Supporting Information for

Hemin-Catalyzed Sulfonium Ylide Formation and Subsequently Reactant-Controlled Chemoselective Rearrangements

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Table of Contents

1. General Information and Materials

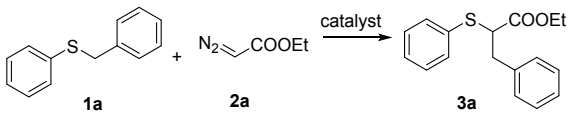
All reagents were purchased at the highest commercial quality and used without further purification. Purification of products was carried out with silica gel (academic grade, 200-300) and a preparative HPLC (Varian ProStar 215 and Shimadzu Shimpack-C 18 column, 250×20mm i.d.). Some NMR spectra were recorded at 400 MHz and 100 MHz with Bruker ARX-400 instrument. The Other NMR spectra were recorded at 600MHz and 150 MHz with Bruker Avance DMX-500 instrument. High resolution mass spectra (HRMS) were recorded on a Shimadzu LC/MS IT-TOF.

2. Preparation of benzyl sulfide [1]

1.2 equiv. of benzyl bromide were added to an ethanolic solution of thiophenol/thiol (3 mmmol) and K_2CO_3 (3.6 mmol) at room temperature, and the reaction was stirred overnight. The resulting mixture was concentrated and extracted with CH_2Cl_2. Then the extract was purified by column chromatography (petroleum ether) to afford the desired sulfide.

3. Screening reaction conditions

Table S1. Screening reaction condition[a]



1a 2a 3a

entry	catalyst (mol%)	solvent	temp(°C)	time(h)	yield[b] (%)
1	hemin(2.5)	Et_2O	40	48	N.R.
2	hemin(2.5)	Pyridine	40	48	N.R.
3	hemin(2.5)	MeCN	40	48	N.R.

4	hemin(2.5)	$CHCl_3$	40	48	19
5	hemin(2.5)	Acetone	40	48	47
6	hemin(2.5)	DMF	40	48	52
7	hemin(2.5)	CH_2Cl_2	40	48	27
8	hemin(2.5)	H_2O	40	48	57
9	hemin(2.5)	EtOH	40	48	36
10	hemin(2.5)	THF	40	48	88
11	hemin(5)	THF	40	48	70
12	hemin(2.5)	THF	80	8	85
13	hemin(2.5)	THF	40	8	23
14	hemin(2.5)	THF	0	8	1
15	hemin(2.5)	THF	80	10	83
16	hemin(2.5)	THF	80	12	77
17[c]	hemin(2.5)	THF	80	12	76
18[d]	hemin(2.5)	THF	80	12	66
19[e]	hemin(2.5)	THF	80	12	79

[a]The molar ratio **2a** / **1a** was 2.

[b]Yield was determined by ^1H NMR analysis of the crude reaction mixture.

[c]The molar ratio **2a** / **1a** was 2.5.

[d]The molar ratio **2a** / **1a** was 1.5.

[e]N_2 protected.

4. General procedures for [1, 2]-Stevens rearrangement

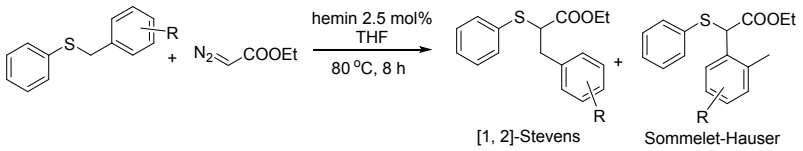
Sulfide (1.5 mmol) was added into a solution of hemin (0.0375 mmol) in 15 mL THF, followed by adding 3 mmol diazo reagent in one portion. The reaction mixture was strirred at 80 °C for 8 hours, then the solvent was removed in vacuum and hemin was removed by a short silica gel column. Finally, the crude reaction mixture was purified by a preparative HPLC with a C-18 column using elution of methanol/ H_2O 80: 20 to obtain the corresponding product.

5. General procedures for Sommelet-Hauser rearrangement

Sulfide (1.5 mmol) was added into 15 mL aqueous solution of 0.0375 mmol hemin, followed by adding 3 mmol diazo reagent in one portion. The reaction was then placed in a constant temperature shaker and left to shake at 200 rpm under 40 °C. After 12 hours, the mixture was extracted thrice with EtOAc. The organic layer was further washed with brine and then dried with Na_2SO_4. Then the organic solvent was removed in vacuum and hemin was removed by a short silica gel column. Finally, the crude reaction mixture was purified by a preparative HPLC with a C-18 column using elution of methanol/ H_2O 80: 20 to obtain the corresponding product.

6. Substrate electronic effects on Stevens/ Sommelet-Hauser rearrangement

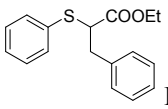
Table S2. Substrate electronic effects of Stevens/ Sommelet-Hauser rearrangement



Entry	R	Hammett constant σ[2]	Yield[b] (%)	
			Stevens	Sommelet-Hauser
1	*p*-NO_2	0.78	0	94
2	*p*-CN	0.66	36	54
3	*p*-CF_3	0.54	71	20
4	*p*-COOMe	0.45	54	23
5	*p*-Br	0.23	76	10
6	*p*-Cl	0.23	87	0
7	*p*-F	0.06	89	0
8	H	0	81	0
9	*p*-Me	−0.17	71	0

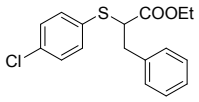
[a]Reaction were carried out under standard reaction conditions as in entry 12 of Table 1. [b]Isolated yield based on sulfide.

7. Experimental Characterization of Products



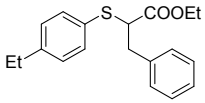
Ethyl 3-phenyl-2-(phenylthio)propionate (**3a**):

Colorless oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.45 – 7.42 (m, 2H), 7.32 – 7.25 (m, 5H), 7.23 – 7.18 (m, 3H), 4.06 – 3.98 (m, 2H), 3.90 (dd, *J* = 9.4, 6.3 Hz, 1H), 3.22 – 3.03 (m, 2H), 1.06 (t, *J* = 7.1 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 171.7, 137.8, 133.3, 133.2, 129.2, 129.1, 128.6, 128.2, 127.0, 61.2, 52.3, 38.1, 14.1. HRMS (ESI) calcd. for $(M+Na)^+$ $(C_{17}H_{18}O_2SNa)^+$: 309.0920, found: 309.0898.



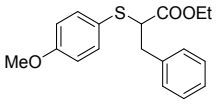
Ethyl 2-((4-chlorophenyl)thio)-3-phenylpropionate (**3b**):

Colorless oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.37 – 7.34 (m, 2H), 7.30 – 7.21 (m, 5H), 7.20 – 7.17 (m, 2H), 4.09 – 3.98 (m, 2H), 3.85 (dd, *J* = 9.1, 6.5 Hz, 1H), 3.21 – 3.01 (m, 2H), 1.08 (t, *J* = 7.1 Hz, 3H).^{13}C NMR (100 MHz, $CDCl_3$) δ 171.5, 137.6, 134.6, 134.5, 131.8, 129.2, 129.2, 128.6, 127.1, 61.3, 52.4, 38.0, 14.1. HRMS (ESI) calcd. for $(M+Na)^+$ $(C_{17}H_{17}ClO_2SNa)^+$: 343.0530, found: 343.0520.



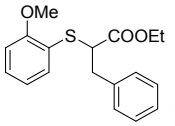
Ethyl 2-((4-ethylphenyl)thio)-3-phenylpropionate (**3c**):

Colorless oil; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.36 (d, *J* = 8.1 Hz, 2H), 7.27 (t, *J* = 7.2 Hz, 2H), 7.22 – 7.18 (m, 3H), 7.13 (d, *J* = 8.1 Hz, 2H), 4.06 – 3.97 (m, 2H), 3.83 (dd, *J* = 9.5, 6.2 Hz, 1H), 3.19 – 3.02 (m, 2H), 2.63 (q, *J* = 7.6 Hz, 2H), 1.22 (t, *J* = 7.6 Hz, 3H), 1.06 (t, *J* = 7.1 Hz, 3H).^{13}C NMR (125 MHz, $CDCl_3$) δ 171.8, 144.9, 138.0, 134.0, 129.7, 129.2, 128.7, 128.6, 126.9, 61.1, 52.6, 38.1, 28.7, 15.5, 14.1. HRMS (ESI) calcd. for $(M+Na)^+$ $(C_{19}H_{22}O_2SNa)^+$: 337.1233, found: 337.1210.



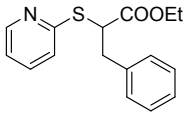
Ethyl 2-((4-methoxyphenyl)thio)-3-phenylpropionate (**3d**):

Colorless oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.29 – 7.16 (m, 8H), 7.08 (d, *J* = 7.4 Hz, 1H), 4.09 – 3.97 (m, 2H), 3.88 (dd, *J* = 9.4, 6.3 Hz, 1H), 3.22 –3.03 (m, 2H), 2.31 (s, 3H), 1.07 (t, *J* = 7.1 Hz, 3H).^{13}C NMR (100 MHz, $CDCl_3$) δ 171.8, 138.8, 137.9, 133.7, 133.1, 130.1, 129.2, 129.0, 128.9, 128.6, 127.0, 61.2, 52.4, 38.2, 21.4, 14.1. HRMS (ESI) calcd. for $(M+Na)^+$ $(C_{18}H_{20}O_3SNa)^+$: 339.1025, found: 339.1003.



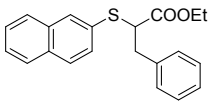
Ethyl 2-((2-methoxyphenyl)thio)-3-phenylpropionate (**3e**):

Colorless oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.44 (dd, *J* = 7.5, 1.6 Hz, 1H), 7.31 – 7.19 (m, 6H), 6.91 – 6.86 (m, 2H), 4.08 – 4.01 (m, 1H), 3.98 – 3.92 (m, 2H), 3.87 (s, 3H), 3.24 – 3.06 (m, 2H), 1.00 (t, *J* = 7.1 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 171.8, 159.2, 138.1, 134.9, 130.0, 129.1, 128.5, 126.8, 120.9, 110.9, 61.0, 55.9, 50.1, 37.9, 14.0. HRMS (ESI) calcd. for $(M+Na)^+$ $(C_{18}H_{20}O_3SNa)^+$: 339.1025, found: 339.1003.



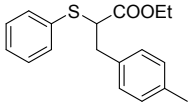
Ethyl 3-phenyl-2-(2-pyridin-2-ylthio)propionate (**3f**):

Yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.42 (d, *J* = 4.4 Hz, 1H), 7.48 (td, *J* = 8.1, 1.6 Hz, 1H), 7.28 (m, *J* = 4.4 Hz, 4H), 7.24 – 7.18 (m, 2H), 7.02 –6.98 (m, 1H), 4.84 (dd, *J* = 8.6, 6.8 Hz, 1H), 4.17 – 4.04 (m, 2H), 3.33 –3.18 (m, 2H), 1.13 (t, *J* = 7.1 Hz, 3H).^{13}C NMR (100 MHz, $CDCl_3$) δ 172.0, 157.2, 149.4, 137.9, 136.3, 129.3, 128.5, 127.0, 122.7, 120.1, 61.4, 48.2, 38.4, 14.1. HRMS (ESI) calcd. for $(M+Na)^+$ $(C_{16}H_{17}NO_2SNa)^+$: 310.0872, found: 310.0849.



Ethyl 2-(naphthalin-2-ylthio)-3-phenylpropionate (**3g**):

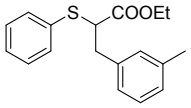
Yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.91 (s, 1H), 7.78 – 7.72 (m, 3H), 7.48 – 7.44 (m, 3H), 7.28 – 7.19 (m, 5H), 4.06 – 3.95 (m, 3H), 3.27 – 3.08 (m, 2H), 1.01 (t, *J* = 7.1 Hz, 3H).^{13}C NMR (100 MHz, $CDCl_3$) δ 171.7, 137.8, 133.6, 132.7, 132.1, 130.8, 130.0, 129.2, 128.6, 128.6, 127.8, 127.6, 127.0, 126.6, 126.6, 61.2, 52.3, 38.1, 14.0. HRMS (ESI) calcd. for $(M+Na)^+$ $(C_{21}H_{20}O_2SNa)^+$: 359.1076, found: 359.1057.



Ethyl 3-(4-methylphenyl)-2-(phenylthio)propionate (**3h**):

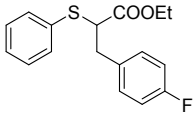
Colorless oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.45 – 7.43 (m, 2H), 7.31 – 7.24 (m, 3H), 7.08 (m, 4H), 4.08 – 3.96 (m, 2H), 3.90 – 3.86 (m, 1H), 3.19 – 2.99 (m, 2H), 2.30 (s, 3H), 1.07 (t, *J* = 7.1 Hz, 3H).^{13}C

NMR (100 MHz, $CDCl_3$) δ 171.8, 136.5, 134.7, 133.1, 129.2, 129.0, 128.1, 61.2, 52.3, 37.6, 21.2, 14.0. HRMS (ESI) calcd. for $(M+Na)^+$ $(C_{18}H_{20}O_2SNa)^+$: 323.1076, found: 323.1053.



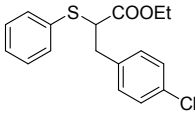
Ethyl 3-(3-methylphenyl)-2-(phenylthio)propionate (**3i**):

Colorless oil; ^1H NMR (400 MHz, $CDCl_3$) δ 7.45 – 7.43 (m, 2H), 7.31 – 7.24 (m, 3H), 7.15 (t, J = 7.5 Hz, 1H), 7.00 (t, J = 9.8 Hz, 3H), 4.07 – 3.98 (m, 2H), 3.89 (dd, J = 9.3, 6.3 Hz, 1H), 3.09 (ddd, J = 20.1, 13.9, 7.8 Hz, 2H), 2.30 (s, 3H), 1.06 (t, J = 7.1 Hz, 3H).^{13}C NMR (100 MHz, $CDCl_3$) δ 171.7, 138.1, 137.7, 133.4, 133.1, 129.9, 129.0, 128.4, 128.1, 127.7, 126.1, 61.1, 52.3, 38.0, 21.4, 14.0. HRMS (ESI) calcd. for $(M+Na)^+$ $(C_{18}H_{20}O_2SNa)^+$: 323.1076, found: 323.1052.



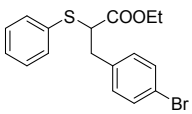
Ethyl 3-(4-fluorophenyl)-2-(phenylthio)propionate (**3j**):

Yellow oil; ^1H NMR (400 MHz, $CDCl_3$) δ 7.46 – 7.43 (m, 2H), 7.32 – 7.28 (m, 3H), 7.19 – 7.14 (m, 2H), 6.99 – 6.94 (m, 2H), 4.08 – 3.98 (m, 2H), 3.86 (dd, J = 9.3, 6.3 Hz, 1H), 3.20 – 3.01 (m, 2H), 1.08 (t, J = 7.1 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 171.6, 163.1, 160.7, 133.5, 133.5, 133.3, 133.2, 130.7, 130.7, 129.1, 128.3, 115.5, 115.3, 61.3, 52.4, 52.4, 37.2, 14.0. HRMS (ESI) calcd. for $(M+Na)^+$ $(C_{17}H_{17}FO_2SNa)^+$: 327.0825, found: 327.0793.



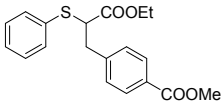
Ethyl 3-(4-chlorophenyl)-2-(phenylthio)propionate (**3k**):

Colorless oil; ^1H NMR (400 MHz, $CDCl_3$) δ 7.45 – 7.41 (m, 2H), 7.31 – 7.27 (m, 3H), 7.25 – 7.22 (m, 2H), 7.13 – 7.11 (m, 2H), 4.08 – 3.97 (m, 2H), 3.84 (dd, J = 9.3, 6.4 Hz, 1H), 3.18 – 2.99 (m, 2H), 1.08 (t, J = 7.1 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 171.5, 136.3, 133.4, 133.0, 132.8, 130.5, 129.1, 128.7, 128.3, 61.3, 52.1, 37.3, 14.1. HRMS (ESI) calcd. for $(M+Na)^+$ $(C_{17}H_{17}ClO_2SNa)^+$: 343.0530, found: 343.0508.



Ethyl 3-(4-bromophenyl)-2-(phenylthio)propionate (**3l**):

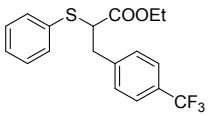
Colorless oil; ^1H NMR (400 MHz, $CDCl_3$) δ 7.46 – 7.38 (m, 4H), 7.34 – 7.29 (m, 3H), 7.08 – 7.06 (m, 2H), 4.06 – 3.99 (m, 2H), 3.83 (dd, J = 9.3, 6.3 Hz, 1H), 3.17– 2.98 (m, 2H), 1.09 (t, J = 7.1 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 171.5, 136.8, 133.4, 133.0, 131.7, 131.0, 129.1, 128.4, 120.9, 61.4, 52.0, 37.4, 14.1. HRMS (ESI) calcd. for $(M+Na)^+$ $(C_{17}H_{17}BrO_2SNa)^+$: 387.0025, found: 387.0007.



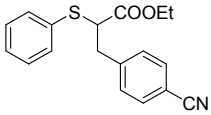
Ethyl 3-(4-methoxycarbonylphenyl)-2-(phenylthio)propionate (**3m**):

Colorless oil; ^1H NMR (400 MHz, $CDCl_3$) δ 7.96 – 7.94 (m, 2H), 7.45 – 7.43 (m, 2H), 7.32 – 7.26 (m, 5H), 4.09 – 3.97 (m, 2H), 3.91 – 3.87 (m, 1H), 3.90 (s, 3H), 3.27 – 3.08 (m, 2H), 1.08 (t, J = 7.1 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 171.4, 167.0, 143.2, 133.5, 132.9, 129.9, 129.3, 129.1, 128.9,

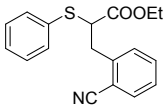
128.5, 61.4, 52.2, 51.9, 38.0, 14.1. HRMS (ESI) calcd. for $(M+Na)^+$ $(C_{19}H_{20}O_4SNa)^+$: 367.0975, found: 367.0954.



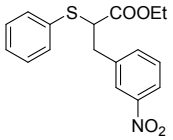
Ethyl 2-(phenylthio)-3-(4-(trifluoromethyl)phenyl)- propionate (**3n**):
Colorless oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.54 – 7.52 (m, 2H), 7.45 – 7.41 (m, 2H), 7.32 – 7.30 (m, 5H), 4.10 – 3.98 (m, 2H), 3.87 (dd, J = 9.2, 6.4 Hz, 1H), 3.28 – 3.08 (m, 2H), 1.08 (t, J = 7.1 Hz, 3H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 171.4, 141.9, 133.5, 132.8, 129.6, 129.3 (q, J_{CF} = 32.3 Hz), 129.2, 128.5, 125.5 (q, J_{CF} = 3.7 Hz), 124.3 (q, J_{CF} = 270.6 Hz), 61.5, 51.9, 37.8, 14.1. HRMS (ESI) calcd. for $(M+Na)^+$ $(C_{18}H_{17}F_3O_2SNa)^+$: 377.0794, found: 377.0780



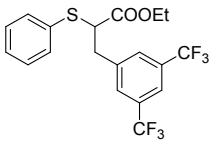
Ethyl 3-(4-cyanophenyl)-2-(phenylthio)propionate (**3o**):
Yellowish oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.58 – 5.56 (m, 2H), 7.45 – 7.41 (m, 2H), 7.32 (m, 5H), 4.08 – 4.00 (m, 2H), 3.85 (dd, J = 9.1, 6.5 Hz, 1H), 3.27 – 3.07 (m, 2H), 1.09 (t, J = 7.1 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 171.2, 143.4, 133.6, 132.4, 130.1, 129.2, 128.7, 118.9, 111.0, 61.6, 51.7, 38.0, 14.1. HRMS (ESI) calcd. for $(M+Na)^+$ $(C_{18}H_{17}NO_2SNa)^+$: 334.0872, found: 334.0863.



Ethyl 3-(2-cyanophenyl)-2-(phenylthio)propionate (**3p**):
Yellowish oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.62 (d, J = 7.7 Hz, 1H), 7.50 (td, J = 7.7, 1.2 Hz, 1H), 7.47– 7.43 (m, 2H), 7.36 – 7.33 (m, 2H), 7.31 – 7.28 (m, 3H), 4.11 – 3.98 (m, 3H), 3.43 – 3.30 (m, 2H), 1.09 (t, J = 7.1 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 171.1, 141.6, 133.6, 133.2, 132.9, 132.8, 130.8, 129.2, 128.6, 127.7, 117.8, 113.1, 61.5, 51.2, 36.6, 14.1. HRMS (ESI) calcd. for $(M+Na)^+$ $(C_{18}H_{17}NO_2SNa)^+$: 334.0872, found: 334.0850.

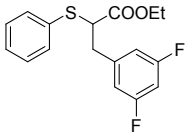


Ethyl 3-(3-nitrophenyl)-2-(phenylthio)propionate (**3r**):
Yellowish oil; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.09 – 8.07 (m, 2H), 7.54 – 7.53 (m, 1H), 7.47 – 7.42 (m, 3H), 7.32 – 7.30 (m, 3H), 4.11 – 4.01 (m, 2H), 3.89 (dd, J = 9.0, 6.6 Hz, 1H), 3.32 – 3.13 (m, 2H), 1.11 (t, J = 7.1 Hz, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 171.1, 148.4, 139.8, 135.6, 133.6, 132.5, 129.5, 129.2, 128.6, 124.1, 122.2, 61.6, 51.8, 37.5, 14.1. HRMS (ESI) calcd. for $(M+Na)^+$ $(C_{17}H_{17}NO_4SNa)^+$: 354.0770, found: 354.0758.



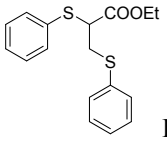
Ethyl 3-(3, 5-bis(trifluoromethyl)phenyl)-2-(phenylthio)propionate (**3s**):

Yellowish oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.75 (s, 1H), 7.65 (s, 2H), 7.45 – 7.42 (m, 2H), 7.34 – 7.31 (m, 3H), 4.12 – 4.05 (m, 2H), 3.88 (dd, J = 8.9, 6.6 Hz, 1H), 3.35 – 3.15 (m, 2H), 1.13 (t, J = 7.1 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 171.0, 140.3, 133.8, 132.3, 131.8 (q, J_{CF} = 33.1 Hz), 129.6, 129.5, 129.3, 128.8, 123.4 (q, J_{CF} = 271.0 Hz), 121.1 (m), 61.7, 51.7, 37.6, 14.0. HRMS (ESI) calcd. for $(M+Na)^+$ $(C_{19}H_{16}F_6O_2SNa)^+$: 445.0667, found: 445.0684.



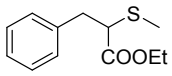
Ethyl 3-(3, 5-difluorophenyl)-2-(phenylthio)propionate (**3t**):

Yellowish oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.47 – 7.43 (m, 2H), 7.33 – 7.30 (m, 3H), 6.75 – 6.64 (m, 3H), 4.09 – 4.04 (m, 2H), 3.84 (dd, J = 9.3, 6.3 Hz, 1H), 3.20 – 3.00 (m, 2H), 1.11 (t, J = 7.1 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 171.2, 164.3, 164.2, 161.9, 161.7, 141.6, 133.6, 132.7, 129.2, 128.6, 112.2, 112.1, 112.0, 112.0, 102.8, 102.5, 102.3, 61.5, 51.7, 37.7, 14.1. HRMS (ESI) calcd. for $(M+Na)^+$ $(C_{17}H_{15}F_2O_2S)^-$: 321.0766, found: 321.0753.



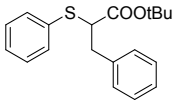
Ethyl 2, 3-bis(phenylthio)propionate (**3u**):

Yellowish oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.42 – 7.40 (m, 2H), 7.33 – 7.19 (m, 8H), 4.12 (q, J = 7.1 Hz, 2H), 3.72 (dd, J = 10.3, 4.9 Hz, 1H), 3.34 – 3.20 (m, 2H), 1.19 (t, J = 7.1 Hz, 3H).^{13}C NMR (100 MHz, $CDCl_3$) δ 170.5, 134.6, 133.8, 132.1, 130.8, 129.2, 129.1, 129.1, 128.6, 127.1, 61.6, 49.9, 35.9, 14.1. HRMS (ESI) calcd. for $(M+Na)^+$ $(C_{17}H_{18}O_2S_2Na)^+$: 341.0640, found: 341.0623.



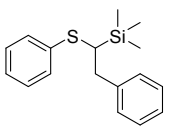
Ethyl 2-(methylthio)-3-phenylpropionate (**3w**):

Yellowish oil; ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.30 – 7.28 (m, 2H), 7.24 – 7.21 (m, 3H), 4.18 – 4.10 (m, 2H), 3.46 (t, J = 7.7 Hz, 1H), 3.23 – 2.95 (m, 2H), 2.18 (s, 3H), 1.21 (t, J = 7.2 Hz, 3H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 138.2, 129.1, 128.6, 126.9, 61.2, 48.9, 37.3, 14.3, 14.2. HRMS (ESI) calcd. for $(M+Na)^+$ $(C_{12}H_{16}O_2SNa)^+$: 247.0763, found: 247.0759.



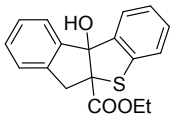
tert-Butyl 3-phenyl-2-(phenylthio)propionate (**3x**):

Colorless oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.46 (d, J = 7.9 Hz, 2H), 7.31 – 7.20 (m, 8H), 3.85 – 3.81 (m, 1H), 3.18 – 3.00 (m, 2H), 1.24 (d, J = 0.6 Hz, 9H).^{13}C NMR (100 MHz, $CDCl_3$) δ 170.8, 138.0, 133.8, 133.0, 129.2, 128.9, 128.5, 127.9, 126.9, 81.5, 52.9, 38.1, 27.8. HRMS (ESI) calcd. for $(M+Na)^+$ $(C_{19}H_{22}O_2SNa)^+$: 337.1233, found: 337.1214.

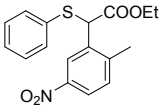


Trimethyl(2-phenyl-1-(phenylthio)ethyl)silane (**3y**):

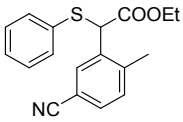
Colorless oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.18 – 7.07 (m, 9H), 7.06 – 7.02 (m, 1H), 2.98 – 2.83 (m, 2H), 2.71 – 2.66 (m, 1H), 0.00 (s, 9H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 140.9, 137.7, 130.0, 129.4, 128.8, 128.3, 126.3, 126.0, 38.2, 36.8, -2.1. HRMS (ESI) calcd. for $(M+Na)^+$ $(C_{17}H_{23}SSi)^+$: 287.1284, found: 287.1287.



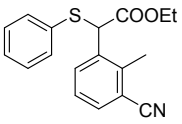
Ethyl 10b-hydroxy-6,10b-dihydro-5aH-benzo[b]indeno[1,2-d]thiophene-5a-carboxylate (**5a**):
White solid; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.63 (d, J = 7.3 Hz, 1H), 7.31 – 7.15 (m, 6H), 7.04 (d, J = 7.4 Hz, 1H), 4.23 (q, J = 7.1 Hz, 2H), 3.60 (dd, J = 153.9, 17.1 Hz, 2H), 1.26 (t, J = 7.1 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 172.6, 141.6, 141.0, 140.1, 137.9, 129.4, 129.2, 127.9, 125.7, 125.0, 124.7, 124.1, 122.4, 95.5, 69.3, 62.0, 38.8, 14.0. HRMS (ESI) calcd. for $(M+Na)^+$ $(C_{18}H_{16}O_3SNa)^+$: 335.0712, found: 335.0696.



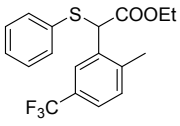
Ethyl 2-(2-methyl-5-nitrophenyl)-2-(phenylthio)acetate (**4q**):
Yellowish oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.45 (d, J = 2.4 Hz, 1H), 8.03 (dd, J = 8.4, 2.4 Hz, 1H), 7.39 – 7.34 (m, 2H), 7.32 – 7.24 (m, 4H), 5.11 (s, 1H), 4.25 – 4.12 (m, 2H), 2.43 (s, 3H), 1.20 (t, J = 7.1 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 169.6, 146.7, 144.1, 136.2, 133.6, 132.6, 131.4, 129.2, 128.8, 124.0, 122.9, 62.3, 52.5, 19.9, 14.1. HRMS (ESI) calcd. for $(M+Na)^+$ $(C_{17}H_{17}NO_4SNa)^+$: 354.0770, found: 354.0767.



Ethyl 2-(5-cyano-2-methylphenyl)-2-(phenylthio)acetate (**4o**):
Colorless oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.87 (d, J = 1.6 Hz, 1H), 7.47 – 7.45 (m, 1H), 7.37 – 7.34 (m, 2H), 7.32 – 7.23 (m, 4H), 5.07 (s, 1H), 4.23 – 4.10 (m, 2H), 2.39 (s, 3H), 1.19 (t, J = 7.1 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 169.8, 142.1, 135.9, 133.6, 132.7, 132.4, 131.5, 131.4, 129.2, 128.8, 118.7, 110.5, 62.3, 52.2, 20.0, 14.1. HRMS (ESI) calcd. for $(M+Na)^+$ $(C_{18}H_{17}NO_2SNa)^+$: 334.0872, found: 334.0861.

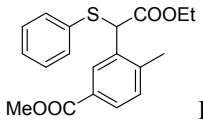


Ethyl 2-(3-cyano-2-methylphenyl)-2-(phenylthio)acetate (**4p**):
Colorless oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.81 (d, J = 7.9 Hz, 1H), 7.55 (dd, J = 7.7, 0.9 Hz, 1H), 7.38 – 7.35 (m, 2H), 7.32 – 7.24 (m, 4H), 5.12 (s, 1H), 4.22 – 4.08 (m, 2H), 2.53 (s, 3H), 1.18 (t, J = 7.1 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 169.8, 140.0, 136.1, 133.4, 133.1, 132.8, 132.5, 129.2, 128.7, 126.9, 118.2, 113.9, 62.2, 52.7, 17.7, 14.0. HRMS (ESI) calcd. for $(M+Na)^+$ $(C_{18}H_{17}NO_2SNa)^+$: 334.0872, found: 334.0868.



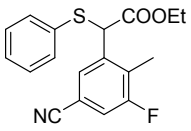
Ethyl 2-(2-methyl-5-(trifluoromethyl)phenyl)-2-(phenylthio)acetate (**4n**):

Colorless oil; ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.78 (s, 1H), 7.42 (d, J = 7.6 Hz, 1H), 7.37 – 7.35 (m, 2H), 7.29 – 7.25 (m, 4H), 5.10 (s, 1H), 4.21 – 4.11 (m, 2H), 2.40 (s, 3H), 1.18 (t, J = 7.1 Hz, 3H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 170.1, 140.5, 135.1, 133.5, 133.1, 131.0, 129.2, 128.9 (q, J_{CF} = 32.5 Hz), 128.6, 125.6 (q, J_{CF} = 3.8 Hz), 124.9 (q, J_{CF} = 3.7 Hz), 124.1 (q, J_{CF} = 270.6 Hz), 125.6, 124.9, 124.9, 62.2, 52.6, 19.7, 14.1. HRMS (ESI) calcd. for $(M+Na)^+$ $(C_{18}H_{17}F_3O_2SNa)^+$: 377.0794, found: 377.0791.



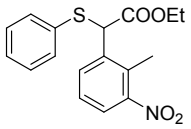
Ethyl 2-(2-methyl-5-(methoxycarbonyl)phenyl)-2-(phenylthio)acetate (**4m**):

Colorless oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.23 (d, J = 1.7 Hz, 1H), 7.87 (dd, J = 7.9, 1.8 Hz, 1H), 7.40 – 7.36 (m, 2H), 7.28 – 7.22 (m, 3H), 7.23 (d, J = 8.0 Hz, 1H), 5.12 (s, 1H), 4.23 – 4.08 (m, 2H), 3.90 (s, 3H), 2.39 (s, 3H), 1.18 (t, J = 7.1 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 170.3, 166.9, 141.8, 134.7, 133.7, 133.1, 130.9, 129.8, 129.4, 129.2, 128.7, 128.3, 62.1, 52.9, 52.2, 19.9, 14.2. HRMS (ESI) calcd. for $(M+Na)^+$ $(C_{19}H_{20}O_4SNa)^+$: 367.0975, found: 367.0963.



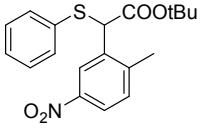
Ethyl 2-(5-cyano-3-fluoro-2-methylphenyl)-2-(phenylthio)acetate (**4f**):

Colorless oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.68 (s, 1H), 7.37 – 7.23 (m, 6H), 5.06 (s, 1H), 4.24 – 4.11 (m, 2H), 2.28 (d, J = 2.2 Hz, 3H), 1.20 (t, J = 7.1 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 169.3, 161.7, 159.2, 138.6, 138.6, 133.8, 132.2, 130.3, 130.1, 129.3, 129.0, 128.4, 128.3, 118.2, 117.9, 117.6, 117.6, 110.9, 110.8, 62.4, 52.2, 52.2, 14.1, 11.1, 11.0. HRMS (ESI) calcd. for $(M+Na)^+$ $(C_{18}H_{16}FNO_2SNa)^+$: 352.0778, found: 352.0780.



Ethyl 2-(2-methyl-3-nitrophenyl)-2-(phenylthio)acetate (**4z'**):

Yellowish oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.82 – 7.80 (m, 1H), 7.68 – 7.65 (m, 1H), 7.39 – 7.36 (m, 2H), 7.33 – 7.28 (m, 4H), 5.16 (s, 1H), 4.22 – 4.09 (m, 2H), 2.40 (s, 3H), 1.18 (t, J = 7.1 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 170.0, 151.6, 137.4, 133.5, 132.9, 132.7, 130.4, 129.3, 128.8, 126.9, 123.8, 62.3, 52.8, 14.8, 14.1. HRMS (ESI) calcd. for $(M+Na)^+$ $(C_{17}H_{17}NO_4SNa)^+$: 354.0770, found: 354.0757.



tert-Butyl 2-(2-methyl-5-nitrophenyl)-2-(phenylthio)acetate (**4q'**):

Colorless oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.47 (s, 1H), 8.02 (d, J = 8.4 Hz, 1H), 7.38 (dd, J = 5.4, 2.2 Hz, 2H), 7.33 – 7.21 (m, 4H), 5.05 (s, 1H), 2.44 (s, 3H), 1.40 (d, J = 0.7 Hz, 9H). ^{13}C NMR (100

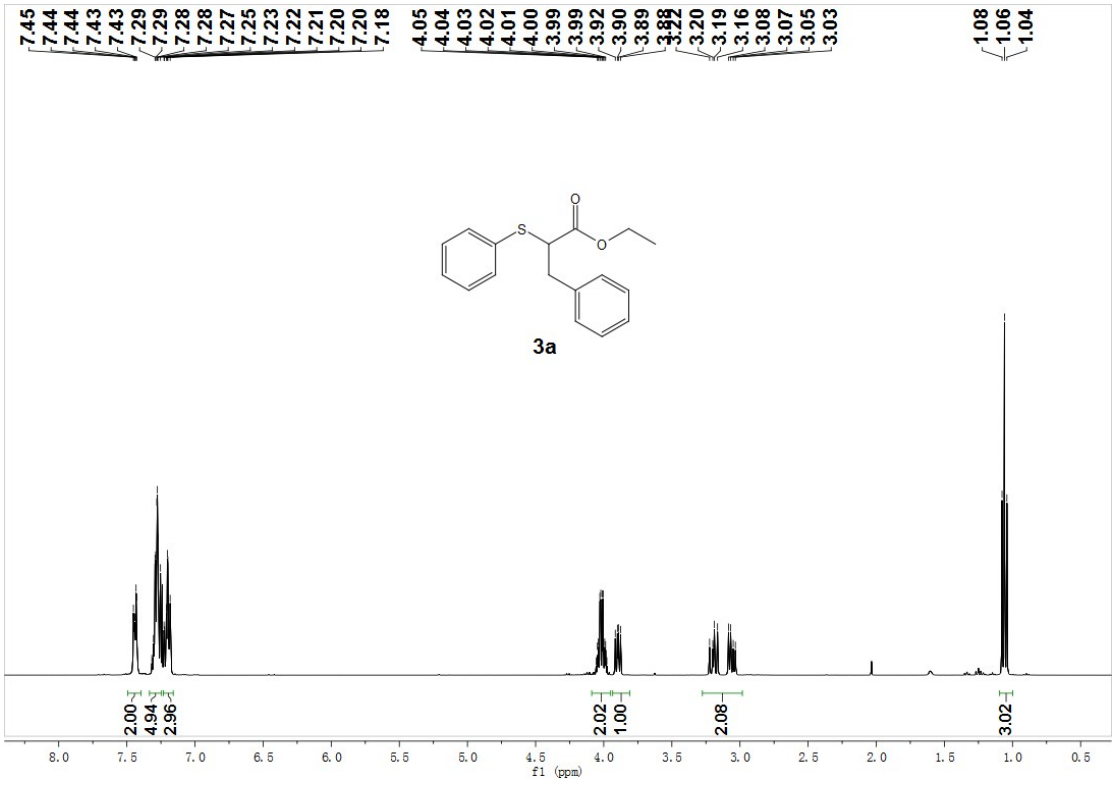
MHz, $CDCl_3$) δ 168.6, 146.7, 144.1, 136.6, 133.3, 133.1, 131.3, 129.2, 128.5, 123.9, 122.8, 83.2, 53.3, 27.9, 19.9. HRMS (ESI) calcd. for $(M+Na)^+$ $(C_{19}H_{21}NO_4SNa)^+$: 382.1083, found: 382.1068.

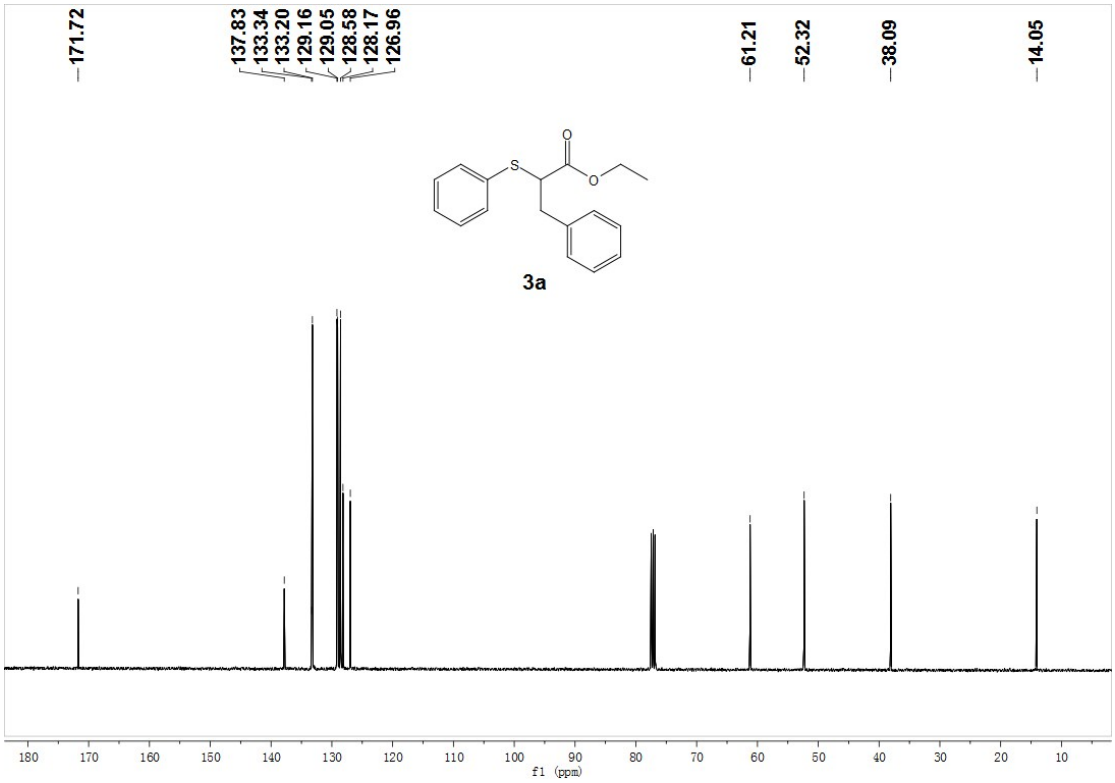
8. References

[1] C. G. Screttas, G. A. Heropoulos, M. Micha-Screttas, B. R. Steele, *Tetrahedron Lett.* **2005**, *46*, 4357-4360.

[2] C. Hansch, A. Leo, R. W. Taft, *Chem. Rev.* **1991**, *91*, 165-195.

9. Copies for ^1H NMR and ^{13}C NMR

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128.17
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S
O
O
3a
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140
130
120
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100
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50
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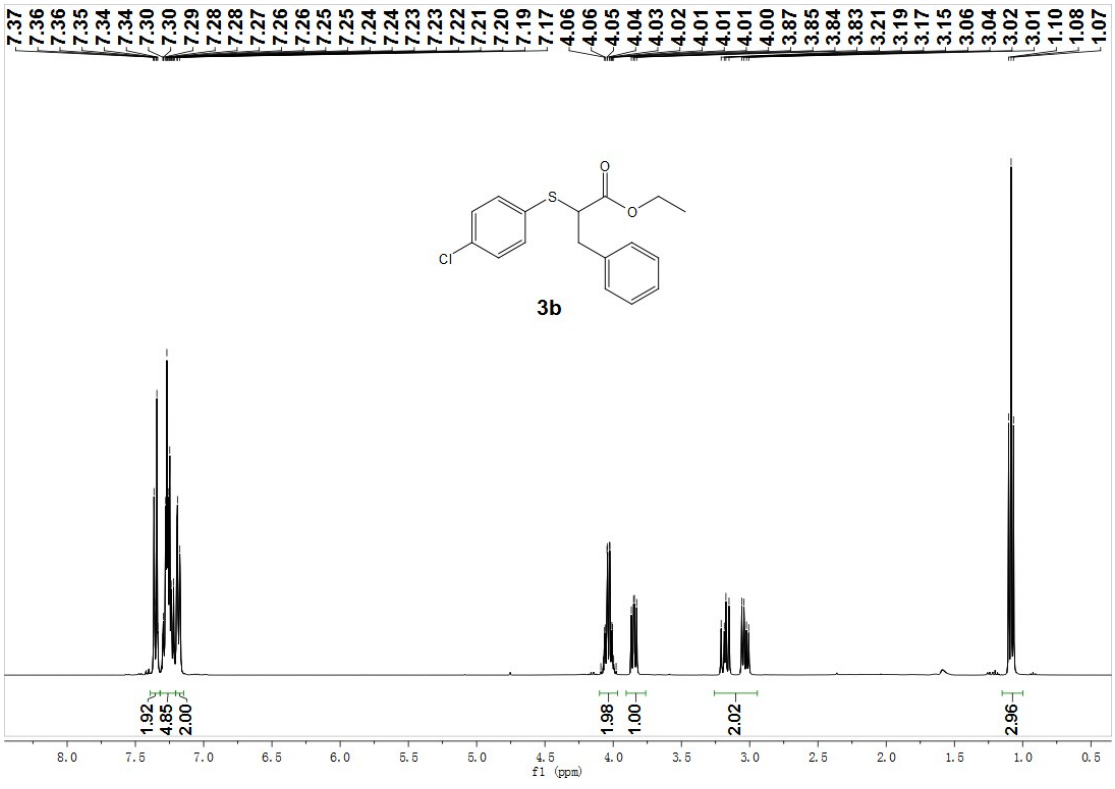
30
20
10
f1 (ppm)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S
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O
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1.00
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7.0
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6.0
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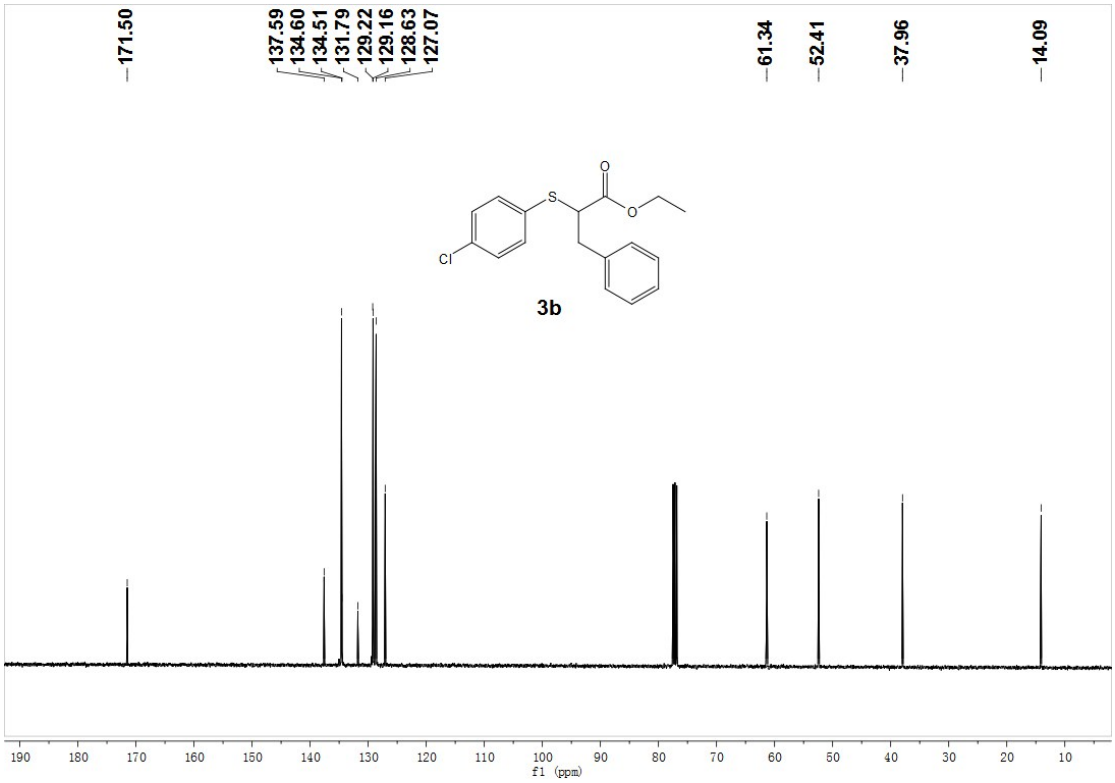
f1 (ppm)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S
O
Cl
3b
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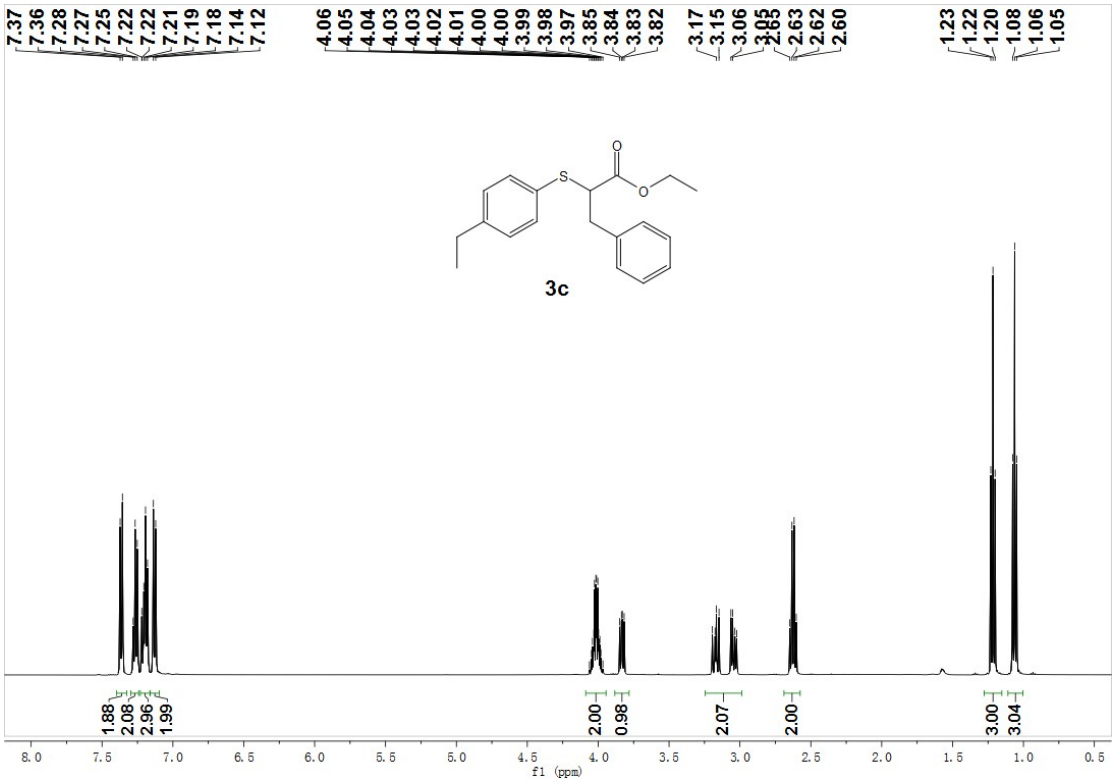
f1 (ppm)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4.00
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3.15
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2.60
1.23
1.22
1.20
1.08
1.06
1.05
O
S
O
3c
1.88
2.08
2.96
1.99
2.00
0.98
2.07
2.00
3.00
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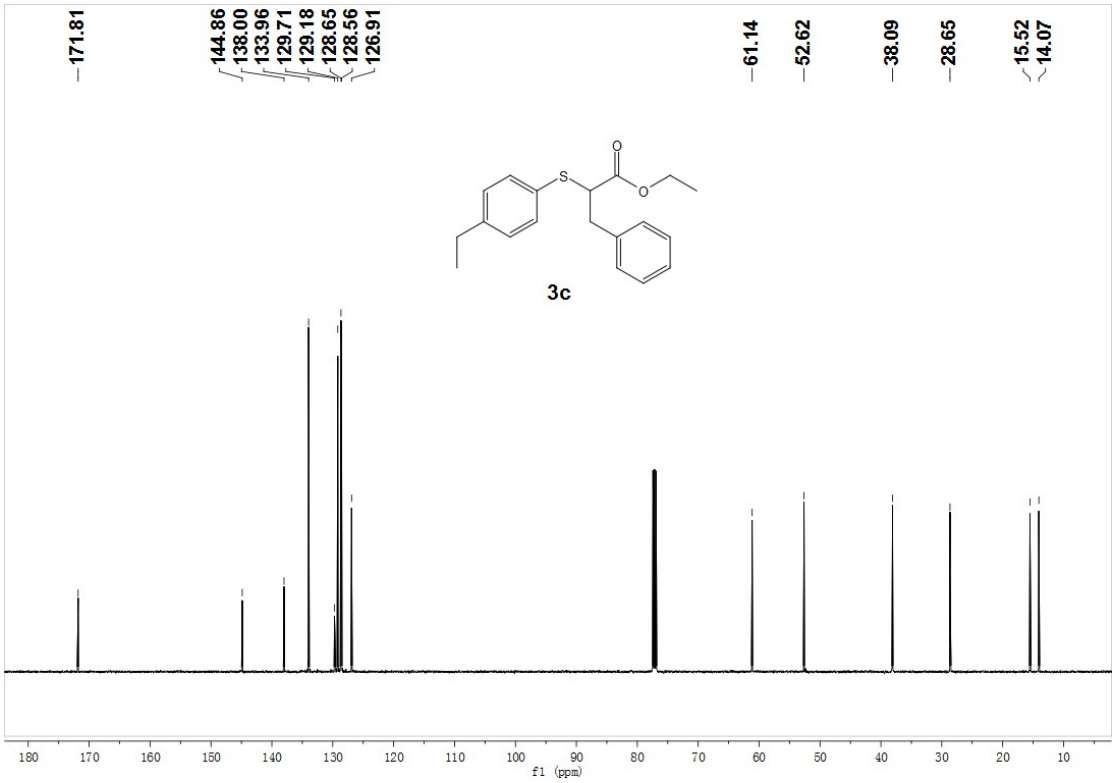
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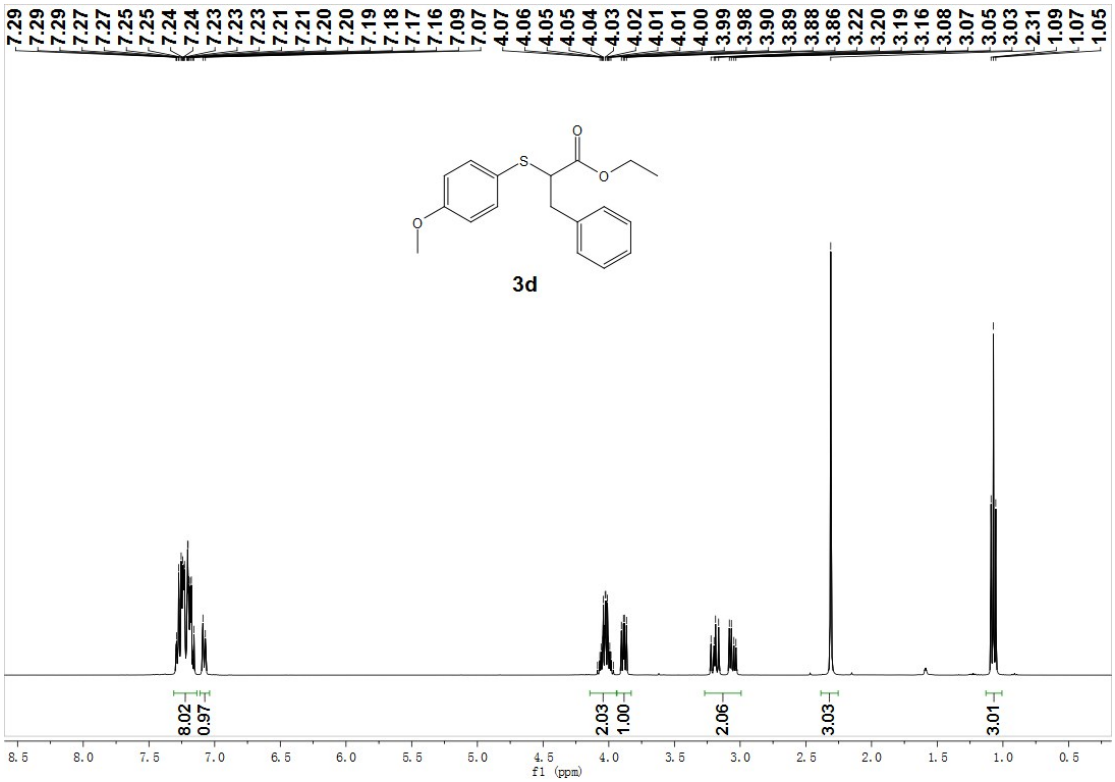
f1 (ppm)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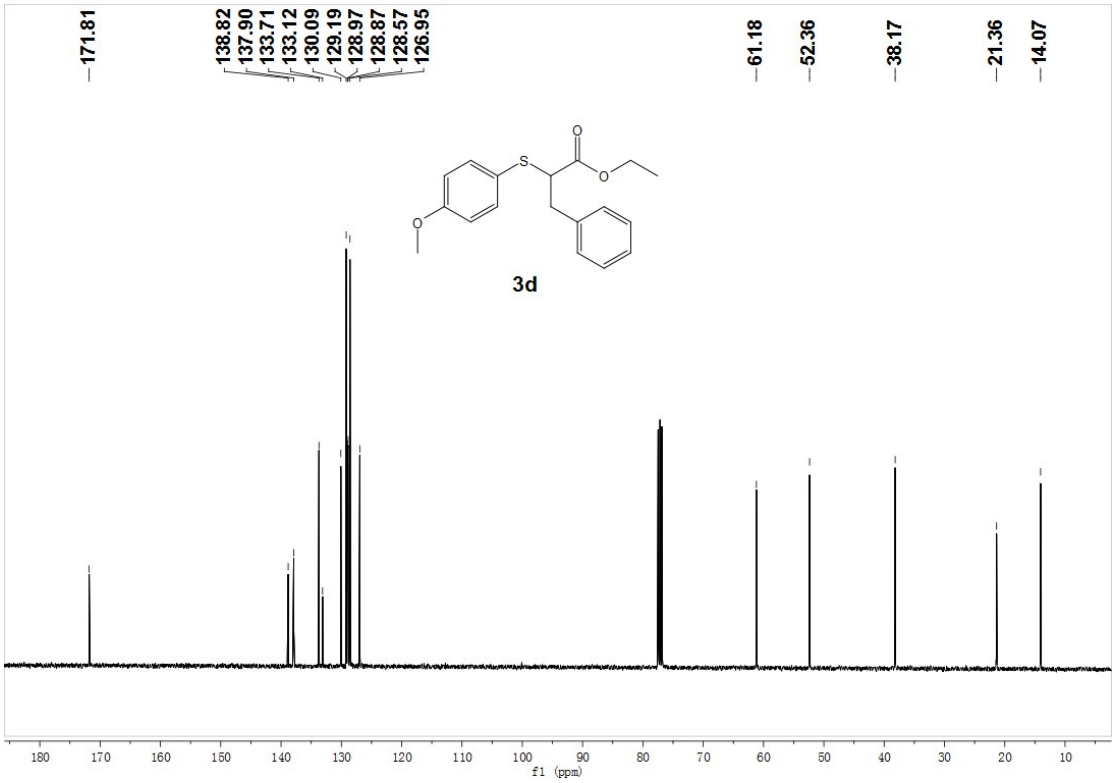
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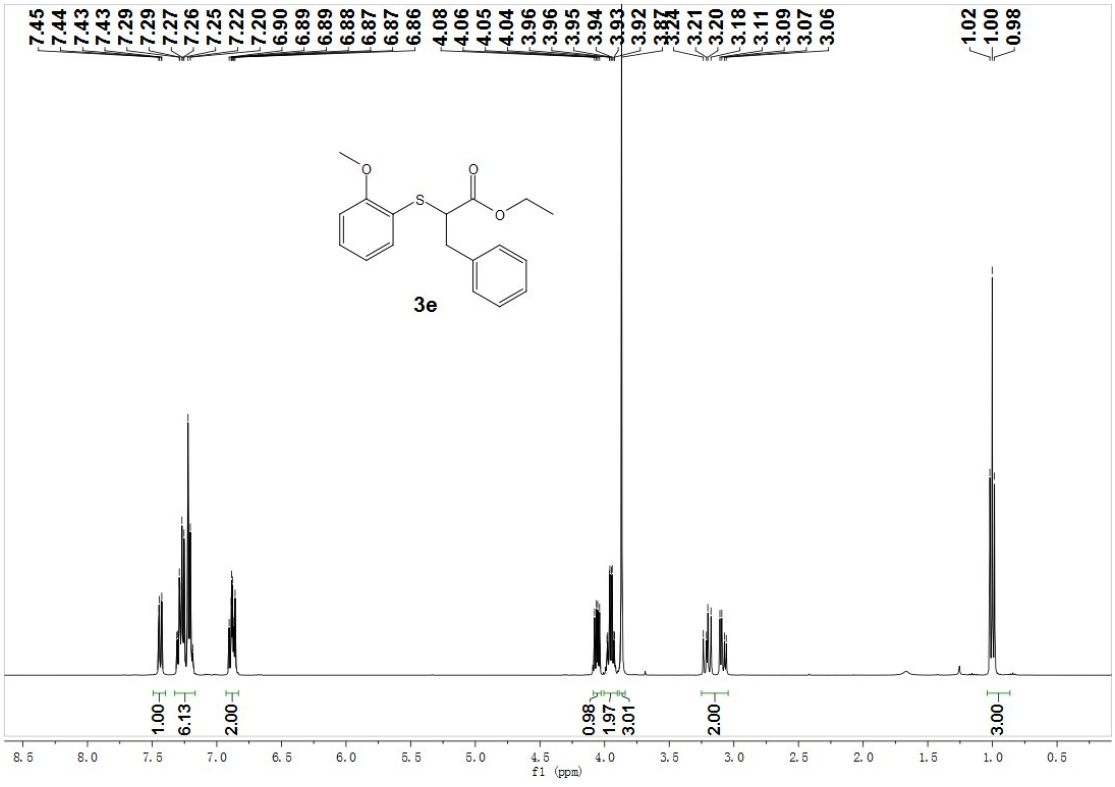
f1 (ppm)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6.87
6.86
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4.05
4.04
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3.07
3.06
1.02
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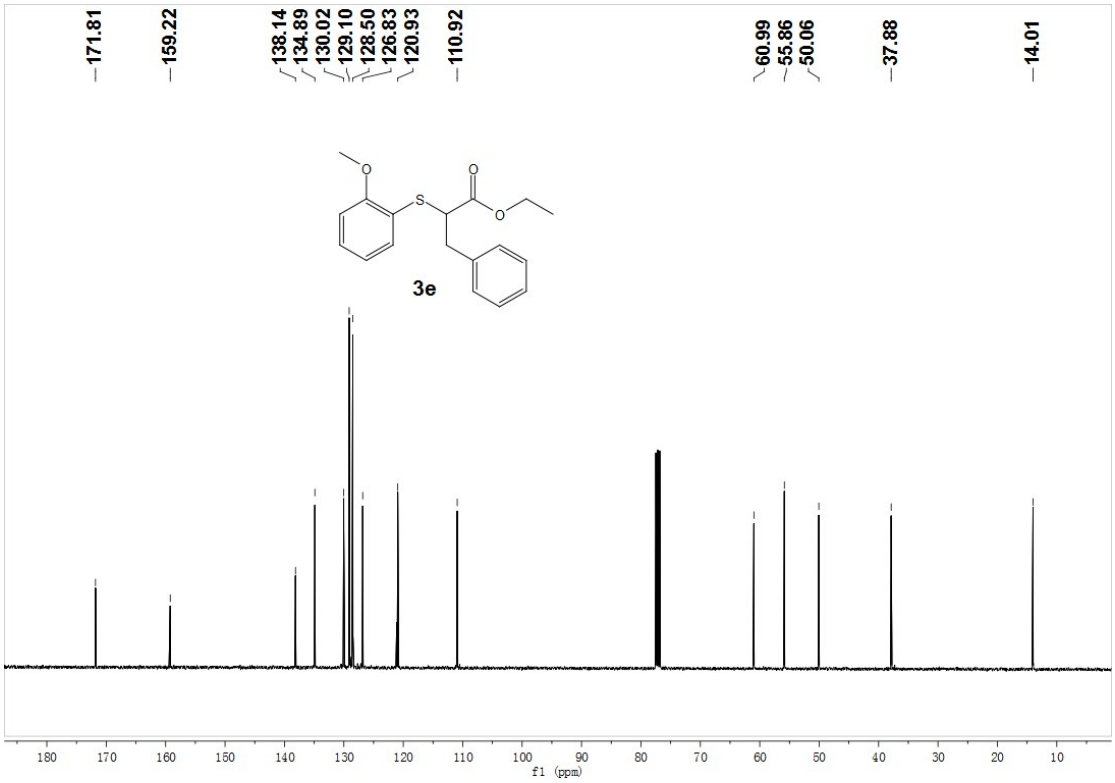
3.00
f1 (ppm)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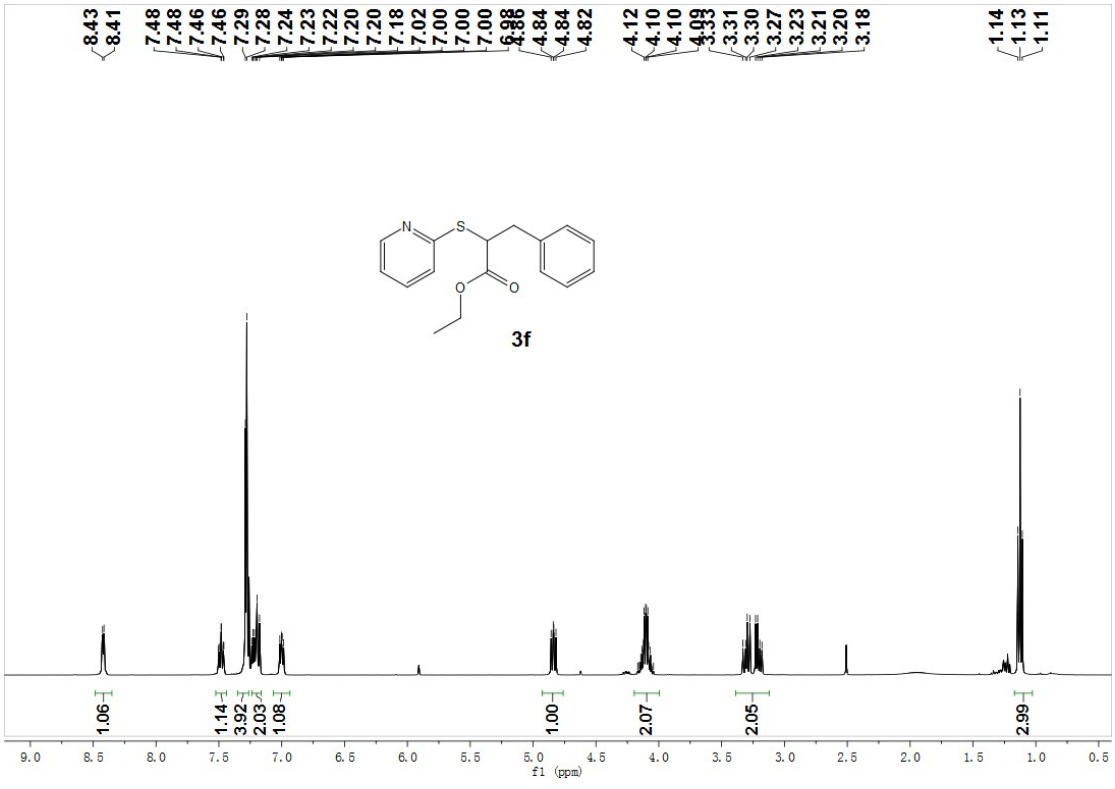
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7.00
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4.10
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3.30
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3.18
1.14
1.13
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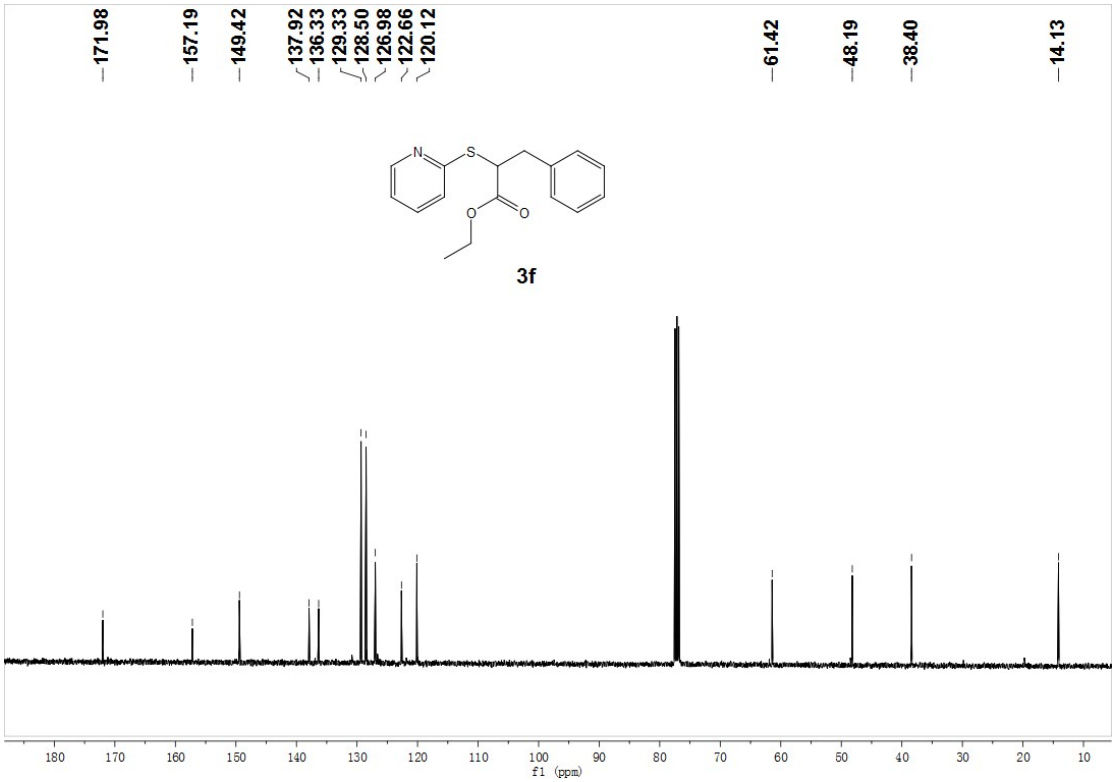
2.07
2.05
2.99
3f
f1 (ppm)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N
S
O
O
3f
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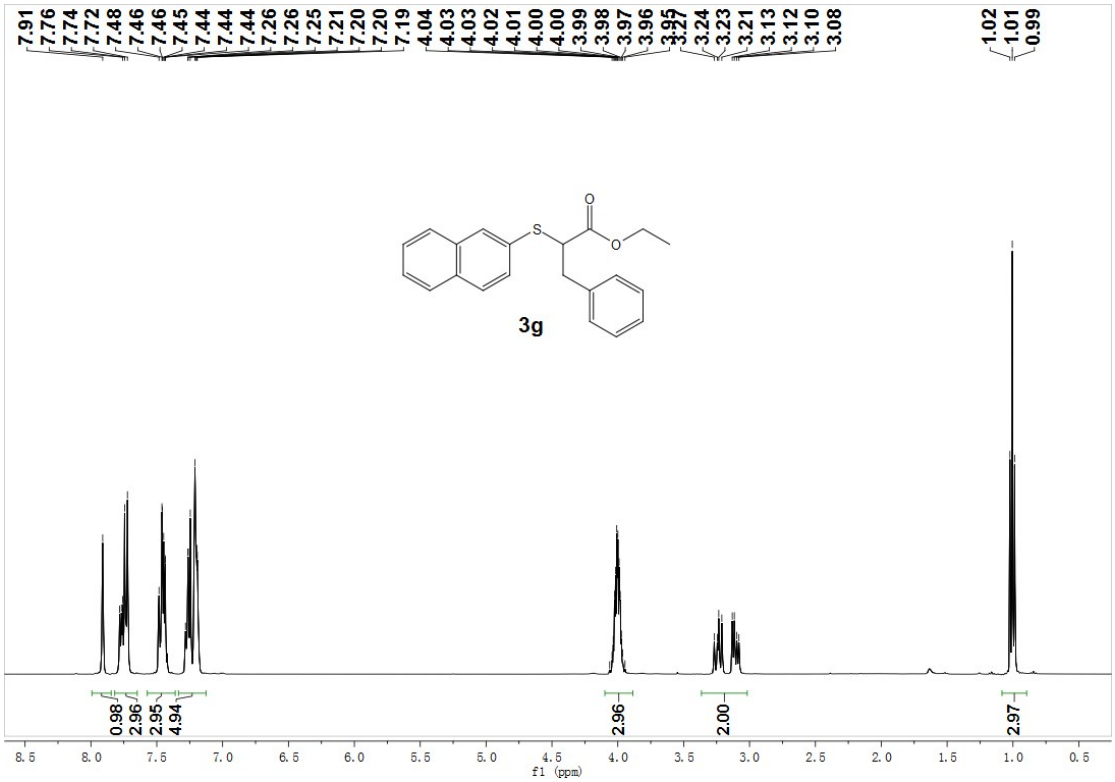
f1 (ppm)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O
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7.0
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6.0
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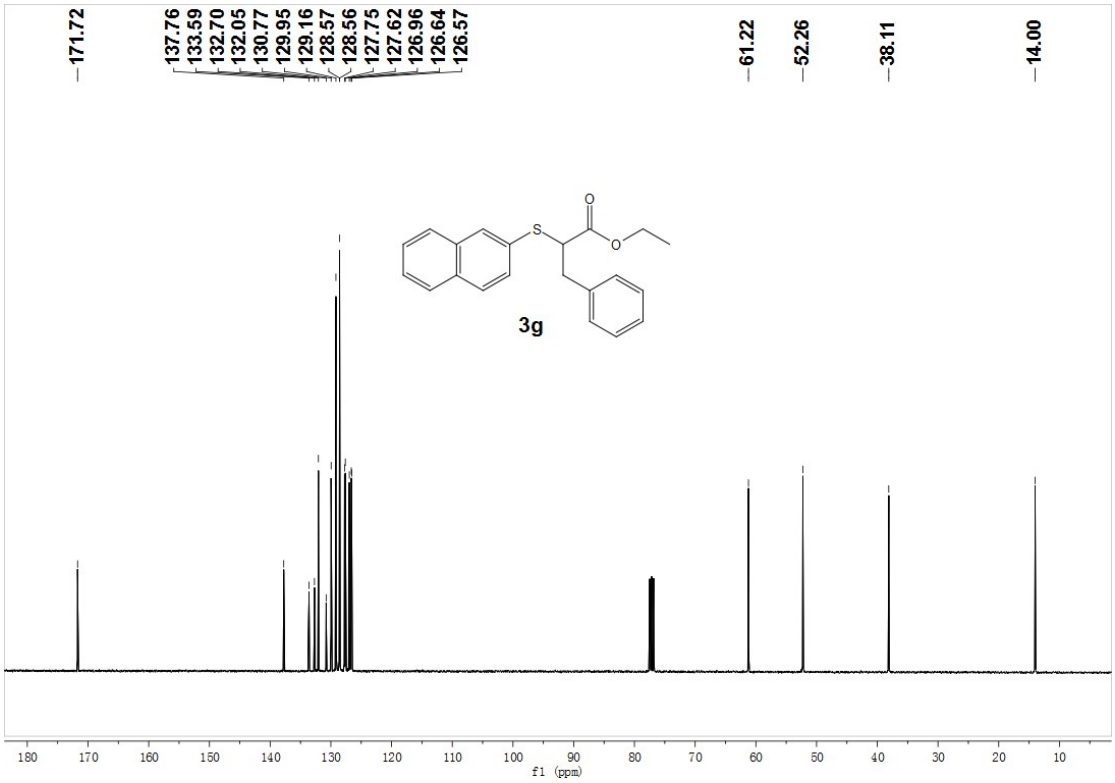
0.5
f1 (ppm)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52.26
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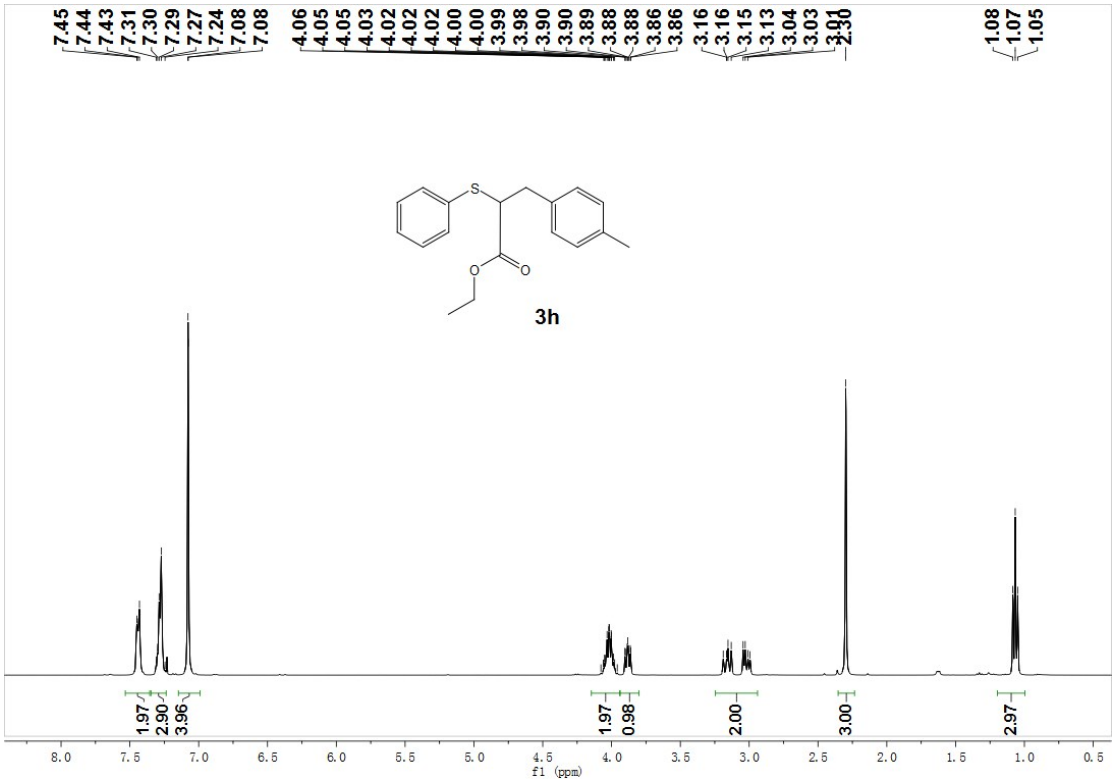
3g
f1 (ppm)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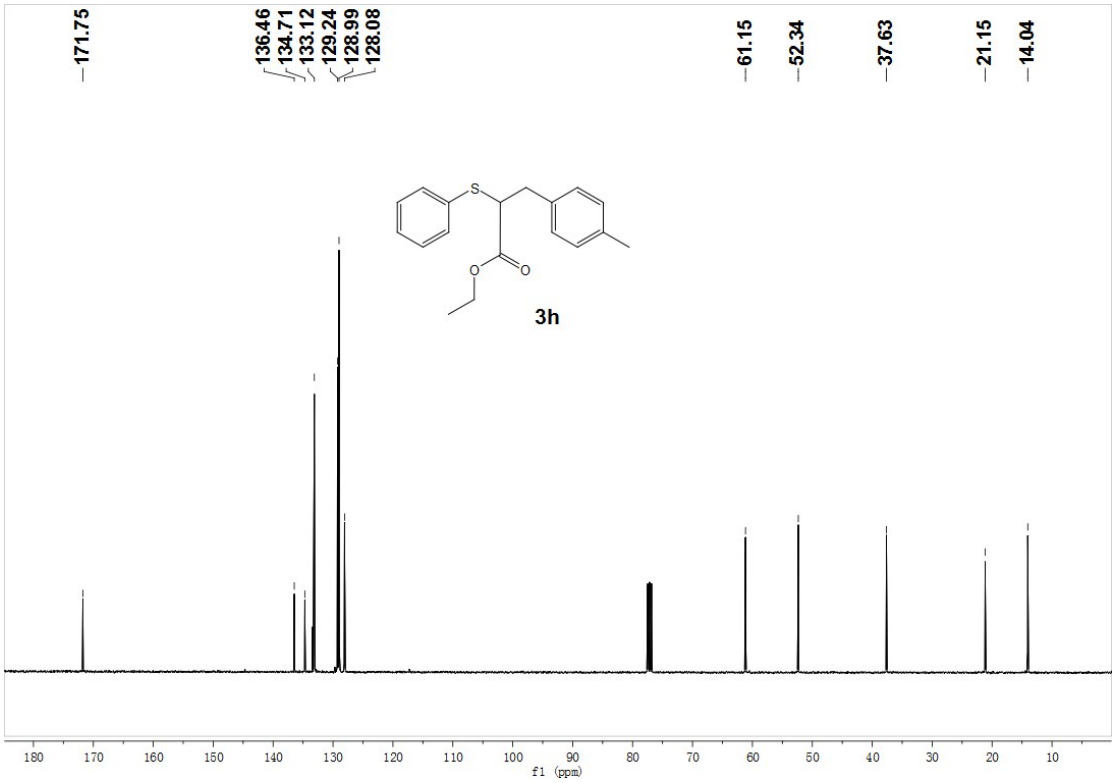
2.97
f1 (ppm)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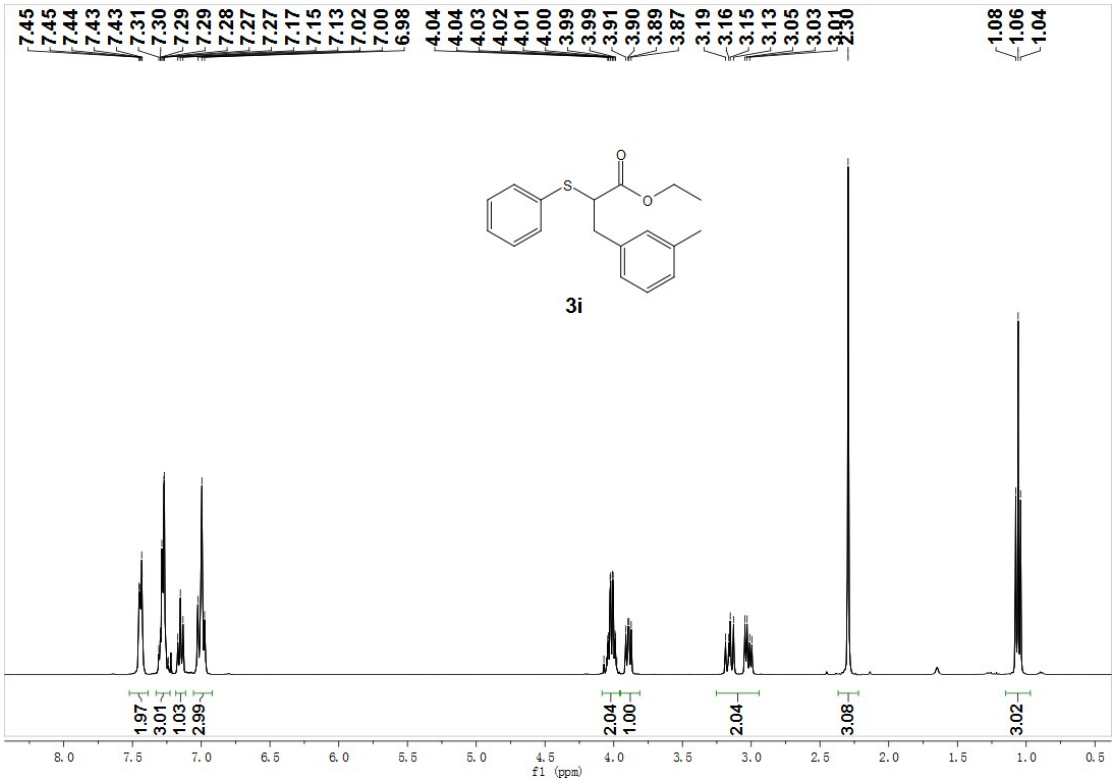
O
3h
f1 (ppm)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S
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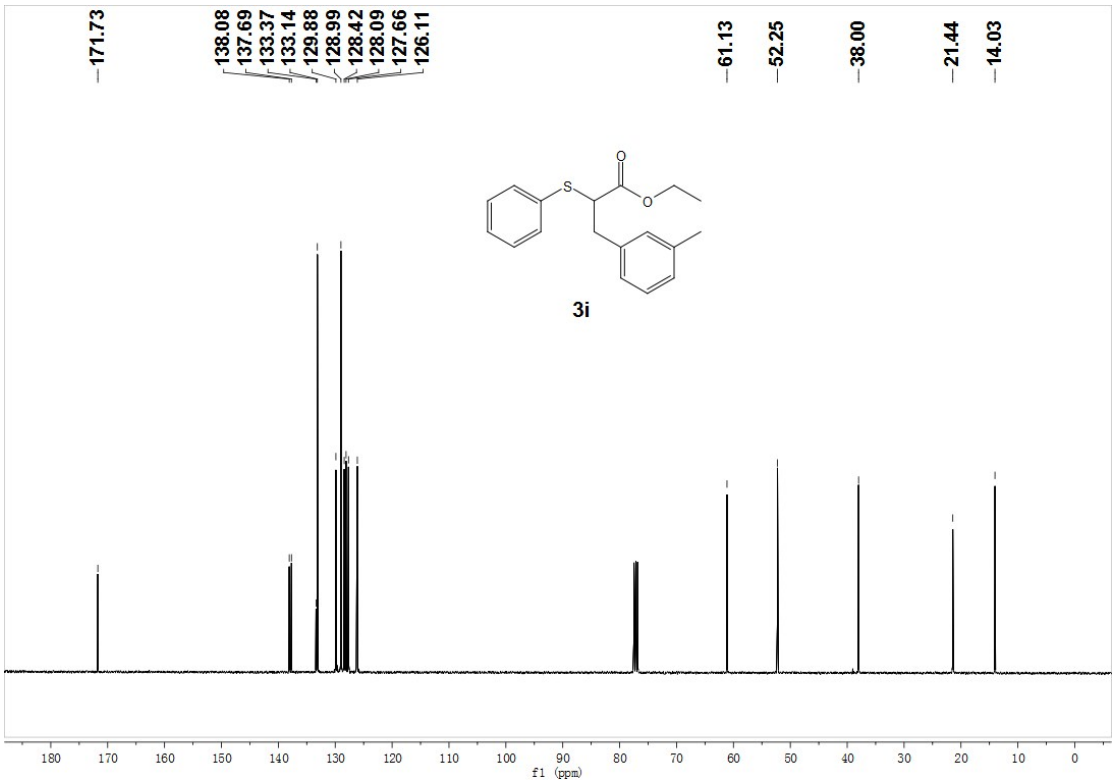
3.02
f1 (ppm)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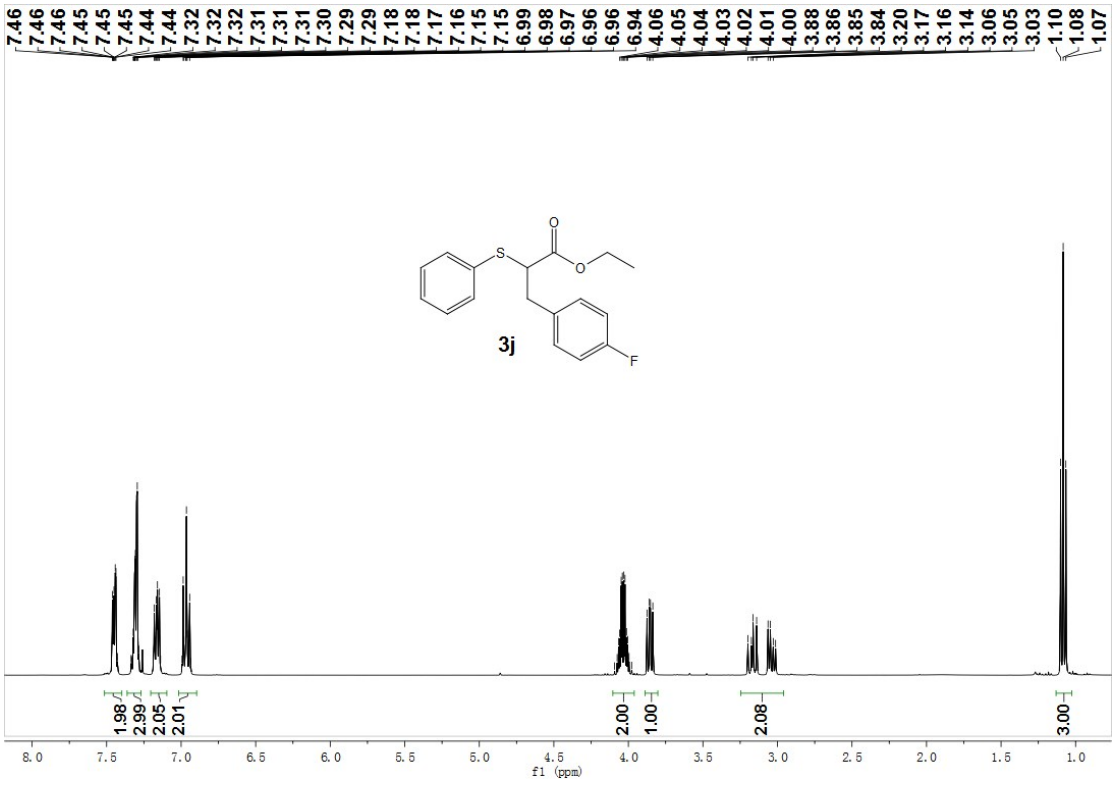
f1 (ppm)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1.08
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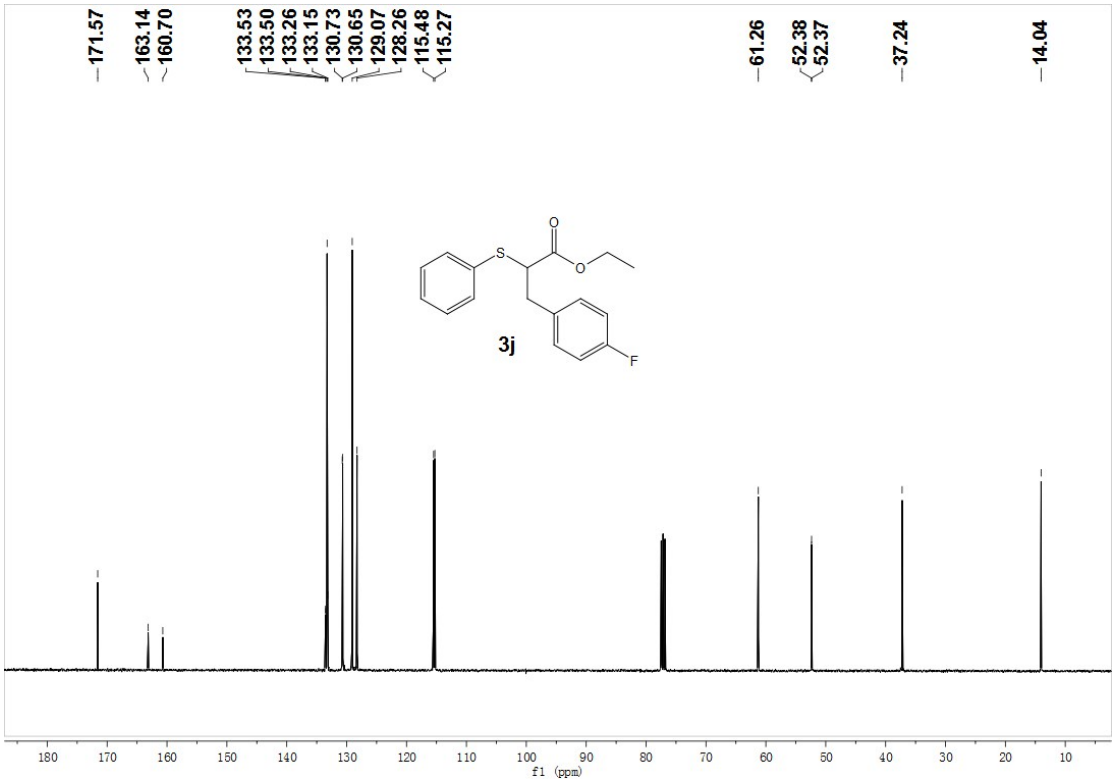
f1 (ppm)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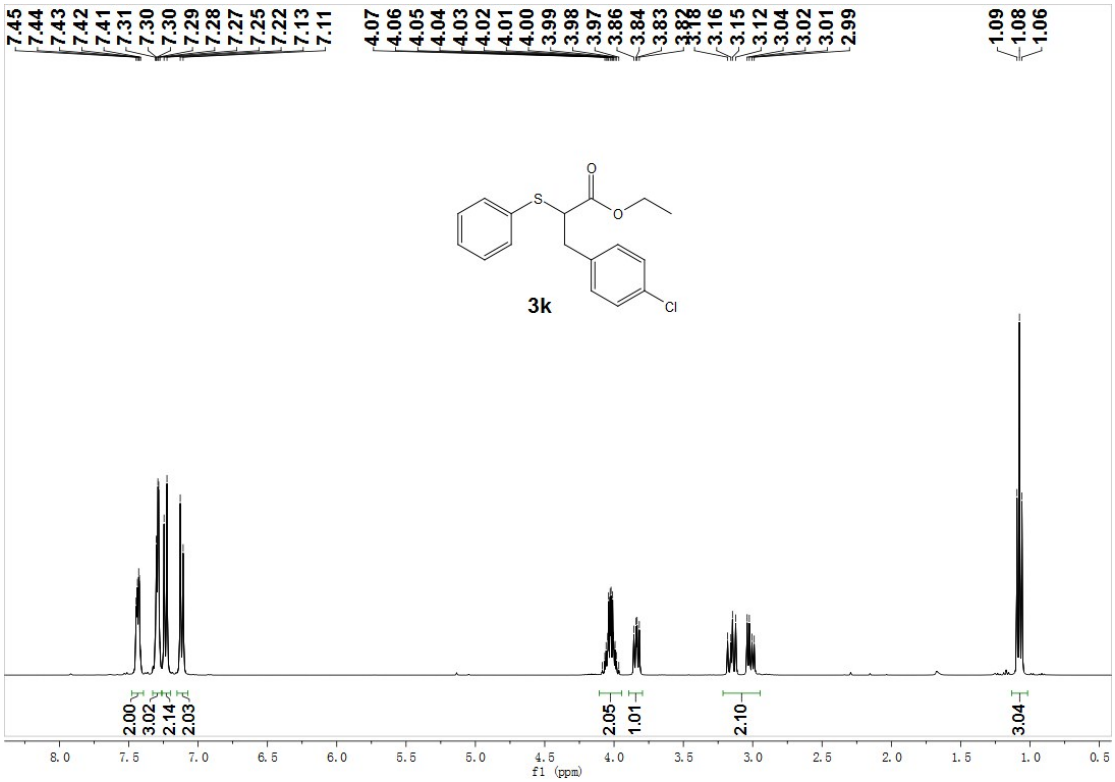
O
S
O
F
3j
f1 (ppm)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3.01
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1.09
1.08
1.06
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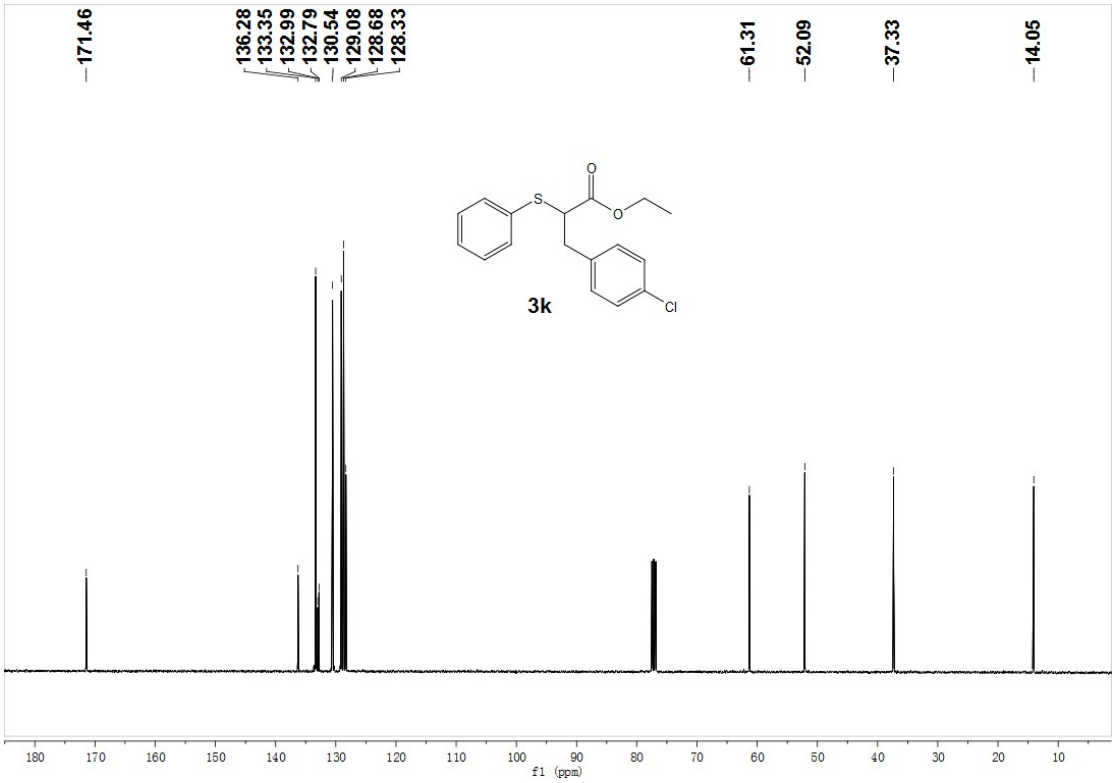
f1 (ppm)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O
Cl
3k
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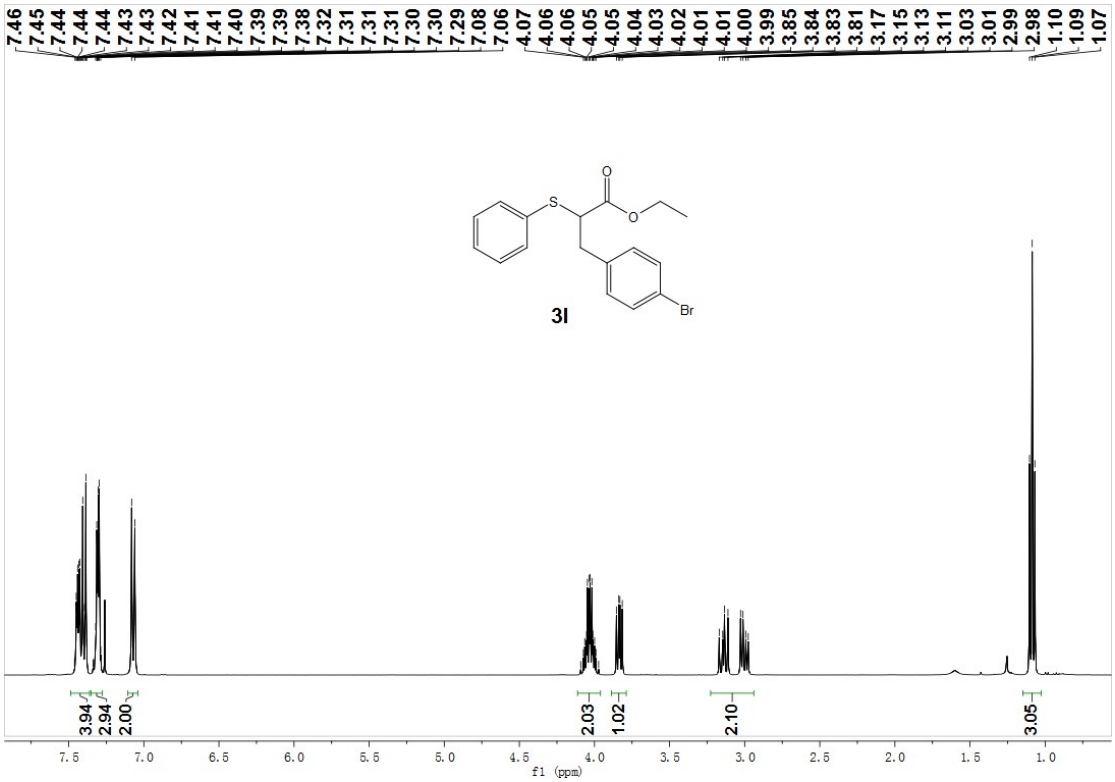
f1 (ppm)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4.07 4.06 4.06 4.05 4.05 4.04 4.03 4.02 4.01 4.01 4.00 3.99 3.85 3.84 3.83 3.81 3.17 3.15 3.13 3.11 3.03 3.01 2.99 2.98 1.10 1.09 1.07
O
S
O
Br
3l
3.94
2.94
2.00
2.03
1.02
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3.05
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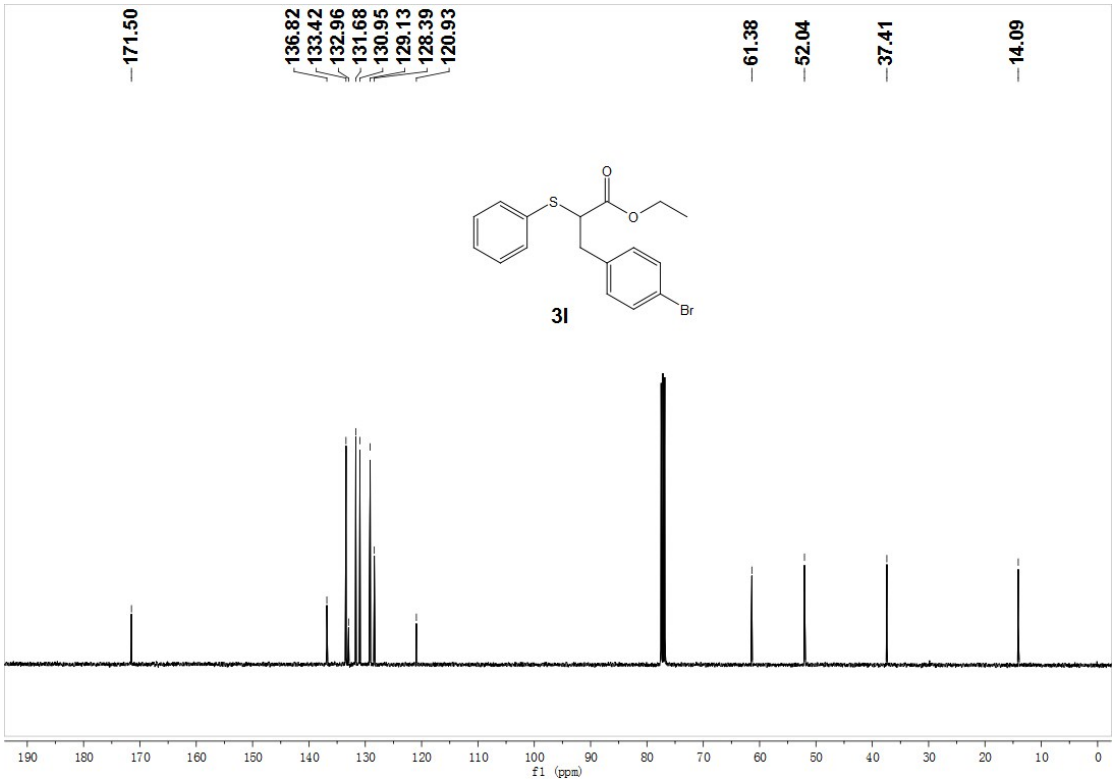
f1 (ppm)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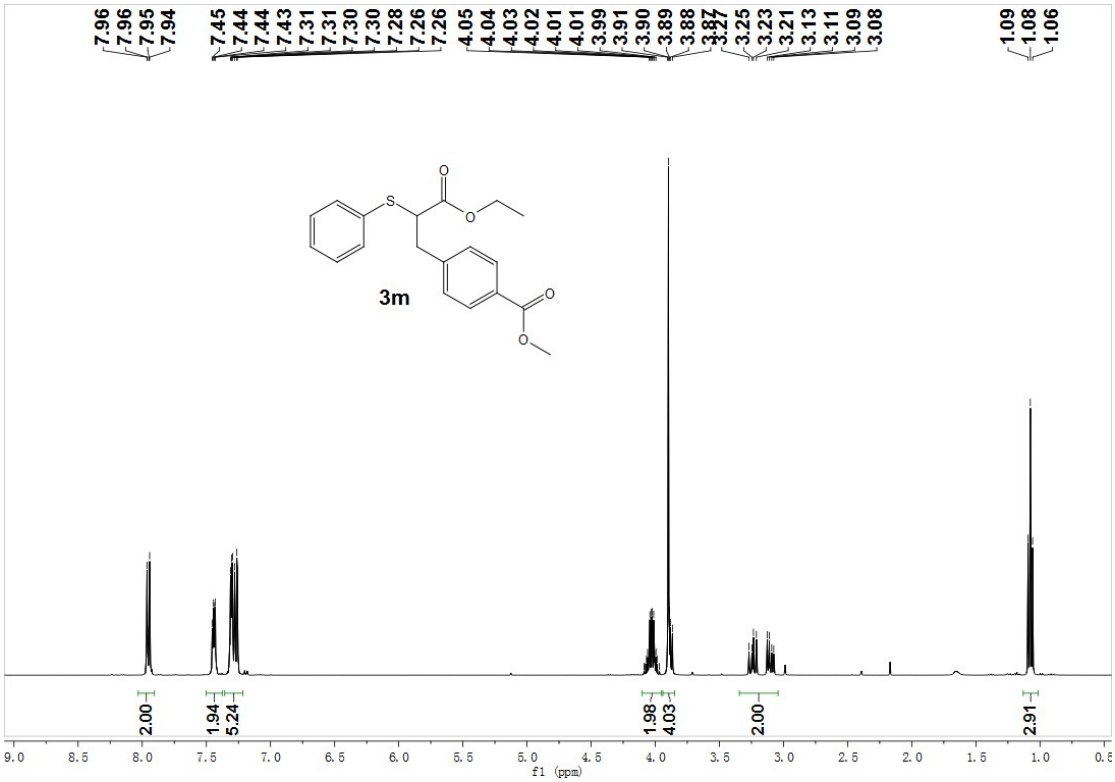
S
O
O
Br
3l
f1 (ppm)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1.06
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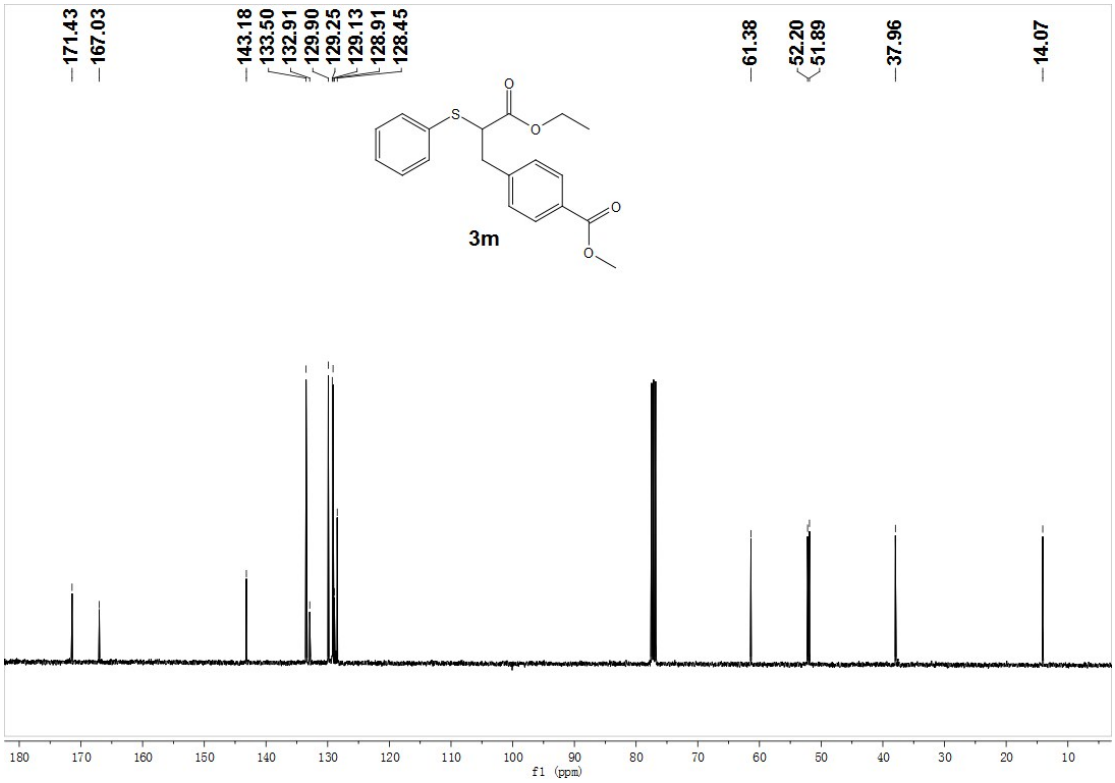
f1 (ppm)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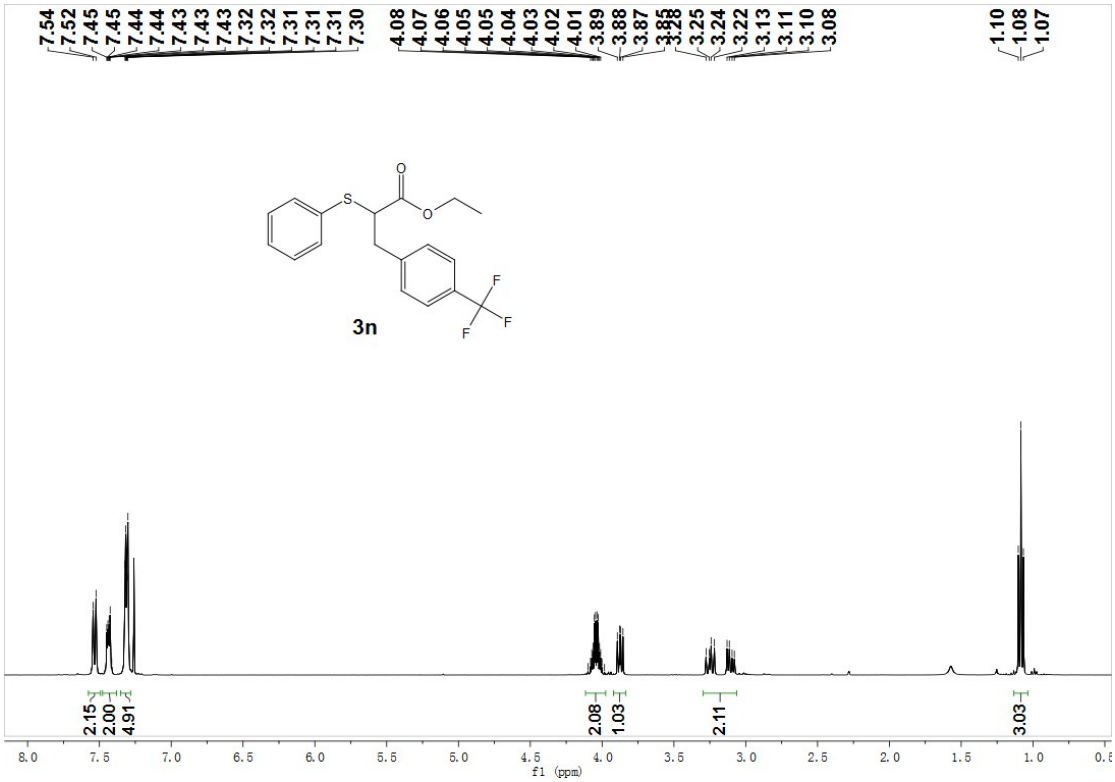
3m
f1 (ppm)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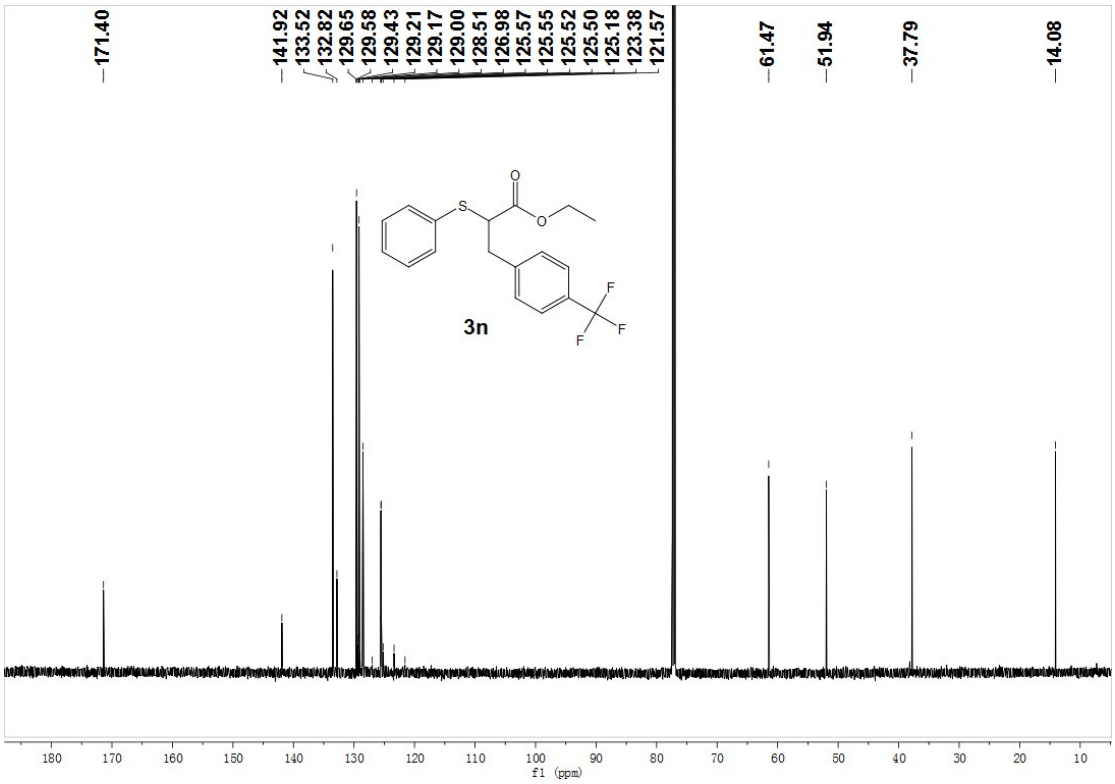
2.11
3.03
f1 (ppm)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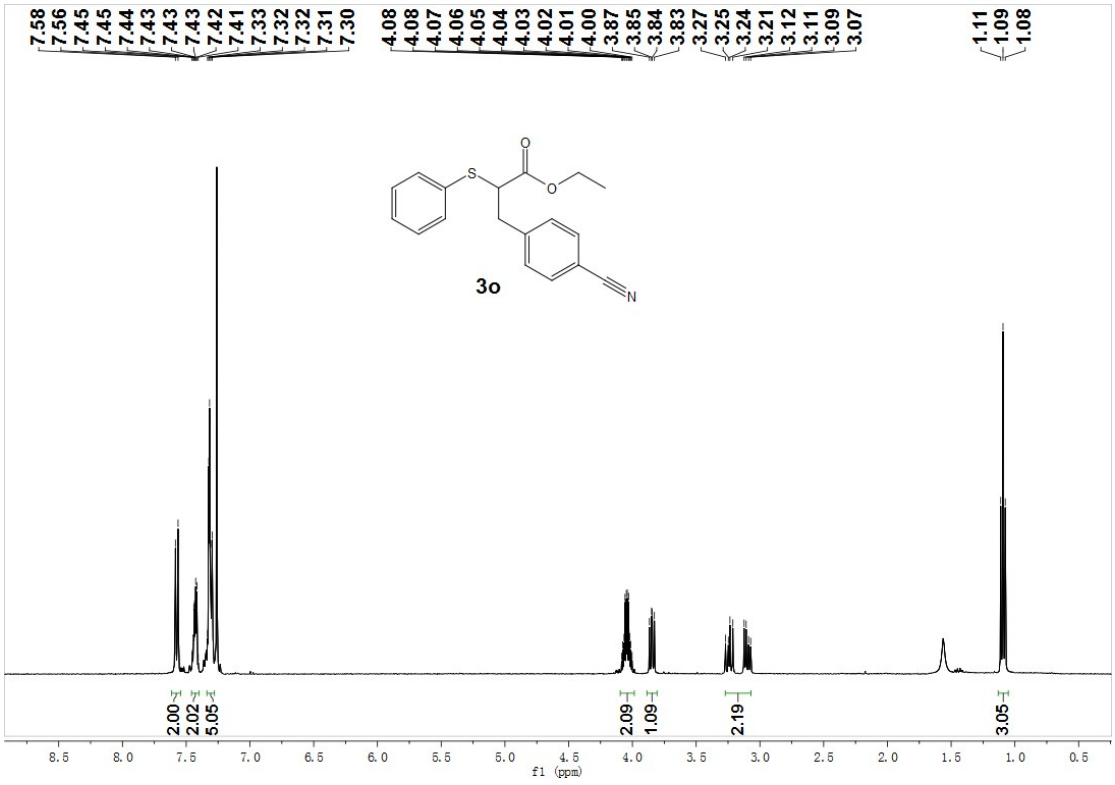
3n
f1 (ppm)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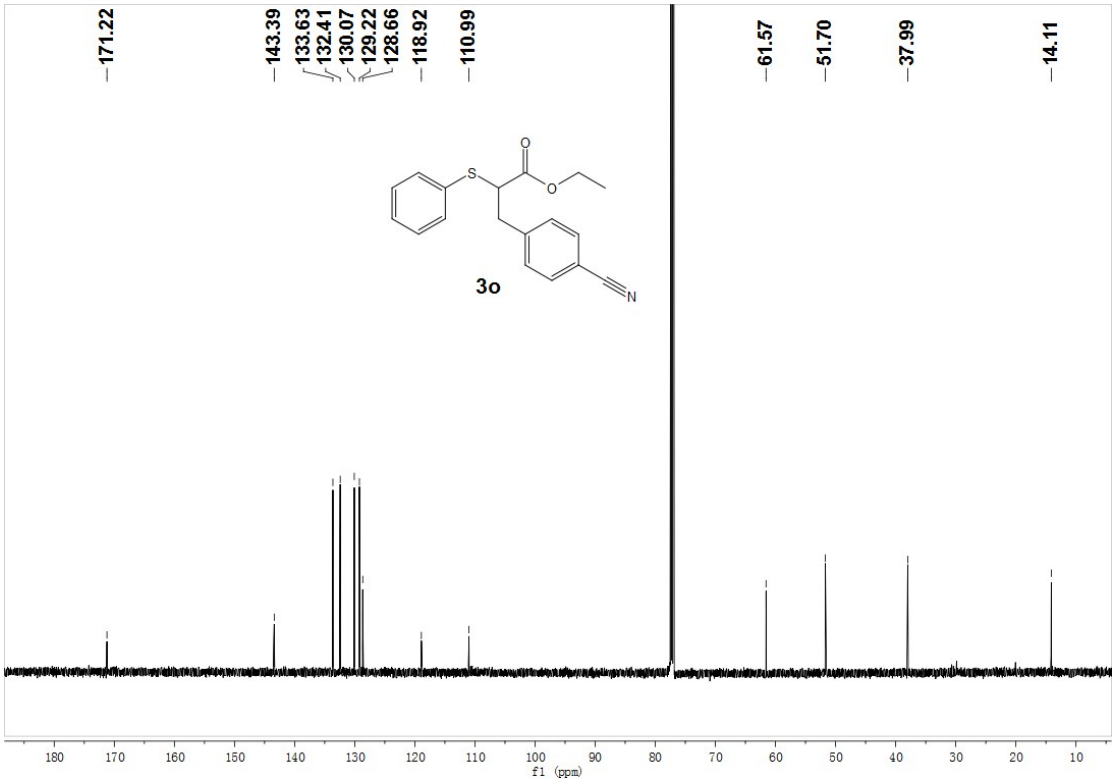
3.05
f1 (ppm)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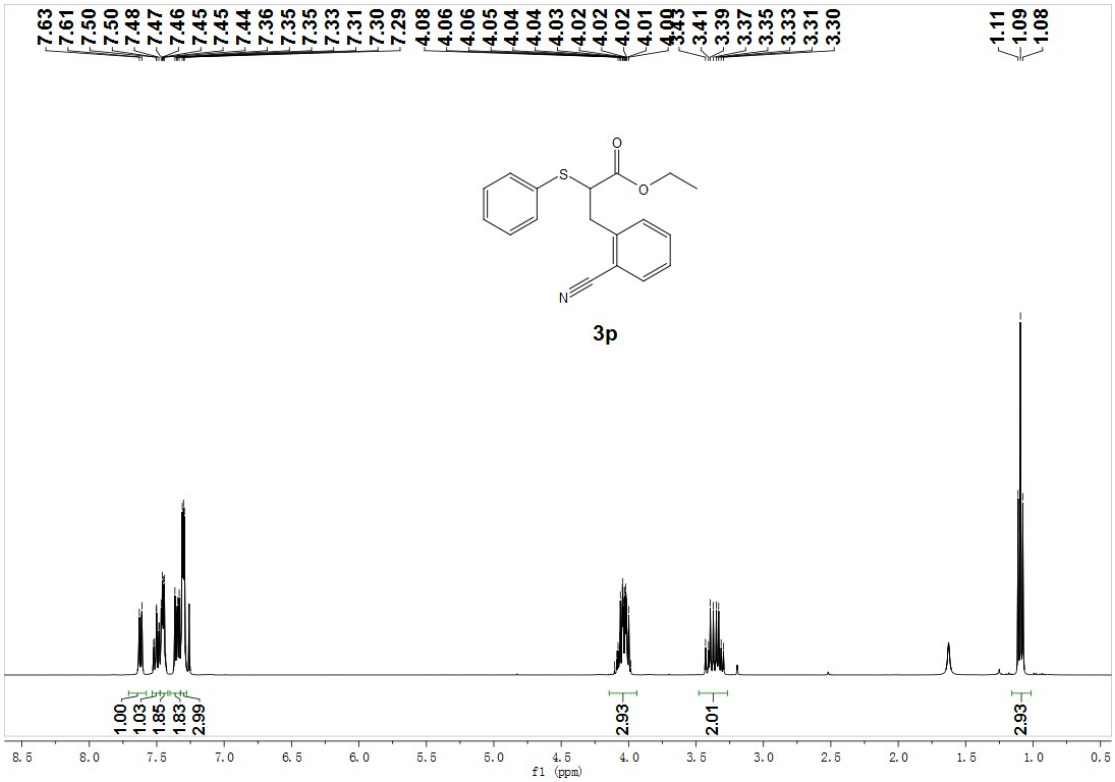
37.99
14.11
3o
f1 (ppm)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7.31
7.30
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4.06
4.06
4.05
4.04
4.04
4.03
4.02
4.02
4.02
4.01
4.00
3.43
3.41
3.39
3.37
3.35
3.33
3.31
3.30
1.11
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1.08
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1.03
1.85
1.83
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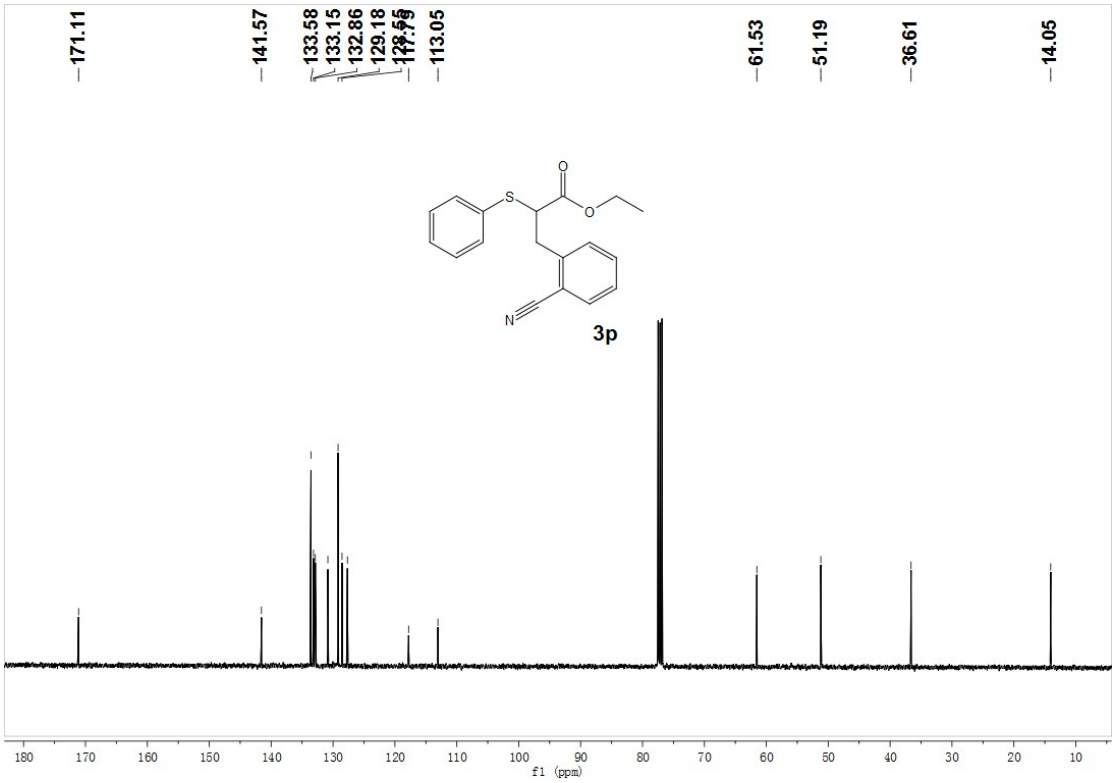
2.93
2.01
2.93
f1 (ppm)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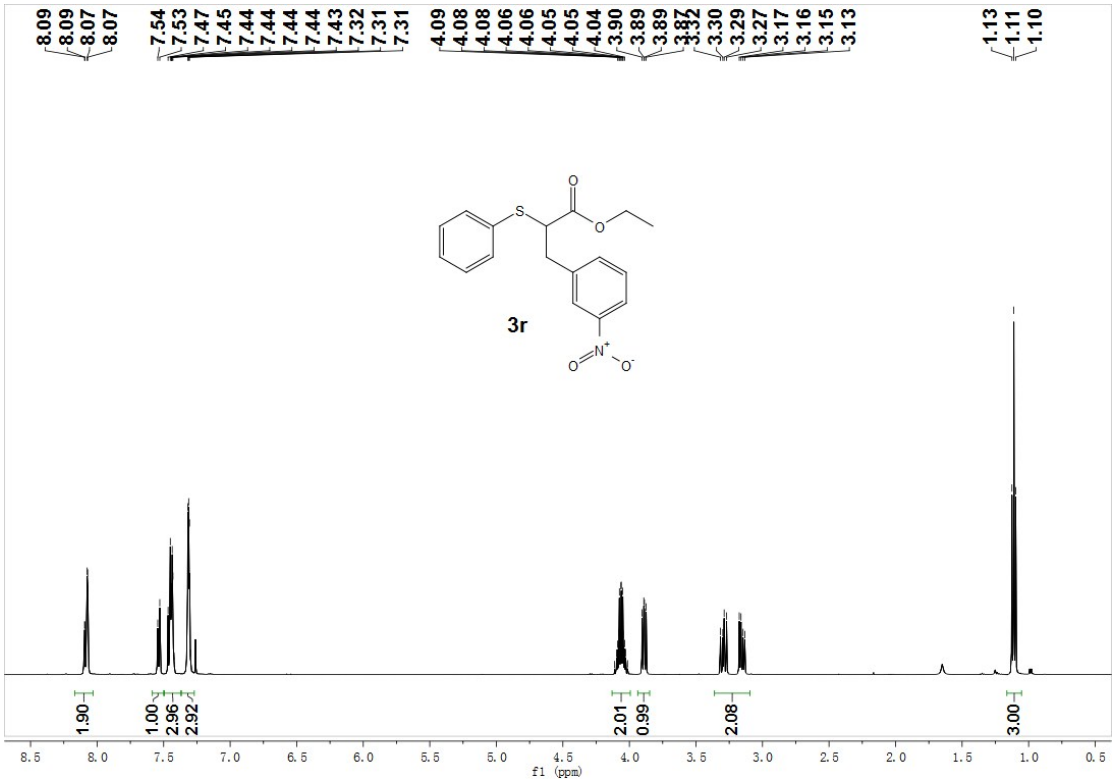
36.61
14.05
3p
f1 (ppm)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7.32
7.31
7.31
4.09
4.08
4.08
4.06
4.06
4.05
4.05
4.04
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3.89
3.89
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3.27
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3.16
3.15
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1.13
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1.10
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2.92
2.01
0.99
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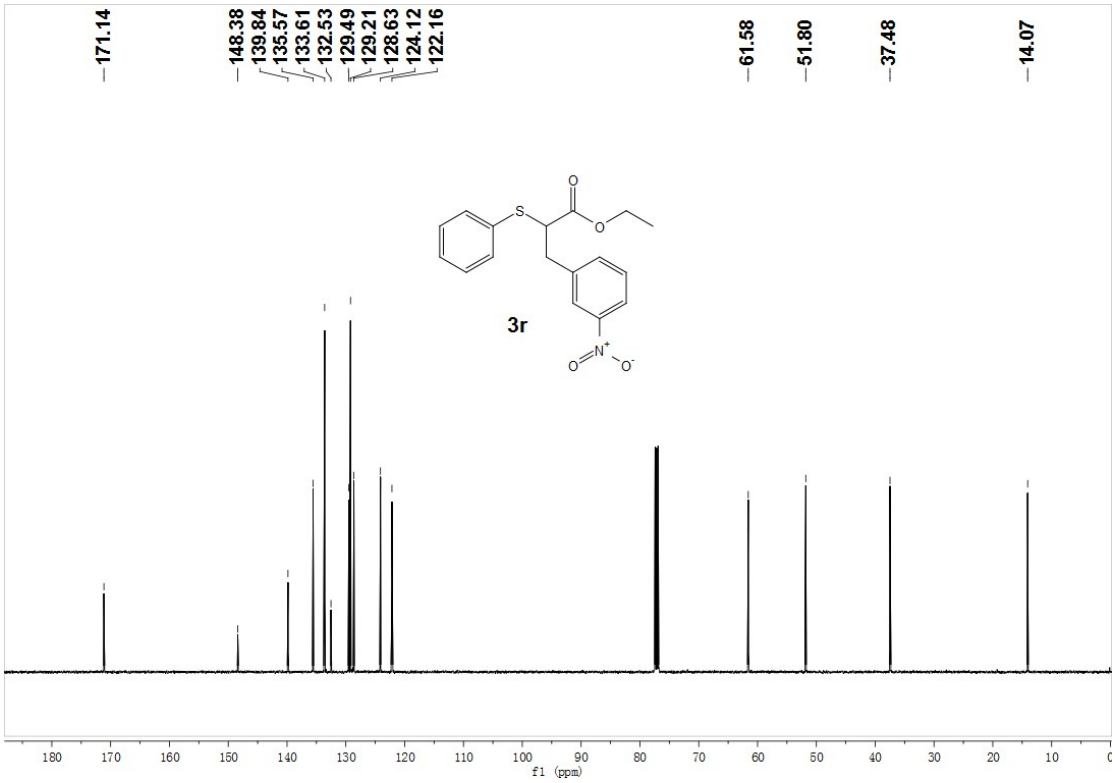
3.00
f1 (ppm)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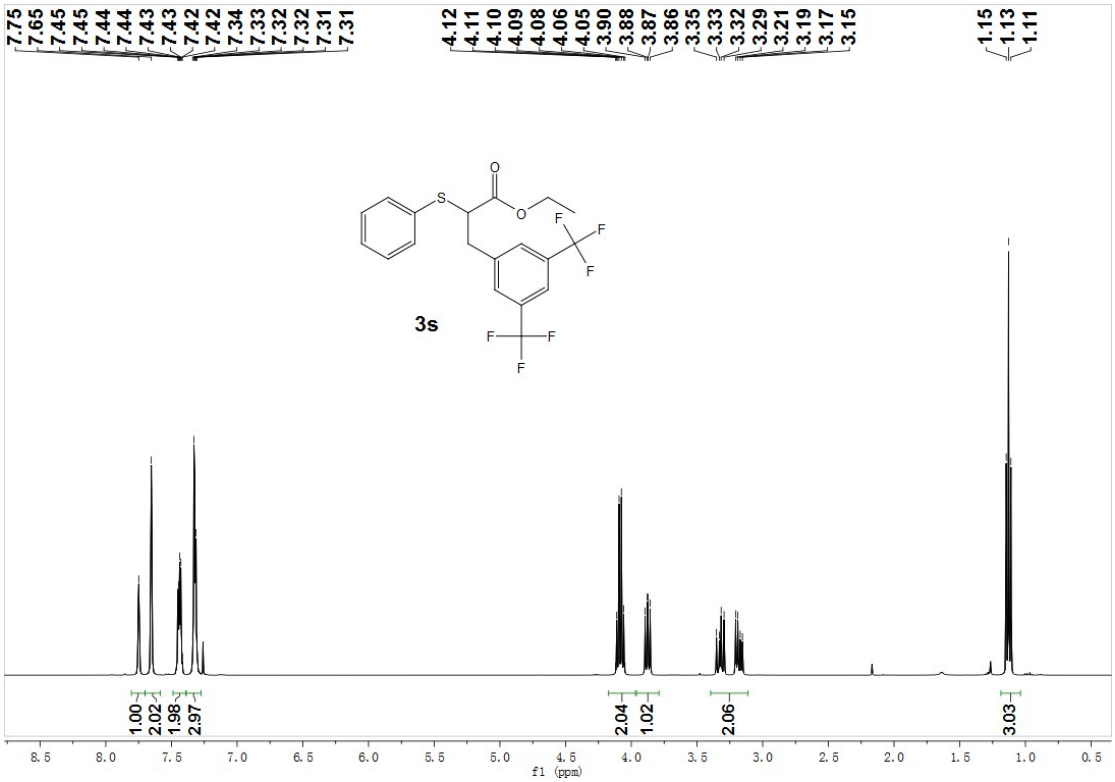
37.48
14.07
3r
f1 (ppm)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7.32
7.31
7.31
4.12
4.11
4.10
4.09
4.08
4.06
4.05
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3.87
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3.35
3.33
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3.19
3.17
3.15
1.15
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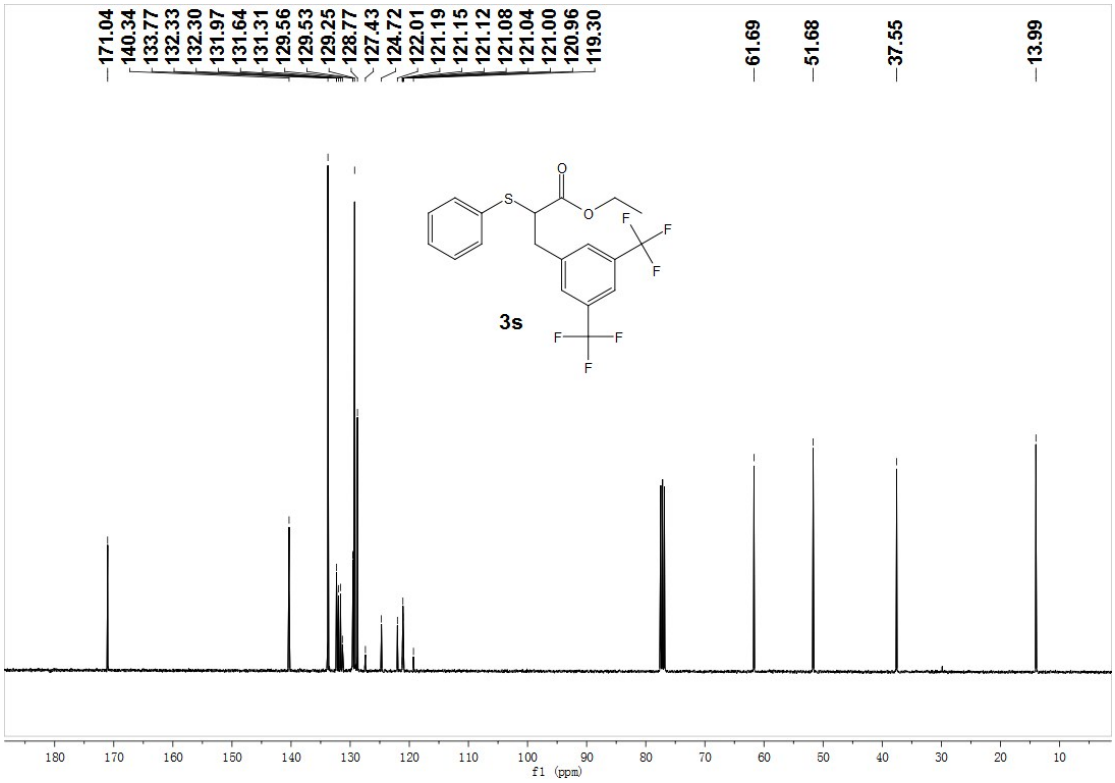
1.98
2.97
2.04
1.02
2.06
3.03
f1 (ppm)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122.01
121.19
121.15
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121.04
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119.30
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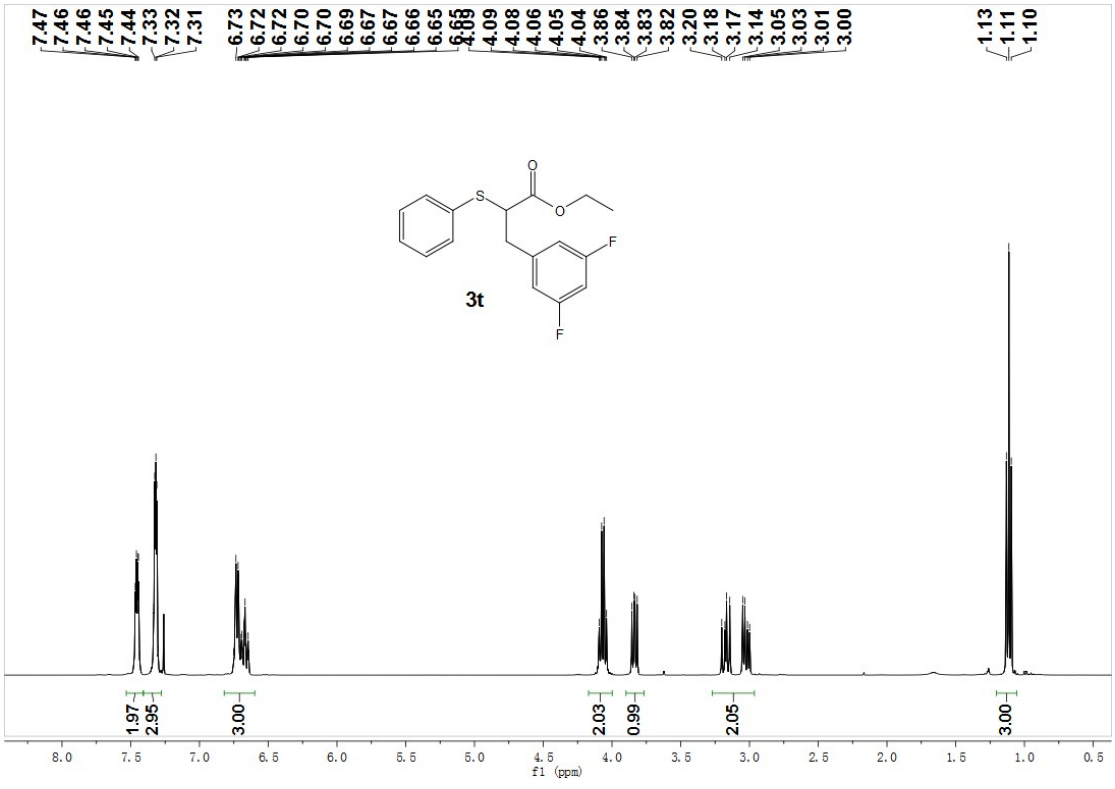
51.68
37.55
13.99
3s
f1 (ppm)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7.31
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6.72
6.72
6.70
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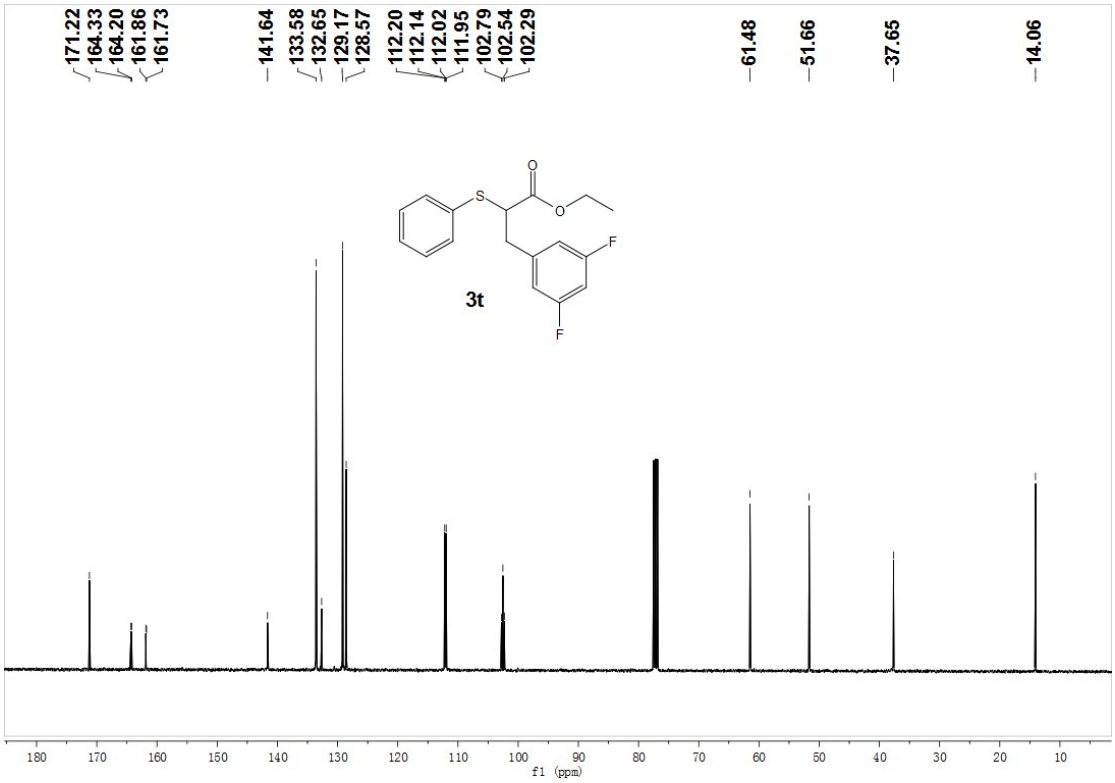
6.69
6.67
6.67
6.66
6.65
4.09
4.08
4.06
4.05
4.04
3.86
3.84
3.83
3.82
3.20
3.18
3.17
3.14
3.05
3.03
3.01
3.00
1.13
1.11
1.10
3t
1.97
2.95
3.00
2.03
0.99
2.05
3.00
f1 (ppm)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133.58
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129.17
128.57
112.20
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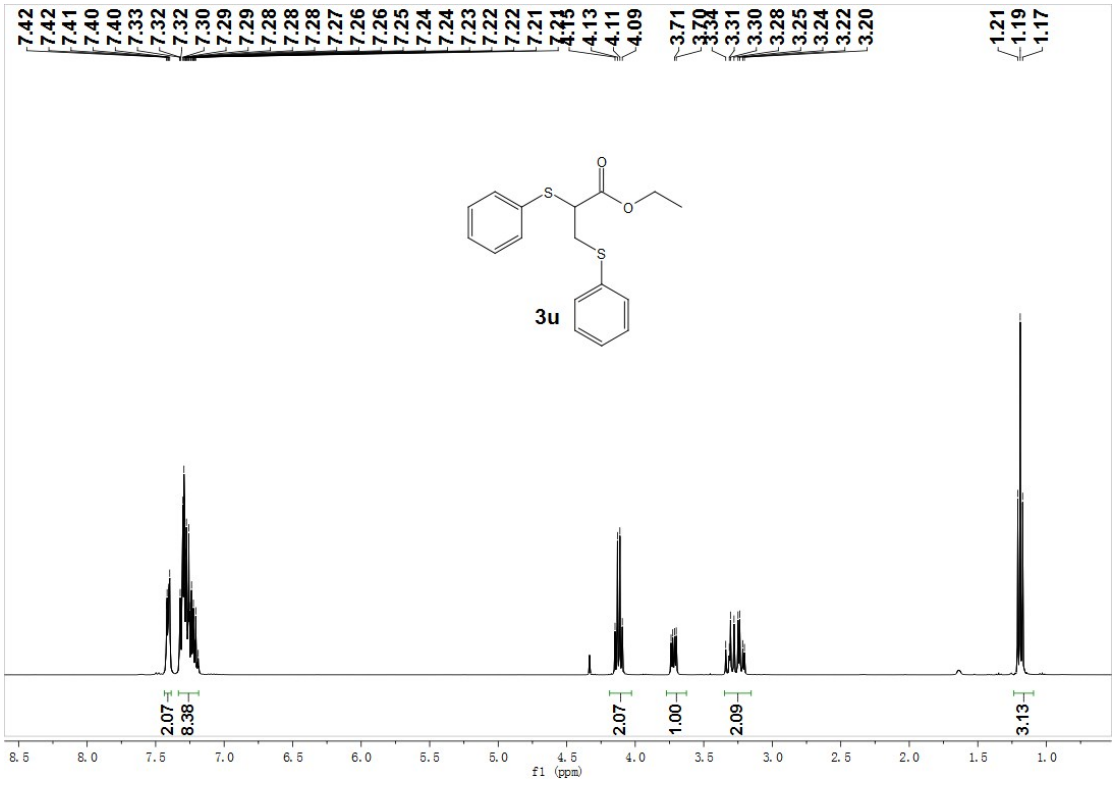
102.54
102.29
61.48
51.66
37.65
14.06
3t
f1 (ppm)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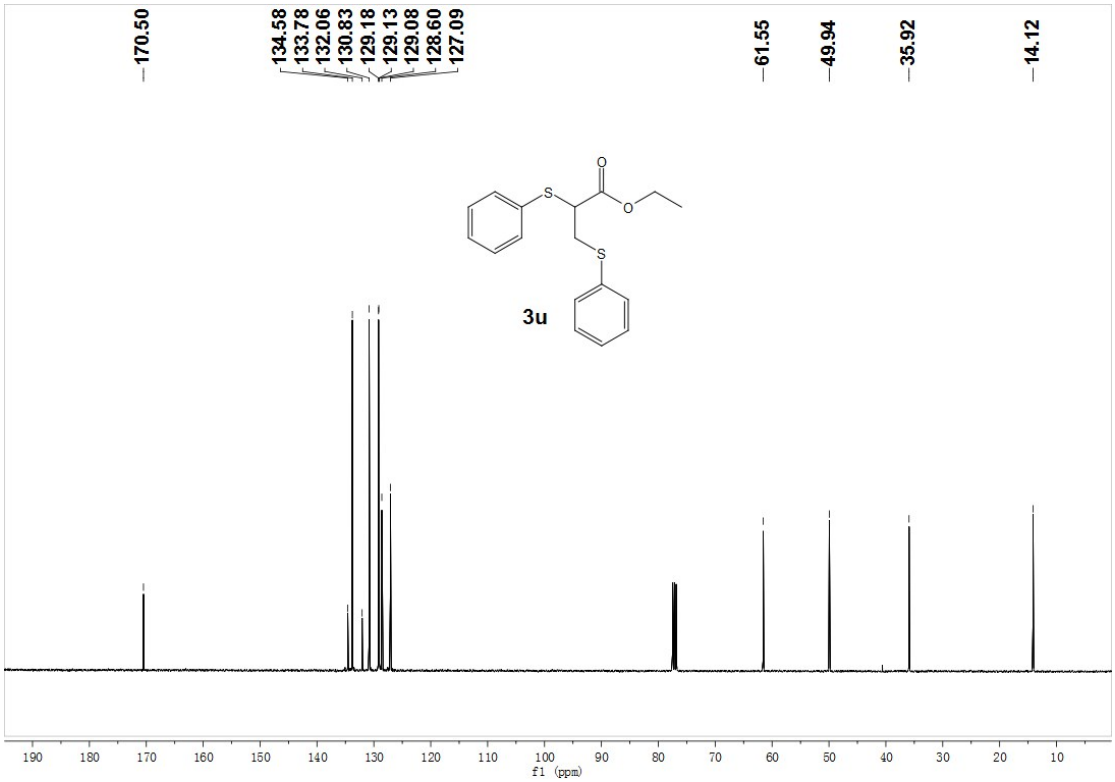
7.26
7.25
7.24
7.24
7.23
7.22
7.22
7.21
4.13
4.11
4.09
3.71
3.31
3.30
3.28
3.25
3.24
3.22
3.20
1.21
1.19
1.17
3u
2.07
8.38
2.07
1.00
2.09
3.13
f1 (ppm)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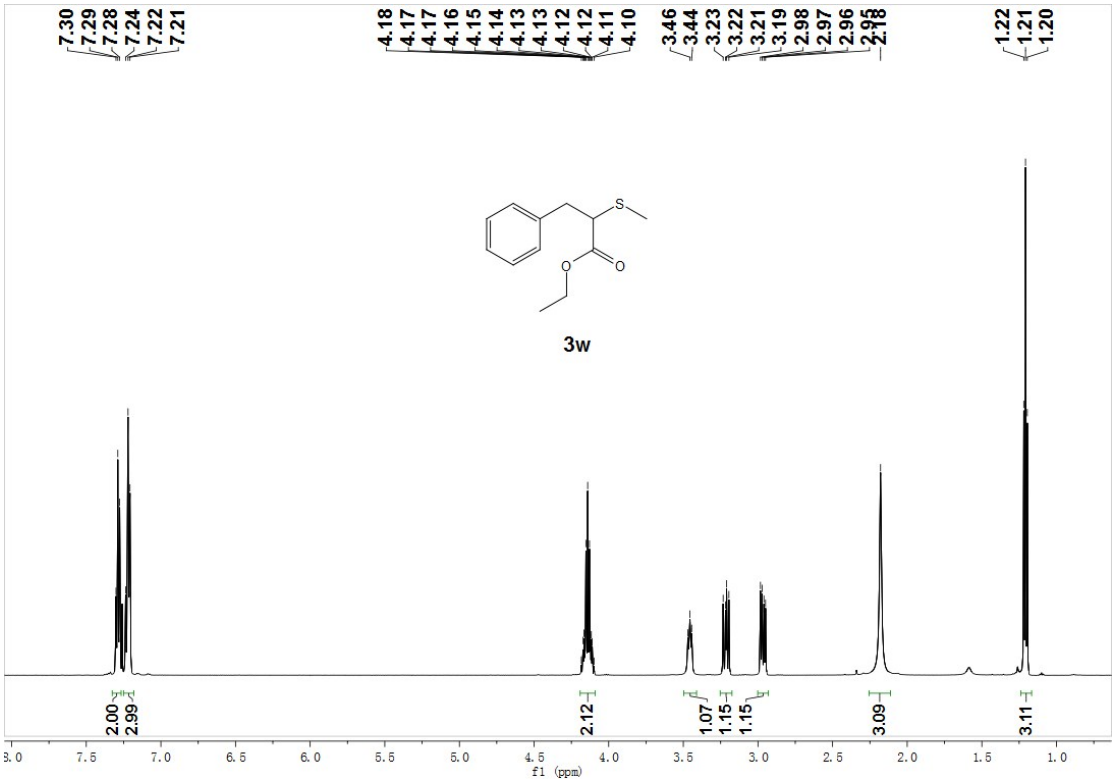
127.09
61.55
49.94
35.92
14.12
3u
f1 (ppm)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4.17
4.17
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4.15
4.14
4.13
4.13
4.12
4.12
4.11
4.10
3.46
3.44
3.23
3.22
3.21
3.19
2.98
2.97
2.96
2.95
2.18
1.22
1.21
1.20
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2.00
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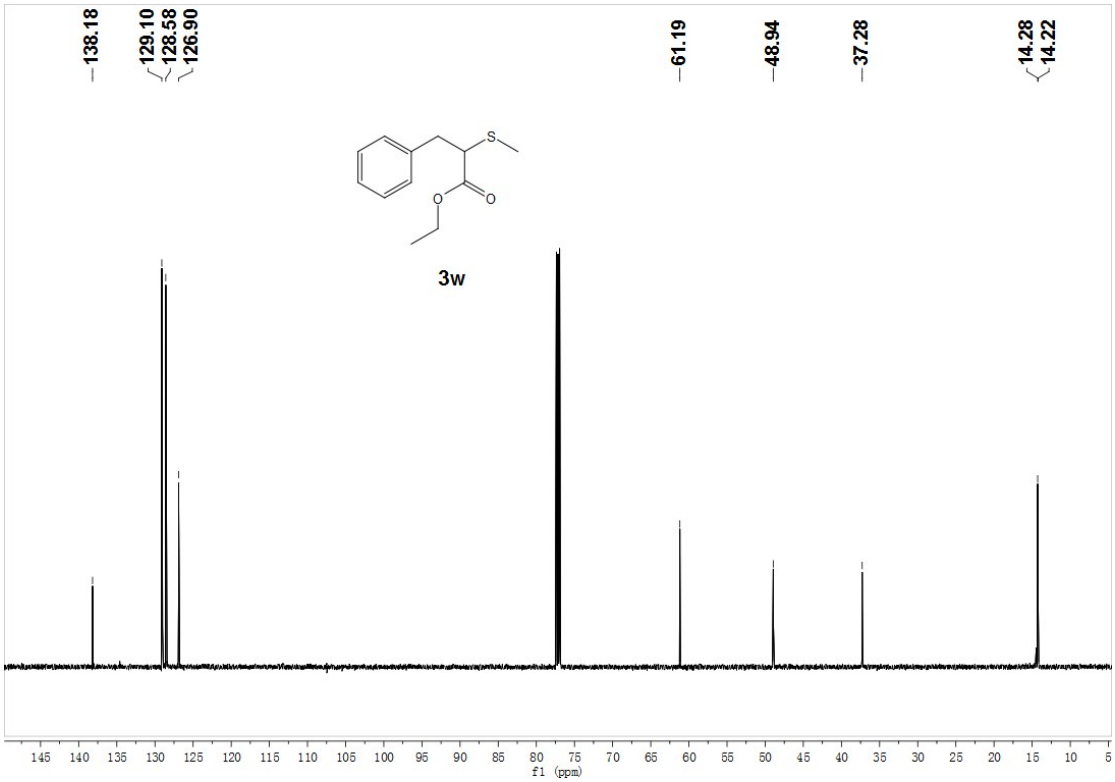
2.12
1.07
1.15
1.15
3.09
3.11
f1 (ppm)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61.19
48.94
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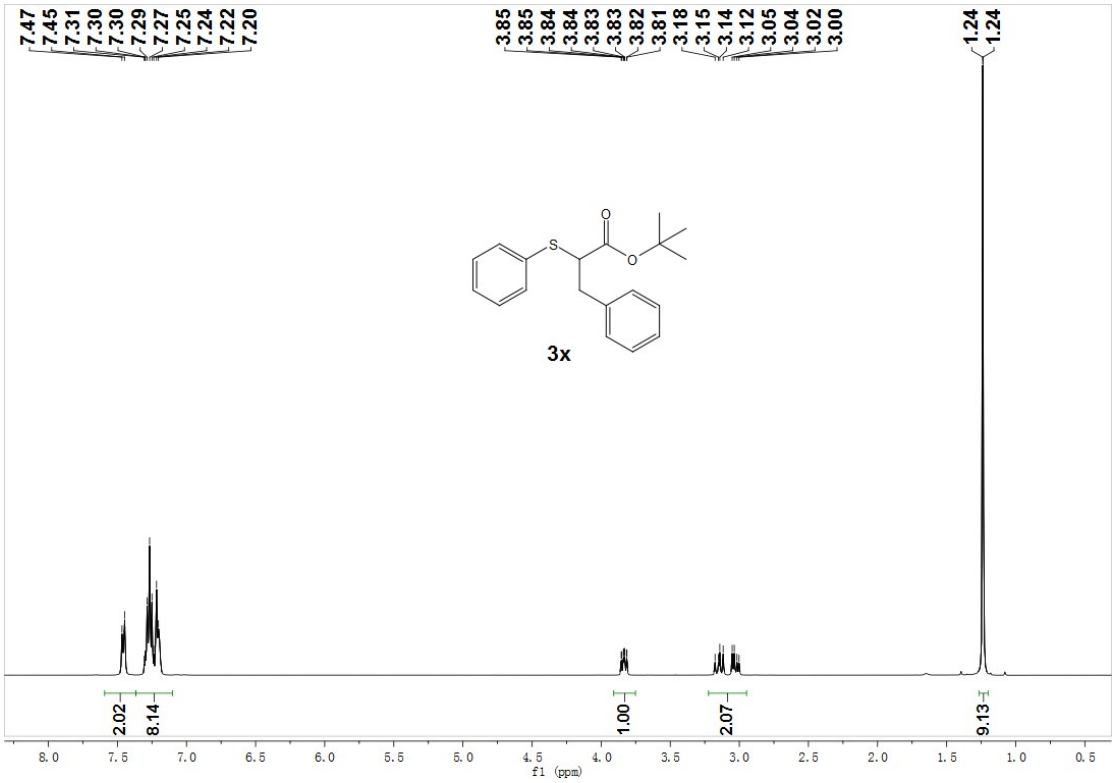
14.22
S
O
O
3w
145 140 135 130 125 120 115 110 105 100 95 90 85 80 75 70 65 60 55 50 45 40 35 30 25 20 15 10 5
f1 (ppm)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7.22
7.20
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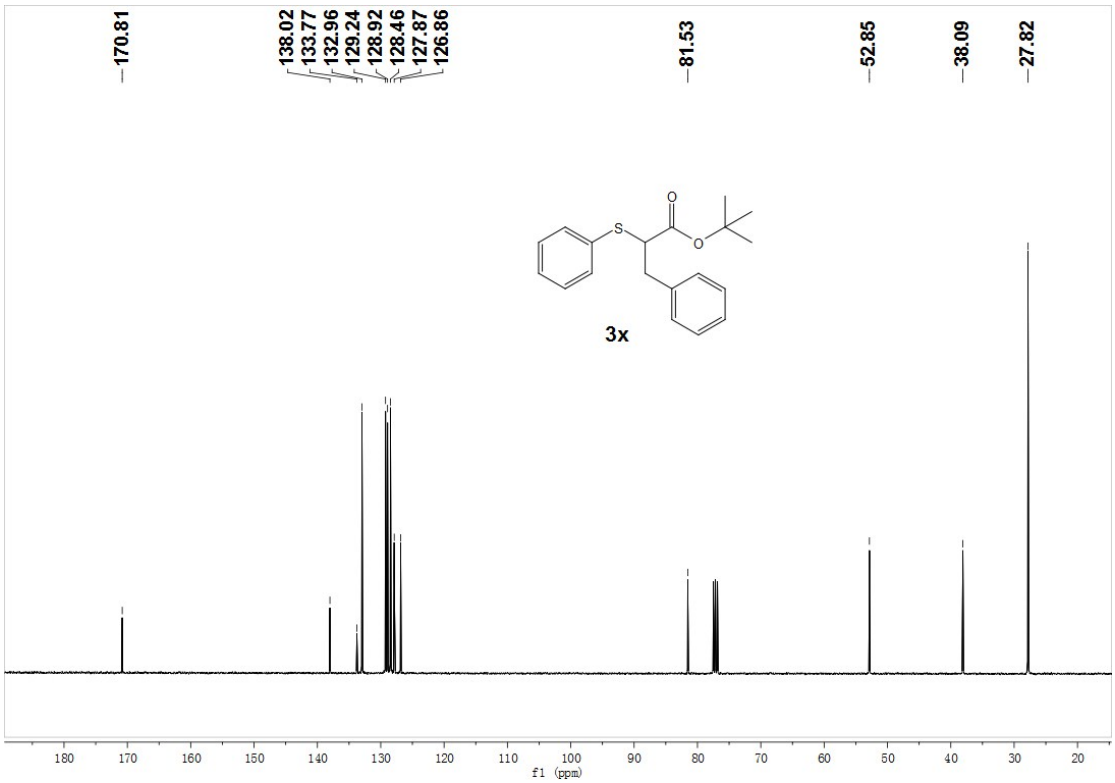
3.85
3.84
3.84
3.83
3.83
3.82
3.81
3.18
3.15
3.14
3.12
3.05
3.04
3.02
3.00
1.24
1.24
S
O
O
3x
2.02
8.14
1.00
2.07
9.13
8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
f1 (ppm)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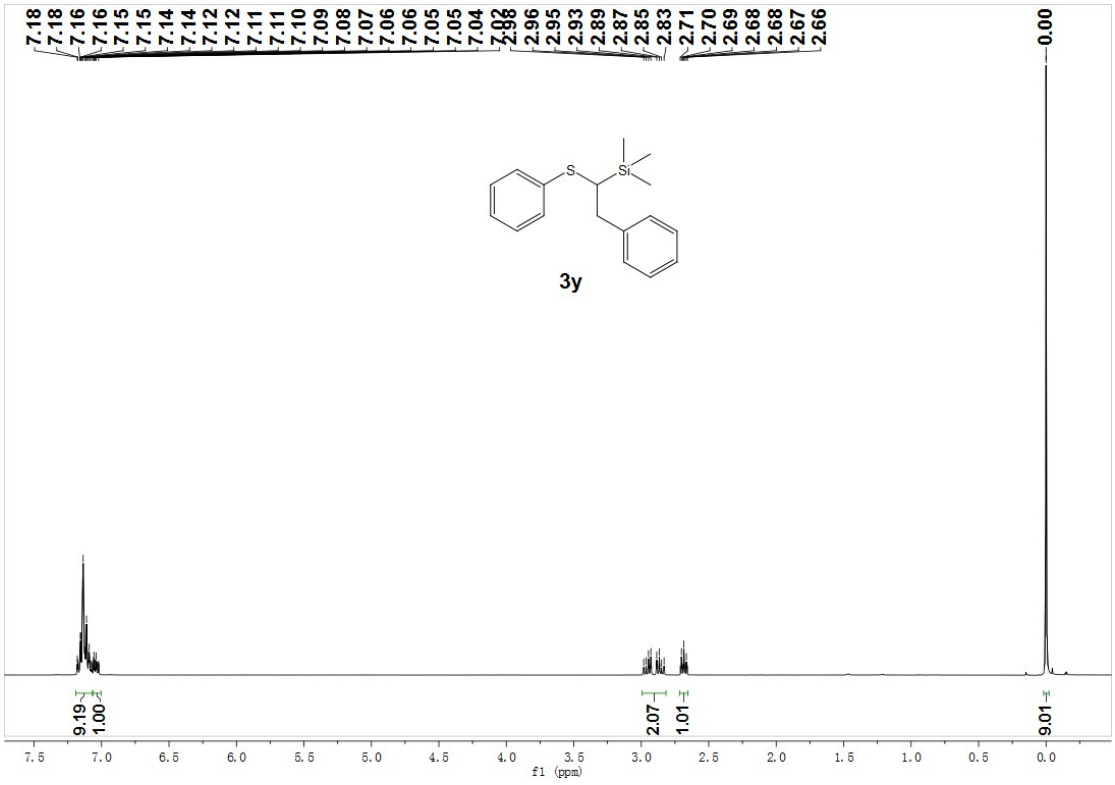
129.24
128.92
128.46
127.87
126.86
81.53
52.85
38.09
27.82
O
S
O
3x
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
f1 (ppm)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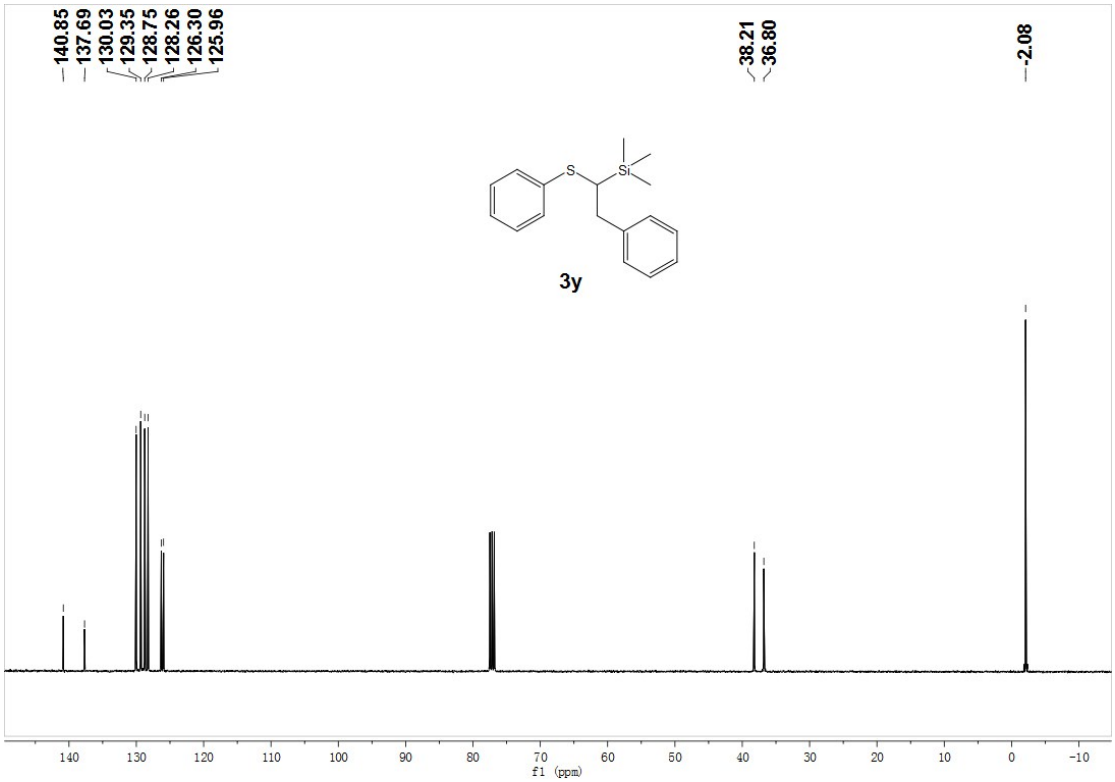
7.11
7.10
7.09
7.08
7.07
7.06
7.06
7.05
7.05
7.04
2.96
2.95
2.93
2.89
2.87
2.85
2.83
2.71
2.70
2.69
2.68
2.68
2.67
2.66
0.00
S
Si
3y
9.19
1.00
2.07
1.01
9.01
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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128.26
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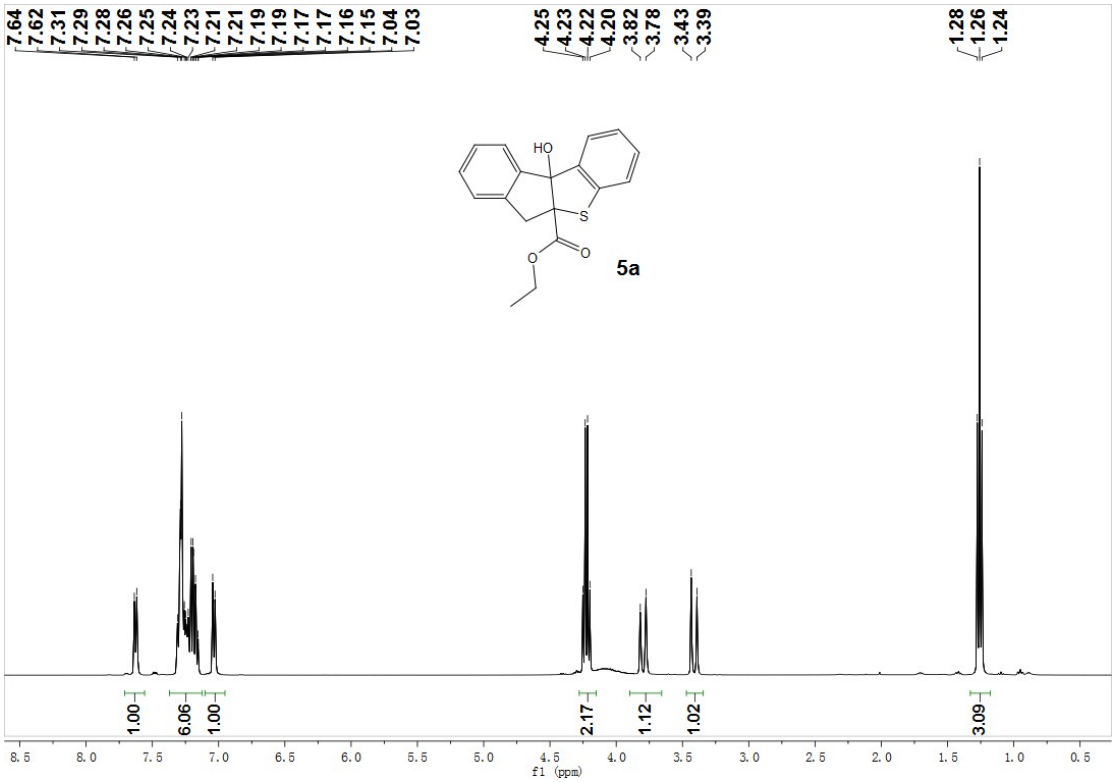
125.96
38.21
36.80
-2.08
S
Si
3y
f1 (ppm)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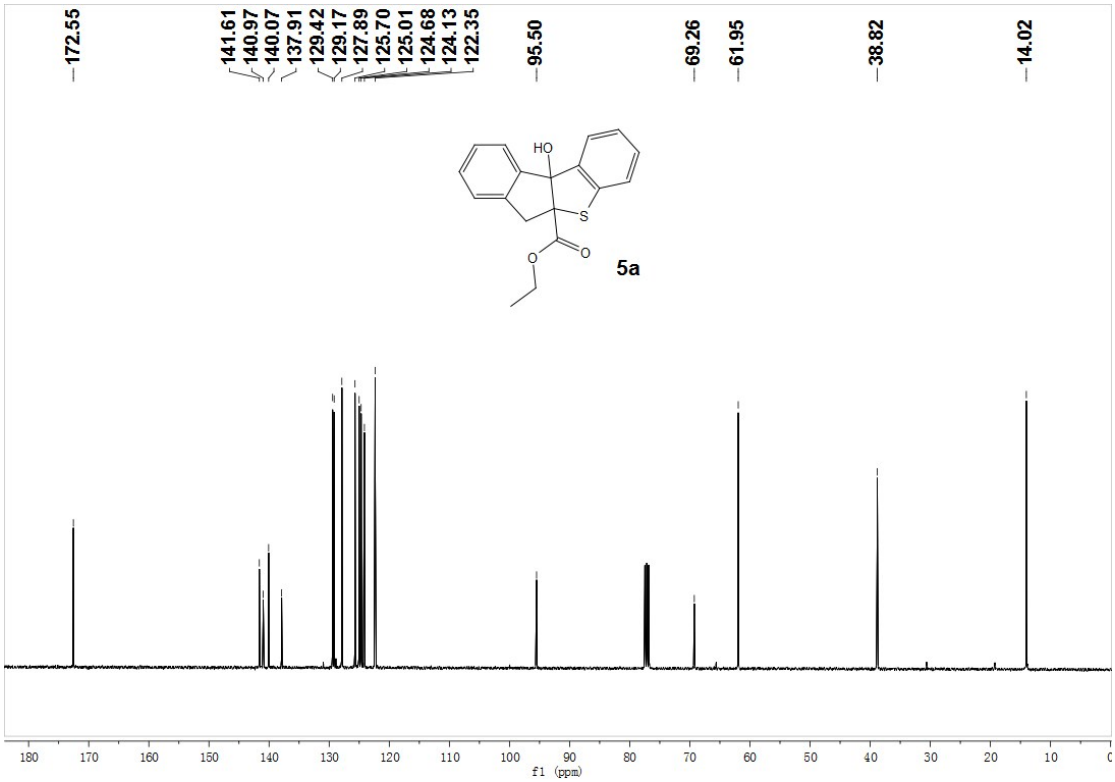
7.19
7.17
7.17
7.16
7.15
7.04
7.03
4.25
4.23
4.22
4.20
3.82
3.78
3.43
3.39
1.28
1.26
1.24
HO
S
O
O
5a
1.00
6.06
1.00
2.17
1.12
1.02
3.09
f1 (ppm)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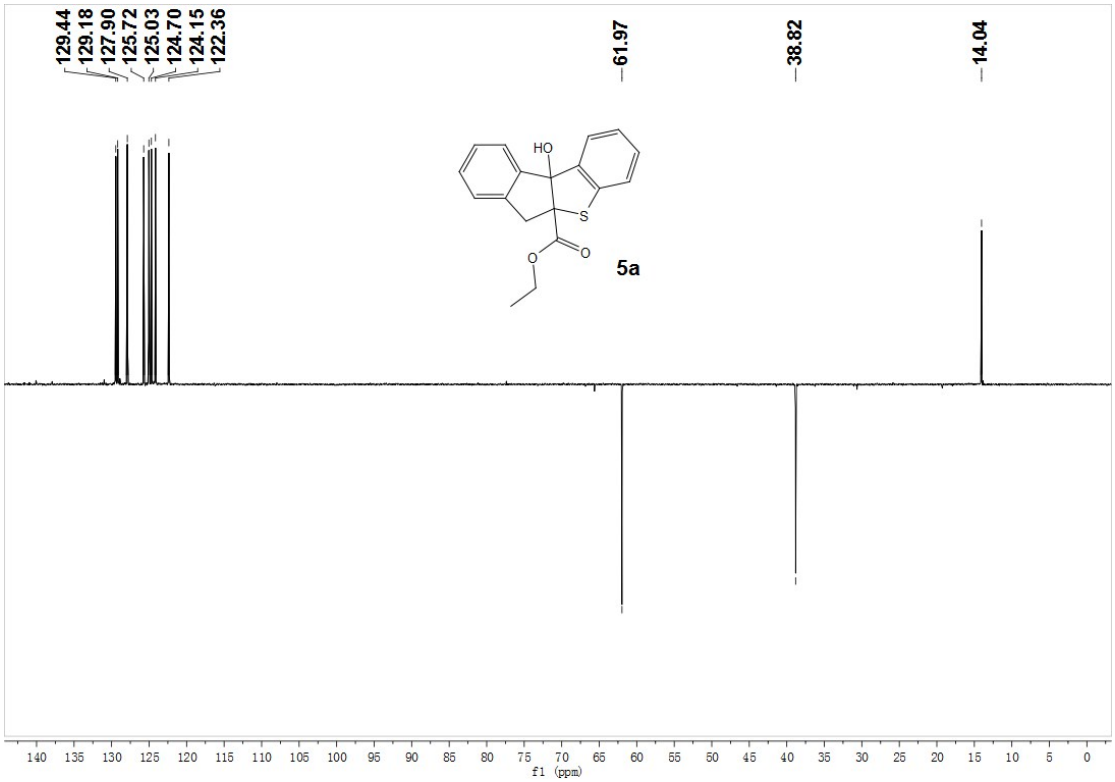
127.89
125.70
125.01
124.68
124.13
122.35
95.50
69.26
61.95
38.82
14.02
HO
S
O
O
5a
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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127.90
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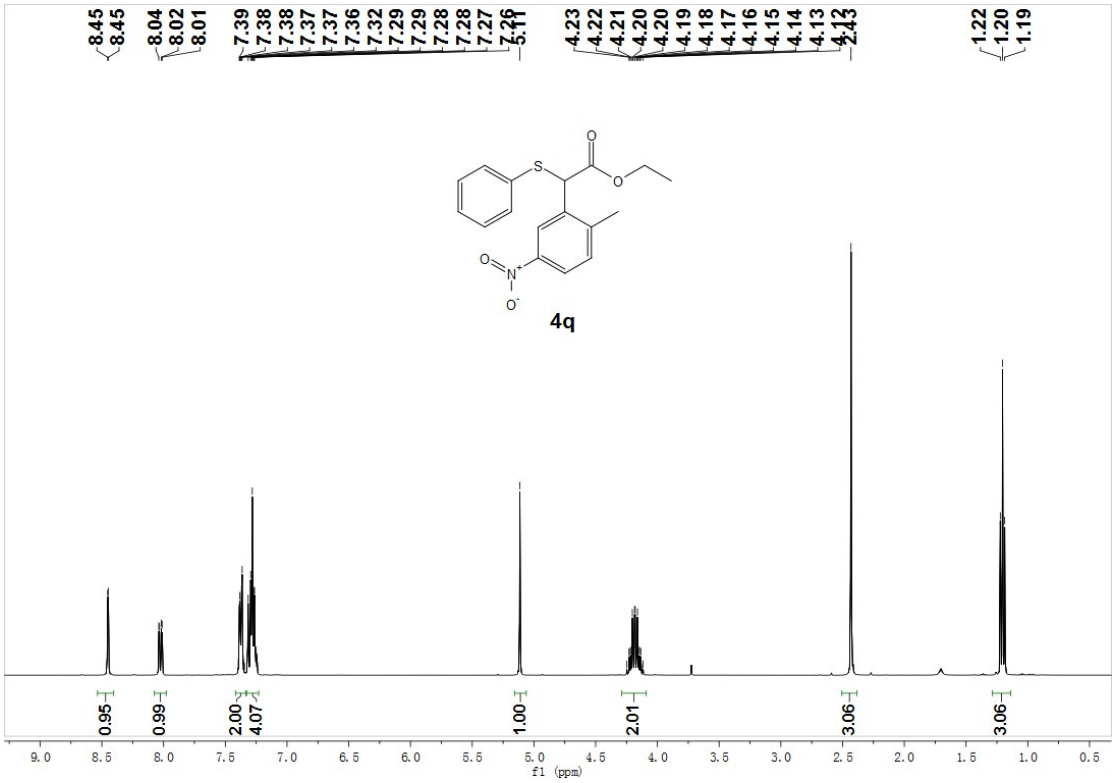
124.70
124.15
122.36
61.97
38.82
14.04
HO
S
O
O
5a
140 135 130 125 120 115 110 105 100 95 90 85 80 75 70 65 60 55 50 45 40 35 30 25 20 15 10 5 0
f1 (ppm)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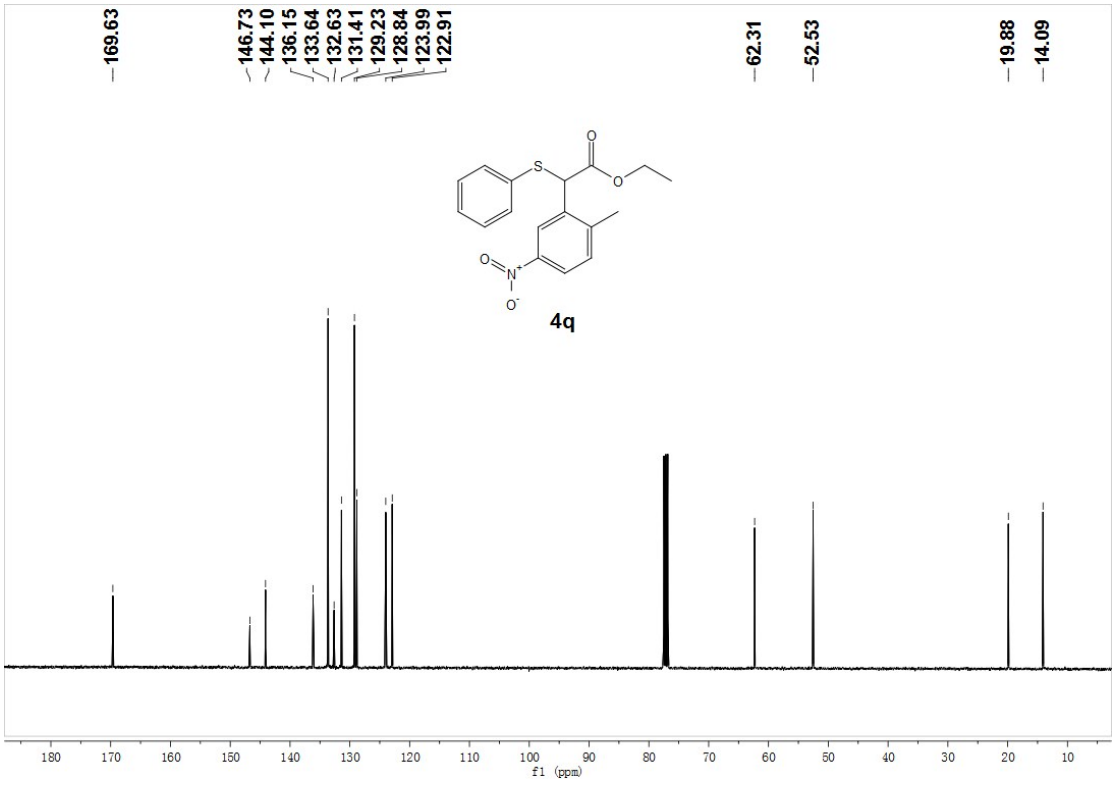
7.29
7.28
7.28
7.27
7.26
5.11
4.23
4.22
4.21
4.20
4.20
4.19
4.18
4.17
4.16
4.15
4.14
4.13
4.12
4.13
1.22
1.20
1.19
4q
0.95
0.99
2.00
4.07
1.00
2.01
3.06
3.06
f1 (ppm)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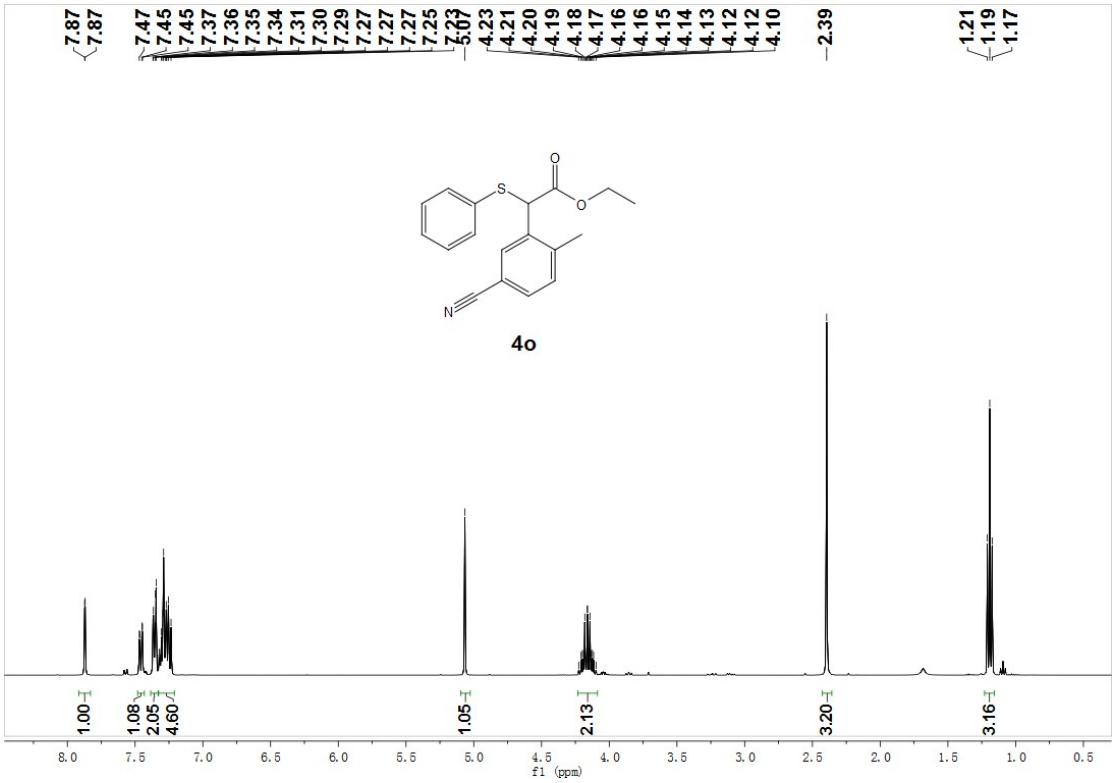
129.23
128.84
123.99
122.91
62.31
52.53
19.88
14.09
4q
f1 (ppm)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5.07
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4.20
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4.17
4.16
4.16
4.15
4.14
4.13
4.12
4.12
4.10
2.39
1.21
1.19
1.17
O
S
O
N
1.00
1.08
2.05
4.60
1.05
2.13
3.20
3.16
8.0
7.5
7.0
6.5
6.0
5.5
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4.5
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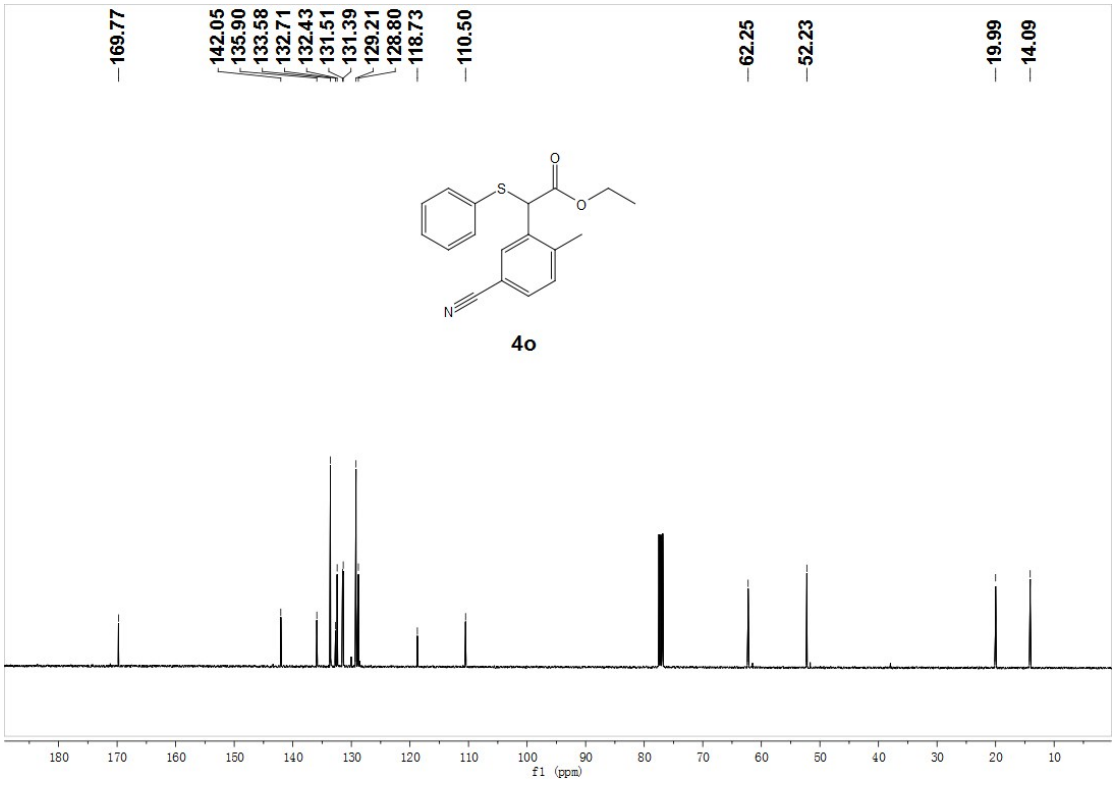
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)

4o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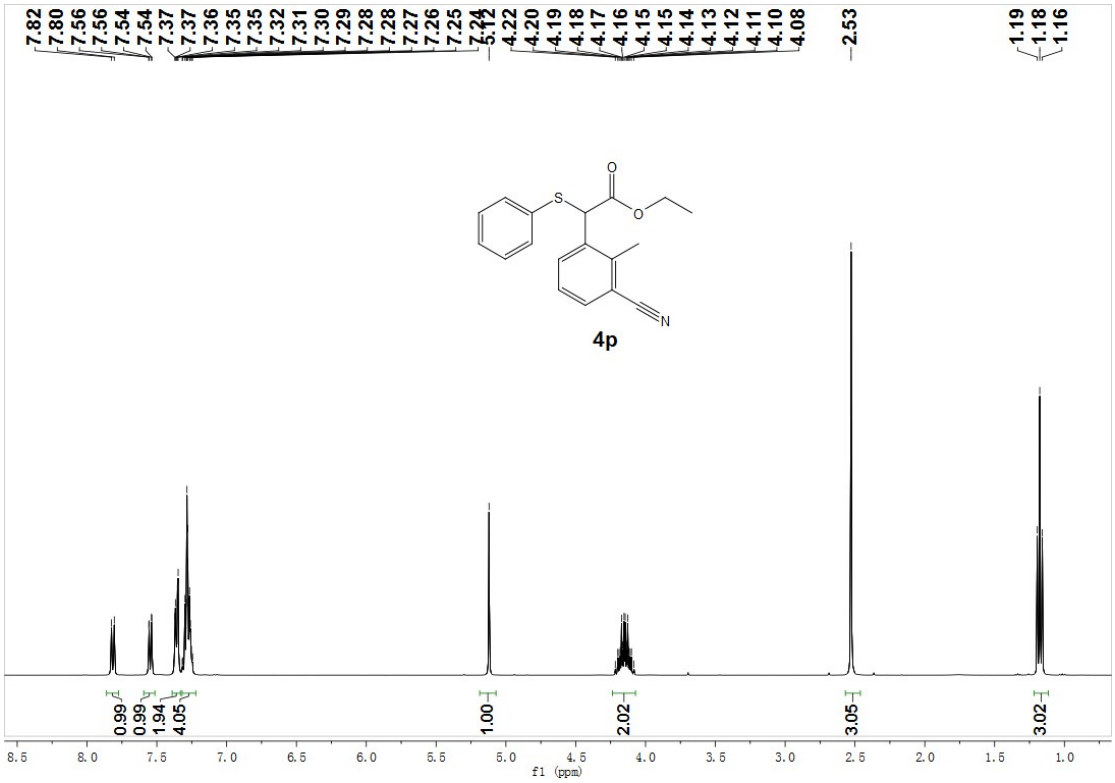
131.51
131.39
129.21
128.80
118.73
110.50
62.25
52.23
19.99
14.09
O
S
O
N
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

4o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7.26
7.25
7.24
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4.19
4.18
4.17
4.16
4.15
4.15
4.14
4.13
4.12
4.11
4.10
4.08
2.53
1.19
1.18
1.16
O
S
O
N
4p
0.99
0.99
1.94
4.05
1.00
2.02
3.05
3.02
8.5
8.0
7.5
7.0
6.5
6.0
5.5
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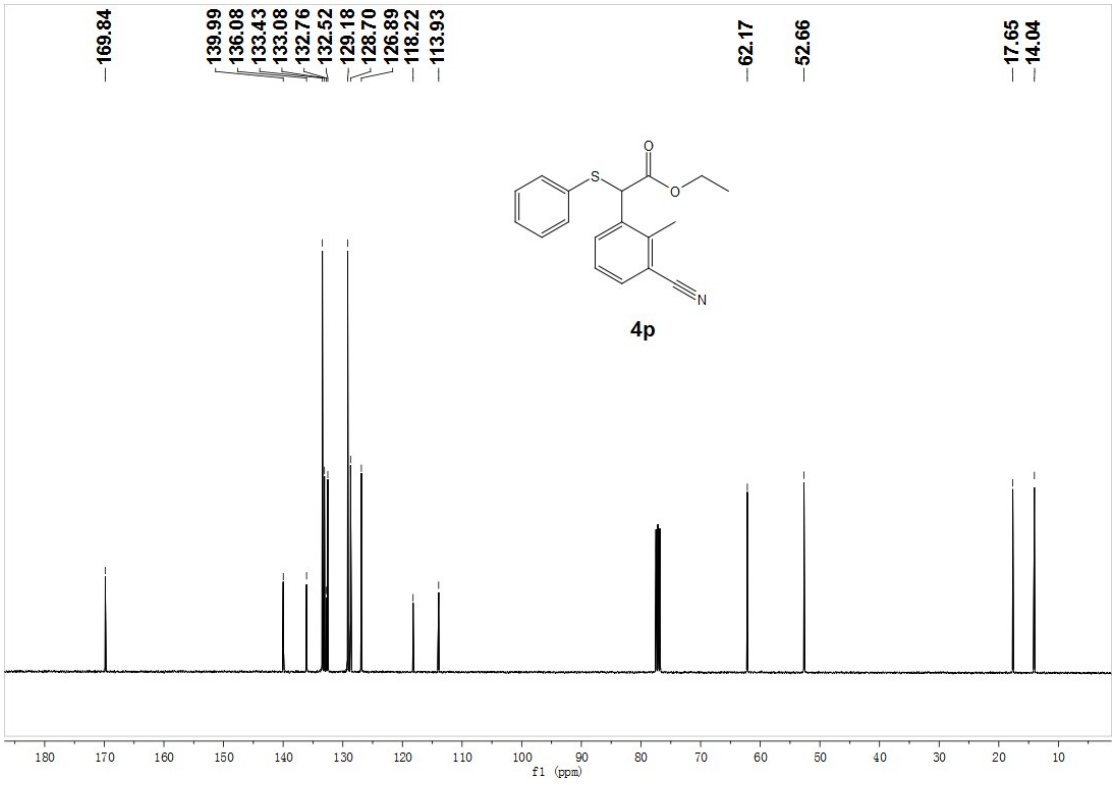
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
f1 (ppm)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128.70
126.89
118.22
113.93
62.17
52.66
17.65
14.04
O
S
O
N
4p
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170
160
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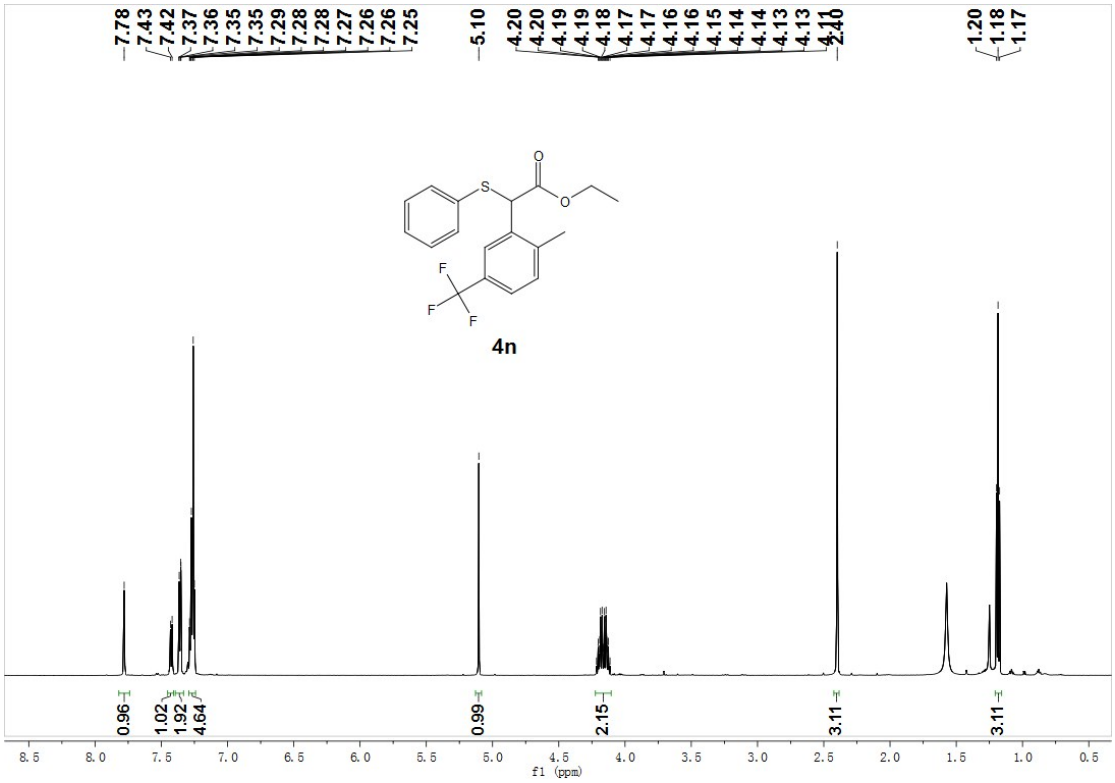
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)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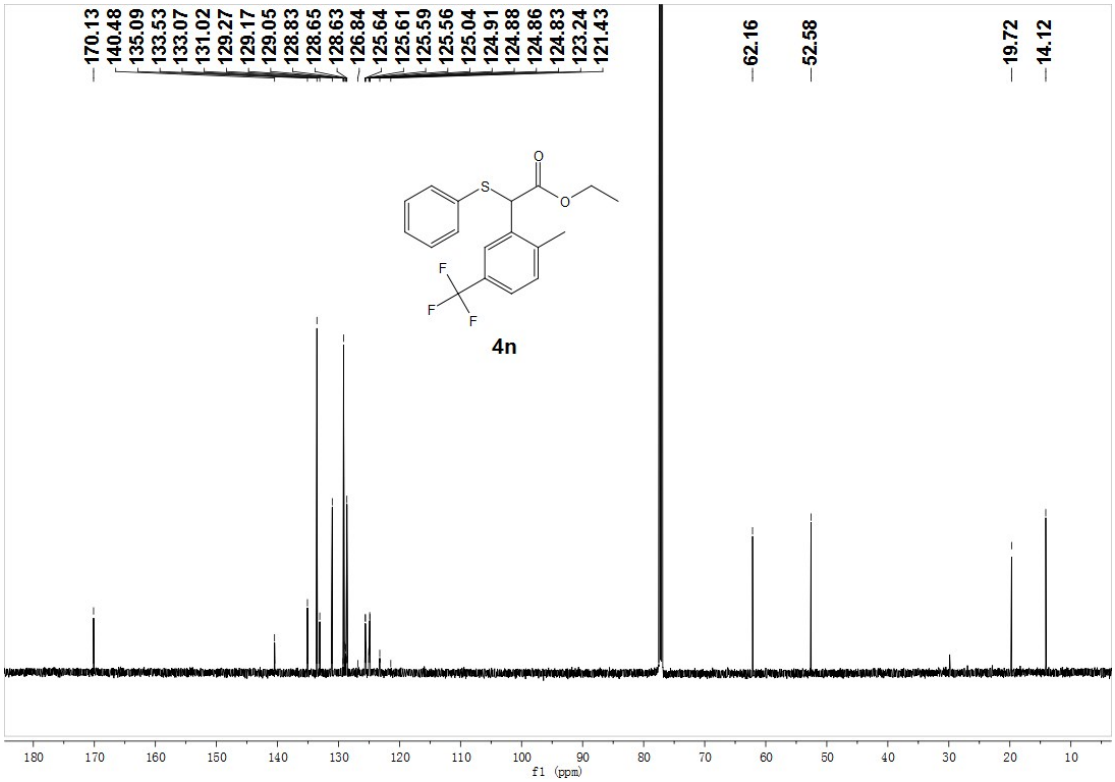
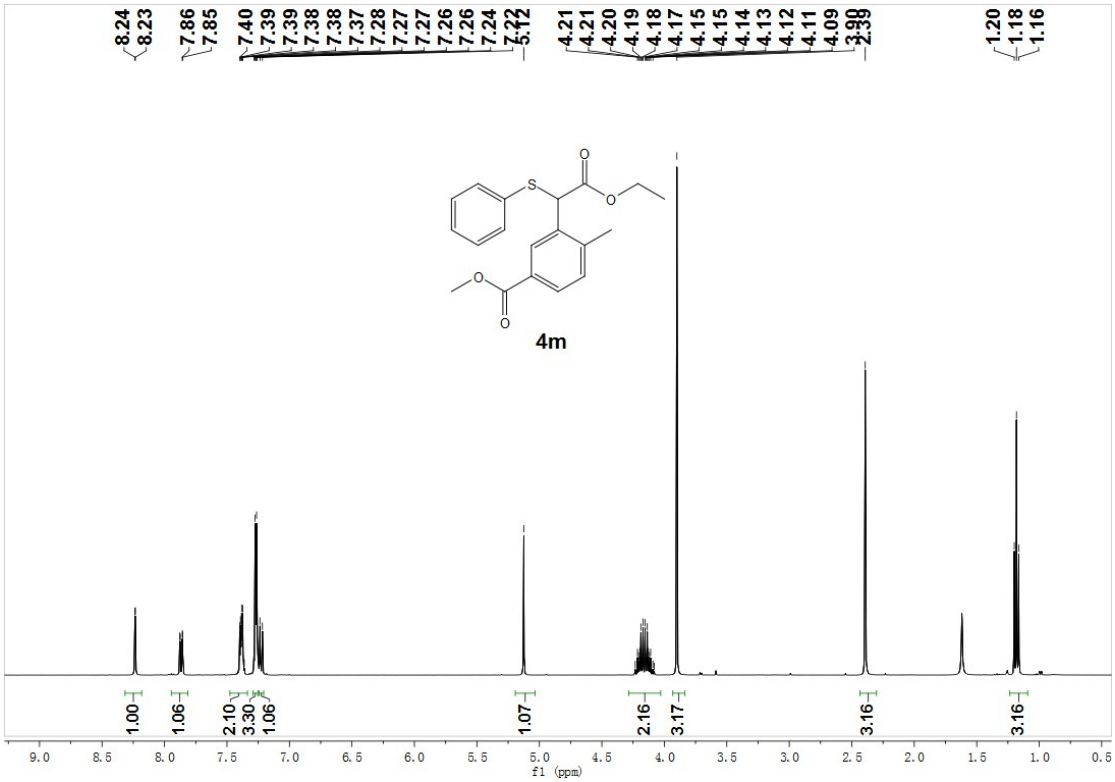
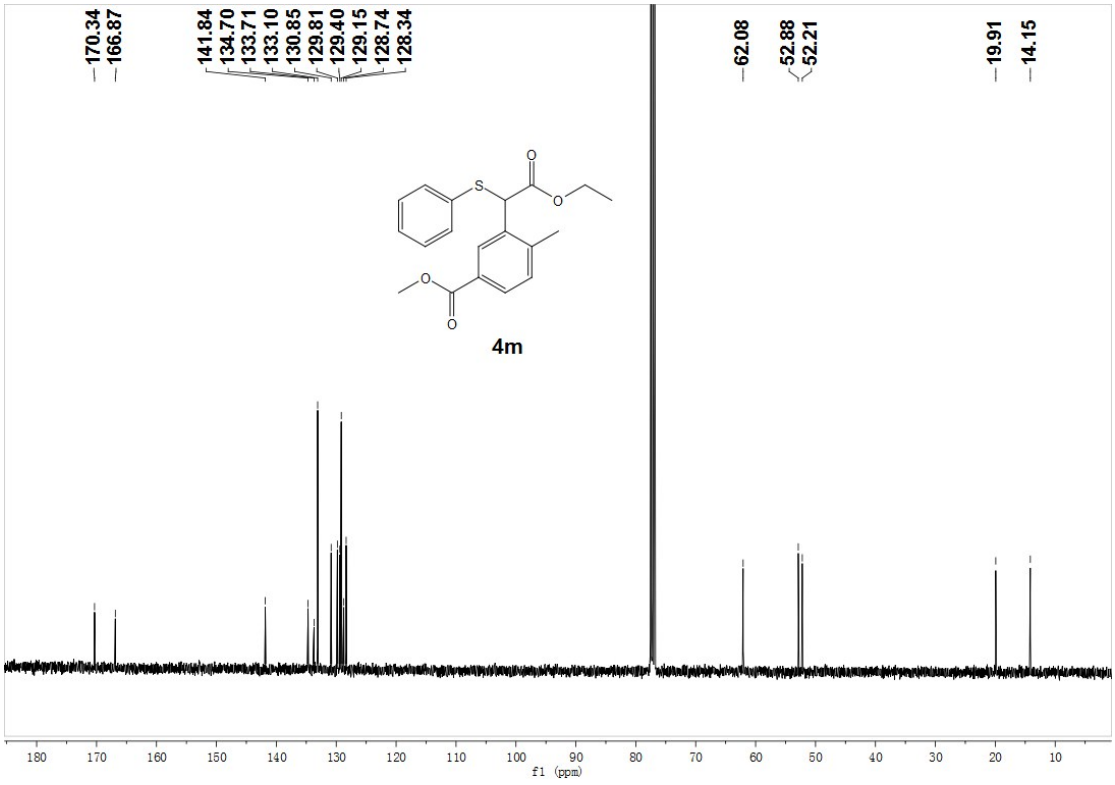
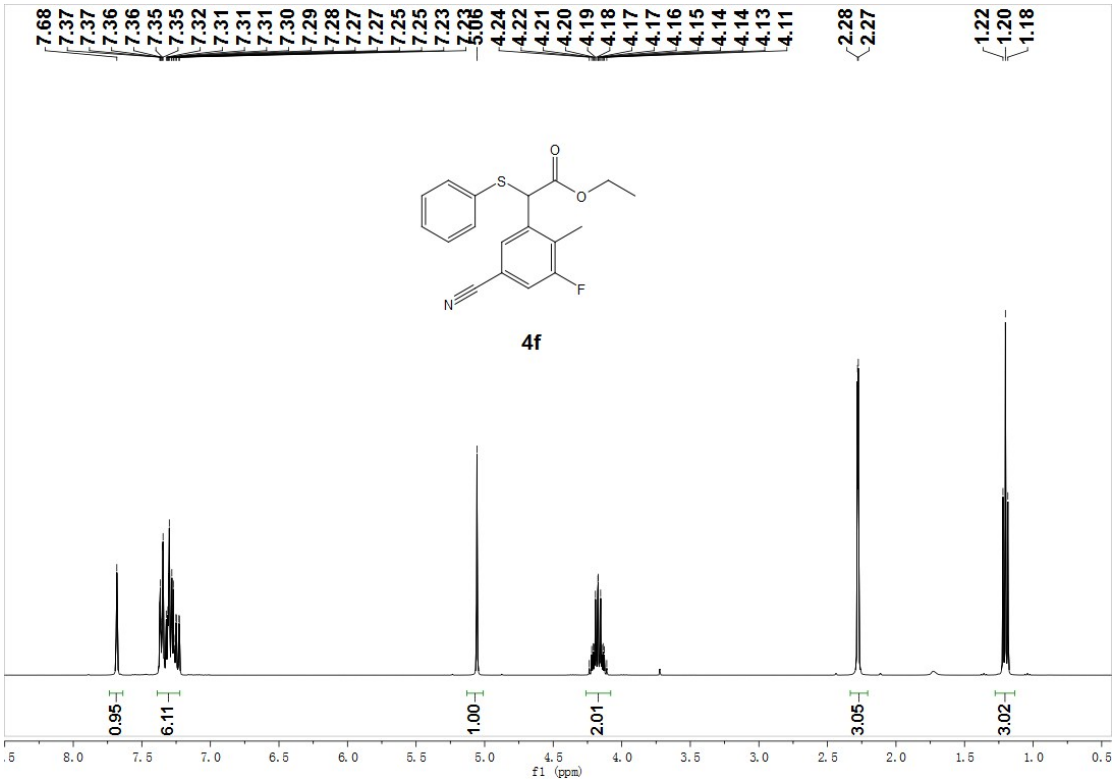
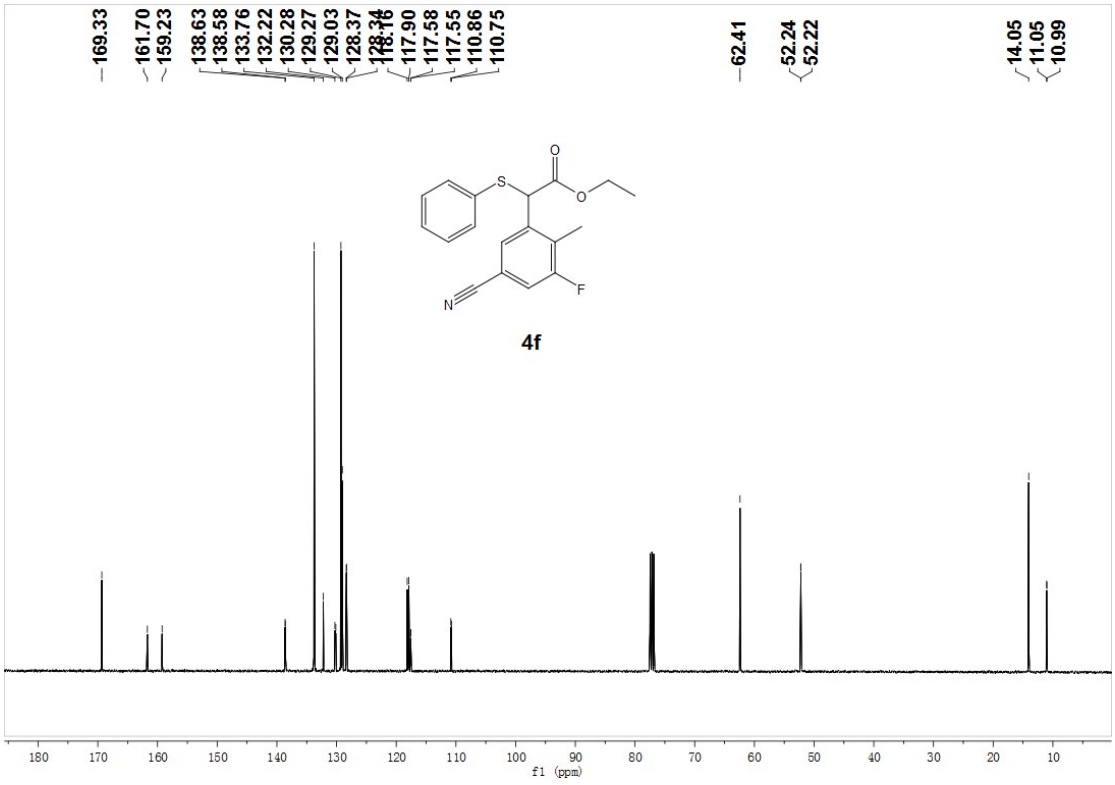
7.25
5.10
4.20
4.20
4.19
4.19
4.18
4.17
4.17
4.16
4.16
4.15
4.14
4.14
4.13
4.13
4.11
4.10
1.20
1.18
1.17
O
S
O
F
F
F
4n
0.96
1.02
1.92
4.64
0.99
2.15
3.11
3.11
f1 (ppm)

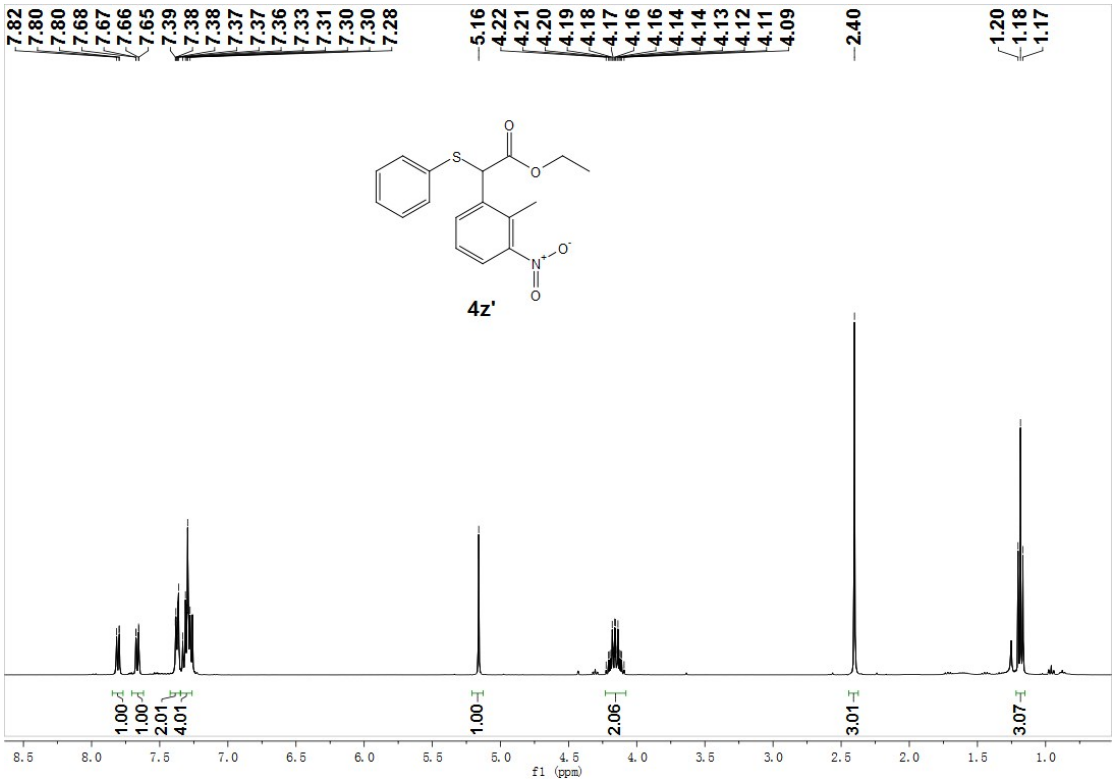

170.13
140.48
135.09
133.53
133.07
131.02
129.27
129.17
129.05
128.83
128.65
128.63
126.84
125.64
125.61
125.59
125.56
125.04
124.91
124.88
124.86
124.83
123.24
121.43
62.16
52.58
19.72
14.12
O
S
O
F
F
F
4n
f1 (ppm)

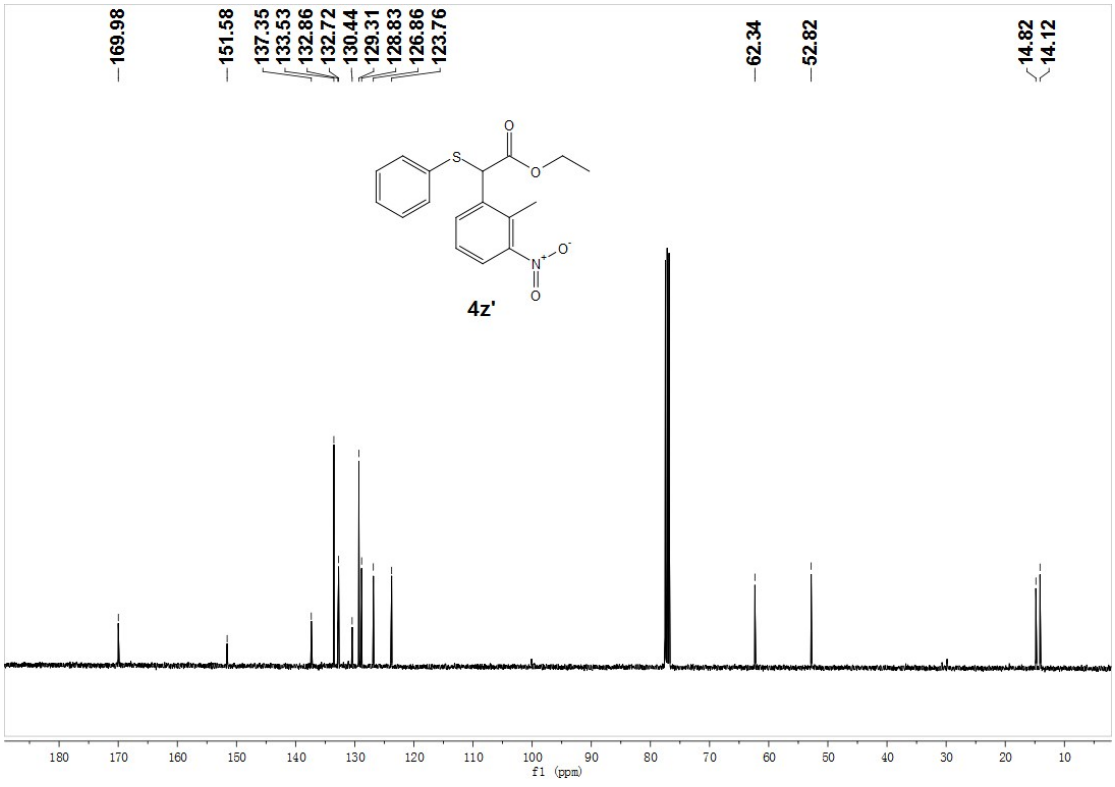

8.24
8.23
7.86
7.85
7.40
7.39
7.39
7.38
7.38
7.37
7.28
7.27
7.27
7.26
7.26
7.24
7.22
5.12
4.21
4.21
4.20
4.19
4.18
4.17
4.15
4.15
4.14
4.13
4.12
4.11
4.09
3.90
2.39
1.20
1.18
1.16
4m
1.00
1.06
2.10
3.30
1.06
1.07
2.16
3.17
3.16
3.16
f1 (ppm)

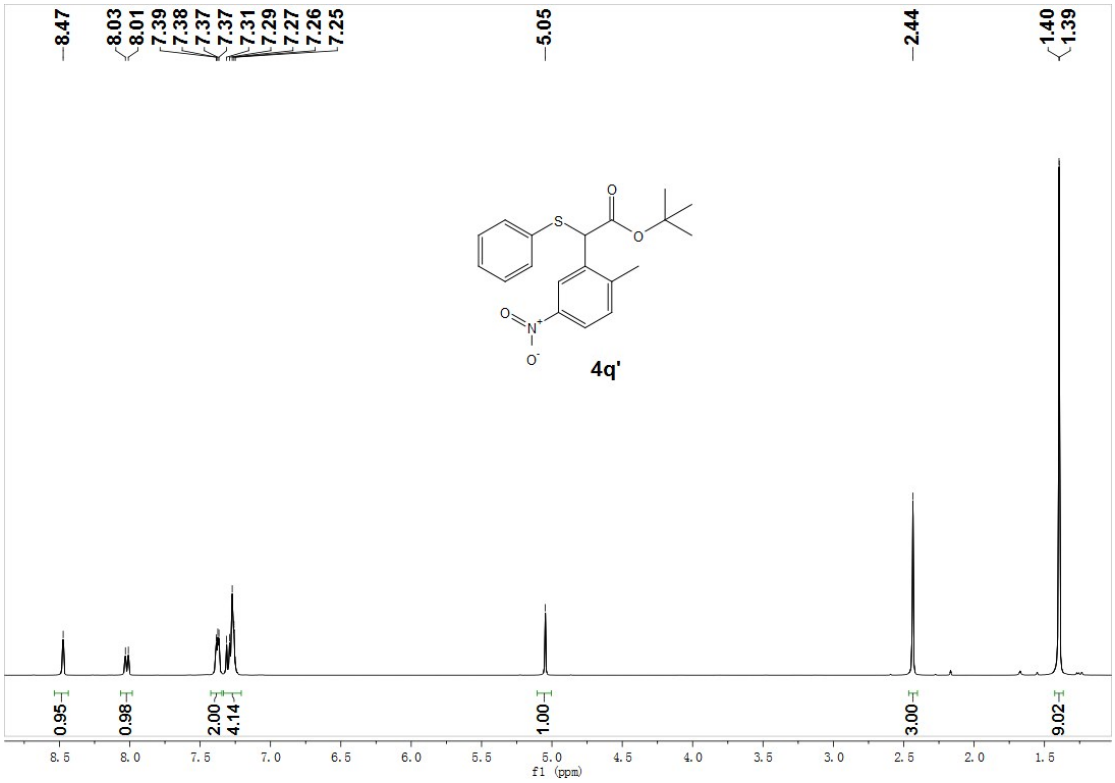

170.34
166.87
141.84
134.70
133.71
133.10
130.85
129.81
129.40
129.15
128.74
128.34
62.08
52.88
52.21
19.91
14.15
4m
f1 (ppm)

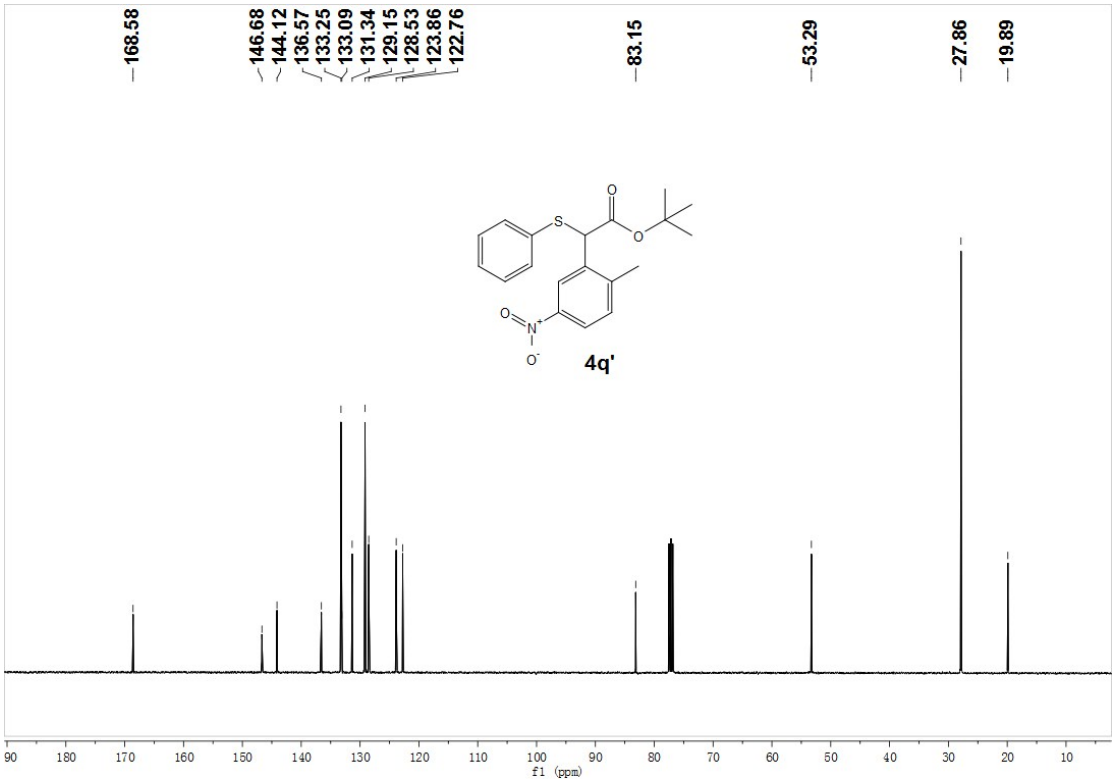

7.68 7.37 7.37 7.36 7.36 7.35 7.35 7.32 7.31 7.31 7.31 7.30 7.29 7.28 7.27 7.27 7.25 7.25 7.23 7.23 5.06 4.24 4.22 4.21 4.20 4.19 4.18 4.17 4.17 4.16 4.15 4.14 4.14 4.13 4.11 2.28 2.27 1.22 1.20 1.18
O
S
O
F
N
4f
0.95 6.11 1.00 2.01 3.05 3.02
f1 (ppm)


169.33 161.70 159.23 138.63 138.58 133.76 132.22 130.28 129.27 129.03 128.37 117.90 117.58 117.55 110.86 110.75 62.41 52.24 52.22 14.05 11.05 10.99
O
S
O
F
N
4f
f1 (ppm)


7.82
7.80
7.80
7.68
7.67
7.66
7.65
7.39
7.38
7.38
7.37
7.37
7.36
7.33
7.31
7.30
7.30
7.28
5.16
4.22
4.21
4.20
4.19
4.18
4.17
4.16
4.16
4.14
4.14
4.13
4.12
4.11
4.09
2.40
1.20
1.18
1.17
4z'
1.00
1.00
2.01
4.01
1.00
2.06
3.01
3.07
f1 (ppm)


169.98
151.58
137.35
133.53
132.86
132.72
130.44
129.31
128.83
126.86
123.76
62.34
52.82
14.82
14.12
4z'
f1 (ppm)


8.47
8.03
8.01
7.39
7.38
7.37
7.37
7.31
7.29
7.27
7.26
7.25
5.05
2.44
1.40
1.39
4q'
0.95
0.98
2.00
4.14
1.00
3.00
9.02
f1 (ppm)


168.58
146.68
144.12
136.57
133.25
133.09
131.34
129.15
128.53
123.86
122.76
83.15
53.29
27.86
19.89
4q'
f1 (ppm)