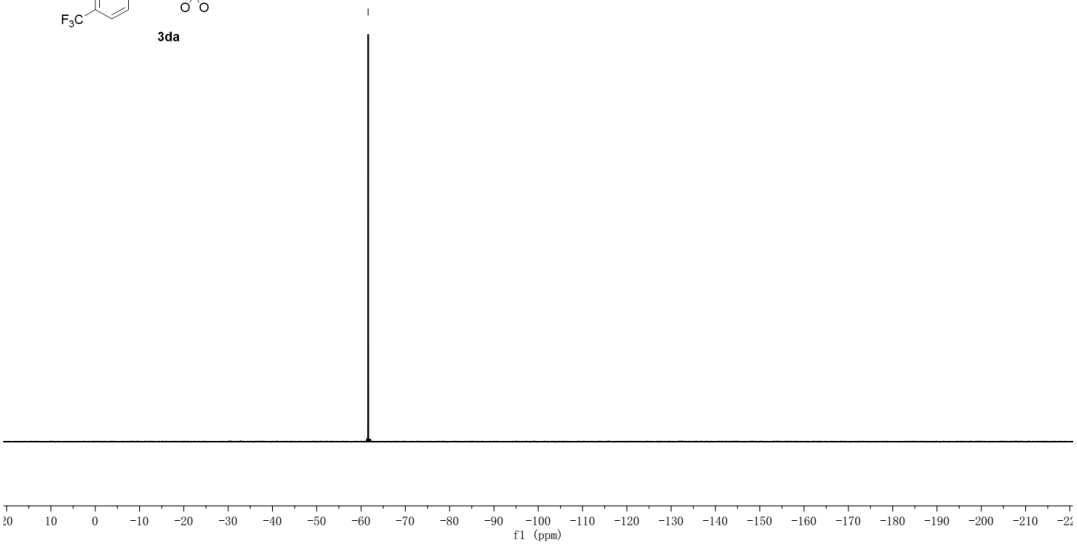
1.02
1.04
1.00
4.11
2.02
2.00
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


-61.60


O
S
O
O
F3C

3da


10
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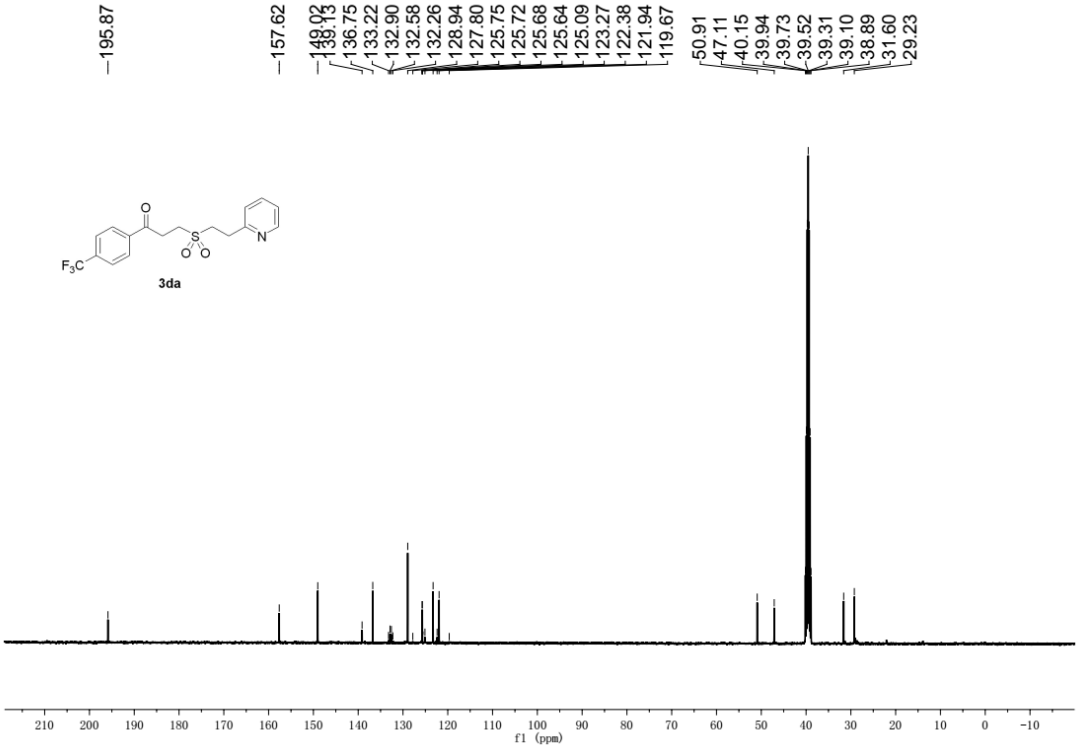
−50
−60
−70
−80
−90
−100
−110
−120
−130
−140
−150
−160
−170
−180
−190
−200
−210
f1 (ppm)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127.80
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125.72
125.68
125.64
125.09
123.27
122.38
121.94
119.67
50.91
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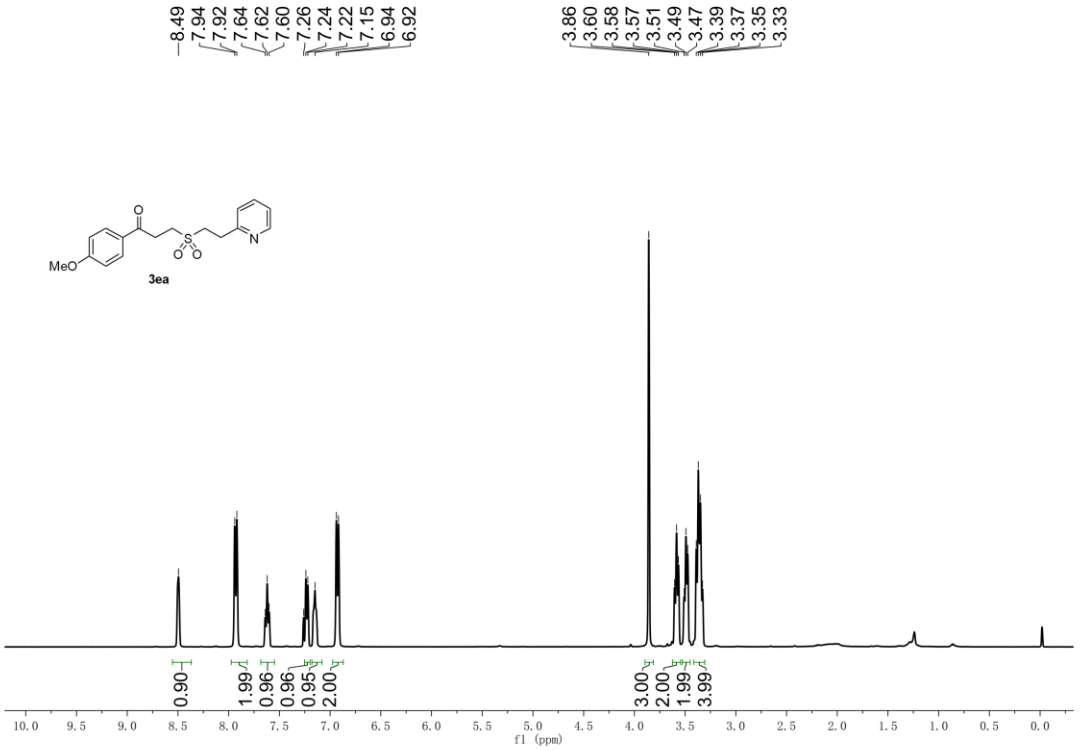
40.15
39.94
39.73
39.52
39.31
39.10
38.89
31.60
29.23
3da
f1 (ppm)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7.15
6.94
6.92
3.86
3.60
3.58
3.57
3.51
3.49
3.47
3.39
3.37
3.35
3.33
MeO
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0.95
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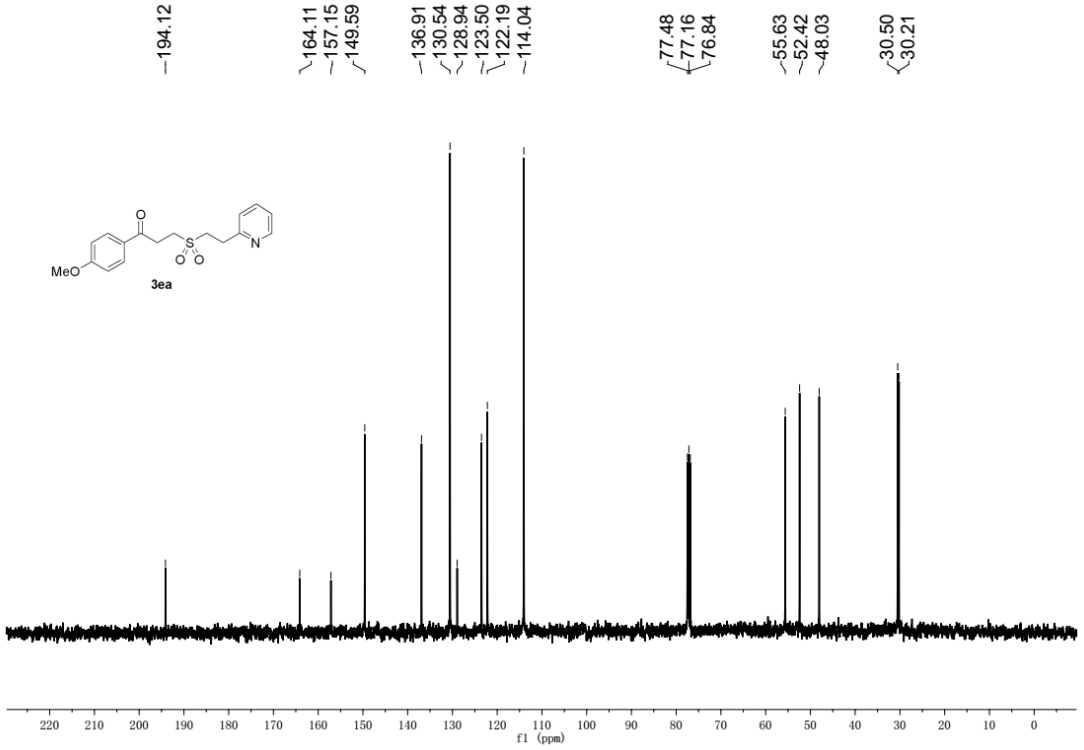
f1 (ppm)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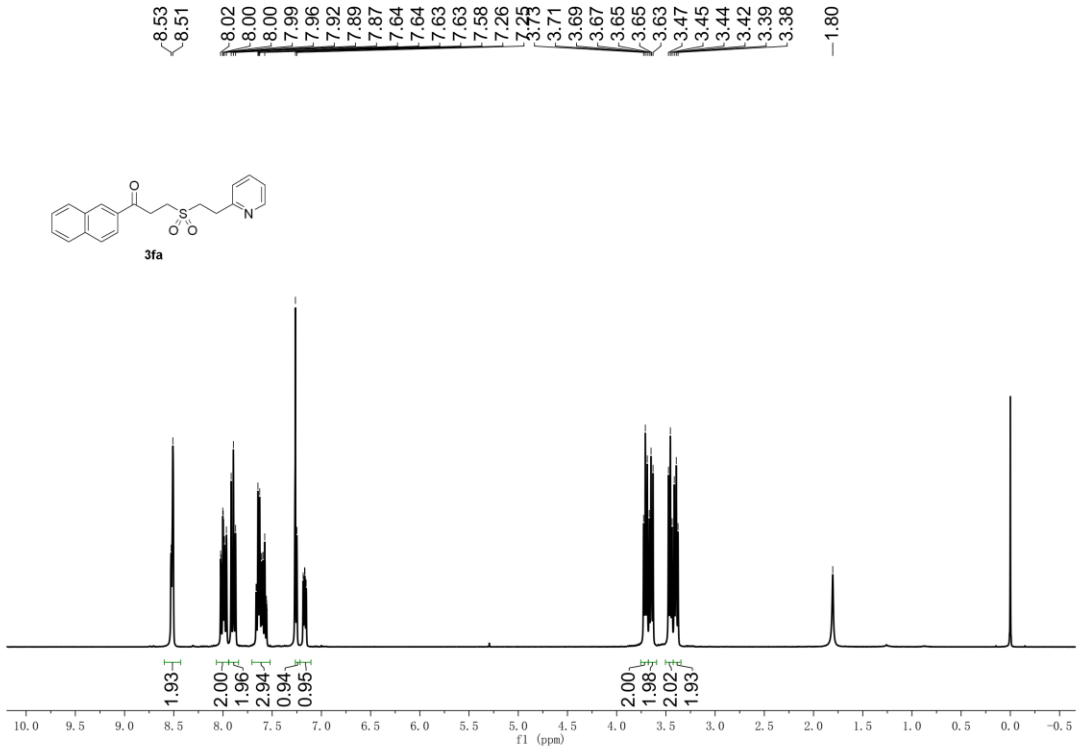
52.42
48.03
30.50
30.21
MeO
3ea
f1 (ppm)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7.63
7.63
7.58
7.26
3.73
3.71
3.69
3.67
3.65
3.65
3.63
3.47
3.45
3.44
3.42
3.39
3.38
1.80
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0.95
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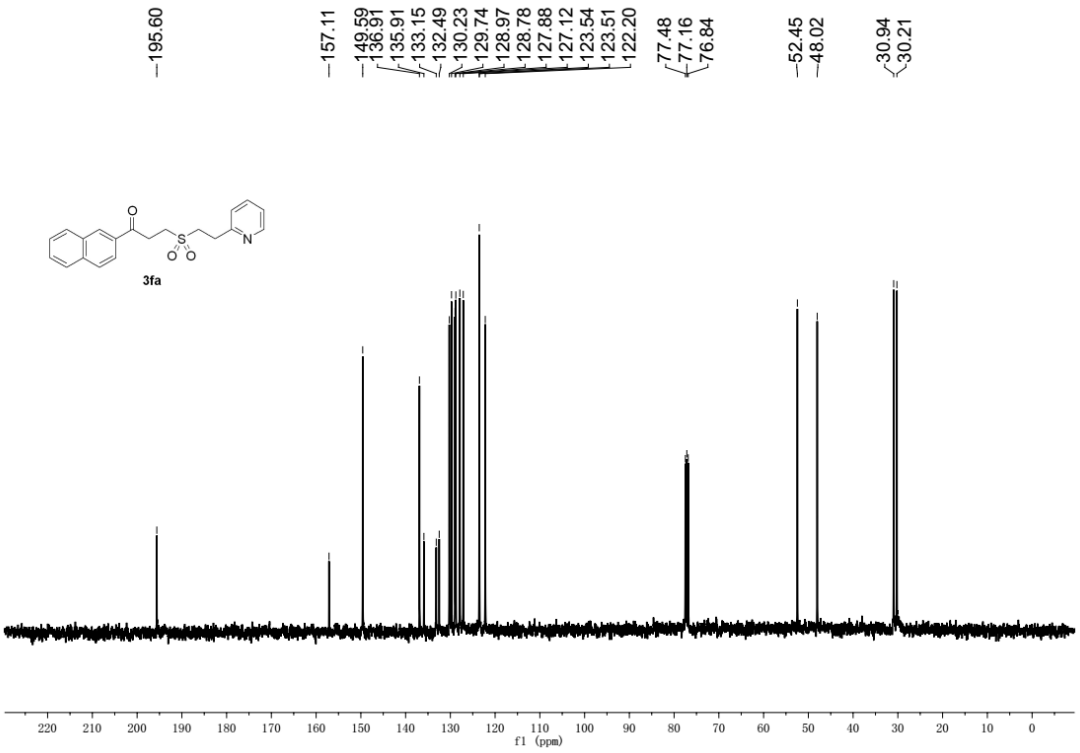
1.93
f1 (ppm)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127.12
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76.84
52.45
48.02
30.94
30.21
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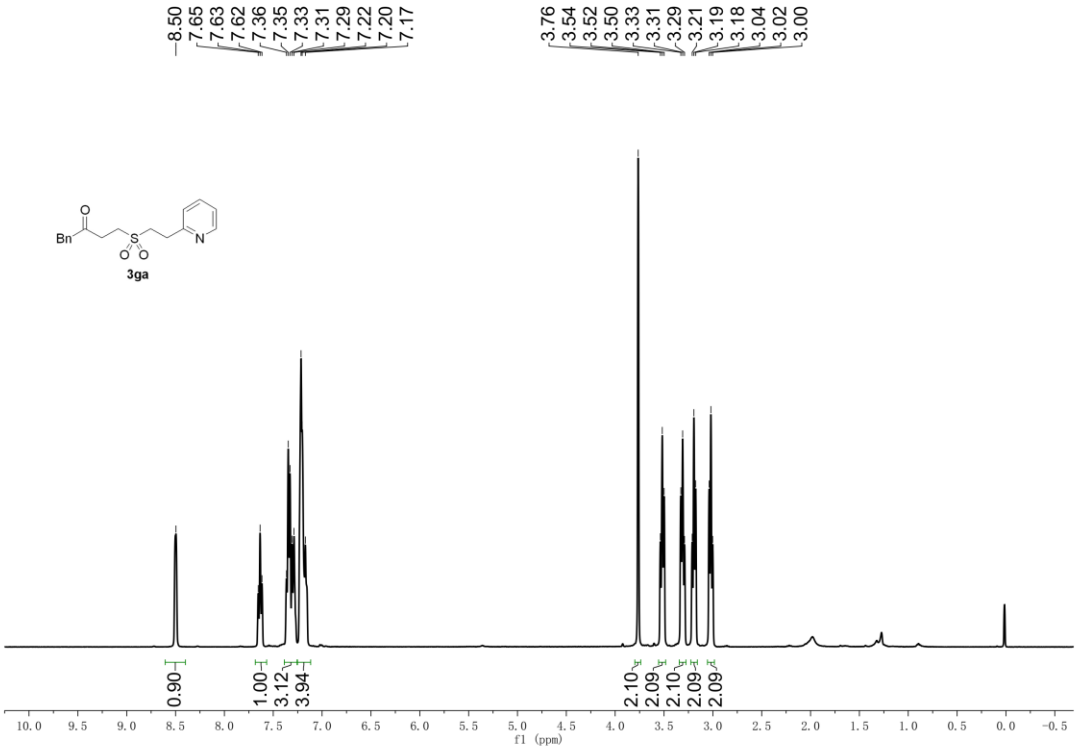
f1 (ppm)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7.35
7.33
7.31
7.29
7.22
7.20
7.17
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3.54
3.52
3.50
3.33
3.31
3.29
3.21
3.19
3.18
3.04
3.02
3.00
Bn
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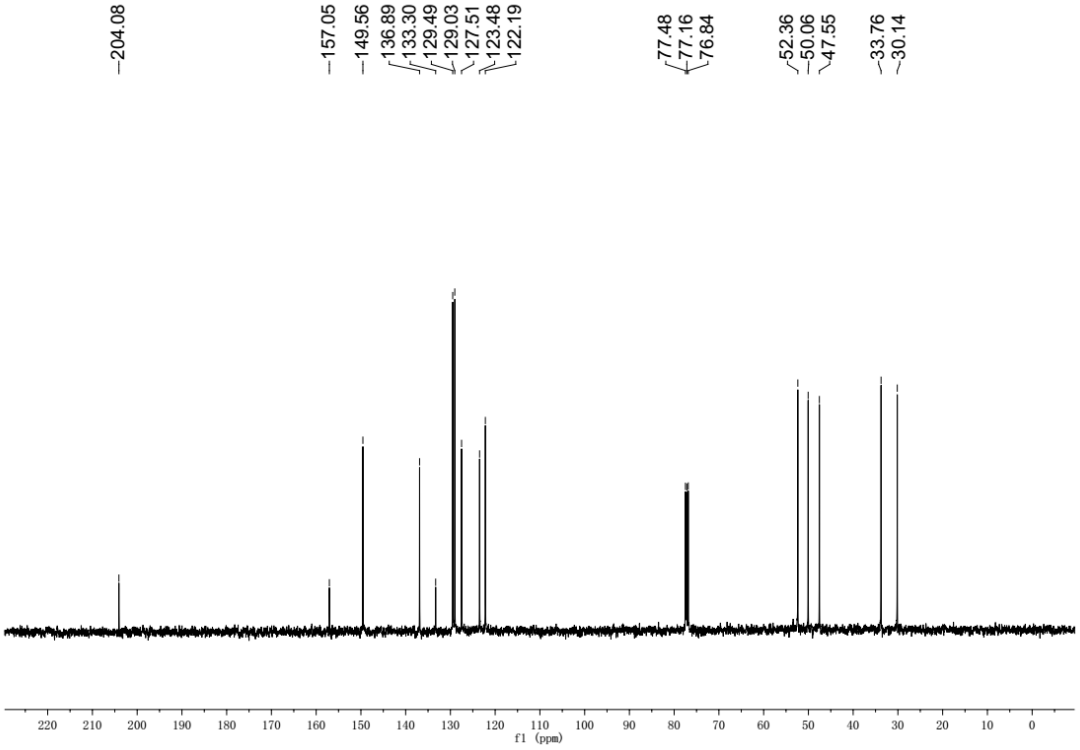
2.09
2.10
2.09
2.09
f1 (ppm)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50.06
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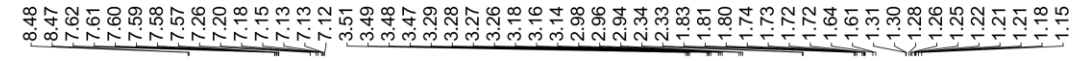
f1 (ppm)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7.15
7.13
7.13
7.12
3.51
3.49
3.48
3.47
3.29
3.28
3.27
3.26
3.18
3.16
3.14
2.98
2.96
2.94
2.34
2.33
1.83
1.81
1.80
1.74
1.73
1.72
1.72
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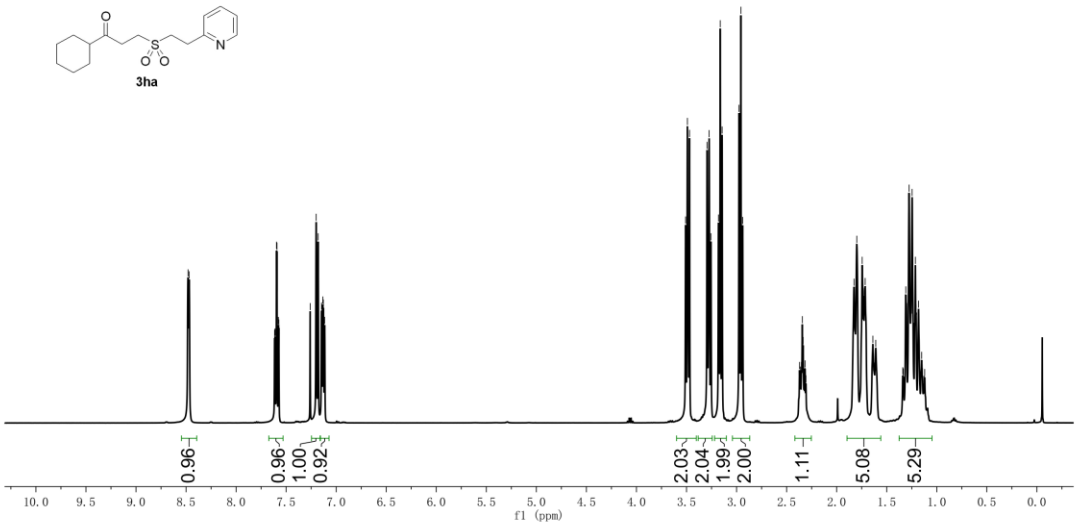
1.30
1.28
1.26
1.25
1.22
1.21
1.21
1.18
1.15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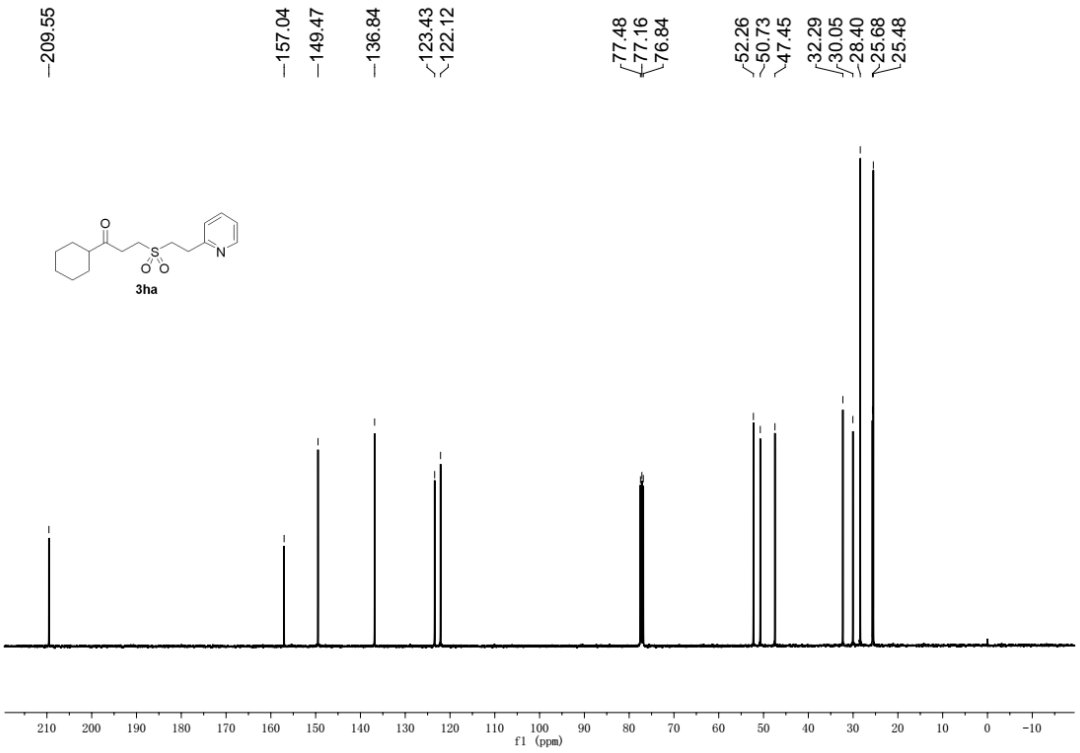
2.04
1.99
2.00
1.11
5.08
5.29
f1 (ppm)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77.16
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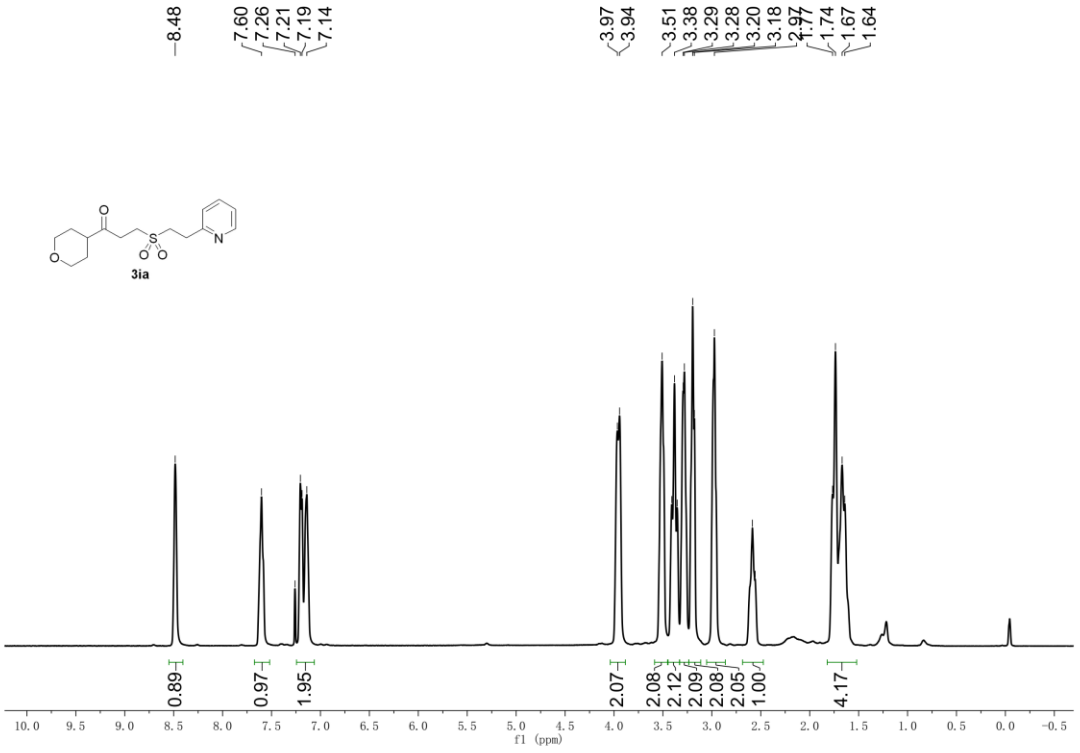
52.26
50.73
47.45
32.29
30.05
28.40
25.68
25.48
3ha
f1 (ppm)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7.26
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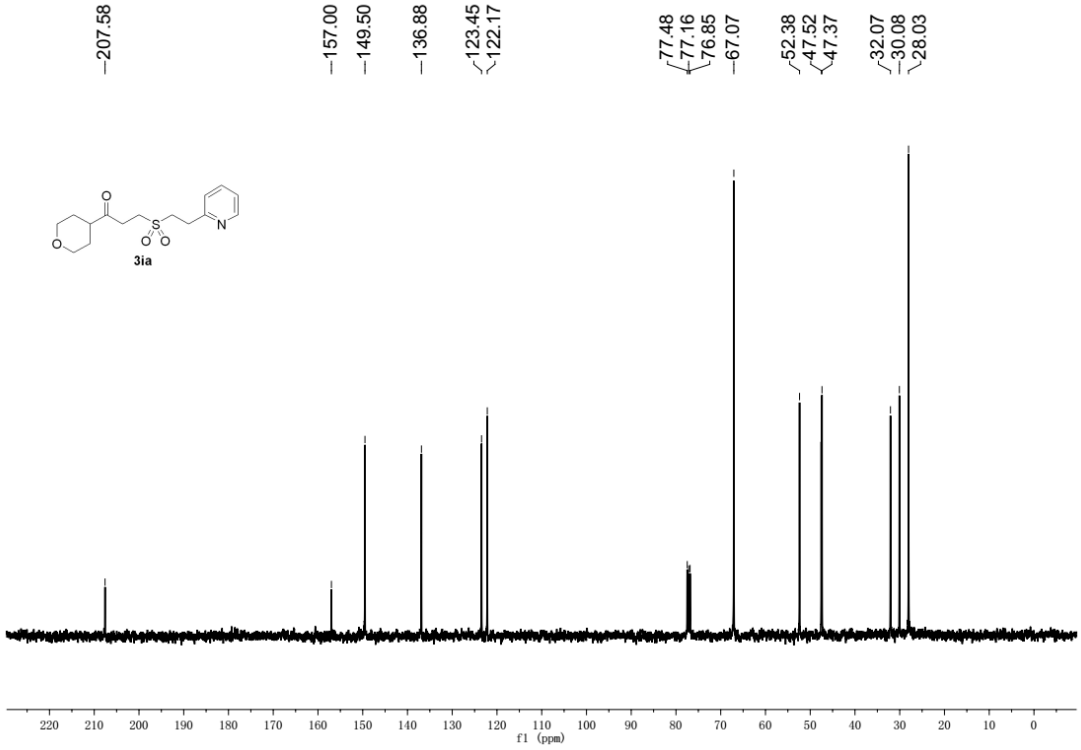
7.19
7.14
3.97
3.94
3.51
3.38
3.29
3.28
3.20
3.18
1.74
1.67
1.64
3ia
0.89
0.97
1.95
2.07
2.08
2.12
2.09
2.08
2.05
1.00
4.17
f1 (ppm)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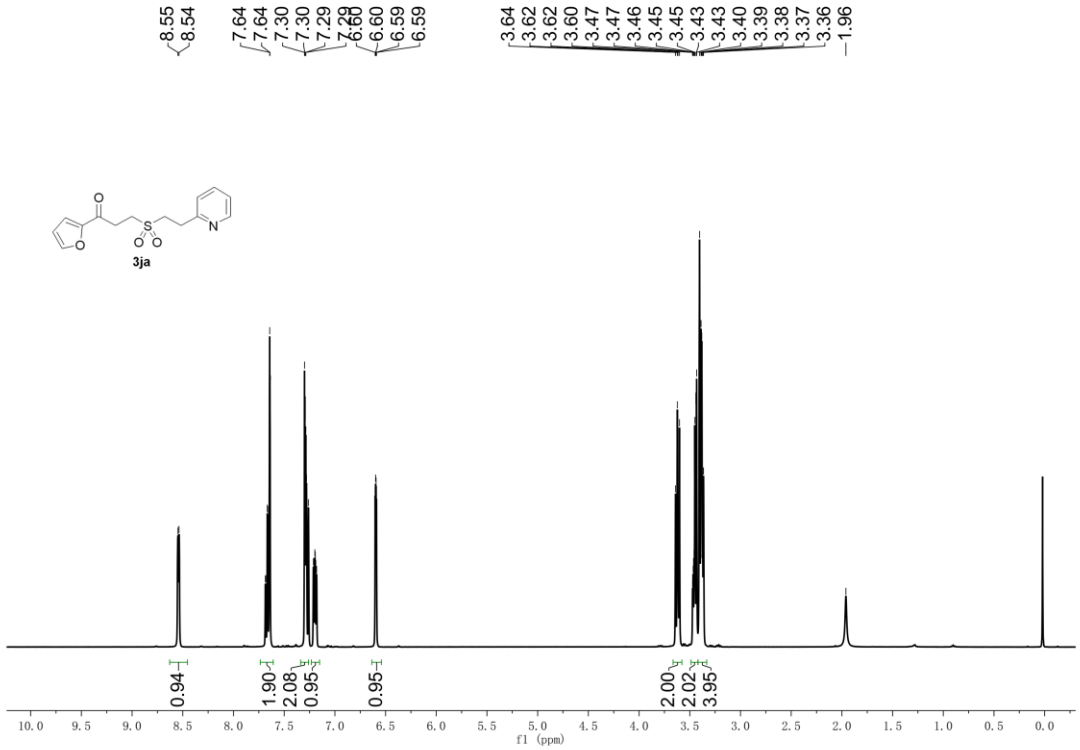
3ia
f1 (ppm)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6.59
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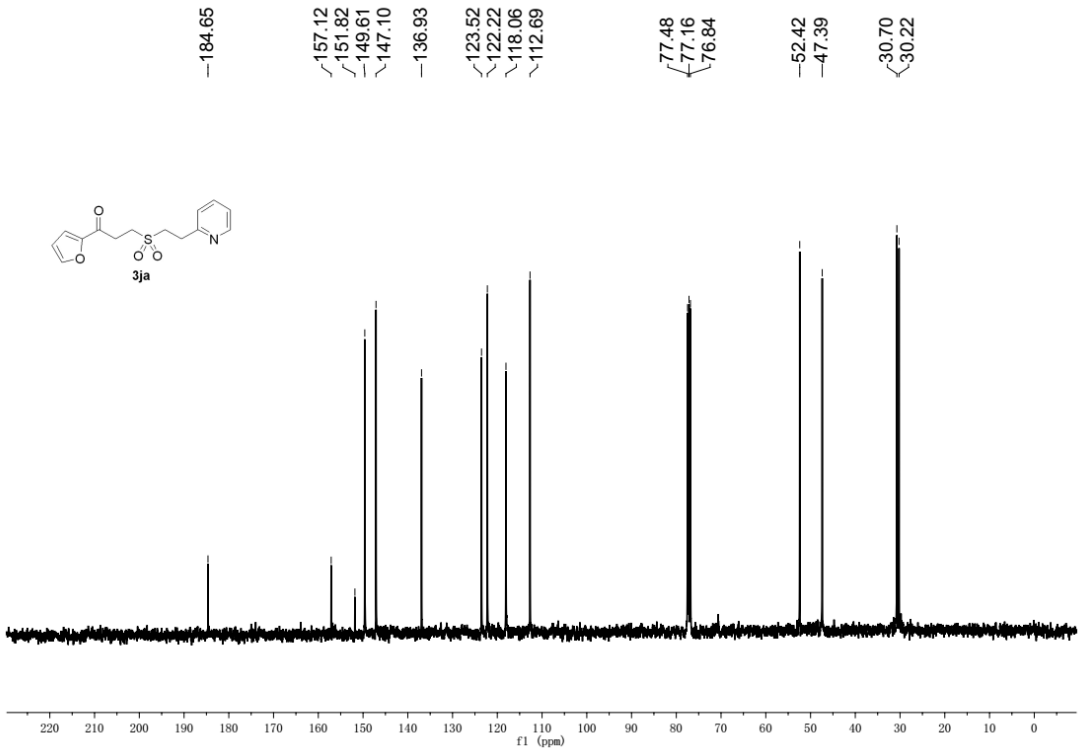
3.62
3.62
3.60
3.47
3.47
3.46
3.45
3.45
3.43
3.43
3.40
3.39
3.38
3.37
3.36
1.96
3ja
0.94
1.90
2.08
0.95
0.95
2.00
2.02
3.95
f1 (ppm)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47.39
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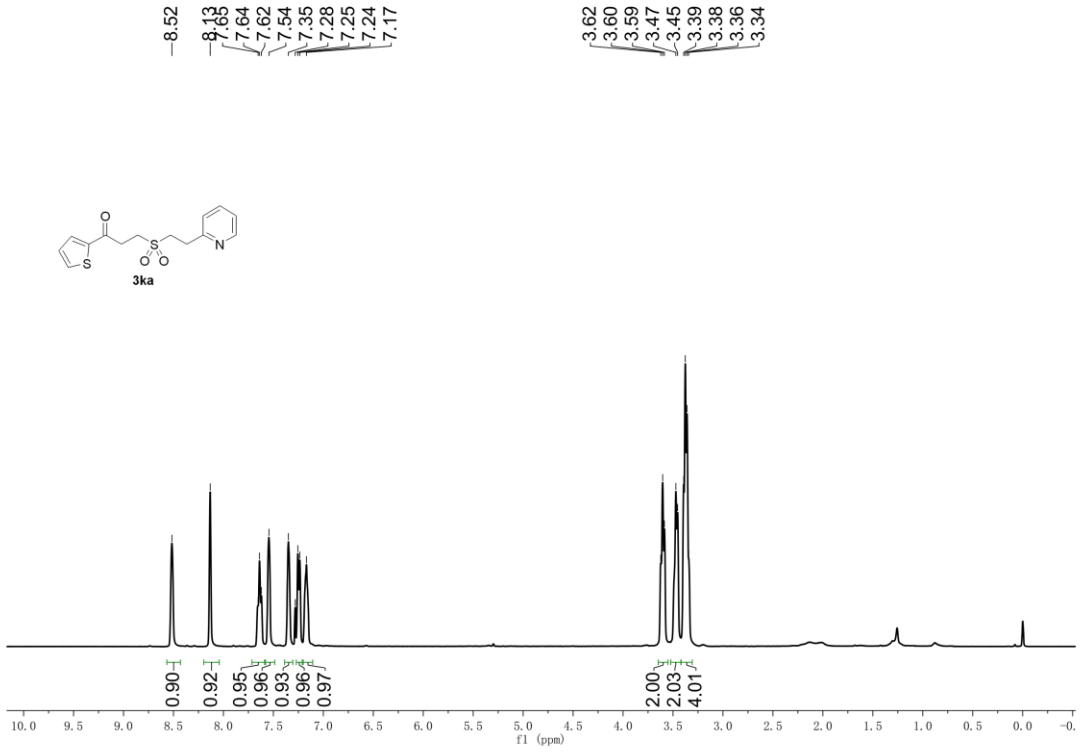
30.22
3ja
f1 (ppm)


8.52
8.13
7.65
7.64
7.62
7.54
7.35
7.28
7.25
7.24
7.17
3.62
3.60
3.59
3.47
3.45
3.39
3.38
3.36
3.34
3ka
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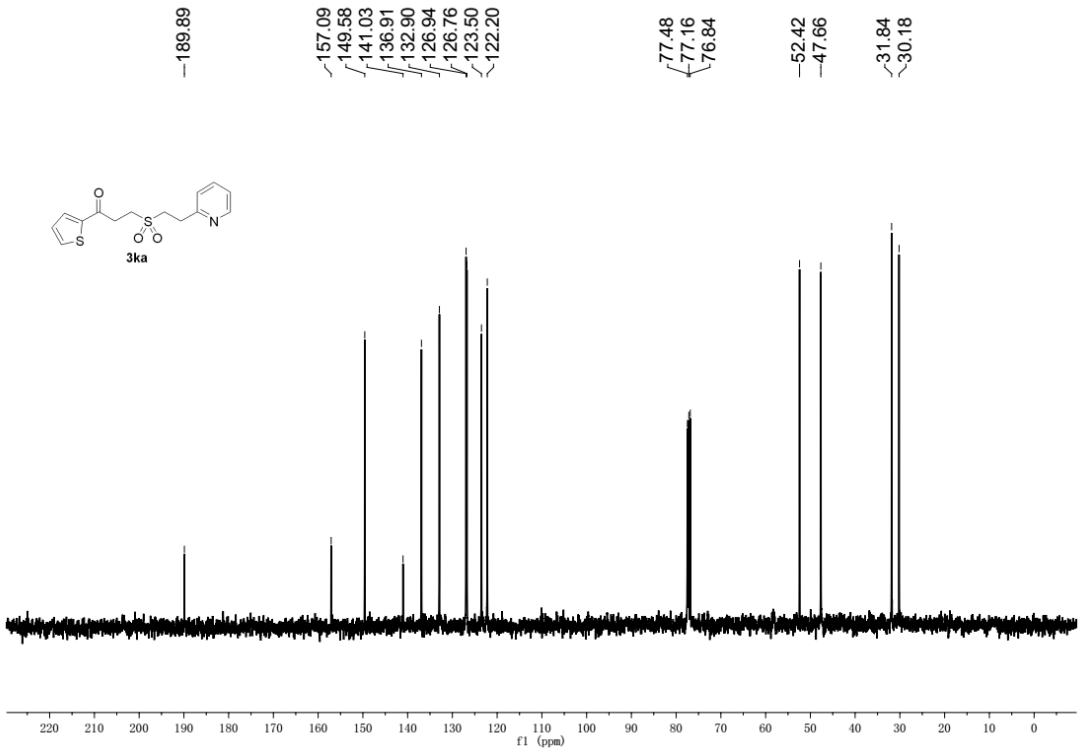
0.95
0.96
0.93
0.96
0.97
2.00
2.03
4.01
f1 (ppm)




X-ray diffraction analysis of **3aa**

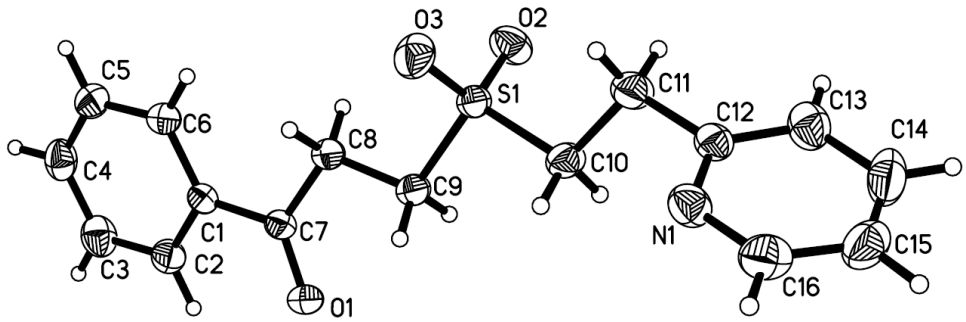



Table 1. Crystal data and structure refinement for ga_200108d_a.

| | |
|---|---|
| Identification code | ga_200108d_a |
| Empirical formula | C16 H21 N O5 S |
| Formula weight | 339.40 |
| Temperature | 296(2) K |

| | | |
|---|---|---|
| Wavelength | 1.34138 Å | |
| Crystal system | Monoclinic | |
| Space group | C2/c | |
| Unit cell dimensions | a = 19.9401(7) Å | a= 90°. |
| | b = 5.3894(2) Å | b= 101.506(2)°. |
| | c = 32.9348(13) Å | g = 90°. |
| Volume | 3468.2(2) $Å^3$ | |
| Z | 8 | |
| Density (calculated) | 1.300 $Mg/m^3$ | |
| Absorption coefficient | 1.222 $mm^{-1}$ | |
| F(000) | 1440 | |
| Crystal size | 0.430 x 0.200 x 0.100 $mm^3$ | |
| Theta range for data collection | 4.768 to 58.491°. | |
| Index ranges | -25<=h<=25, -6<=k<=6, -41<=l<=41 | |
| Reflections collected | 24549 | |
| Independent reflections | 3702 [R(int) = 0.0317] | |
| Completeness to theta = 53.594° | 99.1 % | |
| Absorption correction | Semi-empirical from equivalents | |
| Max. and min. transmission | 0.752 and 0.583 | |
| Refinement method | Full-matrix least-squares on $F^2$ | |
| Data / restraints / parameters | 3702 / 3 / 216 | |
| Goodness-of-fit on $F^2$ | 1.121 | |
| Final R indices [I>2sigma(I)] | R1 = 0.0585, wR2 = 0.1942 | |
| R indices (all data) | R1 = 0.0601, wR2 = 0.1979 | |
| Extinction coefficient | n/a | |

| | |
|---|---|
| Largest diff. peak and hole | 0.991 and -0.401 e.Å$^{-3}$ |