Supporting Information

Rh(III)-Catalyzed Oxime Ether-Directed Heteroarylation of Arene through Oxidative C–H/C–H Cross-Coupling

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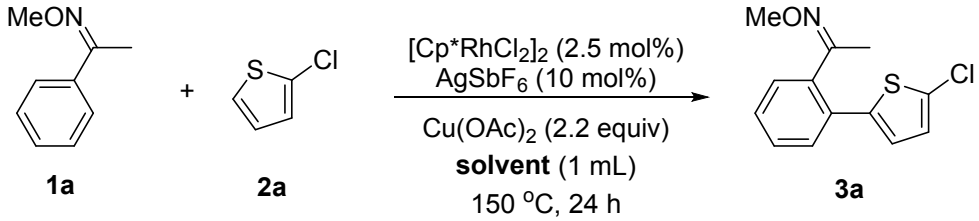
I. General Remarks

Unless otherwise noted, all reagents were obtained from commercial suppliers and used without further purification. $[RhCp^*Cl_2]_2$,[1] oxime ethers[2] were prepared according to the literature procedures. All solvents were dried according to the known methods and distilled prior to use. Unless otherwise indicated, all reactions were carried out under N_2 atmosphere. NMR spectra were obtained on a Bruker AMX-400. The ^1H NMR (400 MHz) chemical shifts were measured using $CDCl_3$ or acetone-d_6 as the internal reference ($CDCl_3$: δ = 7.26 ppm; acetone-d_6: δ = 2.05 ppm). The ^{13}C NMR (100 MHz) chemical shifts are given using $CDCl_3$ or acetone-d_6 as the internal standard ($CDCl_3$: δ = 77.16 ppm; acetone-d_6: δ = 29.84 ppm). High-resolution mass spectra (HR-MS) were obtained with a Waters-Q-TOF-Premier (ESI). Melting points were determined with XRC-1 and are uncorrected.

II. Optimization of the reaction conditions

A flame-dried Schlenk test tube with a magnetic stirring bar was charged with acetophenone *O*-methyl oxime **1a** (37.3 mg, 0.25 mmol), 2-Chlorothiophene **2a** (44.5 mg, 0.375 mmol), [Rh] catalyst (0.00625 mmol, 2.5 mol%), $AgSbF_6$ (10 mol%, if required), oxidant (2.2 equiv), additive (50 mol%) and solvent (1.0 mL) under an N_2 atmosphere. The mixture was stirred for 5 min at room temperature, and then heated at 140-160 ºC for the indicated time. After the reaction was cooled down to ambient temperature, it was diluted with 20 mL of CH_2Cl_2 and filtered through a celite pad, which was then washed with 10-20 mL of CH_2Cl_2. The combined organic phase was concentrated under reduced pressure and the residue was purified by column chromatography on silica gel (petroleum ether/dichloromethane = 15/1-5/1, v/v) to provide the desired product **3a**.

Table S1. Screening of solvents[a]

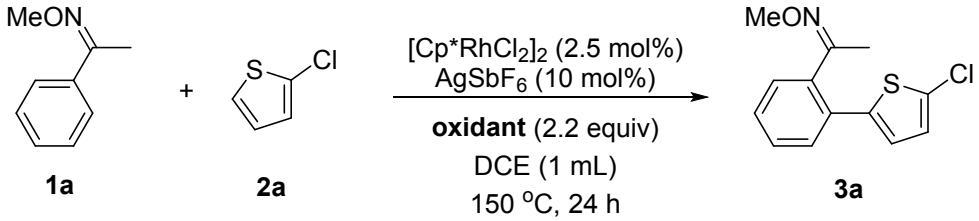


1a **2a** **3a**

Entry	Solvent	Yield (%)[b]	Entry	Solvent	Yield (%)[b]
1	DCE	32	8	DMSO	12
2	mesitylene	12	9	MeOH	20
3	DMF	22	10	NMP	18
4	dioxane	24	11	MeCN	22
5	*o*-DCB	22	12	THF	26
6	*t*-AmylOH	24	13	diglyme	trace
7	DMA	18			

[a] Reaction conditions: acetophenone *O*-methyl oxime (0.25 mmol), 2-Chlorothiophene (0.375 mmol, 1.5 equiv), $[Cp^*RhCl_2]_2$ (2.5 mol%), $AgSbF_6$ (10 mol%), $Cu(OAc)_2$ (2.2 equiv), solvent (1.0 mL) at 150℃ for 24 h under an N_2 atmosphere. [b] Isolated yield.

Table S2. Screening of oxidants[a]

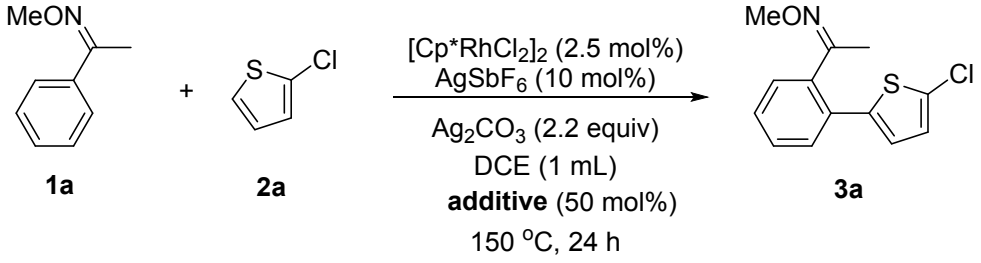


1a **2a** **3a**

Entry	Oxidant	Yield (%)[b]	Entry	Oxidant	Yield (%)[b]
1	$Cu(OAc)_2$	32	8	AgOAc	trace
2	$Cu(OAc)_2 \cdot H_2O$	24	9	AgOTf	trace
3	$CuCl_2 \cdot 2H_20$	N.D	10	Ag_2O	N.D
4	$CuBr_2$	N.D	11	NFSI	trace
5	$Cu(OTf)_2$	trace	12	BQ	N.D
6	$Cu(TFA)_2 \cdot H_2O$	24	13	$K_2S_2O_8$	N.D
7	Ag_2CO_3	36	14	$PhI(OAc)_2$	18

[a] Reaction conditions: acetophenone *O*-methyl oxime (0.25 mmol), 2-Chlorothiophene (0.375 mmol, 1.5 equiv), $[Cp^*RhCl_2]_2$ (2.5 mol%), $AgSbF_6$ (10 mol%), oxidant (2.2 equiv), DCE (1.0 mL) at 150℃ for 24 h under an N_2 atmosphere. [b] Isolated yield.

Table S3. Screening of additives[a]

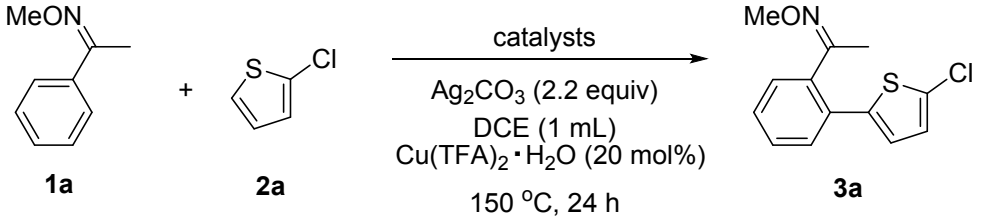


1a **2a** **3a**

Entry	Additive	Yield (%)[b]	Entry	Additive	Yield (%)[b]
1	PivOH	trace	9	K_2CO_3	36
2	TFA	trace	10	*t*-BuOK	trace
3	TfOH	trace	11	KH_2PO_4	trace
4	NaOAc	12	12	$Cu(OAc)_2$	47
5	KOAc	16	13	$Cu(TFA)_2·H_2O$	50
6	CsOAc	19	14	$Cu(TFA)_2·H_2O$[c]	58
7	Cs_2CO_3	28	15	$Cu(TFA)_2·H_2O$[d]	55
8	CsOPiv	25	16	$Cu(TFA)_2·H_2O$[e]	47

[a] Reaction conditions: acetophenone *O*-methyl oxime (0.25 mmol), 2-Chlorothiophene (0.375 mmol, 1.5 equiv), $[Cp^*RhCl_2]_2$ (2.5 mol%), $AgSbF_6$ (10 mol%), Ag_2CO_3 (2.2 equiv), additive (50 mol%) and DCE (1.0 mL) at 150℃ for 24 h under an N_2 atmosphere. [b] Isolated yield. [c] 20 mol% was uesd. [d] 10 mol% was used. [e] 100 mol% was used.

Table S4. Screening of catalysts[a]

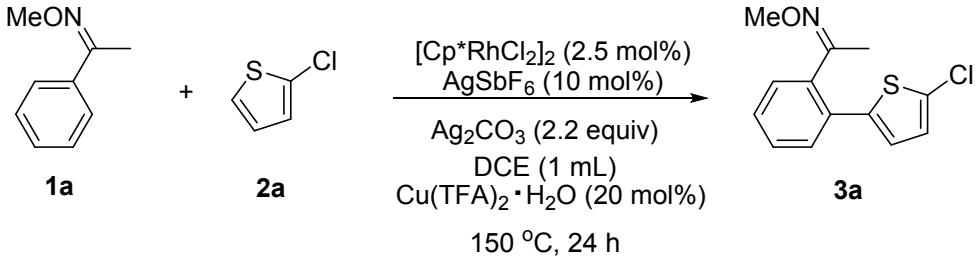


1a **2a** **3a**

Entry	Catalysts	Yield (%)[b]	Entry	Catalysts	Yield (%)[b]
1	$[Cp^*Rh(MeCN)_3][SbF_6]_2$ (5 mol%)	42	4	$[Cp^*RhCl_2]_2$,	trace
2	$Rh(PPh_3)_3Cl$ (5 mol%)	trace	5	$[Cp^*RhCl_2]_2$,	trace
3	$RhCp^*(OAc)_2$ (5 mol%)	16	6	$[Cp^*RhCl_2]_2$,	trace

[a] Reaction conditions: acetophenone *O*-methyl oxime (0.25 mmol), 2-Chlorothiophene (0.375 mmol, 1.5 equiv), Rh source (2.5 mol%), Ag source (10 mol%), Ag_2CO_3 (2.2 equiv), $Cu(TFA)_2·H_2O$ (20 mol%) and DCE (1.0 mL) at 150℃ for 24 h under an N_2 atmosphere. [b] Isolated yield.

Table S5. Other reaction parameters[a]



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

Entry	Variation	Yield (%)[b]	Entry	Variation	Yield (%)[b]
1	no variation	58	7	without Ag_2CO_3	N.D
2	DCE (0.6 mL)	65	8	without $AgSbF_6$	8
3	DCE (2.0 mL)	44	9	0.25 mmol of **2a** and 0.375 mmol of **1a**	48
4	140 °C	56	10	36 h	54
5	160 °C	51	11	20h	50
6	without	N.D			

[a] Reaction conditions: acetophenone *O*-methyl oxime (0.25 mmol), 2-Chlorothiophene (0.375 mmol, 1.5 equiv), $[Cp^*RhCl_2]_2$ (2.5 mol%), $AgSbF_6$ (10 mol%), Ag_2CO_3 (2.2 equiv), $Cu(TFA)_2 \cdot H_2O$ (20 mol%) and DCE (1.0 mL) at 150℃ for 24 h under an N_2 atmosphere. [b] Isolated yield.

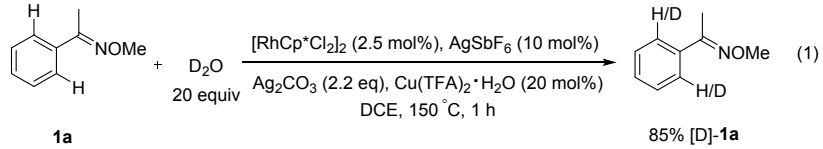
III. General procedure for the oxidative C–H/C–H cross-coupling of oxime ethers with heteroarenes

A flame-dried Schlenk test tube with a magnetic stirring bar was charged with oxime ethers (0.25 mmol), heteroarene (0.375 mmol), $[RhCp^*Cl_2]_2$ (3.9 mg, 0.00625 mmol), $AgSbF_6$ (8.6 mg, 0.025 mmol), Ag_2CO_3 (151.7 mg, 0.55 mmol), $Cu(TFA)_2 \cdot H_2O$ (14.5 mg, 0.05 mmol), and DCE (0.6 mL) under an N_2 atmosphere. The mixture was stirred for 5 min at room temperature, and then heated at 150 ºC for 24 h. After the reaction was cooled down to ambient temperature, it was diluted with 20 mL of CH_2Cl_2 and filtered through a celite pad, which was then washed with 10-20 mL of CH_2Cl_2. The combined organic phase was concentrated under reduced pressure and the residue was purified by column chromatography on silica gel to provide the desired product.

IV. Mechanism study

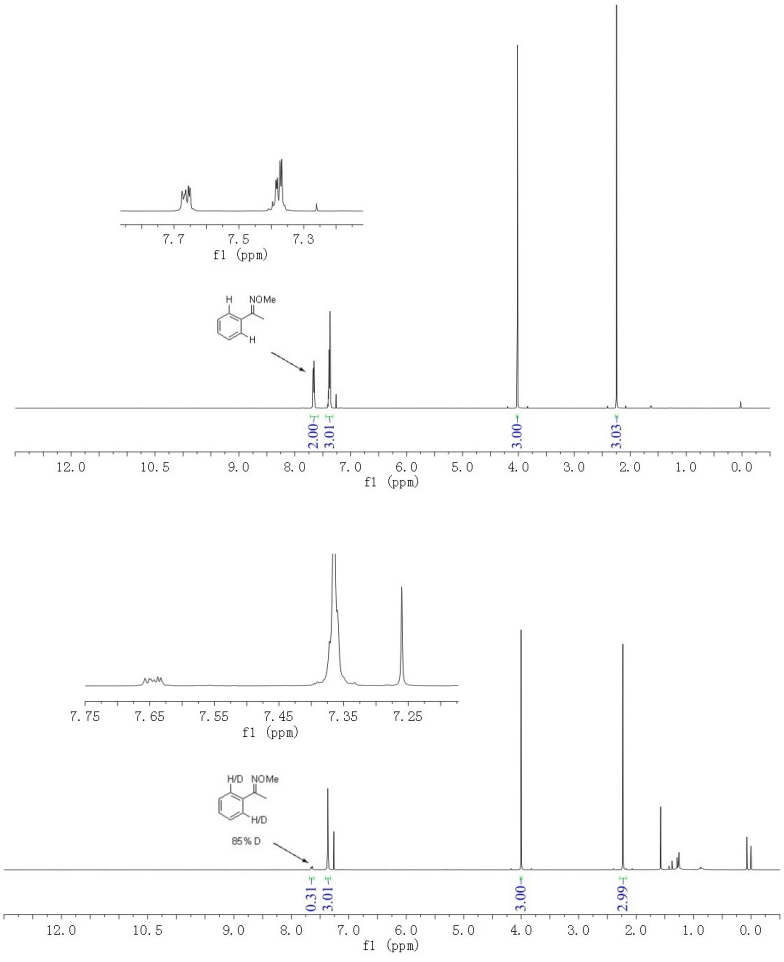
(a) The H/D exchange experiments

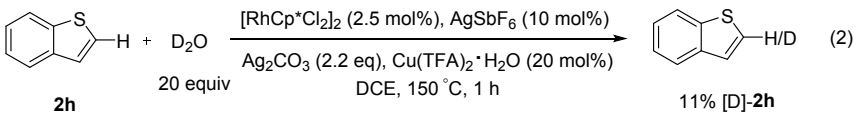
The reactions were conducted by using the general procedure with (1) only **1a**, (2) only **2h** and (3) both in the presence of D_2O (5.0 mmol).



1a 85% [D]-**1a**

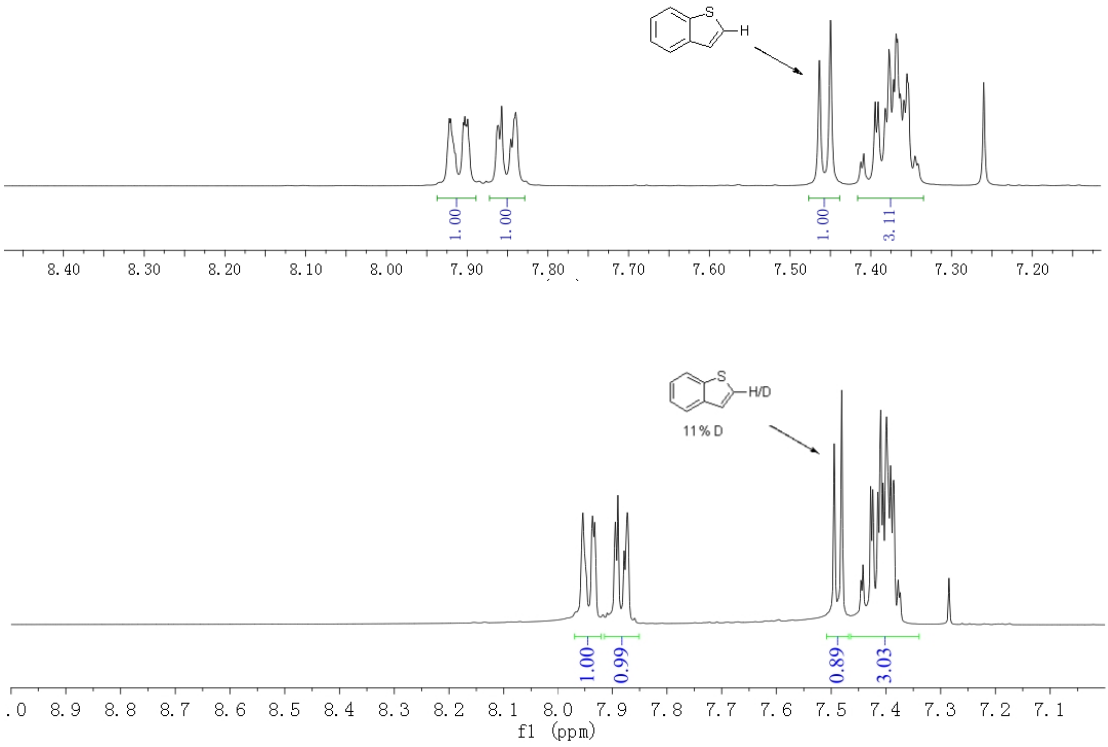
The ^{1}H NMR analysis showed that 85% hydrogen at the *ortho*-position of phenyl ring of acetophenone *O*-methyl oxime was deuterated.

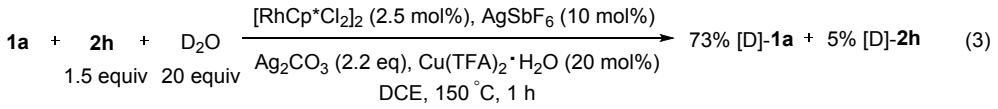




2h 11% [D]-**2h**

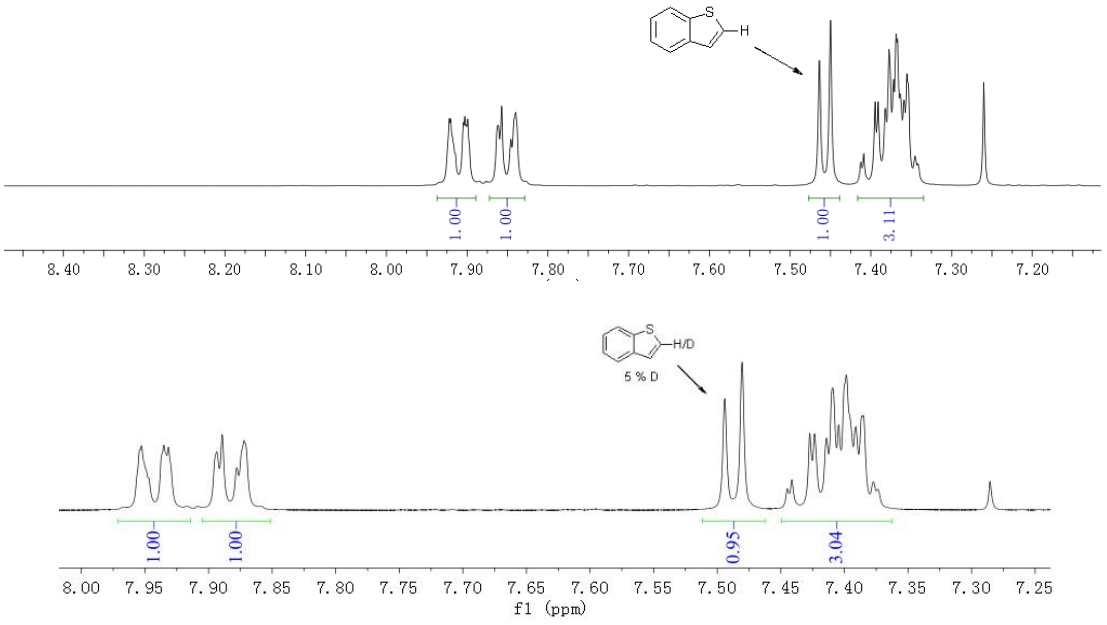
The ^{1}H NMR analysis showed that 11% hydrogen at the C2-position of benzothiophene was deuterated.

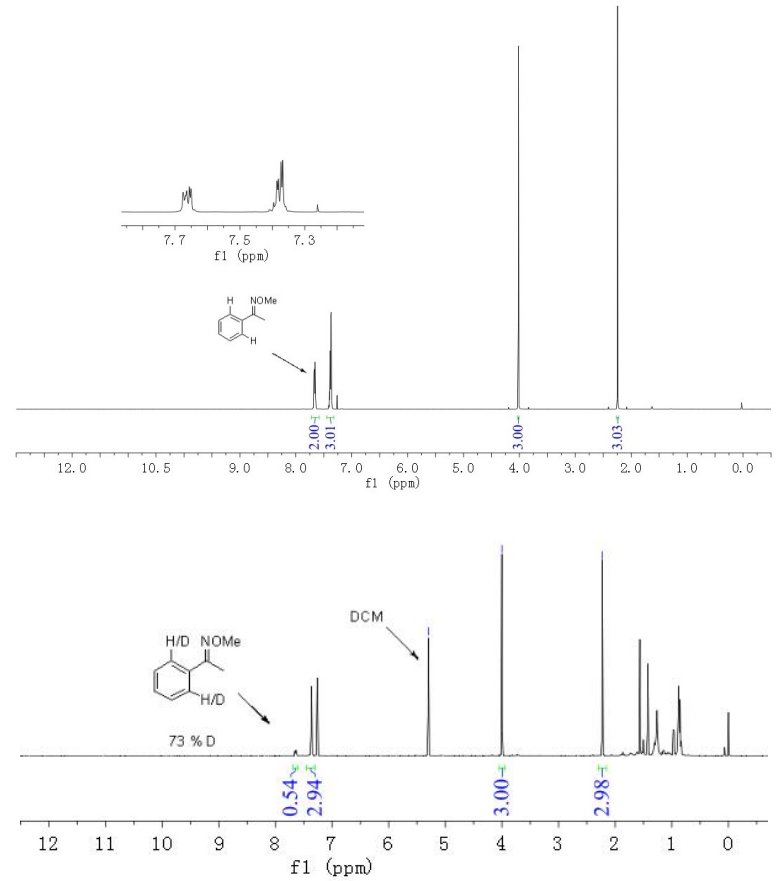




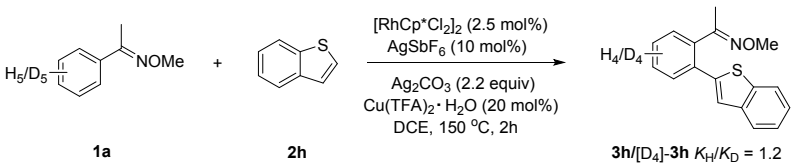
(3)

The ^{1}H NMR analysis showed that 5% hydrogen at the C2-position of benzothiophene and 73% hydrogen at the *ortho*-position of the phenyl ring of acetophenone *O*-methyl oxime were deuterated, respectively.



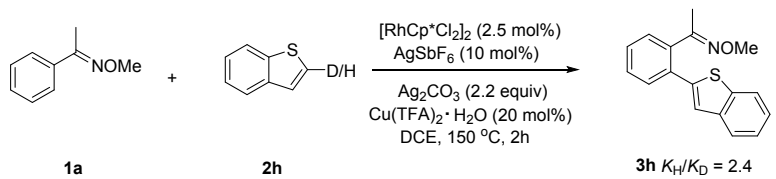


(b) Kinetic isotope experiments



1a **2h** **3h**/[D$_4$]-**3h** K_H/K_D = 1.2

Two sets of reactions were carried out in a parallel manner under the optimal conditions for only 2 h. In each case benzothiophene was allowed to react with acetophenone *O*-methyl oxime and its deuterated derivative, respectively. **3h** was obtained in 17% yield and [D$_4$]-**3h** was obtained in 14% yield. KIE = 1.2.

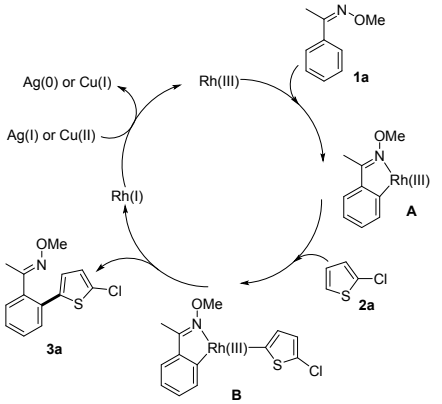


1a **2h** **3h** K_H/K_D = 2.4

Two sets of reactions were carried out in a parallel manner under the optimal conditions for only 2 h. In each case acetophenone *O*-methyl oxime was allowed to react with benzothiophene and 2-deuterio-benzothiophene, respectively. **3h** was

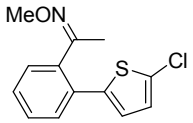
obtained in 17% and 7% yields, respectively. KIE = 2.4.

(c) Plausible mechanism

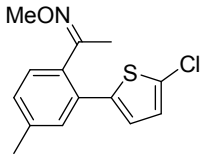


Scheme S1. Plausible mechanism

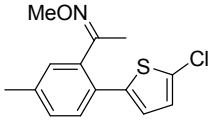
V. Characterization of the products



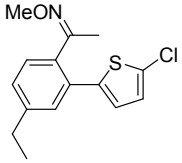
1-(2-(5-chlorothiophen-2-yl)phenyl)ethanone *O*-methyl oxime (3a): Pale yellow oil (40.4 mg, 61%). ^{1}H NMR (400 MHz, $CDCl_3$): δ = 1.87 (s, 3H), 4.00 (s, 3H), 6.86 (d, J = 4.0 Hz, 1H), 6.88 (d, J = 3.6 Hz, 1H), 7.34-7.43 (m, 4H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ = 16.5, 62.0, 126.4, 126.8, 128.4, 129.1, 129.7, 130.2, 130.6, 132.4, 137.0, 140.9, 157.8 ppm. HRMS (ESI$^+$): calcd for $C_{13}H_{12}ClNOS$ $[M+H]^+$ 266.0406, found 266.0406.



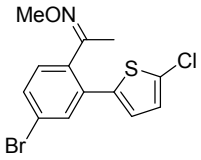
1-(2-(5-chlorothiophen-2-yl)-4-methylphenyl)ethanone *O*-methyl oxime (3b): Pale yellow oil (41.8 mg, 60%). ^{1}H NMR (400 MHz, $CDCl_3$): δ = 1.85 (s, 3H), 2.38 (s, 3H), 3.98 (s, 3H), 6.84 (d, J = 4.0 Hz, 1H), 6.86 (d, J = 4.0 Hz, 1H), 7.16 (dd, J = 8.0 Hz, 1.2 Hz, 1H), 7.22 (s, 1H), 7.26 (d, J = 8.0 Hz, 1H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ = 16.6, 21.3, 62.0, 126.3, 126.7, 129.1, 129.7, 130.4, 130.9, 132.1, 134.3, 139.1, 141.1, 157.8 ppm. HRMS (ESI$^+$): calcd for $C_{14}H_{14}ClNOS$ $[M+H]^+$ 280.0563, found 280.0560.



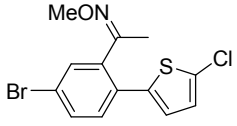
1-(2-(5-chlorothiophen-2-yl)-5-methylphenyl)ethanone *O*-methyl oxime (3c): Pale yellow oil (37.0 mg, 53%). ^{1}H NMR (400 MHz, $CDCl_3$): δ = 1.86 (s, 3H), 2.38 (s, 3H), 4.00 (s, 3H), 6.82 (d, J = 4.0 Hz, 1H), 6.86 (d, J = 3.6 Hz, 1H), 7.18-7.20 (m, 2H), 7.30 (d, J = 8.0 Hz, 1H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ = 16.5, 21.2, 62.0, 126.1, 126.7, 129.5, 129.8, 130.1, 130.2, 130.3, 136.8, 138.4, 141.0, 158.0 ppm. HRMS (ESI$^+$): calcd for $C_{14}H_{14}ClNOS$ $[M+H]^+$ 280.0563, found 280.0560.



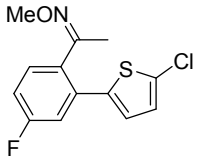
1-(2-(5-chlorothiophen-2-yl)-4-ethylphenyl)ethanone *O*-methyl oxime (3e): Pale yellow oil (51.3 mg, 70%). ^{1}H NMR (400 MHz, $CDCl_3$): δ = 1.25 (t, J = 7.6 Hz, 3H), 1.86 (s, 3H), 2.67 (q, J = 7.6 Hz, 2H), 3.98 (s, 3H), 6.84 (d, J = 4.0 Hz, 1H), 6.87 (d, J = 3.6 Hz, 1H) 7.18 (dd, J = 7.6 Hz, 1.2 Hz, 1H), 7.23 (d, J = 0.8 Hz, 1H), 7.28 (d, J = 8.0 Hz, 1H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ = 15.6, 16.6, 28.7, 62.0, 126.3, 126.7, 127.9, 129.7, 129.8, 130.3, 132.2, 134.5, 141.2, 145.5, 157.8 ppm. HRMS (ESI$^+$): calcd for $C_{15}H_{16}ClNOS$ $[M+Na]^+$ 316.0539, found 316.0539.



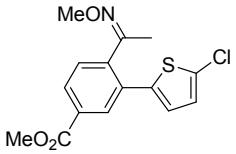
1-(4-bromo-2-(5-chlorothiophen-2-yl)phenyl)ethanone *O*-methyl oxime (3f) : Pale yellow oil (41.1 mg, 48%). ^{1}H NMR (400 MHz, $CDCl_3$): δ = 1.84 (s, 3H), 3.99 (s, 3H), 6.87 (d, J = 3.6 Hz, 1H), 6.88 (d, J = 3.6 Hz, 1H), 7.23 (d, J = 8.4 Hz, 1H), 7.47 (dd, J = 8.0 Hz, 2.0 Hz, 1H), 7.56 (d, J = 2.0 Hz, 1H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ = 16.4, 62.1, 123.0, 126.9, 127.0, 131.2, 131.3, 131.5, 132.8, 134.2, 135.9, 139.1, 156.8 ppm. HRMS (ESI$^+$): calcd for $C_{13}H_{11}BrClNOS$ $[M+H]^+$ 343.9512, found 343.9522.



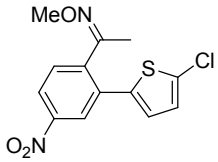
1-(5-bromo-2-(5-chlorothiophen-2-yl)phenyl)ethanone *O*-methyl oxime (3g): Pale yellow oil (44.6 mg, 52%). ^{1}H NMR (400 MHz, $CDCl_3$): δ = 1.84 (s, 3H), 4.00 (s, 3H), 6.84 (d, J = 3.6 Hz, 1H), 6.88 (d, J = 4.0 Hz, 1H), 7.27 (dd, J = 8.0 Hz, 0.4 Hz, 1H), 7.50-7.53 (m, 2H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ = 16.3, 62.2, 122.3, 126.7, 126.9, 131.1, 131.3, 131.6, 132.1, 132.6, 138.5, 139.6, 156.5 ppm. HRMS (ESI^+): calcd for $C_{13}H_{11}BrClNOS$ $[M+H]^+$ 343.9512, found 343.9515.



1-(2-(5-chlorothiophen-2-yl)-4-fluorophenyl)ethanone *O*-methyl oxime (3h): Brown oil (38.9 mg, 55%). ^{1}H NMR (400 MHz, $CDCl_3$): δ = 1.85 (s, 3H), 3.99 (s, 3H), 6.87-6.89 (m, 2H), 7.04 (td, J = 8.4 Hz, 2.8 Hz, 1H), 7.12 (dd, J = 9.2 Hz, 2.4 Hz, 1H),, 7.34 (dd, J = 8.8 Hz, 6.0 Hz, 1H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ = 16.6, 62.1, 115.2 (d, J = 21.0 Hz), 116.9 (d, J = 23.0 Hz), 126.9, 131.4, 131.7 (d, J = 8.0 Hz), 133.1 (d, J = 3.0 Hz), 134.4 (d, J = 9.0 Hz), 139.5 (d, J = 2.0 Hz), 157.0, 161.5, 164.0 ppm. HRMS (ESI^+): calcd for $C_{13}H_{11}ClFNOS$ $[M+H]^+$ 284.0312, found 284.0316.

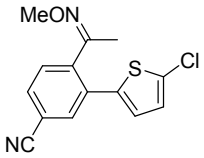


methyl 3-(5-chlorothiophen-2-yl)-4-(1-(methoxyimino)ethyl)benzoate (3i): Pale yellow oil (62.9 mg, 78%). ^{1}H NMR (400 MHz, $CDCl_3$): δ = 1.87 (s, 3H), 3.93 (s, 3H), 4.00 (s, 3H), 6.89-6.91 (m, 2H), 7.45 (d, J = 8.0 Hz, 1H), 7.99 (dd, J = 8.0 Hz, 1.6 Hz, 1H), 8.02 (d, J = 1.6 Hz, 1H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ = 16.3, 52.6, 62.2, 126.9, 127.0, 129.2, 130.0, 130.8, 131.3, 131.4, 132.7, 139.7, 141.0, 157.1, 166.4 ppm. HRMS (ESI^+): calcd for $C_{15}H_{14}ClNO_3S$ $[M+H]^+$ 324.0461, found 324.0457.

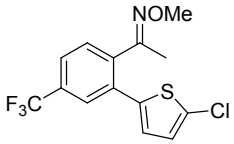


1-(2-(5-chlorothiophen-2-yl)-4-nitrophenyl)ethanone *O*-methyl oxime (3j): A pale

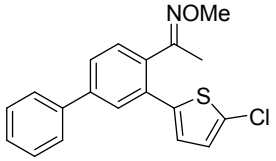
yellow solid (51.3 mg, 70%). M.p.: 110-111 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ = 1.88 (s, 3H), 4.02 (s, 3H), 6.78 (d, J = 4.0 Hz, 1H), 6.96 (d, J = 4.0 Hz, 1H), 7.55 (d, J = 8.4 Hz, 1H), 8.17 (dd, J = 8.4 Hz, 2.4 Hz, 1H), 8.28 (d, J = 2.4 Hz, 1H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ = 16.2, 62.4, 122.8, 125.0, 127.1, 127.7, 131.1, 132.5, 134.0, 138.1, 142.8, 148.1, 156.0 ppm. HRMS (ESI$^+$): calcd for $C_{13}H_{11}ClN_2O_3S$ $[M+Na]^+$ 333.0077, found 333.0077.



3-(5-chlorothiophen-2-yl)-4-(1-(methoxyimino)ethyl)benzonitrile (3k): A brown solid (31.9 mg, 44%). M.p.: 80-82 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ = 1.85 (s, 3H), 4.00 (s, 3H), 6.90 (d, J = 4.0 Hz, 1H), 6.92 (d, J = 3.6 Hz, 1H), 7.48 (d, J = 8.0 Hz, 1H), 7.62 (dd, J = 7.6 Hz, 1.6 Hz, 1H), 7.70 (d, J = 1.2 Hz, 1H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ = 16.1, 62.4, 113.2, 118.1, 127.1, 127.5, 130.8, 131.4, 132.3, 133.6, 133.7, 138.1, 141.2, 156.2 ppm. HRMS (ESI$^+$): calcd for $C_{14}H_{11}ClN_2OS$ $[M+Na]^+$ 313.0178, found 313.0179.

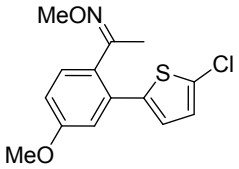


1-(2-(5-chlorothiophen-2-yl)-4-(trifluoromethyl)phenyl)ethanone *O*-methyl oxime (3l): Pale yellow oil (43.3 mg, 52%). ^{1}H NMR (400 MHz, $CDCl_3$): δ = 1.87 (s, 3H), 4.01 (s, 3H), 6.90-6.92 (m, 2H), 7.50 (d, J = 8.0 Hz, 1H), 7.60 (dd, J = 8.0 Hz, 1.2 Hz, 1H), 7.66 (s, 1H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ = 16.3, 62.3, 123.8 (q, J = 270.9 Hz), 124.9 (q, J = 3.6 Hz), 126.99, 127.00 (q, J = 3.7 Hz), 127.3, 130.4, 131.3 (q, J = 32.5 Hz), 131.8, 133.2, 139.1, 140.2, 156.6 ppm. HRMS (ESI$^+$): calcd for $C_{14}H_{11}ClF_3NOS$ $[M+H]^+$ 334.0280, found 334.0280.

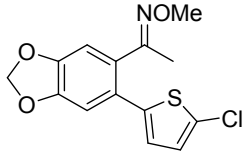


1-(3-(5-chlorothiophen-2-yl)biphenyl-4-yl)ethanone *O*-methyl oxime (3m): Yellow oil (44.0 mg, 51%). ^{1}H NMR (400 MHz, $CDCl_3$): δ = 1.91 (s, 3H), 4.01 (s,

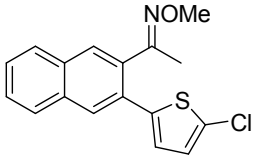
3H), 6.90 (d, J = 4.0 Hz, 1H), 6.91 (d, J = 4.0 Hz, 1H), 7.36-7.40 (m, 1H), 7.44-7.48 (m, 3H), 7.56-7.59 (m, 2H), 7.60-7.61 (m, 1H), 7.62 (d, J = 2.0 Hz, 1H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ = 16.5, 62.1, 126.6, 126.8, 127.0, 127.3, 128.0, 129.0, 130.2, 130.7, 132.8, 135.8, 140.1, 140.8, 142.2, 157.5 ppm. HRMS (ESI$^+$): calcd for $C_{19}H_{16}ClNOS$ $[M+H]^+$ 342.0719, found 342.0719.



1-(2-(5-chlorothiophen-2-yl)-4-methoxyphenyl)ethanone *O*-methyl oxime (3n): Brown oil (37.6 mg, 51%). ^{1}H NMR (400 MHz, $CDCl_3$): δ = 1.84 (s, 3H), 3.83 (s, 3H), 3.98 (s, 3H), 6.85-6.89 (m, 3H), 6.92 (d, J = 2.4 Hz, 1H), 7.30 (d, J = 8.4 Hz, 1H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ = 16.7, 55.6, 61.9, 113.7, 115.6, 126.5, 126.8, 129.8, 130.6, 131.1, 133.6, 140.8, 157.6, 160.0 ppm. HRMS (ESI$^+$): calcd for $C_{14}H_{14}ClNO_2S$ $[M+Na]^+$ 318.0331, found 318.0328.

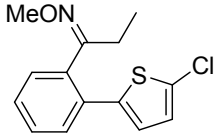


1-(6-(5-chlorothiophen-2-yl)benzo[d][1,3]dioxol-5-yl)ethanone *O*-methyl oxime (3o): Yellow oil (42.5 mg, 55%). ^{1}H NMR (400 MHz, $CDCl_3$): δ = 1.84 (s, 3H), 3.97 (s, 3H), 6.03 (s, 2H), 6.78 (d, J = 8.0 Hz, 1H), 6.87 (d, J = 8.0 Hz, 1H), 6.90 (d, J = 3.6 Hz, 1H), 6.99 (d, J = 4.0 Hz, 1H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ = 16.8, 62.0, 101.7, 108.0, 114.7, 123.3, 126.3, 128.2, 131.2, 131.4, 133.6, 145.6, 148.1, 157.2 ppm. HRMS (ESI$^+$): calcd for $C_{14}H_{12}ClNO_3S$ $[M+Na]^+$ 332.0124, found 332.0127.

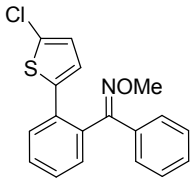


1-(1-(5-chlorothiophen-2-yl)naphthalen-2-yl)ethanone *O*-methyl oxime (3p): Pale yellow oil (44.9 mg, 57%). ^{1}H NMR (400 MHz, $CDCl_3$): δ = 1.92 (s, 3H), 4.04 (s, 3H), 6.92 (d, J = 4.0 Hz, 1H), 6.94 (d, J = 4.0 Hz, 1H), 7.49-7.53 (m, 2H), 7.82-7.87 (m, 3H), 7.88 (s, 1H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ = 16.9, 62.1, 126.5, 126.9,

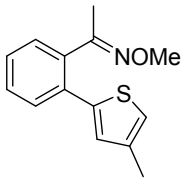
127.1, 127.3, 127.9, 128.2, 129.1, 129.5, 129.9, 130.4, 132.7, 133.2, 134.9, 141.0, 158.1 ppm. HRMS (ESI^+): calcd for $C_{17}H_{14}ClNOS$ $[M+Na]^+$ 338.0382, found 338.0385.



1-(2-(5-chlorothiophen-2-yl)phenyl)propan-1-one *O*-methyl oxime (3q): Pale yellow oil (50.9 mg, 73%). ^1H NMR (400 MHz, $CDCl_3$): δ = 0.83 (t, J = 7.6 Hz, 3H), 2.36 (q, J = 7.6 Hz, 2H), 3.99 (s, 3H), 6.87 (d, J = 4.0 Hz, 1H), 6.90 (d, J = 4.0 Hz, 1H), 7.29-7.44 (m, 4H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ = 10.3, 23.2, 62.0, 126.3, 126.8, 128.1, 129.1, 129.9, 130.4, 130.6, 132.5, 135.4, 141.0, 163.0 ppm. HRMS (ESI^+): calcd for $C_{14}H_{14}ClNOS$ $[M+H]^+$ 280.0563, found 280.0564.

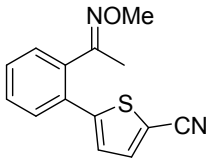


(2-(5-chlorothiophen-2-yl)phenyl)(phenyl)methanone *O*-methyl oxime (3r): A off-white solid (55.6 mg, 68%). M.p.: 47-49 °C. ^1H NMR (400 MHz, $CDCl_3$): δ = 4.01 (s, 3H), 6.68 (d, J = 3.6 Hz, 1H), 6.72 (d, J = 4.0 Hz, 1H), 7.18-7.24 (m, 3H), 7.29-7.31 (m, 2H), 7.39-7.47 (m, 3H), 7.50-7.52 (m, 1H) ppm. ^{13}C NMR (400 MHz, $CDCl_3$): δ = 62.6, 126.0, 126.7, 127.7, 128.3, 129.2, 129.3, 130.0, 130.2, 130.5, 131.1, 133.0, 133.8, 136.7, 140.7, 156.4 ppm. HRMS (ESI^+): calcd for $C_{18}H_{14}ClNOS$ $[M+H]^+$ 328.0563, found 328.0564.

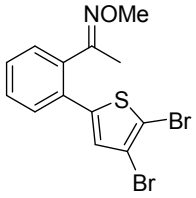


1-(2-(4-methylthiophen-2-yl)phenyl)ethanone *O*-methyl oxime (4a): Pale yellow oil (40.0 mg, 65%).^1H NMR (400 MHz, $CDCl_3$): δ = 1.83 (s, 3H), 2.28 (s, 3H), 4.01 (s, 3H), 6.89-6.92 (m, 2H), 7.30-7.40 (m, 3H), 7.45-7.47 (m, 1H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ = 15.9, 16.5, 62.0, 121.7, 127.8, 129.0, 129.4, 129.6, 130.3, 133.4,

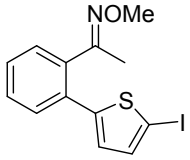
136.8, 138.2, 142.0, 158.4 ppm. HRMS (ESI$^+$): calcd for $C_{14}H_{15}NOS$ $[M+H]^+$ 246.0593, found 246.0593.



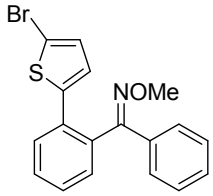
5-(2-(1-(methoxyimino)ethyl)phenyl)thiophene-2-carbonitrile (4b): Yellow oil (32.0 mg, 50%). ^{1}H NMR (400 MHz, $CDCl_3$): δ = 1.86 (s, 3H), 3.97 (s, 3H), 7.09 (d, J = 4.0 Hz, 1H), 7.39-7.48 (m, 4H), 7.57 (d, J = 3.6 Hz, 1H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ = 16.6, 62.1, 110.0, 114.3, 127.2, 129.3, 129.6, 129.9, 130.5, 130.8, 137.5, 137.8, 150.5, 156.8 ppm. HRMS (ESI$^+$): calcd for $C_{14}H_{13}N_2OS$ $[M+H]^+$ 257.0749, found 257.0746.



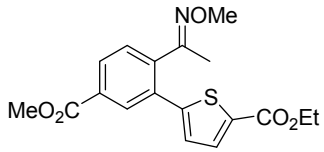
1-(2-(4,5-dibromothiophen-2-yl)phenyl)ethanone *O*-methyl oxime (4c): Pale yellow oil (53.2 mg, 55%). ^{1}H NMR (400 MHz, $CDCl_3$): δ = 1.91 (s, 3H), 4.00 (s, 3H), 6.91 (s, 1H), 7.36-7.40 (m, 4H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ = 16.7, 62.1, 111.8, 114.2, 129.0, 129.2, 129.3, 129.8, 130.1, 131.4, 137.0, 143.7, 157.1 ppm. HRMS (ESI$^+$): calcd for $C_{13}H_{11}Br_2NOS$ $[M+H]^+$ 387.9006, found 387.9006.



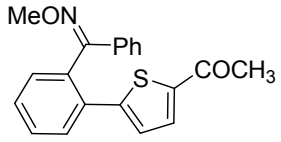
1-(2-(5-iodothiophen-2-yl)phenyl)ethanone *O*-methyl oxime (4d): Pale yellow oil (44.0 mg, 50%). ^{1}H NMR (400 MHz, $CDCl_3$): δ = 1.84 (s, 3H), 4.00 (s, 3H), 6.76 (d, J = 3.6 Hz, 1H), 7.20 (d, J = 4.0 Hz, 1H), 7.35-7.42 (m, 4H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ = 16.4, 62.0, 126.2, 127.2, 127.7, 128.0, 129.0, 129.6, 130.5, 133.2, 137.0, 142.2, 158.4 ppm. HRMS (ESI$^+$): calcd for $C_{13}H_{12}INOS$ $[M+H]^+$ 357.9763, found 357.9758.



(2-(5-bromothiophen-2-yl)phenyl)(phenyl)methanone *O*-methyl oxime (4e): Pale yellow oil (40.8 mg, 44%). ^{1}H NMR (400 MHz, $CDCl_3$): δ = 4.00 (s, 3H), 6.70 (d, J = 4.0 Hz, 1H), 6.82 (d, J = 3.6 Hz, 1H), 7.18-7.24 (m, 3H), 7.28-7.30 (m, 2H), 7.39-7.45 (m, 3H), 7.50-7.52 (m, 1H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ = 62.6, 112.5, 127.68, 127.70, 128.3, 129.2, 129.3, 129.8, 129.9, 130.5, 131.1, 133.0, 133.8, 136.7, 143.7, 156.4 ppm. HRMS (ESI$^+$): calcd for $C_{18}H_{14}BrNOS$ $[M+H]^+$ 372.0058, found 372.0061.

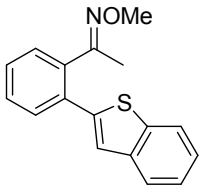


Ethyl 5-(5-(methoxycarbonyl)-2-(1-(methoxyimino)ethyl)phenyl)thiophene-2-carboxylate (4f)： off-white oil (47.0 mg, 52%). ^{1}H NMR (400 MHz, $CDCl_3$): δ = 1.39 (t, J = 7.2 Hz, 3H), 1.82 (s, 3H), 3.94 (s, 3H), 3.99 (s, 3H), 4.37 (q, J = 7.2 Hz, 2H), 7.09 (d, J = 4.0 Hz, 1H), 7.48 (d, J = 8.0 Hz, 1H), 7.74 (d, J = 3.6 Hz, 1H), 8.04 (dd, J = 8.0 Hz, 2.0 Hz, 1H), 8.14 (d, J = 1.6 Hz, 1H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ = 14.5, 16.3, 52.5, 61.5, 62.2, 128.2, 129.8, 130.1, 130.8, 131.6, 132.6, 133.7, 134.7, 141.4, 148.0, 156.7, 162.2, 166.2 ppm. HRMS (ESI$^+$): calcd for $C_{18}H_{19}NO_5S$ $[M+H]^+$ 362.3062, found 362.3054.

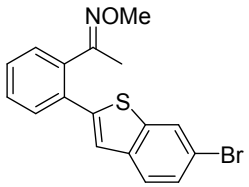


1-(5-(2-((methoxyimino)(phenyl)methyl)phenyl)thiophen-2-yl)ethanone (4g): Yellow oil (45.2 mg, 54%). ^{1}H NMR (400 MHz, $CDCl_3$): δ = 2.48 (s, 3H), 3.98 (s, 3H), 6.97 (d, J = 4.0 Hz, 1H), 7.15-7.23 (m, 3H), 7.28-7.30 (m, 2H), 7.44 (d, J = 3.6 Hz, 1H), 7.46-7.47 (m, 3H), 7.52-7.56 (m, 1H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ = 26.8, 62.7, 127.7, 128.5, 129.0, 129.3, 129.4, 130.0, 130.7, 131.3, 132.4, 132.9, 133.7, 136.8, 144.2, 151.0, 156.1, 190.7 ppm. HRMS (ESI$^+$): calcd for $C_{20}H_{17}NO_2S$

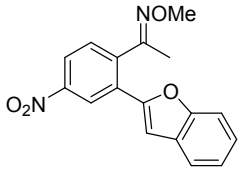
[M+Na]$^+$ 358.0878, found 358.0878.



1-(2-(benzo[b]thiophen-2-yl)phenyl)ethanone *O*-methyl oxime (4h): Pale yellow oil (43.5 mg, 62%). ^{1}H NMR (400 MHz, $CDCl_3$): δ = 1.88 (s, 3H), 4.04 (s, 3H), 7.32 (s, 1H), 7.33-7.47 (m, 5H), 7.58-7.60 (m, 1H), 7.80 (dd, J = 7.2 Hz, 1.6 Hz, 1H), 7.85 (d, J = 7.6 Hz, 1H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ = 16.6, 62.0, 122.2, 123.8, 123.9, 124.5, 124.6, 128.5, 129.1, 129.7, 130.8, 133.2, 137.4, 140.3, 140.5, 142.6, 158.1 ppm. HRMS (ESI$^+$): calcd for $C_{17}H_{15}NOS$ [M+H]$^+$ 282.0953, found 282.0946.

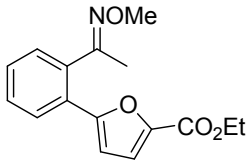


1-(2-(6-bromobenzo[b]thiophen-2-yl)phenyl)ethanone *O*-methyl oxime (4i): Pale yellow oil (55.1 mg, 62%). ^{1}H NMR (400 MHz, acetone-d_6): δ = 1.83 (s, 3H), 3.91 (s, 3H), 7.40 (s, 1H), 7.43-7.54 (m, 4H), 7.61 (d, J = 7.6 Hz, 1H), 7.79 (d, J = 8.4 Hz, 1H), 8.16 (s, 1H) ppm. ^{13}C NMR (100 MHz, acetone-d_6): δ = 16.6, 62.0, 118.6, 124.1, 125.4, 126.1, 128.7, 129.5, 129.9, 130.6, 131.3, 133.2, 138.3, 140.0, 142.7, 144.2, 157.3 ppm. HRMS (ESI$^+$): calcd for $C_{17}H_{14}BrNOS$ [M+H]$^+$ 360.0058, found 360.0058.



1-(2-(benzofuran-2-yl)-4-nitrophenyl)ethanone *O*-methyl oxime (4j): Yellow oil (50.4 mg, 65%). ^{1}H NMR (400 MHz, $CDCl_3$): δ = 2.04 (s, 3H), 4.06 (s, 3H), 6.98 (s, 1H), 7.29 (td, J = 7.6 Hz, 0.8 Hz, 1H), 7.38 (td, J = 8.4 Hz, 1.2 Hz, 1H), 7.57 (d, J = 8.4 Hz, 2H), 7.65 (d, J = 7.6 Hz, 1H), 8.21 (dd, J = 8.4 Hz, 2.0 Hz, 1H), 8.74 (d, J = 2.4 Hz, 1H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ = 16.2, 62.4, 107.4, 111.6, 121.7,

123.0, 123.2, 123.6, 125.7, 128.7, 130.6, 131.3, 141.6, 148.2, 151.7, 155.0, 156.2 ppm. HRMS (ESI$^+$): calcd for $C_{17}H_{14}N_2O_4$ $[M+H]^+$ 311.1032, found 311.1024.



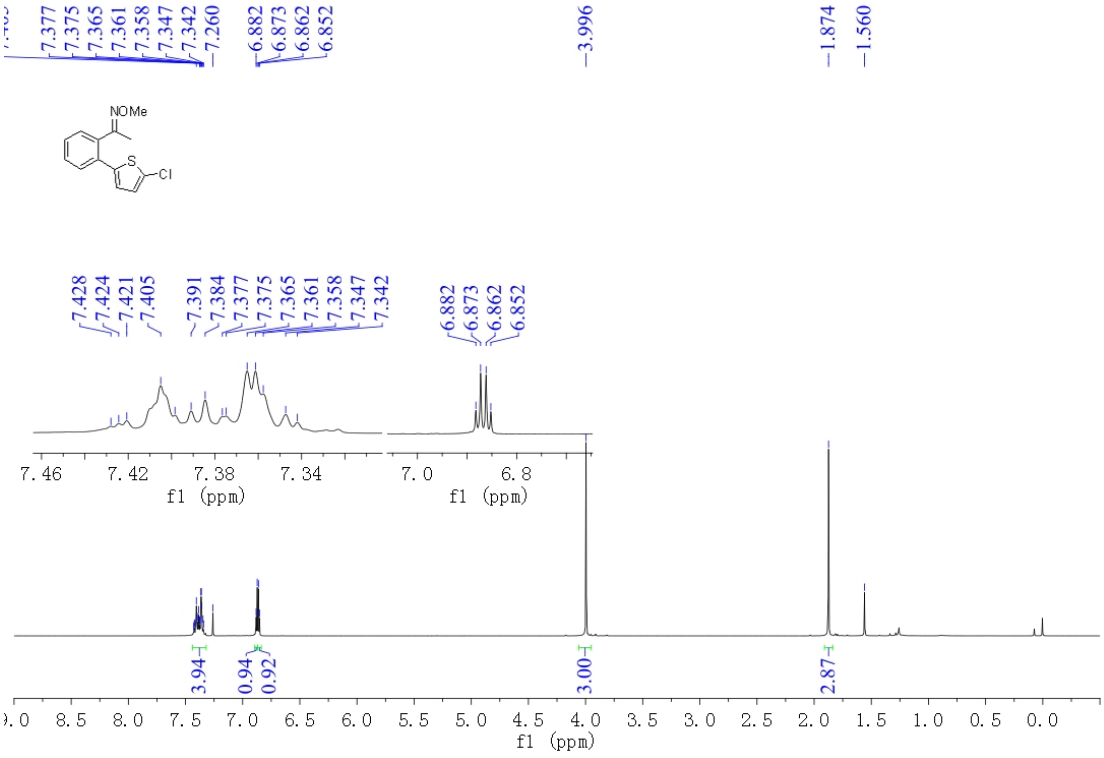
ethyl 5-(2-(1-(methoxyimino)ethyl)phenyl)furan-2-carboxylate (4k): Pale yellow oil (32.3 mg, 45%). ^{1}H NMR (400 MHz, $CDCl_3$): δ = 1.40 (t, J = 7.2 Hz, 3H), 2.02 (s, 3H), 3.98 (s, 3H), 4.38 (q, J = 7.2 Hz, 2H), 6.58 (d, J = 3.6 Hz, 1H), 7.22 (d, J = 3.6 Hz, 1H), 7.34 (dd, J = 7.6 Hz, 1.6 Hz, 1H), 7.37 (td, J = 7.6 Hz, 1.2 Hz, 1H), 7.44 (td, J = 7.2 Hz, 1.6 Hz, 1H), 7.79 (dd, J = 8.0 Hz, 1.2 Hz, 1H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ = 14.5, 16.7, 61.1, 62.0, 110.7, 119.6, 128.1, 129.0, 129.1, 129.7, 136.2, 144.3, 155.9, 157.6, 158.9 ppm. HRMS (ESI$^+$): calcd for $C_{16}H_{17}NO_4$ $[M+Na]^+$ 310.1055, found 310.1058.

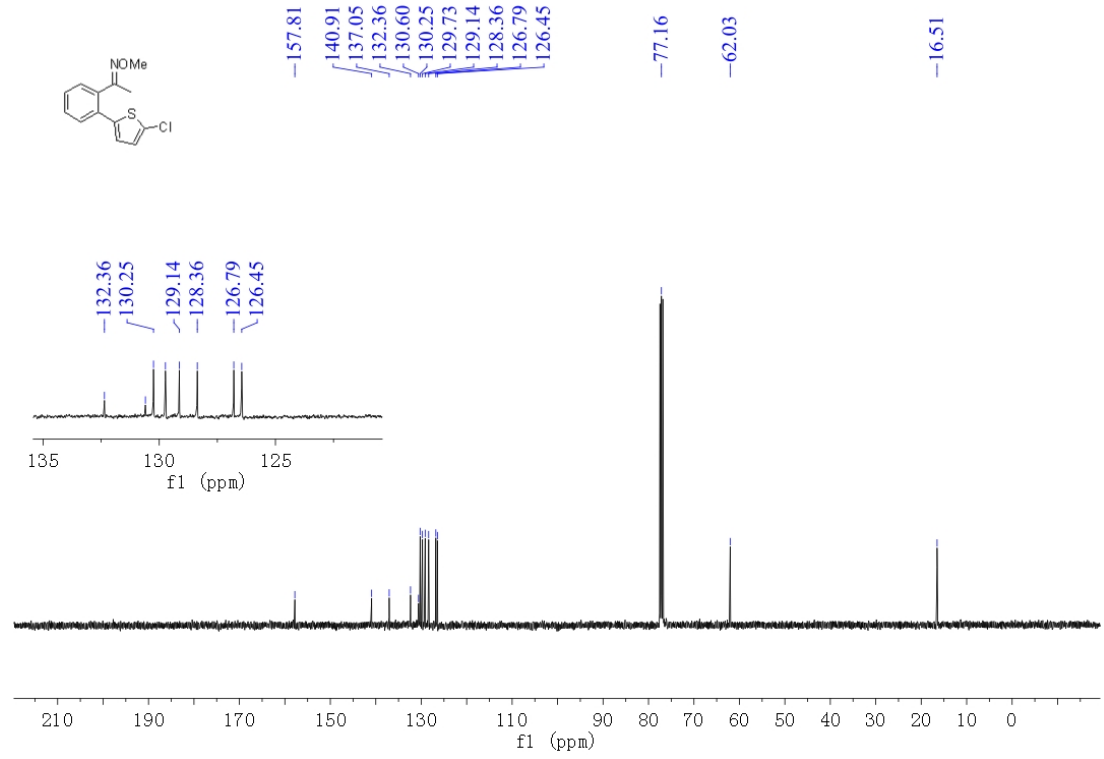
XII. References

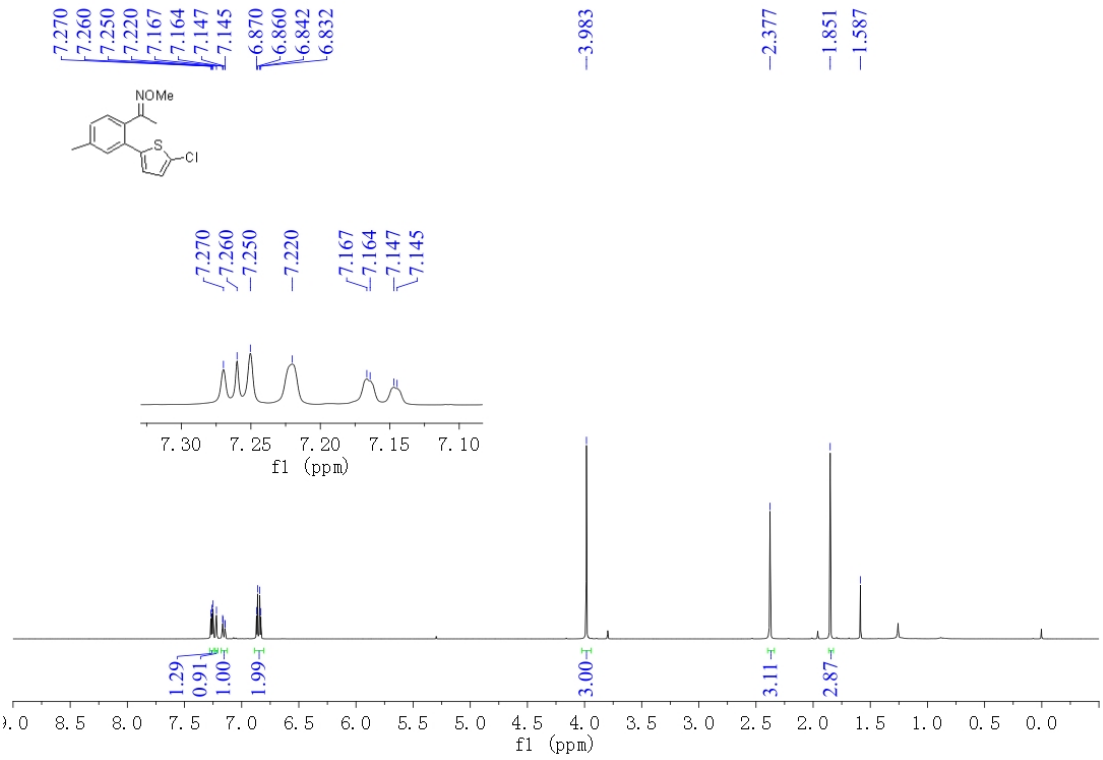
[1] K.-I. Fujita, Y. Takahashi, M. Owaki, K. Yamamoto, R. Yamaguchi, *Org. Lett.* **2004**, *6*, 2785-2788.

[2] A. S. Tsai, M. Brasse, R. G. Bergman, J. A. Ellman, *Org. Lett.* **2011**, 13, 540.

XIII. Copies of ^{1}H and ^{13}C NMR spectra



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7.250
7.220
7.167
7.164
7.147
7.145
6.870
6.860
6.842
6.832
3.983
2.377
1.851
1.587
NOMe
S
Cl
7.30
7.25
7.20
7.15
7.10
f1 (ppm)
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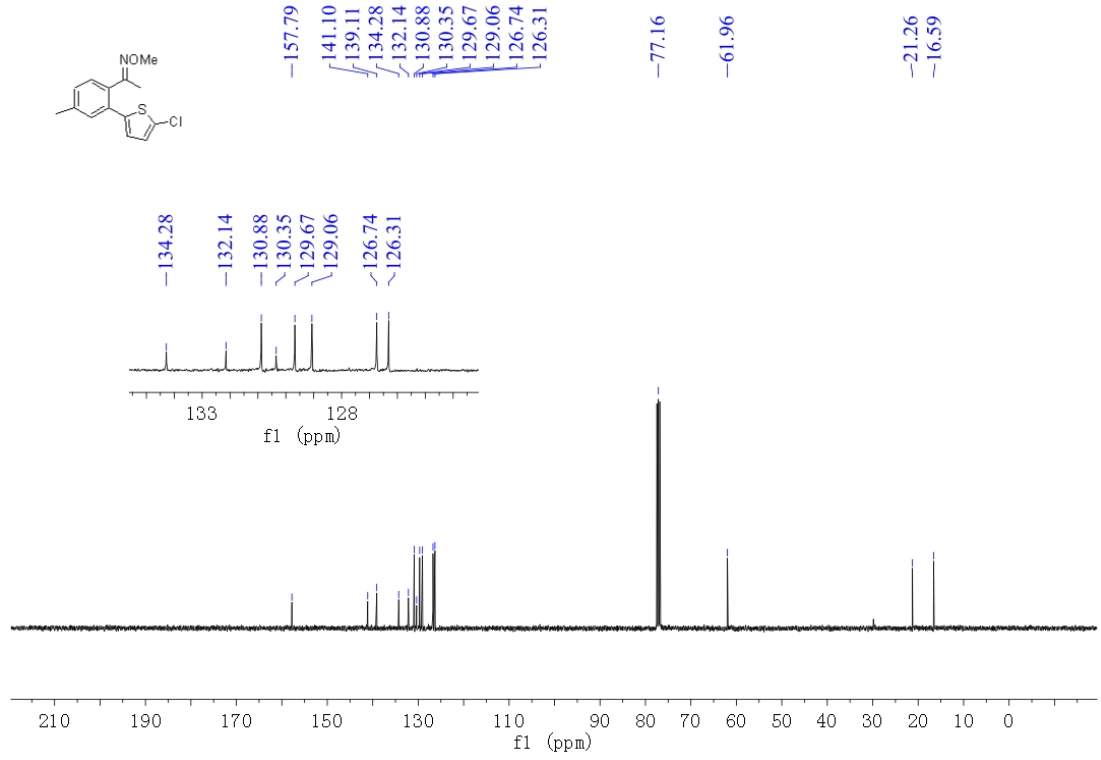
0.91
1.00
1.99
3.00
3.11
2.87
f1 (ppm)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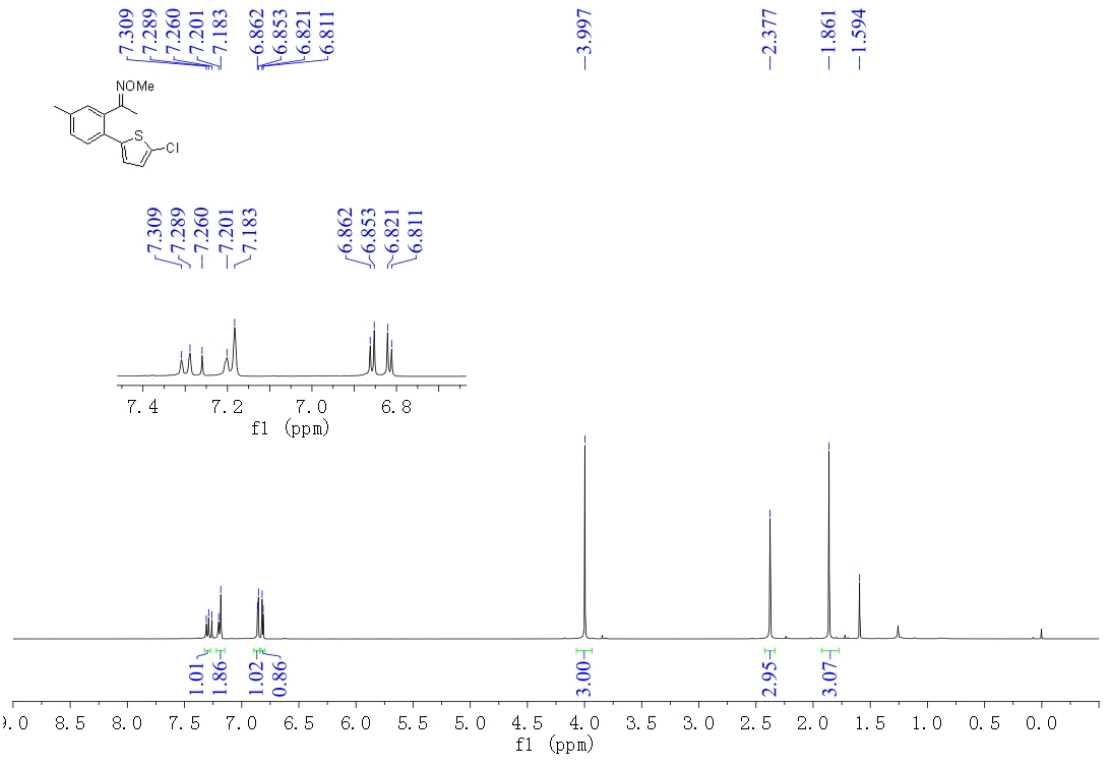
141.10
139.11
134.28
132.14
130.88
130.35
129.67
129.06
126.74
126.31
77.16
61.96
21.26
16.59
NOMe
S
Cl
133
128
f1 (ppm)
f1 (ppm)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7.289
7.260
7.201
7.183
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6.853
6.821
6.811
3.997
2.377
1.861
1.594
NOMe
S
Cl
f1 (ppm)
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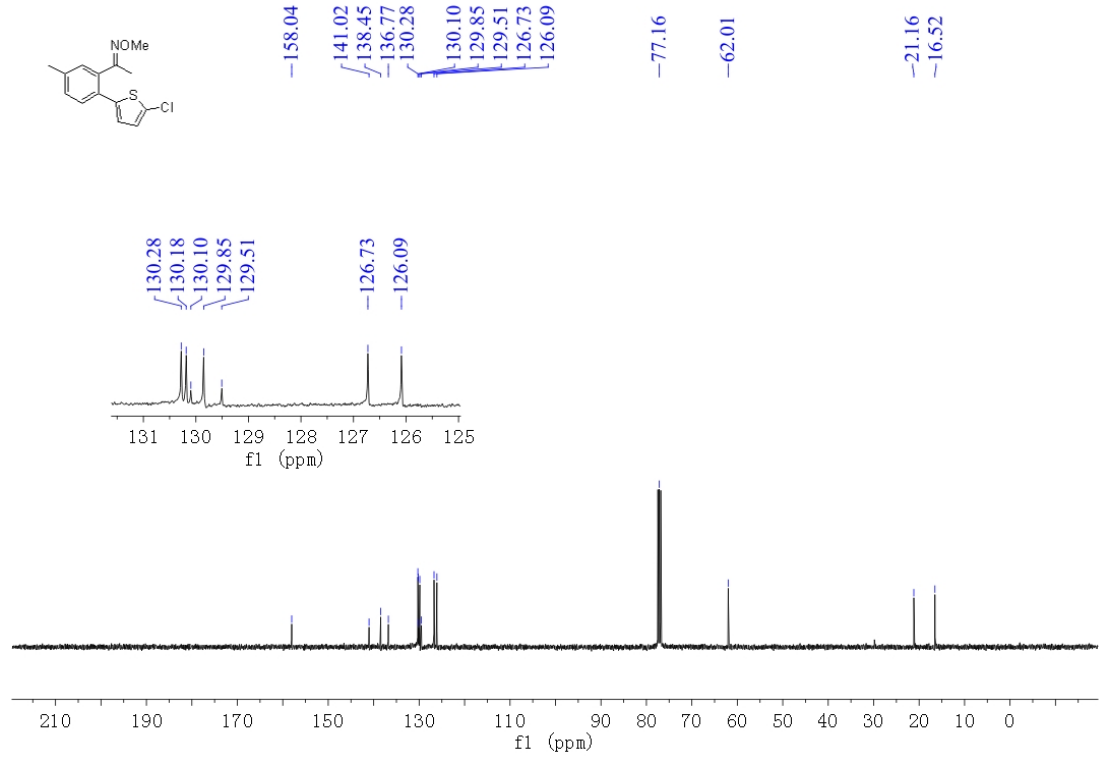
1.86
1.02
0.86
3.00
2.95
3.07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141.02
138.45
136.77
130.28
130.10
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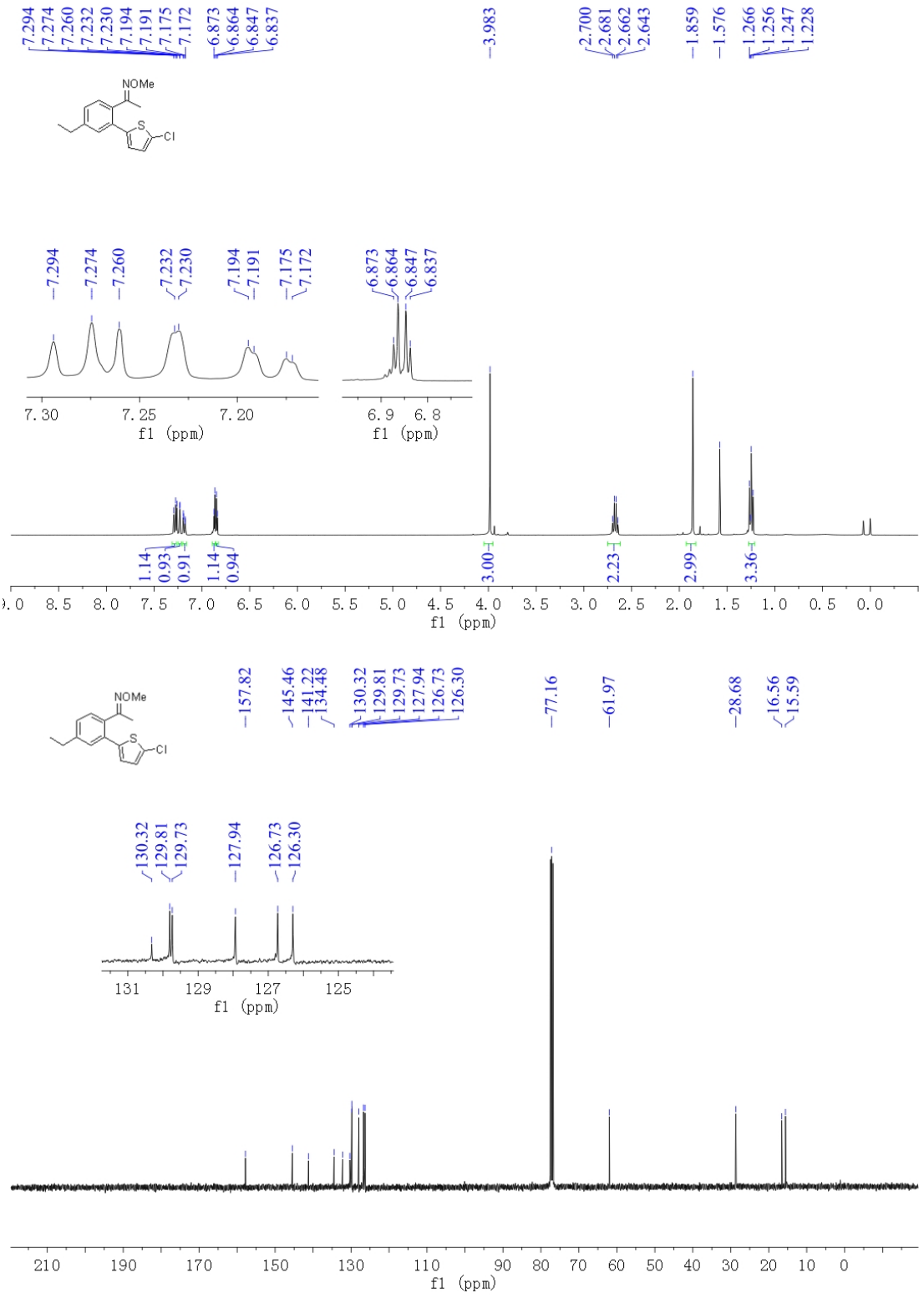
126.09
77.16
62.01
21.16
16.52
NOMe
S
Cl
f1 (ppm)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7.230
7.194
7.191
7.175
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6.873
6.864
6.847
6.837
3.983
2.700
2.681
2.662
2.643
1.859
1.576
1.266
1.256
1.247
1.228
NOMe
S
Cl
f1 (ppm)
1.14
0.93
0.91
1.14
0.94
3.00
2.23
2.99
3.36
157.82
145.46
141.22
134.48
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129.73
127.94
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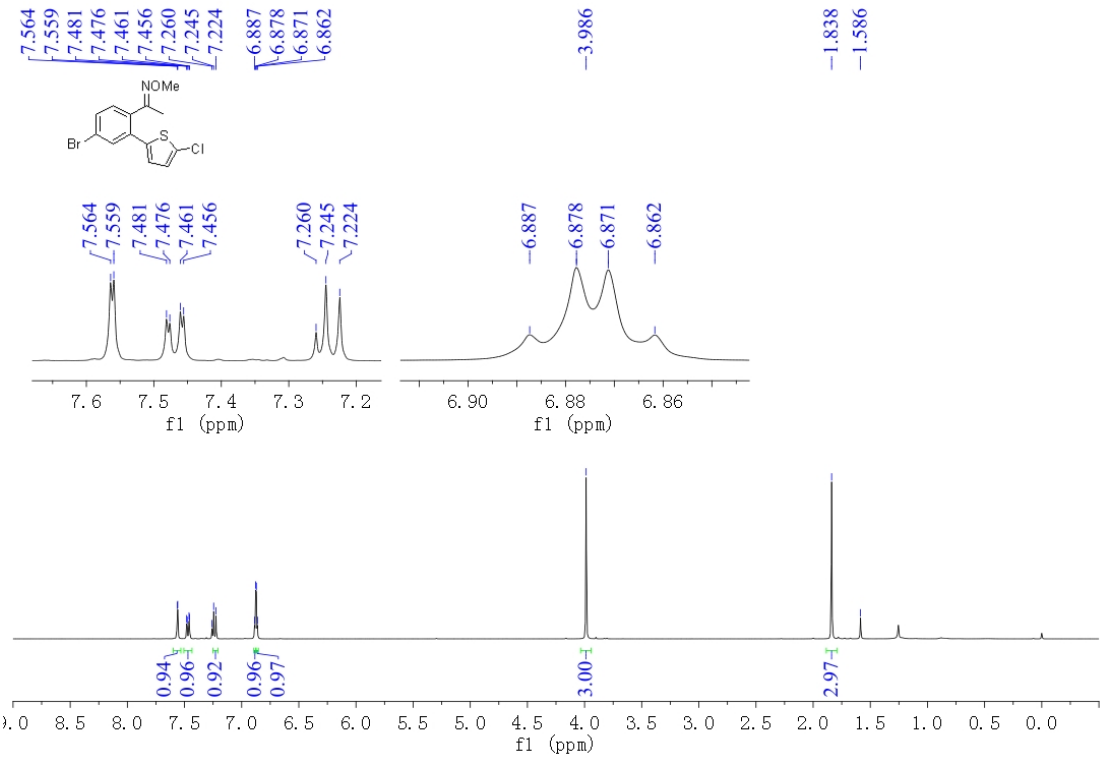
16.56
15.59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7.245
7.224
6.887
6.878
6.871
6.862
3.986
1.838
1.586
NOMe
Br
S
Cl
f1 (ppm)
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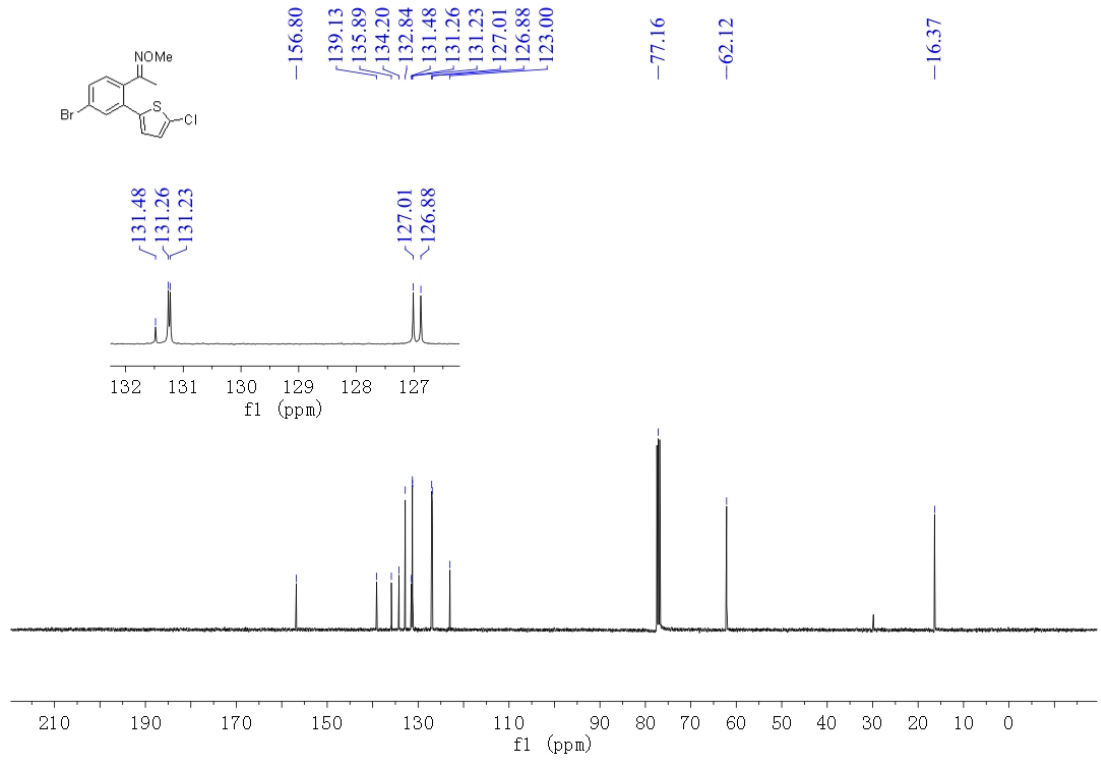
0.96
0.92
0.96
0.97
3.00
2.97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134.20
132.84
131.48
131.26
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127.01
126.88
123.00
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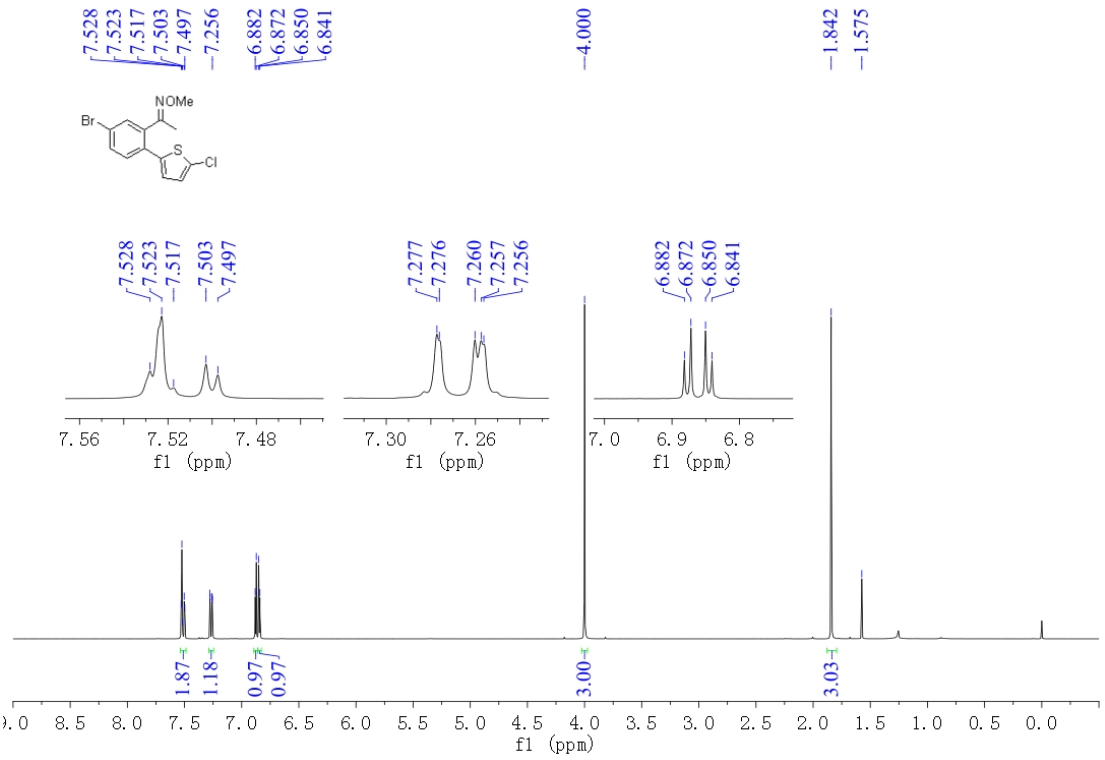
62.12
16.37
NOMe
Br
S
Cl
f1 (ppm)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6.872
6.850
6.841
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1.575
NOMe
Br
S
Cl
7.56
7.52
7.48
f1 (ppm)
7.30
7.26
f1 (ppm)
7.0
6.9
6.8
f1 (ppm)
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1.18
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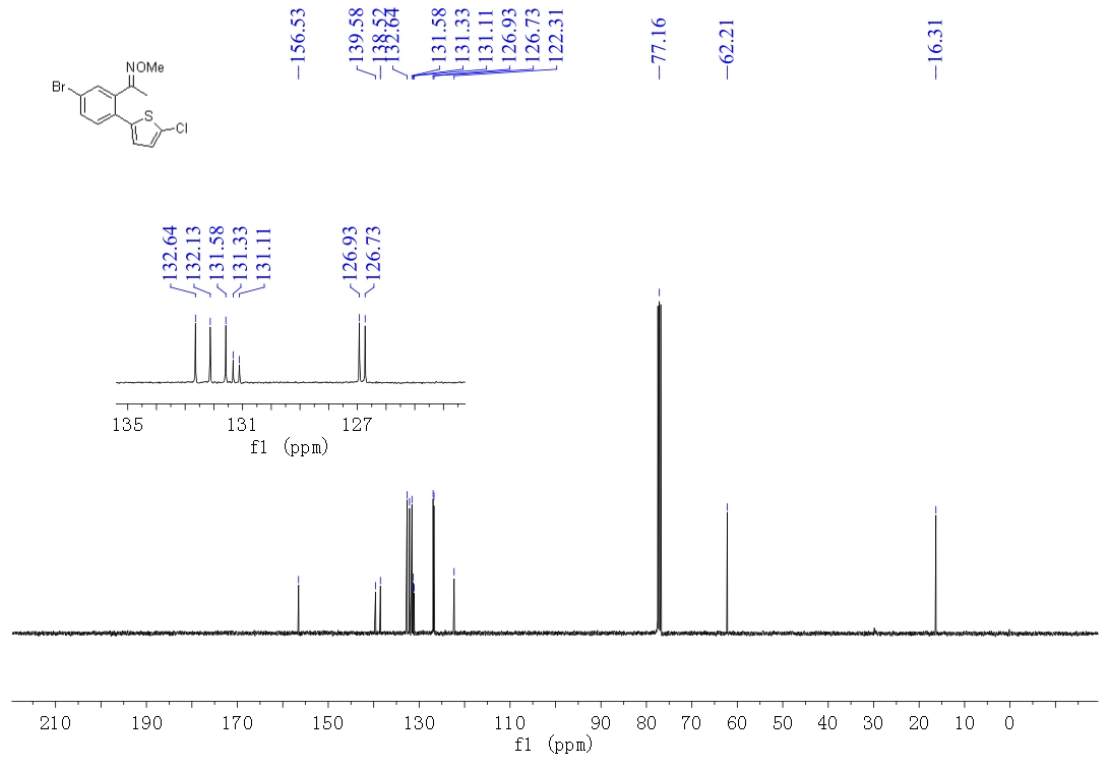
0.97
3.00
3.03
f1 (ppm)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131.33
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126.93
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122.31
77.16
62.21
16.31
NOMe
Br
S
Cl
132.64
132.13
131.58
131.33
131.11
126.93
126.73
135
131
127
f1 (ppm)
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170
150
130
110
90
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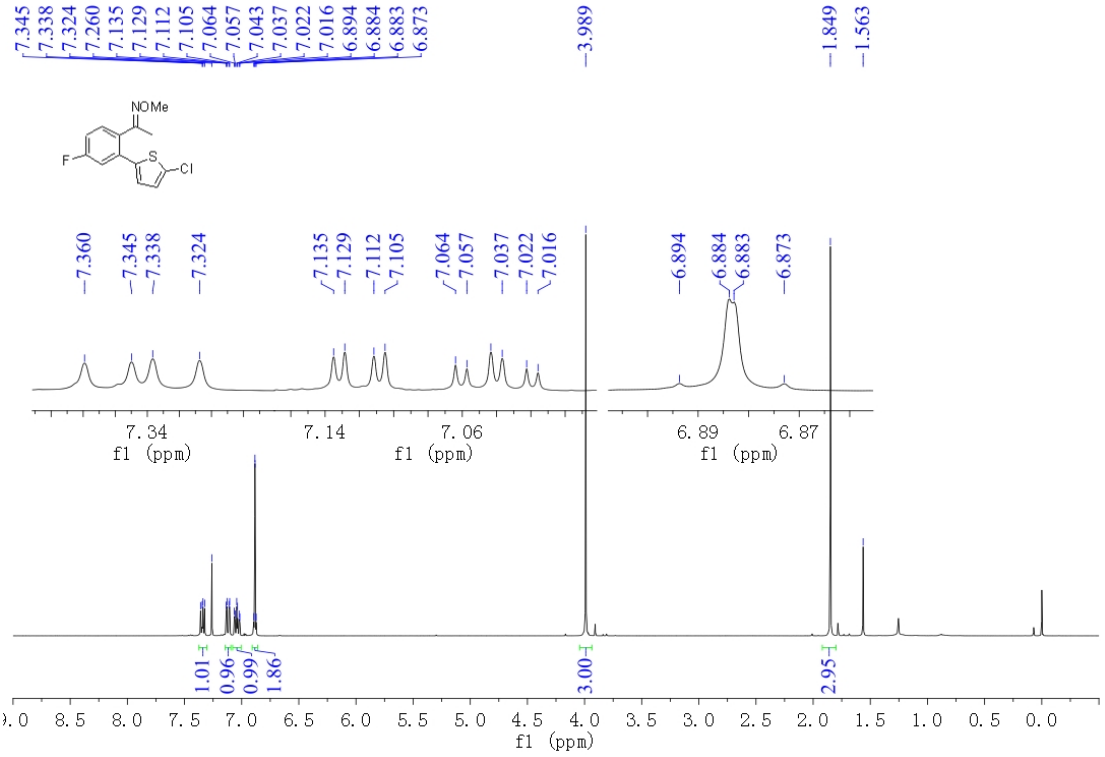
70
60
50
40
30
20
10
0
f1 (ppm)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7.129
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7.057
7.043
7.037
7.022
7.016
6.894
6.884
6.883
6.873
3.989
1.849
1.563
NOMe
F
S
Cl
7.34
f1 (ppm)
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7.06
6.89
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0.99
1.86
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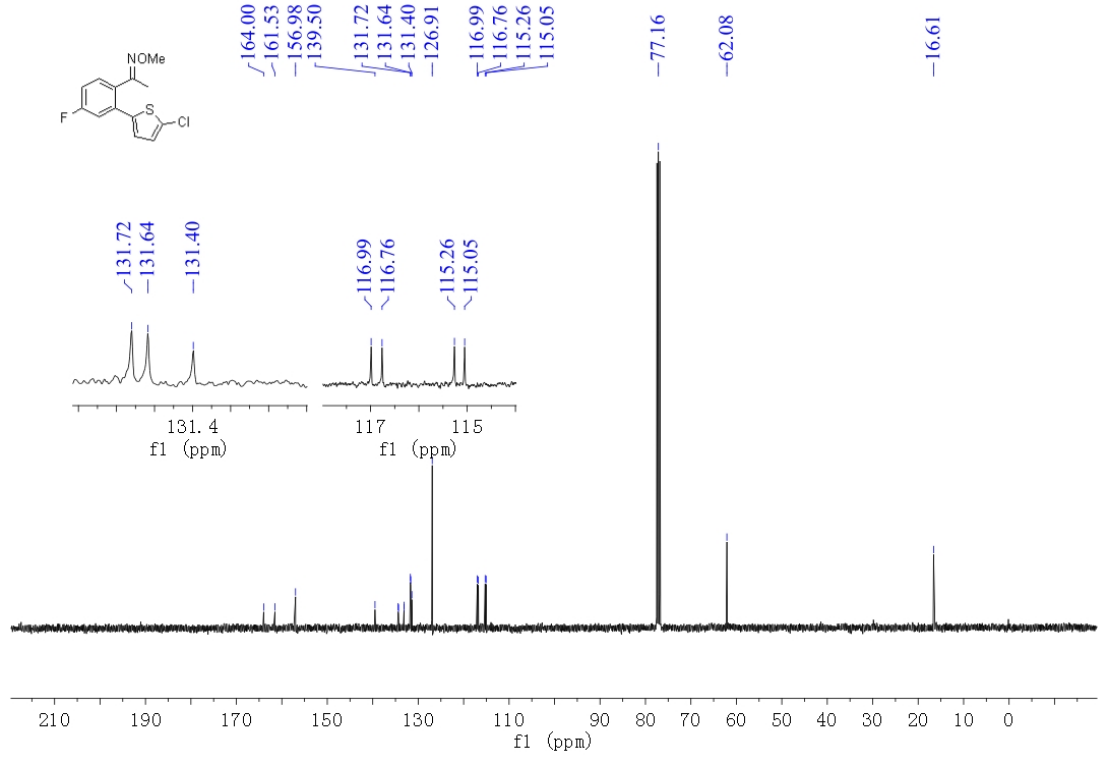
2.95
f1 (ppm)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115.26
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F
S
Cl
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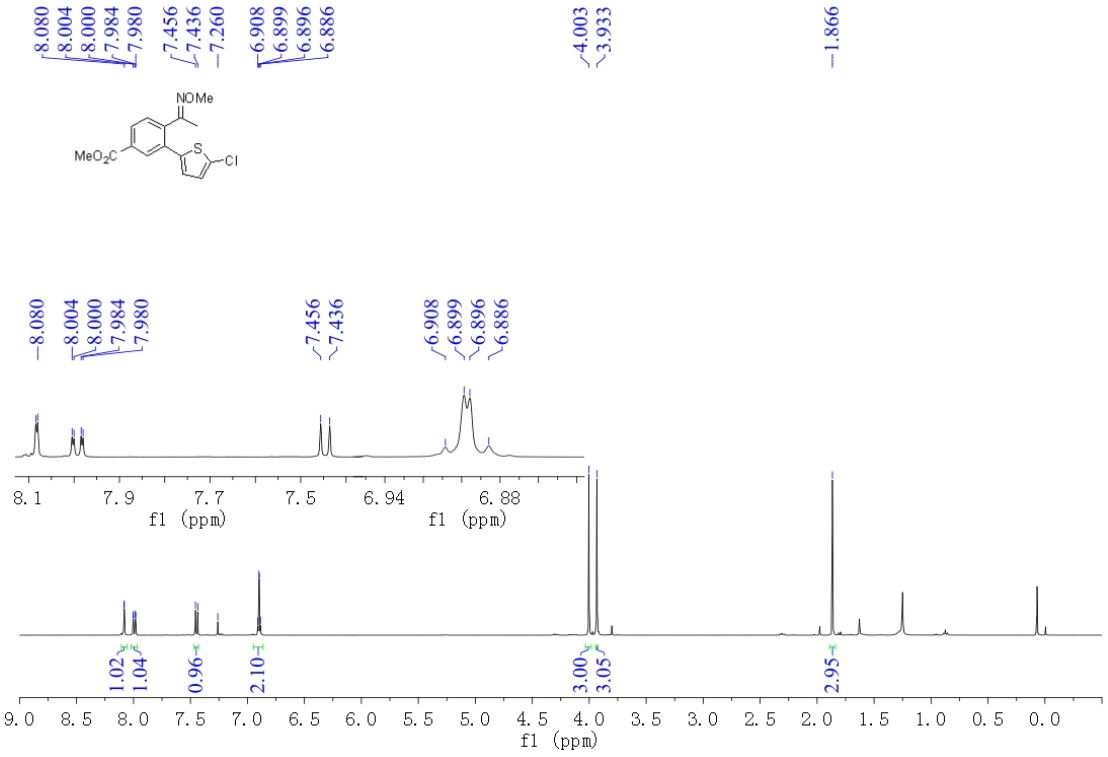
f1 (ppm)
117
115
f1 (ppm)
f1 (ppm)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3.933
1.866
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S
Cl
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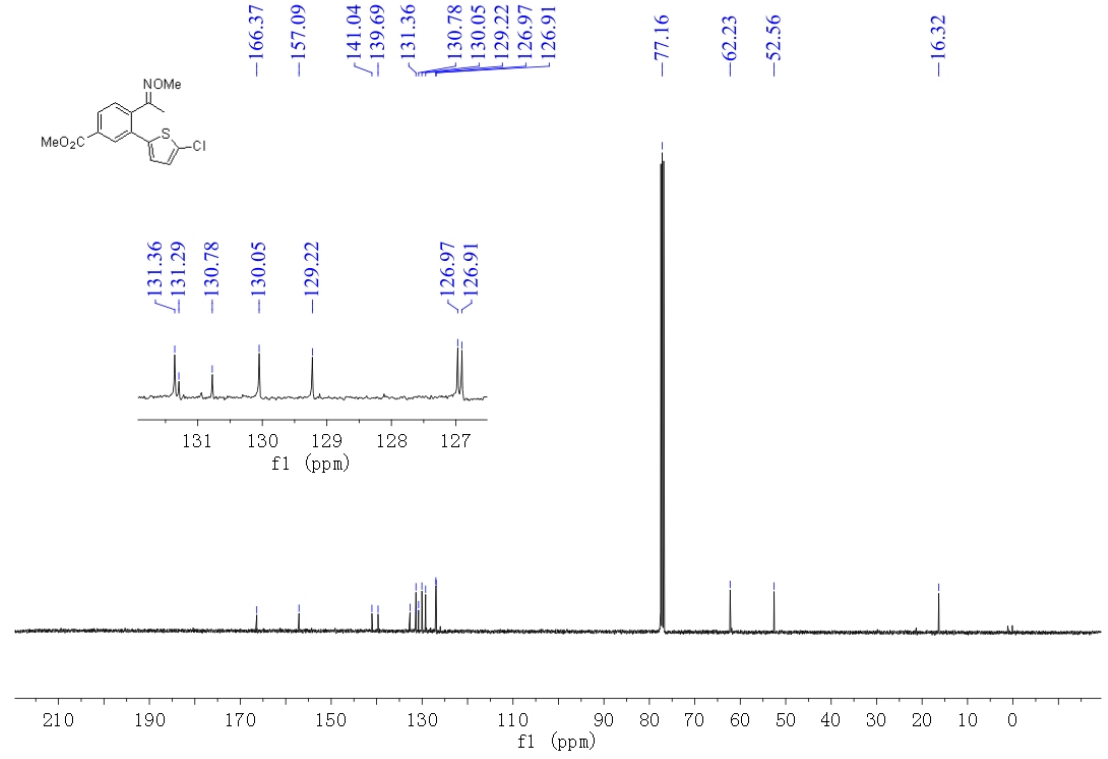
3.00
3.05
2.95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129.22
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77.16
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52.56
16.32
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S
Cl
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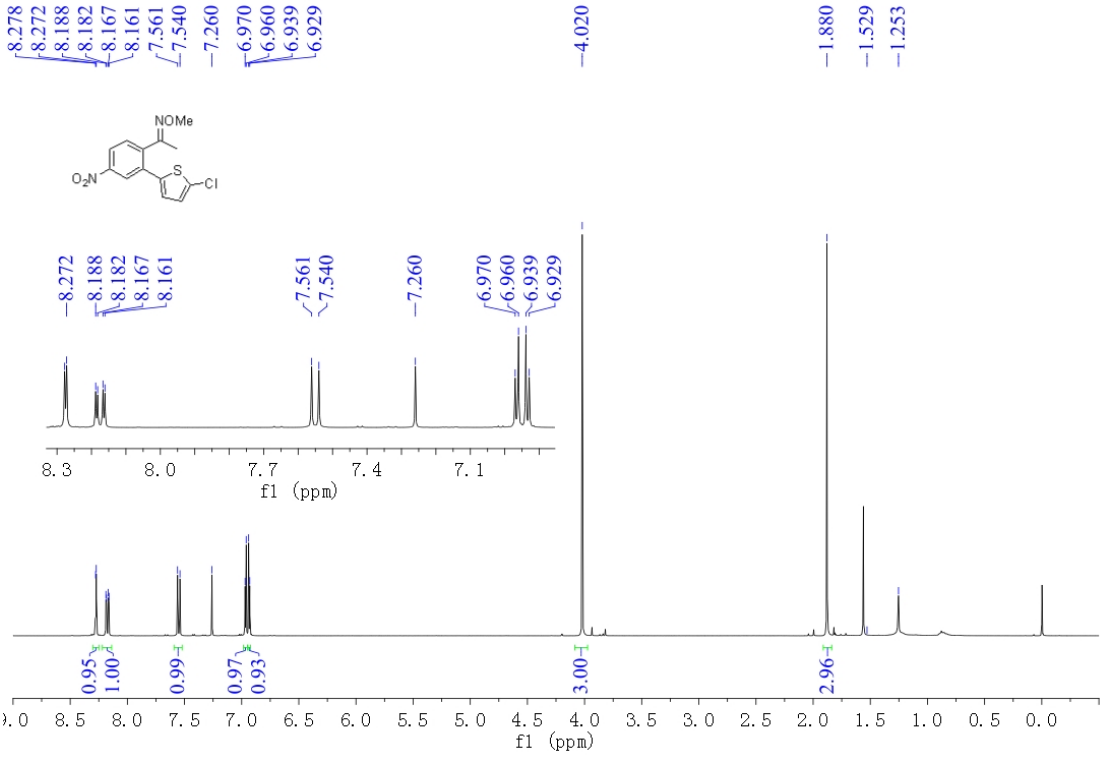
131.29
130.78
130.05
129.22
126.97
126.91
f1 (ppm)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1.529
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S
Cl
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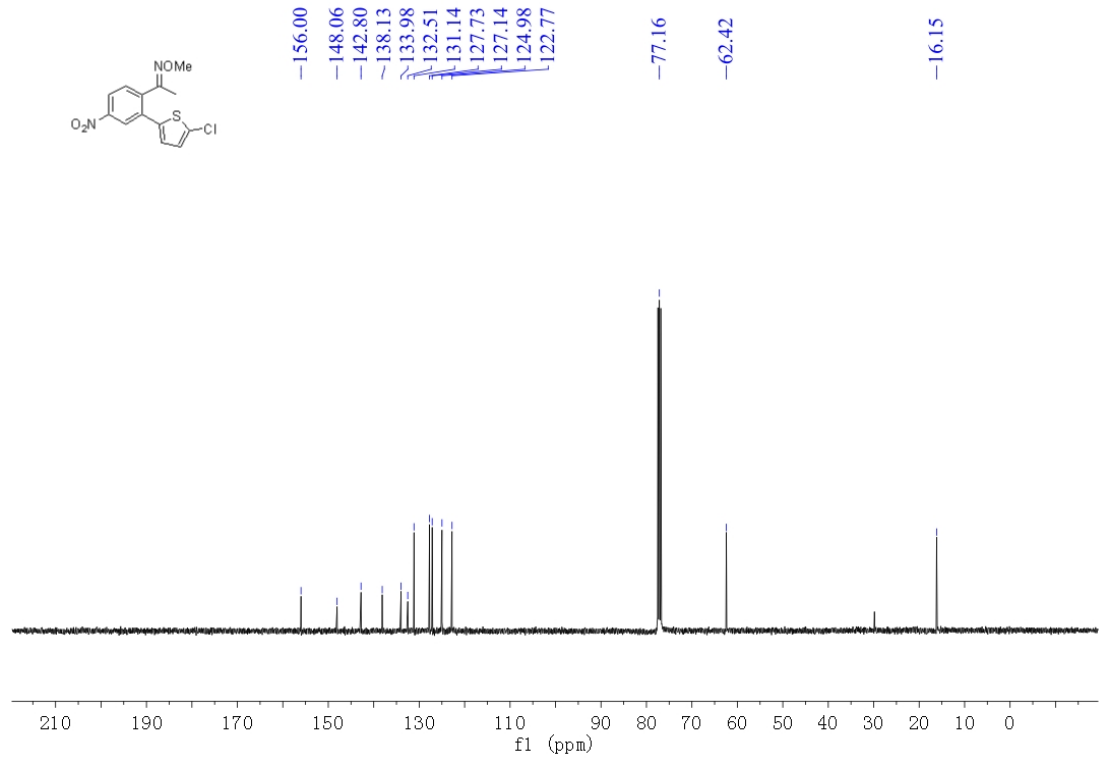
3.00
2.96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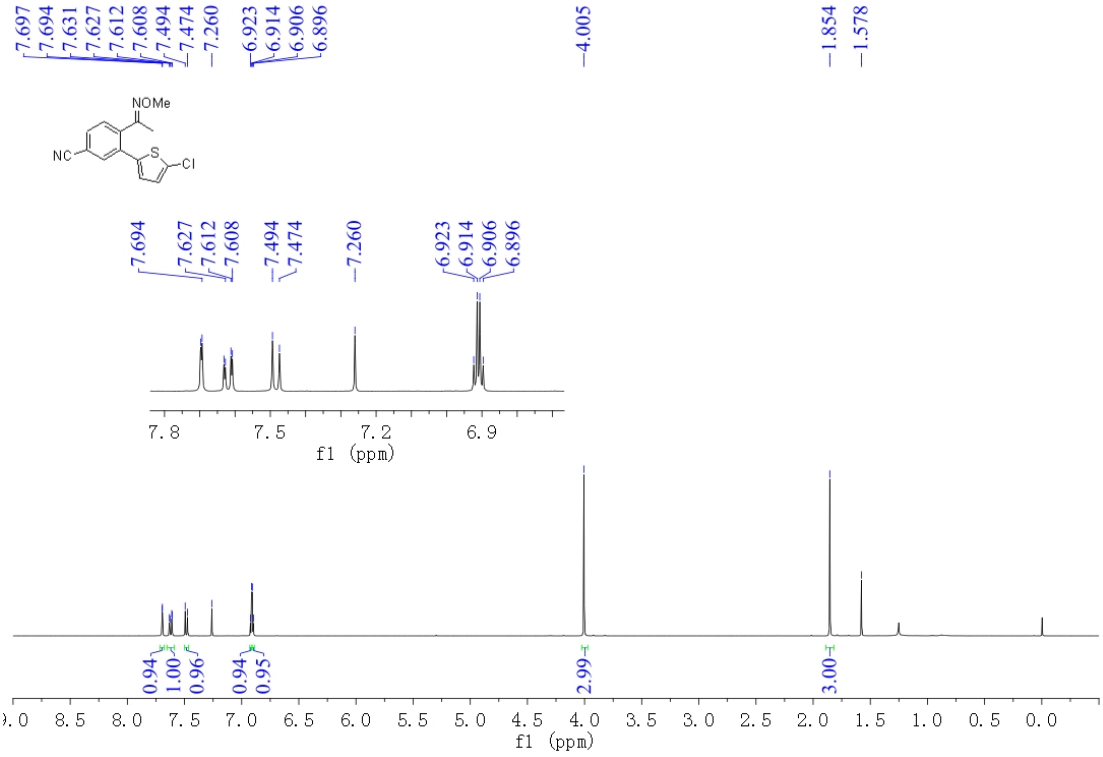
NOMe
O2N
S
Cl
f1 (ppm)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4.005
1.854
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NC
S
Cl
7.8
7.5
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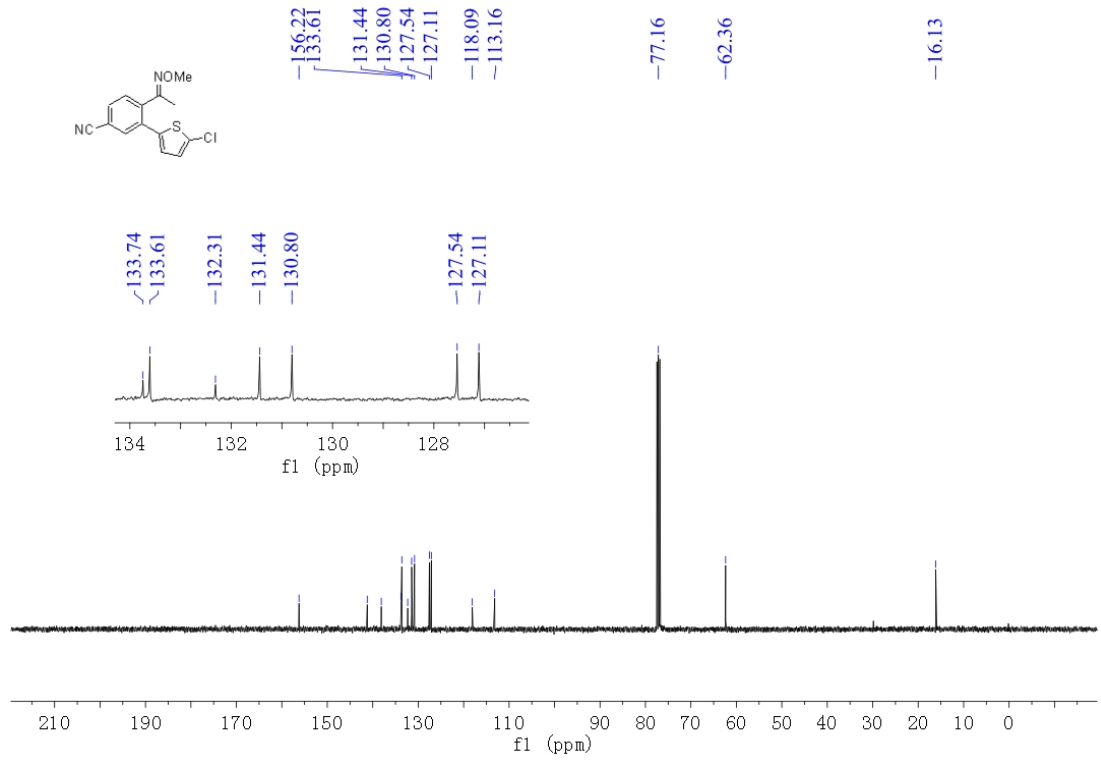
f1 (ppm)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NC
S
Cl
133.74
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132.31
131.44
130.80
127.54
127.11
134
132
130
128
f1 (ppm)
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50
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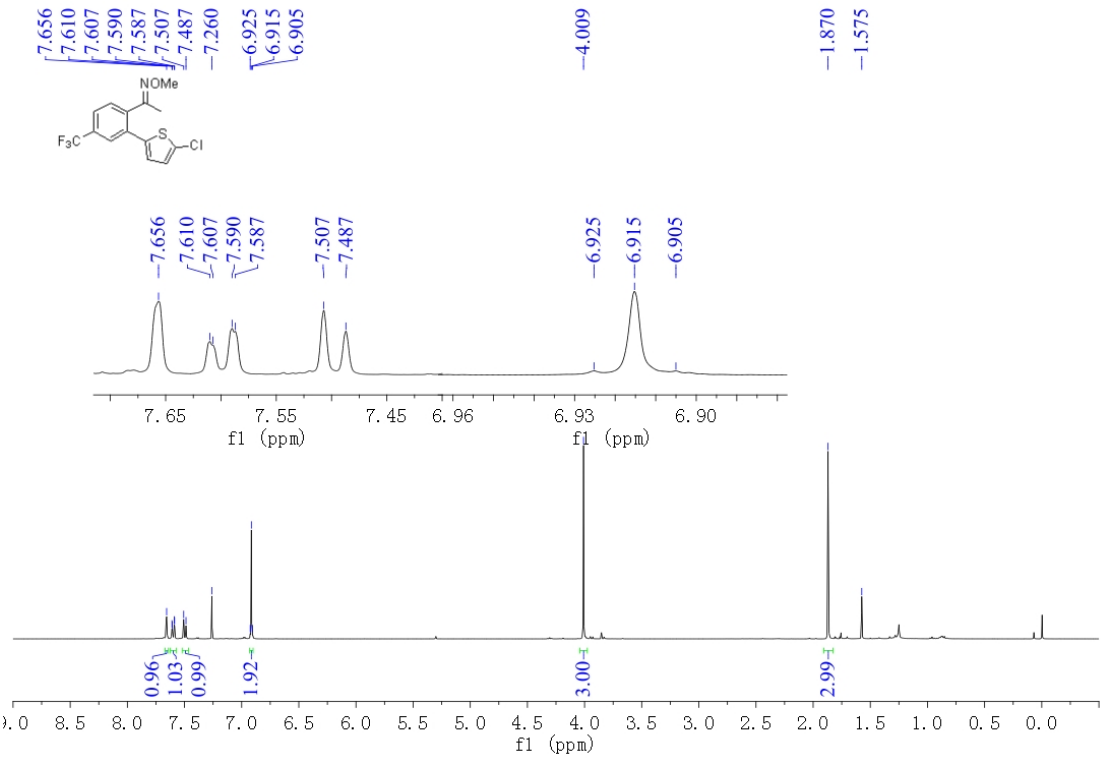
f1 (ppm)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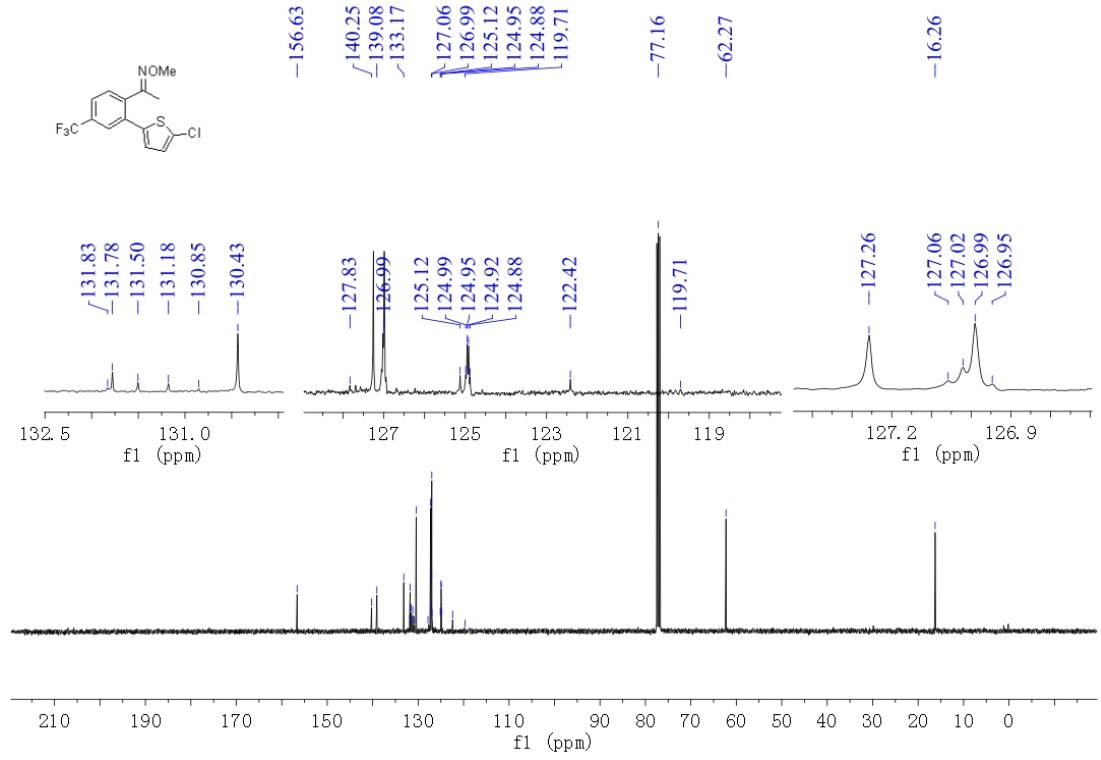
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F3C
S
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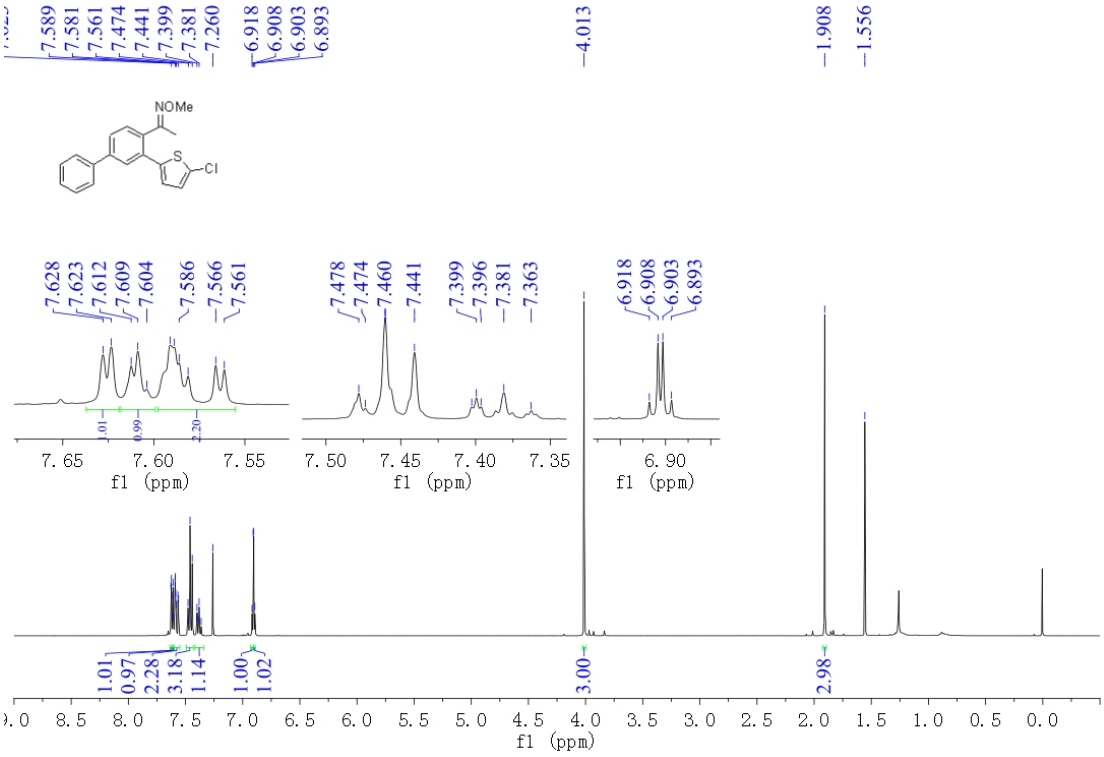
f1 (ppm)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4.013
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1.556
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S
Cl
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7.586
7.566
7.561
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7.399
7.396
7.381
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6.908
6.903
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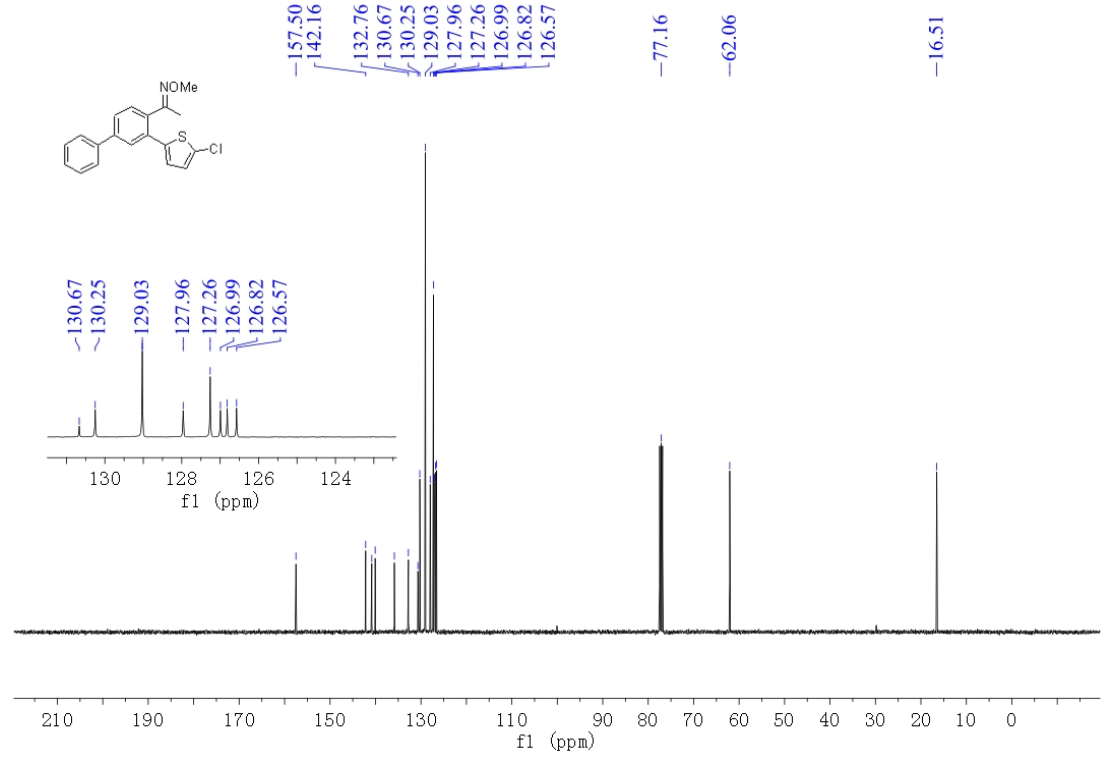
3.00
2.98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127.26
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126.82
126.57
77.16
62.06
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S
Cl
130.67
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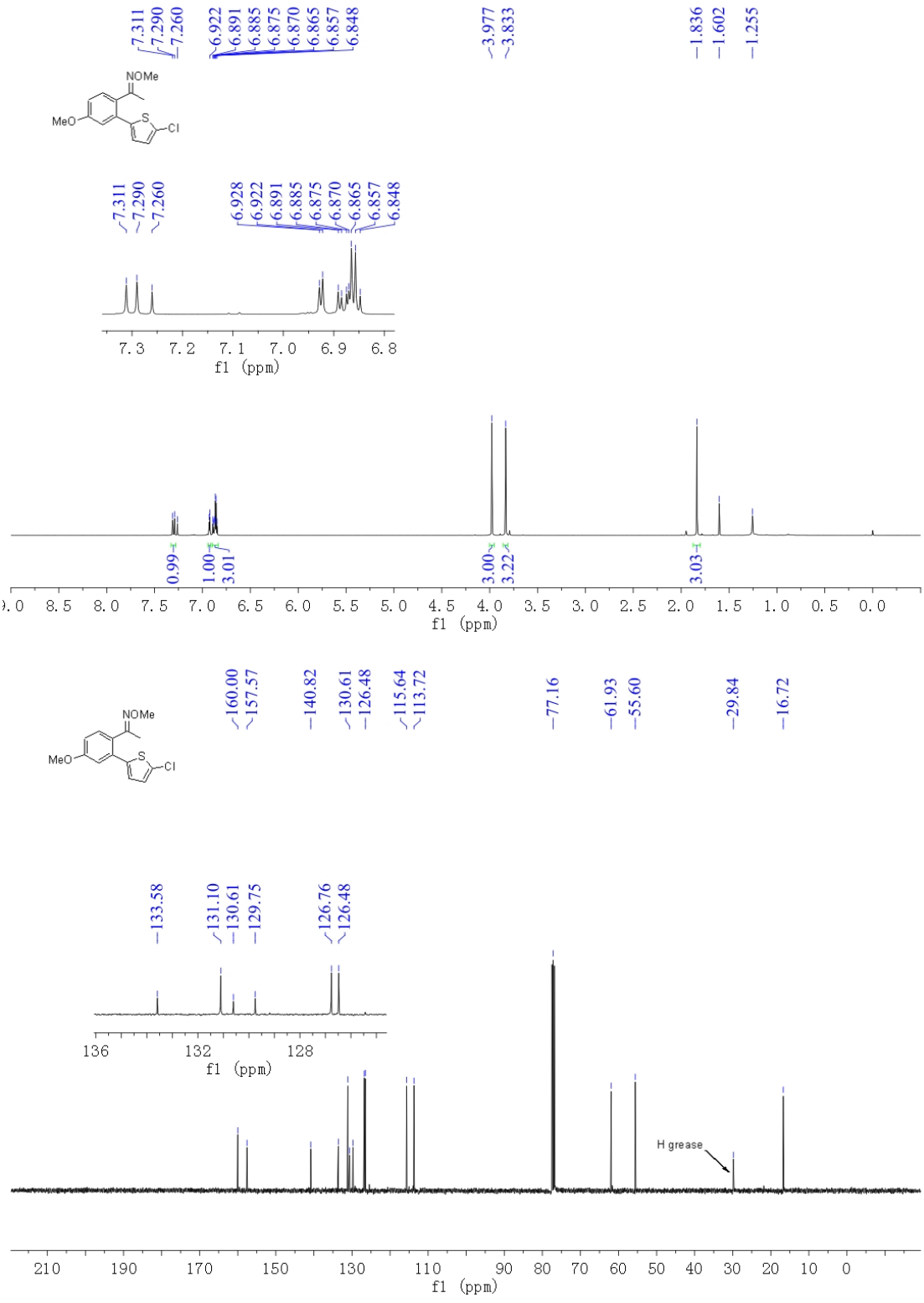
127.26
126.99
126.82
126.57
f1 (ppm)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6.857
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1.602
1.255
NOMe
MeO
S
Cl
6.928
7.3 7.2 7.1 7.0 6.9 6.8
f1 (ppm)
0.99
1.00
3.01
3.00
3.22
3.03
f1 (ppm)
160.00
157.57
140.82
130.61
126.48
115.64
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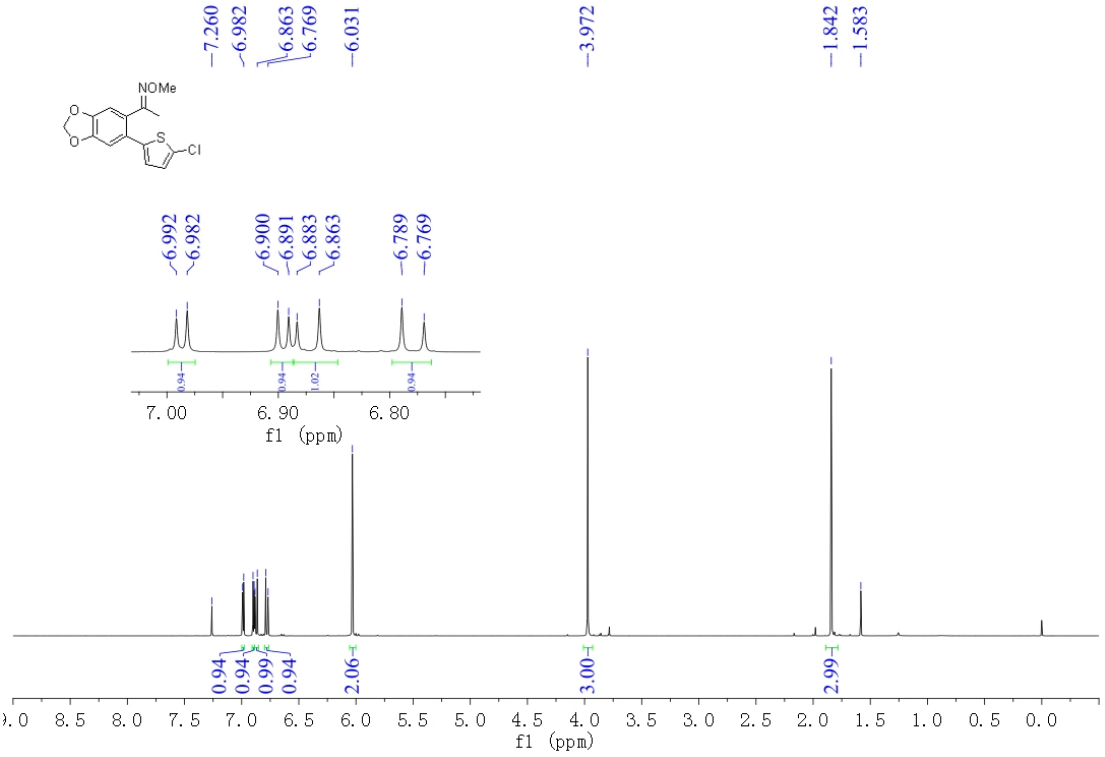
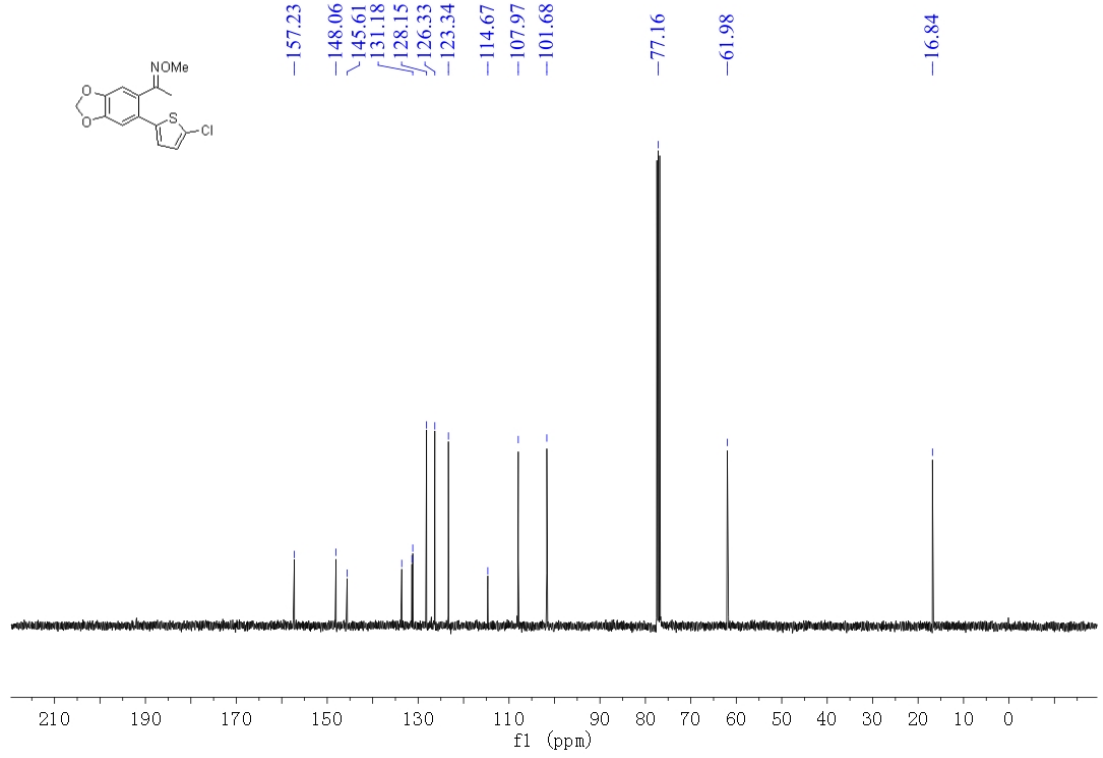
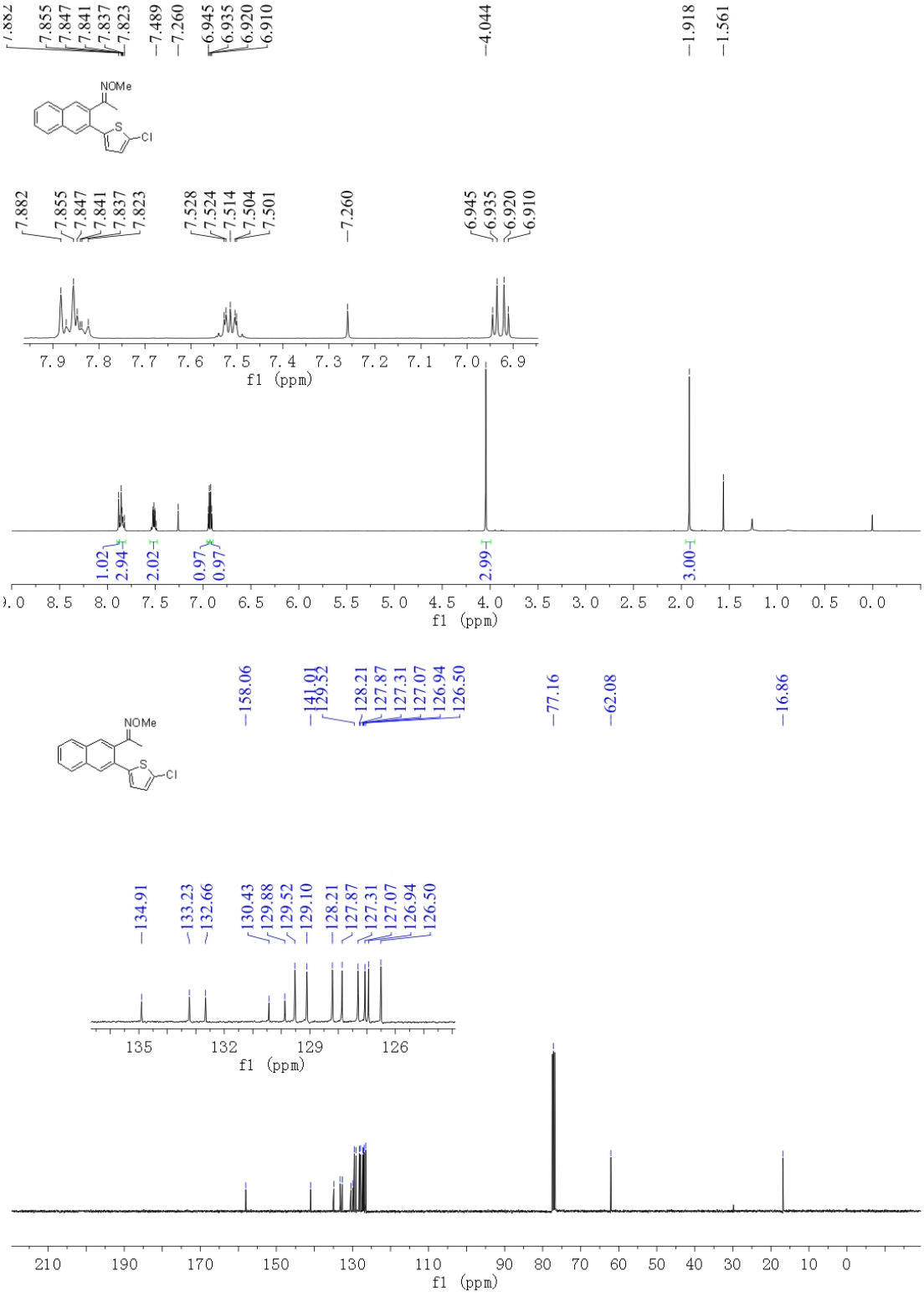
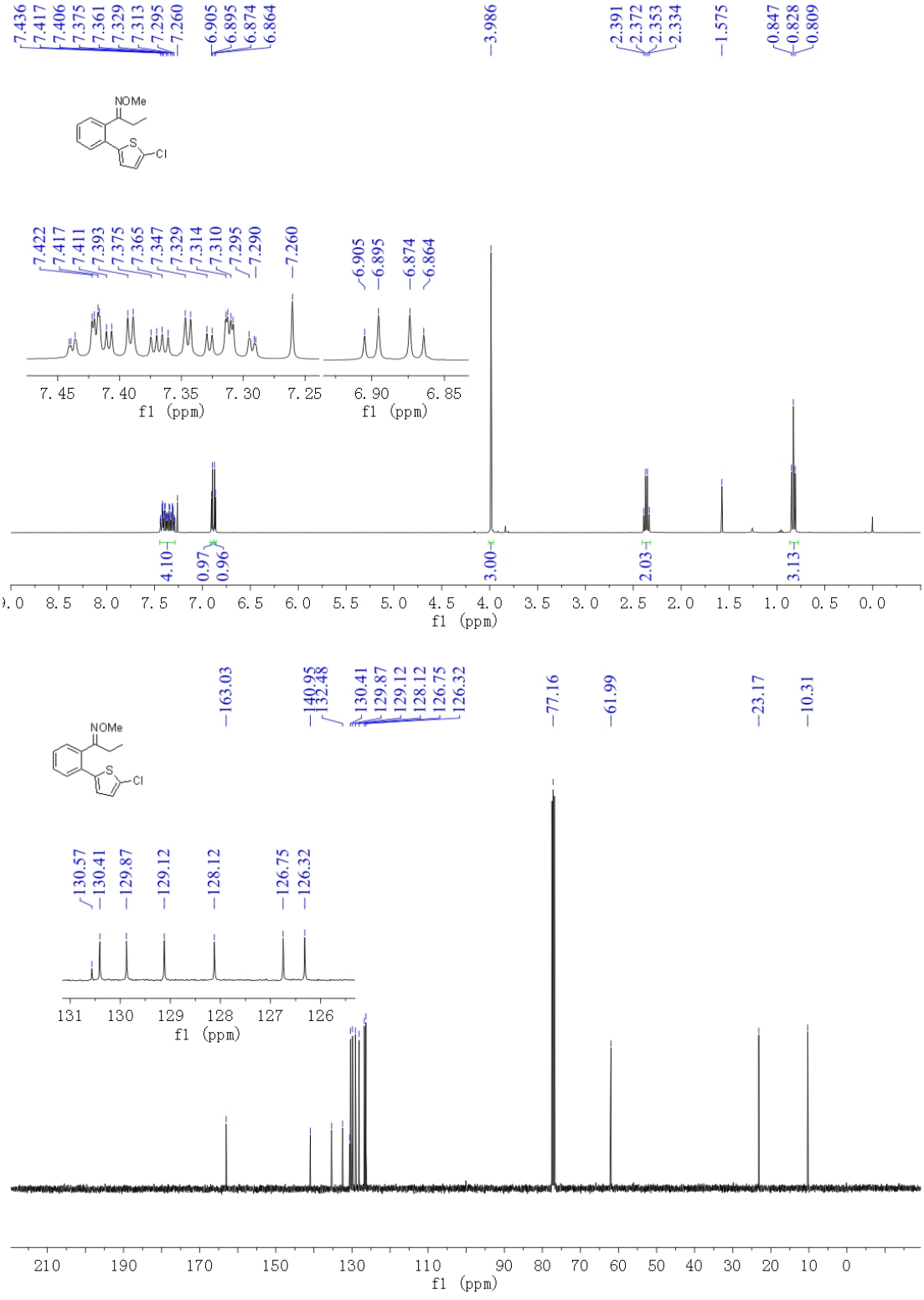
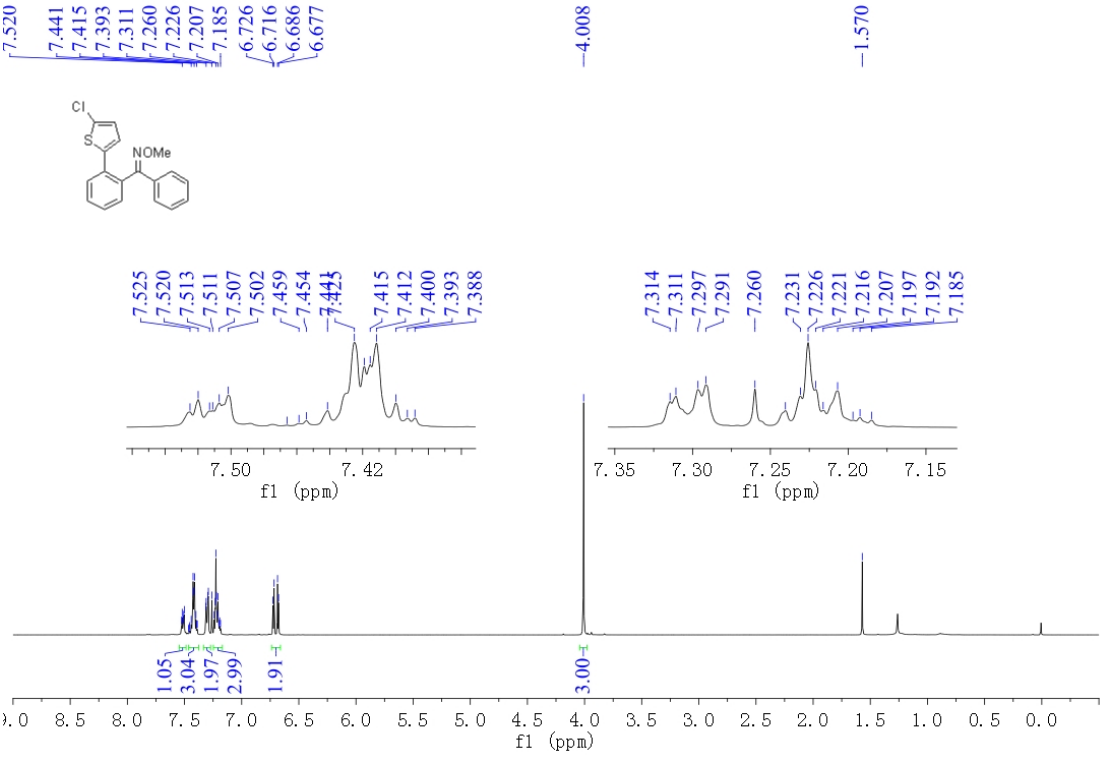
133.58
131.10
130.61
129.75
126.76
126.48
136 132 128
f1 (ppm)
H grease
210 190 170 150 130 110 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

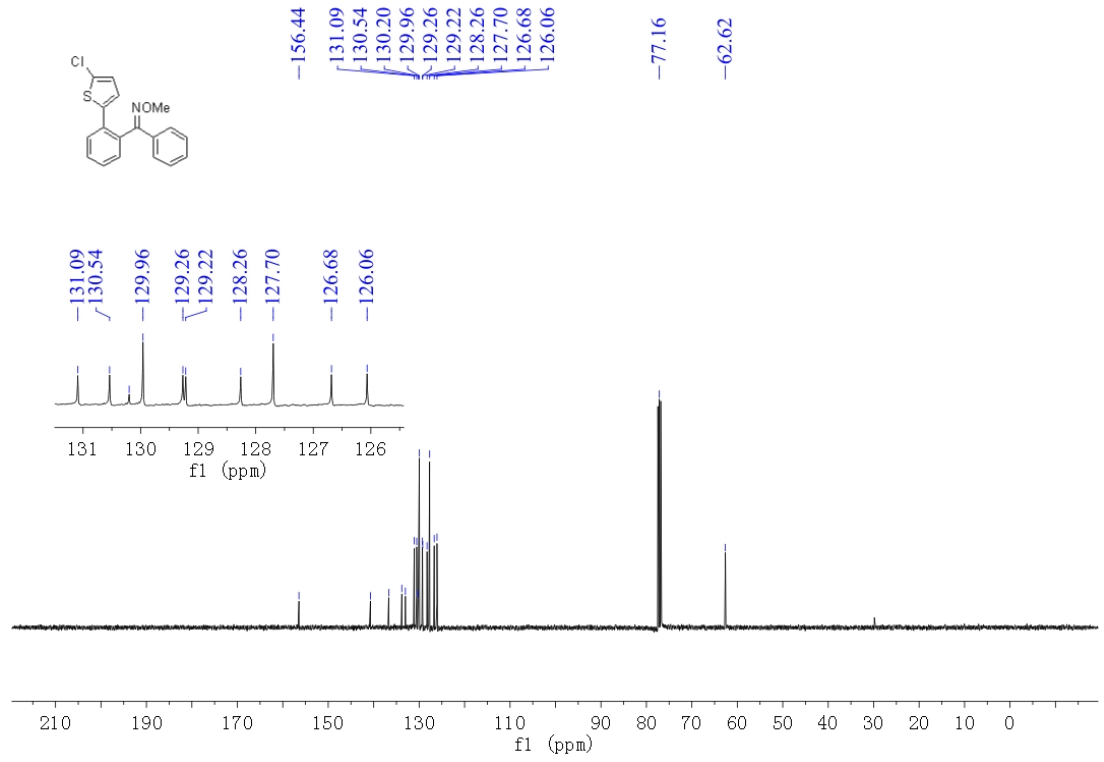

7.260
6.982
6.863
6.769
6.031
3.972
1.842
1.583
NOMe
O
O
S
Cl
6.992
6.982
6.900
6.891
6.883
6.863
6.789
6.769
0.94
0.94
1.02
0.94
7.00
6.90
6.80
f1 (ppm)
0.94
0.94
0.99
0.94
2.06
3.00
2.99
f1 (ppm)

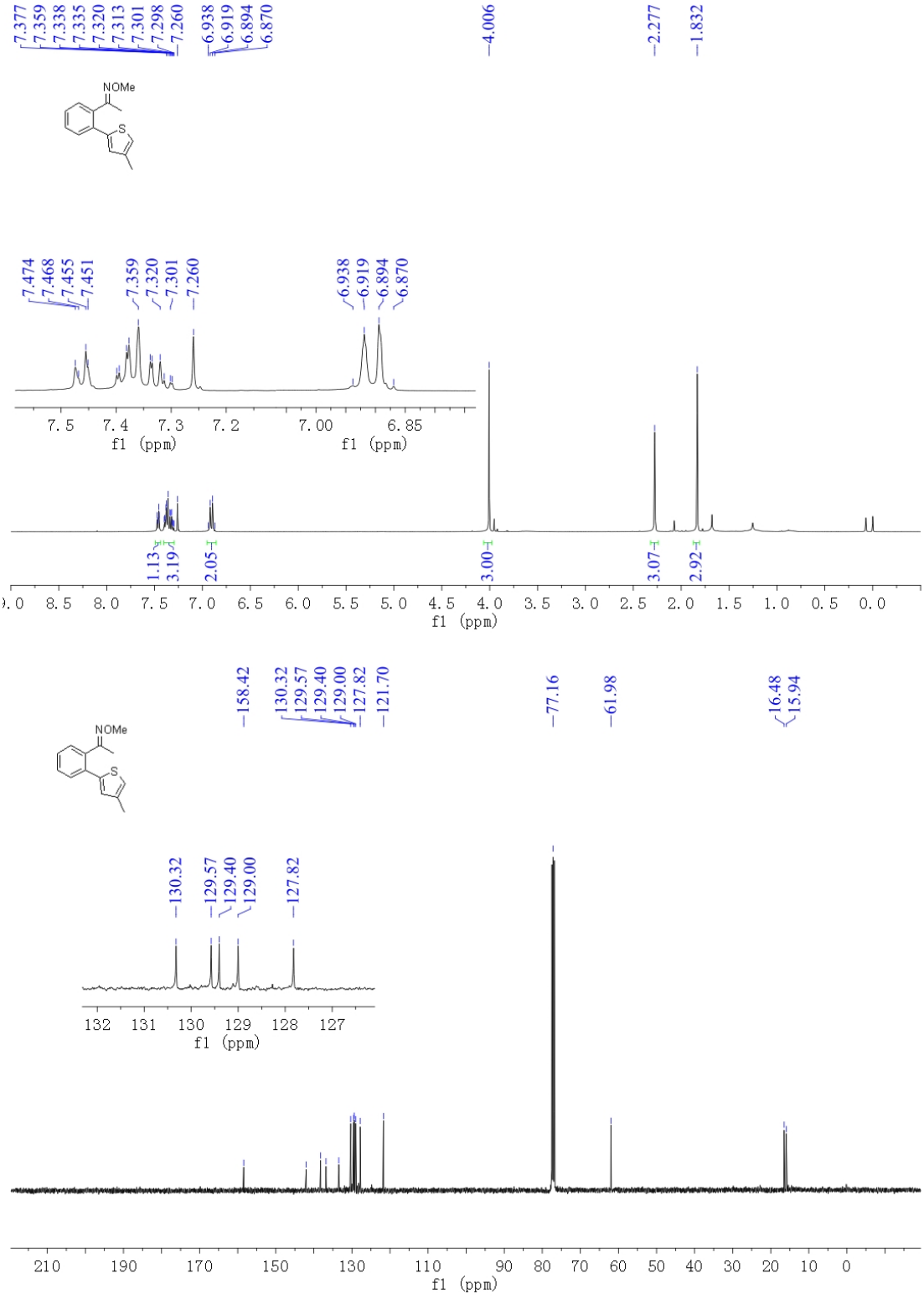

157.23
148.06
145.61
131.18
128.15
126.33
123.34
114.67
107.97
101.68
77.16
61.98
16.84
NOMe
O
O
S
Cl
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

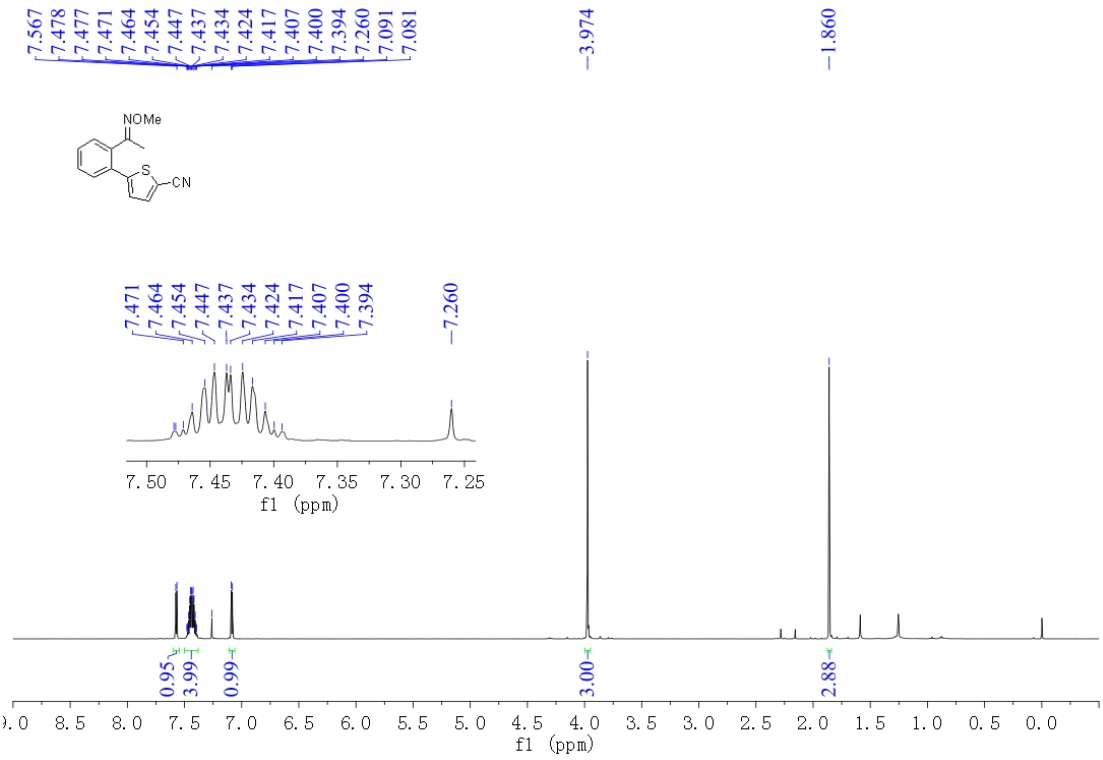

7.882
7.855
7.847
7.841
7.837
7.823
7.489
7.260
6.945
6.935
6.920
6.910
4.044
1.918
1.561
NOMe
S
Cl
7.528
7.524
7.514
7.504
7.501
f1 (ppm)
1.02
2.94
2.02
0.97
0.97
2.99
3.00
158.06
141.01
129.52
128.21
127.87
127.31
127.07
126.94
126.50
77.16
62.08
16.86
134.91
133.23
132.66
130.43
129.88
129.52
129.10
128.21
127.87
127.31
127.07
126.94
126.50

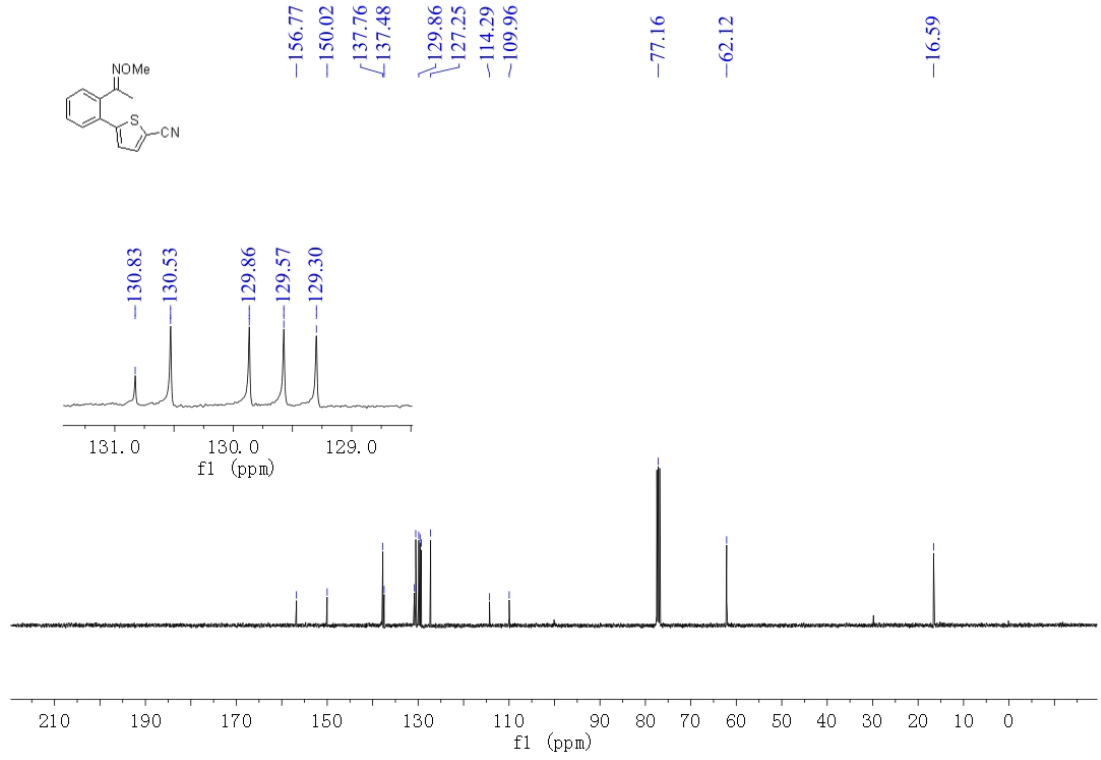

7.436
7.417
7.406
7.375
7.361
7.329
7.313
7.295
7.260
6.905
6.895
6.874
6.864
3.986
2.391
2.372
2.353
2.334
1.575
0.847
0.828
0.809
NOMe
S
Cl
7.422
7.417
7.411
7.393
7.375
7.365
7.347
7.329
7.314
7.310
7.295
7.290
7.260
6.905
6.895
6.874
6.864
7.45 7.40 7.35 7.30 7.25
f1 (ppm)
6.90 6.85
f1 (ppm)
4.10
0.97
0.96
3.00
2.03
3.13
f1 (ppm)
163.03
140.95
132.48
130.41
129.87
129.12
128.12
126.75
126.32
77.16
61.99
23.17
10.31
NOMe
S
Cl
130.57
130.41
129.87
129.12
128.12
126.75
126.32
131 130 129 128 127 126
f1 (ppm)
f1 (ppm)

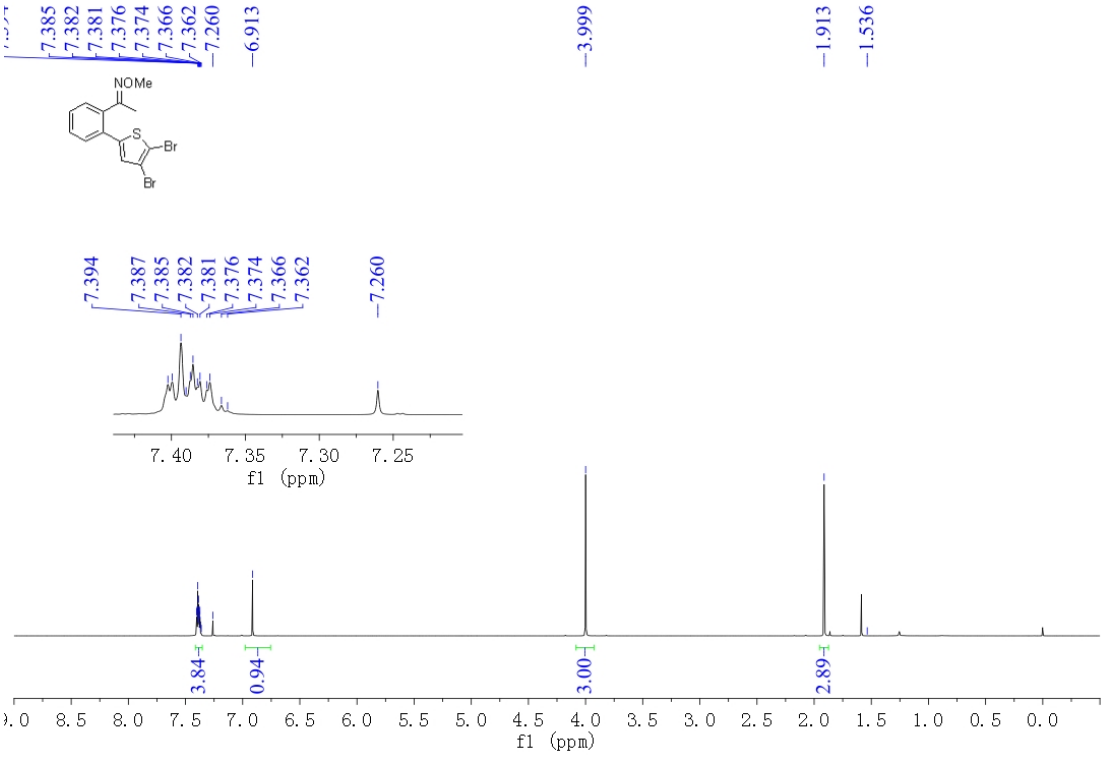

7.520
7.441
7.415
7.393
7.311
7.260
7.226
7.207
7.185
6.726
6.716
6.686
6.677
4.008
1.570
Cl
S
NOMe
7.525
7.520
7.513
7.511
7.507
7.502
7.459
7.454
7.415
7.412
7.400
7.393
7.388
7.314
7.311
7.297
7.291
7.260
7.231
7.226
7.221
7.216
7.207
7.197
7.192
7.185
7.50
7.42
f1 (ppm)
7.35
7.30
7.25
7.20
7.15
f1 (ppm)
1.05
3.04
1.97
2.99
1.91
3.00
f1 (ppm)

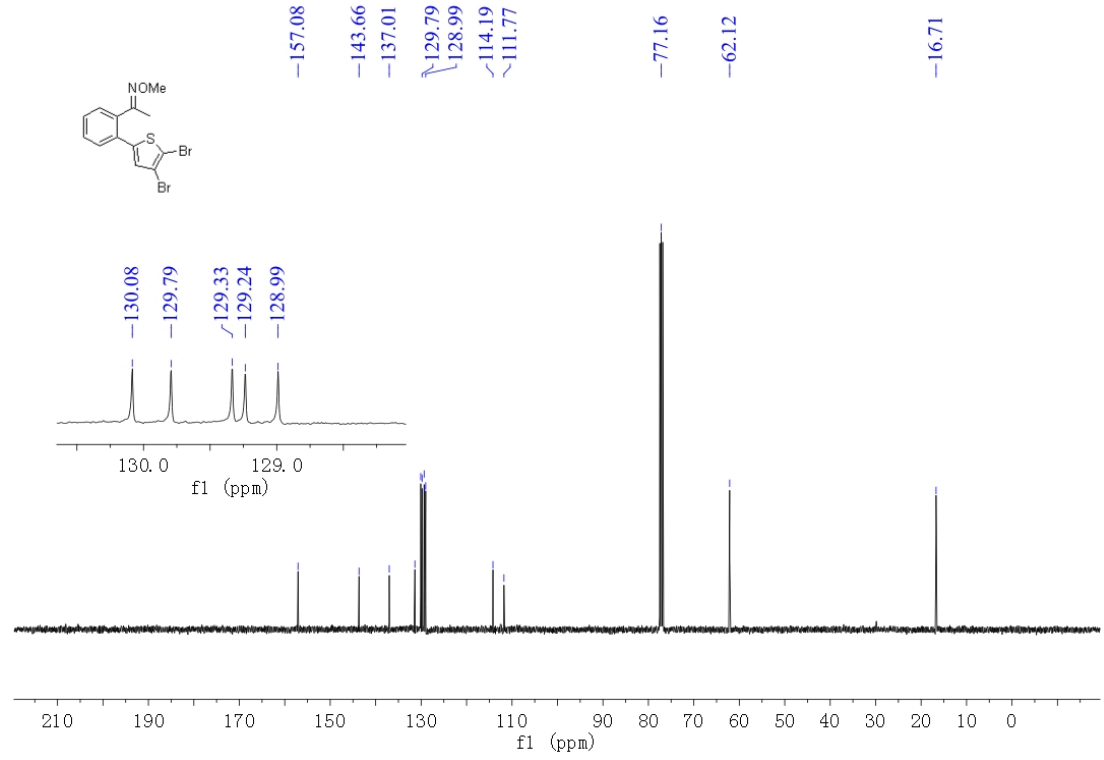

156.44
131.09
130.54
130.20
129.96
129.26
129.22
128.26
127.70
126.68
126.06
77.16
62.62
Cl
S
NOMe
131.09
130.54
129.96
129.26
129.22
128.26
127.70
126.68
126.06
131
130
129
128
127
126
f1 (ppm)
f1 (ppm)

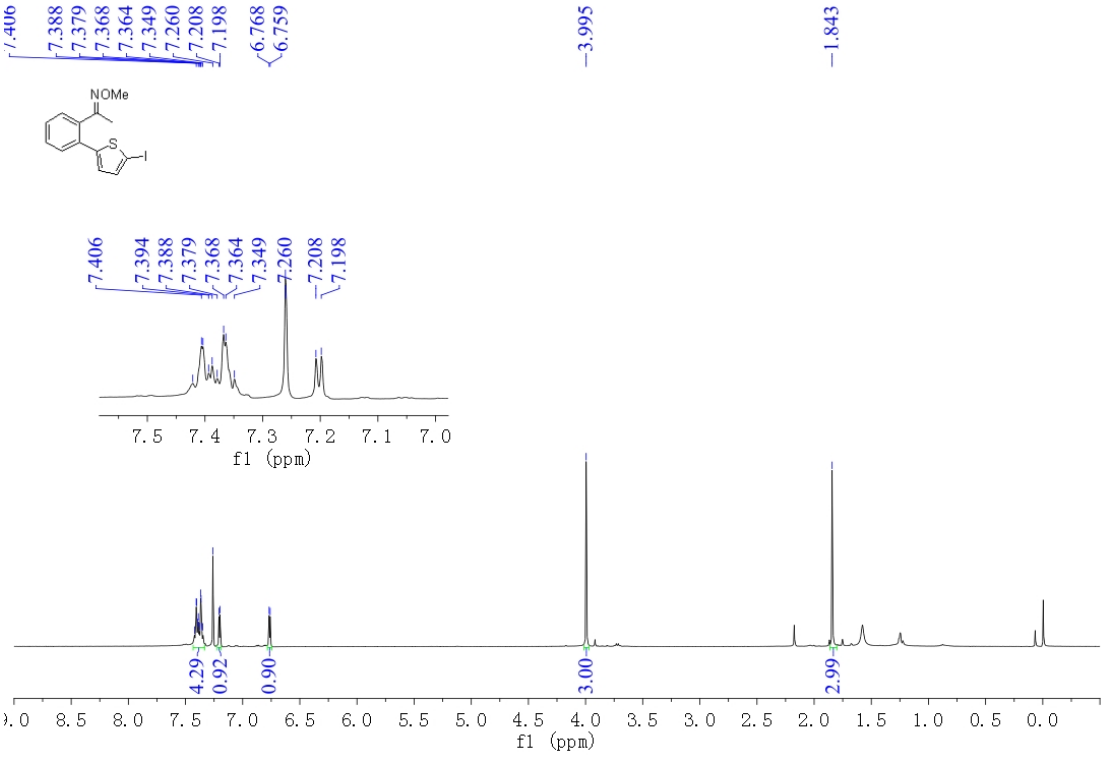

7.377
7.359
7.338
7.335
7.320
7.313
7.301
7.298
7.260
6.938
6.919
6.894
6.870
4.006
2.277
1.832
NOMe
S
7.474
7.468
7.455
7.451
7.359
7.320
7.301
7.260
6.938
6.919
6.894
6.870
7.5 7.4 7.3 7.2
f1 (ppm)
7.00 6.85
f1 (ppm)
1.13
3.19
2.05
3.00
3.07
2.92
f1 (ppm)
158.42
130.32
129.57
129.40
129.00
127.82
121.70
77.16
61.98
16.48
15.94
NOMe
S
130.32
129.57
129.40
129.00
127.82
132 131 130 129 128 127
f1 (ppm)
210 190 170 150 130 110 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

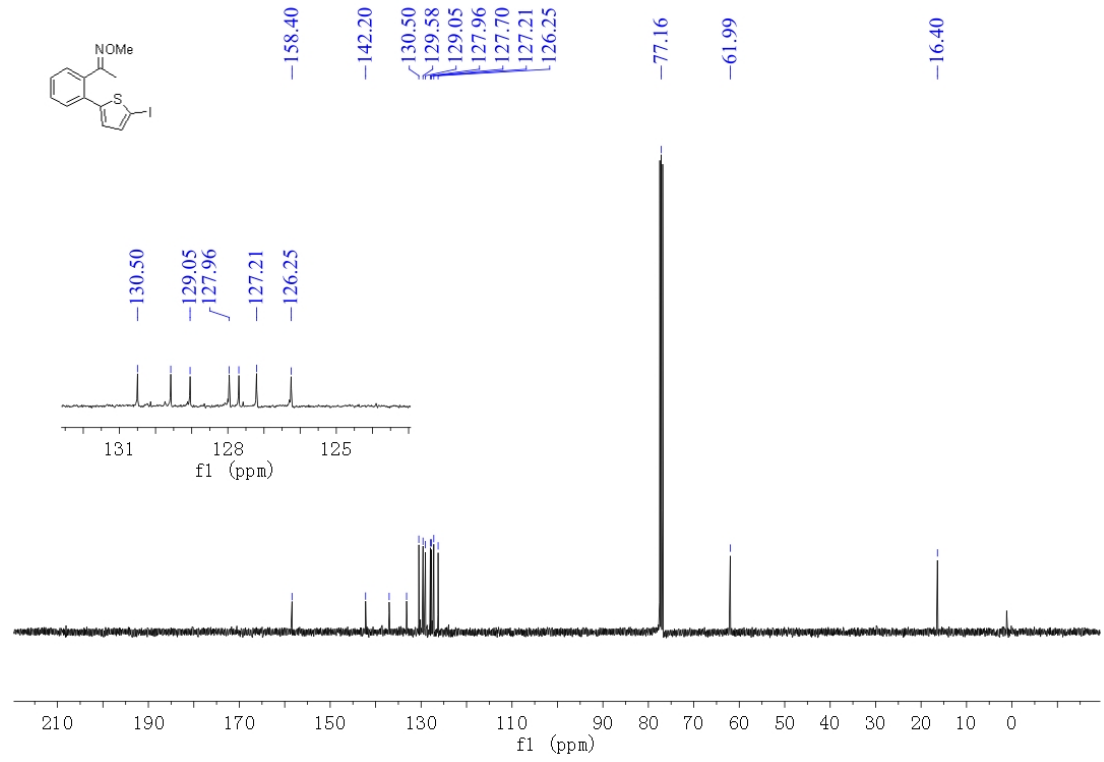

7.567
7.478
7.477
7.471
7.464
7.454
7.447
7.437
7.434
7.424
7.417
7.407
7.400
7.394
7.260
7.091
7.081
3.974
1.860
NOMe
S
CN
7.471
7.464
7.454
7.447
7.437
7.434
7.424
7.417
7.407
7.400
7.394
7.260
7.50 7.45 7.40 7.35 7.30 7.25
f1 (ppm)
0.95
3.99
0.99
3.00
2.88
f1 (ppm)

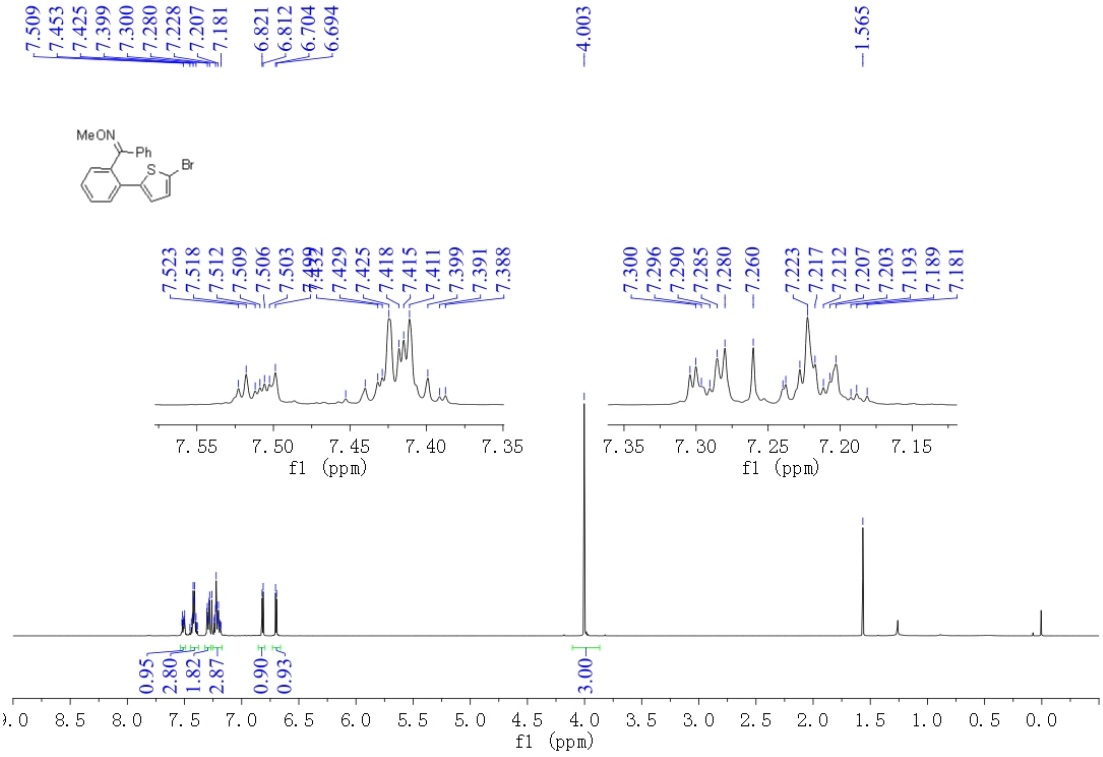

156.77
150.02
137.76
137.48
129.86
127.25
114.29
109.96
77.16
62.12
16.59
NOMe
S
CN
130.83
130.53
129.86
129.57
129.30
131.0 130.0 129.0
f1 (ppm)
210 190 170 150 130 110 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

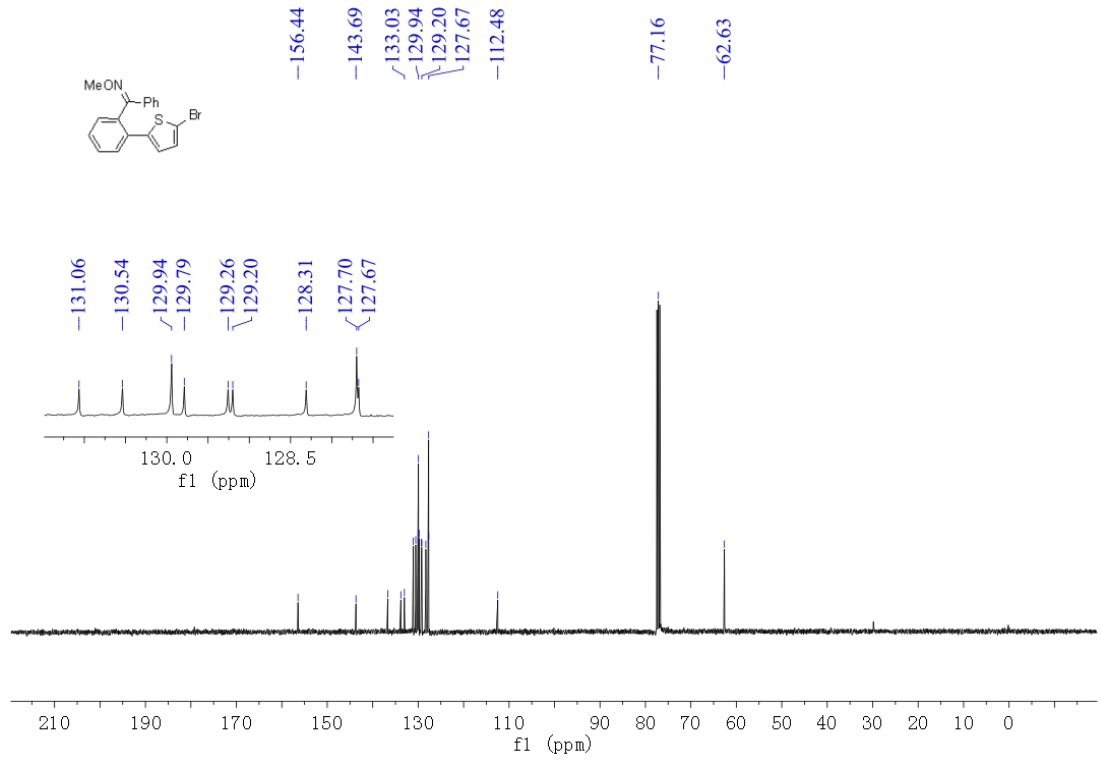

7.385
7.382
7.381
7.376
7.374
7.366
7.362
7.260
6.913
3.999
1.913
1.536
NOMe
S
Br
Br
7.394
7.387
7.385
7.382
7.381
7.376
7.374
7.366
7.362
7.260
7.40
7.35
7.30
7.25
f1 (ppm)
3.84
0.94
3.00
2.89
f1 (ppm)

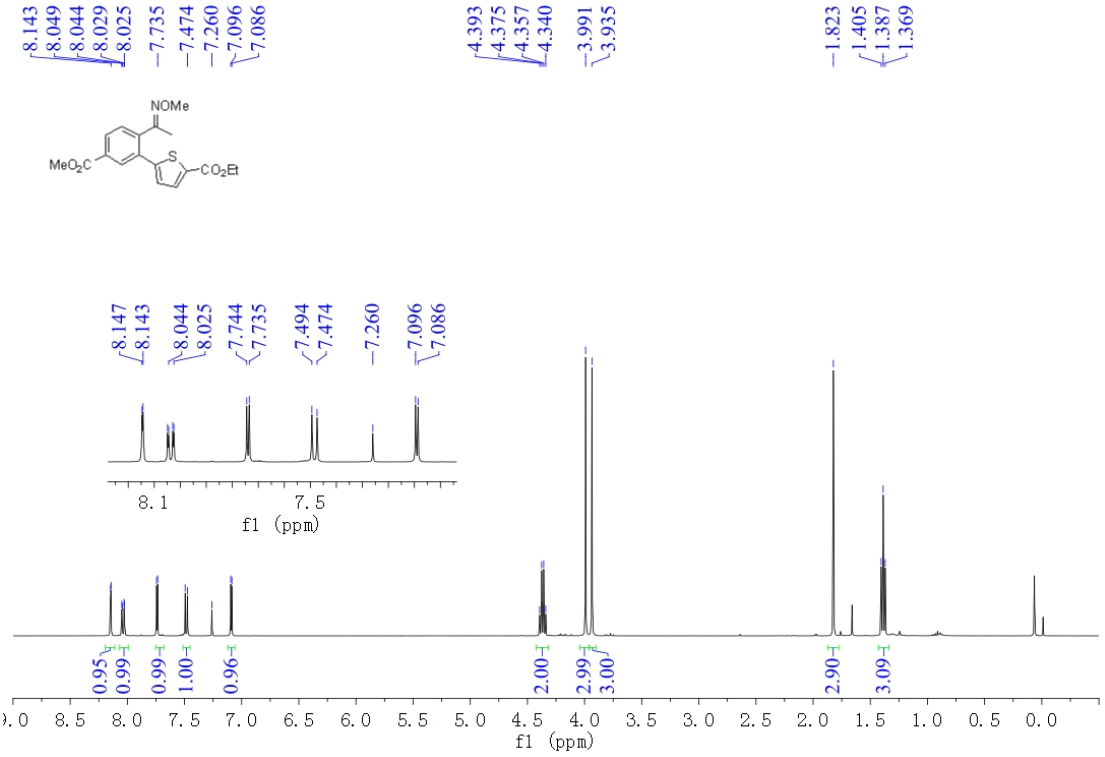

157.08
143.66
137.01
129.79
128.99
114.19
111.77
77.16
62.12
16.71
NOMe
S
Br
Br
130.08
129.79
129.33
129.24
128.99
130.0
129.0
f1 (ppm)
f1 (ppm)

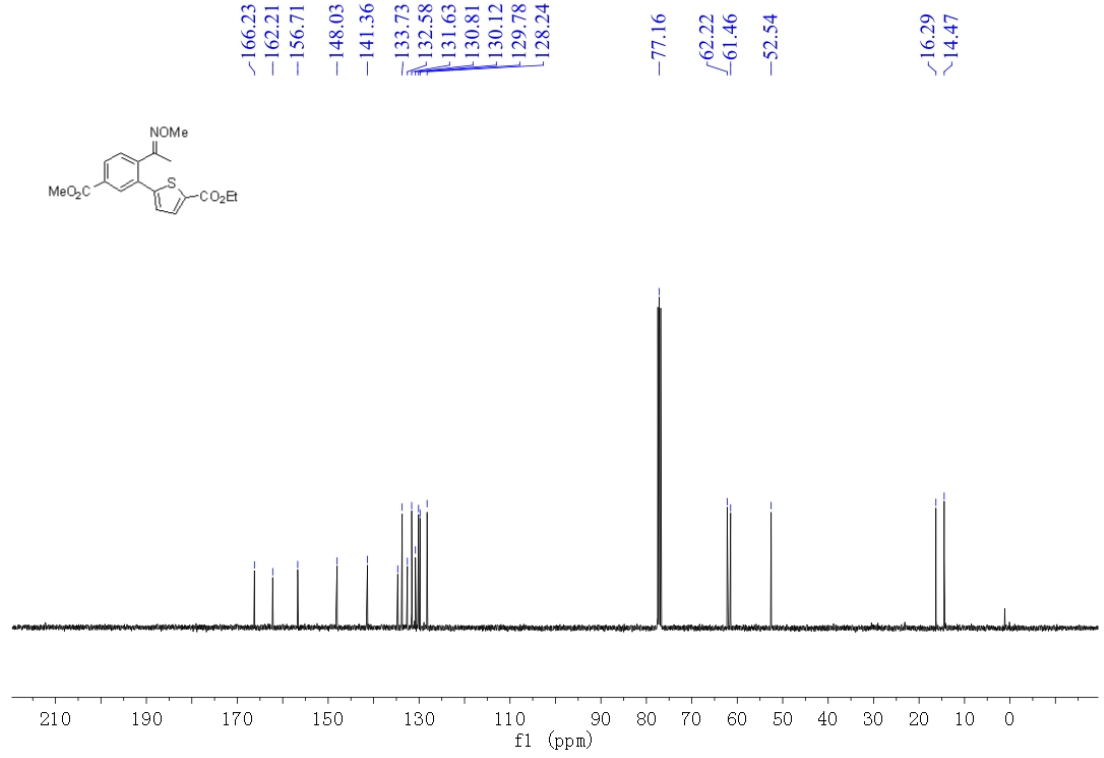

7.406
7.388
7.379
7.368
7.364
7.349
7.260
7.208
7.198
6.768
6.759
3.995
1.843
NOMe
S
I
7.406
7.394
7.388
7.379
7.368
7.364
7.349
7.260
7.208
7.198
7.5 7.4 7.3 7.2 7.1 7.0
f1 (ppm)
4.29
0.92
0.90
3.00
2.99
f1 (ppm)

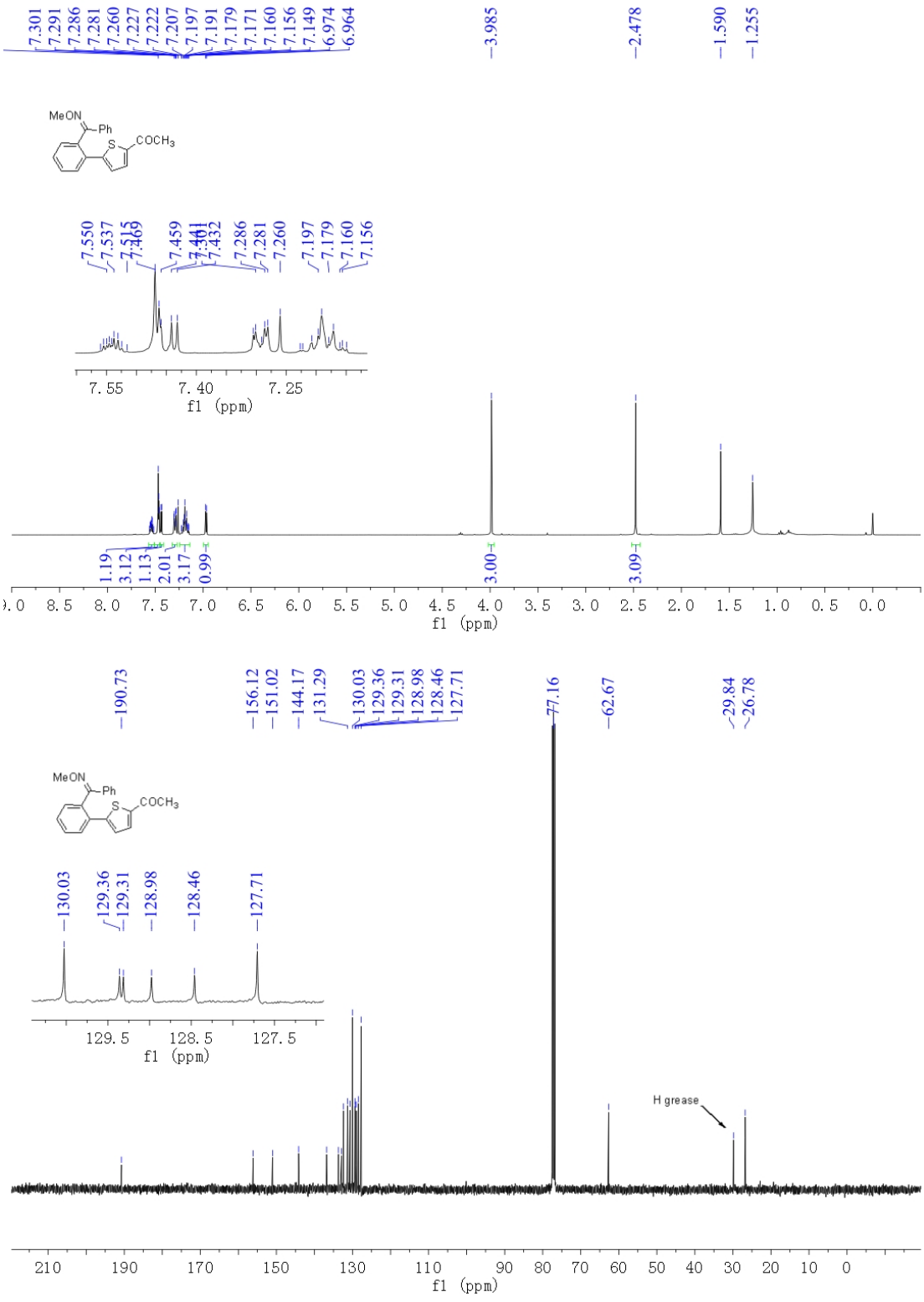

158.40
142.20
130.50
129.58
129.05
127.96
127.70
127.21
126.25
77.16
61.99
16.40
NOMe
S
I
130.50
129.05
127.96
127.21
126.25
131
128
125
f1 (ppm)
210 190 170 150 130 110 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

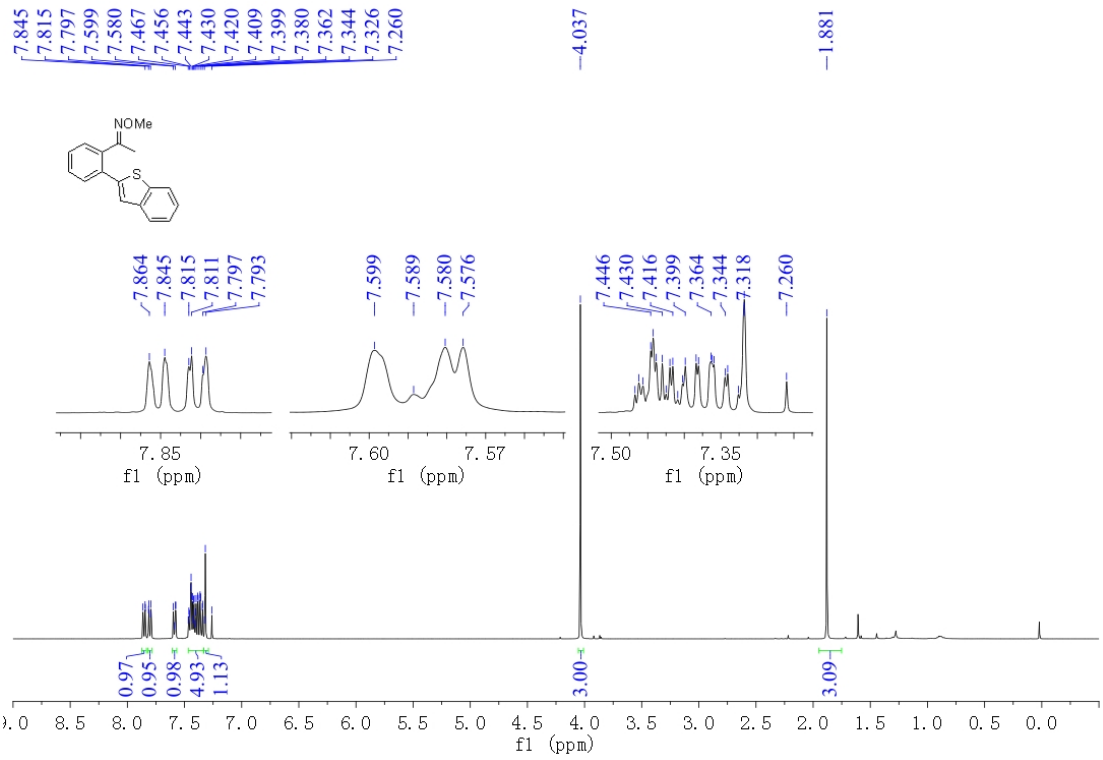

7.509
7.453
7.425
7.399
7.300
7.280
7.228
7.207
7.181
6.821
6.812
6.704
6.694
4.003
1.565
MeON
Ph
S
Br
7.523
7.518
7.512
7.509
7.506
7.503
7.429
7.425
7.418
7.415
7.411
7.399
7.391
7.388
7.300
7.296
7.290
7.285
7.280
7.260
7.223
7.217
7.212
7.207
7.203
7.193
7.189
7.181
7.55 7.50 7.45 7.40 7.35
f1 (ppm)
7.35 7.30 7.25 7.20 7.15
f1 (ppm)
0.95
2.80
1.82
2.87
0.90
0.93
3.00
f1 (ppm)

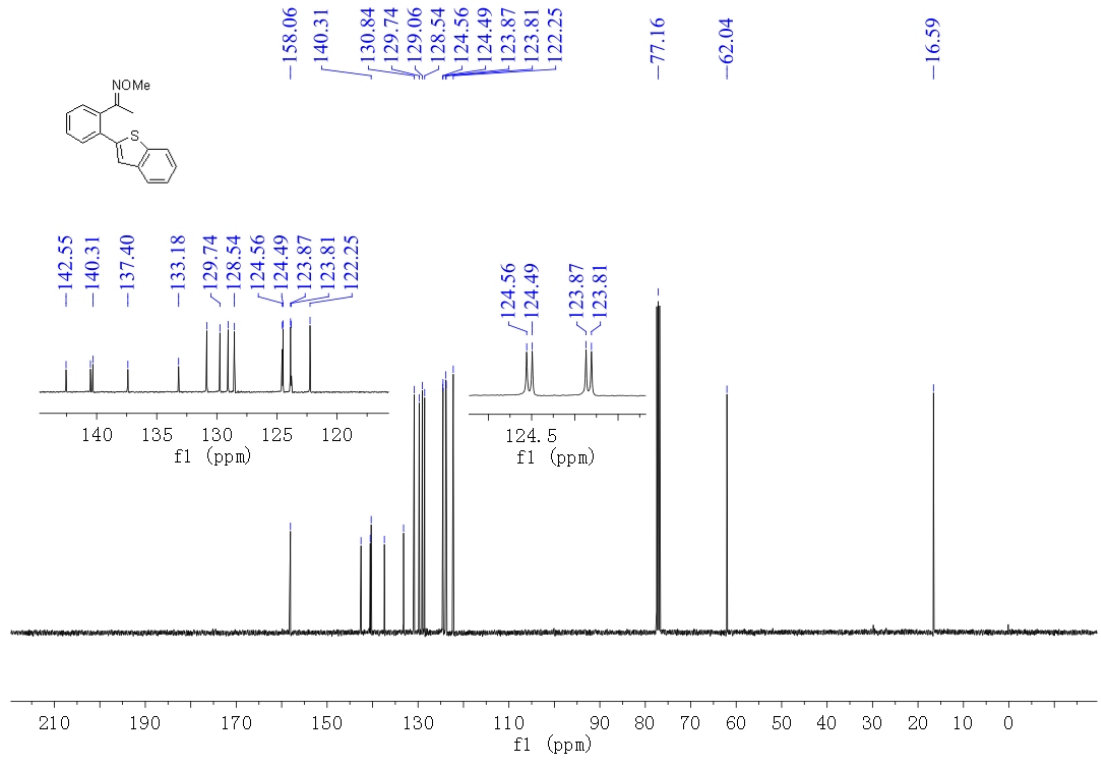

156.44
143.69
133.03
129.94
129.20
127.67
112.48
77.16
62.63
MeON
Ph
S
Br
131.06
130.54
129.94
129.79
129.26
129.20
128.31
127.70
127.67
130.0 128.5
f1 (ppm)
f1 (ppm)

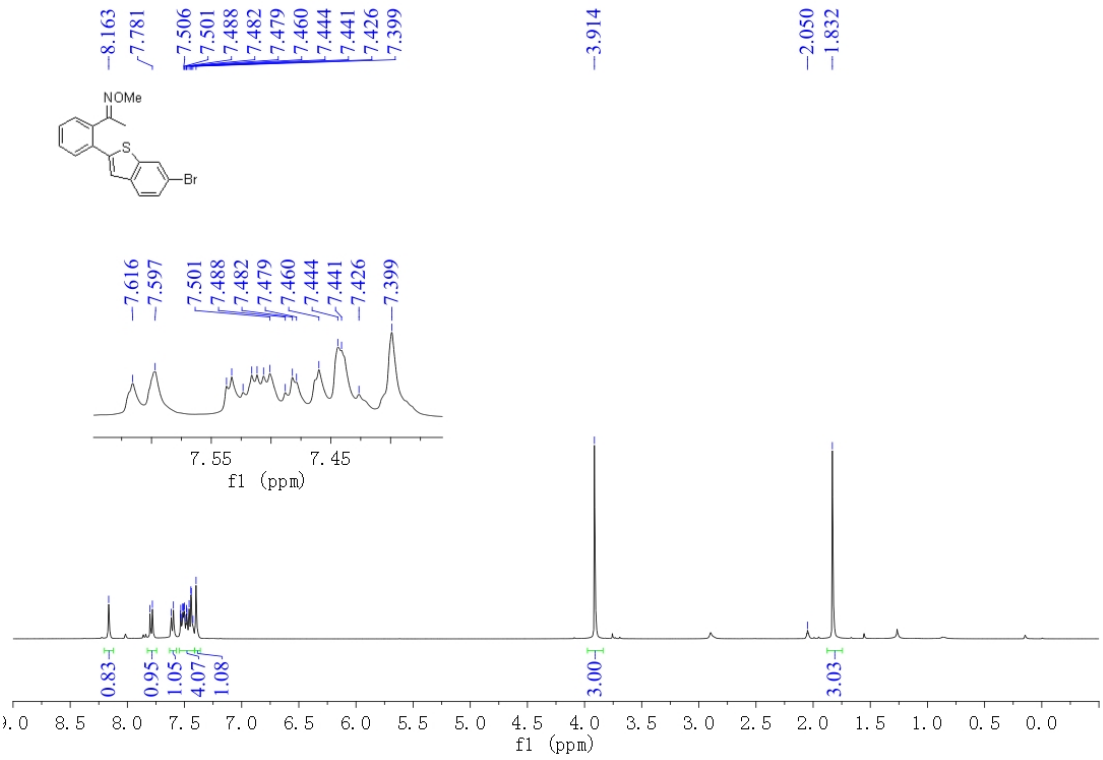

8.143
8.049
8.044
8.029
8.025
7.735
7.474
7.260
7.096
7.086
4.393
4.375
4.357
4.340
3.991
3.935
1.823
1.405
1.387
1.369
NOMe
MeO2C
CO2Et
8.147
8.143
8.044
8.025
7.744
7.735
7.494
7.474
7.260
7.096
7.086
8.1
7.5
f1 (ppm)
0.95
0.99
0.99
1.00
0.96
2.00
2.99
3.00
2.90
3.09
f1 (ppm)

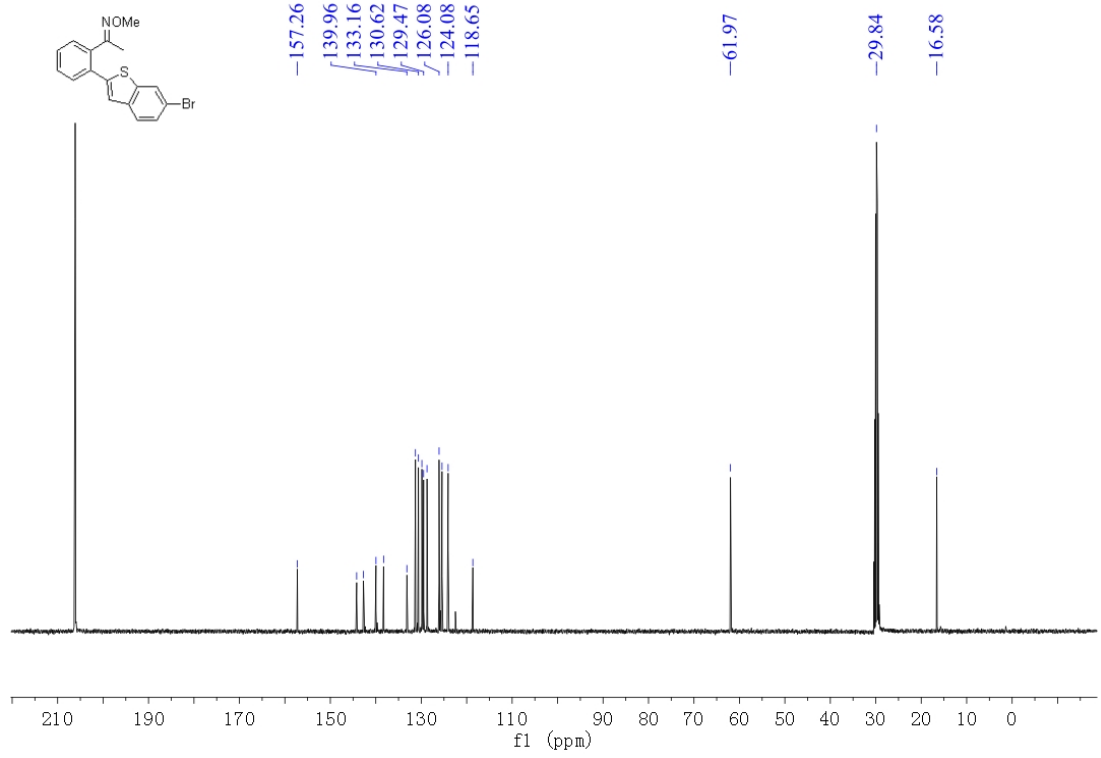

166.23
162.21
156.71
148.03
141.36
133.73
132.58
131.63
130.81
130.12
129.78
128.24
77.16
62.22
61.46
52.54
16.29
14.47
NOMe
MeO2C
CO2Et
f1 (ppm)

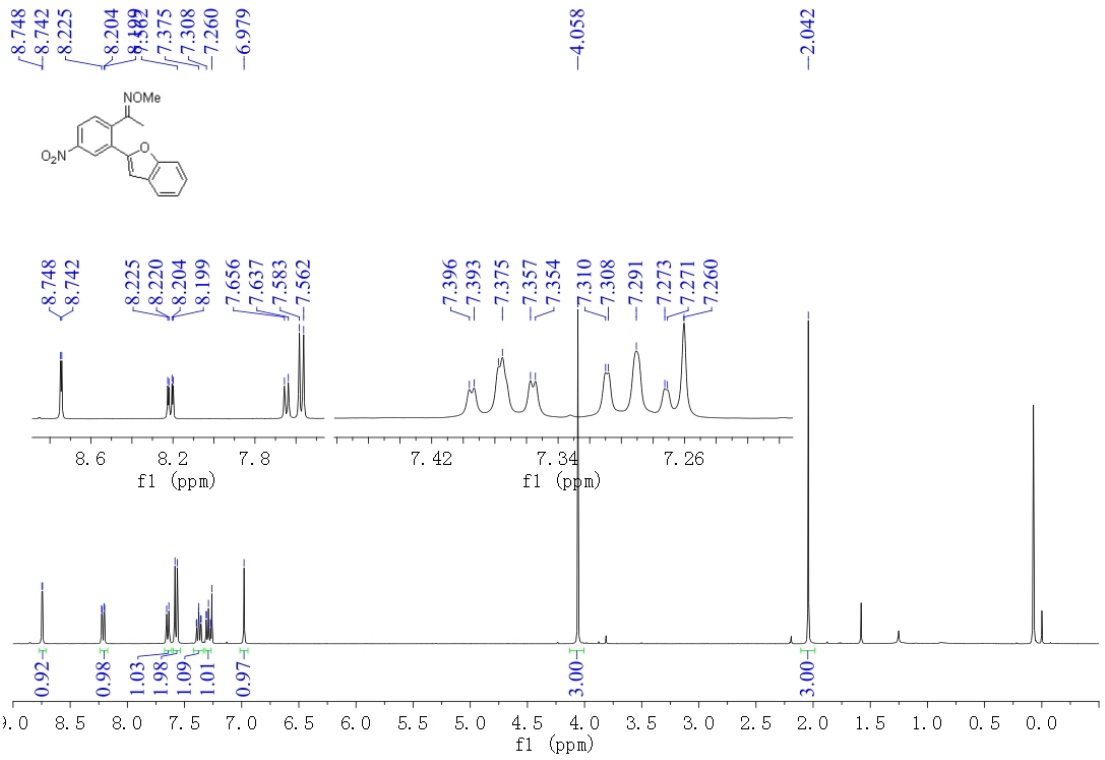

7.301
7.291
7.286
7.281
7.260
7.227
7.222
7.207
7.197
7.191
7.179
7.171
7.160
7.156
7.149
6.974
6.964
3.985
2.478
1.590
1.255
MeON
Ph
S
COCH3
7.550
7.537
7.515
7.469
7.459
7.441
7.432
7.286
7.281
7.260
7.197
7.179
7.160
7.156
7.55
7.40
7.25
f1 (ppm)
1.19
3.12
1.13
2.01
3.17
0.99
3.00
3.09
f1 (ppm)
190.73
156.12
151.02
144.17
131.29
130.03
129.36
129.31
128.98
128.46
127.71
77.16
62.67
29.84
26.78
H grease
129.5
128.5
127.5
f1 (ppm)
f1 (ppm)

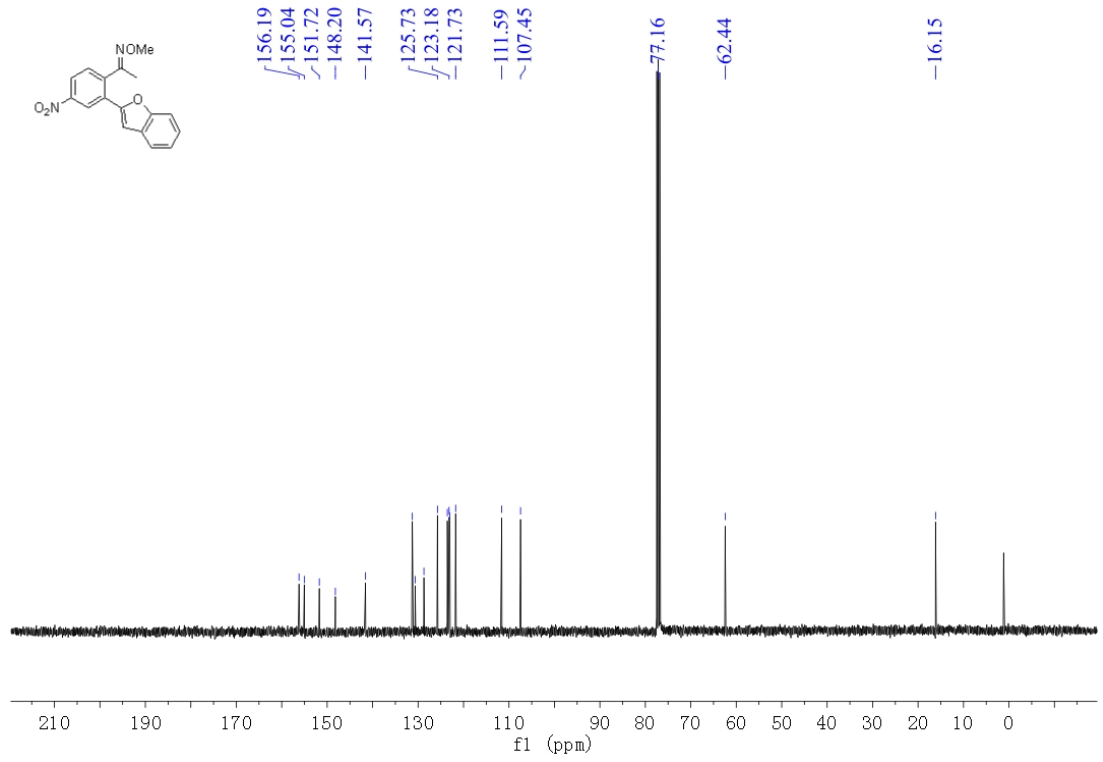

7.845
7.815
7.797
7.599
7.580
7.467
7.456
7.443
7.430
7.420
7.409
7.399
7.380
7.362
7.344
7.326
7.260
4.037
1.881
NOMe
S
7.85
f1 (ppm)
7.60
7.57
7.50
7.35
0.97
0.95
0.98
4.93
1.13
3.00
3.09
f1 (ppm)

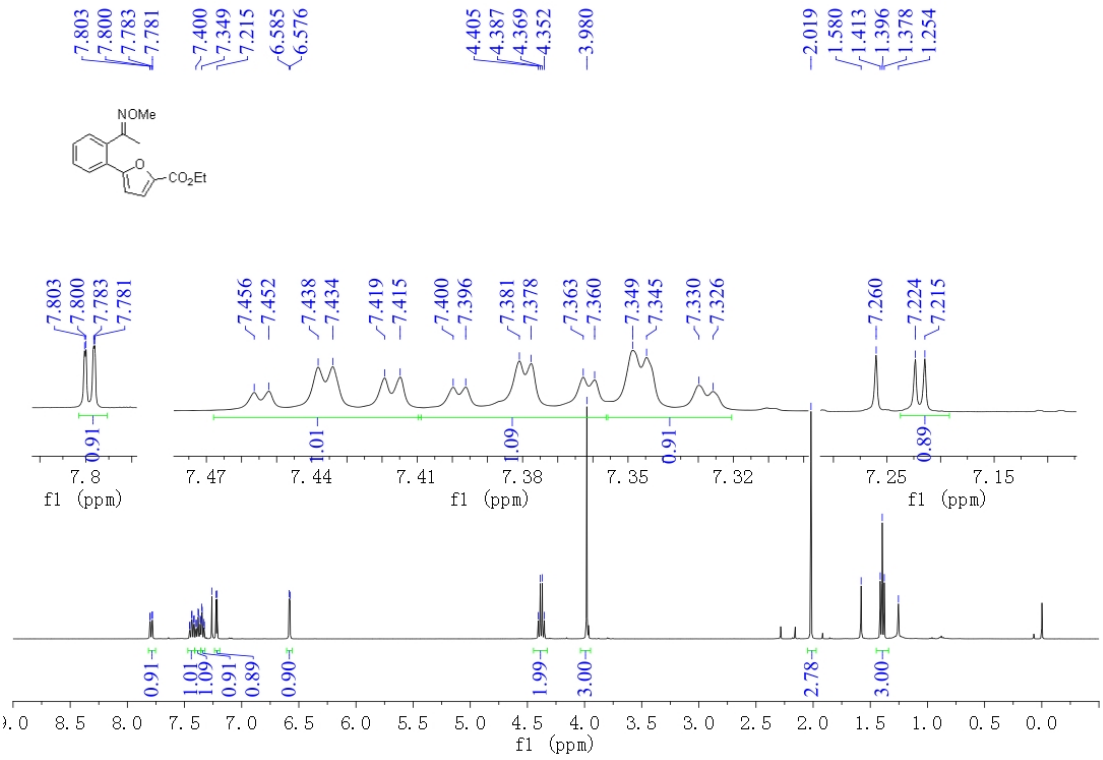

158.06
140.31
130.84
129.74
129.06
128.54
124.56
124.49
123.87
123.81
122.25
77.16
62.04
16.59
NOMe
S
142.55
140.31
137.40
133.18
129.74
128.54
124.56
124.49
123.87
123.81
122.25
140
135
130
125
120
f1 (ppm)
124.5
f1 (ppm)
f1 (ppm)

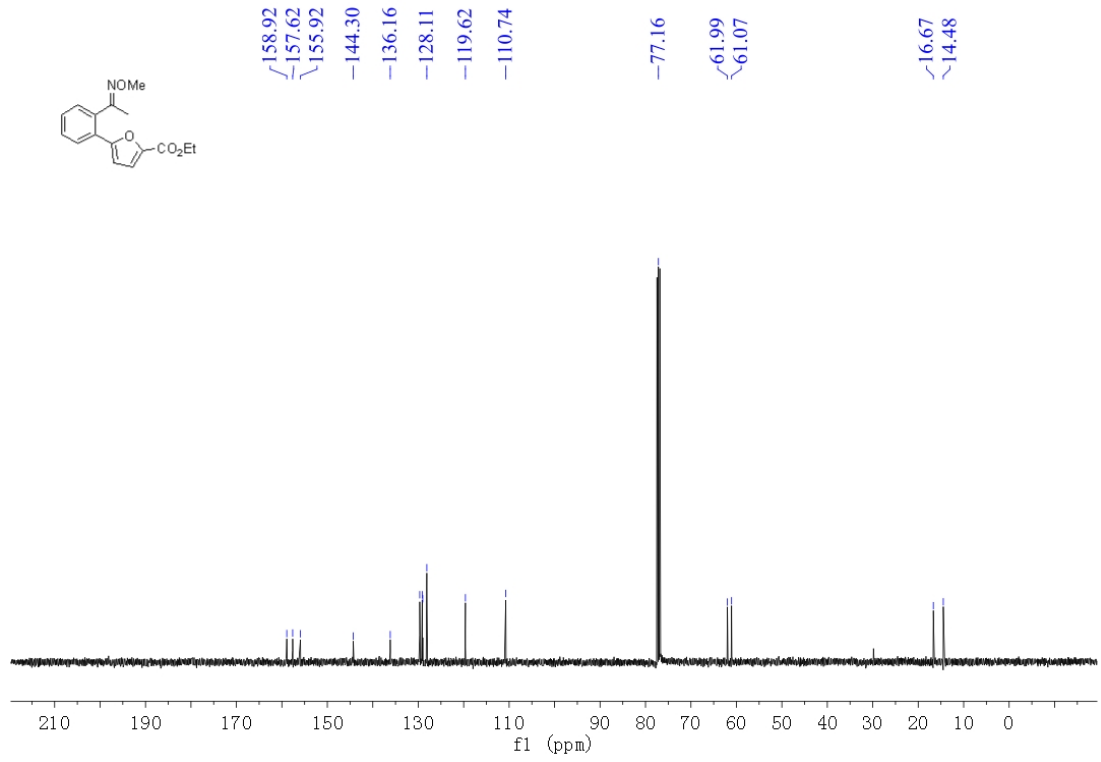

8.163
7.781
7.506
7.501
7.488
7.482
7.479
7.460
7.444
7.441
7.426
7.399
3.914
2.050
1.832
NOMe
S
Br
7.616
7.597
7.501
7.488
7.482
7.479
7.460
7.444
7.441
7.426
7.399
7.55
7.45
f1 (ppm)
0.83
0.95
1.05
4.07
1.08
3.00
3.03
f1 (ppm)


NOMe
S
Br
157.26
139.96
133.16
130.62
129.47
126.08
124.08
118.65
61.97
29.84
16.58
f1 (ppm)


8.748
8.742
8.225
8.204
7.375
7.308
7.260
6.979
4.058
2.042
NOMe
O2N
8.748
8.742
8.225
8.220
8.204
8.199
7.656
7.637
7.583
7.562
7.396
7.393
7.375
7.357
7.354
7.310
7.308
7.291
7.273
7.271
7.260
8.6
8.2
7.8
7.42
7.34
7.26
f1 (ppm)
0.92
0.98
1.03
1.98
1.09
1.01
0.97
3.00
3.00
f1 (ppm)


NOMe
O2N
156.19
155.04
151.72
148.20
141.57
125.73
123.18
121.73
111.59
107.45
77.16
62.44
16.15
f1 (ppm)


7.803
7.800
7.783
7.781
7.400
7.349
7.215
6.585
6.576
4.405
4.387
4.369
4.352
3.980
2.019
1.580
1.413
1.396
1.378
1.254
NOMe
CO2Et
f1 (ppm)


158.92
157.62
155.92
144.30
136.16
128.11
119.62
110.74
77.16
61.99
61.07
16.67
14.48
NOMe
CO2Et
f1 (ppm)