Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.

Autoinductive Thiolation/Oxygenation of Alkenes at Room Temperature

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Supporting Information

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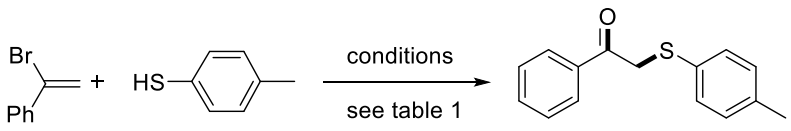
General information

All reactions were run under a dry air atmosphere with a dry air balloon fitted on a Schlenk tube. All glassware was oven dried at 110 °C for hours and cooled down under vacuum. All the solvents were purified according to the solvents handbook. Unless otherwise noted, materials were obtained from commercial suppliers and used without further purification. α-Bromostyrene derivatives and α-chlorostyrene derivatives were all prepared following literature procedures.[1] Thin layer chromatography (TLC) employed glass 0.25 mm silica gel plates. Flash chromatography columns were packed with 200-300 mesh silica gel in petroleum (bp. 60-90 °C). GC-MS spectra were recorded on a Varian GC-MS 3900-2100T or a Varian GCMS-QP2010SE. EPR spectra were recorded on a Bruker A-200 spectrometer. GC yields were recorded with a Varian GC 3900 gas chromatography instrument with a FID detector. IR spectra were recorded on a Mettler Toledo React IR TM 15 spectrometer using a diamond comb. All new compounds were characterized by ^{1}H NMR, ^{13}C NMR and HRMS. The known compounds were characterized by ^{1}H NMR, ^{13}C NMR. ^{1}H and ^{13}C NMR data were recorded with ADVANCE III 400 MHz with tetramethylsilane as an internal standard. High resolution mass spectra (HRMS) were measured with a Waters Micromass GCT instrument. All chemical shifts (δ) were reported in ppm and coupling constants (*J*) in Hz. All chemical shifts were reported relative to tetramethylsilane (0 ppm for ^{1}H), CD_3OD (3.31 ppm for ^{1}H), and $CDCl_3$ (77.16 ppm for ^{13}C), respectively.

Experimental section

1) Impact of reaction parameters

Table S1. Impact of Reaction Parameters[a]



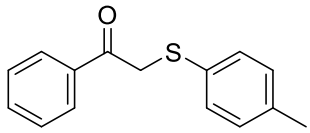
1a **2a** **3aa**

entry	solvent	conditions	yield (%)[b]
1	THF	1 atm of air	73
2	THF	1 atm of air	56[c]
3	CH_2Cl_2	1 atm of air	47
4	MeCN	1 atm of air	30
5	Toluene	1 atm of air	71
6	DMSO	1 atm of air	87

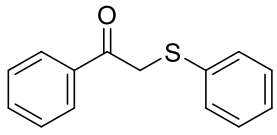
7	NMP	1 atm of air	74
8	H_2O	1 atm of air	69
9	DMF/H_2O (1:1)	1 atm of air	58
10	DMF	1 atm of air	89
11	DMF	1 atm of air	26[d]
12	DMF	1 atm of O_2	93
13	DMF	1 atm of N_2	trace
14	**DMF**	**1 atm of air**	**93 (83)[e]**

[a]Unless otherwise specified, all reactions were carried out using **1a** (0.2 mmol), **2a** (0.6 mmol), in solvent (4.0 mL) at room temperature for 1 h. [b]Yield was determined by ^{1}H NMR analysis using diphenylmethane as internal standard, isolated yield in parenthesis. [c]**2a** (0.4 mmol). [d]**2a** (0.2 mmol). [e]DMF (2.0 mL).

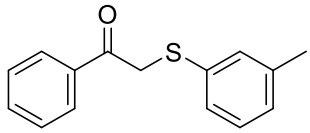
2) Procedure and analytical data of compounds 3aa-3ga.



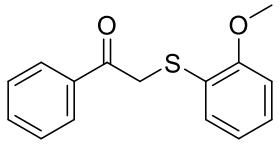
1-phenyl-2-(*p*-tolylthio)ethan-1-one (3aa).[2a] Typical procedure: To an oven-dried Schlenk tube equipped with a stir bar was added *p*-toluenethiol (**2a**, 0.60 mmol), and a balloon filled with dry air was connected to the Schlenk tube through the side arm and purged one time. Then, α-bromostyrene (0.20 mmol), and DMF (2.0 mL) were successively injected in the reaction tube with magnetic stirring. The reaction mixture was allowed to stir vigorously at room temperature in a warm room for 1 h. Thereafter, water was added and the mixture was extracted with ethyl acetate (x 4). The combined organic layers were dried on Na_2SO_4 and concentrated under reduced pressure. The resulting crude product was separated on a silica gel column with petroleum ether and ethyl acetate as eluent to afford the desired product. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.92-7.94 (m, 2H), 7.57 (dt, *J* = 8.8, 1.2 Hz, 1H), 7.45 (t, *J* = 8.0 Hz, 2H), 7.29 (d, *J* = 8.4 Hz, 2H), 7.09 (t, *J* = 7.6 Hz, 2H), 4.21 (s, 2H) 2.31 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 194.3, 137.7, 135.5, 133.5, 131.7, 130.9, 130.0, 128.8, 128.7, 42.0, 21.2.



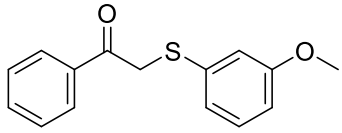
1-phenyl-2-(phenylthio)ethan-1-one (3ab):[2a] The synthesis procedure is the same as for **3aa**. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.93 (d, *J* = 7.6 Hz, 2H), 7.56 (t, *J* = 7.2 Hz, 1H), 7.45 (t, *J* = 7.6 Hz, 2H), 7.38 (d, *J* = 7.6 Hz, 2H), 7.27 (t, *J* = 7.4 Hz, 2H), 7.21 (t, *J* = 7.2 Hz, 1H), 4.27 (s, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 194.1, 135.4, 134.8, 133.6, 130.5, 129.1, 128.8, 127.2, 41.3.



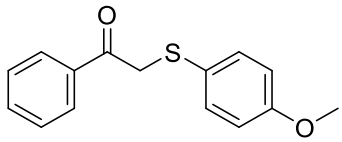
1-phenyl-2-(*m*-tolylthio)ethan-1-one (3ac): The synthesis procedure is the same as for **3aa**. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.93 (m, 2H), 7.57 (t, *J* = 7.4 Hz, 1H), 7.45 (t, *J* = 7.6 Hz, 2H), 7.14-7.20 (m, 3H), 7.02 (d, *J* = 6.0 Hz, 1H), 4.26 (s, 2H) 2.29 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 194.2, 138.9, 135.5, 134.6, 133.5, 131.2, 129.0, 128.7 (7), 128.7 (5), 128.1, 127.5, 41.3, 21.4. HRMS (ESI+) calculated for $C_{15}H_{15}OS$ (M+H): 243.0844; found: 243.0842.



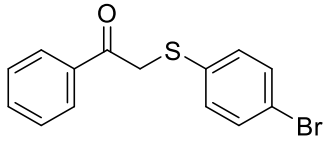
2-((2-methoxyphenyl)thio)-1-phenylethan-1-one (3ad): The synthesis procedure is the same as for **3aa**. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.94 (d, *J* = 7.6 Hz, 2H), 7.56 (t, *J* = 7.6 Hz, 1H), 7.44 (t, *J* = 7.2 Hz, 2H), 7.34 (dd, *J* = 7.6, 0.9 Hz, 1H), 7.25 (t, *J* = 7.8 Hz, 1H), 6.84-6.89 (m, 2H), 4.22 (s, 2H) 3.83 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 194.6, 158.4, 135.7, 133.4, 132.7, 129.2, 128.7, 128.6 (7), 122.1, 121.1, 110.8, 55.8, 39.6. HRMS (ESI+) calculated for $C_{15}H_{15}O_2S$ (M+H): 259.0793; found: 259.0785.



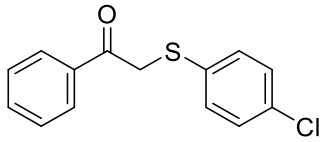
2-((3-methoxyphenyl)thio)-1-phenylethan-1-one (3ae): The synthesis procedure is the same as for **3aa**. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.94-7.96 (m, 2H), 7.58 (t, *J* = 7.4 Hz, 1H), 7.46 (t, *J* = 7.6 Hz, 2H), 7.19 (t, *J* = 8.0 Hz, 1H), 6.96 (ddd, *J* = 7.8, 1.6, 0.6 Hz, 1H), 6.93 (t, *J* = 2.0 Hz, 1H), 6.76 (ddd, *J* = 8.0, 2.4, 0.6 Hz, 1H), 4.29 (s, 2H) 3.77 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 194.2, 159.9, 136.2, 135.5, 133.6, 130.0, 128.8 (1), 128.8 (0), 122.4, 115.5, 113.0, 55.4, 41.2. HRMS (ESI+) calculated for $C_{15}H_{15}O_2S$ (M+H): 259.0793; found: 259.0788.



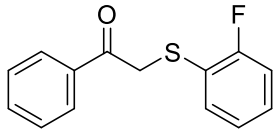
2-((4-methoxyphenyl)thio)-1-phenylethanone (3af).[2b] The synthesis procedure is the same as for **3aa**. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.93-7.90 (m, 2H), 7.57 (t, *J* = 7.4 Hz, 1H), 7.45 (t, *J* = 7.6 Hz, 2H), 7.35 (d, *J* = 8.8 Hz, 2H), 6.82 (d, *J* = 8.8 Hz, 2H), 4.13 (s, 2H), 3.78 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 194.4, 159.8, 135.6, 134.8, 133.4, 128.8, 128.7, 124.6, 114.8, 55.4, 42.9.



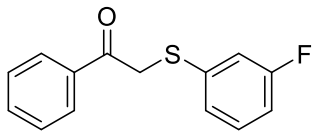
2-((4-bromophenyl)thio)-1-phenylethan-1-one (3ag).[2a] The synthesis procedure is the same as for **3aa**. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.99-7.89 (m, 2H), 7.58 (t, *J* = 7.2 Hz, 1H), 7.46 (t, *J* = 7.6 Hz, 2H), 7.38 (d, *J* = 8.6 Hz, 2H), 7.24 (d, *J* = 8.6 Hz, 2H), 4.25 (s, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 193.8, 135.3, 133.9, 133.7, 132.2, 132.0, 128.8, 128.7, 121.2, 41.1.



2-((4-chlorophenyl)thio)-1-phenylethan-1-one (3ah).[2c] The synthesis procedure is the same as for **3aa**. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.92-7.95 (m, 2H), 7.59 (t, *J* = 7.4 Hz, 1H), 7.47 (t, *J* = 7.6 Hz, 2H), 7.32 (d, *J* = 8.4 Hz, 2H), 7.24 (d, *J* = 8.4 Hz, 2H), 4.25 (s, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 193.9, 135.3, 133.7, 133.4, 133.3, 132.1, 129.3, 128.9, 128.8, 41.3.

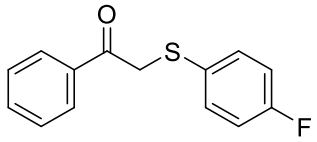


2-((2-fluorophenyl)thio)-1-phenylethan-1-one (3ai). The synthesis procedure is the same as for **3aa**. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.93 (m, 2H), 7.58 (tt, *J* = 7.4, 1.2 Hz, 1H), 7.45 (t, *J* = 7.0 Hz, 2H), 7.40 (dt, *J* = 7.6, 1.2 Hz, 1H), 7.23-7.29 (m, 1H), 7.04-7.09 (m, 2H), 4.28 (s, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 193.9, 162.1 (d, $^{1}J_{C\text{-}F}$ = 247.2 Hz), 135.4, 133.9 (d, $^{4}J_{C\text{-}F}$ = 1.3 Hz), 133.6, 129.9 (d, $^{3}J_{C\text{-}F}$ = 8.0 Hz), 128.8, 128.7, 124.7 (d, $^{3}J_{C\text{-}F}$ = 3.7 Hz), 121.3 (d, $^{2}J_{C\text{-}F}$ = 17.7 Hz), 116.0 (d, $^{2}J_{C\text{-}F}$ = 22.5 Hz), 40.5 (d, $^{4}J_{C\text{-}F}$ = 2.7 Hz). HRMS (ESI+) calculated for $C_{14}H_{12}OSF$ (M+H): 246.0593; found: 247.0591.

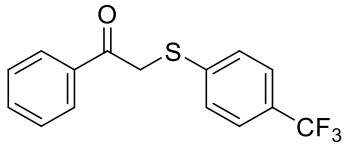


2-((3-fluorophenyl)thio)-1-phenylethan-1-one (3aj). The synthesis procedure is the same as for **3aa**. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.96 (d, *J* = 8.4 Hz, 2H), 7.60 (tt, *J* = 7.4, 1.2 Hz, 1H), 7.48 (t, *J* = 6.8 Hz, 2H), 7.24 (ddd, *J* = 8.0, 8.0, 2.0 Hz, 1H), 7.14 (ddd, *J* = 7.6, 1.6, 0.8 Hz, 1H), 7.14 (dt,

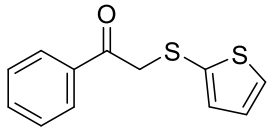
J = 9.2, 2.4 Hz, 1H), 6.90 (ddt, J = 8.4, 2.4, 0.8 Hz, 1H), 4.32 (s, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 193.7, 162.8 (d, $^{1}J_{C\text{-}F}$ = 249.4 Hz), 137.4 (d, $^{3}J_{C\text{-}F}$ = 7.9 Hz), 135.3, 133.8, 130.4 (d, $^{3}J_{C\text{-}F}$ = 8.6 Hz), 128.9, 128.8, 125.3 (d, $^{4}J_{C\text{-}F}$ = 3.0 Hz), 116.6 (d, $^{2}J_{C\text{-}F}$ = 23.2 Hz), 113.9 (d, $^{2}J_{C\text{-}F}$ = 21.3 Hz), 40.8. HRMS (ESI+) calculated for $C_{14}H_{12}OSF$ (M+H): 246.0593; found: 247.0587.



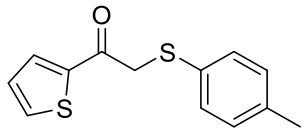
2-((4-fluorophenyl)thio)-1-phenylethan-1-one (3ak).[2d] The synthesis procedure is the same as for **3aa**. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.91-7.93 (m, 2H), 7.59 (tt, J = 7.2, 0.9 Hz, 1H), 7.46 (t, J = 7.6 Hz, 2H), 7.36-7.41 (m, 2H), 6.98 (tt, J = 8.6, 2.0 Hz, 2H), 4.20 (s, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 194.1, 162.6 (d, $^{1}J_{C\text{-}F}$ = 248.9 Hz), 135.4, 134.1(d, $^{3}J_{C\text{-}F}$ = 8.3 Hz), 133.7, 129.5 (d, $^{4}J_{C\text{-}F}$ = 3.4 Hz), 128.8, 116.4 (d, $^{2}J_{C\text{-}F}$ = 22.0 Hz), 42.2.



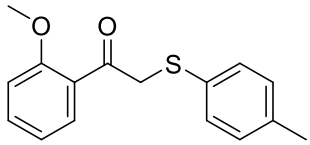
1-phenyl-2-((4-(trifluoromethyl)phenyl)thio)ethan-1-one (3al). The synthesis procedure is the same as for **3aa**. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.97 (d, J = 7.2 Hz, 2H), 7.61 (tt, J = 7.2, 0.9 Hz, 1H), 7.47-7.53 (m, 4H), 7.43 (d, J = 8.4 Hz, 2H), 4.37 (s, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 193.5, 140.5, 135.2, 134.0, 129.0, 128.8, 128.6, 128.5 (q, $^{2}J_{C\text{-}F}$ = 32.8 Hz), 125.9 (q, $^{3}J_{C\text{-}F}$ = 3.8 Hz), 124.1 (q, $^{1}J_{C\text{-}F}$ = 272.9 Hz), 39.9. HRMS (ESI+) calculated for $C_{15}H_{12}SOF_3$ (M+H): 297.0561; found: 297.0554.



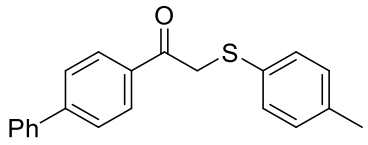
1-phenyl-2-(thiophen-2-ylthio)ethan-1-one (3am). The synthesis procedure is the same as for **3aa**. ^{1}H NMR (400 MHz, CD3OD) δ 7.92-7.94 (m, 2H), 7.58-7.63 (m, 1H), 7.45-7.50 (m, 3H), 7.08 (dd, J = 3.6, 0.8 Hz, 1H), 6.96 (dd, J = 5.2, 3.6 Hz, 1H), 4.22 (s, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 194.0, 135.5, 133.6, 132.2, 130.8, 128.8, 128.7, 127.8, 45.5. HRMS (ESI+) calculated for $C_{12}H_{13}S_2O$ (M+H): 235.0251; found: 235.0238.



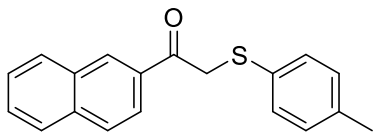
1-phenyl-2-(thiophen-2-ylthio)ethan-1-one (3ba).[2e] The synthesis procedure is the same as for **3aa**. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.68 (dd, *J* = 4.0, 1.2 Hz, 1H), 7.65 (dd, *J* = 5.0, 1.0 Hz, 1H), 7.32 (d, *J* = 8.0 Hz, 2H), 7.08-7.12 (m, 3H), 4.09 (s, 2H), 2.31 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 187.6, 142.6, 137.8, 134.4, 133.0, 131.7, 130.9, 130.0, 128.3, 42.5, 21.2.



1-(2-methoxyphenyl)-2-(*p*-tolylthio)ethan-1-one (3ca). The synthesis procedure is the same as for **3aa**. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.71 (dd, *J* = 7.6, 1.2 Hz, 1H), 7.45 (ddd, *J* = 8.4, 7.6, 2.0 Hz, 1H), 7.22 (d, *J* = 8.4 Hz, 2H), 7.04 (d, *J* = 8.0 Hz, 2H), 7.00 (dt, *J* = 7.6, 0.8 Hz, 1H), 6.93 (d, *J* = 8.4 Hz, 1H), 4.26 (s, 2H), 3.86 (s, 3H), 2.28 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 196.2, 158.6, 136.8, 134.1, 131.8, 131.3, 130.7, 129.7, 126.3, 120.9, 111.5, 55.6, 46.4, 21.1. HRMS (ESI+) calculated for $C_{16}H_{17}SO_2$ (M+H): 273.0949; found: 273.0946.

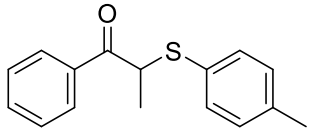


1-([1,1'-biphenyl]-4-yl)-2-(*p*-tolylthio)ethan-1-one (3da). The synthesis procedure is the same as for **3aa**. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.00 (d, *J* = 8.4 Hz, 2H), 7.66 (d, *J* = 8.4 Hz, 2H), 7.61 (d, *J* = 7.2 Hz, 2H), 7.47 (t, *J* = 7.2 Hz, 2H), 7.40 (tt, *J* = 7.2, 0.9 Hz, 1H), 7.31 (d, *J* = 8.0 Hz, 2H), 7.09 (d, *J* = 8.0 Hz, 2H), 4.22 (s, 2H), 2.31 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 193.9, 146.1, 139.8, 137.6, 134.1, 131.6, 130.9, 130.0, 129.4, 129.1, 128.4, 127.4, 41.9, 21.2. HRMS (ESI+) calculated for $C_{21}H_{19}SO$ (M+H): 319.1157; found: 319.1150.

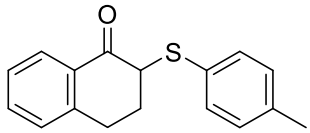


1-(naphthalen-2-yl)-2-(*p*-tolylthio)ethan-1-one (3ea). The synthesis procedure is the same as for **3aa**. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.38 (s, 1H), 7.99 (dd, *J* = 8.6, 1.8 Hz, 1H), 7.89 (t, *J* = 6.8 Hz,

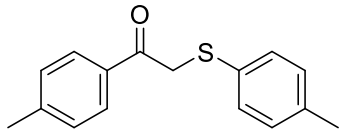
2H), 7.86 (d, *J* = 5.6 Hz, 1H), 7.60 (ddd, *J* = 8.0, 6.8, 0.9 Hz, 1H), 7.54 (ddd, *J* = 8.0, 6.8, 0.9 Hz, 1H), 7.31 (d, *J* = 8.0 Hz, 2H), 7.08 (d, *J* = 8.0 Hz, 2H), 4.32 (s, 2H), 2.30 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 194.3, 137.7, 135.7, 132.8, 132.5, 131.8, 131.0, 130.7, 130.0, 129.7, 128.8, 128.6, 127.9, 126.9, 124.3, 42.1, 21.2. HRMS (ESI+) calculated for $C_{19}H_{17}SO$ (M+H): 293.1000; found: 293.0997.



1-phenyl-2-(*p*-tolylthio)propan-1-one (3fa).[3f] The synthesis procedure is the same as for **3aa**. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.95-7.97 (m, 2H), 7.55 (d, *J* = 7.4 Hz, 1H), 7.44 (t, *J* = 7.6 Hz, 2H), 7.22 (d, *J* = 8.0 Hz, 2H), 7.08 (d, *J* = 8.0 Hz, 2H), 4.55 (q, *J* = 6.8 Hz, 2H), 2.32 (s, 3H), 1.49 (d, *J* = 6.8 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 196.2, 139.1, 135.8, 135.3, 133.1, 129.8, 128.7, 128.6, 127.7, 46.2, 21.3, 16.9.

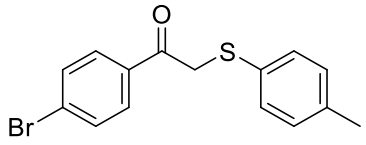


2-(*p*-tolylthio)-3,4-dihydronaphthalen-1(2H)-one (3ga). The synthesis procedure is the same as for **3aa**. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.05 (dd, *J* = 8.0, 0.8 Hz, 1H), 7.48 (dt, *J* = 7.4, 0.9 Hz, 1H), 7.38 (d, *J* = 8.0 Hz, 2H), 7.32 (t, *J* = 7.6 Hz, 1H), 7.23 (d, *J* = 7.6 Hz, 1H), 7.12 (d, *J* = 7.6 Hz, 2H), 4.02 (dd, *J* = 6.2, 4.2 Hz, 1H), 3.26 (ddd, *J* = 16.8, 9.6, 4.4 Hz, 1H), 2.89 (dt, *J* = 17.2, 5.0 Hz, 1H), 2.43-2.52 (m, 1H), 2.29-2.36 (m, 4H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 193.4, 143.1, 138.3, 133.8, 133.7, 131.5, 130.0, 129.2, 128.8, 128.3, 127.0, 54.0, 29.2, 26.6, 21.3. HRMS (ESI+) calculated for $C_{19}H_{17}SO$ (M+H): 269.0922; found: 269.1001.

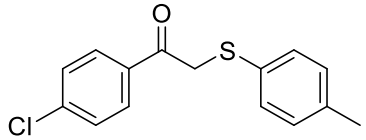


1-(*p*-tolyl)-2-(*p*-tolylthio)ethan-1-one (3ha). Typical procedure: To an oven-dried Schlenk tube equipped with a stir bar was added *p*-toluenethiol (**2a**, 0.80 mmol), and a balloon filled with dry air was connected to the Schlenk tube through the side arm and purged one time. Then, 1-(1-chlorovinyl)-4-methylbenzene (0.20 mmol), and DMF (2.0 mL) were successively injected in

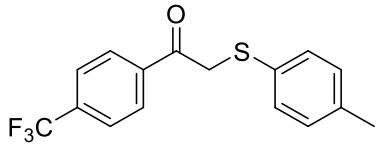
the reaction tube with magnetic stirring. The reaction mixture was allowed to stir vigorously at room temperature in a warm room for 1 h. Thereafter, water was added and the mixture was extracted with ethyl acetate (x 4). The combined organic layers were dried on Na_2SO_4 and concentrated under reduced pressure. The resulting crude product was separated on a silica gel column with petroleum ether and ethyl acetate as eluent to afford the desired product. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.83 (d, *J* = 8.4 Hz, 2H), 7.29 (d, *J* = 8.4 Hz, 2H), 7.25 (d, *J* = 8.0 Hz, 2H), 7.09 (d, *J* = 8.0 Hz, 2H), 4.19 (s, 2H), 2.41 (s, 3H), 2.31 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 194.0, 144.4, 137.5, 133.0, 131.5, 131.1, 130.0, 129.5, 128.9, 41.9, 21.8, 21.2. HRMS (ESI+) calculated for $C_{16}H_{17}SO$ (M+H): 257.1000; found: 257.1000.



1-(4-bromophenyl)-2-(*p*-tolylthio)ethan-1-one (3ia). The synthesis procedure is the same as for **3ha**. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.78 (d, *J* = 8.4 Hz, 2H), 7.59 (d, *J* = 8.4 Hz, 2H), 7.27 (d, *J* = 8.4 Hz, 2H), 7.09 (d, *J* = 8.4 Hz, 2H), 4.14 (s, 2H), 2.31 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 193.3, 137.9, 134.2, 132.1, 131.9, 130.4, 130.3, 130.0, 128.7, 41.8, 21.2. HRMS (ESI+) calculated for $C_{15}H_{14}OSBr$ (M+H): 320.9949; found: 320.9944.



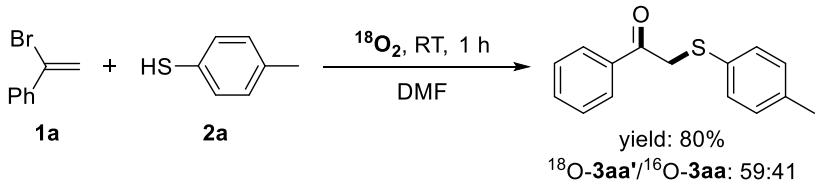
1-(4-chlorophenyl)-2-(*p*-tolylthio)ethan-1-one (3ja). The synthesis procedure is the same as for **3ha**. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.87 (d, *J* = 8.4 Hz, 2H), 7.43 (d, *J* = 8.4 Hz, 2H), 7.28 (d, *J* = 7.6 Hz, 2H), 7.10 (d, *J* = 8.0 Hz, 2H), 4.15 (s, 2H), 2.32 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 193.1, 140.0, 138.0, 133.8, 131.9, 130.5, 130.3, 130.1, 129.1, 41.8, 21.3. HRMS (ESI+) calculated for $C_{15}H_{14}SOCl$ (M+H): 277.0454; found: 277.0454.



2-(*p*-tolylthio)-1-(4-(trifluoromethyl)phenyl)ethan-1-one (3ka). The synthesis procedure is the same as for **3ha**. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.02 (d, *J* = 8.4 Hz, 2H), 7.71 (d, *J* = 8.4 Hz, 2H),

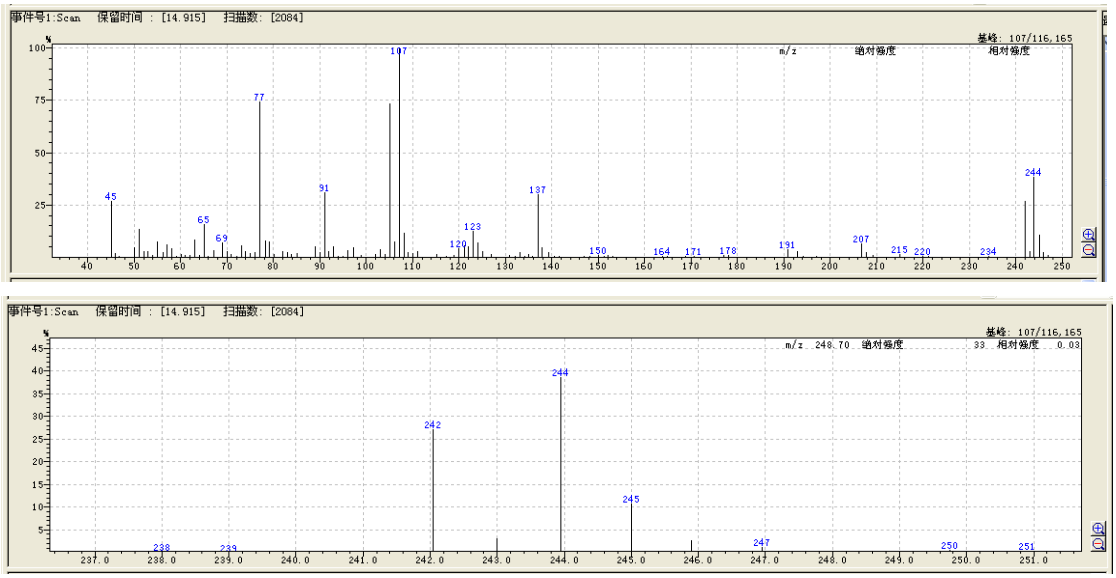
7.27 (d, J = 8.0 Hz, 2H), 7.10 (d, J = 8.0 Hz, 2H), 4.18 (s, 2H), 2.32 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 193.3, 138.2, 134.7 (q, $^2J_{C\text{-}F}$ = 32.7 Hz), 132.1, 130.1, 129.2, 125.8 (q, $^3J_{C\text{-}F}$ = 3.7 Hz), 123.7 (q, $^1J_{C\text{-}F}$ = 273.6 Hz), 42.0, 21.3. HRMS (ESI+) calculated for $C_{16}H_{14}SOF_3$ (M+H): 311.0717; found: 311.0709.

3) Labeling experiments.

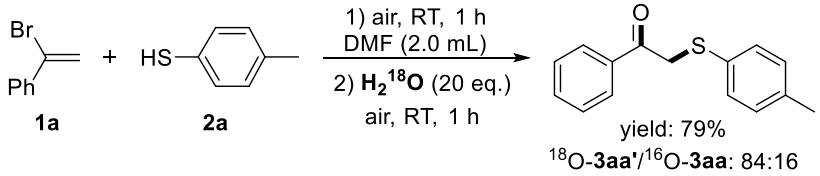


Typical procedure for labeling experiment: An oven-dried Schlenk tube equipped with a stir bar were capped by septa for injections and a three way cock which was connected to a nitrogen line and a balloon filled with $^{18}O_2$ respectively. After evacuation under vacuum and flushing with N_2 for one time, *p*-toluenethiol (**2a**, 0.60 mmol) and DMF (2.0 mL) was quickly added under N_2, and the reaction mixture was degassed the air by the method of freeze-pump-thaw cycle for 4 times. Then, $^{18}O_2$ was purged one time, α-Bromostyrene (0.20 mmol) was further injected into the reaction tube with magnetic stirring. The reaction mixture was vigorous stirred at RT (warm room) for 1 h. Thereafter, the reaction mixture was analyzed by GC-MS and was further separated on a silica gel column with petroleum ether and ethyl acetate as eluent to afford the desired product in 80% yield.

The EI-MS spectral of **3aa'**

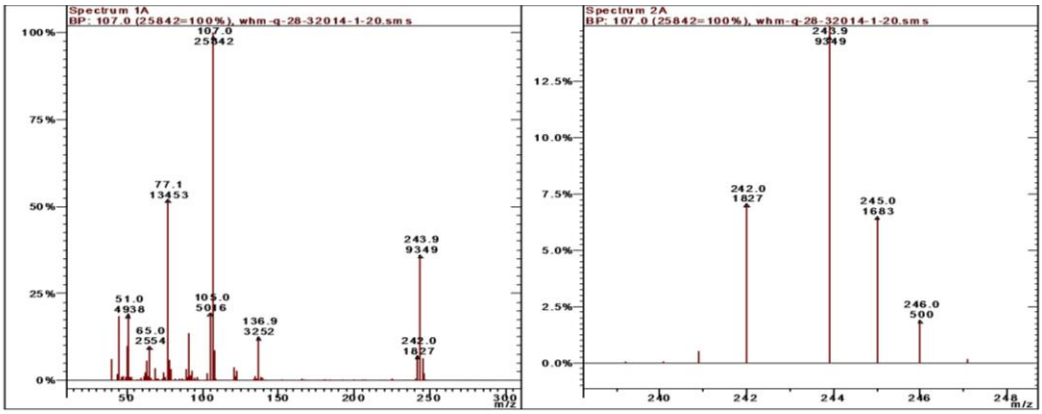


The relative intensity of m/z 244 and m/z 242are 45120 and 31729 respectively.



Typical procedure for labeling experiment: To an oven-dried Schlenk tube equipped with a stir bar was added *p*-toluenethiol (**2a**, 0.60 mmol), and a balloon filled with dry air was connected to the Schlenk tube through the side arm and purged one time. Then, α-bromostyrene (0.20 mmol), and DMF (2.0 mL) were successively injected in the reaction tube with magnetic stirring. The reaction mixture was allowed to stir vigorously at RT in a warm room for 1 h. Thereafter, H_2O^{18} (20 eq.) was added and the mixture was allowed to stir for another 1 h. after completion, the reaction mixture was analyzed by GC-MS and was further separated on a silica gel column with petroleum ether and ethyl acetate as eluent to afford the desired product in 79% yield.

The EI-MS spectral of **3aa'**



4) EPR experiments.

EPR spectra was recorded at 298 K on EPR spectrometer operated at 9.4158 GHz. Typical spectrometer parameters are shown as follows, scan range: 100 G; center field set: 3359.8 G; time constant: 163.84 ms; scan time: 30.72 s; modulation amplitude: 1.0 G; modulation frequency: 100 kHz; receiver gain: 1.00×105; microwave power: 19.05 mW.

4.1 The interaction between 1a (α-bromostyrene) / 2a (*p*-toluenethiol) was investigated by electron paramagnetic resonance (EPR) (X band, 9.4GHz, RT): (1) To an oven-dried Schlenk tube equipped with a stir bar was added *p*-toluenethiol (**2a**, 0.30 mmol), the Schlenk tube through

the side arm and purged one time. Then, DMF (2.0 mL) were successively injected in the reaction tube with magnetic stirring. The reaction mixture was allowed to stir vigorously at room temperature in a warm room for 15 mintues. Thereafter, 10 uL of DMPO (5,5-dimethyl-1-pyrroline N-oxide) was added and well mixed. Afterwards, 20 uL of the mixture was quickly taken out into a small tube and analyzed by EPR. (2) An oven-dried Schlenk tube equipped with a stir bar was evacuated under vacuum and flushed with air through a dry air balloon for one times. Then, **1a** (0.1 mmol) and DMF (2.0 mL) were successively injected in the reaction tube with magnetic stirring. The reaction mixture was allowed to stir vigorously at room temperature in a warm room for 15 mintues. Thereafter, 10 uL of DMPO (5,5-dimethyl-1-pyrroline N-oxide) was added and well mixed. Afterwards, 20 uL of the mixture was quickly taken out into a small tube and analyzed by EPR.

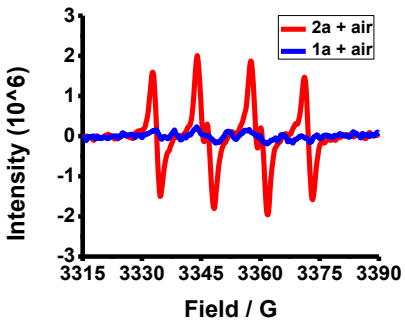


Figure S1. DMPO spin trapping of radical formed from (a) **2a** (0.30 mmol) in DMF (2.0 mL) at RT under 1 atm of air (balloon), (b) **1a** (0.10 mmol) in DMF (2.0 mL) at RT was monitored by electron paramagnetic resonance (EPR) (X band, 9.4GHz, RT).

4.2 Comparison of DMPO-radical adduct formed from the interaction between 2a and air with the DMPO-thiyl radical adduct.

4.2.1 The generation of the DMPO-thiyl radical adduct from the reaction between 2a and AIBN under N_2: (1) An oven-dried Schlenk tube equipped with a stir bar were capped by septa for injections and a nitrogen line, after evacuation under vacuum and flushing with N_2 for one time. Then, *p*-toluenethiol (**2a**, 0.30 mmol) and DMF (2.0 mL) was quickly added under N_2, and the reaction mixture was degassed the air by the method of freeze-pump-thaw cycle for 2 times. Subsequently, AIBN (azodiisobutyronitrile, 0.10 mmol) was added under N_2 and the reaction mixture was degassed the air by the method of freeze-pump-thaw cycle for 3 times. The reaction mixture was allowed to stir vigorously at 70 °C for 15 mintues. Thereafter, 10 uL of DMPO (5,5-dimethyl-1-pyrroline N-oxide) was added and well mixed. Afterwards, 20 uL of the mixture was quickly taken out into a small tube and analyzed by EPR.

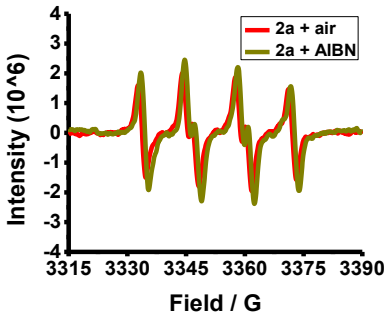


Figure S2. Comparison of the DMPO-radical adducts formed from (a) **2a** (0.30 mmol) in DMF (2.0 mL) at RT under 1 atm of air (balloon), (b) **2a** (0.30 mmol) and AIBN (0.1 mmol) in DMF (2.0 mL) at 70 °C was monitored by electron paramagnetic resonance (EPR) (X band, 9.4GHz, RT).

4.2.2 Blank control experiments.

(1) **The interaction between 2a (*p*-toluenethiol) and DMF under N_2**: An oven-dried Schlenk tube equipped with a stir bar were capped by septa for injections and a nitrogen line, after evacuation under vacuum and flushing with N_2 for one time. Then, *p*-toluenethiol (**2a**, 0.30 mmol) and DMF (2.0 mL) was quickly added under N_2, and the reaction mixture was degassed the air by the method of freeze-pump-thaw cycle for 4 times. The reaction mixture was allowed to stir vigorously at 70 °C for 15 mintues. Thereafter, 10 uL of DMPO (5,5-dimethyl-1-pyrroline N-oxide) was added and well mixed. Afterwards, 20 uL of the mixture was quickly taken out into a small tube and analyzed by EPR.

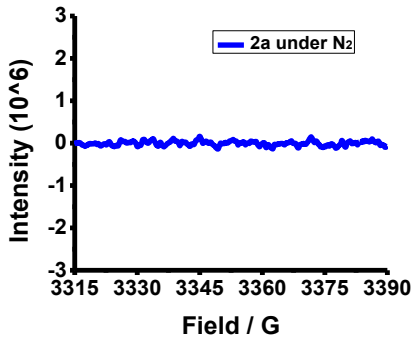


Figure S3. DMPO spin trapping of radical formed from **2a** (0.30 mmol) in degassed DMF (2.0 mL) at 70 °C under N_2.

(2) **The interaction between AIBN and DMF under N_2**: An oven-dried Schlenk tube equipped with a stir bar were capped by septa for injections and a nitrogen line, after evacuation under vacuum and flushing with N_2 for one time. Then, AIBN (**2a**, 0.10 mmol) and DMF (2.0 mL) was quickly added under N_2, and the reaction mixture was degassed the air by the method of freeze-pump-thaw cycle for 4 times. The reaction mixture was allowed to stir vigorously at 70 °C for 15 mintues. Thereafter, 10 uL of DMPO (5,5-dimethyl-1-pyrroline N-oxide) was added and well mixed. Afterwards, 20 uL of the mixture was quickly taken out into a small tube and analyzed by EPR.

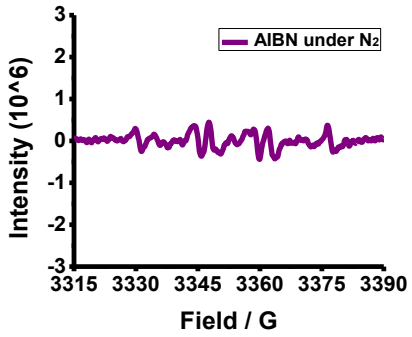


Figure S4. DMPO spin trapping of radical formed from AIBN (0.10 mmol) in degassed DMF (2.0 mL) at 70 °C under N_2.

5) ReactIR experiments.

5.1 The interaction between 1a (α-bromostyrene) / 2a (*p*-toluenethiol) and air was explored by operando IR: an oven-dried three-necked reaction vessel was equipped with a stir bar, the operando IR probe was inserted through an adapter into the middle neck, the other two necks were capped by septa for injections and a nitrogen line, after evacuation under vacuum and flushing with air through a dry air balloon for three times. At room temperature, THF (4.0 mL) was added to the vessel via a springe and the reaction was monitored by operando IR. Afterwards, **1a** (0.2 mmol) or **2a** (0.6 mmol) was added and the reaction mixture was allowed to stir vigorously at room temperature for 1 h.

The kinetic profiles of the reactions:

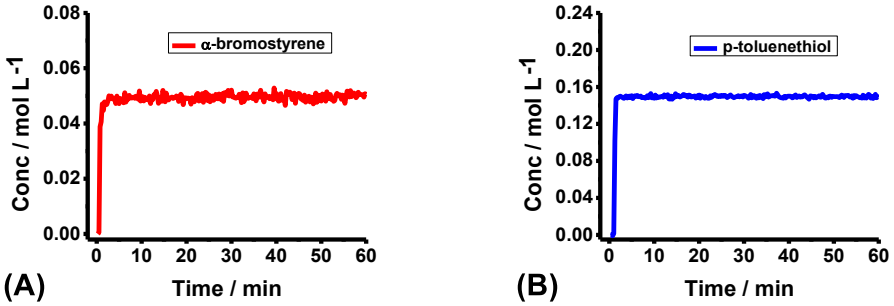
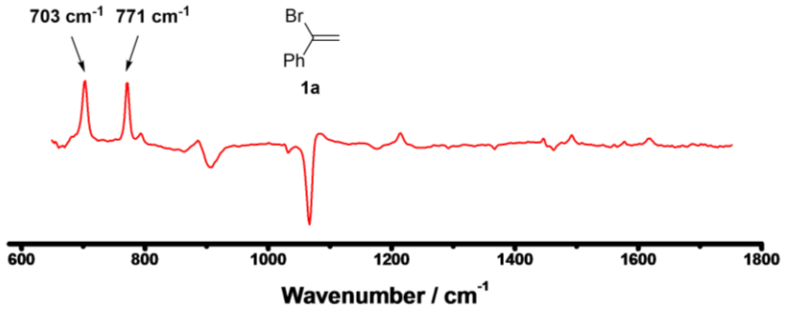


Figure S5. (A) The kinetic profile of the reaction of **1a** (0.20 mmol) in THF (4.0 mL) at RT for 1 h under 1 atm of air (balloon). (B) The kinetic profile of the reaction of **2a** (0.60 mmol) in THF (4.0 mL) at RT for 1 h under 1 atm of air (balloon).



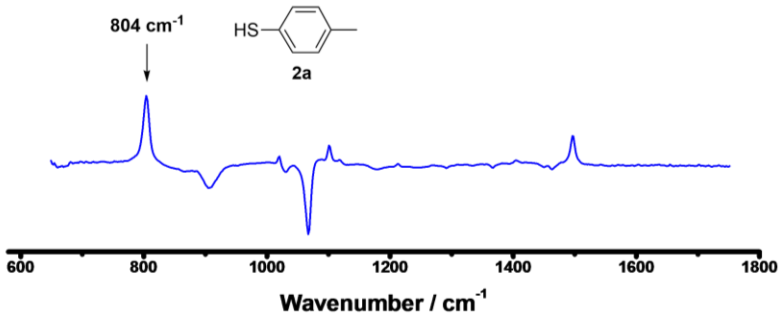


Figure S6. The Characteristic IR band of the different species (in THF).

5.2.1 The model reaction between 1a and 2a under argon was monitored by operando IR: an oven-dried three-necked reaction vessel was equipped with a stir bar, the operando IR probe was inserted through an adapter into the middle neck, the other two necks were capped by septa for injections and a argon line, after evacuation under vacuum and flushing with argon for three times. At room temperature, degassed THF (4.0 mL) was added to the vessel via a springe and the reaction was monitored by operando IR. Afterwards, **1a** (0.2 mmol) or **2a** (0.6 mmol) was added and the reaction mixture was allowed to stir vigorously at room temperature for 1 h.

5.2.2 The model reaction between 1a and 2a in the presence of dioxygen was monitored by operando IR: an oven-dried three-necked reaction vessel was equipped with a stir bar, the operando IR probe was inserted through an adapter into the middle neck, the other two necks were capped by septa for injections and dry air balloon, after evacuation under vacuum and flushing with air through the dry air balloon for three times. At room temperature, THF (4.0 mL) was added to the vessel via a springe and the reaction was monitored by operando IR. Afterwards, **1a** (0.2 mmol) and **2a** (0.6 mmol) were added and the reaction mixture was allowed to stir vigorously at room temperature for 1 h. Thereafter, the mixture was analyzed by GC, **3aa** was obtained in 85% yield, and the conversions of **1a** and **2a** were 99% and 97% respectively. Additionally, aryl disulfide **4a** was obtained in 0.187 mmol, which is approximately equal to the expected β-keto sulfide **3aa**.

The kinetic profiles of the reactions:

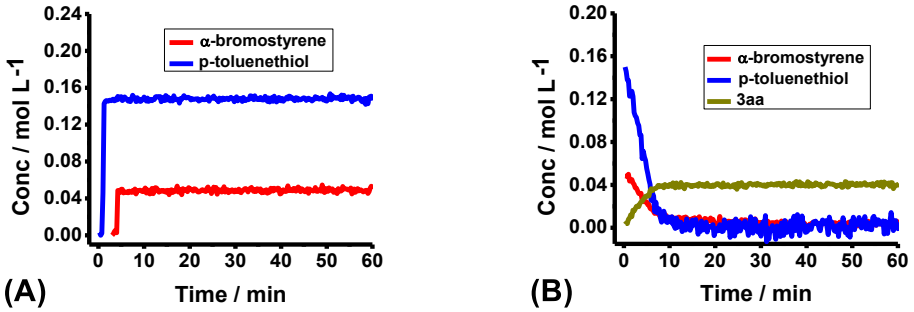


Figure S7. The kinetic profile of the reaction of **1a** (0.20 mmol) and **2a** (0.60 mmol) in THF (4.0 mL) at RT for 1 h. (A) Under argon atmosphere. (B) Under 1 atm of air (balloon).

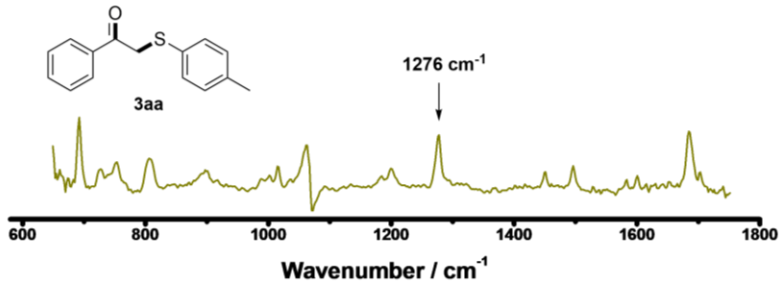
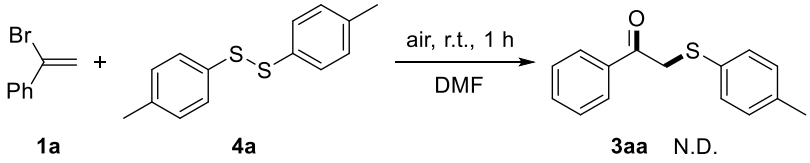


Figure 8. The Characteristic IR band of the desired product **3aa** (in THF).

6) Diaryl disulfide as the starting material.



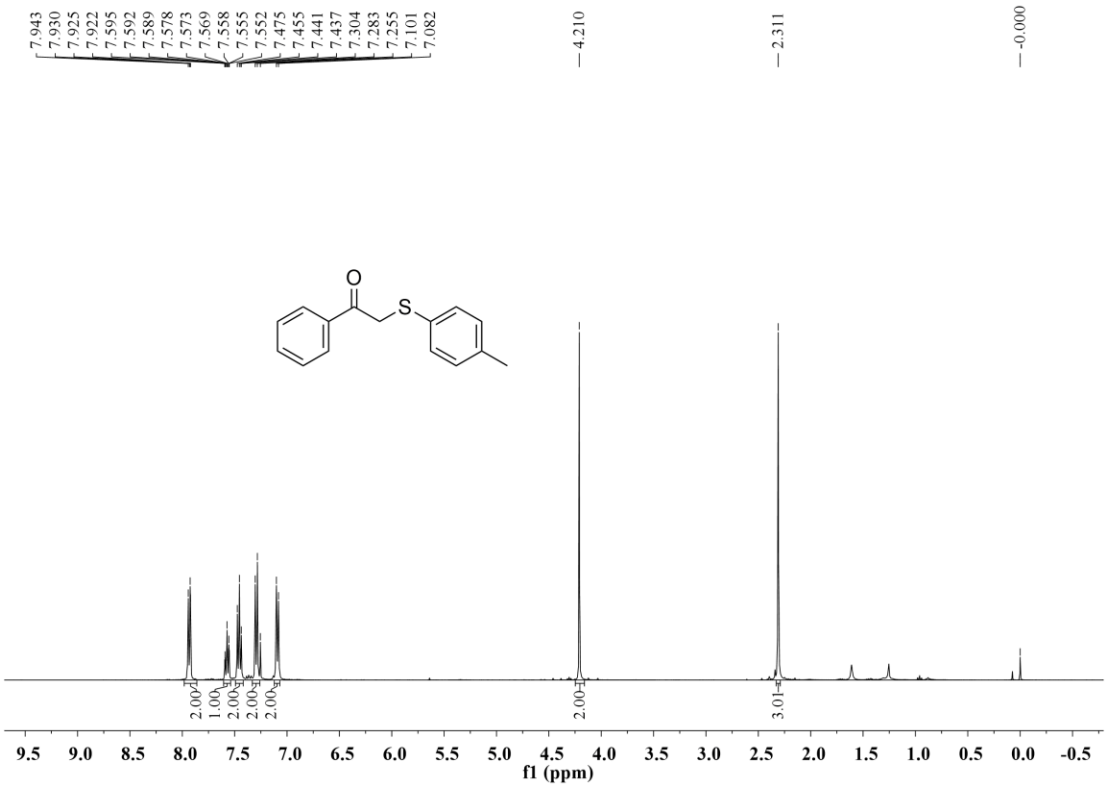
Typical procedure: To an oven-dried Schlenk tube equipped with a stir bar was added aryl disulfide (**4a**, 0.15 mmol), and a balloon filled with dry air was connected to the Schlenk tube through the side arm and purged one time. Then, α-bromostyrene (0.10 mmol) and DMF (1.0 mL) were successively injected in the reaction tube with magnetic stirring. The reaction mixture was allowed to stir vigorously at room temperature in a warm room for 1 h. Thereafter, **3aa** was not detected by GC-MS analysis, and 97% of **4a** was recovered by GC analysis.

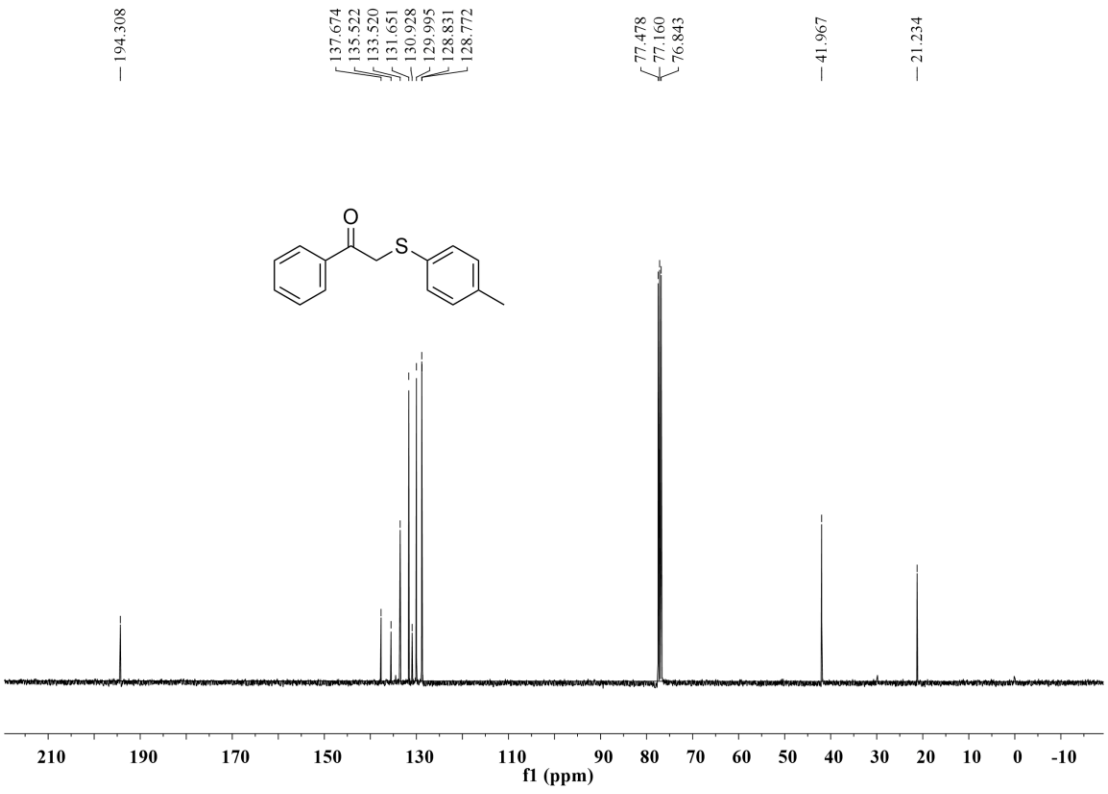
References

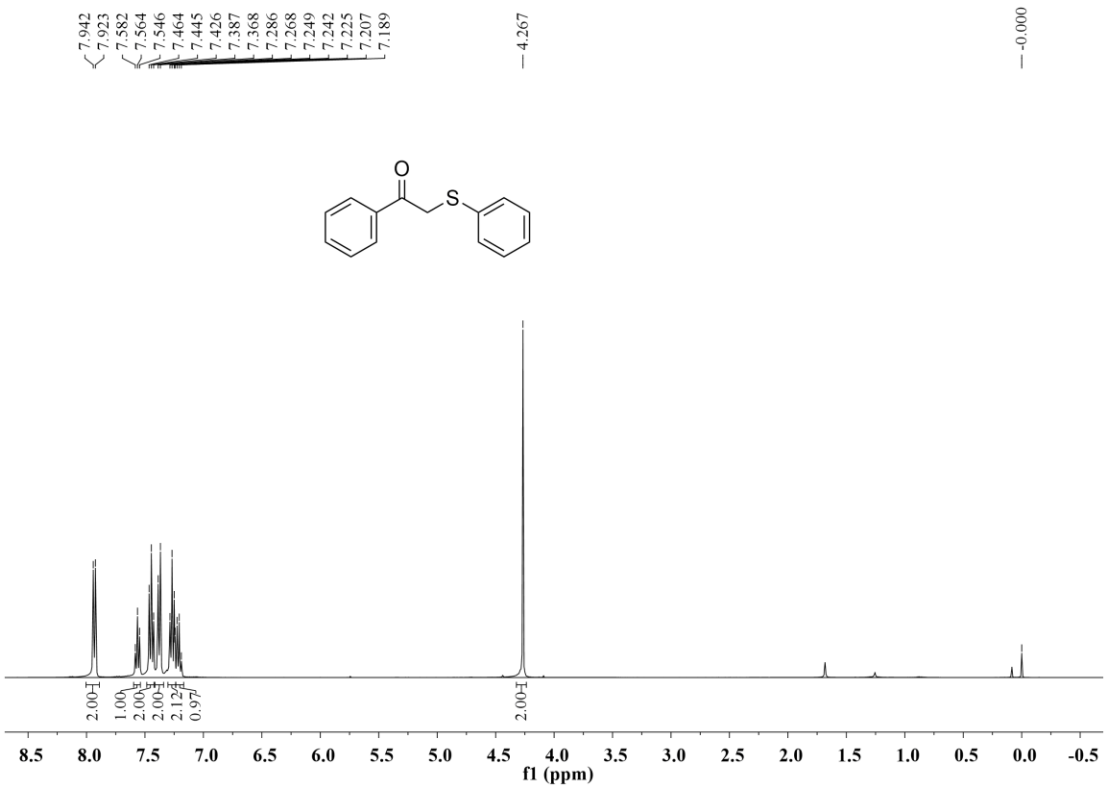
(1) a) A. Lilienkampf, M. P. Johansson, K. Wähälä, *Org. Lett.* **2003**, *5*, 3387-3390; b) A. K. Macharla, R. Chozhiyath Nappunni, N. Nama, *Tetrahedron Lett.* **2012**, *53*, 1401-1405; c) P. B. Silveira, A. L. Monteiro, *Journal of Molecular Catalysis A: Chemical* **2006**, *247*, 1-6; d) M. Kodomari, T. Nagaoka, Y. Furusawa, *Tetrahedron Letters* **2001**, *42*, 3105-3107; e) T. Takeda, R. Sasaki, S. Yamauchi, T. Fujiwara, *Tetrahedron* **1997**, *53*, 557-566; f) A. Hamze, J.-D. Brion, M. Alami, *Org. Lett.* **2012**, *14*, 2782-2785.

(2) a) H. Loghmani-Khouzani, M. R. Poorheravi, M. M. M. Sadeghi, L. Caggiano, R. F. W. Jackson, *Tetrahedron* **2008**, *64*, 7419-7425; b) K. Huang, M. Ortiz-Marciales, V. Stepanenko, M. De Jesús, W. Correa, *J Org Chem* **2008**, *73*, 6928-6931; c) A. Stroba, F. Schaeffer, V. Hindie, L. Lopez-Garcia, I. Adrian, W. Fröhner, R. W. Hartmann, R. M. Biondi, M. Engel, *J Med Chem* **2009**, *52*, 4683-4693; d) O. Fatunsin, M. Shkoor, A. Riahi, M. Hussain, A. Villinger, C. Fischer, P. Langer, *Helv. Chim. Acta* **2010**, *93*, 1610-1621; e) H. Ishibashi, I. Takamuro, Y. Mizukami, M. Irie, M. Ikeda, *Synth. Commun.* **1989**, *19*, 443-452. f) M. Aveniente, E. F. Pinto, L. S. Santos, B. Rossi-Bergmann, L. E. S. Barata, *Bioorg. Med. Chem.* **2007**, *15*, 7337-7343.

NMR Spectra of Products



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7.189
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-0.000
O
S
2.00
1.00
2.00
2.00
2.12
0.97
2.00
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
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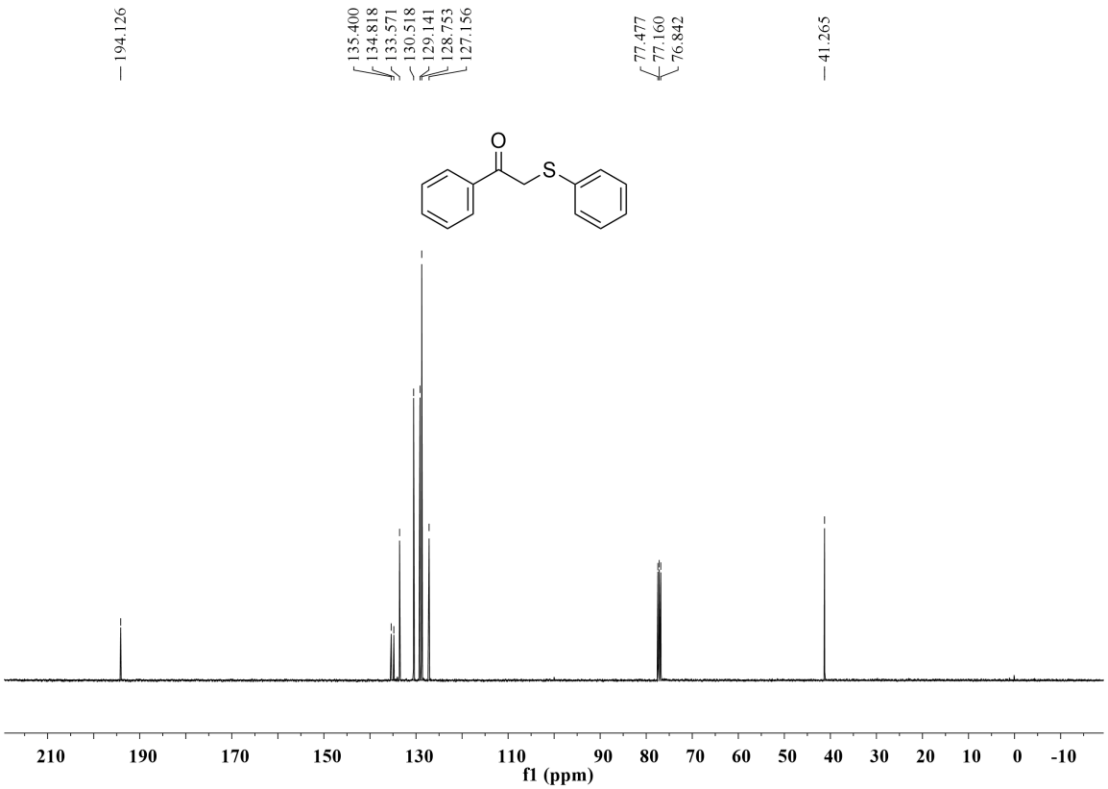
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S
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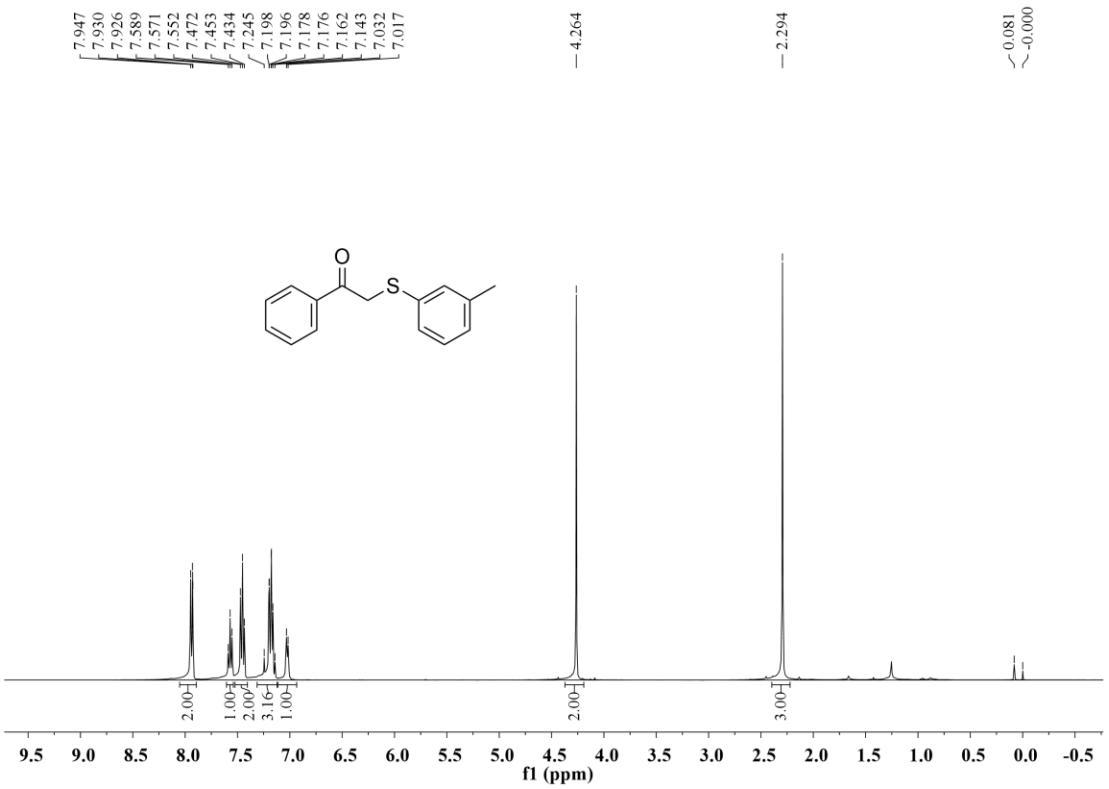
f1 (ppm)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7.176
7.162
7.143
7.032
7.017
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0.081
-0.000
O
S
2.00
1.00
2.00
3.16
1.00
2.00
3.00
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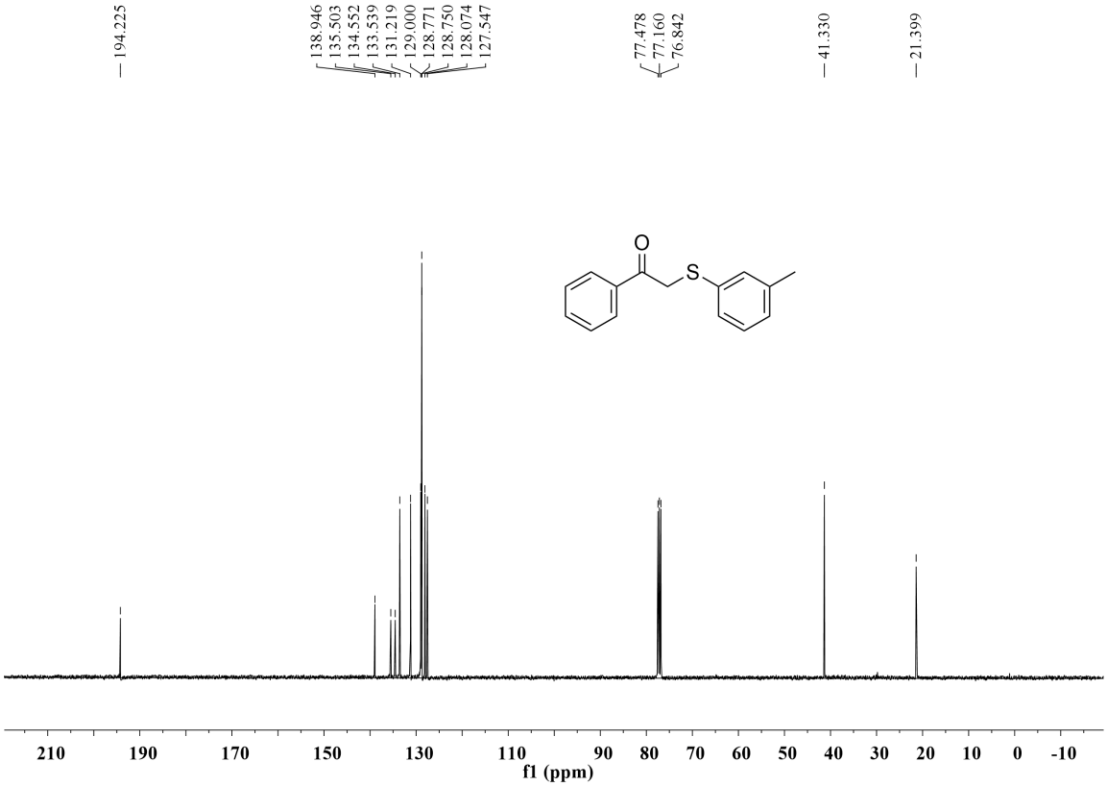
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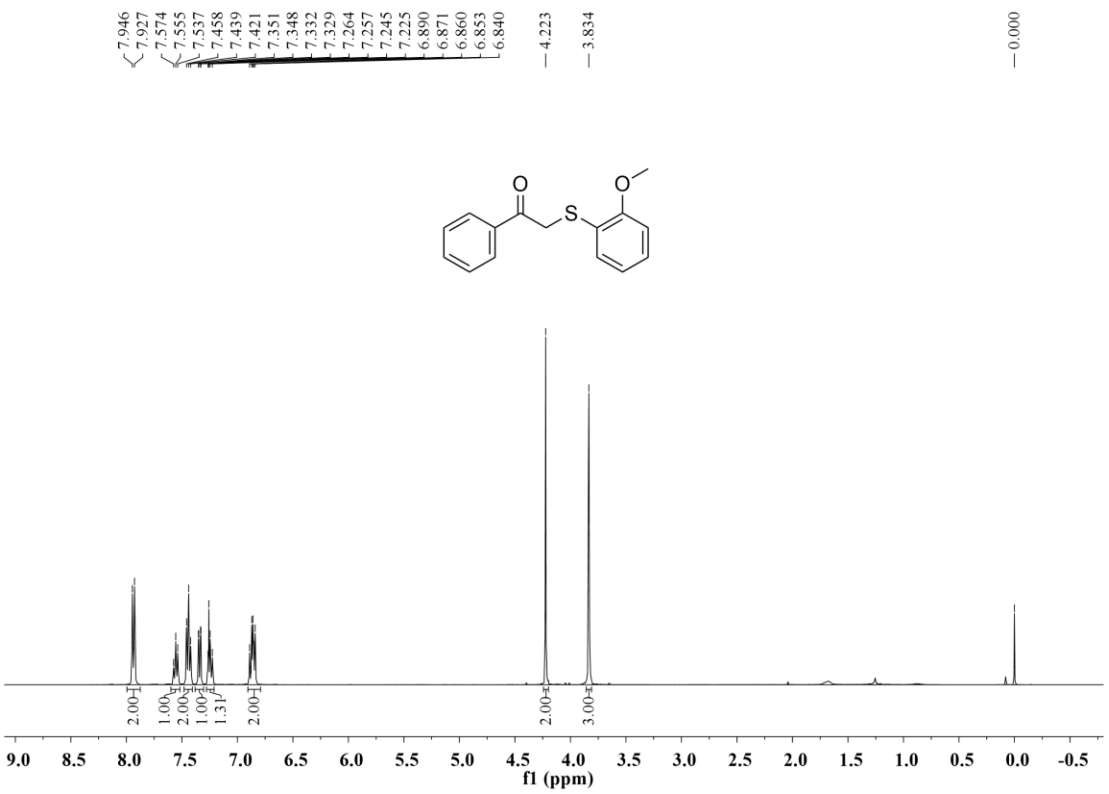
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7.257
7.245
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1.00
2.00
1.00
1.31
2.00
2.00
3.00
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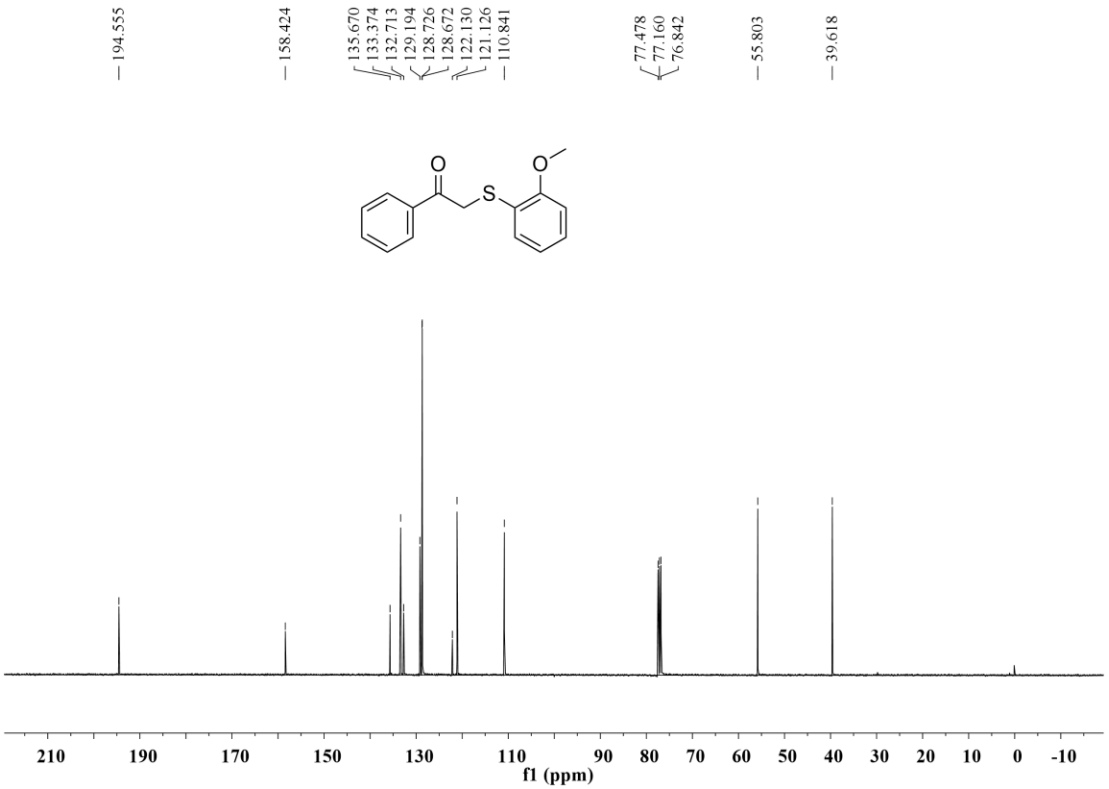
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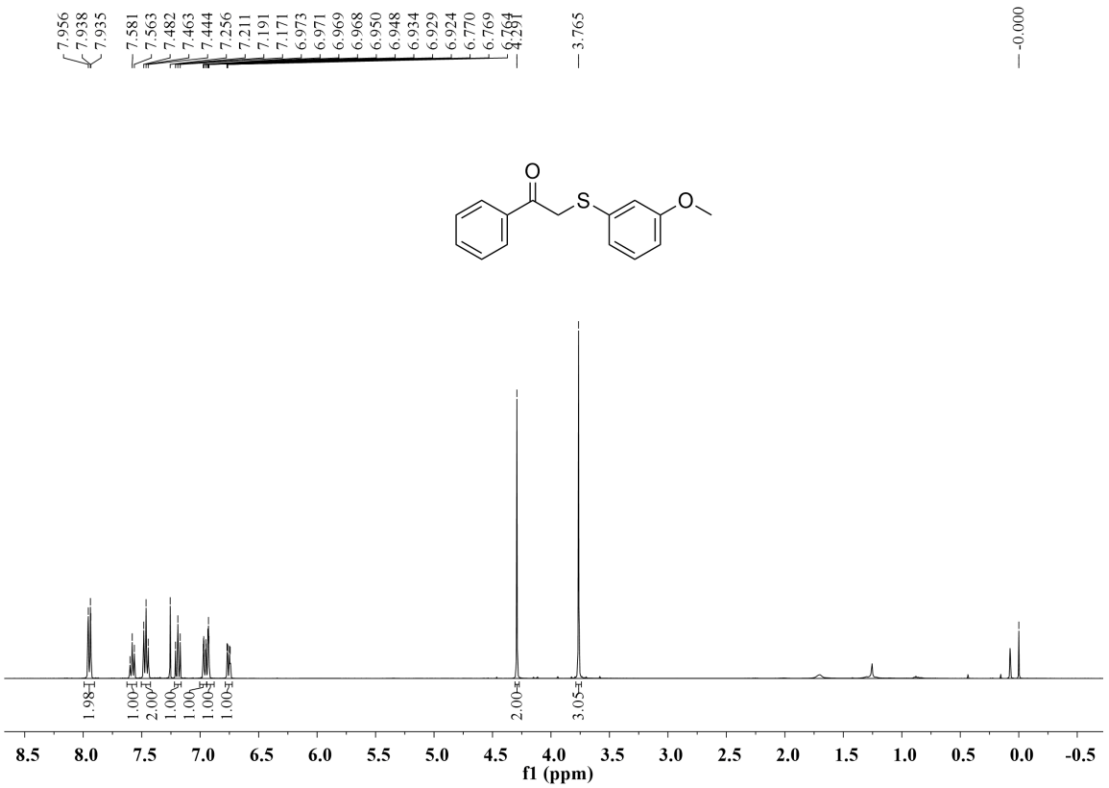
f1 (ppm)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6.969
6.968
6.950
6.948
6.934
6.929
6.924
6.770
6.769
6.764
4.291
3.765
-0.000
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S
O
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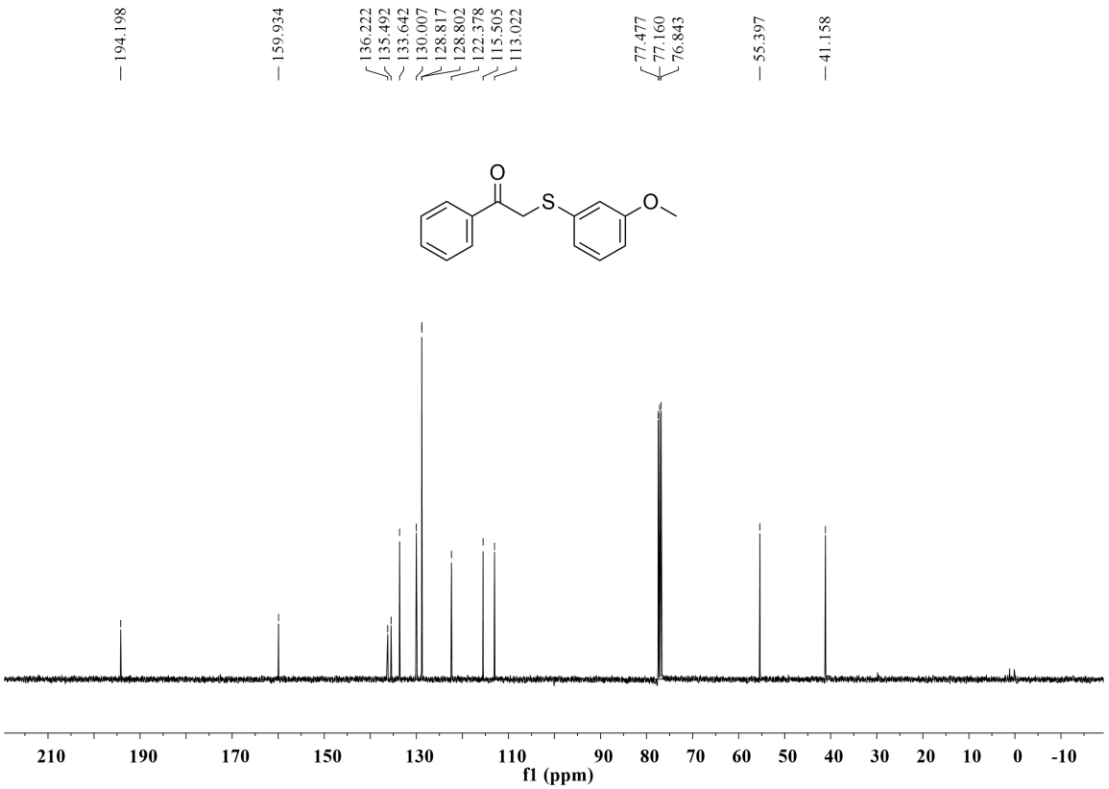
1.00
2.00
1.00
1.00
1.00
2.00
3.05
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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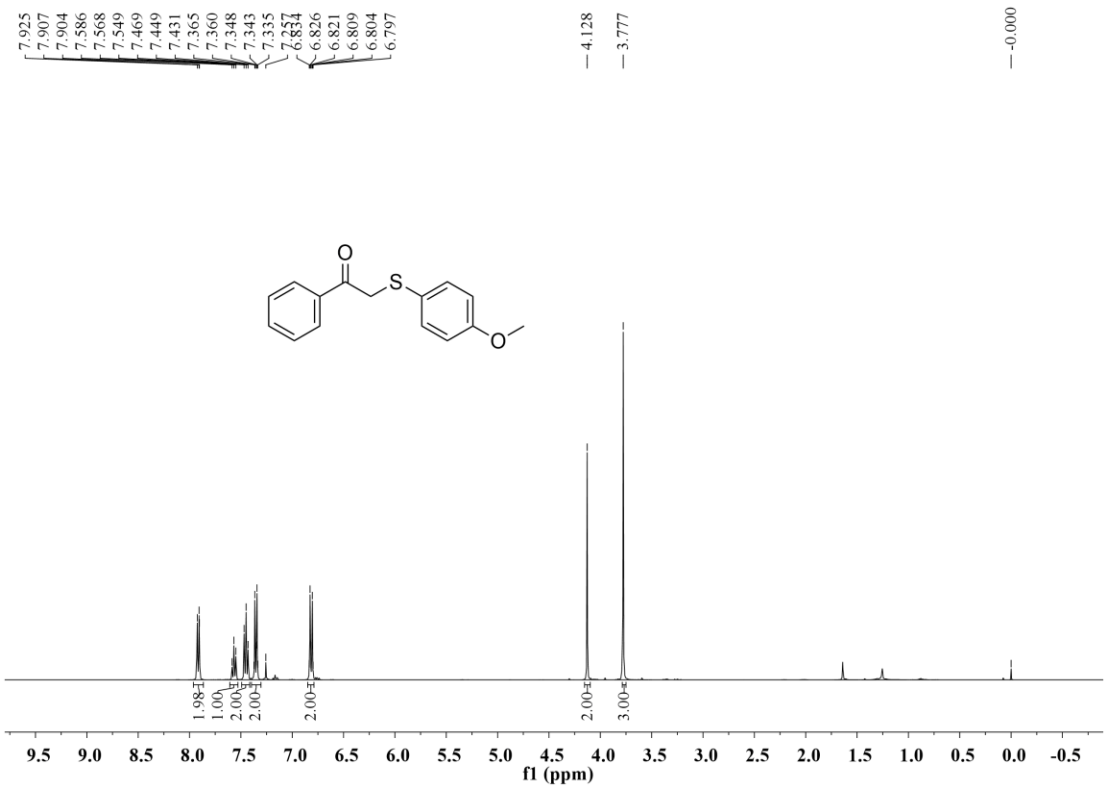
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6.821
6.809
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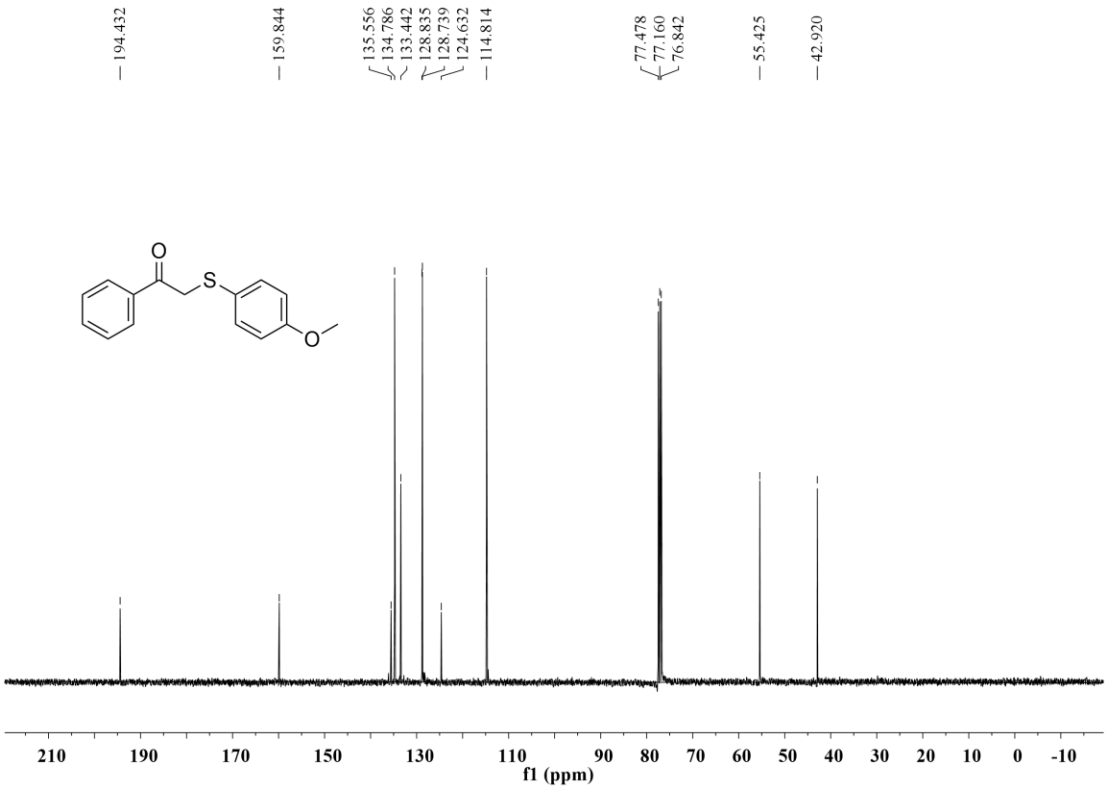
f1 (ppm)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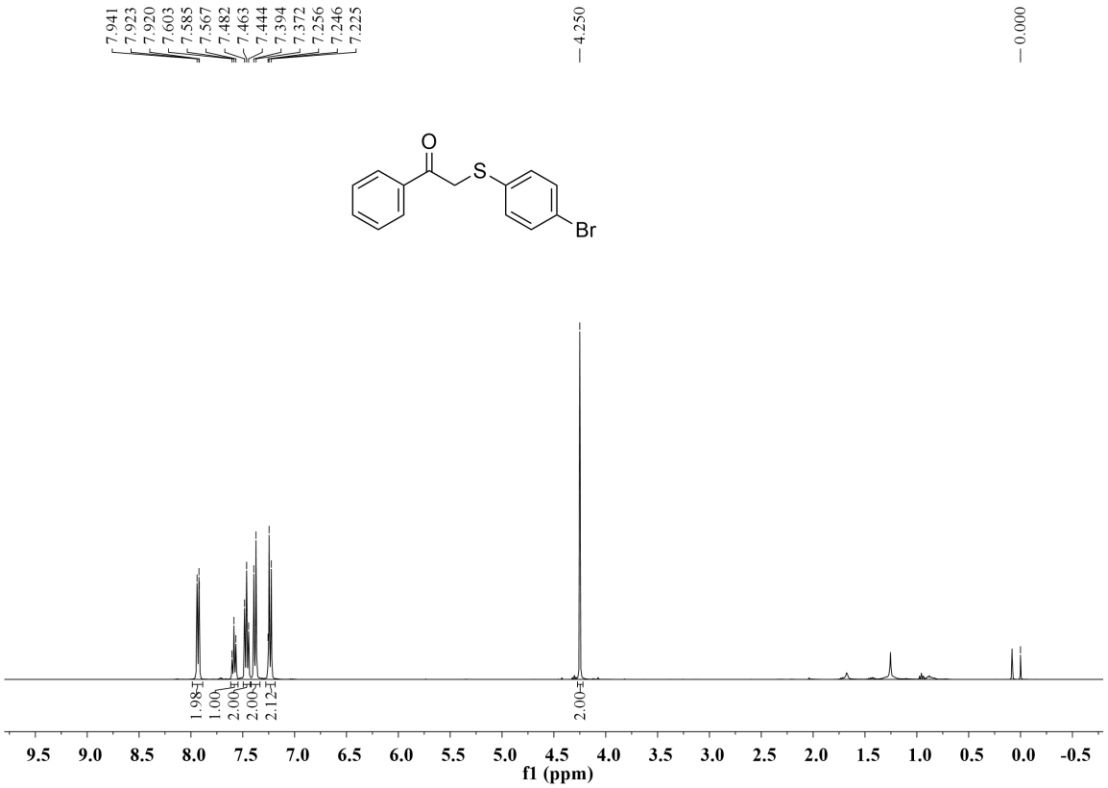
f1 (ppm)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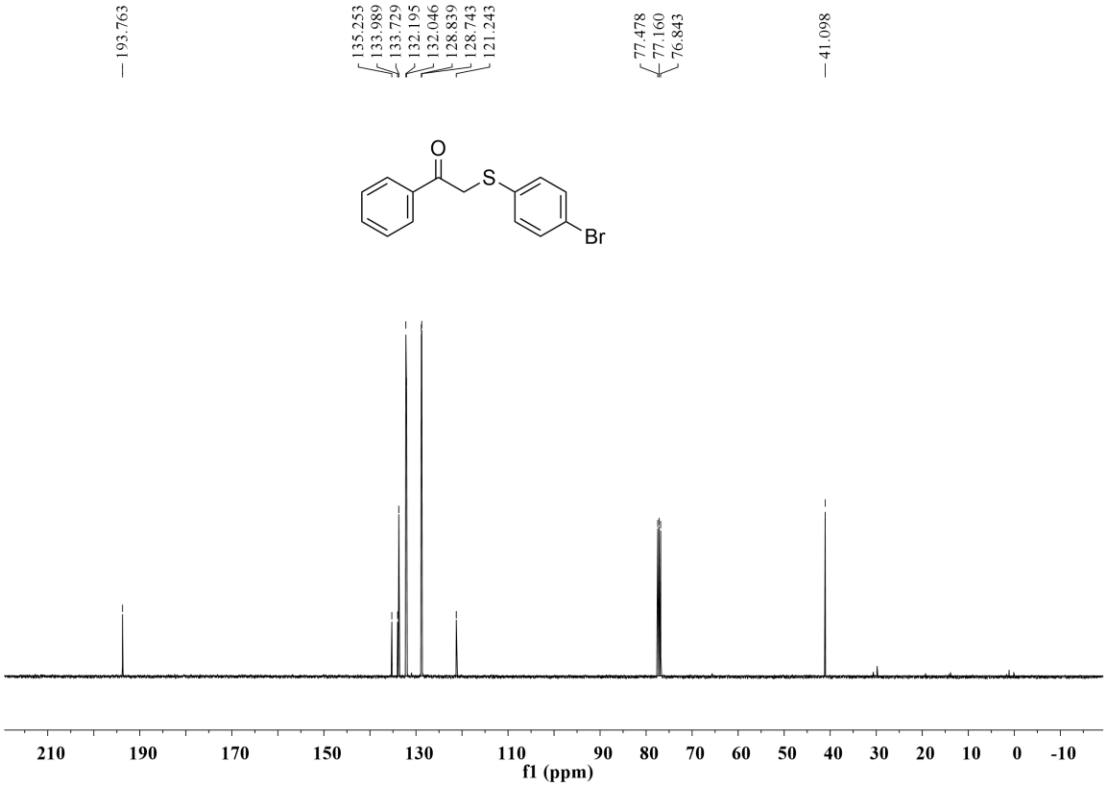
7.225
4.250
0.000
O
S
Br
1.98
1.00
2.00
2.00
2.12
2.00
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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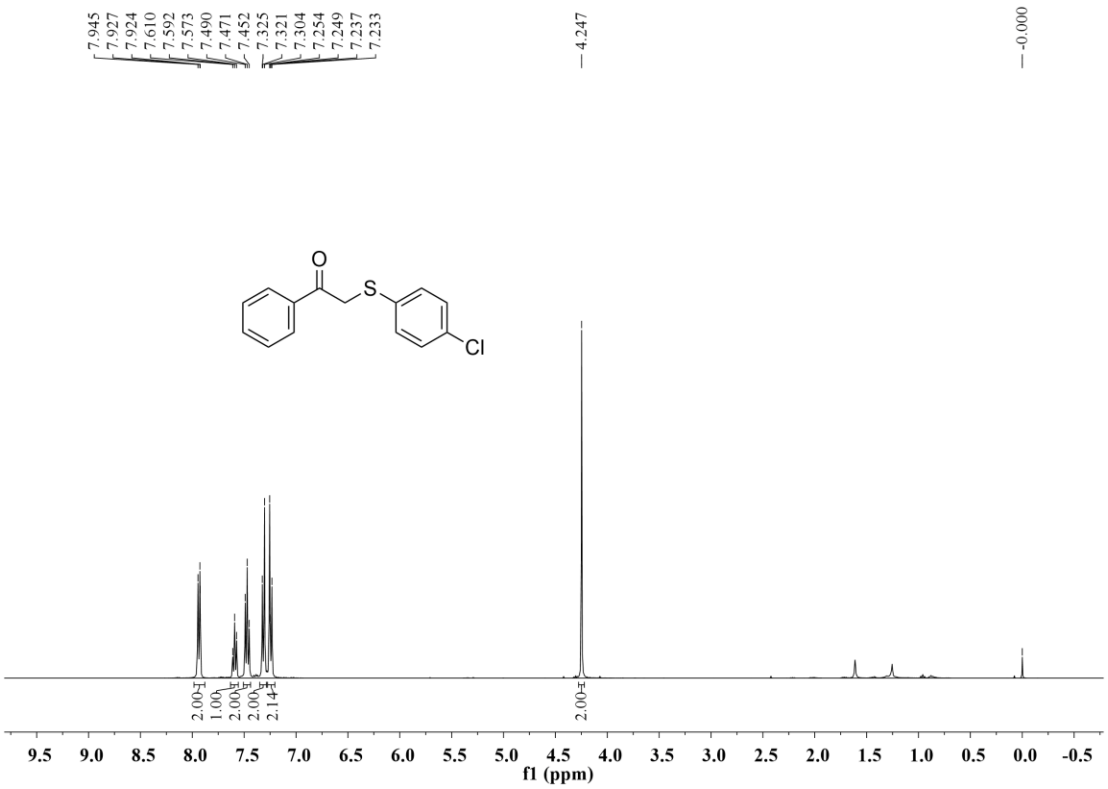
f1 (ppm)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7.249
7.237
7.233
4.247
-0.000
O
S
Cl
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2.00
2.00
2.14
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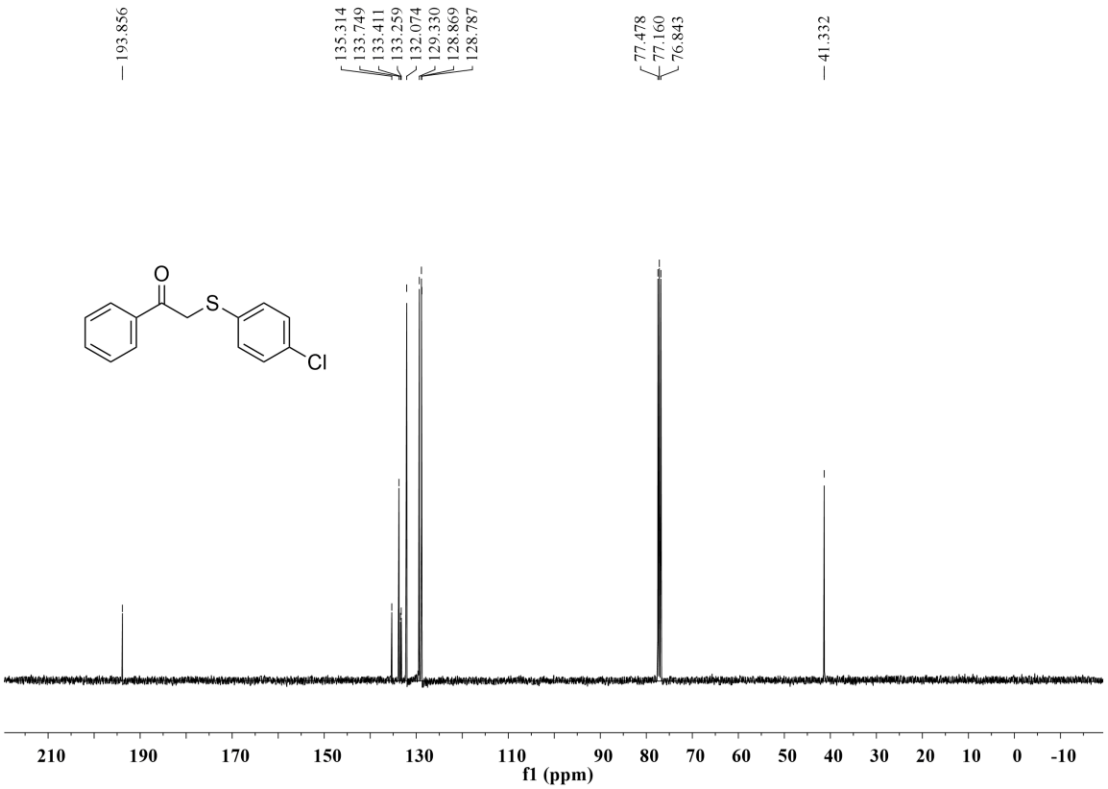
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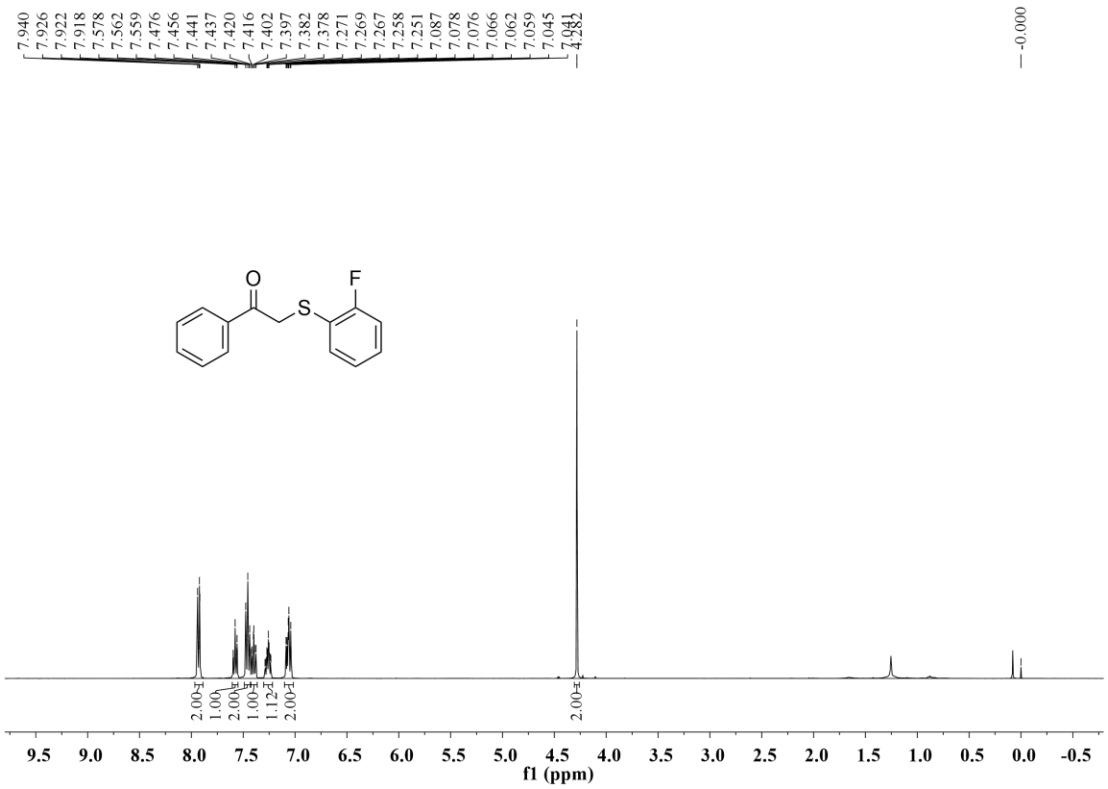
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7.269
7.267
7.258
7.251
7.087
7.078
7.076
7.066
7.062
7.059
7.045
7.041
4.282
-0.000
O
F
S
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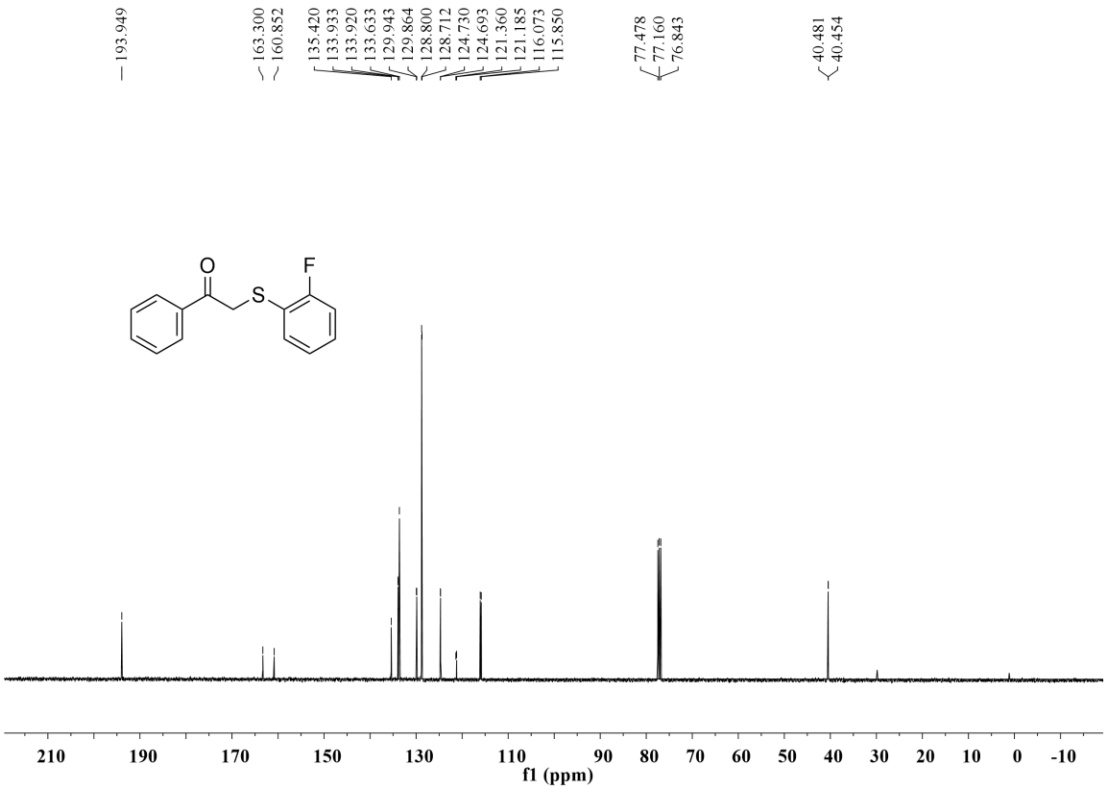
2.00
1.00
1.12
2.00
2.00
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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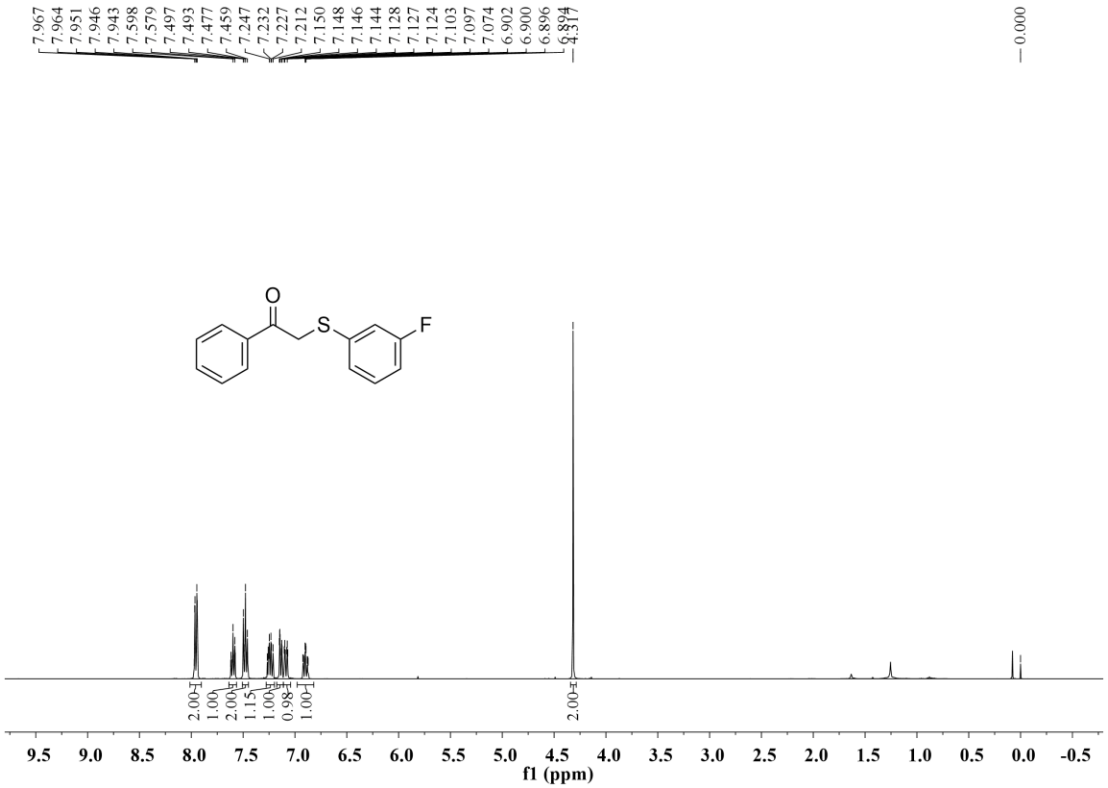
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7.074
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6.900
6.896
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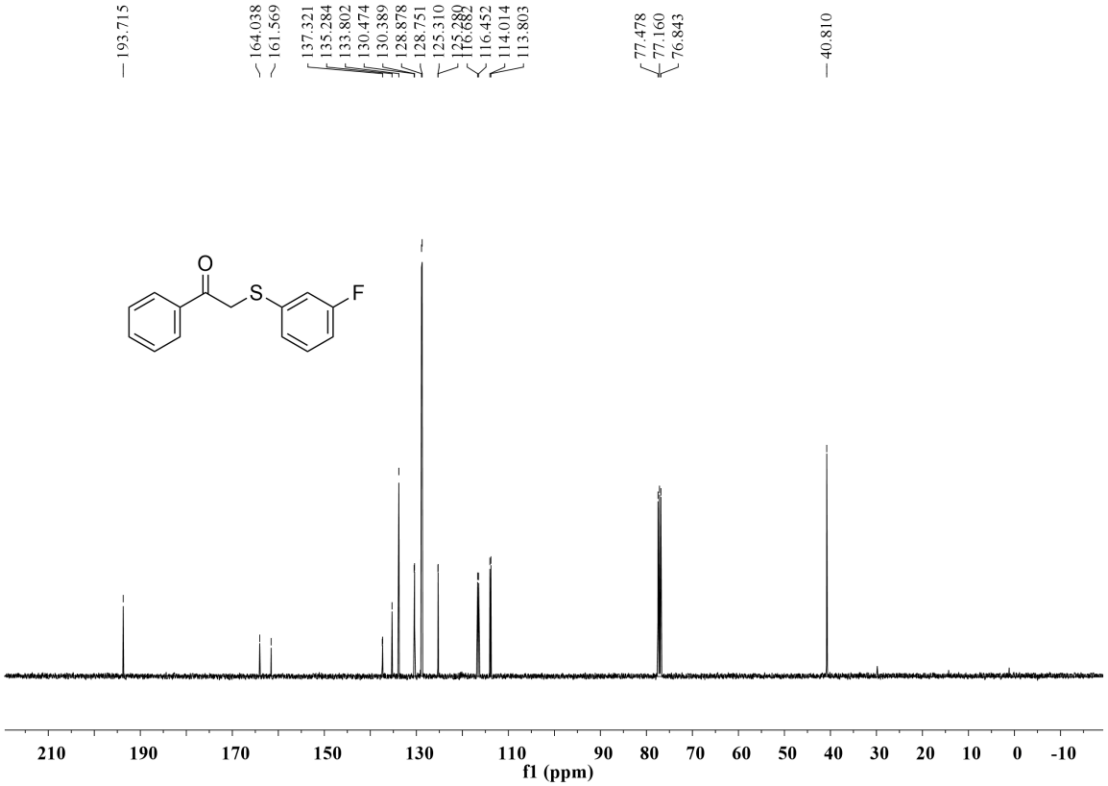
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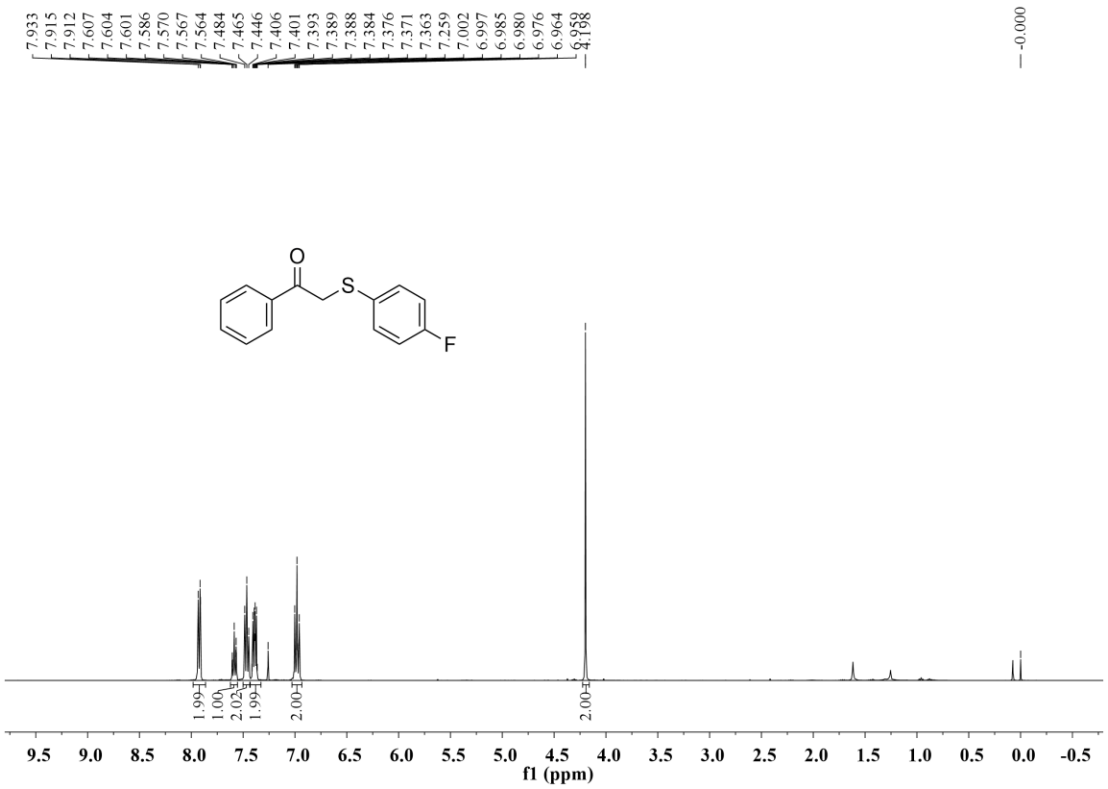
F
f1 (ppm)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7.446
7.406
7.401
7.393
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7.388
7.384
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7.371
7.363
7.259
7.002
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6.980
6.976
6.964
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2.02
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2.00
2.00
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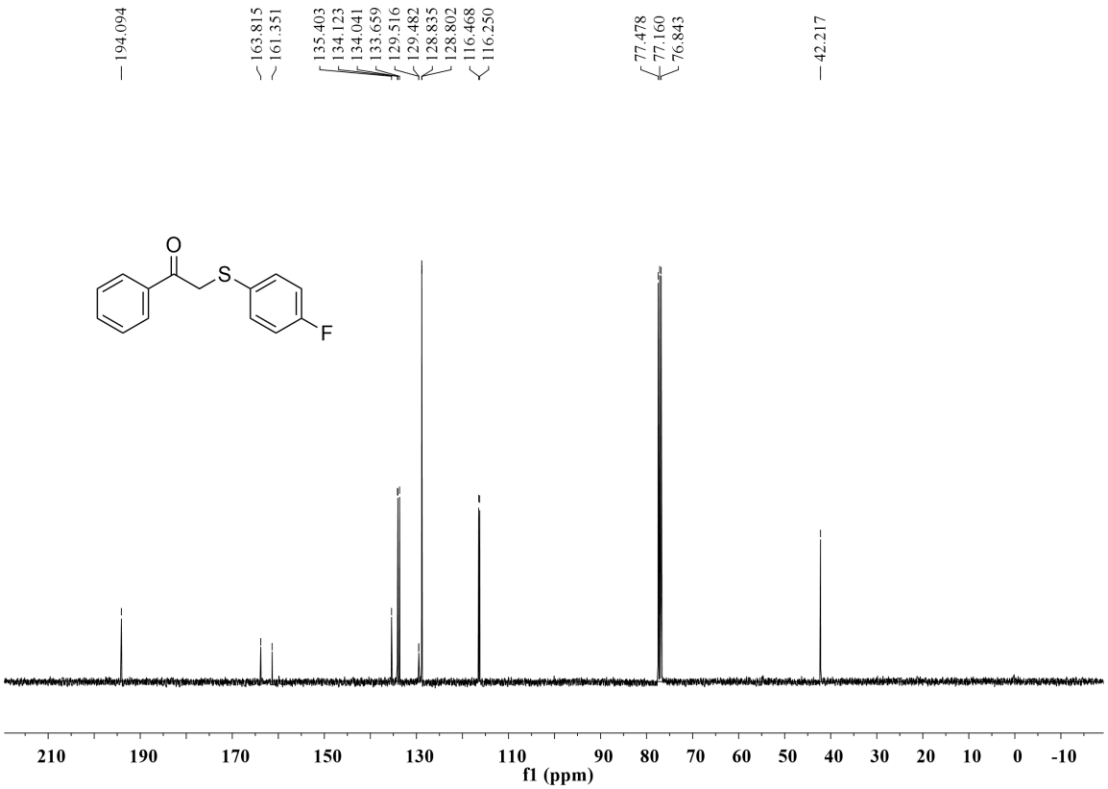
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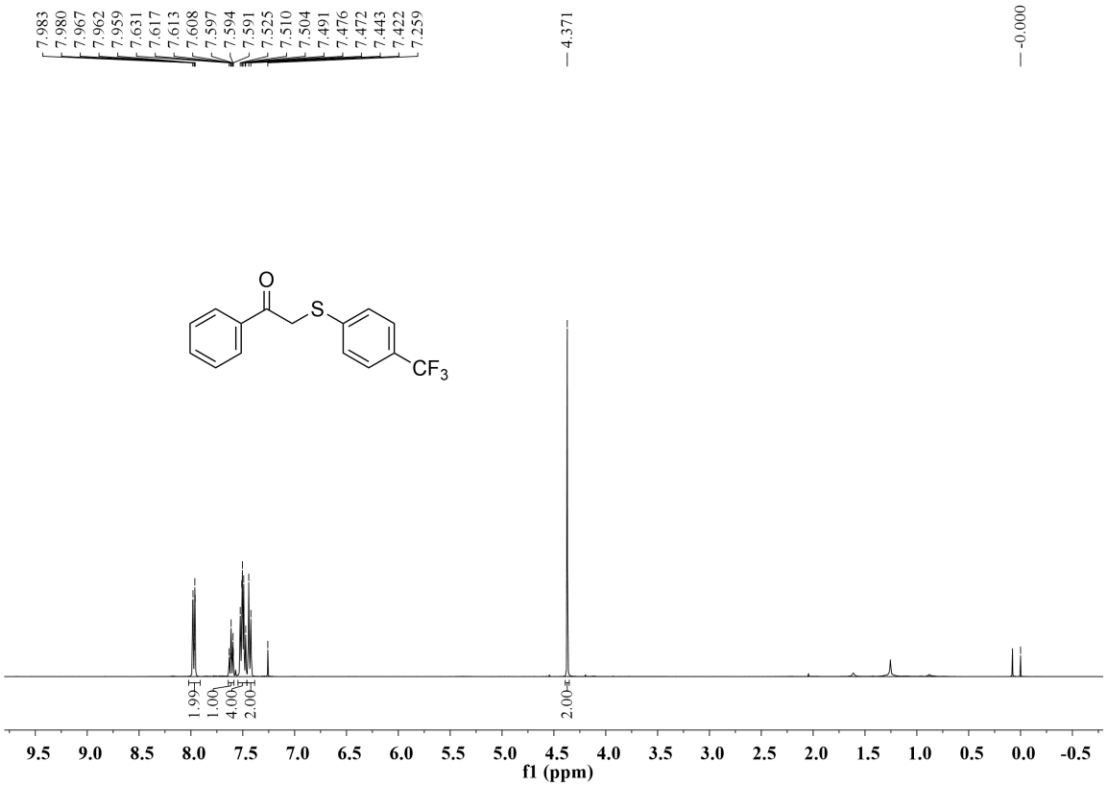
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7.443
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O
S
CF3
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2.00
2.00
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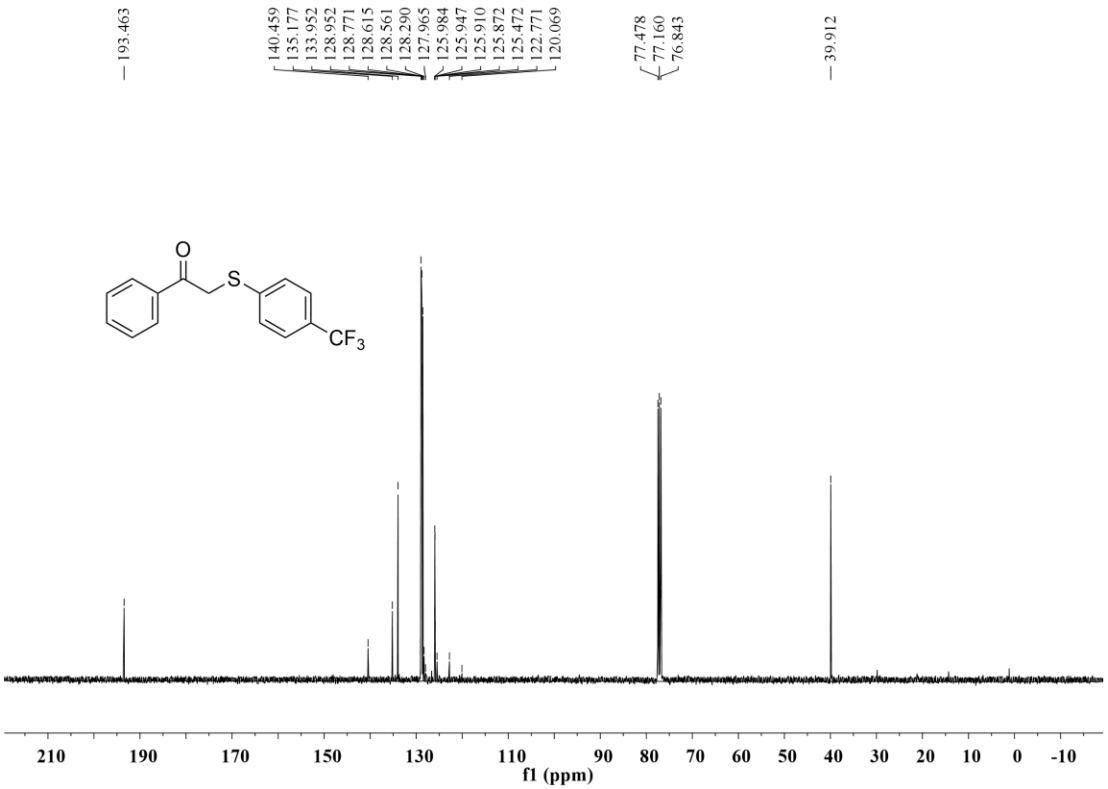
f1 (ppm)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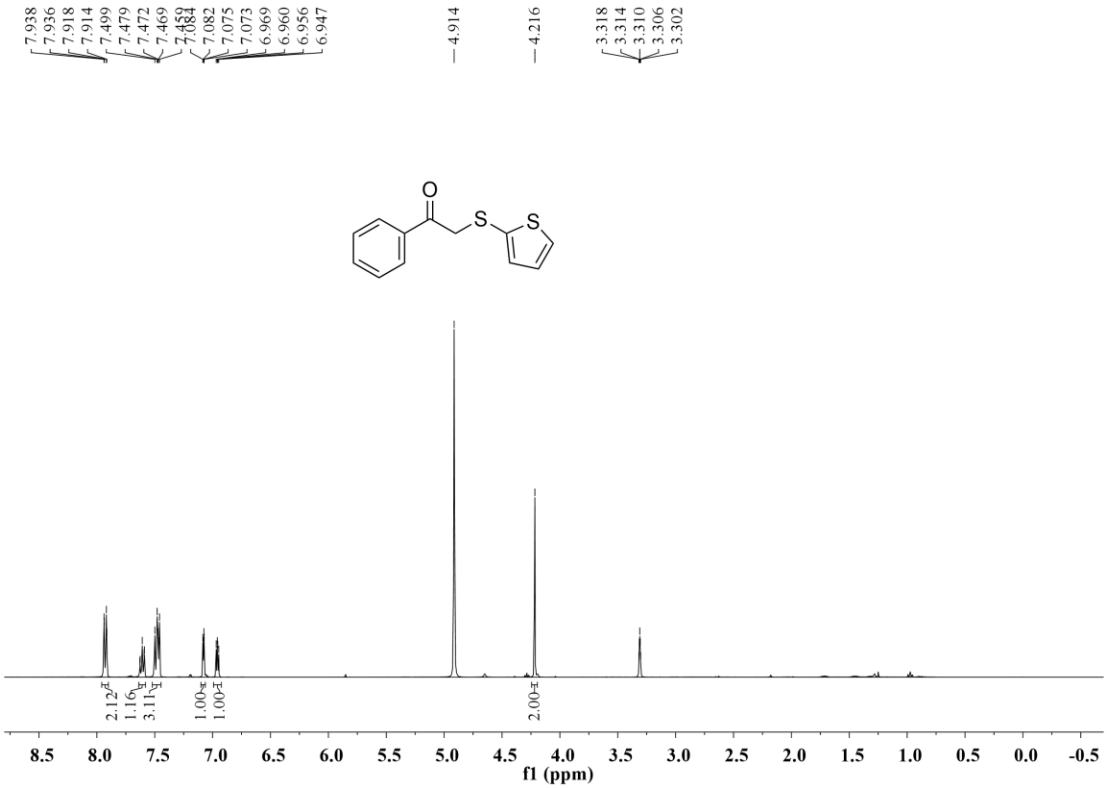
f1 (ppm)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3.310
3.306
3.302
O
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1.16
3.11
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1.00
2.00
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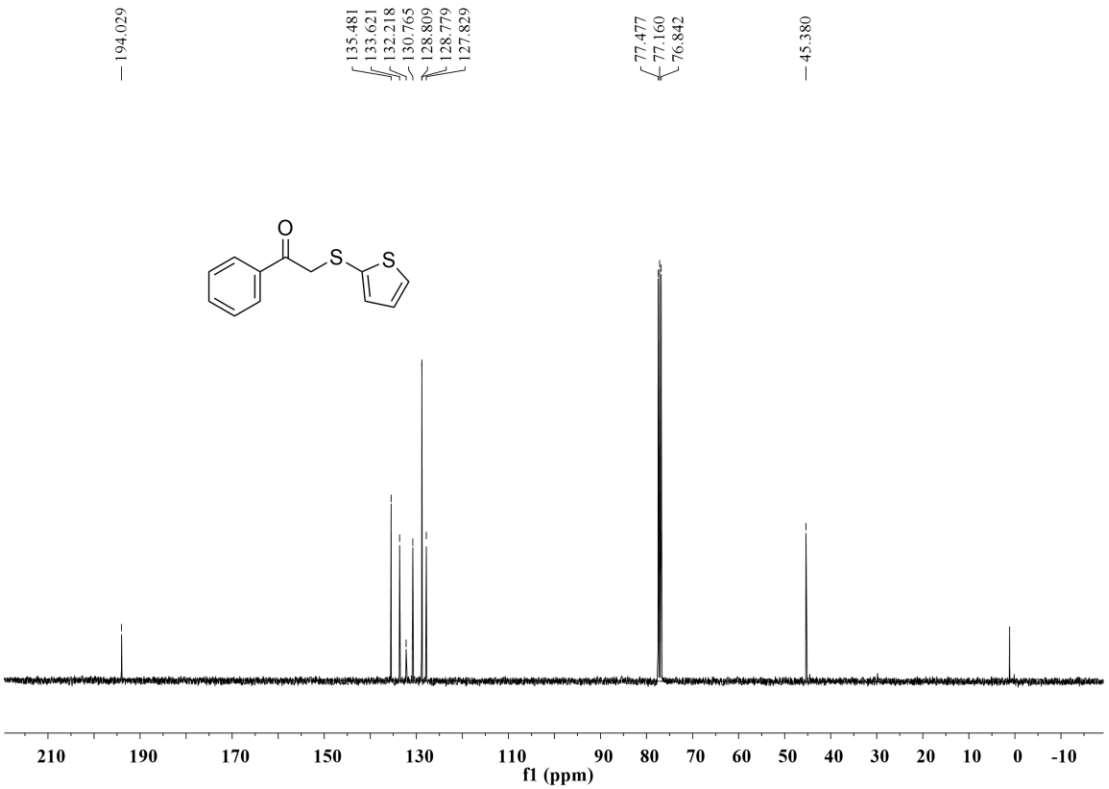
f1 (ppm)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S
S
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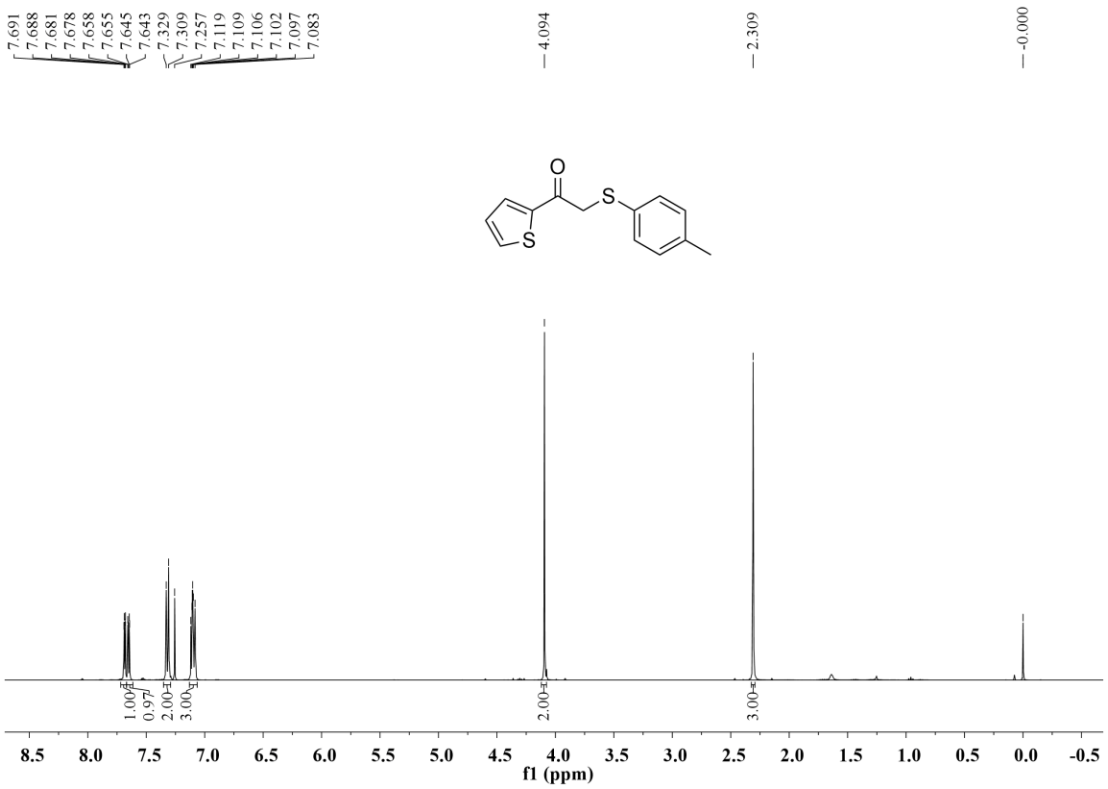
f1 (ppm)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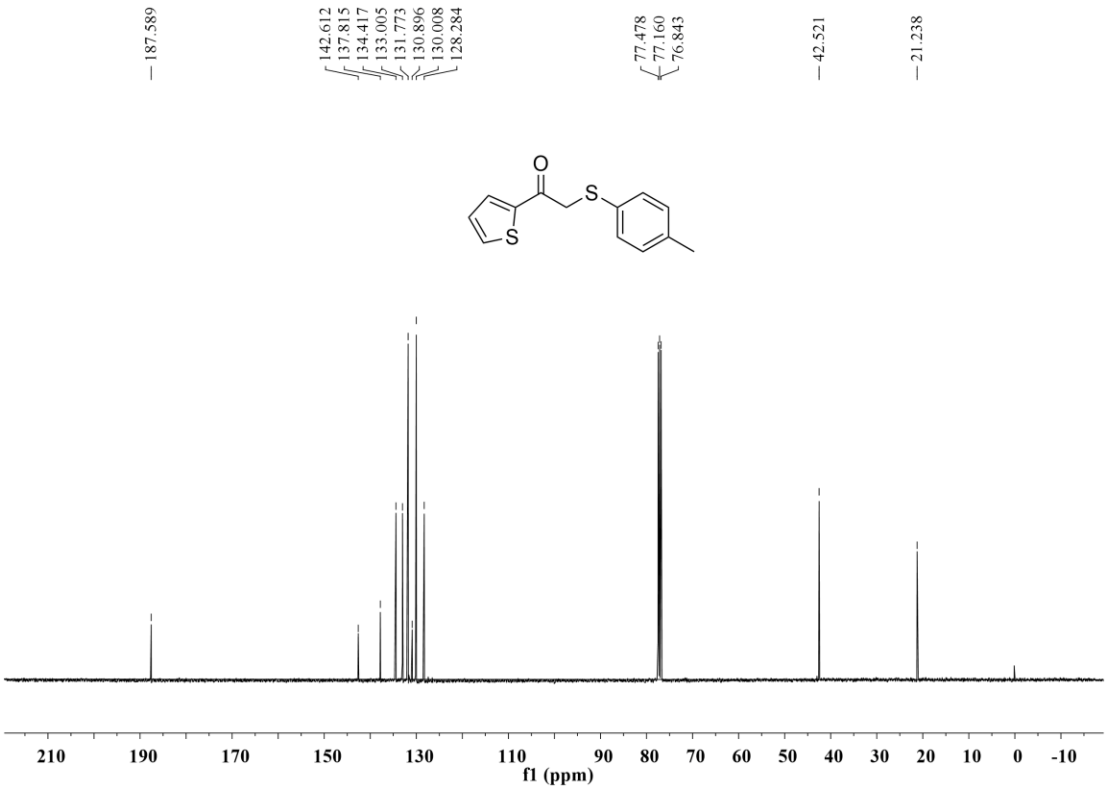
7.643
7.329
7.309
7.257
7.119
7.109
7.106
7.102
7.097
7.083
4.094
2.309
-0.000
O
S
S
1.00
0.97
2.00
3.00
2.00
3.00
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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142.612
137.815
134.417
133.005
131.773
130.896
130.008
128.284
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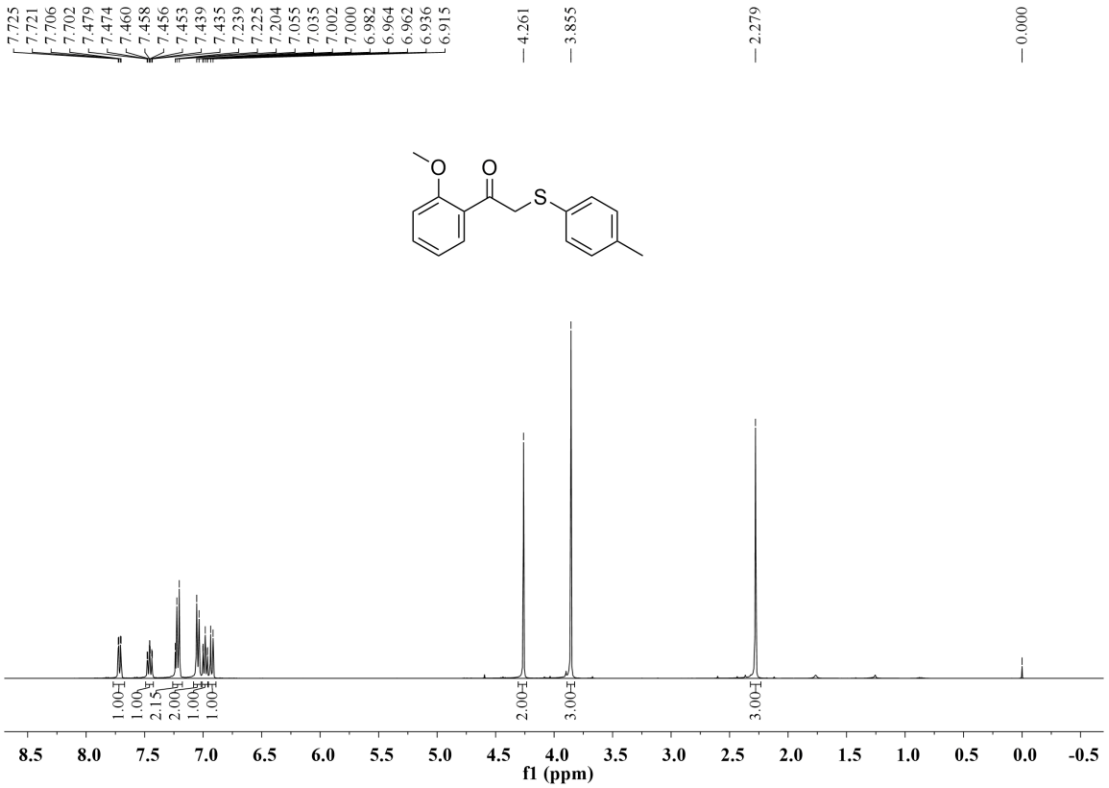
77.160
76.843
42.521
21.238
O
S
S
210 190 170 150 130 110 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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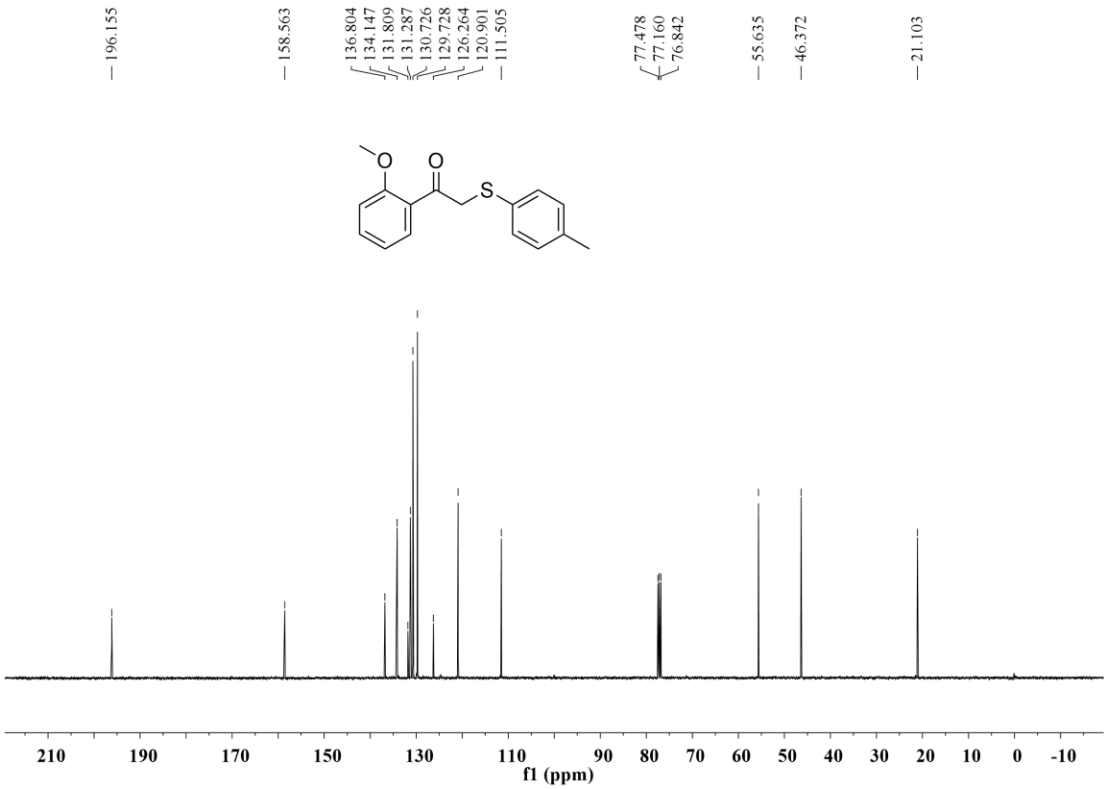
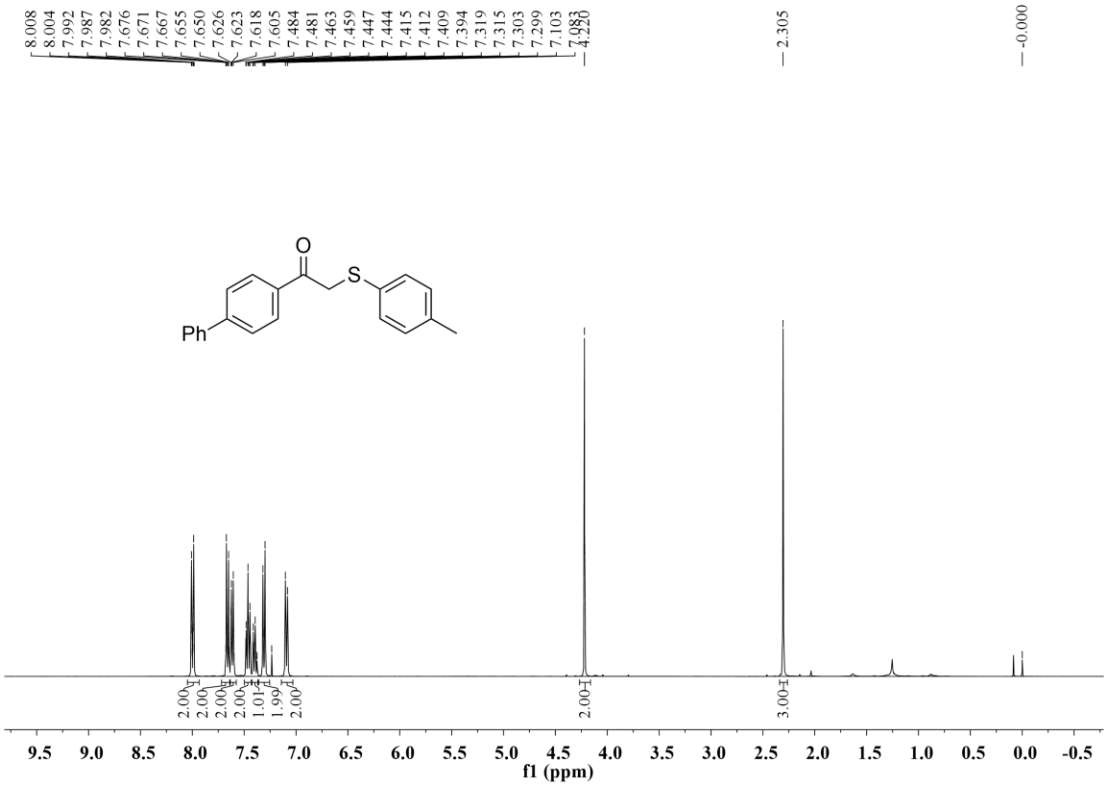
7.721
7.706
7.702
7.479
7.474
7.460
7.458
7.456
7.453
7.439
7.435
7.239
7.225
7.204
7.055
7.035
7.002
7.000
6.982
6.964
6.962
6.936
6.915
4.261
3.855
2.279
0.000
O
O
S
1.00
1.00
2.15
2.00
1.00
1.00
2.00
3.00
3.00
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)


196.155
158.563
136.804
134.147
131.809
131.287
130.726
129.728
126.264
120.901
111.505
77.478
77.160
76.842
55.635
46.372
21.103
O
O
S
210 190 170 150 130 110 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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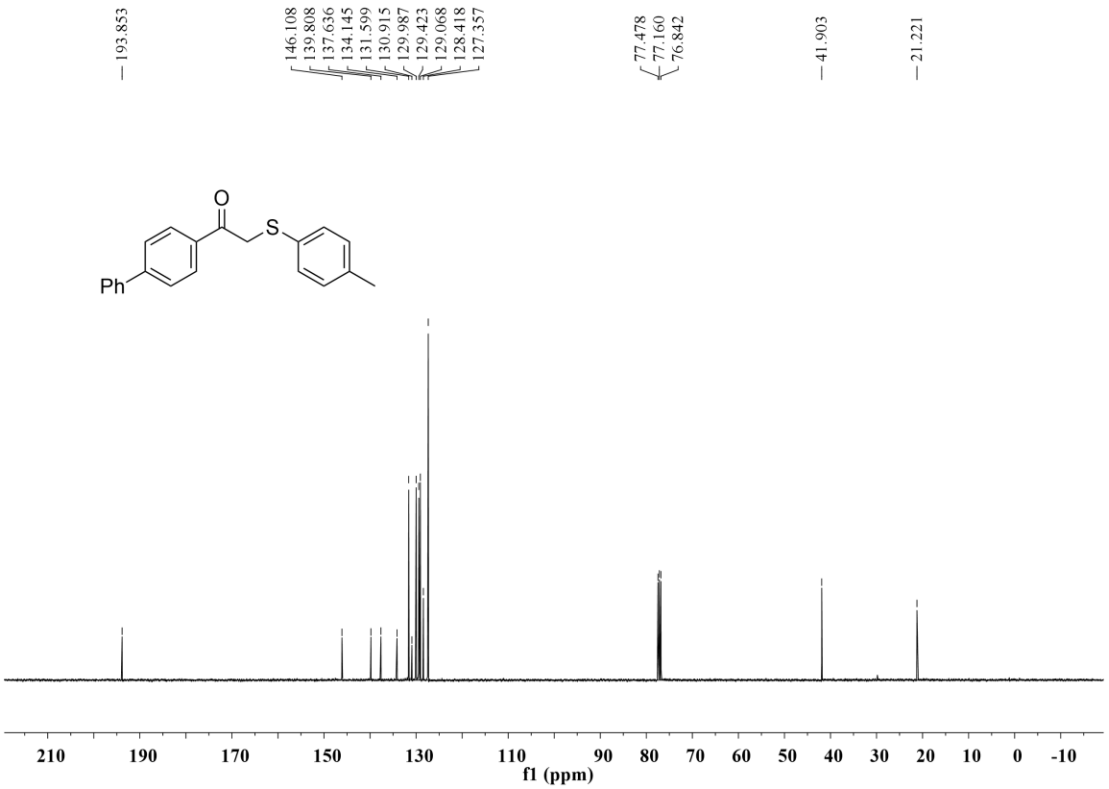
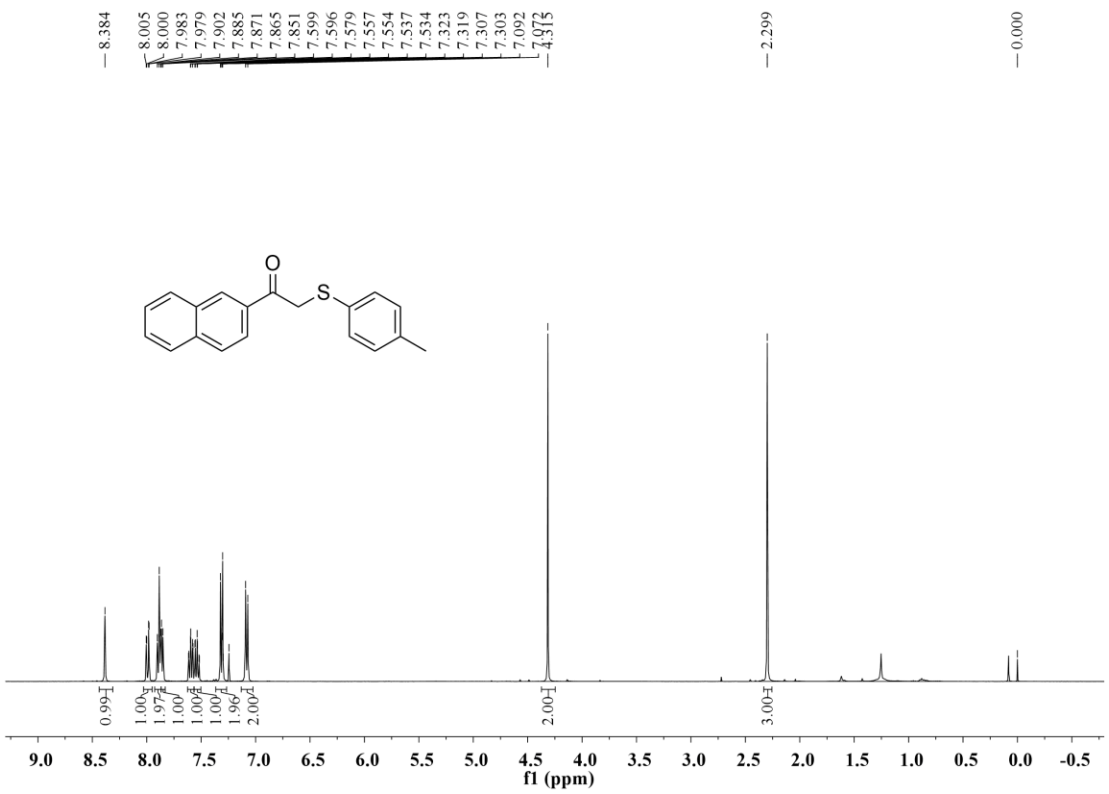
8.004
7.992
7.987
7.982
7.676
7.671
7.667
7.655
7.650
7.626
7.623
7.618
7.605
7.484
7.481
7.463
7.459
7.447
7.444
7.415
7.412
7.409
7.394
7.319
7.315
7.303
7.299
7.103
4.220
2.305
-0.000
O
S
Ph
2.00
2.00
2.00
2.00
1.01
1.99
2.00
2.00
3.00
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)


193.853
146.108
139.808
137.636
134.145
131.599
130.915
129.987
129.423
129.068
128.418
127.357
77.478
77.160
76.842
41.903
21.221
O
S
Ph
210 190 170 150 130 110 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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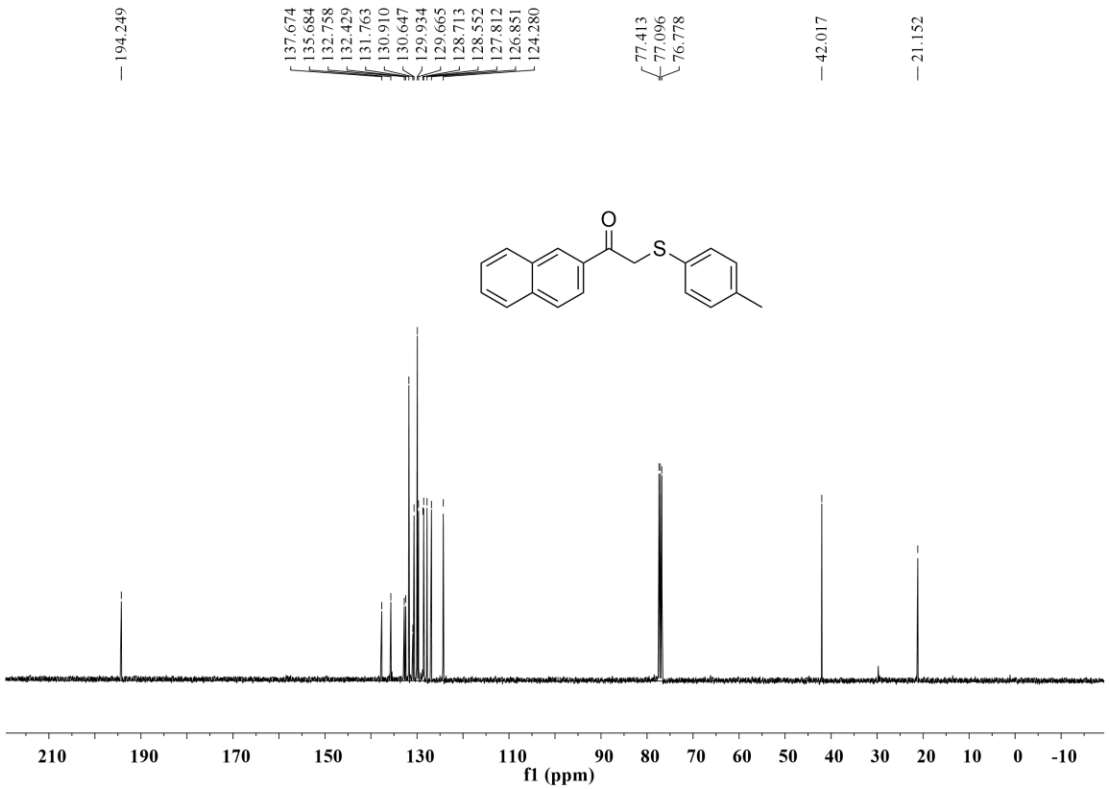
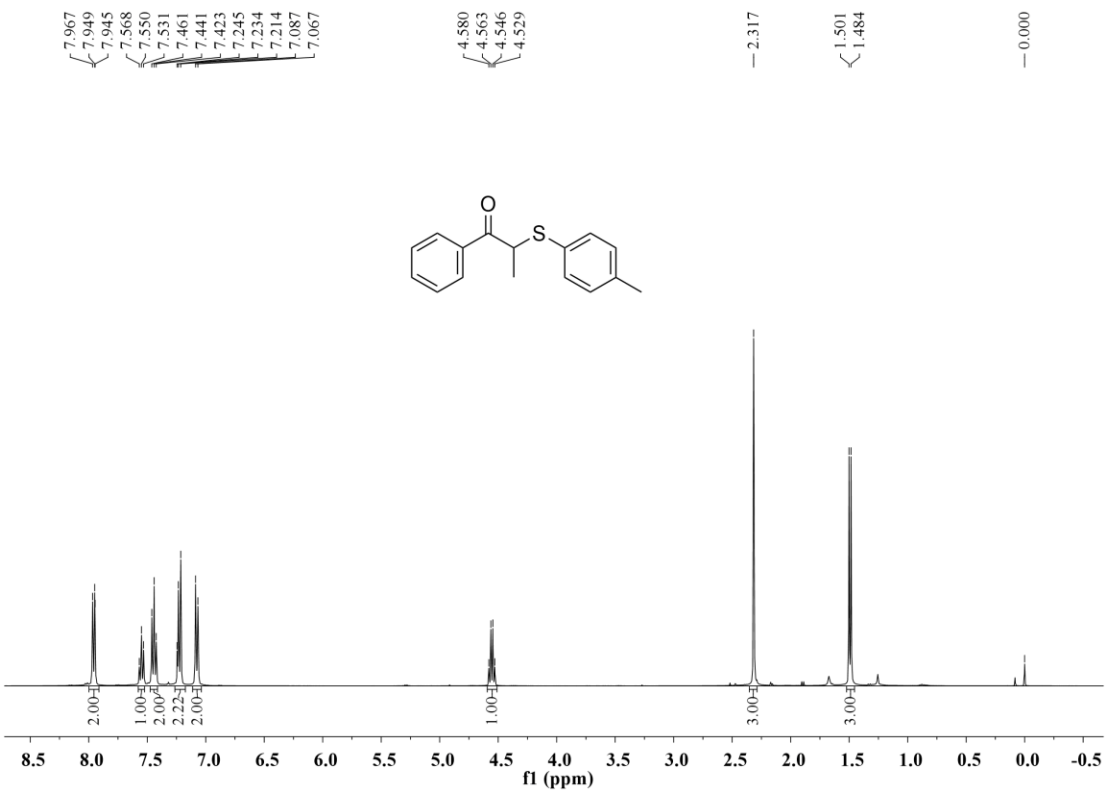
8.005
8.000
7.983
7.979
7.902
7.885
7.871
7.865
7.851
7.599
7.596
7.579
7.557
7.554
7.537
7.534
7.323
7.319
7.307
7.303
7.092
7.072
4.315
2.299
0.000
O
S
0.99
1.00
1.97
1.00
1.00
1.00
1.96
2.00
2.00
3.00
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)


194.249
137.674
135.684
132.758
132.429
131.763
130.910
130.647
129.934
129.665
128.713
128.552
127.812
126.851
124.280
77.413
77.096
76.778
42.017
21.152
O
S
210 190 170 150 130 110 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


7.967
7.949
7.945
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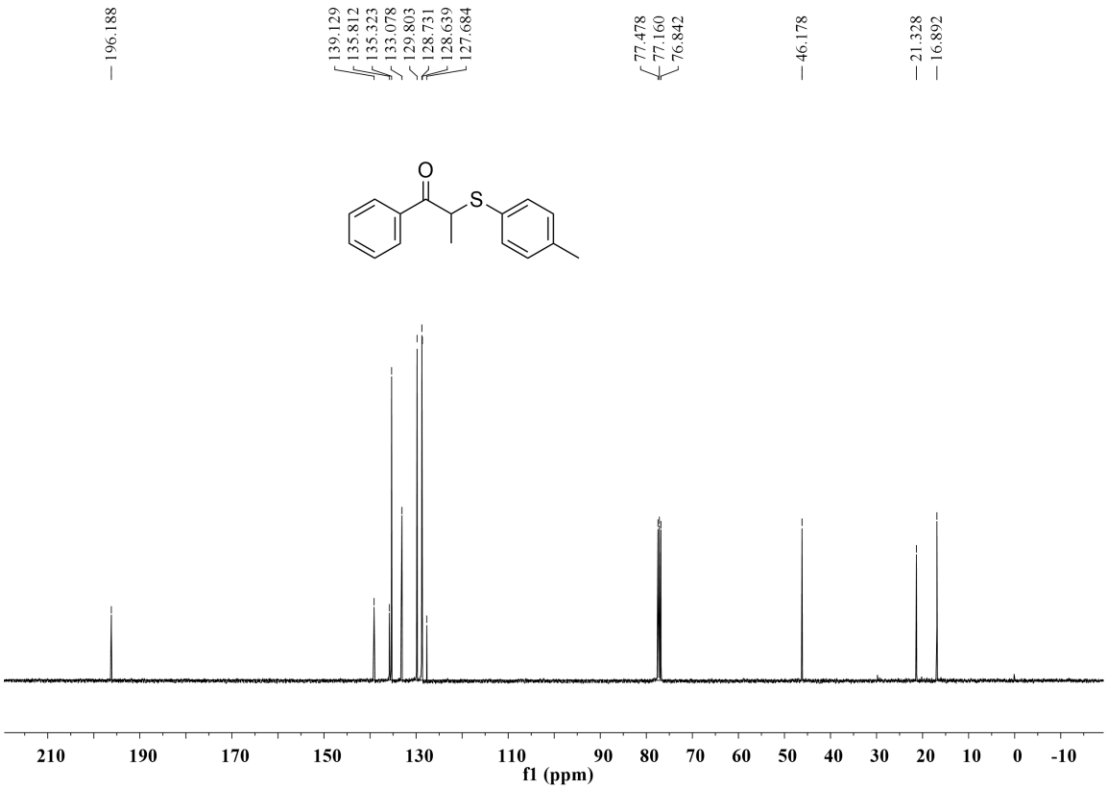
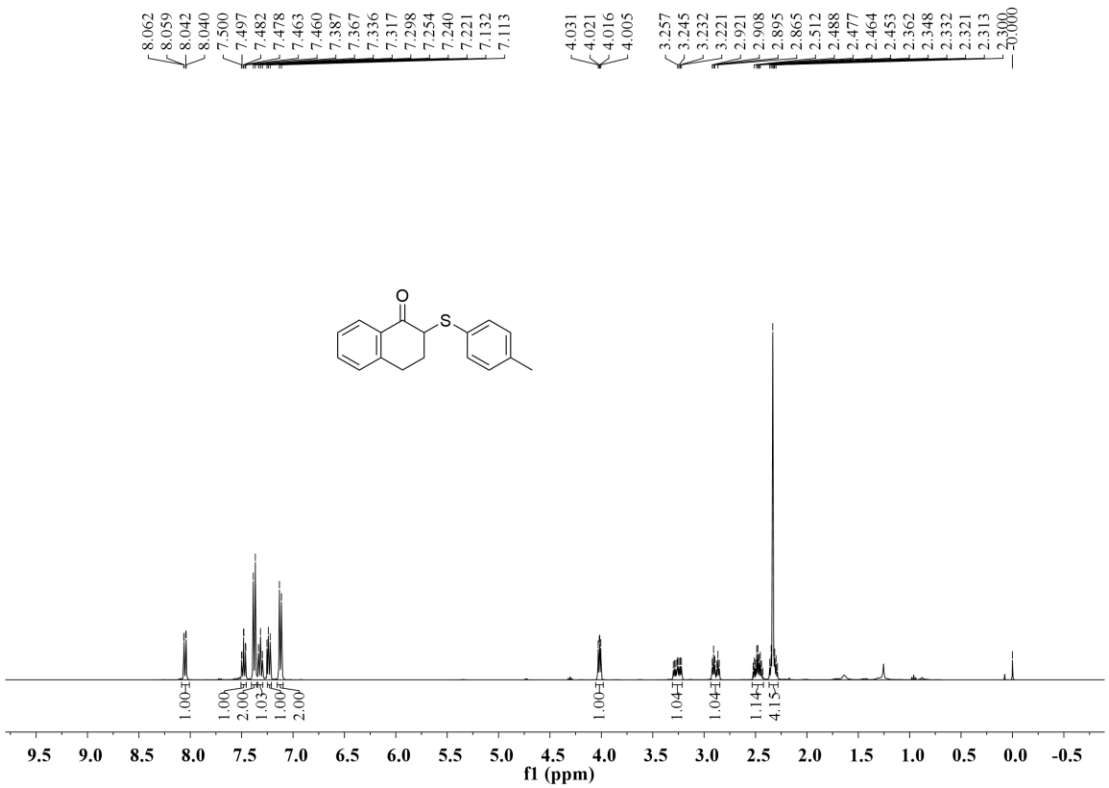
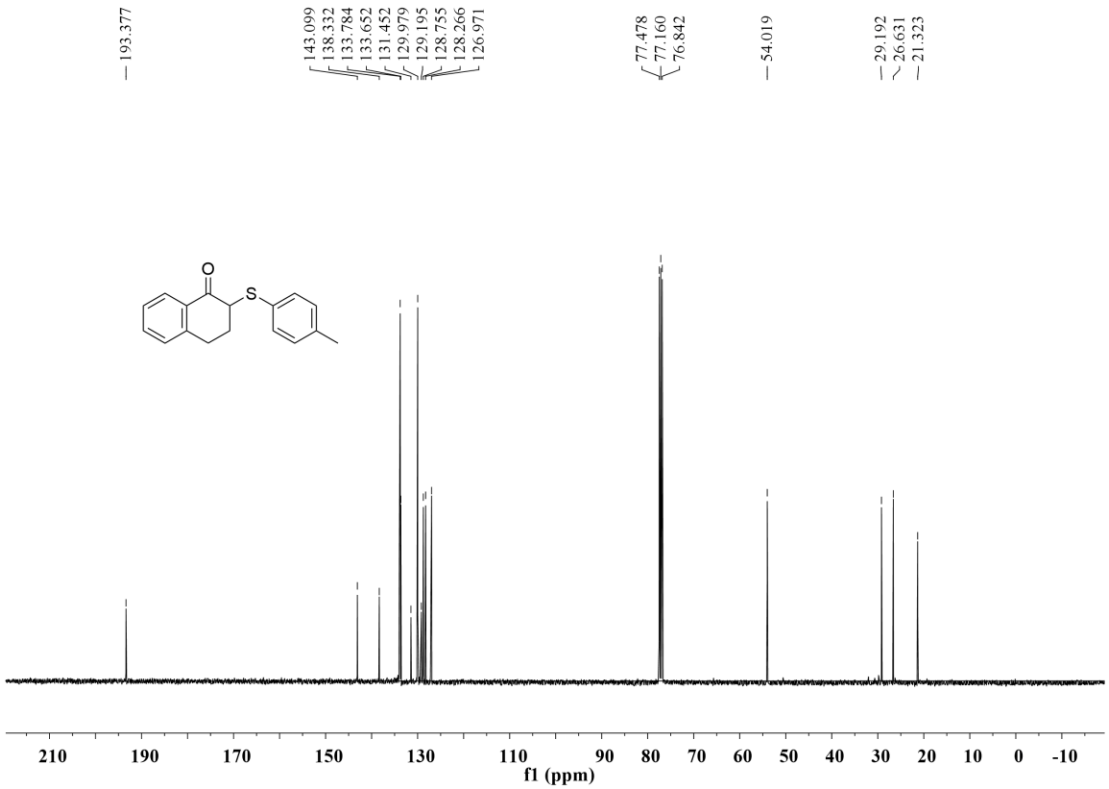
7.550
7.531
7.461
7.441
7.423
7.245
7.234
7.214
7.087
7.067
4.580
4.563
4.546
4.529
2.317
1.501
1.484
0.000
O
S
2.00
1.00
2.00
2.22
2.00
1.00
3.00
3.00
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)


196.188
139.129
135.812
135.323
133.078
129.803
128.731
128.639
127.684
77.478
77.160
76.842
46.178
21.328
16.892
O
S
210 190 170 150 130 110 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


8.062
8.059
8.042
8.040
7.500
7.497
7.482
7.478
7.463
7.460
7.387
7.367
7.336
7.317
7.298
7.254
7.240
7.221
7.132
7.113
4.031
4.021
4.016
4.005
3.257
3.245
3.232
3.221
2.921
2.908
2.895
2.865
2.512
2.488
2.477
2.464
2.453
2.362
2.348
2.332
2.321
2.313
2.300
0.000
O
S
1.00
1.00
2.00
1.03
1.00
2.00
1.00
1.04
1.04
1.14
4.15
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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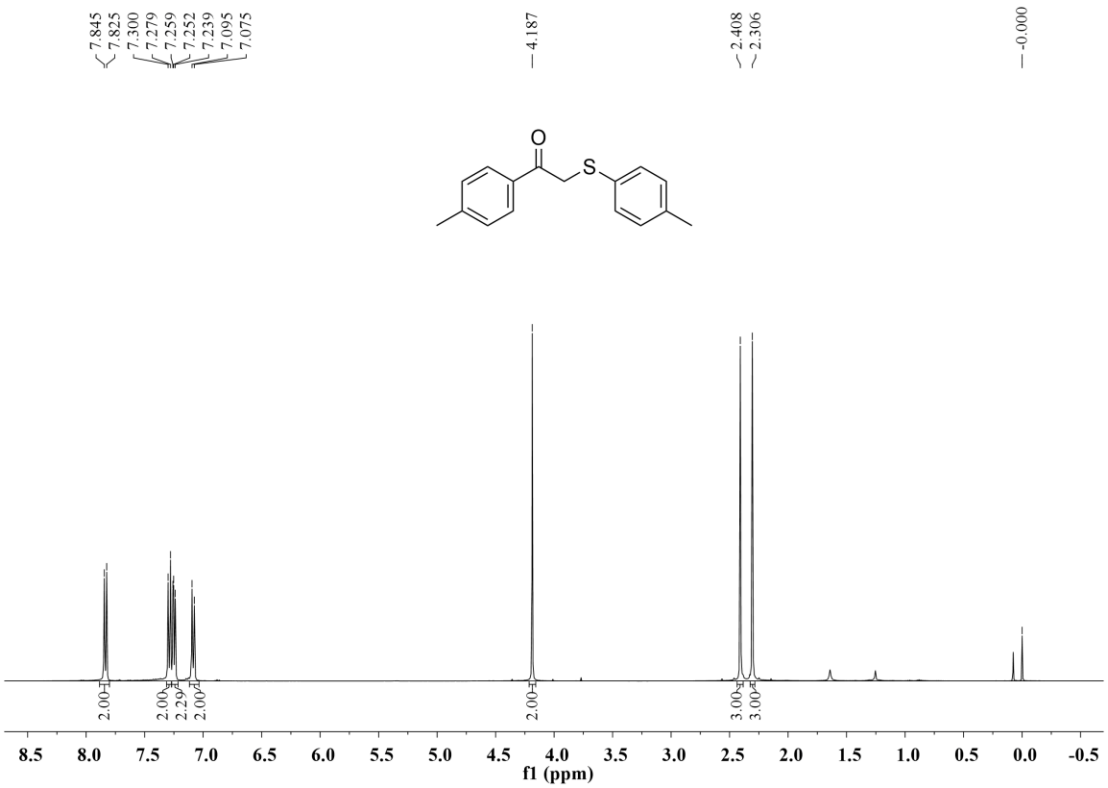
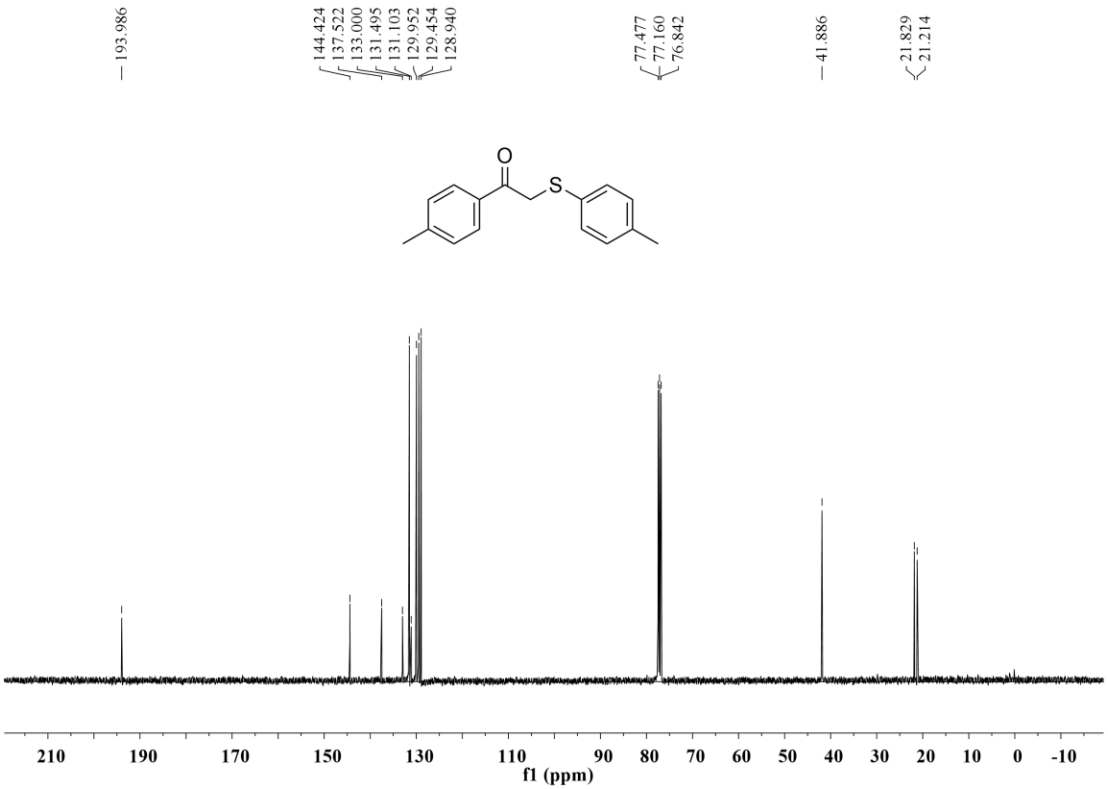
129.195
128.755
128.266
126.971
77.478
77.160
76.842
54.019
29.192
26.631
21.323
O
S
210 190 170 150 130 110 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


7.845
7.825
7.300
7.279
7.259
7.252
7.239
7.095
7.075
4.187
2.408
2.306
-0.000
O
S
2.00
2.00
2.29
2.00
2.00
3.00
3.00
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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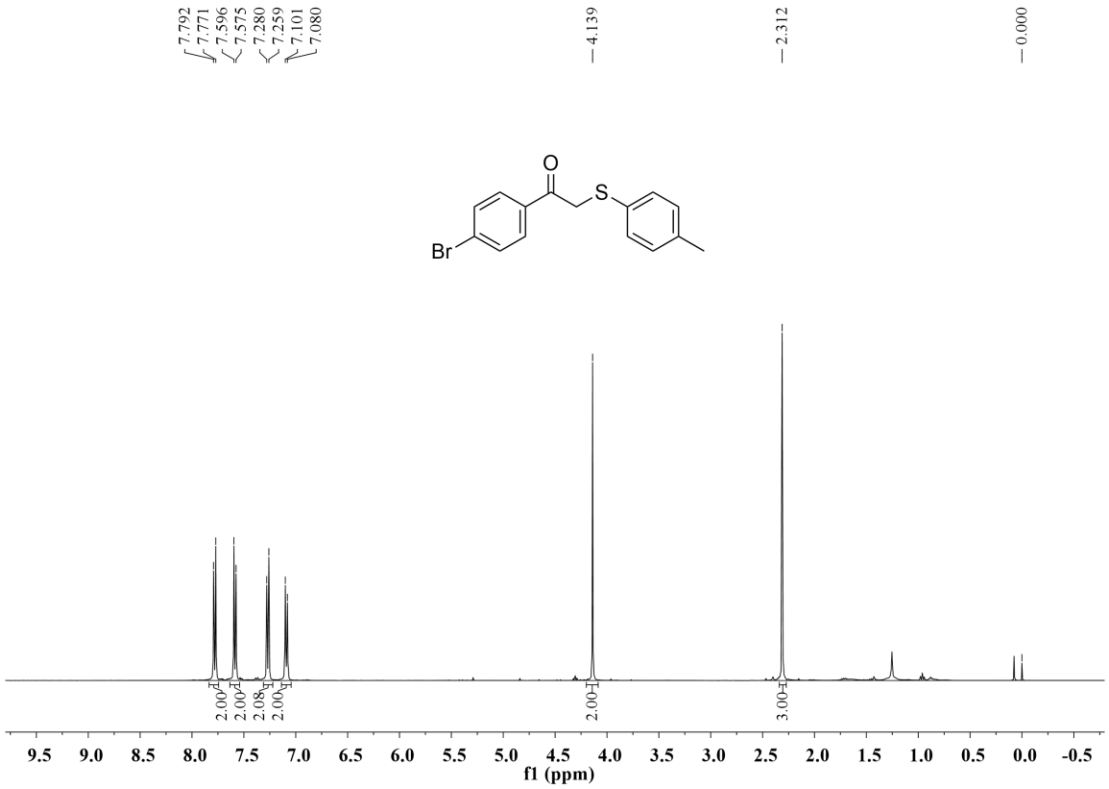
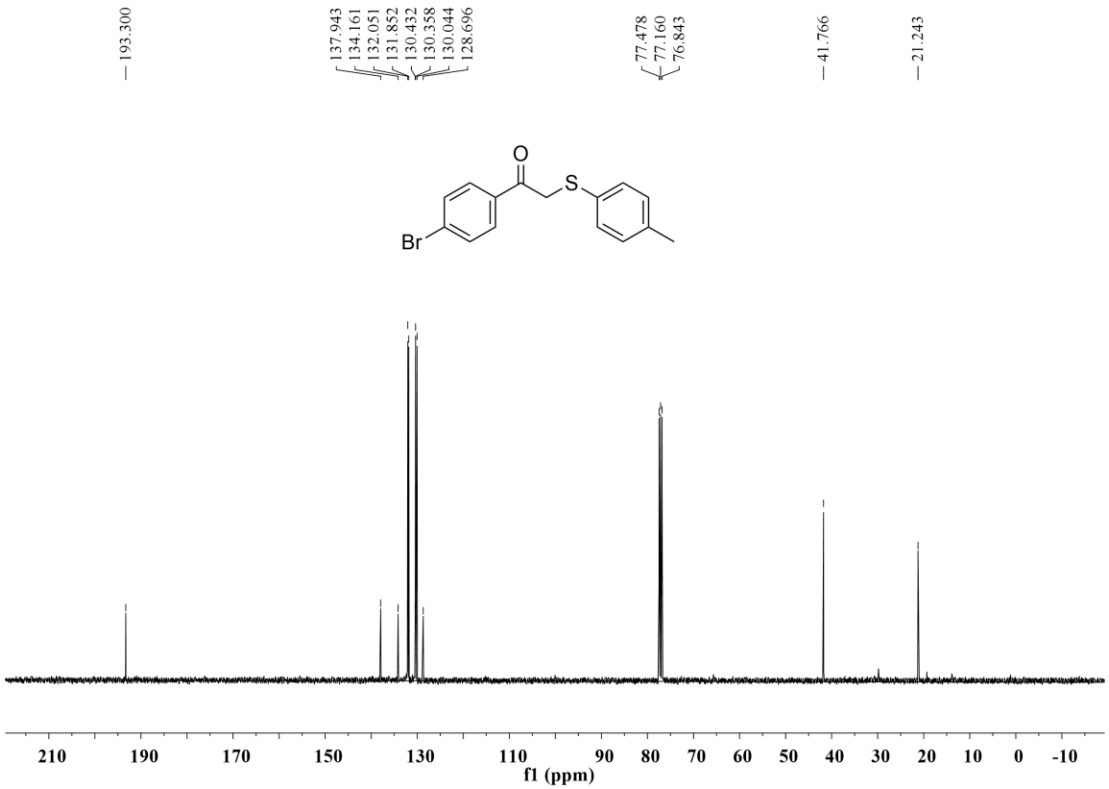
144.424
137.522
133.000
131.495
131.103
129.952
129.454
128.940
77.477
77.160
76.842
41.886
21.829
21.214
O
S
210 190 170 150 130 110 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


7.792
7.771
7.596
7.575
7.280
7.259
7.101
7.080
4.139
2.312
0.000
O
S
Br
2.00
2.00
2.08
2.00
2.00
3.00
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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134.161
132.051
131.852
130.432
130.358
130.044
128.696
77.478
77.160
76.843
41.766
21.243
O
S
Br
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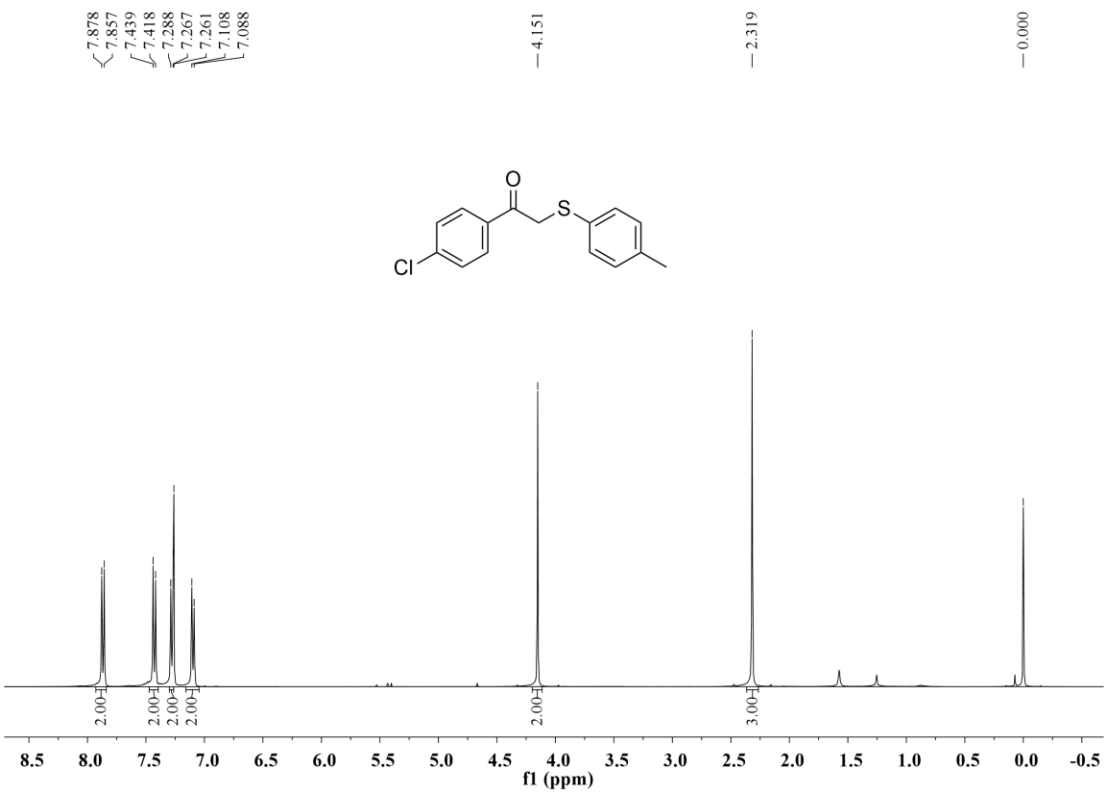
f1 (ppm)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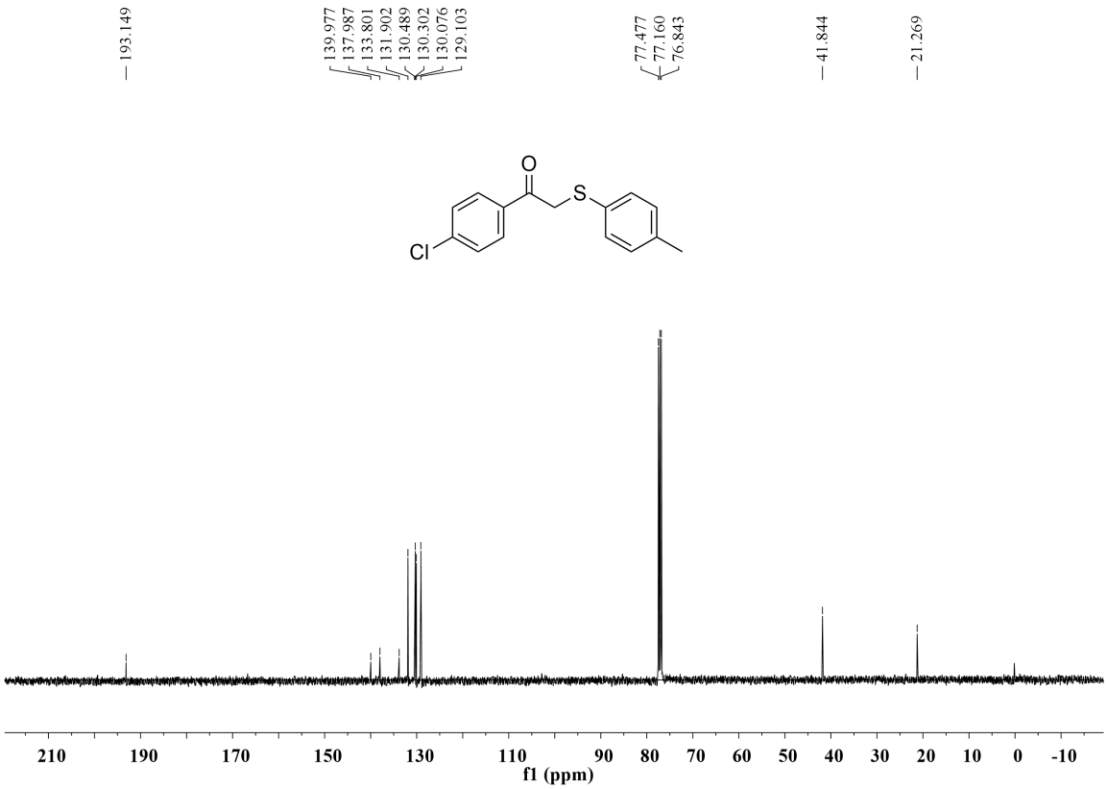
7.288
7.267
7.261
7.108
7.088
4.151
2.319
0.000
O
S
Cl
2.00
2.00
2.00
2.00
2.00
3.00
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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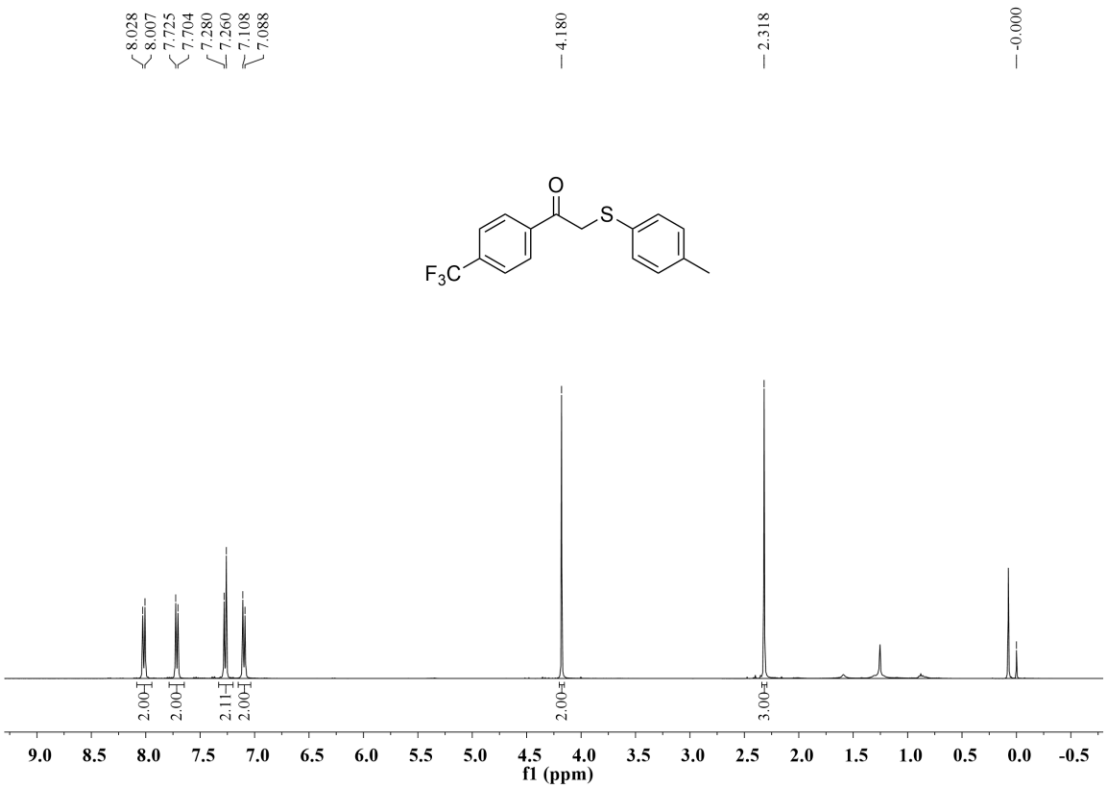
139.977
137.987
133.801
131.902
130.489
130.302
130.076
129.103
77.477
77.160
76.843
41.844
21.269
O
S
Cl
210 190 170 150 130 110 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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8.007
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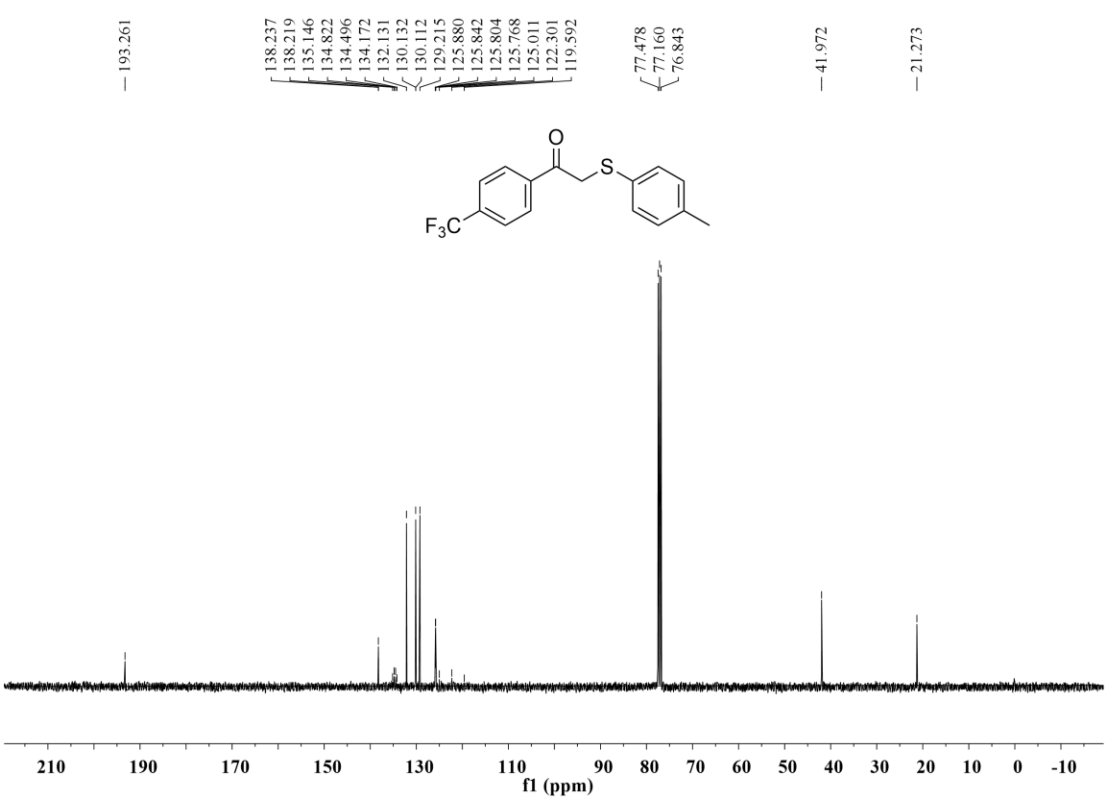
7.704
7.280
7.260
7.108
7.088
4.180
2.318
-0.000
O
S
F3C
2.00
2.00
2.11
2.00
2.00
3.00
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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138.219
135.146
134.822
134.496
134.172
132.131
130.132
130.112
129.215
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125.842
125.804
125.768
125.011
122.301
119.592
77.478
77.160
76.843
41.972
21.273
O
S
F3C
210 190 170 150 130 110 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)