Supporting Information

The General Method for *E*-Selective Olefination of Acylsilanes with Isocyanides via Silver Catalysis

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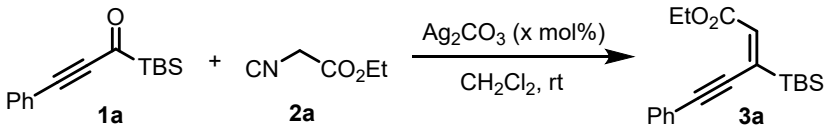
1. General information

Chemicals and analytical grade solvents were purchased from commercial suppliers and used without further purification unless otherwise stated. Flash column chromatography was performed on silica gels (200–300 mesh). General ^{1}H and ^{13}C NMR spectra were recorded on a Bruker 600 MHz NMR spectrometer. Chemical shifts were reported in ppm and the coupling constants *J* are given in Hz. Tetramethylsilane (TMS, δ = 0.00 ppm) or $CHCl_3$ (δ = 7.26 ppm) served as an internal standard for ^{1}H NMR; while $CDCl_3$ was used as an internal standard (δ = 77.0 ppm) for ^{13}C NMR. HRMS data were obtained on a Bruker Apex II mass instrument (ESI) or an Agilent Technologies 6540 UHD Accurate-Mass Q-TOF LC/MS (ESI). X-ray crystallography analysis was performed on PANalytical X'Pert PRO MPD system (PW3040/60).

Acylsilanes were prepared according to the literature procedure.[1-4] Isocyanides was purchased from commercial suppliers.

2. The reoptimization of the reaction conditions with acylsilanes

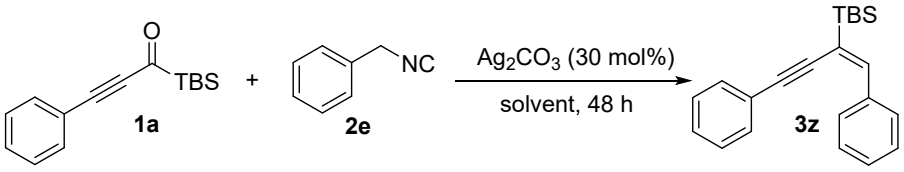
Table S1. Optimization of the reaction conditions for catalyst loading[a]



Entry	Ag_2CO_3 (x mol%)	**2a** (x equiv.)	Time (h)	Yield (%)[b]	*E*/*Z*[c]
1	30	1.2	48	82	17:1
2	15	1.5	72	71	-
3	15	2.0	72	76	-
4	15	3.0	72	80	17:1
5	10	3.0	72	76	17:1

[a]Reactions were performed with 0.20 mmol of alkynyl acylsilanes **1a**, isocyanoacetate **2a** (x equiv.) and Ag_2CO_3 (x mol%) in 2 mL CH_2Cl_2 at room temperature. [b]Isolated yield after purification by column chromatography. [c]Determined by ^{1}H NMR analysis of crude mixture.

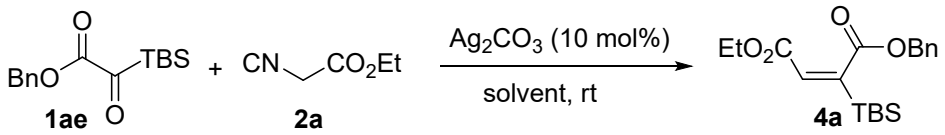
Table S2. Optimization of the reaction conditions for benzyl isonitrile[a]



Entry	Solvent	Temperature	Yield (%)[b]	*E*/*Z*[c]
1	CH_2Cl_2	rt	38	4:1
2	THF	rt	41	3:1
3	1,4-dioxane	rt	39	3:1
4	CH_3CN	rt	57	5:1
5	EtOAc	rt	45	4:1
6	DMSO	rt	53	4:1
7	CH_3CN	40 °C	54	6:1
8	CH_3CN[d]	40 °C	62	6:1

[a]Reactions were performed with 0.20 mmol of alkynyl acylsilanes **1**, 0.24 mmol of benzyl isonitrile **2e**, and 30 mol% of Ag_2CO_3 in 2 mL solvent at room temperature. [b]Isolated yield after purification by column chromatography. [c]Determined by ^{1}H NMR analysis of crude mixture. [d]1.5 eq. benzyl isonitrile was used.

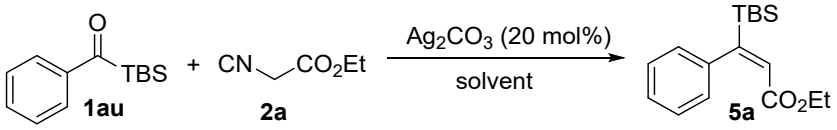
Table S3. Optimization of the reaction conditions for silylglyoxylates[a]



Entry	Solvent	Time (h)	Yield (%)[b]	*E*/*Z*[c]
1	CH_2Cl_2	7	38	10:1
2	THF	4	86	16:1
3	CH_3CN	12	49	10:1
4	acetone	9	77	13:1
5	CH_3OH	13	43	ND
6	DMF	15	34	12:1
7	THF[d]	3	87	16:1

[a]Reactions were performed with 0.20 mmol of silylglyoxylate **1ae**, 0.24 mmol of **2a**, and 10 mol% of Ag_2CO_3 in 2 mL solvent at room temperature. [b]Isolated yield after purification by column chromatography. [c]Determined by ^{1}H NMR analysis of crude mixture. [d]30 mol% of catalyst was used. ND = not determined.

Table S4. Optimization of the reaction conditions for unactive aroylsilane[a]

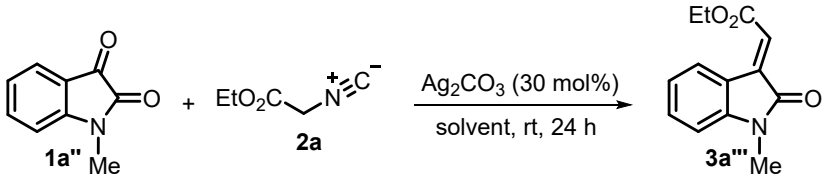


Entry	Solvent	temperature	Time (h)	Yield (%)[b]	*E*/*Z*[c]
1	THF[d]	rt	24	trace	ND
2	THF	rt	24	trace	ND
3	THF	80 °C	24	6	4:1
4	CH_3CN	80 °C	24	52	6:1
5	EtOAc	80 °C	24	trace	ND
6	DMF	80 °C	24	60	4:1
7	DCE	80 °C	24	45	4:1
8	DMSO	80 °C	24	58	4:1
9	DMSO	120 °C	23	64	4:1
10	DMSO[d]	140 °C	7	65	5:1
11	DMSO[e]	140 °C	10	61	5:1

[a]Reactions were performed with 0.20 mmol of aroylsilane **1au**, 0.24 mmol of **2a**, and 20 mol% of Ag_2CO_3 in 2 mL solvent at room temperature. [b]Isolated yield after purification by column chromatography. [c]Determined by ^{1}H NMR analysis of crude mixture. [d]10 mol% of catalyst was used. [e]5 mol% of catalyst was used. ND = not determined.

3. The optimization of the reaction conditions with 1-methylisatin

Table S5. Optimization of the reaction conditions with 1-methylisatin[a]



Entry	Solvent	Yield (%)[b]	*E*/*Z*[c]
1	CH_2Cl_2	17	-
2	CH_3CN	48	>20:1
3	toluene	20	-
4	DMSO	24	-
5	DCE	7	-
6	1,4-dioxane	21	-
7	DMF	25	-
8	DMAc	66	>20:1
9	THF	55	>20:1

[a]Reactions were performed with 0.20 mmol of **1a''**, 0.24 mmol of **2a**, and 30 mol% of Ag_2CO_3 in 2 mL solvent at room temperature. [b]Isolated yield after purification by column chromatography. [c]Determined by ^{1}H NMR analysis of crude mixture.

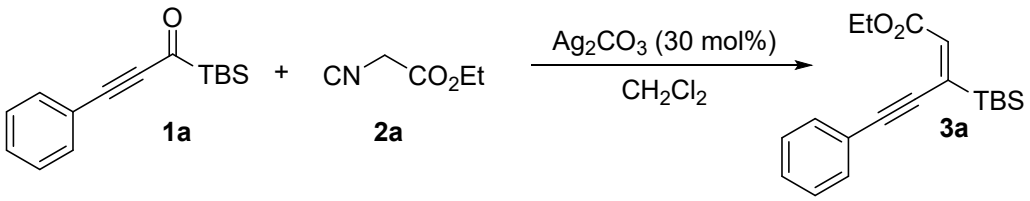
Representative procedure for silver-catalyzed olefination reaction of 1-methylisatin with ethyl isocyanoacetate

The mixture of isatin **1a''** (32.2 mg, 0.2 mmol), ethyl isocyanoacetate **2a** (27.1 mg, 0.24 mmol), 30 mol% of Ag_2CO_3 in solvent (2 mL) was stirred at room temperature for 24 h. After the reaction was finished, the mixture was purified by silica gel column chromatography (PE/EA = 4:1) to afford the desired product **3a'''**.

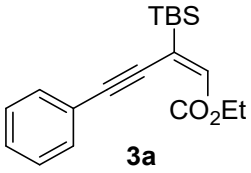
3a''': Ethyl (*E*)-2-(1-methyl-2-oxoindolin-3-ylidene)acetate; isolated by column chromatography (EtOAc/petroleum ether = 1:5); bright orange soild, m.p. 91–92 ºC; (30.5 mg, 66% yield); ^{1}H NMR (600 MHz, $CDCl_3$): δ 8.54 (d, *J* = 7.8 Hz, 1H), 7.34–7.37 (m, 1H), 7.05 (d, *J* = 15.6 Hz, 1H), 6.89 (s, 1H), 6.78 (d, *J* = 7.8 Hz, 1H), 4.31 (q, *J* = 7.2 Hz, 2H), 3.21 (s, 3H), 1.36 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (150 MHz,

$CDCl_3$): δ 167.5, 165.6, 145.9, 137.8, 132.4, 128.7, 122.8, 122.4, 119.8, 108.1, 61.1, 26.2, 14.1; The data are consistent with previous report.[5]

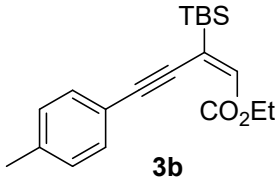
4. Representative procedure for silver-catalyzed olefination reaction of alkynyl acylsilanes with ethyl isocyanoacetate



Alkynyl acylsilane **1a** (48.8 mg, 0.20 mmol) and ethyl isocyanoacetate **2a** (27.1 mg, 0.24 mmol) were dissolved in CH_2Cl_2 (2 mL). Then Ag_2CO_3 (16.5 mg, 0.06 mmol) was added at room temperature. After stirring for 48 h, the reaction mixture was extracted with EtOAc, the combined organic phases were washed with brine, dried over anhydrous Na_2SO_4, filtered, and concentrated. The residue was purified by flash chromatography to afford the product **3a** (51.5 mg, 82% yield).

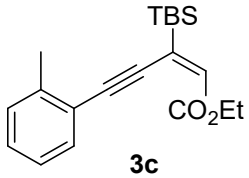


3a: (*E*)-2-(*tert*-butyldimethylsilyl)-4-phenylbut-1-en-3-yn-1-yl propionate; isolated by column chromatography (EtOAc/petroleum ether = 1:30); colorless oil; (51.5 mg, 82% yield); ^{1}H NMR (600 MHz, $CDCl_3$): δ 7.50–7.49 (m, 2H), 7.34–7.33 (m, 3H), 6.29 (s, 1H), 4.26 (dd, 14.4 Hz, *J* =7.2, 2H), 1.34 (t, *J* =7.2 Hz, 3H), 1.00 (s, 9H), 0.26 (s, 6H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 164.3, 141.2, 131.7, 128.7, 128.3, 123.7, 108.0, 89.9, 60.3, 26.6, 17.5, 14.3, -6.4; HRMS (ESI) m/z calcd for $[C_{19}H_{26}OSi + Na]^+$ 337.1600, found 337.1605.



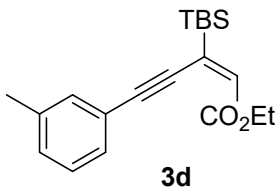
3b

3b: (*E*)-2-(*tert*-butyldimethylsilyl)-4-(*p*-tolyl)but-1-en-3-yn-1-yl propionate; isolated by column chromatography (EtOAc/petroleum ether = 1:30); colorless oil; (54.4 mg, 83% yield); ^{1}H NMR (600 MHz, $CDCl_3$): δ 7.39 (d, *J* = 7.8 Hz, 2H), 7.14 (d, *J* = 7.8 Hz, 2H), 6.27 (s, 1H), 4.26 (dd, 14.4, *J* = 7.2 Hz, 2H), 2.36 (s, 3H), 1.34 (t, *J* = 6.6 Hz, 3H), 0.99 (s, 9H), 0.25 (s, 6H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 164.3, 141.4, 139.1, 133.8, 131.7, 129.1, 120.6, 108.6, 89.5, 60.3, 26.6, 21.6, 17.5, 14.4, -6.4; HRMS (ESI) m/z calcd for $[C_{20}H_{28}O_2Si + Na]^+$ 351.1756, found 351.1758.



3c

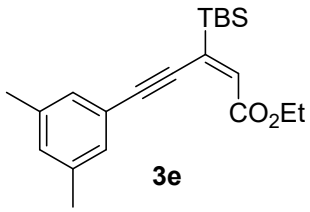
3c: (*E*)-2-(*tert*-butyldimethylsilyl)-4-(*o*-tolyl)but-1-en-3-yn-1-yl propionate; isolated by column chromatography (EtOAc/petroleum ether = 1:30); colorless oil; (51.8 mg, 79% yield); ^{1}H NMR (600 MHz, $CDCl_3$): δ 7.50 (d, *J* = 7.2 Hz, 1H), 7.28–7.23 (m, 2H), 7.18–7.16 (m, 1H), 6.32 (s, 1H), 4.28 (dd, 14.4, *J* =7.2 Hz, 2H), 2.55 (s, 3H), 1.34 (t, *J* = 7.2 Hz, 3H), 1.02 (s, 9H), 0.29 (s, 6H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 164.2, 141.0, 140.5, 134.2, 132.5, 128.8, 125.5, 123.5, 106.9, 93.5, 60.3, 26.7, 20.8, 17.5, 14.4, -6.3; HRMS (ESI) m/z calcd for $[C_{20}H_{28}O_2Si + Na]^+$ 351.1756, found 351.1758.



3d

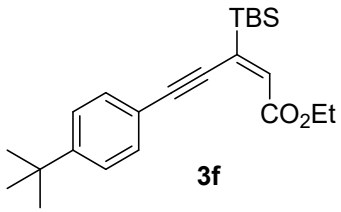
3d: (*E*)-2-(*tert*-butyldimethylsilyl)-4-(*m*-tolyl)but-1-en-3-yn-1-yl propionate; isolated by column chromatography (EtOAc/petroleum ether = 1:30); colorless oil; (52.4 mg, 80% yield); ^{1}H NMR(600 MHz, $CDCl_3$): δ 7.12 (s, 2H), 6.97 (s, 1H), 6.28 (s, 1H), 4.27

(dd, J =14.4, 7.2 Hz, 2H), 2.30 (s, 6H), 1.34 (t, J = 7.2 Hz, 3H), 0.99 (s, 9H), 0.26 (s, 6H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 164.3, 141.5, 137.9, 134.0, 130.7, 129.3, 123.3, 108.8, 89.2, 60.3, 26.6, 21.1, 17.5, 14.3, -6.4; HRMS (ESI) m/z calcd for $[C_{20}H_{28}O_2Si + Na]^+$ 351.1756, found 351.1754.



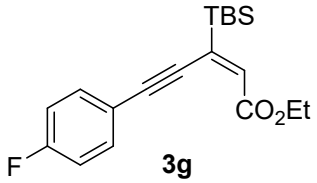
3e

3e: ethyl (*E*)-3-(*tert*-butyldimethylsilyl)-5-(3,5-dimethylphenyl)pent-2-en-4-ynoate; isolated by column chromatography (EtOAc/petroleum ether = 1:30); colorless oil; (52.6 mg, 77% yield); ^{1}H NMR (600 MHz, $CDCl_3$): δ 7.12 (s, 2H), 6.97 (s, 1H), 6.28 (s, 1H), 4.27 (dd, J =14.4, 7.2 Hz, 2H), 2.30 (s, 6H), 1.34 (t, J = 7.2 Hz, 3H), 0.99 (s, 9H), 0.26 (s, 6H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 164.3, 141.5, 137.9, 134.0, 130.7, 129.3, 123.3, 108.8, 89.2, 60.3, 26.6, 21.1, 17.5, 14.3, -6.4; HRMS (ESI) m/z calcd for $[C_{21}H_{30}O_2Si + Na]^+$ 365.1913, found 365.1907.



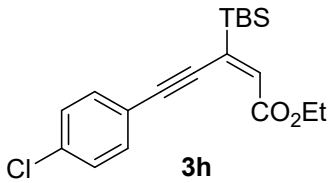
3f

3f: ethyl (*E*)-5-(4-(*tert*-butyl)phenyl)-3-(*tert*-butyldimethylsilyl)pent-2-en-4-ynoate; isolated by column chromatography (EtOAc/petroleum ether = 1:30); colorless oil; (65.1 mg, 88% yield); ^{1}H NMR (600 MHz, $CDCl_3$): δ 7.45–7.43 (m, 2H), 7.37–7.35 (m, 2H), 6.27 (s, 1H), 4.27 (dd, J =14.4, 7.2 Hz, 2H), 1.35 (t, J = 7.2 Hz, 3H), 1.31 (s, 9H), 0.26 (s, 6H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 164.3, 152.1, 141.3, 133.8, 131.4, 125.3, 120.7, 108.5, 89.4, 60.2, 34.8, 31.1, 26.6, 17.4, 14.3, -6.4; HRMS (ESI) m/z calcd for $[C_{23}H_{34}O_2Si + Na]^+$ 393.2226, found393.2220.



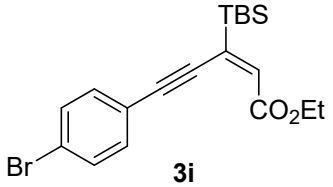
3g

3g: ethyl (*E*)-3-(*tert*-butyldimethylsilyl)-5-(4-fluorophenyl)pent-2-en-4-ynoate;isolated by column chromatography (EtOAc/petroleum ether = 1:30); colorless oil; (54.4 mg, 82% yield); ^{1}H NMR (600 MHz, $CDCl_3$): δ 7.49–7.45 (m, 2H), 7.40–7.00 (m, 2H), 6.29 (s, 1H), 4.25 (dd, *J* =13.8, 6.6 Hz, 2H), 1.33 (t, *J* = 6.6 Hz, 3H), 0.98 (s, 9H), 0.25 (s, 6H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 164.2, 162.8 ($J_{C\text{-}F}$ = 249.0 Hz), 141.0, 134.4, 133.7 ($J_{C\text{-}F}$ = 7.5 Hz), 119.8 ($J_{C\text{-}F}$ = 3.0 Hz), 115.6 ($J_{C\text{-}F}$ = 22.5 Hz), 106.8, 89.7, 60.3, 26.6, 17.4, 14.3, -6.4; HRMS (ESI) m/z calcd for $[C_{19}H_{25}FO_2Si + Na]^+$ 355.1506, found 355.1499.



3h

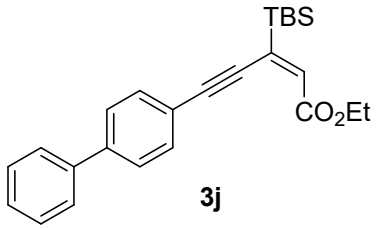
3h: ethyl (*E*)-3-(*tert*-butyldimethylsilyl)-5-(4-chlorophenyl)pent-2-en-4-ynoate; isolated by column chromatography (EtOAc/petroleum ether = 1:30); colorless oil; (61.1 mg, 88% yield); ^{1}H NMR(600 MHz, $CDCl_3$): δ 7.42–7.41 (m, 2H), 7.31–7.30 (m, 2H), 6.30 (s, 1H), 4.26 (dd, *J* =14.4, 7.2 Hz, 2H), 1.33 (t, *J* = 7.2 Hz, 3H), 0.98 (s, 9H), 0.25 (s, 6H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 164.2, 140.8, 134.8, 132.8, 128.7, 122.1, 106.5, 90.8, 60.4, 26.6, 17.5, 14.3, -6.4; HRMS (ESI) m/z calcd for $[C_{19}H_{25}ClO_2Si + Na]^+$371.1210, found 371.1215.



3i

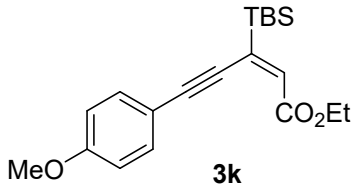
3i: ethyl (*E*)-5-(4-bromophenyl)-3-(*tert*-butyldimethylsilyl)pent-2-en-4-ynoate; isolated by column chromatography (EtOAc/petroleum ether = 1:30); colorless oil;

(63.5 mg, 81% yield); ^{1}H NMR (600 MHz, $CDCl_3$): δ 7.47–7.46 (m, 2H), 7.35–7.34 (m, 2H), 6.31 (s, 1H), 4.25 (dd, *J* =13.8, 6.6 Hz, 2H), 1.33 (t, *J* = 7.2 Hz, 3H), 0.98 (s, 9H), 0.25 (s, 6H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 164.2, 140.8, 134.8, 133.0, 131.6, 123.1, 120.6, 106.6, 90.9, 60.4, 26.6, 17.5, 14.3, -6.4; HRMS (ESI) m/z calcd for $[C_{19}H_{25}BrO_2Si + Na]^+$ 415.0705, found 415.0696.



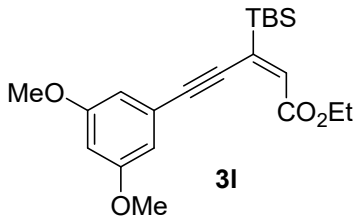
3j

3j: ethyl (*E*)-5-([1,1'-biphenyl]-4-yl)-3-(*tert*-butyldimethylsilyl)pent-2-en-4-ynoate; isolated by column chromatography (EtOAc/petroleum ether = 1:30); colorless oil; (63.2 mg, 82% yield); ^{1}H NMR (600 MHz, $CDCl_3$): δ 7.61–7.58 (m, 6H), 7.46–7.44 (m, 2H), 6.31 (s, 1H), 4.29 (dd, *J* =14.4, 7.2 Hz, 2H), 1.36 (t, *J* = 7.2 Hz, 2H), 1.02 (s, 9H), 0.28 (s, 6H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 164.3, 141.5, 141.2, 140.3, 134.2, 132.1, 128.8, 127.7, 127.0, 122.6, 108.0, 90.6, 60.3, 26.6, 17.5, 14.4, -6.4; HRMS (ESI) m/z calcd for $[C_{25}H_{30}O_2Si + Na]^+$ 413.1913, found 413.1912.



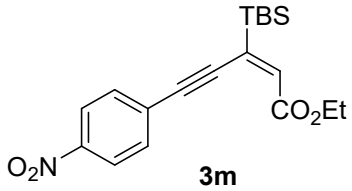
3k

3k: ethyl (*E*)-3-(*tert*-butyldimethylsilyl)-5-(4-methoxyphenyl)pent-2-en-4-ynoate; isolated by column chromatography (EtOAc/petroleum ether = 1:30); colorless oil; (53.6 mg, 78% yield); ^{1}H NMR (600 MHz, $CDCl_3$): δ 7.45–7.44 (m, 2H), 6.86–6.84 (m, 2H), 6.24 (s, 1H), 4.25 (dd, *J* =14.4, 7.2 Hz, 2H), 3.79 (s, 3H), 1.33 (t, *J* = 7.2 Hz, 3H), 0.98 (s, 9H), 0.24 (s, 6H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 164.3, 160.1, 141.5, 133.4, 133.1, 115.8, 114.0, 108.7, 89.2, 60.1, 55.2, 26.6, 17.4, 14.3, -6.4; HRMS (ESI) m/z calcd for $[C_{20}H_{28}O_3Si + Na]^+$ 367.1705, found 367.1698.



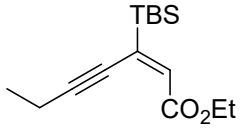
3l

3l: ethyl (*E*)-3-(*tert*-butyldimethylsilyl)-5-(3,5-dimethoxyphenyl)pent-2-en-4-ynoate;isolated by column chromatography (EtOAc/petroleum ether = 1:30); colorless oil; (53.1 mg, 71% yield); ^{1}H NMR (600 MHz, $CDCl_3$): δ 6.64 (d, *J* = 2.4 Hz, 1H), 6.46 (t, *J* = 2.4 Hz, 1H), 6.29 (s, 1H), 4.26 (dd, *J* =14.4, 7.2 Hz, 2H), 3.79 (s, 6H), 1.34 (t, *J* = 7.2 Hz, 3H), 0.99 (s, 9H), 0.25 (s, 6H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 164.2, 160.5, 141.7, 134.5, 125.0, 109.4, 108.0, 102.0, 89.3, 60.4, 55.4, 26.6, 17.5, 14.3, -6.4; HRMS (ESI) m/z calcd for $[C_{21}H_{30}O_4Si + Na]^+$ 397.1811, found 397.1803.



3m

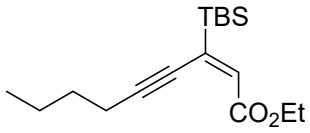
3m: ethyl (*E*)-3-(*tert*-butyldimethylsilyl)-5-(4-nitrophenyl)pent-2-en-4-ynoate;isolated by column chromatography (EtOAc/petroleum ether = 1:30); colorless oil; (50.2 mg, 70% yield); ^{1}H NMR (600 MHz, $CDCl_3$): δ 8.20 (d, *J* = 9 Hz, 2H), 7.61 (d, *J* = 9 Hz, 2H), 6.38 (s, 1H), 4.26 (dd, *J* =14.4, 7.2 Hz, 2H), 1.33 (t, *J* = 7.2 Hz, 3H), 0.99 (s, 9H), 0.26 (s, 6H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 164.0, 147.2, 140.0, 136.4, 132.1, 130.4, 123.6, 104.7, 94.5, 60.6, 26.5, 17.5, 14.3, -6.4; HRMS (ESI) m/z calcd for $[C_{19}H_{25}NO_4Si + Na]^+$ 382.1451, found 382.1450.



3n

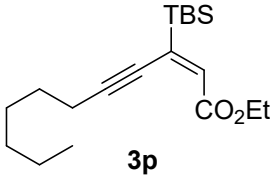
3n: ethyl (*E*)-3-(*tert*-butyldimethylsilyl)hept-2-en-4-ynoate;isolated by column chromatography (EtOAc/petroleum ether = 1:30); colorless oil; (44.1 mg, 83% yield);

^{1}H NMR (600 MHz, $CDCl_3$): δ 7.18 (s, 1H), 4.19 (dd, *J* =14.4, 7.2 Hz, 2H), 2.50 (dd, *J* = 15, 7.2 Hz, 2H), 1.28 (t, *J* = 7.2 Hz, 3H), 1.19 (t, *J* = 7.8 Hz, 3H), 0.91 (s, 9H), 0.15 (s, 6H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 164.2, 143.0, 133.5, 112.3, 80.5, 60.0, 26.6, 17.2, 14.2, 14.1 13.6, -6.5; HRMS (ESI) m/z calcd for $[C_{15}H_{26}O_2Si + Na]^+$ 289.1600, found 289.1602.



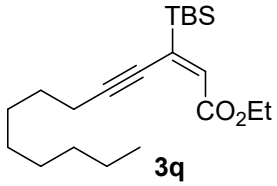
3o

3o: ethyl (*E*)-3-(*tert*-butyldimethylsilyl)non-2-en-4-ynoate;isolated by column chromatography (EtOAc/petroleum ether = 1:30); colorless oil; (52.3 mg, 89% yield); ^{1}H NMR (600 MHz, $CDCl_3$): δ 6.20 (s, 1H), 4.21 (dd, *J* =14.4, 7.2 Hz, 2H), 2.5 (t, *J* = 6.6 Hz, 2H), 1.61–1.55 (m, 3H), 1.47–1.41 (m, 2H), 1.3 (t, *J* = 7.2 Hz, 3H), 0.91 (t, *J* = 7.2 Hz, 3H), 0.93 (s, 9H), 0.17 (s, 6H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 164.3, 143.0, 133.7, 111.2, 81.0, 60.1, 30.7, 26.6, 20.3, 17.3, 14.3, 13.6, -6.4; HRMS (ESI) m/z calcd for $[C_{17}H_{30}O_2Si + Na]^+$ 317.1913, found 317.1907.



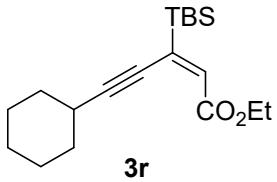
3p

3p: ethyl (*E*)-3-(*tert*-butyldimethylsilyl)undec-2-en-4-ynoate;isolated by column chromatography (EtOAc/petroleum ether = 1:30); colorless oil; (52.3 mg, 82% yield); ^{1}H NMR (600 MHz, $CDCl_3$): δ 6.18 (s, 1H), 4.19 (dd, *J* =14.4, 7.2 Hz, 2H), 1.58–1.54 (m, 2H), 1.43–1.38 (m, 2H), 1.31–1.25 (m, 7H), 0.92 (s, 9H), 0.86 (t, *J* = 6.6 Hz, 3H), 0.15 (s, 6H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 164.2, 142.9, 133.6, 111.1, 81.0, 60.0, 31.3, 26.6, 20.5, 17.2, 14.2, 14.0, -6.5; HRMS (ESI) m/z calcd for $[C_{19}H_{34}O_2Si + Na]^+$ 345.2226, found 345.2231.



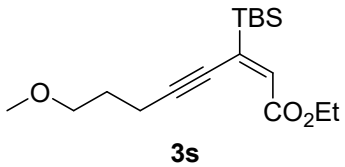
3q

3q: ethyl (*E*)-3-(*tert*-butyldimethylsilyl)tridec-2-en-4-ynoate;isolated by column chromatography (EtOAc/petroleum ether = 1:30); colorless oil; (54.6 mg, 78% yield); ^{1}H NMR (600 MHz, $CDCl_3$): δ 6.18 (s, 1H), 4.18 (dd, *J* =14.4, 7.2 Hz, 2H), 2.47 (t, *J* = 6.6 Hz, 2H), 1.58–1.53 (m, 2H), 1.42–1.37 (m, 2H), 1.29–1.24 (m, 11H), 0.91 (s, 9H) 0.85 (t, *J* = 6.6 Hz, 3H), 0.15 (s, 6H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 164.2, 142.8, 133.6, 111.1, 81.0, 60.0, 31.8, 29.1, 29.0, 28.6, 26.6, 22.6, 20.5, 17.2, 14.2, 14.0, -6.5; HRMS (ESI) m/z calcd for $[C_{21}H_{38}O_2Si + Na]^+$ 373.2539, found 373.2537.



3r

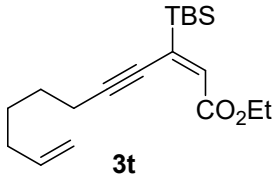
3r: ethyl (*E*)-3-(*tert*-butyldimethylsilyl)-5-cyclohexylpent-2-en-4-ynoate; isolated by column chromatography (EtOAc/petroleum ether = 1:30; colorless oil; (58.2 mg, 91% yield); ^{1}H NMR (600 MHz, $CDCl_3$): δ 6.19 (s, 1H), 4.21 (dd, *J* = 13.8, 6.6 Hz, 2H), 1.89–1.87 (m, 2H), 1.74–1.71 (m, 2H), 1.55–1.49 (m, 2H), 1.32–1.29 (m, 6H), 0.94 (s, 9H), 0.17 (s, 6H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 164.3, 142.8, 133.5, 115.1, 81.0, 32.5, 30.8, 26.6, 25.9, 25.0, 17.3, 14.3, -6.4; HRMS (ESI) m/z calcd for $[C_{19}H_{32}O_2Si + Na]^+$ 343.2069, found 343.2063.



3s

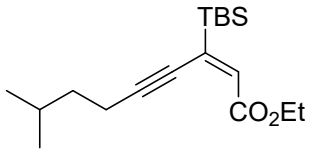
3s: ethyl (*E*)-3-(*tert*-butyldimethylsilyl)-7-methoxyhept-2-en-4-ynoate;isolated by column chromatography (EtOAc/petroleum ether = 1:30); colorless oil; (41.4 mg, 70% yield); ^{1}H NMR (600 MHz, $CDCl_3$): δ 6.21 (s, 1H), 4.21 (dd, *J* = 13.8, 7.2 Hz, 2H), 3.49 (t, *J* = 6.6 Hz, 2H), 3.33 (s, 3H), 2.59 (t, *J* = 7.2 Hz, 2H), 1.87–1.82 (m, 2H), 1.30

(t, *J* = 7.2 Hz, 3H), 10.93 (s, 9H), 0.17 (s, 6H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 164.2, 142.7, 134.0, 110.0, 81.3, 60.1, 58.6, 28.7, 26.6, 17.3, 14.3, -6.4; HRMS (ESI) m/z calcd for $[C_{16}H_{28}O_3Si + Na]^+$ 319.1705, found 319.1710.



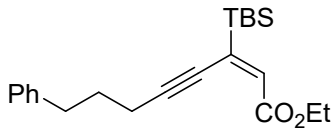
3t

3t: ethyl (*E*)-3-(*tert*-butyldimethylsilyl)undeca-2,10-dien-4-ynoate;isolated by column chromatography (EtOAc/petroleum ether = 1:30); colorless oil; (54.4 mg, 85% yield); ^{1}H NMR (600 MHz, $CDCl_3$): δ 6.17 (s, 1H), 5.79–5.77 (m, 2H), 4.98–4.94 (m, 1H), 4.91–4.89 (m, 1H), 4.17 (dd, *J* =14.4, 7.2 Hz, 2H), 2.48 (t, *J* = 6.6 Hz, 2H), 2.05–2.01 (m, 2H), 1.59–1.54 (m, 2H), 1.53–1.47 (m, 2H), 1.26 (t, *J* = 7.2 Hz, 3H), 0.90 (s, 9H), 0.13 (s, 6H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 164.1, 142.6, 138.4, 133.7, 114.4, 110.6, 81.1, 59.9, 33.1, 28.1, 28.0, 26.5, 20.3, 17.2, 14.2, -6.6; HRMS (ESI) m/z calcd for $[C_{19}H_{32}O_2Si + Na]^+$ 343.2069, found 343.2067.



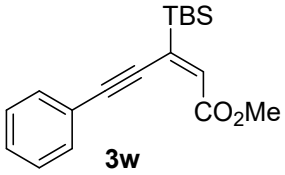
3u

3u: ethyl(*E*)-3-(*tert*-butyldimethylsilyl)-8-methylnon-2-en-4-ynoate; isolated by column chromatography (EtOAc/petroleum ether = 1:30); colorless oil; (51.7 mg, 84% yield); ^{1}H NMR (600 MHz, $CDCl_3$): δ 6.20 (s, 1H), 4.21 (dd, *J* =14.4, 7.2 Hz, 2H), 2.51 (t, *J* = 7.2 Hz, 2H), 1.73–1.69 (m, 1H), 1.48 (dd, *J* = 7.2, 14.4 Hz, 2H), 1.30 (t, *J* = 7.2 Hz, 3H), 0.93 (s, 9H), 0.90 (s, 9H), 0.89 (s, 9H), 0.17 (s, 6H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 164.3, 143.0, 133.7, 111.2, 81.0, 60.1, 37.5, 27.3, 26.6, 22.1, 17.3, 14.3, -6.5; HRMS (ESI) m/z calcd for $[C_{18}H_{32}O_2Si + Na]^+$ 331.2069, found 331.2065.



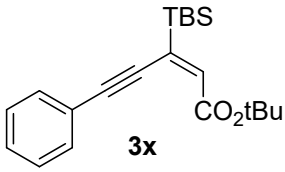
3v

3v: ethyl (*E*)-3-(tert-butyldimethylsilyl)-8-phenyloct-2-en-4-ynoate;isolated by column chromatography (EtOAc/petroleum ether = 1:30); colorless oil; (56.9 mg, 80% yield); ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.27–7.24 (m, 2H), 7.19–7.16 (m, 3H), 6.21 (s, 1H), 4.20 (dd, *J* =14.4, 7.2 Hz, 2H), 2.75 (t, *J* = 7.2 Hz, 2H), 2.52 (t, *J* = 6.6 Hz, 2H), 1.91–1.86 (m, 2H), 1.28 (t, *J* = 7.2 Hz, 3H), 0.93 (s, 9H), 0.18 (s, 6H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 164.2, 142.7, 141.7, 134.0, 128.5, 128.3, 125.9, 110.3, 81.5, 60.1, 35.0, 30.4, 26.6, 20.1, 17.3, 14.3, -6.4; HRMS (ESI) m/z calcd for $[C_{22}H_{32}O_2Si + Na]^+$ 379.2069, found 379.2061.



3w

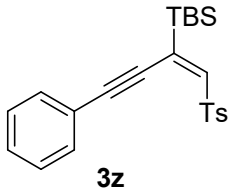
3w: methyl (*E*)-3-(*tert*-butyldimethylsilyl)-5-phenylpent-2-en-4-ynoate; isolated by column chromatography (EtOAc/petroleum ether = 1:100); colorless oil; (41.9 mg, 71% yield); ^{1}H NMR (600 MHz, $CDCl_3$): δ 7.51–7.49 (m, 2H), 7.34–7.33 (m, 3H), 6.30 (s, 1H), 3.80 (s, 3H), 0.99 (s, 9H), 0.25 (s, 6H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 164.6, 141.6, 133.8, 131.7, 128.3, 123.6, 108.2, 89.8, 51.4, 45.9, 26.6, 17.4, -6.4; HRMS (ESI) m/z calcd for $[C_{18}H_{24}O_2Si + Na]^+$ 323.1443, found 323.1443.



3x

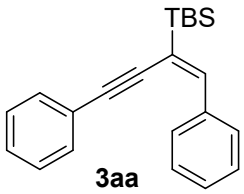
3x: *tert*-butyl (*E*)-3-(*tert*-butyldimethylsilyl)-5-phenylpent-2-en-4-ynoate; isolated by column chromatography (EtOAc/petroleum ether = 1:100); colorless oil; (36.1 mg, 54% yield); ^{1}H NMR (600 MHz, $CDCl_3$): δ 7.51–7.47 (m, 2H), 7.34–7.32 (m, 3H), 6.20 (s, 1H), 1.54 (s, 9H), 0.99 (s, 9H), 0.25 (s, 6H); ^{13}C NMR (150 MHz, $CDCl_3$): δ

163.6, 139.0, 136.5, 131.5, 128.3, 123.9, 107.2, 89.9, 80.6, 28.3, 26.7, 17.5, -6.3; HRMS (ESI) m/z calcd for $[C_{21}H_{30}O_2Si + Na]^+$ 365.1913, found 365.1918.



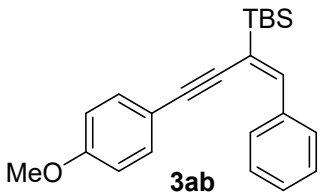
3z

3z: (*E*)-*tert*-butyl(1,4-diphenylbut-1-en-3-yn-2-yl)dimethylsilane; isolated by column chromatography (EtOAc/petroleum ether = 1:100); colorless oil; (52 mg, 68% yield);^{1}H NMR (600 MHz, $CDCl_3$): δ7.69 (d, *J* = 7.9 Hz, 2H), 7.24 (d, *J* = 7.9 Hz, 2H), 7.16 (s, 2H), 7.06 (d, *J* = 7.9 Hz, 2H), 7.04 (s, 1H), 6.56 (s, 1H), 2.18 (s, 3H), 0.68 (s, 9H), -0.00 (s, 6H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 144.4, 143.2, 140.1, 138.4, 131.9, 129.7, 129.5, 128.6, 128.2, 123.0, 111.7, 86.6, 26.6, 21.8, 17.8, -6.4; HRMS (ESI) m/z calcd for $[C_{23}H_{28}O_2SSi + Na]^+$ 419.1471, found 419.1483.



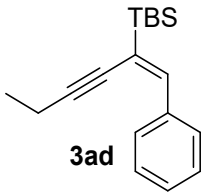
3aa

3aa: (*E*)-*tert*-butyl(1,4-diphenylbut-1-en-3-yn-2-yl)dimethylsilane; isolated by column chromatography (EtOAc/petroleum ether = 1:100); colorless oil; (39.4 mg, 62% yield);^{1}H NMR (600 MHz, $CDCl_3$): δ 8.12–8.10 (m, 2H), 7.55–7.53 (m, 2H), 7.48–7.45 (m, 2H), 7.43–7.37 (m, 4H), 6.96 (s, 1H), 1.11 (s, 9H), 0.38 (s, 6H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 145.7, 137.8, 131.1, 128.9, 128.5, 128.4, 128.2, 127.9, 124.4, 121.3, 101.1, 91.4, 26.8, 17.8, -6.2; HRMS (ESI) m/z calcd for $[C_{22}H_{26}Si + H]^+$ 319.1882, found 319.1884.



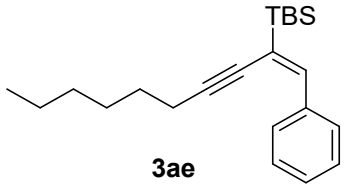
3ab

3ab: (*E*)-*tert*-butyl(4-(4-methoxyphenyl)-1-phenylbut-1-en-3-yn-2-yl)dimethylsilane; isolated by column chromatography (EtOAc/petroleum ether = 1:100); colorless oil; (27.4 mg, 39% yield); ^{1}H NMR (600 MHz, $CDCl_3$): δ 8.04–8.03 (m, 2H), 7.41–7.38 (m, 4H), 7.31–7.29 (m, 1H), 6.89–6.83 (m, 2H), 6.83 (s, 1H), 3.83 (s, 3H), 1.03 (s, 9H), 0.29 (s, 6H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 159.5, 144.8, 137.9, 132.6, 128.8, 128.3, 128.2, 121.6, 116.7, 114.0, 101.2, 90.2, 55.3, 26.8, 17.8, -6.2; HRMS (ESI) m/z calcd for $[C_{23}H_{28}OSi + H]^+$ 349.1988, found 349.1982.



3ad

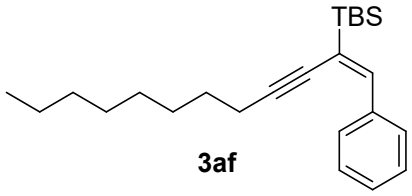
3ad: (*E*)-*tert*-butyldimethyl(1-phenylhex-1-en-3-yn-2-yl)silane; isolated by column chromatography (EtOAc/petroleum ether = 1:100); colorless oil; (25.9 mg, 48% yield); ^{1}H NMR (600 MHz, $CDCl_3$): δ 7.89–7.87 (m, 2H), 7.27–7.25 (m, 2H), 7.19–7.16 (m, 1H), 6.56 (s, 1H), 1.15 (t, *J* = 15.6 Hz, 3H), 0.88 (s, 9H), 0.13 (s, 6H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 144.4, 137.9, 128.6, 128.1, 122.6, 104.3, 81.6, 26.8, 17.7, 14.0, 13.9, -6.3; HRMS (ESI) m/z calcd for $[C_{18}H_{26}Si + Na]^+$ 293.1701, found 293.1697.



3ae

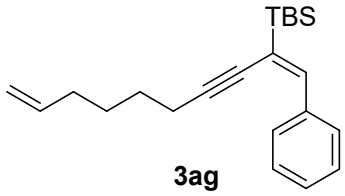
3ae: (*E*)-*tert*-butyldimethyl(1-phenyldec-1-en-3-yn-2-yl)silane; isolated by column chromatography (EtOAc/petroleum ether = 1:100); colorless oil; (36.5 mg, 56% yield); ^{1}H NMR (600 MHz, $CDCl_3$): δ 8.00–7.99 (m, 2H), 7.38–7.35 (m, 2H), 7.30–7.27 (m, 1H), 6.77 (s, 1H), 2.50 (t, *J* = 7.2 Hz, 3H), 1.65–1.60 (m, 2H), 1.52–1.47 (m, 2H), 1.38–1.32 (m, 4H), 1.00 (s, 9H), 0.94 (t, *J* = 6.6 Hz, 3H), 0.25 (s, 6H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 144.5, 137.9, 128.6, 128.1, 128.0, 122.6, 103.2, 82.1, 31.5, 28.81,

28.76, 26.8, 22.6, 20.3, 17.7, 14.1, -6.2; HRMS (ESI) m/z calcd for $[C_{22}H_{34}Si + H]^+$ 327.2508, found 327.2506.



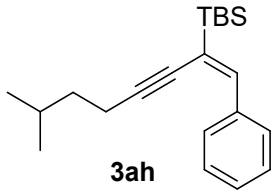
3af

3af: (*E*)-*tert*-butyldimethyl(1-phenyldodec-1-en-3-yn-2-yl)silane; isolated by column chromatography (EtOAc/petroleum ether = 1:100); colorless oil; (34.7 mg, 49% yield); ^{1}H NMR (600 MHz, $CDCl_3$): δ 7.97–7.96 (m, 2H), 7.35–7.33 (m, 2H), 7.29–7.27 (m, 1H), 6.73 (s, 1H), 2.47 (t, *J* = 7.2 Hz, 3H), 1.62–1.55 (m, 2H), 1.47–1.43 (m, 2H), 1.31–1.28 (m, 7H), 0.96 (s, 9H), 0.89 (t, *J* = 6.6 Hz, 3H), 0.21 (s, 6H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 144.5, 137.9, 128.6, 128.1, 128.0, 122.7, 103.2, 82.0, 31.9, 29.3, 29.2, 29.1, 28.8, 26.8, 22.7, 20.3, 17.7, 14.1, -6.2; HRMS (ESI) m/z calcd for $[C_{24}H_{38}Si+ H]^+$ 355.2821, found 355.2814.



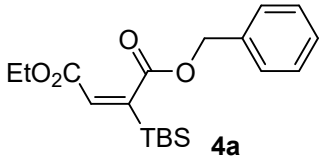
3ag

3ag: (*E*)-*tert*-butyldimethyl(1-phenyldeca-1,9-dien-3-yn-2-yl)silane; isolated by column chromatography (EtOAc/petroleum ether = 1:100); colorless oil; (35.6 mg, 55% yield); ^{1}H NMR (600 MHz, $CDCl_3$): δ 7.89–7.87 (m, 2H), 7.27–7.25 (m, 2H), 7.19–7.17 (m, 1H), 6.66 (s, 1H), 5.77–5.71 (m, 1H), 4.96–4.93 (m, 1H), 4.89–4.88 (m, 1H), 2.42–2.40 (m, 2H), 2.04–2.00 (m, 2H), 1.54–1.47 (m, 4H), 0.89 (s, 9H), 0.13 (s, 6H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 144.6, 138.6, 128.5, 128.1, 122.6, 114.6, 102.8, 82.2, 33.3, 28.3, 28.2, 26.8, 20.1, 17.7, -6.2; HRMS (ESI) m/z calcd for $[C_{22}H_{32}Si + H]^+$ 325.2352, found 325.2348.



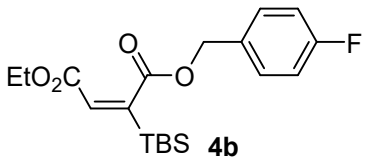
3ah

3ah: (*E*)-*tert*-butyldimethyl(7-methyl-1-phenyloct-1-en-3-yn-2-yl)silane; isolated by column chromatography (EtOAc/petroleum ether = 1:100); colorless oil; (37.4 mg, 60% yield); ^{1}H NMR (600 MHz, $CDCl_3$): δ 8.04–8.02 (m, 2H), 7.42–7.39 (m, 2H), 7.34–7.31 (m, 1H), 6.80 (s, 1H), 2.55 (t, *J* = 7.2 Hz, 2H), 1.88–1.81 (m, 1H), 1.58–1.54 (m, 2H), 1.03 (s, 9H), 1.00 (s, 3H), 0.99 (s, 3H), 0.28 (s, 6H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 144.5, 137.9, 128.6, 128.1, 122.6, 103.1, 82.0, 37.7, 27.2, 26.8, 22.2, 18.3, 17.7, -6.2; HRMS (ESI) m/z calcd for $[C_{21}H_{32}Si + H]^+$ 313.2352, found 313.2353.



4a

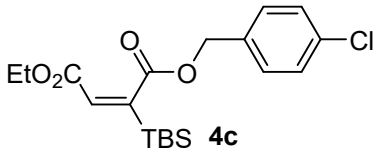
4a: 1-benzyl 4-ethyl 2-(*tert*-butyldimethylsilyl)maleate; isolated by column chromatography (EtOAc/petroleum ether = 1:30); colorless oil; (59.1 mg, 86% yield); ^{1}H NMR (600 MHz, $CDCl_3$): δ 7.41–7.38 (m, 2H), 7.37–7.30 (m, 3H), 6.10 (s, 1H), 5.24 (s, 2H), 4.16 (dd, *J* =14.4, 7.2 Hz, 2H), 1.26 (t, *J* = 7.2 Hz, 3H), 0.91 (s, 9H), 0.13 (s, 6H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 170.7, 163.7, 153.3, 135.5, 130.7, 128.8, 128.4, 128.2, 66.8, 60.9, 26.3, 17.3, 14.0, -6.4; HRMS (ESI) m/z calcd for $[C_{19}H_{28}O_4Si + Na]^+$ 371.1655, found 371.1646.



4b

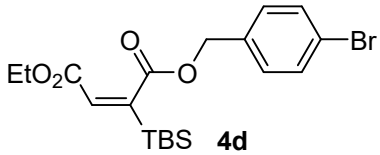
4b: 4-ethyl 1-(4-fluorobenzyl) 2-(*tert*-butyldimethylsilyl)maleate;isolated by column chromatography (EtOAc/petroleum ether = 1:30); colorless oil; (66.6 mg, 91% yield); ^{1}H NMR (600 MHz, $CDCl_3$): δ 7.39–7.37 (m, 2H), 7.05–7.02 (m, 2H), 6.09 (s, 1H),

5.20 (s, 2H), 4.16 (dd, J =14.4, 7.2 Hz, 2H), 1.26 (t, J = 7.2 Hz, 3H), 0.90 (s, 9H), 0.11 (s, 6H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 170.7, 163.8, 162.7 ($J_{C\text{-}F}$ = 246.0 Hz), 153.3, 131.5 ($J_{C\text{-}F}$ = 3.0 Hz), 130.9, 130.8 ($J_{C\text{-}F}$ = 4.5 Hz), 115.3 ($J_{C\text{-}F}$ = 7.0 Hz), 66.0, 61.0, 26.3, 17.4, 14.1, -6.4; HRMS (ESI) m/z calcd for $[C_{19}H_{27}FO_2Si + Na]^+$ 389.1560, found 389.1562.



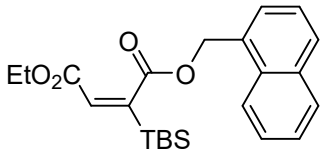
4c

4c: 1-(4-chlorobenzyl) 4-ethyl 2-(*tert*-butyldimethylsilyl)maleate; isolated by column chromatography (EtOAc/petroleum ether = 1:30); colorless oil; (67.2 mg, 88% yield); ^{1}H NMR (600 MHz, $CDCl_3$): δ 7.35–7.31 (m, 4H), 6.10 (s, 1H), 5.19 (s, 2H), 4.17 (dd, J =14.4, 7.2 Hz, 2H), 1.27 (t, J = 3 Hz, 3H), 0.91 (s, 9H), 0.12 (s, 6H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 170.7, 163.8, 153.3, 134.2, 134.1, 130.9, 130.2, 128.6, 66.0, 61.0, 26.3, 17.4, 14.1, -6.4; HRMS (ESI) m/z calcd for $[C_{19}H_{27}ClO_4Si + Na]^+$ 405.1265, found 405.1264.



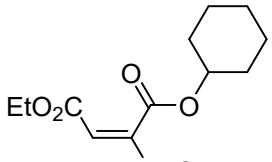
4d

4d: 1-(4-bromobenzyl) 4-ethyl 2-(*tert*-butyldimethylsilyl)maleate;isolated by column chromatography (EtOAc/petroleum ether = 1:30); colorless oil; (79.2 mg, 93% yield); ^{1}H NMR (600 MHz, $CDCl_3$): δ 7.34–7.31 (m, 4H), 6.09 (s, 1H), 5.19 (s, 2H), 4.16 (dd, J =14.4, 7.2 Hz, 2H), 1.26 (t, J = 7.2 Hz, 3H), 0.90 (s, 9H), 0.12 (s, 6H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 170.7, 163.8, 153.3, 134.2, 134.1, 130.9, 130.2, 128.6, 66.0, 61.0, 26.3, 17.4, 14.1, -6.4 ; HRMS (ESI) m/z calcd for $[C_{19}H_{27}BrO_4Si + Na]^+$ 449.0760, found 449.0764.



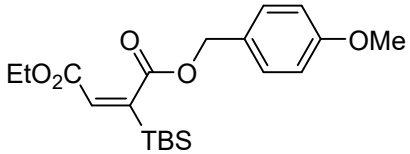
4e

4e: 4-ethyl 1-(naphthalen-1-ylmethyl) 2-(*tert*-butyldimethylsilyl)maleate; isolated by column chromatography (EtOAc/petroleum ether = 1:30); colorless oil; (62.1 mg, 78% yield); ^{1}H NMR (600 MHz, $CDCl_3$): δ 8.12 (d, *J* = 8.4 Hz, 1H), 7.88–7.84 (m, 2H), 7.59 (d, *J* = 6.6 Hz, 1H), 7.54–7.49 (m, 2H), 7.45 (t, *J* = 7.8 Hz, 1H), 6.08 (s, 1H), 5.69 (s, 2H), 4.15 (dd, *J* = 13.8, 4.2 Hz, 2H), 1.25 (t, *J* = 7.2 Hz, 3H), 0.86 (s, 9H), 0.08 (s, 6H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 170.9, 163.9, 153.5, 133.7, 130.8, 128.5, 128.0, 126.4, 125.9, 125.2, 124.1, 65.1, 61.0, 26.3, 17.4, 14.1, -6.4; HRMS (ESI) m/z calcd for $[C_{23}H_{30}O_4Si + Na]^+$ 421.1811, found 421.1804.



4f

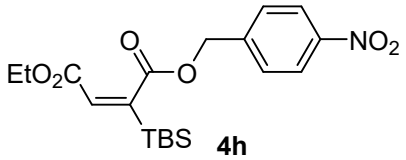
4f: 1-cyclohexyl 4-ethyl 2-(*tert*-butyldimethylsilyl)maleate; isolated by column chromatography (EtOAc/petroleum ether = 1:30); colorless oil; (47.6 mg, 70% yield); ^{1}H NMR (400 MHz, $CDCl_3$): δ 6.04 (s, 1H), 4.93–4.89 (m, 1H), 4.17 (d, *J* = 7.2 Hz, 2H), 1.97–1.94 (m, 2H), 1.75–1.71 (m, 2H), 1.56–1.49 (m, 2H), 1.47–1.40 (m, 2H), 1.39–1.33 (m, 2H), 1.27 (t, *J* = 7.2 Hz, 3H), 0.94 (s, 9H), 0.16 (s, 6H); ^{13}C NMR (101 MHz, $CDCl_3$): δ 170.3, 163.8, 153.9, 130.1, 73.4, 60.8, 31.6, 26.4, 25.4, 23.9, 17.4, 14.1, -6.3; HRMS (ESI) m/z calcd for $[C_{18}H_{32}O_4Si + Na]^+$ 363.1968, found 363.1966.



4g

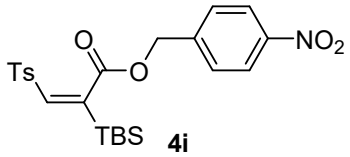
4g: 4-ethyl 1-(4-methoxybenzyl) 2-(*tert*-butyldimethylsilyl)maleate;isolated by column chromatography (EtOAc/petroleum ether = 1:30); colorless oil; (66.5 mg, 88% yield);

^{1}H NMR (600 MHz, $CDCl_3$): δ 7.33 (d, *J*=8.4 Hz, 2H), 6.87 (d, *J* = 9.0 Hz, 2H), 6.07 (s, 1H), 5.17 (s, 2H), 4.16 (dd, *J* =14.4, 7.2 Hz, 2H), 3.80 (s, 3H), 1.26 (t, *J* = 7.2 Hz, 3H), 0.90 (s, 9H), 0.12 (s, 6H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 170.8, 163.8, 159.6, 153.4, 130.59, 130.57, 127.7, 113.8, 66.6, 60.9, 55.2, 26.3, 17.4, 14.1, -6.4 ; HRMS (ESI) m/z calcd for $[C_{20}H_{30}O_5Si + Na]^+$ 401.1760, found 401.1760.



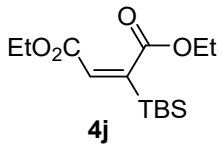
4h

4h: 4-ethyl 1-(4-nitrobenzyl) 2-(*tert*-butyldimethylsilyl)maleate; isolated by column chromatography (EtOAc/petroleum ether = 1:30); colorless oil; (63.6 mg, 81% yield); ^{1}H NMR (600 MHz, $CDCl_3$): δ 8.20 (d, *J* = 3 Hz, 2H), 7.57 (d, *J* = 8.4 Hz, 2H), 6.12 (s, 1H), 5.31 (s, 2H), 4.16 (dd, *J* =14.4, 7.2 Hz, 2H), 1.26 (t, *J* = 7.2 Hz, 3H), 0.91 (s, 9H), 0.14 (s, 6H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 170.6, 163.7, 153.1, 147.7, 142.9, 131.1, 129.0, 123.6, 65.2, 60.1, 26.3, 17.4, 14.0, -6.4; HRMS (ESI) m/z calcd for $[C_{19}H_{27}NO_6Si + Na]^+$ 416.1505, found 416.1498.



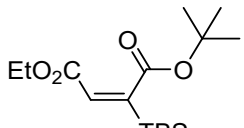
4i

4i: 4-nitrobenzyl (*E*)-2-(tert-butyldimethylsilyl)-3-tosylacrylate; isolated by column chromatography (EtOAc/petroleum ether = 1:30); colorless oil; (50 mg, 53% yield); ^{1}H NMR (600 MHz, $CDCl_3$): δ 8.24 (d, *J* = 8.0 Hz, 2H), 7.79 (d, *J* = 7.7 Hz, 2H), 7.64 (d, *J* = 8.1 Hz, 2H), 7.32 (d, *J* = 7.9 Hz, 2H), 6.39 (s, 1H), 3.84 (s, 2H), 2.44 (s, 3H), 0.86 (s, 9H), 0.12 (s, 6H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 168.6, 148.9, 148.0, 145.2, 142.5, 138.4, 136.6, 130.2, 129.5, 128.2, 123.9, 66.1, 26.4, 21.8, 17.9, -6.2; HRMS (ESI) m/z calcd for $[C_{23}H_{29}NO_6SSi + Na]^+$ 498.1377, found 498.1342.



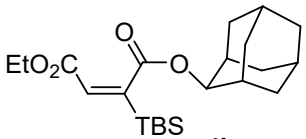
4j

4j: diethyl 2-(*tert*-butyldimethylsilyl)maleate; isolated by column chromatography (EtOAc/petroleum ether = 1:30); colorless oil; (48.5 mg, 82% yield); ^{1}H NMR (600 MHz, $CDCl_3$): δ 6.07 (s, 1H), 4.27 (dd, *J* = 7.2, 14.4 Hz, 2H), 4.18 (dd, *J* =14.4, 7.2 Hz, 2H), 1.31 (t, *J* = 6.6 Hz, 3H), 1.28 (t, *J* = 7.2 Hz, 3H), 0.94 (s, 9H), 0.16 (s, 6H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 170.9, 163.9, 153.8, 130.4, 60.9, 60.8, 26.4, 17.4, 14.11, 14.07, -6.4; HRMS (ESI) m/z calcd for $[C_{14}H_{26}O_4Si + Na]^+$ 309.1498, found 309.1503.



4k

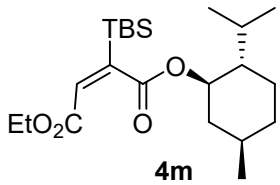
4k: 1-(*tert*-butyl) 4-ethyl 2-(*tert*-butyldimethylsilyl)maleate;isolated by column chromatography (EtOAc/petroleum ether = 1:30); colorless oil; (30.8 mg, 72% yield); ^{1}H NMR (600 MHz, $CDCl_3$): δ 6.00 (s, 1H), 4.20 (dd, *J* =14.4, 7.2 Hz, 2H), 1.53 (s, 9H), 1.28 (t, *J* = 7.2 Hz, 3H), 0.95 (s, 9H), 0.17 (s, 6H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 169.7, 163.9, 154.2, 129.6, 81.8, 60.7, 28.2, 26.5, 17.5, 14.2, -6.2; HRMS (ESI) m/z calcd for $[C_{16}H_{30}O_4Si + Na]^+$ 337.1811, found 337.1803.



4l

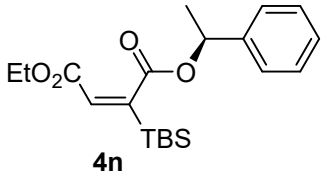
4l: 1-(adamantan-2-yl) 4-ethyl 2-(*tert*-butyldimethylsilyl)maleate; isolated by column chromatography (EtOAc/petroleum ether = 1:30); colorless oil; (39.2 mg, 50% yield); ^{1}H NMR (600 MHz, $CDCl_3$): δ 6.05 (s, 1H), 5.11–5.10 (m, 1H), 4.15 (dd, *J* =14.4, 7.2 Hz, 2H), 2.07 (s, 2H), 1.99 (d, *J* = 12.6 Hz, 2H), 1.85–1.79 (m, 6H), 1.71 (s, 2H), 1.25 (d, *J* = 12 Hz, 2H), 1.99 (t, *J* = 6.6 Hz, 3H), 0.94 (s, 9H), 0.16 (s, 6H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 170.2, 163.7, 153.9, 130.0, 60.7, 37.4, 36.4, 31.71, 31.69, 27.2, 27.0,

26.4, 17.4, 14.1, -6.3; HRMS (ESI) m/z calcd for $[C_{22}H_{36}O_4Si + Na]^+$ 415.2281, found 415.2272.



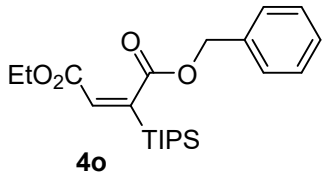
4m

4m: 4-ethyl 1-((1*R*,2*S*,6*R*)-2-isopropyl-6-methylcyclohexyl) 2-(*tert*-butyldimethylsilyl)maleate;isolated by column chromatography (EtOAc/petroleum ether = 1:30); colorless oil; (44.1 mg, 56% yield); ^{1}H NMR (600 MHz, $CDCl_3$): δ 6.04 (s, 1H), 4.78–4.73 (m, 1H), 4.16 (dd, *J* =14.4, 7.2 Hz, 2H), 2.27–2.25 (m, 1H), 2.03–1.98 (m, 1H), 1.68–1.65 (m, 2H), 1.51–1.44 (m, 1H), 1.38–1.33 (m, 1H), 1.25 (t, *J* = 7.2 Hz, 3H), 1.08–1.01 (m, 1H), 1.08–1.01 (m, 1H), 0.93–0.76 (m, 17H), 0.93 (s, 9H), 0.89 (d, *J* = 6.6 Hz, 3H), 0.85 (d, *J* = 7.2 Hz, 3H), 0.76 (d, *J* = 7.2 Hz, 3H), 0.14 (d, *J* = 3.6 Hz, 6H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 169.3, 162.7, 152.3, 129.6, 59.7, 46.1, 39.5, 33.3, 30.4, 25.5, 21.1, 20.0, 16.5, 14.9, 13.2, -7.1, -7.2; HRMS (ESI) m/z calcd for $[C_{22}H_{40}O_4Si + Na]^+$ 419.2594, found 419.2588.



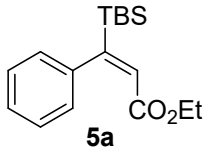
4n

4n: (*S*)-4-ethyl-1-(1-phenylethyl)-2-(*tert*-butyldimethylsilyl)maleate; isolated by column chromatography (EtOAc/petroleum ether = 1:30); colorless oil; (44.2 mg, 61% yield); ^{1}H NMR (600 MHz, $CDCl_3$): δ 7.38–7.37 (m, 2H), 7.34–7.29 (m, 2H), 7.25–7.23 (m, 1H), 6.07–6.03 (m, 1H), 4.12–4.07 (m, 1H), 4.06–4.00 (m, 1H), 1.60 (d, *J* = 6.6 Hz, 3H), 1.17 (t, *J* = 7.2 Hz, 3H), 0.87 (s, 9H), 0.08 (s, 3H), 0.06 (s, 3H) ; ^{13}C NMR (150 MHz, $CDCl_3$): δ 169.9, 163.7, 153.2, 141.0, 130.6, 128.2, 127.8, 126.7, 72.8, 60.8, 26.3, 21.5, 17.3, 14.0, -6.3, -6.4; HRMS (ESI) m/z calcd for $[C_{20}H_{30}O_4Si + Na]^+$ 385.1811, found385.1812.



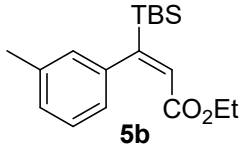
4o

4o: 1-benzyl 4-ethyl 2-(triisopropylsilyl)maleate; isolated by column chromatography (EtOAc/petroleum ether = 1:30); colorless oil; (60.8 mg, 78% yield); ^{1}H NMR (600 MHz, $CDCl_3$): δ 7.37–7.35 (m, 5H), 6.12 (s, 1H), 5.22 (s, 2H), 4.19 (dd, *J* =14.4, 7.2 Hz, 2H), 1.31–1.26 (m, 6H), 1.06 (d, *J* = 7.8 Hz, 18H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 164.7, 164.0, 150.5, 134.8, 128.64, 128.61, 106.2, 67.8, 60.0, 18.3, 18.0, 17.7, 14.3, 13.7; HRMS (ESI) m/z calcd for $[C_{22}H_{34}O_4Si + Na]^+$ 413.2124, found 413.2125.



5a

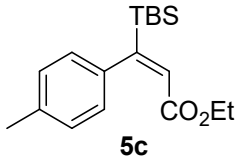
5a: ethyl (*E*)-3-(*tert*-butyldimethylsilyl)-3-phenylacrylate; isolated by column chromatography (EtOAc/petroleum ether = 1:30); colorless oil; (37.7 mg, 65% yield); ^{1}H NMR (600 MHz, $CDCl_3$): δ 7.29–7.28 (m, 2H), 7.23–7.20 (m, 1H), 7.06–7.05 (m, 2H), 6.38 (s, 1H), 4.20 (dd, *J* =14.4, 7.2 Hz, 2H), 1.31 (t, *J* = 7.2 Hz, 3H), 0.95 (s, 9H), 0.11 (s, 6H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 166.6, 161.6, 146.4, 135.1, 127.8, 126.9, 126.3, 60.3, 28.1, 18.7, 14.3, -2.8 ; HRMS (ESI) m/z calcd for $[C_{17}H_{26}O_2Si + Na]^+$ 313.1600, found 313.1594.



5b

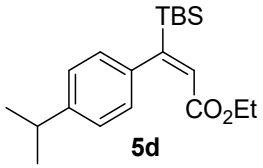
5b: ethyl (*E*)-3-(*tert*-butyldimethylsilyl)-3-(m-tolyl)acrylate; isolated by column chromatography (EtOAc/petroleum ether = 1:30); colorless oil; (38.3 mg, 63% yield); ^{1}H NMR (600 MHz, $CDCl_3$): δ 7.17 (t, *J* = 7.2 Hz, 1H), 7.01 (d, *J* = 7.2 Hz, 1H), 6.79–6.78 (m, 2H), 7.25 (s, 1H), 3.96 (dd, *J* =14.4, 7.2 Hz, 2H), 2.33 (s, 3H), 1.01 (t, *J* = 7.2 Hz, 3H), 0.84 (s, 9H), 0.14 (s, 6H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 165.4, 161.1,

142.3, 137.0, 127.5, 126.8, 126.7, 123.3, 59.8, 26.9, 21.5, 17.5, 13.8, -5.7; HRMS (ESI) m/z calcd for $[C_{18}H_{28}O_2Si + Na]^+$ 327.1756, found 327.1749.



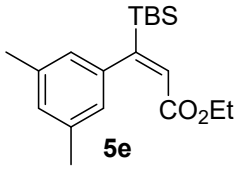
5c

5c: ethyl (*E*)-3-(*tert*-butyldimethylsilyl)-3-(p-tolyl)acrylate; isolated by column chromatography (EtOAc/petroleum ether = 1:30); colorless oil; (48.6 mg, 80% yield); ^{1}H NMR (600 MHz, $CDCl_3$): δ 7.09 (d, *J* = 7.8 Hz, 2H), 6.87 (d, *J* = 7.8 Hz, 2H), 6.25 (s, 1H), 3.98 (dd, *J* =14.4, 7.2 Hz, 2H), 2.33 (s, 3H), 1.05 (t, *J* = 7.2 Hz, 3H), 0.83 (s, 9H), 0.14 (s, 6H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 165.3, 161.5, 139.2, 135.5, 130.0, 128.4, 126.1, 59.9, 26.9, 21.2, 17.5, 13.9, -5.7; HRMS (ESI) m/z calcd for $[C_{18}H_{28}O_2Si + Na]^+$ 327.1756, found 327.1759.



5d

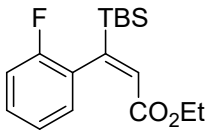
5d: ethyl (*E*)-3-(*tert*-butyldimethylsilyl)-3-(4-isopropylphenyl)acrylate; isolated by column chromatography (EtOAc/petroleum ether = 1:30); colorless oil; (48.5 mg, 73% yield); ^{1}H NMR (600 MHz, $CDCl_3$): δ 7.13 (d, *J* = 7.8 Hz, 2H), 6.99–6.97 (m, 2H), 6.38 (s, 1H), 4.19 (dd, *J* =14.4, 7.2 Hz, 2H), 2.91–2.86 (m, 1H), 1.30 (t, *J* = 7.2 Hz, 3H), 1.25 (d, *J* = 7.2 Hz, 6H), 0.95 (s, 9H), 0.11 (s, 6H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 166.7, 161.6, 146.9, 143.7, 134.9, 126.9, 125.7, 60.3, 33.6, 28.2, 24.0, 18.7, 14.3, -2.7; HRMS (ESI) m/z calcd for $[C_{20}H_{32}O_2Si + Na]^+$ 355.2069, found 355.2065.



5e

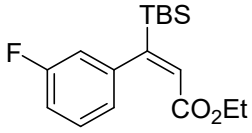
5e: ethyl (*E*)-3-(*tert*-butyldimethylsilyl)-3-(3,5-dimethylphenyl)acrylate; isolated by column chromatography (EtOAc/petroleum ether = 1:30); colorless oil; (30.8 mg, 50%

yield); ^{1}H NMR (600 MHz, $CDCl_3$): δ 6.83 (s, 1H), 6.59 (s, 2H), 6.23 (s, 1H), 3.97 (dd, *J* =14.4, 7.2 Hz, 2H), 2.28 (s, 6H), 1.02 (t, *J* = 7.2 Hz, 3H), 0.84 (s, 9H), 0.13 (s, 6H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 165.5, 161.1, 142.2, 136.9 , 129.9, 127.6, 123.9, 59.8, 26.9, 21.3, 17.5, 13.8, -5.6; HRMS (ESI) m/z calcd for $[C_{20}H_{32}O_2Si + Na]^+$ 341.1913, found 341.1906.



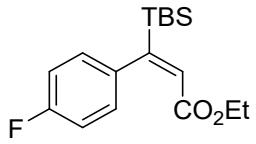
5f

5f: ethyl (*E*)-3-(*tert*-butyldimethylsilyl)-3-(2-fluorophenyl)acrylate; isolated by column chromatography (EtOAc/petroleum ether = 1:30); colorless oil; (27 mg, 45% yield);^{1}H NMR (600 MHz, $CDCl_3$): δ 7.21–7.18 (m, 1H), 7.09–7.05 (m, 1H), 7.03–7.00 (m, 1H), 6.95–6.93 (m, 1H), 6.36 (s, 1H), 3.99 (dd, *J* = 13.8, 7.2 Hz, 2H), 1.05 (t, *J* = 7.2 Hz, 3H), 0.88 (s, 9H), 0.13 (s, 6H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 165.5, 161.1, 142.2, 138.4 ($J_{C\text{-}F}$ = 478.5), 136.9, 130.0, 127.6, 127.4, 123.9, 59.8, 26.9, 21.3, 17.5, 13.8, -5.6; HRMS (ESI) m/z calcd for $[C_{17}H_{25}FO_2Si + Na]^+$ 331.1506, found 331.1508.



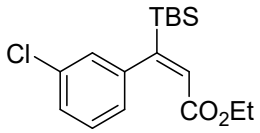
5g

5g: ethyl (*E*)-3-(*tert*-butyldimethylsilyl)-3-(3-fluorophenyl)acrylate; isolated by column chromatography (EtOAc/petroleum ether = 1:30); colorless oil; (37.0 mg, 60% yield); ^{1}H NMR (600 MHz, $CDCl_3$): δ 7.30–7.27 (m, 1H), 6.95–6.91 (m, 1H), 6.79–6.78 (m, 1H), 6.74–6.72 (m, 1H), 6.30 (s, 1H), 4.00 (dd, *J* =14.4, 7.2 Hz, 2H), 1.07 (t, *J* = 7.2 Hz, 3H), 0.88 (s, 9H), 0.17 (s, 6H); ^{13}C NMR (150 MHz, $CDCl_3$):δ 165.0, 162.4 ($J_{C\text{-}F}$ = 244.5), 159.8, 144.7 ($J_{C\text{-}F}$ = 7.5), 130.8, 129.2 ($J_{C\text{-}F}$ = 9.0), 122.0 ($J_{C\text{-}F}$ = 3.0), 113.3 ($J_{C\text{-}F}$ = 21.0), 112.8 ($J_{C\text{-}F}$ = 19.5), 60.1, 26.8,17.5, 13.8, 1.00, -5.7; HRMS (ESI) m/z calcd for $[C_{17}H_{25}FO_2Si + Na]^+$ 331.1506, found 331.1507.



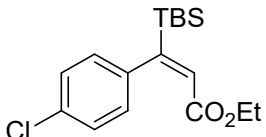
5h

5h:ethyl (*E*)-3-(*tert*-butyldimethylsilyl)-3-(4-fluorophenyl)acrylate; isolated by column chromatography (EtOAc/petroleum ether = 1:30); colorless oil; (42.5 mg, 69% yield); ^{1}H NMR (600 MHz, $CDCl_3$): δ 7.05–6.98 (m, 2H), 6.95–6.93 (m, 2H), 6.27 (s, 1H), 3.97 (dd, *J* =14.4, 7.2 Hz, 2H), 1.05 (t, *J* = 7.2 Hz, 3H), 0.83 (s, 9H), 0.13 (s, 6H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 165.1, 161.5 ($J_{C\text{-}F}$ = 243.0 Hz), 160.2, 138.1 ($J_{C\text{-}F}$ = 3.0 Hz), 130.8, 127.8 ($J_{C\text{-}F}$ = 7.5 Hz), 114.7 ($J_{C\text{-}F}$ = 21.0 Hz), 60.0, 26.8, 17.5, 13.9, -5.7; HRMS (ESI) m/z calcd for $[C_{17}H_{25}FO_2Si + Na]^+$ 331.1506, found 331.1501.



5i

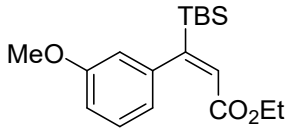
5i: ethyl (*E*)-3-(*tert*-butyldimethylsilyl)-3-(3-chlorophenyl)acrylate; isolated by column chromatography (EtOAc/petroleum ether = 1:30); colorless oil; (42.1 mg, 65% yield); ^{1}H NMR (600 MHz, $CDCl_3$): δ 7.23–7.17 (m, 2H), 6.98–6.97 (m, 1H), 6.87–6.86 (m, 1H), 6.27 (s, 1H), 3.97 (dd, *J* =14.4, 7.2 Hz, 2H), 1.03 (t, *J* = 7.2 Hz, 3H), 0.85 (s, 9H), 0.13 (s, 6H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 165.0, 159.6, 144.3, 133.6, 129.0, 126.2, 126.1, 124.5, 60.1, 26.9, 17.6, 13.8, -5.7; HRMS (ESI) m/z calcd for $[C_{17}H_{25}ClO_2Si + Na]^+$ 347.1210, found 347.1211.



5j

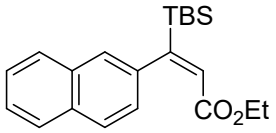
5j: ethyl (*E*)-3-(*tert*-butyldimethylsilyl)-3-(4-chlorophenyl)acrylate; isolated by column chromatography (EtOAc/petroleum ether = 1:30); colorless oil; (42.1 mg, 65% yield); ^{1}H NMR (600 MHz, $CDCl_3$): δ 7.27–7.26 (m, 2H), 7.01–7.00 (m, 2H), 6.37 (s, 1H), 4.21 (dd, *J* =14.4, 7.2 Hz, 2H), 1.32 (t, *J* = 7.2 Hz, 3H), 0.95 (s, 9H), 0.11 (s, 6H);

^{13}C NMR (150 MHz, $CDCl_3$): δ 166.4, 160.3, 144.8, 135.6, 132.3, 128.3, 128.0, 60.5, 28.1, 18.8, 14.2, -2.8; HRMS (ESI) m/z calcd for $[C_{17}H_{25}ClO_2Si + Na]^+$ 347.1210, found 347.1207.



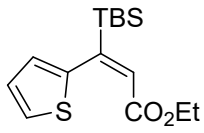
5k

5k: ethyl (*E*)-3-(*tert*-butyldimethylsilyl)-3-(3-methoxyphenyl)acrylate; isolated by column chromatography (EtOAc/petroleum ether = 1:30); colorless oil; (33.3 mg, 52% yield); ^{1}H NMR (600 MHz, $CDCl_3$): δ 7.19 (t, *J* = 7.8 Hz, 2H), 6.77–6.75 (m, 1H), 6.65–6.64 (m, 1H), 6.60–6.59 (m, 1H), 6.39 (s, 1H), 4.20 (dd, *J* =14.4, 7.2 Hz, 2H), 3.80 (s, 3H), 1.30 (t, *J* = 7.2 Hz, 3H), 0.95 (s, 9H), 0.11 (s, 6H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 166.6, 161.3, 159.0, 147.8, 135.0, 128.8, 119.4, 112.6, 111.7, 60.4, 55.2, 28.2, 18.8, 14.3, -2.8; HRMS (ESI) m/z calcd for $[C_{18}H_{28}O_3Si + Na]^+$ 342.1705, found 342.1702.



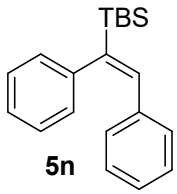
5l

5l: ethyl (*E*)-3-(*tert*-butyldimethylsilyl)-3-(naphthalen-2-yl)acrylate; isolated by column chromatography (EtOAc/petroleum ether = 1:30); colorless oil; (35.3 mg, 52% yield); ^{1}H NMR (600 MHz, $CDCl_3$): δ 7.83–7.79 (m, 2H), 7.77–7.75 (m, 1H), 7.50 (s, 1H), 7.49–7.44 (m, 2H), 7.23–7.21 (m, 1H), 6.47 (s, 1H), 4.23 (dd, *J* = 13.8, 6.6 Hz, 2H), 1.32 (t, *J* = 7.2 Hz, 3H), 0.98 (s, 9H), 0.14 (s, 6H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 166.6, 161.7, 144.1, 135.5, 133.1, 132.0, 127.8, 127.6, 127.2, 126.2, 125.9, 125.6, 125.0, 60.4, 28.2, 18.8, 14.3, -2.7; HRMS (ESI) m/z calcd for $[C_{21}H_{28}O_2Si + H]^+$ 363.1756, found 363.1760.



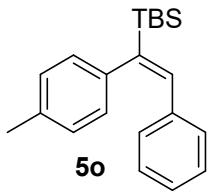
5m

5m: ethyl (*E*)-3-(*tert*-butyldimethylsilyl)-3-(thiophen-2-yl)acrylate; isolated by column chromatography (EtOAc/petroleum ether = 1:30); colorless oil; (23 mg, 38% yield); ^{1}H NMR (600 MHz, $CDCl_3$): δ 7.24 (d, *J* = 5.0 Hz, 1H), 6.97 (t, *J* = 3.7 Hz, 1H), 6.72 (d, *J* = 3.1 Hz, 1H), 6.28 (s, 1H), 4.04 (q, *J* = 7.0 Hz, 2H), 1.10 (t, *J* = 7.1 Hz, 3H), 0.83 (s, 9H), 0.20 (s, 6H), 0.07 (s, 6H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 165.7, 151.8, 142.4, 132.8, 127.0, 124.8, 124.6, 60.4, 26.9, 17.6, 14.1, -5.5; HRMS (ESI) m/z calcd for $[C_{15}H_{24}O_2SSi + H]^+$ 297.1339, found 297.1347.



5n

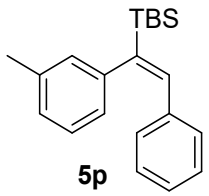
5n: (*E*)-*tert*-butyl(1,2-diphenylvinyl)dimethylsilane; isolated by column chromatography (EtOAc/petroleum ether = 1:100); colorless oil; (35.3 mg, 60% yield); ^{1}H NMR (600 MHz, $CDCl_3$): δ 7.28–7.24 (m, 3H), 7.21–7.16 (m, 2H), 7.08–7.05 (m, 3H), 7.03–7.01 (m, 2H), 6.92–6.91 (m, 2H), 6.84 (s, 1H), 0.86 (s, 9H), 0.15 (s, 6H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 147.1, 145.0, 144.4, 139.8, 137.4, 129.5, 128.5, 127.9, 127.8, 127.7, 126.9, 125.6, 27.1, -5.2; HRMS (ESI) m/z calcd for $[C_{20}H_{26}Si + H]^+$ 295.1882, found 295.1877.



5o

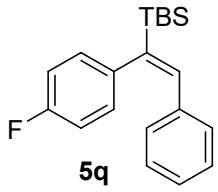
5o: (*E*)-*tert*-butyldimethyl(2-phenyl-1-(*p*-tolyl)vinyl)silane; isolated by column chromatography (EtOAc/petroleum ether = 1:100); colorless oil; (48.2 mg, 62% yield);

^{1}H NMR (600 MHz, $CDCl_3$): δ 7.32–7.27 (m, 1H), 7.10–7.08 (m, 4H), 6.95–6.94 (m, 2H), 6.92–6.91 (m, 2H), 6.83 (s, 1H), 2.34 (s, 3H), 0.87 (s, 9H), 0.15 (s, 6H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 145.0, 139.7, 135.0, 129.5, 129.2, 128.6, 128.4, 127.80, 127.78, 126.8, 27.1, 21.2, 17.9, -5.2 ; HRMS (ESI) m/z calcd for $[C_{21}H_{28}Si + Na]^+$ 331.1858, found 331.1845.



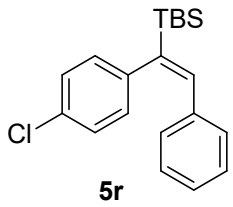
5p

5p: (*E*)-*tert*-butyldimethyl(2-phenyl-1-(*m*-tolyl)vinyl)silane; isolated by column chromatography (EtOAc/petroleum ether = 1:100); colorless oil; (33.4 mg, 54% yield); ^{1}H NMR (600 MHz, $CDCl_3$): δ 7.31–7.28 (m, 1H), 7.18–7.15 (m, 1H), 7.10–7.08 (m, 2H), 7.07–6.99 (m, 1H), 6.95–6.94 (m, 2H), 6.86 (s, 1H), 6.83–6.82 (m, 2H), 2.30 (s, 3H), 0.88 (s, 9H), 0.15 (s, 6H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 145.2, 143.3, 139.5, 137.9, 137.5, 129.5, 128.4, 128.3, 127.8, 126.9, 126.3, 124.9, 27.1, 21.5, 17.9, -5.2 ; HRMS (ESI) m/z calcd for $[C_{21}H_{28}Si+ H]^+$ 309.2039, found 309.2043.



5q

5q: (*E*)-*tert*-butyl(1-(4-fluorophenyl)-2-phenylvinyl)dimethylsilane; isolated by column chromatography (EtOAc/petroleum ether = 1:100); colorless oil; (36.2 mg, 58% yield); ^{1}H NMR (600 MHz, $CDCl_3$): δ 7.33–7.28 (m, 1H), 7.12–7.11 (m, 1H), 7.10–6.98 (m, 4H), 6.94–6.93 (m, 2H), 6.88 (s, 1H), 0.87 (s, 9H), 0.17 (s, 6H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 161.2 ($J_{C\text{-}F}$ = 243.0 Hz), 147.6, 143.9, 140.5, 139.1 ($J_{C\text{-}F}$ = 3.0 Hz), 137.2, 129.5 ($J_{C\text{-}F}$ = 7.5 Hz), 127.9, 127.1, 115.4 ($J_{C\text{-}F}$ = 21.0 Hz), 27.1, 17.9, -5.3; HRMS (ESI) m/z calcd for $[C_{20}H_{25}FSi + H]^+$ 313.1788, found 313.1800.

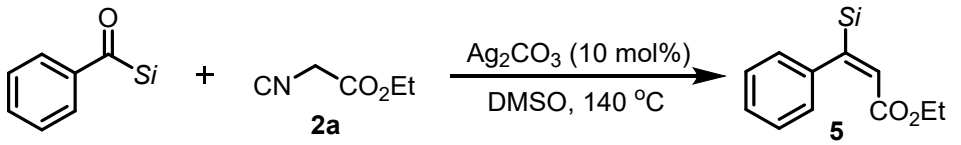


5r

5r: (*E*)-*tert*-butyl(1-(4-chlorophenyl)-2-phenylvinyl)dimethylsilane; isolated by column chromatography (EtOAc/petroleum ether = 1:100); colorless oil; (42.6 mg, 65% yield); ^{1}H NMR (600 MHz, $CDCl_3$): δ 7.31–7.27 (m, 1H), 7.25–7.25 (m, 1H), 7.15–7.11 (m, 3H), 6.98–6.96 (m, 2H), 6.94–6.93 (m, 2H), 6.87 (s, 1H), 0.87 (s, 9H), 0.16 (s, 6H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 147.6, 143.6, 141.9, 140.5, 137.1, 131.4, 129.5, 129.4, 128.7, 128.0, 127.2, 27.1, 17.9, -5.3; HRMS (ESI) m/z calcd for $[C_{20}H_{25}ClSi + Na]^+$ 351.1312, found 351.1321.

5. Control experiments

a) Size effect of silyl moiety



Si = TMS (**1av'**)
TES (**1av''**)

Si = TMS (**5a'**), *E*:*Z* = 3:1 (6h, 59% yield)
TES (**5a''**), *E*:*Z* = 5:1 (7h, 63% yield)

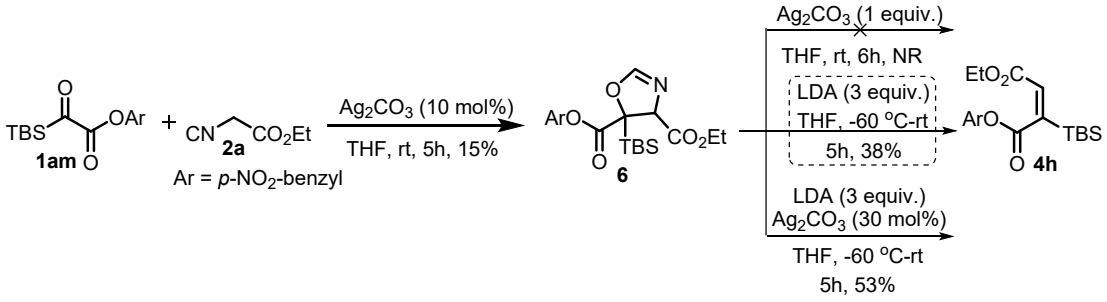
Acylsilane **1** (0.2 mmol, 1.0 eq.) and isocyanoacetate **2a** (26 μL, 0.24 mmol) were dissolved in DMSO (2.0 mL). Then Ag_2CO_3 (5.5 mg, 0.02 mmol) was added at room temperature. The reaction mixture was then stirred at 140 ℃ for appropriate time, the reaction mixture was extracted with EtOAc, and the combined organic phases were washed with brine, dried over anhydrous Na_2SO_4, filtered, and concentrated. The residue was purified by flash chromatography to afford the desired product.

5a': ethyl (*E*)-3-phenyl-3-(trimethylsilyl)acrylate; isolated by column chromatography (EtOAc/petroleum ether = 1:30); colorless oil; (29.26 mg, 59% yield); ^{1}H NMR (600 MHz, $CDCl_3$): δ 7.27–7.24 (m, 2H), 7.21–7.18 (m, 1H), 7.00 (d, *J* = 7.2 Hz, 2H), 6.29

(s, 1H), 4.18 (dd, J = 13.8, 7.2 Hz, 2H), 1.28 (t, J = 7.2 Hz, 3H), 0. 14 (s, 9H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 166.8, 165.7, 145.4, 132.9, 127.9, 126.5, 126.2, 60.4, 14.3; HRMS (ESI) m/z calcd for $[C_{14}H_{21}O_2Si + H]^+$ 249.1311, found 249.1312.

5a'': ethyl (*E*)-3-phenyl-3-(triethylsilyl)acrylate; isolated by column chromatography (EtOAc/petroleum ether = 1:30); colorless oil; (37.7 mg, 65% yield); ^{1}H NMR (600 MHz, $CDCl_3$): δ 7.30–7.28 (m, 2H), 7.21–7.19 (m, 1H), 6.94 (d, J = 7.8 Hz, 2H), 3.95 (dd, J =14.4, 7.2 Hz, 2H), 1.02 (d, J = 7.2 Hz, 3H), 0.93 (t, J = 7.8 Hz, 9H), 0.64 (dd, J = 15.6, 7.8 Hz, 6H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 165.1, 161.1, 142.1, 129.1, 127.8, 125.8, 125.5, 59.9, 13.8, 7.1, 2.3.

b) Oxazoline intermediate (byproduct)



For **6**:

To a mixture of 4-nitrobenzyl 2-(*tert*-butyldimethylsilyl)-2-oxoacetate **1am** (64.6 mg, 0.2 mmol) and isocyanoacetate (**2a**) (26 μL, 0.24 mmol) in THF (2.0 mL) was added Ag_2CO_3 (5.5 mg, 0.02 mmol,) at room temperature. After stirring for 5 h, the reaction mixture was extracted with EtOAc, and the combined organic phases were washed with brine, dried over anhydrous Na_2SO_4, filtered, and concentrated. The residue was purified by flash chromatography to afford the product **6** in 15% yield.

6: ethyl 5-((l1-oxidaneyl)carbonyl)-5-(*tert*-butyldimethylsilyl)-4,5-dihydrooxazole-4-carboxylate; isolated by column chromatography (EtOAc/petroleum ether = 1:5); colorless oil; (9.5 mg, 15% yield); ^{1}H NMR (600 MHz, $CDCl_3$): δ 8.22 (d, J = 9.0 Hz,

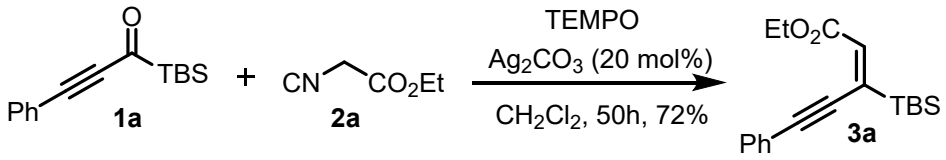
2H), 7.53 (d, J = 9.0 Hz, 2H), 7.06 (d, J = 1.8 Hz, 1H), 5.24 (d, J = 13.2 Hz, 1H), 5.12 (d, J = 1.8 Hz, 1H), 4.85 (d, J = 1.8 Hz, 1H), 4.09–4.00 (m, 1H), 1.20 (t, J = 7.2 Hz, 3H), 0.90 (s, 9H), 0.21 (s, 3H), 0.08 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 171.1, 169.5, 156.8, 147.8, 141.8, 128.9, 123.8, 83.7, 74.5, 65.7, 61.8, 26.7, 18.0, 13.9, -8.1, -8.8; HRMS (ESI) m/z calcd for $[C_{20}H_{29}N_2O_7Si + H]^+$ 437.1744, found 437.1751.

For **4h**：

(1) To a mixture of **6** (43.6 mg, 0.1 mmol) in THF (2.0 mL) was added Ag_2CO_3 (27.5 mg, 0.1 mmol) at room temperature. The reaction mixture was then stirred for 6 h at room temperature and no reaction was detected.

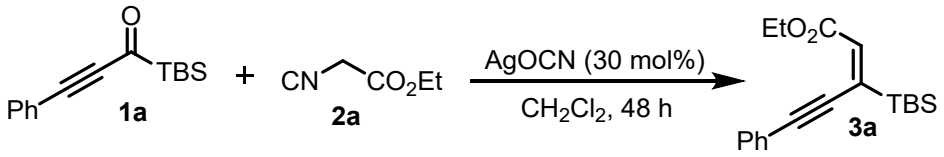
(2) To a mixture of **6** (43.6 mg, 0.1 mmol) and Ag_2CO_3 (8.3 mg, 0.03 mmol) in THF (2.0 mL) was added LDA (0.3 mmol) at -60 °C, and the reaction mixture was then stirred at room temperature for 5 h and the desired product of **4h** was obtained in 53% yield.

c) TEMPO as additive



To a mixture of 1-(*tert*-butyldimethylsilyl)-3-phenylprop-2-yn-1-one (**1a**) (48 mg, 0.2 mmol), isocyanoacetate (**2a**) (26 μL, 0.24 mmol,) and Ag_2CO_3 (16.5 mg, 0.06 mmol) in CH_2Cl_2 (2.0 mL) was added TEMPO (62.4 mg, 0.4 mmol) at room temperature. After stirring for 50h, the reaction mixture was extracted with EtOAc, the combined organic phases were washed with brine, dried over anhydrous Na_2SO_4, filtered, and concentrated. The residue was purified by flash chromatography (silica gel; petroleum ether: ethyl acetate = 30: 1) to afford the product **3a** in 72% yield.

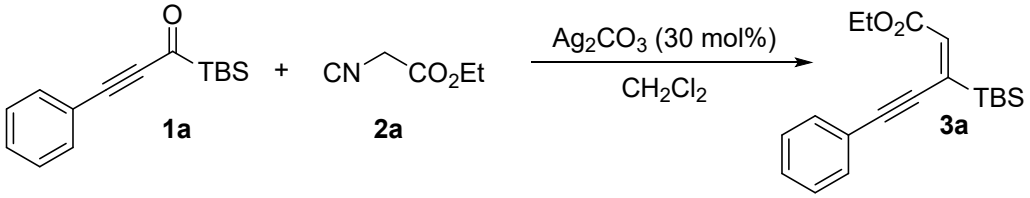
d) AgOCN as additive



To a mixture of 1-(*tert*-butyldimethylsilyl)-3-phenylprop-2-yn-1-one (**1a**) (0.2 mmol, 48.8 mg), isocyanoacetate (**2a**) (0.24 mmol, 26 μL) in CH_2Cl_2 (2.0 mL) was added AgOCN (0.06 mmol, 9.0 mg) at room temperature. After stirring for 48 h, the reaction mixture was extracted with EtOAc, the combined organic phases were washed with brine, dried over anhydrous Na_2SO_4, filtered, and concentrated. The residue was purified by flash chromatography (silica gel; petroleum ether : ethyl acetate = 30:1) to afford the product **3a** in 81% yield (*E*/*Z* = 6:1) (based on recovered starting materials).

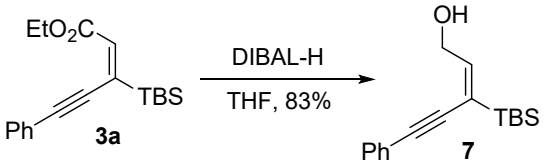
6. Gram-Scale synthesis and further chemical transformations

6.1 Gram-Scale synthesis of product of 3a



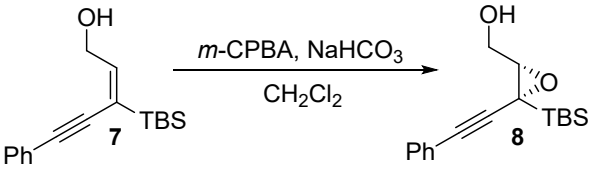
Alkynyl acylsilanes **1a** (1.0 g, 4.1 mmol) and ethyl isocyanoacetate **2a** (554 mg, 4.9 mmol) were dissolved in CH_2Cl_2 (40 mL). Then Ag_2CO_3 (339.2 mg, 1.23 mmol) was added at room temperature. After stirring for 78h, the reaction mixture was extracted with EtOAc, the combined organic phases were washed with brine, dried over anhydrous Na_2SO_4, filtered, and concentrated. The residue was purified by flash chromatography to afford the product **3a** (1.004 g, 78% yield).

6.2 The procedure for Further Chemical Transformations



To a solution of ethyl (*E*)-3-(*tert*-butyldimethylsilyl)-5-phenylpent-2-en-4-ynoate **3a** (536 mg, 1.7 mmol) in THF (8 mL) was added dropwise a solution of diisobutylaluminium hydride (3.3 mL, 5mmol, 1.5 M in hexane) at -78 ^{o}C under argon. After stirring for 20 min at 0 ^{o}C, diethyl ether and water were successively added at 0 ^{o}C. After stirring for 2h, the mixture was filtered through celite pad. The filtrate was dried over Na_2SO_4, filtered and concentrated. The resulting residue was chromatographed over silica gel to yield 385 mg (83%) of the alcohol **7**.

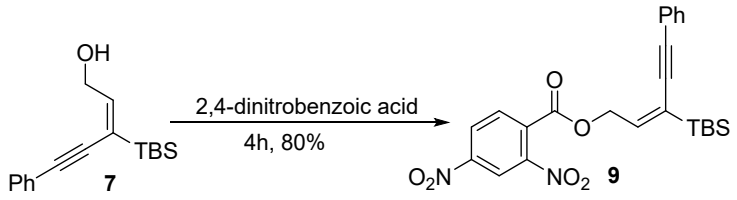
7: (*E*)-3-(*tert*-butyldimethylsilyl)-5-phenylpent-2-en-4-yn-1-ol; isolated by column chromatography (EtOAc/petroleum ether = 1:5); yellow oil; (147 mg, 83% yield); ^{1}H NMR (600 MHz, $CDCl_3$): δ 7.50–7.48 (m, 2H), 7.33–7.30 (m, 3H), 6.36 (s, 1H), 1.01 (s, 9H), 0.28 (s, 6H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 168.8, 144.0, 133.6, 131.8, 129.1, 128.4, 123.3, 110.1, 89.6, 26.6, 17.5, -6.4; HRMS (ESI) m/z calcd for $[C_{17}H_{24}OSi + Na]^+$ 295.1494, found 295.1491.



(*E*)-3-(*tert*-butyldimethylsilyl)-5-phenylpent-2-en-4-yn-1-ol **7** (43.0 mg, 0.158 mmol) was dissolved in CH_2Cl_2 (2 mL). Then, $NaHCO_3$ (31.8 mg, 0.379 mmol) was added, followed by *m*CPBA (58.7 mg, 0.34 mmol). After stirring for 2 hours at room temperature, then the reaction was quenched with a saturated aqueous Na_2SO_3 (2 mL). The aqueous phase was extracted with CH_2Cl_2 (2 x 20 mL) and the organic fractions were combined, dried over Na_2SO_4 and filtered. The solvent was evaporated under

reduced pressure and the resulting residue was chromatographed over silicagel to give epoxide **8**.

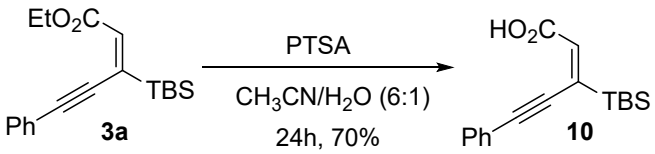
8: ((*2S*,*3S*)-3-(*tert*-butyldimethylsilyl)-3-(phenylethynyl)oxiran-2-yl)methanol; isolated by column chromatography (EtOAc/petroleum ether = 1:10); yellow oil; (37.8 mg, 83% yield); ^{1}H NMR (600 MHz, $CDCl_3$): δ 7.40–7.39 (m, 2H), 7.31–7.29 (m, 3H), 4.08–3.98 (m, 2H), 3.26 (dd, *J* = 6, 4.8 Hz, 1H), 1.06 (s, 9H), 0.17 (s, 3H), 0.08 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 131.6, 128.5, 128.3, 122.5, 87.1, 87.0, 63.4, 60.8, 47.8, 27.0, 17.5, -8.1, -8.2; HRMS (ESI) m/z calcd for $[C_{17}H_{24}NaO_2Si + Na]^+$ 311.1443, found 311.1440.



To a solution of (*E*)-3-(*tert*-butyldimethylsilyl)-5-phenylpent-2-en-4-yn-1-ol **7** (239.4 mg, 0.88 mmol) in dry CH_2Cl_2 (8 mL), were added 2,4-dinitrobenzoic acid (212.1 mg, 1.0 mmol), 4-dimethylaminopyridine (206 mg, 1.0 mmol) and dicyclohexylcarbodiimide (10.7 mg, 0.088 mmol). After stirring for 4h, thereaction was extracted with CH_2Cl_2 and the organic fractions were dried over Na_2SO_4, filtered and concentrated. The resulting residue was chromatographed over silicagel to yield **9**.

9: (*E*)-3-(*tert*-butyldimethylsilyl)-5-phenylpent-2-en-4-yn-1-yl 2,4-dinitrobenzoate; isolated by column chromatography (EtOAc/petroleum ether = 1:5); yellow solid; (328.1mg, 80% yield); ^{1}H NMR (600 MHz, $CDCl_3$): δ 8.76–8.76 (m, 1H), 8.4 (dd, *J* = 8.4, 1.8 Hz, 1H), 7.94 (d, *J* = 8.4 Hz, 1H), 7.43–7.41 (m, 2H), 7.33–7.29 (m, 3H), 6.30 (t, *J* = 12 Hz, 1H), 5.31 (d, *J* = 6 Hz, 2H), 1.02 (s, 9H), 0.25 (s, 6H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 163.5, 148.8, 147.9, 141.5, 132.7, 131.14, 131.12, 127.4, 123.4, 119.5, 100.9, 87.6, 66.2, 26.5, 17.2, -6.6; HRMS (ESI) m/z calcd for

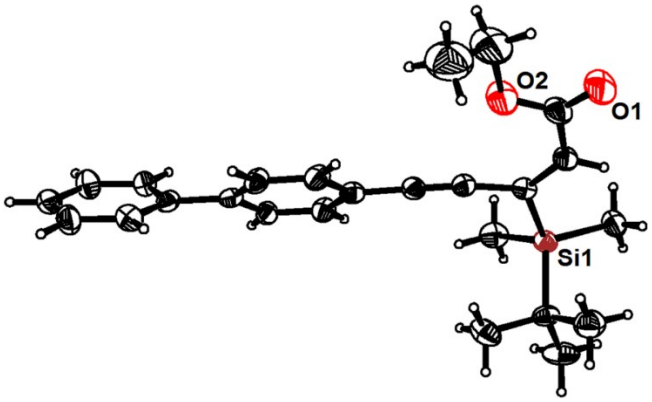
$[C_{24}H_{26}N_2O_6Si + Na]^+$ 489.1458, found 489.1460.



To a solution of ethyl (*E*)-3-(*tert*-butyldimethylsilyl)-5-phenylpent-2-en-4-ynoate **3a** (314.0 mg, 1.0 mmol) in CH_3CN and H_2O (6:1, 6 mL), heated reflux to 90 °C, then was added *p*-toluenesulfonic acid (34.4 mg, 2.0 mmol). After stirring for 24 h at 90 °C, the resulting mixture was concentrated and taken up by ethyl acetate. The aqueous phase was extracted with ethyl acetate and the organic fractions were combined. The filtrate was dried over Na_2SO_4, filtered and concentrated. The resulting residue was chromatographed over silica gel to yield **10**.

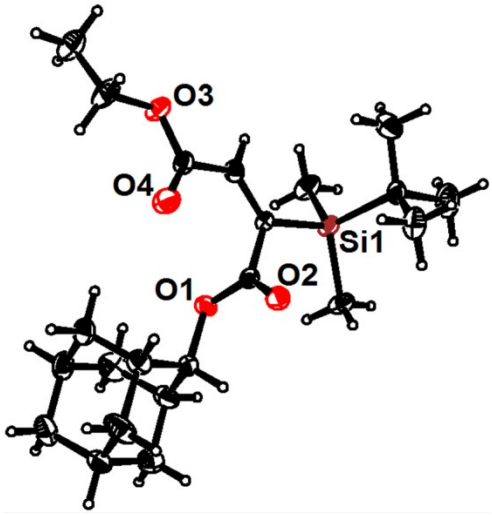
10: (*E*)-3-(*tert*-butyldimethylsilyl)-5-phenylpent-2-en-4-ynoic acid; isolated by column chromatography (EtOAc/petroleum ether = 1:10); white solid; (200.2 mg, 70% yield); ^{1}H NMR (600 MHz, $CDCl_3$): δ 7.50–7.48 (m, 2H), 7.36–7.30 (m, 3H), 6.36 (s, 1H), 1.01 (s, 9H), 0.28 (s, 6H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 168.8, 144.0, 133.6, 131.8, 129.1, 128.4, 123.3, 110.1, 89.6, 26.6, 17.5, -6.4; HRMS (ESI) m/z calcd for $[C_{17}H_{22}O_2Si + Na]^+$ 309.1287, found 309.1282.

7. The crystal structure and data of 3j, 4l and 6



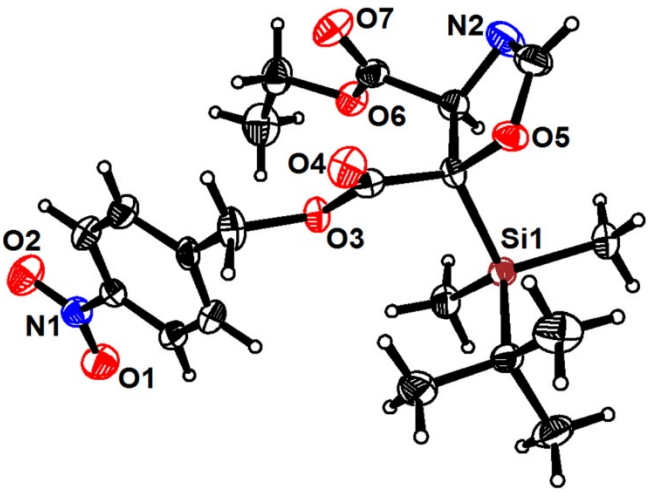
Single crystal data of 3j:

Bond precision:	C-C = 0.0121 A	Wavelength = 0.71073
Cell:	a = 6.3035(2)	b = 9.3843(8) c = 19.8035(6)
	alpha = 89.16(2)	beta = 83.61(2) gamma = 88.49(2)
Temperature:	296 K	
	Calculated	Reported
Volume	1163.69(12)	1163.68(11)
Space group	P -1	P -1
Hall group	-P 1	
Moiety formula	$C_{25}H_{30}O_2Si$	
Sum formula	$C_{25}H_{30}O_2Si$	$C_{25}H_{30}O_2Si$
Mr	390.58	390.58
Dx, g cm-3	1.115	1.115
Z	2	2
Mu (mm-1)	0.117	0.117
F000	420.0	420.0
F000’	420.32	
h, k, lmax	7,11,23	7,11,23
Nref	4116	4034
Tmin, Tmax	0.967,0.976	0.967,0.976
Tmin’	0.967	



Single crystal data of 4l:

Bond precision:	C-C = 0.0078 A	Wavelength = 0.71073
Cell:	a = 15.450(11)	b = 6.749(5) c = 24.159(15)
	alpha = 90	beta = 112.04(4) gamma = 90
Temperature:	293 K	
	Calculated	Reported
Volume	2335(3)	2335(3)
Space group	P 21/c	P21/c
Hall group	-P 2ybc	
Moiety formula	$C_{22}H_{36}O_4Si$	
Sum formula	$C_{22}H_{36}O_4Si$	$C_{22}H_{36}O_4Si$
Mr	392.60	392.60
Dx, g cm-3	1.117	1.117
Z	4	4
Mu (mm-1)	0.117	0.117
F000	0.123	0.123
F000’	856.69	
h, k, lmax	18,8,28	18,8,28
Nref	4102	4099
Tmin, Tmax	0.965,0.976	0.965,0.976
Tmin’	0.965	



Single crystal data of 6:

Bond precision:	C-C = 0.0060 A	Wavelength = 0.71073	
Cell:	a = 9.0411(16)	b = 24.0685(12)	c = 10.800(2)
	alpha = 90	beta = 103.45(3)	gamma = 90
Temperature:	296 K		
	Calculated	Reported	
Volume	2285.7(7)	2285.8(7)	
Space group	P 21/n	P2(1)/n	
Hall group	-P 2yn		
Moiety formula	$C_{20}H_{28}N_2O_7Si$		
Sum formula	$C_{20}H_{28}N_2O_7Si$	$C_{20}H_{28}N_2O_7Si$	
Mr	436.53	436.53	
Dx, g cm-3	1.269	1.269	
Z	4	4	
Mu (mm-1)	0.144	0.144	
F000	928.0	928.0	
F000’	928.80		
h, k, lmax	10,28,12	10,28,12	
Nref	4033	4026	
Tmin, Tmax	0.959,0.970	0.959,0.970	
Tmin’	0.959		

8. DFT Calculation results

As shown in **Figure S1**, simplified model (ester ethyl in substrate were simplified to methyl) were adopted to explore the reaction mechanism.

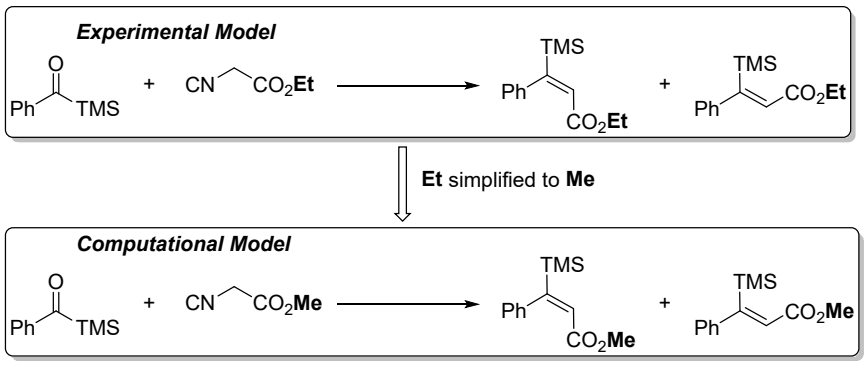


Figure S1. Experimental model versus simplified model used in reaction mechanism exploration.

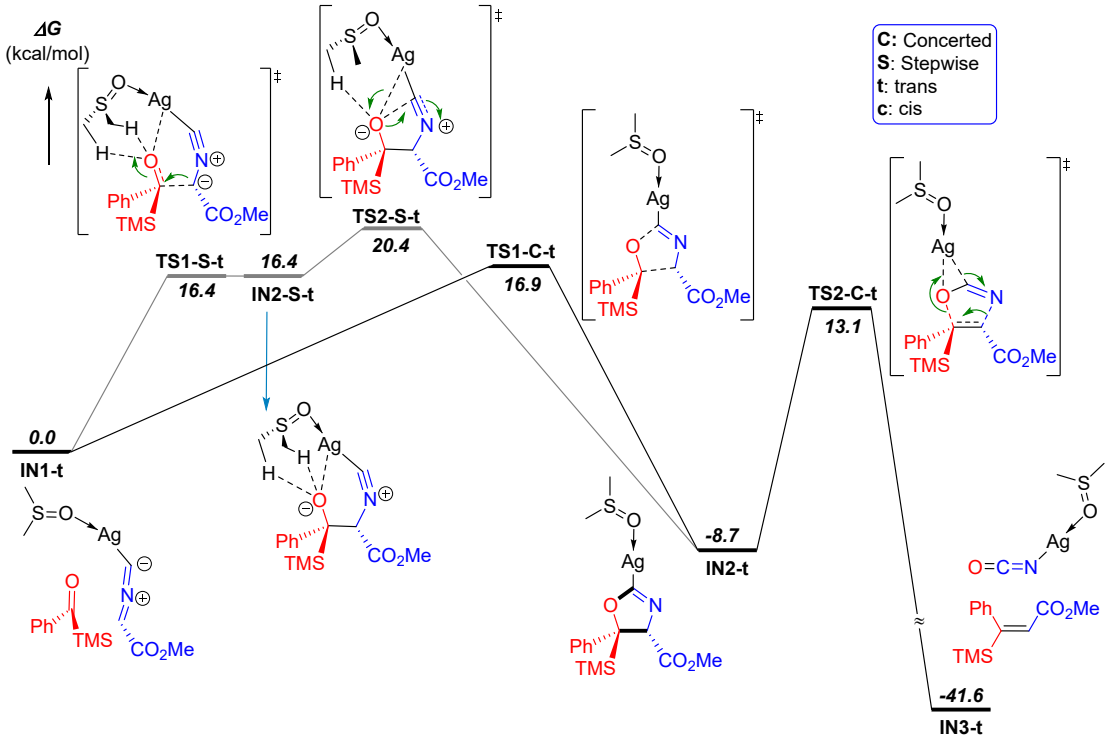


Figure S2. DFT calculation results on *trans*-alkene product pathway. Relative solvated Gibbs free energies are shown in Italic bold, unit: kcal/mol. Calculated at B3LYP-GD3/def2-TZVP//B3LYP-GD3/6-31G(d)/SDD level with SMD solvation model

(solvent = dimethylsulfoxide).

Two cyclization pathways (**C**oncerted and **S**tepwise cyclization pathways) were found. *Trans*- and *cis*- pathways were shown in **Figure S2** and **Figure S3**. And the rate-determining-step is the ring-opening step (**TS2-C-t**, 13.1 kcal/mol; **TS2-C-c**, 14.2 kcal/mol), and chem-selectivity step is cyclization step (**TS2-S-t**, 20.4 kcal/mol; **TS1-C-t**, 16.9 kcal/mol; **TS2-S-t**, 20.4 kcal/mol; **TS1-C-c**, 19.1 kcal/mol).

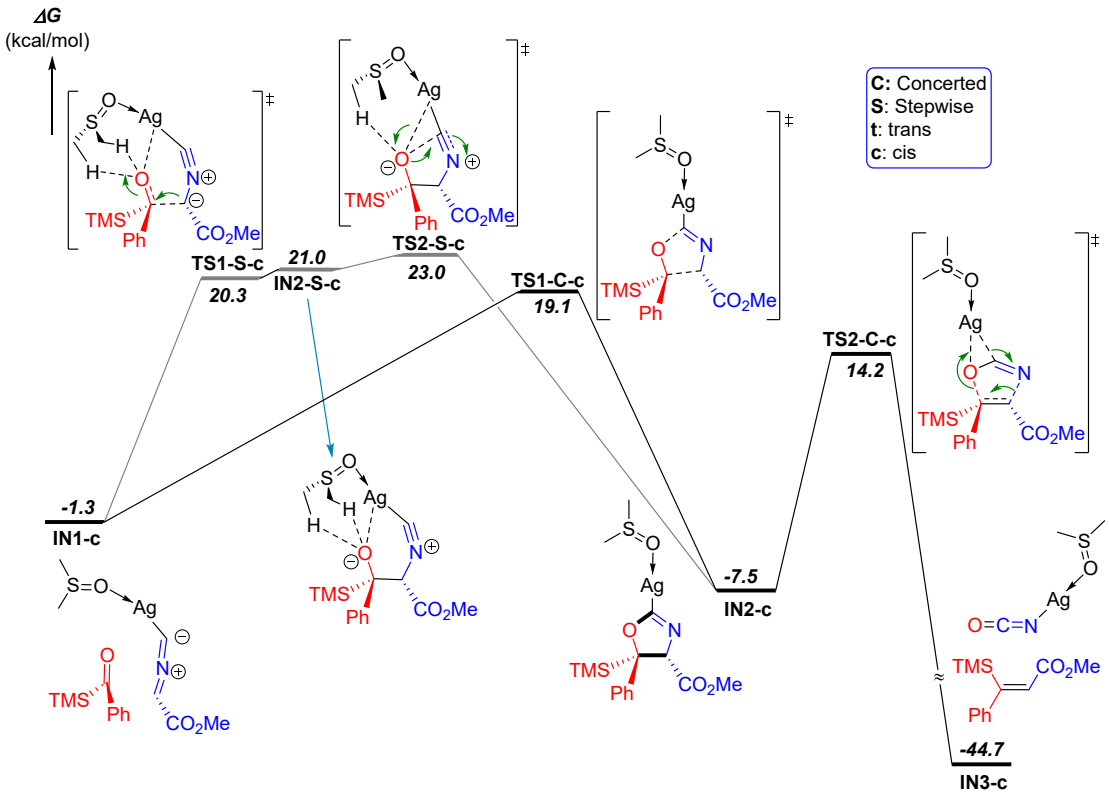


Figure S3. DFT calculation results on *cis*-alkene product pathway. Relative solvated Gibbs free energies are shown in Italic bold, unit: kcal/mol. Calculated at B3LYP-GD3/def2-TZVP//B3LYP-GD3/6-31G(d)/SDD level with SMD solvation model (solvent = dimethylsulfoxide).

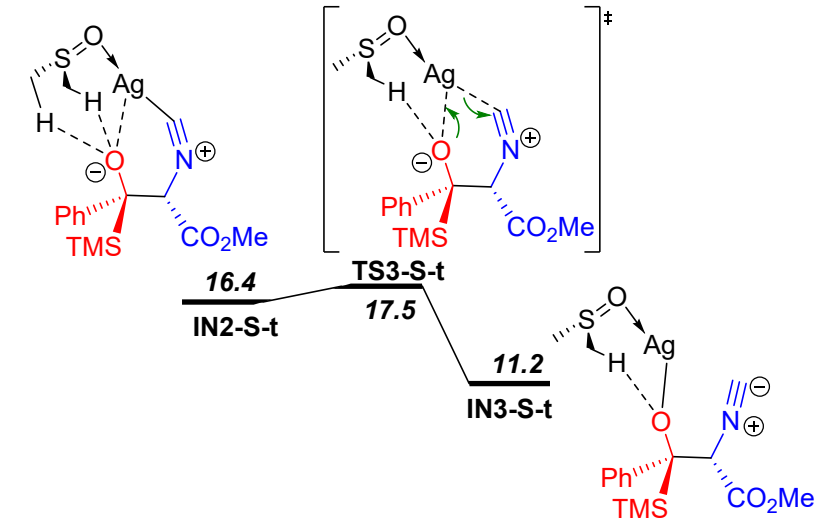


Figure S4. DFT calculation results on coordination of Ag between O and C. Relative solvated Gibbs free energies are shown in Italic bold, unit: kcal/mol. Calculated at B3LYP-GD3/def2-TZVP//B3LYP-GD3/6-31G(d)/SDD level with SMD solvation model (solvent = dimethylsulfoxide).

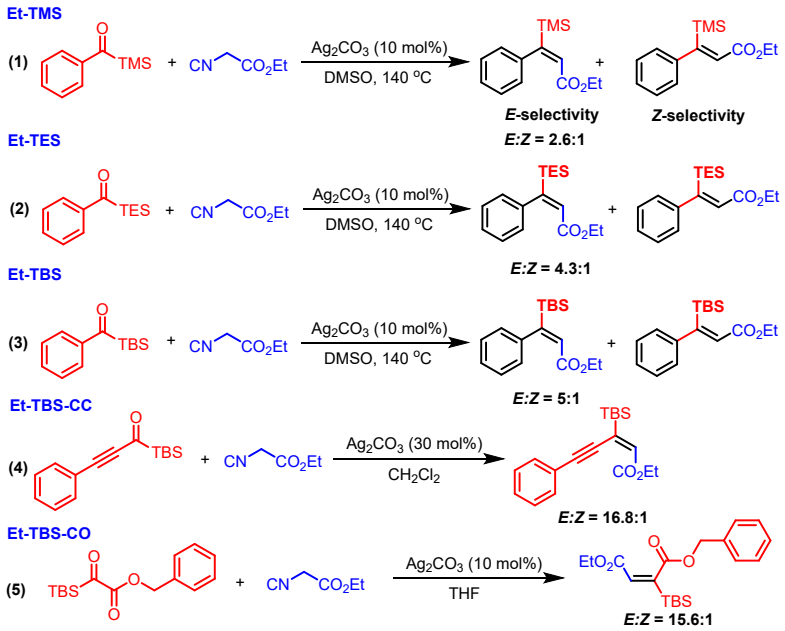


Figure S5. Experimental results on substituent effects on chem-selectivity.

As shown in **Table S6**, computational results on chemselectivity influenced by substituent effects agree well with experimental observation (**Figure S5**).

Table S6. Computational results of substituent effects on chem-selectivity. Calculated at B3LYP-GD3/def2-TZVP//B3LYP-GD3/6-31G(d)/SDD level with SMD solvation model (solvent = dimethylsulfoxide).

Entry	**ΔΔE** (kcal/mol)	***ΔΔG*** (kcal/mol)	***Experimental chem-selectivity (trans: cis or E:Z)***
TS1-C-c-Et-TMS[a]	**2.2**	***4.2***	***2.55***
TS2-S-c-Et-TMS[a]	**-2.8**	***3.8***	
TS1-C-t-Et-TMS[b]	**0.0**	***0.0***	
TS2-S-t-Et-TMS[b]	**0.0**	***4.9***	
/	/	/	/
TS1-C-c-Et-TES[a]	**0.9**	***4.4***	***4.29***
TS2-S-c-Et-TES[a]	**-1.1**	***3.6***	
TS1-C-t-Et-TES[b]	**0.0**	***0.0***	
TS2-S-t-Et-TES[b]	**-0.9**	***3.1***	
/	/	/	/
TS1-C-c-Et-TBS[a]	**2.0**	***4.8***	***major***
TS2-S-c-Et-TBS[a]	**0.8**	***5.9***	
TS1-C-t-Et-TBS[b]	**0.0**	***0.0***	
TS2-S-t-Et-TBS[b]	**2.9**	***7.3***	

Note: [a.] leading to *Z* product; [b.] leading to *E* product.

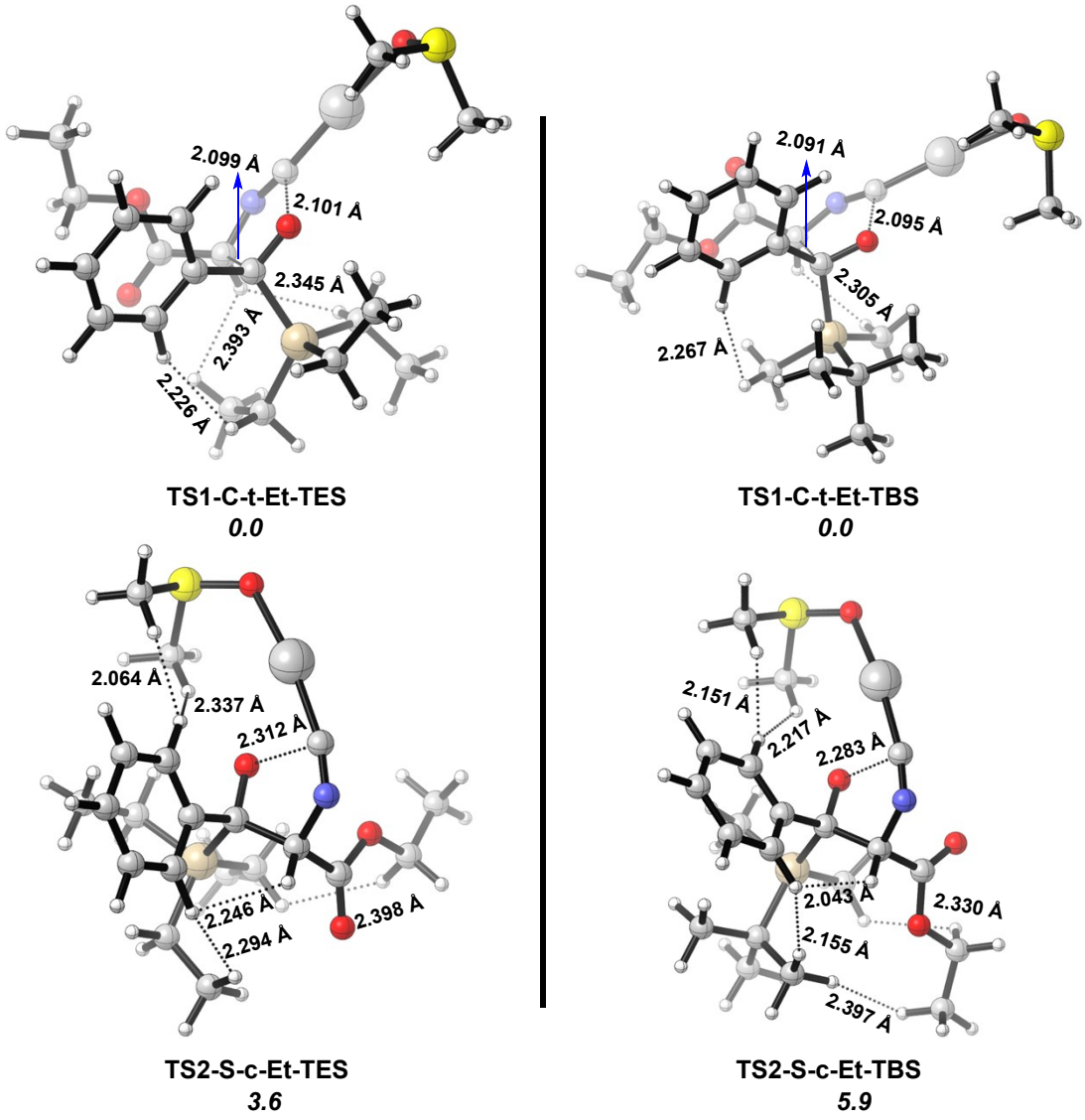


Figure S6. 3d representations of RDS transition states on concerted pathway and stepwise pathway for Et-TES (left) and Et-TBS substrate (right), respectively. Relative solvated Gibbs free energies are shown in Italic bold, unit: kcal/mol. Calculated at B3LYP-GD3/def2-TZVP//B3LYP-GD3/6-31G(d)/SDD level with SMD solvation model (solvent = dimethylsulfoxide).

As shown in **Figure S6**, the steric effects are less severe in **TS1-C-t-Et-TBS** than those in **TS1-C-t-Et-TES**, while such effects are more dramatic in **TS2-S-c-Et-TBS** than those in **TS2-S-c-Et-TES**, accounting for better *E*:*Z* ratio for Et-TBS than Et-TES substrate.

Table S7. Absolute electronic energies and Gibbs free energies for all the intermediates and transition states structures in this article, unit: Hartree. Calculated at B3LYP-

GD3/def2-TZVP//B3LYP-GD3/6-31G(d)/SDD level with SMD solvation model (solvent = dimethylsulfoxide).

Entry	E[a]	G[a]	E[b]
IN1-t	-1814.5380954	-1814.2313430	-1815.0588563
TS1-S-t	-1814.5206832	-1814.2097710	-1815.0369159
IN2-S-t	-1814.5222025	-1814.2110470	-1815.0371571
TS3-S-t	-1814.5199602	-1814.2096990	-1815.0345384
IN3-S-t	-1814.5292322	-1814.2191070	-1815.0443407
TS2-S-t	-1814.5147041	-1814.2027740	-1815.0314632
TS1-C-t	-1814.5106214	-1814.2045750	-1815.0311761
IN2-t	-1814.5648571	-1814.2515170	-1815.0793526
TS2-C-t	-1814.5176181	-1814.2108960	-1815.0379135
IN3-t	-1814.6023218	-1814.2933610	-1815.1273665
IN1-c	-1814.5378236	-1814.2316000	-1815.0603476
TS1-C-c	-1814.5075220	-1814.2013590	-1815.0277769
IN2-c	-1814.5645147	-1814.2508830	-1815.0777641
TS2-C-c	-1814.5181972	-1814.2109390	-1815.0366601
IN3-c	-1814.6082414	-1814.2998990	-1815.1316462
TS1-S-c	-1814.5161816	-1814.2040270	-1815.0319050
IN2-S-c	-1814.5183714	-1814.2038740	-1815.0331767
TS2-S-c	-1814.5124741	-1814.1995730	-1815.0283539
TS1-C-c-Et-TMS	-1853.8304004	-1853.4959810	-1854.3651276
TS2-S-c-Et-TMS	-1853.8428962	-1853.5012120	-1854.3730132
TS1-C-t-Et-TMS	-1853.8334491	-1853.5022420	-1854.3685729
TS2-S-t-Et-TMS	-1853.8374623	-1853.4983480	-1854.3686427
TS1-C-c-Et-TBS	-1971.7798061	-1971.3587030	-1972.3540552
TS2-S-c-Et-TBS	-1971.7841515	-1971.3594270	-1972.3559519
TS1-C-t-Et-TBS	-1971.7798953	-1971.3633820	-1972.3571835
TS2-S-t-Et-TBS	-1971.7788964	-1971.3554890	-1972.3525154
TS1-C-c-Et-TES	-1971.7739972	-1971.3517760	-1972.3481871
TS2-S-c-Et-TES	-1971.7793809	-1971.3552510	-1972.3513812
TS1-C-t-Et-TES	-1971.7738289	-1971.3571620	-1972.3496957

TS2-S-t-Et-TES	-1971.7778142	-1971.3547510	-1972.3512047
TS1-C-c-Et-TBS-CC	-2454.4012175	-2454.0287410	-2454.9736305
TS2-S-c-Et-TBS-CC	-2454.4077876	-2454.0376780	-2454.9812472
TS1-C-t-Et-TBS-CC	-2454.4092329	-2454.0344510	-2454.9789475
TS2-S-t-Et-TBS-CC	-2454.4134290	-2454.0353880	-2454.9797149

Note: [a.] Calculated at B3LYP-GD3/6-31G(d)/SDD level; [b.] Obtained by single point calculation at B3LYP-GD3/def2-TZVP level.

Computational details

All geometry optimizations were performed at B3LYP [6-9]-GD3 [10]/6-31G(d)(for C, H, N, O, S)/SDD (for Ag atoms) level with the Gaussian 16 [11] packages. SMD solvation model (solvent=dimethylsulfoxide) was utilized, in accordance with the experiments [12-15]. To save computational costs, "g09defaults" keyword was used in all calculations. Frequency calculations were performed with the optimized geometries to ensure only one imaginary frequency for transition state structures and zero imaginary frequencies for reactant or product intermediate structures. Single point calculations at B3LYP-GD3/def2-TZVP level were performed on the optimized structures obtained at B3LYP-GD3/6-31G(d)/SDD level to correct the Gibbs free energies.

Total energies (Electronic energies, Gibbs free energies, Unit: Hartree), charge, multiplicity, and geometrical coordinates for structures involved in DFT calculations of this article, calculated at B3LYP-GD3/6-31G(d) level with SMD solvation model (solvent = dimethylsulfoxide).

IN1-t

Electronic_Energy=-1814.53809542

Sum of electronic and thermal Free Energies = -1814.231343

Charge=0 Multiplicity=1

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H,2.8267541554,-1.3367017396,1.2217215119
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O,4.7250451422,-0.491203988,-1.1032477751
S,5.0777269084,-0.3917281895,0.4116373585
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H,4.4540971477,1.1404278764,2.142066322
H,4.763654446,1.9676156741,0.5860974928
H,3.2049374264,1.098281754,0.8342135905
H,4.3232746178,-2.5981735711,0.9257657108
H,4.2134091771,-1.5152163589,2.3485063049
H,2.9800783458,-1.4095002708,1.0408988982
---end---

IN3-S-t

Electronic_Energy=-1814.52923220
Sum of electronic and thermal Free Energies = -1814.219107
Charge=0 Multiplicity=1
---Coordinates start---
C,0.2251390005,0.6527205438,0.6481698971
C,1.731067995,0.5527125306,1.1973287761
N,2.6403963583,1.0715168916,0.2265934224
C,3.3216961429,1.5078690744,-0.620632159
Ag,0.5623993101,3.3110399812,-0.7559729848
C,2.3016506215,-0.7792646117,1.7058482174
O,3.0467831601,-1.5163108274,1.0938441316
O,1.8911563509,-0.9994468154,2.9601209474
C,2.3399822189,-2.2315575148,3.5698875131
O,-0.1416955321,1.9945587045,0.7123389774
C,0.0658096748,0.0471963561,-0.7523185416
C,-0.8952527612,0.6058004956,-1.6165825695
C,0.7998013492,-1.0550434515,-1.2236614649
C,-1.0969885425,0.1037643239,-2.9048660444
C,0.6033225683,-1.5549342339,-2.5139417126
C,-0.3416315054,-0.9767281194,-3.365456853
Si,-1.095759876,-0.1776989253,1.8247352297
C,-2.793012191,0.3135715097,1.1560396161
C,-0.9201110587,0.5160748091,3.57272344
C,-1.011822896,-2.0701796963,1.8039176785
O,1.1910927883,4.6498482989,-2.3418464012
S,1.1413246038,4.2496590576,-3.8513394031
C,1.899304484,2.6049654952,-3.9921700816
C,-0.5721424052,3.7628738421,-4.1988210563
H,1.733880531,1.2387812975,2.0468098427
H,2.0648344786,-3.0899326616,2.952493877
H,3.4246034841,-2.2079303076,3.7045713736
H,1.8359290514,-2.2760671672,4.5350486944
H,-1.4965522899,1.4360306283,-1.2650963607
H,1.549056357,-1.5241655377,-0.5990818598
H,-1.8450489013,0.5620596356,-3.5471607001
H,1.1986771351,-2.3991093931,-2.8535162638
H,-0.4896676579,-1.3659070249,-4.3694229033
H,-3.5758168293,-0.0344872965,1.8436223768
H,-2.8762411899,1.4018754176,1.0663929679
H,-2.9948443005,-0.1269657369,0.1730830685
H,-1.7451268936,0.1658100469,4.2073816116
H,0.0209843761,0.2162472757,4.0436443001
H,-0.9587179122,1.6115932691,3.5488124093
H,-0.0945036443,-2.4694386707,2.2464583175
H,-1.8581663205,-2.4878682114,2.366305994
H,-1.0818897452,-2.4486431731,0.7763791102
H,1.8302768503,2.2909146973,-5.0390493778
H,2.9479750995,2.697754766,-3.6992272623
H,1.376680455,1.8969824715,-3.3415157206
H,-1.1970656119,4.6533111397,-4.0914897951
H,-0.6236617715,3.3914373501,-5.2275703593
H,-0.8791046085,2.9867094666,-3.4908119156
---end---

TS2-S-t

Electronic_Energy=-1814.51470408
Sum of electronic and thermal Free Energies = -1814.202774
Charge=0 Multiplicity=1
---Coordinates start---
C,0.1001799612,1.0259875504,-0.4421769951
C,-0.5827837006,0.9416660754,-1.9326524868
N,0.2456311118,0.0336148516,-2.6853128501
C,1.3898463436,-0.2646517457,-2.5130896946
Ag,3.2283529039,-0.6731642851,-1.7231510805
C,-0.5527049045,2.2990477215,-2.6296414232
O,0.4354358202,2.8205477013,-3.103520885

O,-1.7671452282,2.8726198204,-2.5911154263
C,-1.8165976787,4.2622180784,-2.9721547075
O,1.4545519095,0.8974073453,-0.5448642933
C,-0.3214198332,2.3540114236,0.2041336506
C,0.6638632562,3.2107853926,0.7159787745
C,-1.6693034757,2.7292468633,0.3567435413
C,0.3197399066,4.4087421885,1.3490310389
C,-2.0154969853,3.924680686,0.9879772828
C,-1.0215530827,4.7727731527,1.4889917114
Si,-0.4791175865,-0.4478516322,0.6900703143
C,0.3524272346,-0.167619703,2.3661280096
C,0.0783650925,-2.1044922049,-0.0384651279
C,-2.3563189624,-0.5656957867,0.9503165307
O,5.0268625981,-0.8587540876,-0.5342945397
S,5.018744261,-0.5607041316,1.0051763096
C,4.095478463,0.9863708887,1.2331511545
C,3.8104138736,-1.7022945824,1.7326634721
H,-1.6103264728,0.5790177041,-1.8929845107
H,-1.1593413027,4.8542469683,-2.3288689123
H,-1.5184309101,4.3878659191,-4.01674319
H,-2.8544398361,4.5670499122,-2.8341524417
H,1.7025477043,2.9191572396,0.6039630057
H,-2.4547170221,2.0942782362,-0.0393373548
H,1.1026849916,5.0572592395,1.7361996051
H,-3.0641304813,4.1957274506,1.0857342695
H,-1.2916029912,5.7023816888,1.9837210536
H,0.2904977963,-1.0646485873,2.9961144596
H,1.4095753721,0.0854002107,2.2376834028
H,-0.12582954,0.6563825372,2.9106027404
H,-0.1389103938,-2.9128083676,0.6733631765
H,-0.4503106726,-2.3341634948,-0.9719581071
H,1.1528022605,-2.1225653535,-0.2500470433
H,-2.9030113298,-0.6039394008,-0.0010713233
H,-2.5986713241,-1.4845062715,1.5024016259
H,-2.7460680952,0.2793909636,1.5290922599
H,4.0010403076,1.165138945,2.3096518113
H,4.6926731826,1.7836688483,0.7811652294
H,3.1098407184,0.916009926,0.7501146221
H,4.2064623765,-2.7151371221,1.6201389649
H,3.7000511594,-1.4603360253,2.7944275359
H,2.8545682046,-1.6028437473,1.2113048403
---end---

TS1-C-t

Electronic_Energy=-1814.51062137
Sum of electronic and thermal Free Energies = -1814.204575
Charge=0 Multiplicity=1
---Coordinates start---
C,-0.151162481,0.8941913106,0.131869003
C,-0.476918469,0.8281161139,-1.925560331
N,0.8112011065,0.4339215536,-2.2609758399
C,1.8221250904,0.1394875028,-1.694489633
Ag,3.7335343487,-0.4068102848,-1.2849259049
C,-0.8622765938,2.1594285277,-2.4282018414
O,-0.1058383248,3.0359445427,-2.8126701518
O,-2.2060957623,2.3207136379,-2.3361059696
C,-2.6929578774,3.6403956581,-2.630801692
O,1.0421982333,0.3811931277,0.2599849396
C,-0.2576479287,2.379505305,0.417492407
C,0.9161522842,3.1435386471,0.5169611461
C,-1.4887596324,3.0293938055,0.6033433314
C,0.8650111323,4.5117438544,0.7843329118
C,-1.543982127,4.3985735557,0.8761920812
C,-0.3673958016,5.14825794,0.9666027267
Si,-1.4818425309,-0.3693185813,0.6958609683
C,-1.4444991662,-0.436294387,2.5888852912
C,-0.9328338331,-2.0364177455,-0.0041216704
C,-3.2606391354,-0.0165061394,0.1346733266
O,5.7366891594,-0.9828032296,-0.7661397446
S,6.3391447512,-0.8698990354,0.6738550624
C,6.0274707956,0.8308920524,1.2206866346
C,5.1753466846,-1.7157479449,1.7777825572
H,-1.2182607679,0.0556917224,-2.1185484104
H,-2.2136790897,4.3823463131,-1.9865976665
H,-2.5104385494,3.8959285525,-3.6792861006
H,-3.7658429499,3.6086478724,-2.4340631269
H,1.8684725085,2.6389031615,0.3846342602
H,-2.4146583906,2.4718507406,0.5166242042
H,1.7875327526,5.0842117485,0.8532589767
H,-2.5090741739,4.8792828151,1.0181887026
H,-0.4102636968,6.2134484636,1.1794582683
H,-2.142032671,-1.189782681,2.978495174
H,-0.440564597,-0.6877026141,2.9537911318
H,-1.7246653886,0.531849635,3.0243089483
H,-1.5558589638,-2.8506975574,0.3885504865
H,-1.00128829,-2.0653498244,-1.0990245871
H,0.1088368836,-2.2346749299,0.271071
H,-3.3016138306,0.4094740551,-0.8740353384
H,-3.8423602867,-0.9485035023,0.1316072921
H,-3.7693423044,0.6809315655,0.8117477931

H,6.3457107005,0.9231283174,2.2641536511
H,6.6223814576,1.4950686408,0.5881101178
H,4.9598279728,1.0545853288,1.1172831869
H,5.1833517877,-2.7766033637,1.5138738308
H,5.5181619383,-1.5844696034,2.8093056632
H,4.1740490262,-1.2925456431,1.6430049336
---end---

IN2-t

Electronic_Energy=-1814.56485707
Sum of electronic and thermal Free Energies = -1814.251517
Charge=0 Multiplicity=1
---Coordinates start---
C,-0.489427665,0.9966251675,-0.0941368503
C,-0.5182883096,0.9001690072,-1.6630197524
N,0.7084166172,0.1547613048,-2.0106997259
C,1.4332109498,0.0360294588,-0.9509092377
Ag,3.3120478698,-0.8072023119,-0.8053528539
C,-0.4777410098,2.2684268792,-2.3407258846
O,0.4920549271,2.9970448925,-2.3792745071
O,-1.672611812,2.581929405,-2.8776609296
C,-1.782360551,3.9133197423,-3.420949732
O,0.8842951524,0.5410811541,0.2036607605
C,-0.7153842676,2.363278397,0.5125910931
C,0.1975943988,2.9204987383,1.420843693
C,-1.8901471512,3.081809939,0.2218825642
C,-0.0465870315,4.1652869492,2.006704103
C,-2.130464748,4.3268025951,0.8054627597
C,-1.2095673002,4.8762440268,1.7020039309
Si,-1.6204198622,-0.3375301726,0.7448386744
C,-1.3094135719,-0.2515187655,2.6019238399
C,-1.1170712651,-2.0189131636,0.0515394994
C,-3.432410201,0.0076885289,0.3452192099
O,5.2677840356,-1.7243727773,-0.7258263105
S,6.4161277401,-1.3110816133,0.2485325469
C,6.6195485077,0.4821545158,0.063909667
C,5.6999812095,-1.3182819226,1.915659772
H,-1.403237009,0.3689264472,-2.0241092525
H,-1.6018624752,4.6566111367,-2.6387982332
H,-1.0673642224,4.058588987,-4.235430585
H,-2.804028154,3.995991776,-3.7938179645
H,1.1035740553,2.3769073784,1.6638079834
H,-2.6140563411,2.6746234517,-0.4760261973
H,0.6778183771,4.5788446002,2.7041396934
H,-3.0413127178,4.8660982537,0.5578972499
H,-1.3977020251,5.8446520624,2.1579587477
H,-1.8751726845,-1.0293335159,3.1308765302
H,-0.2460536961,-0.396867428,2.8283111063
H,-1.6113946984,0.720201804,3.0107398301
H,-1.7289689459,-2.8150069553,0.4955402378
H,-1.2488555514,-2.0633083664,-1.0363338845
H,-0.0657812941,-2.23716698,0.2732584649
H,-3.5987630722,0.0986087677,-0.7356206608
H,-4.0579958221,-0.8193405237,0.7066310415
H,-3.788806214,0.927730128,0.8219401117
H,7.3567167251,0.8267216662,0.7964650487
H,6.9846465263,0.6683716725,-0.9496070221
H,5.653405655,0.9737348032,0.2202557141
H,5.4413150961,-2.3524155647,2.1586278618
H,6.4524234023,-0.9461554019,2.6185929631
H,4.8066942644,-0.684750434,1.9289253654
---end---

TS2-C-t

Electronic_Energy=-1814.51761805
Sum of electronic and thermal Free Energies = -1814.210896
Charge=0 Multiplicity=1
---Coordinates start---
C,-0.9371804476,1.149237077,0.0176607494
C,-0.7257539734,1.0774958943,-1.3872495933
N,0.987875586,0.2606951863,-1.674010148
C,1.3886357609,0.1082447773,-0.4926733084
Ag,3.3426862433,-0.7185211364,-0.7890859909
C,-0.4741170525,2.3076618459,-2.1936616271
O,0.2037937866,3.2634062841,-1.8657739814
O,-1.0919195552,2.2161627081,-3.3938256715
C,-0.8880519599,3.3310189558,-4.2806072252
O,0.9436986479,0.3246206747,0.6590620067
C,-0.9851431548,2.4517518269,0.7481375735
C,-0.1873412882,2.7448364847,1.8665937197
C,-1.9771826615,3.3829923279,0.3797365429
C,-0.3581165146,3.9371368879,2.5744663688
C,-2.1521132062,4.569282044,1.0925384562
C,-1.3401017225,4.8550834349,2.1938234116
Si,-1.9065190899,-0.2739871895,0.8339689795
C,-1.5455429925,-0.3310473211,2.6824835433
C,-1.4502824897,-1.9093931437,0.0102398916
C,-3.7430046253,0.0963832053,0.5619671752
O,5.3363703426,-1.578769262,-1.0012110602
S,6.5742987211,-1.1419135516,-0.1555043326

C,6.6917212327,0.6605435559,-0.3194694578
C,6.053242387,-1.207965123,1.580530633
H,-1.2736128027,0.3147930519,-1.9319837085
H,-1.2626076706,4.2562868828,-3.8324329012
H,0.1739172716,3.4502527746,-4.5167208363
H,-1.4509349229,3.0960102751,-5.1853875365
H,0.5772002048,2.0381851188,2.1653909231
H,-2.6172652581,3.1679542979,-0.472032006
H,0.2804150288,4.1463275152,3.4293938442
H,-2.9239595125,5.2705512443,0.7851091469
H,-1.4731828124,5.7798928635,2.7490573079
H,-2.1280048802,-1.1298235016,3.1603298154
H,-0.483462421,-0.5257307994,2.8678463415
H,-1.8081792743,0.6129740381,3.1741004075
H,-2.0570748383,-2.7256882817,0.4238286306
H,-1.6216597232,-1.8866622289,-1.0727474848
H,-0.3947957078,-2.1504382095,0.1814315495
H,-3.9926440531,0.1204449738,-0.5064559086
H,-4.3725198689,-0.6682797585,1.0363206084
H,-4.0169305871,1.0684532627,0.991123933
H,7.4883841375,1.0196711099,0.3402393663
H,6.9411043818,0.8809320322,-1.3608294776
H,5.7292739522,1.1103434573,-0.051273343
H,5.864255851,-2.255759808,1.8282740884
H,6.8645876514,-0.8166768098,2.2028170585
H,5.1421528798,-0.6124529448,1.7069055262
---end---

IN3-t

Electronic_Energy=-1814.60232175
Sum of electronic and thermal Free Energies = -1814.293361
Charge=0 Multiplicity=1
---Coordinates start---
C,-0.827071924,1.0312011718,0.2096717842
C,0.1146694833,0.8871332301,-0.7460408725
N,1.2596163549,-1.4845972545,1.9064798414
C,0.7108978132,-1.2174894899,2.9401175013
Ag,2.9874878743,-1.0785022319,0.8403659714
C,1.1940518902,1.8658999217,-1.0322267034
O,1.7653212504,2.5868359541,-0.2314416847
O,1.4780013404,1.8603877623,-2.3561998597
C,2.4056429368,2.8667030362,-2.810922411
O,0.1078205079,-0.9852590287,3.9563186566
C,-0.9242658591,2.245883489,1.0654620263
C,-0.7805624141,2.1660435488,2.4612864972
C,-1.2278250494,3.4911202703,0.4881036321
C,-0.9054589774,3.3106732088,3.2518599724
C,-1.3676582111,4.6300845453,1.282207711
C,-1.2019940235,4.5454553462,2.667731605
Si,-2.2552264683,-0.2381312802,0.3096678448
C,-2.8355702578,-0.469087772,2.0883650269
C,-1.6919660217,-1.8836910122,-0.4188621938
C,-3.667531913,0.5027202391,-0.7062967895
O,4.9501509693,-1.0403200335,-0.0346380302
S,5.5229683877,-0.0084560217,-1.0575730266
C,4.3708244817,-0.0023888019,-2.4568784708
C,5.1575137476,1.6325503353,-0.3815364854
H,0.0929488312,0.0354373009,-1.4218921942
H,1.9840155939,3.8642613047,-2.6531256304
H,3.3609846482,2.7928321197,-2.2890586434
H,2.5411628107,2.6795537931,-3.8767316291
H,-0.5591416454,1.211621071,2.9293027503
H,-1.3511743364,3.5585434311,-0.5897499663
H,-0.7764277036,3.2342075715,4.3286406045
H,-1.6034901294,5.5842301165,0.817593373
H,-1.307397772,5.4325196417,3.2867522543
H,-3.6717081182,-1.1812202598,2.1043255271
H,-2.0487582026,-0.8572423113,2.7438240546
H,-3.1946076137,0.4740001341,2.5166279027
H,-2.4963924832,-2.6264172856,-0.3374067266
H,-1.425346138,-1.8004151187,-1.4794260971
H,-0.8201995617,-2.2669209231,0.1253818392
H,-3.3802076304,0.6261451071,-1.7579980369
H,-4.5544709173,-0.1435554831,-0.6714702226
H,-3.9562176935,1.4883216878,-0.3194611779
H,4.6652911408,0.7894611459,-3.1524111293
H,4.4499372078,-0.976416148,-2.9474516319
H,3.352829336,0.1572009274,-2.0890852193
H,5.7172902411,1.7269042874,0.5529953675
H,5.5030424857,2.3865895974,-1.0962256063
H,4.0826067318,1.7321081602,-0.1985333051
---end---

IN1-c

Electronic_Energy=-1814.53782357
Sum of electronic and thermal Free Energies = -1814.231600
Charge=0 Multiplicity=1
---Coordinates start---
C,-0.9410839697,1.0093992736,1.4755019328
C,-1.8349381829,1.00275734,-2.0940942912

N,-0.5180733233,0.8556179875,-1.8921730271
C,0.6385219197,0.7025947091,-1.719193713
Ag,2.1483449865,0.1844282028,-0.433608674
C,-2.6100572711,-0.1445585177,-2.4111193432
O,-2.2087687808,-1.2980016577,-2.604990339
O,-3.950567521,0.1738867336,-2.4760720871
C,-4.8226970585,-0.9330836483,-2.7158325145
O,0.2526523076,0.8633040339,1.7777985366
C,-1.4193344328,2.3470540358,1.0246955337
C,-0.4831205165,3.2763398681,0.5359745631
C,-2.7790885118,2.6949054854,1.0548678672
C,-0.902247997,4.5173750344,0.0647721574
C,-3.1960084249,3.9480854458,0.6045302182
C,-2.2609359137,4.8559329291,0.0988549176
Si,-1.9672218446,-0.6456825015,1.6093894908
C,-1.8664469218,-1.1073844645,3.4382685346
C,-0.992147922,-1.8793117632,0.5708563481
C,-3.7615539213,-0.5845290331,1.0249169139
O,3.8107161009,-0.3588035892,0.8317629917
S,3.8277993726,-1.4991189283,1.9017808834
C,2.4836164089,-1.1386962089,3.0660133403
C,3.102872692,-2.9594448379,1.1076807507
H,-2.2670424551,1.9770828224,-1.9119116302
H,-4.6119934243,-1.4088464549,-3.6798919775
H,-4.7368065418,-1.6869630634,-1.9255894724
H,-5.8339118194,-0.5193499684,-2.7218627138
H,0.5662259712,2.9994363992,0.511683208
H,-3.5135009037,1.9959921206,1.439236731
H,-0.1758069969,5.222987862,-0.3297432327
H,-4.2491909593,4.2126498405,0.6401952329
H,-2.5883339596,5.8250980423,-0.2680636499
H,-2.3258903009,-2.0883560258,3.6164118795
H,-0.8196994165,-1.1597045044,3.7632334085
H,-2.3822652586,-0.3750779165,4.0720343503
H,-1.2685131138,-2.9064869683,0.8452698506
H,-1.1926516604,-1.7484157505,-0.4986264561
H,0.082409882,-1.7593198257,0.7459805712
H,-3.8649555415,-0.0820233116,0.0574459179
H,-4.1297541893,-1.6130501763,0.9077076521
H,-4.418658236,-0.0829668205,1.7455966441
H,2.3472462235,-2.0125864164,3.7112889004
H,2.7895140905,-0.2773221112,3.665869209
H,1.5716467297,-0.9028170889,2.5102350418
H,3.764014826,-3.2472759384,0.2861561157
H,3.053166425,-3.7657787369,1.8468704301
H,2.1039493549,-2.7165159377,0.7320279985
---end---

TS1-C-c

Electronic_Energy=-1814.50752203
Sum of electronic and thermal Free Energies = -1814.201359
Charge=0 Multiplicity=1
---Coordinates start---
C,0.0076449165,1.3203120742,-0.1553665853
C,-0.1656556325,1.1378192113,-2.1767842704
N,1.1004320028,0.6135441399,-2.417146869
C,2.1135944706,0.3992999606,-1.8308524488
Ag,3.9554932119,-0.2055777083,-1.2381992353
C,-1.2667694489,0.298092084,-2.7038055173
O,-1.2111072154,-0.8949659398,-2.9585688101
O,-2.3963214289,1.0325456302,-2.851749668
C,-3.5415707055,0.3247317717,-3.360030507
O,1.2653483833,1.0654964504,0.0871595176
C,-0.4385437079,2.7646107448,0.0042520472
C,0.4390431058,3.695020252,0.5799073844
C,-1.7311215055,3.1937572274,-0.346985168
C,0.0432096489,5.0178811648,0.795406716
C,-2.1294325275,4.5132838588,-0.1297289324
C,-1.2443196992,5.4331160236,0.4448303856
Si,-1.019380824,-0.0533783077,0.7177979229
C,-0.7405420012,0.2260043873,2.5714139162
C,-0.2844026735,-1.716637246,0.2088048916
C,-2.8934752628,-0.0469407131,0.4314383462
O,5.8905139775,-0.8667236004,-0.5875285754
S,6.1967452857,-1.4357110362,0.8381189671
C,5.6025748036,-0.1939588251,2.0185911267
C,4.9464891435,-2.7111934879,1.1531893783
H,-0.242763971,2.1720595954,-2.5075410749
H,-3.3619877649,0.0001988816,-4.3897693056
H,-3.7754578132,-0.5484122719,-2.7453842536
H,-4.3650930382,1.0395138618,-3.3292806706
H,1.4335641775,3.358825648,0.8568612857
H,-2.4139762498,2.4950777746,-0.8204825684
H,0.739305896,5.7241390248,1.2427315868
H,-3.131159787,4.8272141315,-0.414249681
H,-1.5560542996,6.4604863205,0.615629475
H,-1.2401178118,-0.5464434058,3.1712797733
H,0.3290597406,0.2043195891,2.8122958796
H,-1.1339080789,1.2000785446,2.8906883323
H,-0.7497847251,-2.5426804929,0.7628366125

H,-0.4281186324,-1.8963876357,-0.8619695602
H,0.792008472,-1.7276062264,0.4161771399
H,-3.1694081572,-0.1946250837,-0.6168064185
H,-3.3568219603,-0.8570105769,1.011801375
H,-3.3433023854,0.8953630298,0.7668364323
H,5.7149907886,-0.5968745326,3.0305464615
H,6.2238506412,0.6976962019,1.9004509853
H,4.5530862393,0.0365077866,1.8057260331
H,5.1208395715,-3.5254055716,0.4450175025
H,5.0705194019,-3.0733859686,2.1789711691
H,3.948326079,-2.2827775904,1.009753396
---end---

IN2-c

Electronic_Energy=-1814.56451467
Sum of electronic and thermal Free Energies = -1814.250883
Charge=0 Multiplicity=1
---Coordinates start---
C,-0.325794406,1.4495403937,-0.3230418184
C,-0.3392077157,1.40352783,-1.8951140863
N,1.0026525346,0.9300795686,-2.2749402892
C,1.7354901791,0.8689989558,-1.216899079
Ag,3.7008959376,0.2452973823,-1.0923419856
C,-1.420273866,0.5237646882,-2.5131472471
O,-1.323722965,-0.6609243059,-2.7626635293
O,-2.5311301398,1.2452310861,-2.7613171402
C,-3.6353654488,0.5340348639,-3.357526437
O,1.1078105939,1.2129543119,-0.0410220298
C,-0.7419067885,2.7967389619,0.2250410626
C,0.0455029834,3.4881081906,1.1582881
C,-1.9715282671,3.357102268,-0.1628350208
C,-0.3825428151,4.7096614013,1.6843990993
C,-2.3992547654,4.5755855644,0.3678231477
C,-1.6072898203,5.2580425072,1.2954844634
Si,-1.164427607,0.0139876337,0.6952746903
C,-0.9081745909,0.4388839939,2.5158385523
C,-0.2850088261,-1.6018986596,0.2809679471
C,-3.0151891879,-0.1075986639,0.3358504721
O,5.7580678323,-0.4160426586,-1.0318854198
S,6.4054621542,-1.2077340396,0.148824498
C,6.0637899146,-0.2531052184,1.6536958076
C,5.3078182965,-2.6128628603,0.483801284
H,-0.4971771624,2.414783078,-2.2893506093
H,-3.3452088001,0.130114438,-4.331501124
H,-3.9700455565,-0.280771648,-2.7107829036
H,-4.4286470502,1.2731697626,-3.4743965368
H,0.9959774957,3.0674141263,1.4670148911
H,-2.5899617809,2.8417683158,-0.8915430662
H,0.2450873693,5.2323451387,2.4020712985
H,-3.3519930498,4.99275515,0.0513992939
H,-1.9397302179,6.2069847936,1.7079593773
H,-1.23924557,-0.3970664752,3.1462483846
H,0.1487314899,0.6276587575,2.7388897652
H,-1.4794206562,1.326818259,2.8101922653
H,-0.7456725828,-2.4387478412,0.8226470168
H,-0.3404985683,-1.8142384294,-0.7913870933
H,0.7717713023,-1.5518372705,0.5689222087
H,-3.215864939,-0.6185451528,-0.6111054497
H,-3.5016567941,-0.6882694047,1.1309555321
H,-3.4948277321,0.8773719796,0.3059132917
H,6.4169480863,-0.8276491416,2.5162647448
H,6.6155766229,0.6879142447,1.5803360637
H,4.9873648473,-0.0631236254,1.7254035268
H,5.3415428551,-3.2725556279,-0.3872344449
H,5.6798394211,-3.1408444852,1.3677920478
H,4.2893801439,-2.244585137,0.6476326376
---end---

TS2-C-c

Electronic_Energy=-1814.51819721
Sum of electronic and thermal Free Energies = -1814.210939
Charge=0 Multiplicity=1
---Coordinates start---
C,-0.9924733895,1.2428152409,-0.0408035781
C,-0.7630794087,1.4244014159,-1.4359305685
N,1.0195292874,0.8668996174,-1.8078739307
C,1.4040158889,0.4628622529,-0.6791321626
Ag,3.4022177637,-0.1872422757,-1.1091502203
C,-1.4168535708,0.5769672009,-2.4686789074
O,-1.8128949778,-0.5698723235,-2.3385715219
O,-1.5204701472,1.2562898892,-3.6300901452
C,-2.1128103835,0.5317729017,-4.7236075817
O,0.9237621816,0.3868070029,0.4747141667
C,-0.9675512389,2.504486889,0.7662615218
C,-0.1869923035,2.6724034433,1.9245103517
C,-1.8185851247,3.5613466016,0.3853269785
C,-0.2478229443,3.8537140387,2.6644481537
C,-1.8853221648,4.7399246038,1.1323404634
C,-1.0984661316,4.893149523,2.2755345328
Si,-1.9154071679,-0.2366454085,0.7652776549

C,-1.8946233297,-0.0010879481,2.6428800465
C,-1.1424193977,-1.9216525242,0.4129342685
C,-3.7249928823,-0.1371869452,0.2173622181
O,5.4361614309,-0.8626887557,-1.5169113497
S,6.5868912096,-0.8587537122,-0.4610170294
C,6.6482789748,0.82237085,0.2177970883
C,5.9334908967,-1.7024227969,1.0056379164
H,-0.6415571081,2.4527003616,-1.7656927055
H,-1.5217559769,-0.3567101255,-4.965552325
H,-3.13547192,0.2289695361,-4.4793252782
H,-2.1160281776,1.2233801669,-5.567451013
H,0.4844675937,1.8780020696,2.2248890698
H,-2.4440727962,3.4497978523,-0.4962453587
H,0.3754659471,3.9626153422,3.548621336
H,-2.5537130823,5.5371092711,0.816799609
H,-1.1455270967,5.8106256956,2.8561788992
H,-2.4482710267,-0.8298033157,3.1059054516
H,-0.8774029382,-0.0159177369,3.0507312215
H,-2.3713035588,0.9337985345,2.9587606181
H,-1.8304665207,-2.724369744,0.7124180539
H,-0.9171666619,-2.0409073581,-0.6490877254
H,-0.2163819389,-2.0345125508,0.9871089279
H,-3.826193089,-0.2912765732,-0.8611497587
H,-4.3263780943,-0.8992669494,0.731386962
H,-4.1524369144,0.8432442474,0.4660438506
H,7.3756085486,0.8420309808,1.0359760818
H,6.9705396948,1.4906521518,-0.5850714746
H,5.6516696041,1.1040263488,0.575491572
H,5.7638434262,-2.7481756565,0.7359692444
H,6.6779841541,-1.6382464418,1.8060199147
H,4.9942325616,-1.2250717778,1.3065518208
---end---

IN3-c

Electronic_Energy=-1814.60824144
Sum of electronic and thermal Free Energies = -1814.299899
Charge=0 Multiplicity=1
---Coordinates start---
C,-2.0122867732,0.7284210948,0.4703953064
C,-1.1473874626,0.751658517,-0.5733453088
N,0.1698698478,-1.4051934587,3.3896012628
C,-0.860765604,-1.402280026,4.008430904
Ag,0.7191690947,-1.3837082628,1.3809748722
C,-1.0544240516,-0.2535990545,-1.6500619238
O,-1.686185408,-1.2942837526,-1.7406941299
O,-0.155746837,0.1403846701,-2.5818630569
C,0.0830200367,-0.7960079236,-3.6488541738
O,-1.8654883852,-1.3864625195,4.6700097783
C,-1.948213199,1.9003263071,1.3912557017
C,-1.8450744204,1.7396275401,2.784939213
C,-1.9803359142,3.2093833954,0.8733318565
C,-1.7485451344,2.8476023553,3.6274257083
C,-1.9019061123,4.3176877068,1.7184997856
C,-1.779559631,4.1416003362,3.099214351
Si,-3.4156342674,-0.5766063245,0.7280053984
C,-4.4385047688,-0.0936965918,2.2447002538
C,-2.7697459433,-2.3260727191,1.0238618652
C,-4.5699188458,-0.4432093231,-0.7625942516
O,1.4821443924,-1.5503099928,-0.6360883947
S,2.7515615026,-0.8159734028,-1.1711007613
C,2.5425292495,0.9437181401,-0.7843562959
C,4.0756719459,-1.1782439995,0.0152718548
H,-0.4377943786,1.5711186773,-0.6640928266
H,0.4406494172,-1.7461685677,-3.2436161598
H,-0.8304672451,-0.9648291466,-4.2263593708
H,0.8473075582,-0.3367775402,-4.2773283691
H,-1.8294687171,0.7455161067,3.2141191019
H,-2.0861443026,3.3535772046,-0.1983347058
H,-1.655975783,2.6969884178,4.6999476987
H,-1.938916599,5.3187499349,1.2965940722
H,-1.7169507861,5.0035362295,3.7580700031
H,-5.3593256654,-0.6937182164,2.2429688596
H,-3.9164219952,-0.2981275218,3.1857208236
H,-4.7323949226,0.9623808662,2.2363526724
H,-3.5905381495,-3.0441480019,0.8864439103
H,-1.968536982,-2.5912571441,0.3295914402
H,-2.4058460569,-2.4359462679,2.0514978635
H,-4.0551619187,-0.6695670534,-1.6998374823
H,-5.4099826626,-1.1421170715,-0.6521703398
H,-4.9894879666,0.5689232187,-0.8311685751
H,3.492191875,1.4534523234,-0.9766322122
H,1.7654400803,1.3328976169,-1.4434633799
H,2.2515001612,1.0473439639,0.2666660086
H,4.2644456347,-2.25441079,-0.0214345615
H,4.974180926,-0.6295629141,-0.285587675
H,3.7539291669,-0.8783370359,1.0187403887
---end---

TS1-S-c

Electronic_Energy=-1814.51618155
Sum of electronic and thermal Free Energies = -

1814.204027

Charge=0 Multiplicity=1

---Coordinates start---

C,0.1271742347,0.7022523817,0.0533869806

C,-0.5449600774,0.9266915769,-1.7359604446

N,0.2433387652,0.0630218248,-2.4850264246

C,1.1459243332,-0.628370139,-2.7838791962

Ag,2.6856336244,-1.12849426,-1.4052947413

C,-1.999680301,0.6428622163,-1.9276734055

O,-2.4803609085,-0.4571808207,-2.1439489689

O,-2.7289813585,1.7670219401,-1.8028646926

C,-4.1606289766,1.5999283535,-1.8495204148

O,1.414824774,0.4189265971,-0.0209239986

C,-0.1619122841,2.0823571828,0.6460706506

C,0.9161971665,2.8902587115,1.04247573

C,-1.4641267055,2.5553720615,0.8843523357

C,0.7033410846,4.1345642949,1.6400962871

C,-1.679205267,3.7972689457,1.4845810282

C,-0.5964347003,4.5957768801,1.8652389158

Si,-0.7513891187,-0.8061827776,0.9104128208

C,0.1161521893,-0.9920098268,2.5847460585

C,-0.483517319,-2.3684357775,-0.1186663226

C,-2.6098246105,-0.6477630243,1.2607226932

O,4.5330324496,-1.3806321068,-0.1992263321

S,4.9966640189,-0.3122667323,0.8421853844

C,4.7299063871,1.3125194209,0.0720324627

C,3.6842201127,-0.2001616767,2.0913920941

H,-0.2907090956,1.9620900964,-1.9596449454

H,-4.4646323319,1.1497751833,-2.7983928441

H,-4.5033958401,0.9732126681,-1.0213218065

H,-4.5732711549,2.6050839573,-1.7561849561

H,1.9239774736,2.5220673598,0.8843458432

H,-2.3198915449,1.9613477742,0.5918882053

H,1.5553525263,4.7413569659,1.9386309528

H,-2.6969507042,4.1400538812,1.6554464328

H,-0.7646439937,5.5609287993,2.3363118484

H,1.1070641758,-1.4448979951,2.4756292292

H,0.2423344039,-0.0223787286,3.0831111425

H,-0.4746781525,-1.6342160889,3.2513430538

H,-0.954251366,-3.2262200842,0.3813200662

H,-0.935539945,-2.2628658933,-1.1101752102

H,0.5814489588,-2.6006942559,-0.242305274

H,-3.2015812327,-0.5032354665,0.3511852711

H,-2.9543840845,-1.5806761715,1.7293145287

H,-2.835042104,0.1680245734,1.9569825575

H,4.9859823088,2.0867599922,0.8030716222

H,5.3958911621,1.3821936601,-0.7923363475

H,3.6802046585,1.3944632981,-0.2305149237

H,3.6544217758,-1.1564113479,2.619960717

H,3.9478001526,0.6010373143,2.790459342

H,2.7361064406,0.0098752623,1.5831669951

---end---

IN2-S-c

Electronic_Energy=-1814.51837140

Sum of electronic and thermal Free Energies = -1814.203874

Charge=0 Multiplicity=1

---Coordinates start---

C,-0.8066248745,0.3677807295,0.1481919993

C,-1.3275741664,0.5529940048,-1.4101824956

N,-0.7646788557,-0.4964799639,-2.1983113474

C,0.1115627617,-1.2575703982,-2.4050737001

Ag,1.7221152662,-1.4766662004,-0.9923667844

C,-2.8328516195,0.5689209945,-1.6148431447

O,-3.5380593008,-0.4216766644,-1.5892793947

O,-3.281642708,1.8149386763,-1.8053376345

C,-4.7165632123,1.964516538,-1.8762959721

O,0.5409320831,0.131259201,0.1514230304

C,-1.1259325653,1.7131728343,0.83319029

C,-0.0664324804,2.5214087015,1.2750642228

C,-2.4368915145,2.1588218824,1.0802124488

C,-0.3048274729,3.7356415895,1.9241723958

C,-2.6784149226,3.3699799865,1.7310869244

C,-1.6124777731,4.1683212254,2.155989987

Si,-1.5939381999,-1.1319805393,1.1335216909

C,-0.5310231055,-1.3028407139,2.6897615589

C,-1.5117475772,-2.7474604257,0.1493620731

C,-3.3928242586,-0.9401044427,1.7143698032

O,3.7191682855,-1.4769737441,0.0382387933

S,4.1524549523,-0.2739560544,0.9345307168

C,3.7431479242,1.2357375091,0.006770896

C,2.8895016179,-0.1032511722,2.2287368745

H,-0.8932855257,1.4897728229,-1.7703937207

H,-5.1191957793,1.3956338017,-2.7183866526

H,-5.1809300944,1.6228502615,-0.9468073151

H,-4.8910112668,3.0312409542,-2.0179619054

H,0.9475739791,2.178309523,1.1079967611

H,-3.287016583,1.5604594887,0.7757582464

H,0.5357259757,4.3413956981,2.2556187208

H,-3.7035316162,3.6865413114,1.9076490787

H,-1.8001206444,5.1095502068,2.666457308
H,0.4489412869,-1.7316105602,2.457205665
H,-0.3668471756,-0.3321257085,3.1742854754
H,-1.0258497725,-1.9600815619,3.4174499664
H,-1.9246340279,-3.5594290765,0.7643344277
H,-2.1084399426,-2.6800800946,-0.7662716559
H,-0.4884641224,-3.0301449194,-0.1254451047
H,-4.0848126708,-0.7500725788,0.8872302997
H,-3.70294732,-1.8768203419,2.1989544362
H,-3.5067190465,-0.1378285063,2.4523880859
H,3.9934832466,2.1013844266,0.6290963651
H,4.3547138544,1.2411729924,-0.8997756596
H,2.67452746,1.2244638963,-0.2357611639
H,2.9460462621,-0.9940462835,2.8598723425
H,3.1312326932,0.7854490207,2.8220470456
H,1.9082535463,-0.0092023263,1.7470007214
---end---

TS2-S-c

Electronic_Energy=-1814.51247412
Sum of electronic and thermal Free Energies = -1814.199573
Charge=0 Multiplicity=1
---Coordinates start---
C,-0.8558481109,0.5226402103,0.0857648759
C,-1.4551477928,0.7039883395,-1.4628913278
N,-0.6724129316,-0.1644604307,-2.2967878542
C,0.3844213648,-0.6892691333,-2.1459409378
Ag,2.1891389675,-1.3362728391,-1.4467968859
C,-2.9258191807,0.386636059,-1.6755343699
O,-3.3742893456,-0.72979035,-1.8518214214
O,-3.6772793633,1.4970095098,-1.6330048278
C,-5.1055182888,1.2979897247,-1.7188974547
O,0.4629594767,0.176149529,0.0023358869
C,-1.0578235382,1.8719116494,0.7945283281
C,0.0616611436,2.5422546539,1.3128744063
C,-2.3248710203,2.4408171803,1.0167805135
C,-0.0737433765,3.747881106,2.0062081271
C,-2.4628263392,3.6459972846,1.7088069917
C,-1.3372516327,4.3091620048,2.2071545075
Si,-1.64401502,-0.9270356807,1.116464528
C,-0.7214727526,-0.9566222237,2.7732861523
C,-1.3549240494,-2.5611838185,0.210365659
C,-3.4948982193,-0.7697497917,1.5237579619
O,4.0071542787,-1.4477490921,-0.2710016315
S,4.2236503596,-0.4583978474,0.9277949198
C,3.8169964884,1.1998101321,0.3072600586
C,2.7899413212,-0.6578073351,2.022866309
H,-1.2595127486,1.7316208149,-1.7835008942
H,-5.367062482,0.811966901,-2.6624544135
H,-5.4573880891,0.6888331138,-0.881755711
H,-5.5407240856,2.296454769,-1.6702551238
H,1.0382951196,2.0952203851,1.1680518254
H,-3.2143585122,1.9461400866,0.6471859733
H,0.811233897,4.2461793892,2.3962690246
H,-3.454887087,4.0649658566,1.8609455795
H,-1.4456360769,5.2449705751,2.7496563031
H,0.2177138085,-1.5147094822,2.6994425246
H,-0.4853082285,0.0556883158,3.1237422171
H,-1.3356465536,-1.4409580522,3.5440627691
H,-1.685551456,-3.409393253,0.8253360273
H,-1.9072686335,-2.5864244549,-0.7351058358
H,-0.2890014715,-2.6948827647,-0.0083924981
H,-4.1227084202,-0.7214888103,0.6277048615
H,-3.8136771774,-1.6497813079,2.1003860202
H,-3.7030194438,0.1145542467,2.1378607864
H,3.9214022735,1.9074714765,1.1366092188
H,4.5321491667,1.4440111315,-0.4827650019
H,2.7892266655,1.1967161512,-0.0731646561
H,2.8111059286,-1.6840538125,2.3992431514
H,2.904030075,0.0434310457,2.8566716799
H,1.8718820927,-0.4491241619,1.4561276573
---end---

TS1-C-c-Et-TMS

Electronic_Energy=-1853.83040036
Sum of electronic and thermal Free Energies = -1853.495981
Charge=0 Multiplicity=1
---Coordinates start---
C,0.182113329,1.4388674285,-0.3565693993
C,-0.0482231895,1.2563067213,-2.2824196516
N,1.2029119552,0.735633225,-2.6208780978
C,2.2623160668,0.4933924642,-2.1532659833
Ag,3.9766181839,-0.1993861307,-1.3219337145
C,-1.1671723666,0.3868822862,-2.7434793759
O,-1.0921467371,-0.8079176156,-2.9826116264
O,-2.3112915192,1.0976210148,-2.8311490229
C,-3.5109826309,0.3855461145,-3.2242807102
O,1.4640509406,1.3011312473,-0.1197422723
C,-0.3903915231,2.8356931584,-0.1285032501
C,0.4321859264,3.8233035365,0.4332654216

C,-1.7324090106,3.1609923141,-0.3949086433
C,-0.0626919148,5.0998475334,0.7128862236
C,-2.2299457439,4.4346564055,-0.1141690831
C,-1.3979039328,5.4123527391,0.4428465689
Si,-0.667861785,-0.0188845383,0.5792716296
C,-0.3698993757,0.3434177992,2.4152395103
C,0.2381275889,-1.6022441453,0.0845967813
C,-2.5358569125,-0.2659301107,0.3504408544
O,5.7046191297,-0.9915520443,-0.3245138633
S,5.688927296,-1.5763987143,1.1277714689
C,4.9156689128,-0.3148834195,2.1765405445
C,4.3513847343,-2.8002787053,1.166783812
H,-0.1578170364,2.2782057501,-2.643831354
H,-3.4689939886,0.2188258437,-4.3066786765
H,-3.5343749351,-0.5905659333,-2.7334792274
H,1.4648027872,3.5658954984,0.6473530238
H,-2.3827425203,2.4213238884,-0.8484798603
H,0.593990778,5.8504108758,1.1478019087
H,-3.2698963255,4.6655251337,-0.3342100059
H,-1.7868802743,6.4031634726,0.6641120942
H,-0.699071306,-0.4921583574,3.0473405596
H,0.6960908811,0.5160521305,2.6055467148
H,-0.9160802324,1.2389689034,2.739418461
H,-0.093199723,-2.4601032569,0.6849177442
H,0.0643202494,-1.8337926813,-0.9722234886
H,1.3155884367,-1.4700461976,0.2334899655
H,-2.7931172895,-0.594211371,-0.6610300458
H,-2.8870116008,-1.0427835262,1.0443236696
H,-3.1000567404,0.6479841849,0.5699287376
H,4.8306557751,-0.7154400376,3.1920404242
H,5.5704263165,0.5605792412,2.1743572245
H,3.9289173961,-0.0603975229,1.7755766938
H,4.6341423775,-3.6197941015,0.5010252837
H,4.250296331,-3.1701863965,2.1922945205
H,3.4203029075,-2.3325074071,0.8289046249
C,-4.6941822921,1.2447305576,-2.8289905551
H,-4.640705106,2.2304160982,-3.3039273469
H,-5.6236189595,0.7579562493,-3.1451858467
H,-4.7270569783,1.3807810372,-1.7423776841
---end---

TS2-S-c-Et-TMS

Electronic_Energy=-1853.84289622

Sum of electronic and thermal Free Energies = -1853.501212

Charge=0 Multiplicity=1

---Coordinates start---
C,0.0309230005,0.8377006532,-0.5793100241
C,-0.4182656046,0.8625944983,-2.1071536714
N,0.6389854961,0.1377043147,-2.8150184694
C,1.7844781093,0.0312624848,-2.478545138
Ag,3.5673166527,-0.089179746,-1.5061726459
C,-0.508275,2.2568501935,-2.7251030275
O,0.376687351,2.8292896694,-3.3260938868
O,-1.7260782595,2.7739592469,-2.4961902268
C,-1.9542574499,4.1346464752,-2.9552773461
O,1.3654742744,1.1116111397,-0.4894692196
C,-0.3533668436,-0.5474228577,-0.0146246393
C,-1.6489402105,-1.085716169,-0.1074736408
C,0.6156880254,-1.2843549745,0.6786641701
C,-1.9530533331,-2.3268195479,0.4568028014
C,0.3177287636,-2.5262650127,1.2451827333
C,-0.9702732106,-3.0562916262,1.1347361579
Si,-0.7521997034,2.1905635842,0.5821823913
C,-2.6463743948,2.1390596245,0.6584725121
C,-0.1517082828,3.9143802712,0.066515057
C,-0.093369346,1.8146681496,2.3146928206
O,5.3137342647,-0.0192526935,-0.2348347747
S,5.2063455349,0.0119114797,1.3280397894
C,3.8587319072,1.1580594627,1.742557468
C,4.4082276324,-1.5461655287,1.801847726
H,-1.3746347042,0.3638337383,-2.2621999735
H,-1.1356414108,4.7670869104,-2.6027736334
H,-1.9400047713,4.1325485348,-4.0502252833
H,-2.4340748292,-0.5340893401,-0.618805278
H,1.6053458331,-0.8544419232,0.7679609743
H,-2.9612850311,-2.7244201672,0.3675288523
H,1.0917281814,-3.076162127,1.776532994
H,-1.2092545378,-4.0211899609,1.5746314984
H,-3.0235634775,2.9843318826,1.2509268682
H,-3.0894651839,2.2050016032,-0.3404064837
H,-3.0041240283,1.2177627595,1.1334889701
H,0.4220590093,4.3702487413,0.8837221344
H,0.5073087707,3.864171466,-0.8055954321
H,-0.9863669712,4.5855765751,-0.16616199
H,1.0003330827,1.8849501207,2.3407735625
H,-0.4957653631,2.5385148583,3.0364970569
H,-0.3766346654,0.8117703964,2.6555704445
H,3.6475435103,1.0552755059,2.8120525309
H,4.2210826354,2.1687775704,1.5338796538
H,2.9679104647,0.9455222652,1.1369781553

H,5.1113821042,-2.353214144,1.5797690333
H,4.1972456589,-1.5187606411,2.8755569524
H,3.4867893154,-1.6737200115,1.2271852932
C,-3.2928051175,4.5792521127,-2.4052679093
H,-3.2830311728,4.5890336449,-1.3102698007
H,-3.5112538744,5.5931019062,-2.7589187757
H,-4.096191371,3.9152617215,-2.7424882416
---end---

TS1-C-t-Et-TMS

Electronic_Energy=-1853.83344910
Sum of electronic and thermal Free Energies = -1853.502242
Charge=0 Multiplicity=1
---Coordinates start---
C,-0.1522908063,0.8783654132,0.1105510661
C,-0.4595804648,0.8025978378,-1.9500174032
N,0.8318429062,0.4095126637,-2.2732314676
C,1.8381120732,0.1186561714,-1.6966557924
Ag,3.7478418129,-0.4186392986,-1.2678622458
C,-0.8462511655,2.1322374294,-2.4565829726
O,-0.0893060467,3.004902025,-2.8506200266
O,-2.1870362107,2.2933278672,-2.3502097318
C,-2.6982030696,3.6204789981,-2.610784954
O,1.0391799526,0.3642971821,0.2509974154
C,-0.2590370943,2.3653441529,0.3860985046
C,0.9124129962,3.1359510344,0.4586616569
C,-1.4898697531,3.0110357752,0.586320485
C,0.858262266,4.5068839462,0.7110572334
C,-1.5484845946,4.3831317582,0.8431558979
C,-0.3745125712,5.1397217034,0.9045628483
Si,-1.4954319575,-0.3761005671,0.6654558926
C,-1.4820928877,-0.4338191343,2.5593305542
C,-0.945273,-2.0498114899,-0.0177580989
C,-3.2662375223,-0.0178954129,0.0804627661
O,5.7482930944,-0.9841728718,-0.7272520078
S,6.3404432317,-0.8456970916,0.7148622718
C,6.0146883707,0.8612650791,1.2334933512
C,5.1741248352,-1.6821891738,1.8232462137
H,-1.1980223383,0.027798965,-2.1446979365
H,-2.0991068583,4.3472654094,-2.0548153838
H,-2.5931006785,3.8371666983,-3.6799205075
H,1.8652757892,2.6349278877,0.3165912541
H,-2.4137538464,2.4473405328,0.5243505016
H,1.7787072035,5.0848664139,0.7585045202
H,-2.5139682728,4.8602427382,0.9944363807
H,-0.4192534019,6.2073246738,1.104584403
H,-2.1895260981,-1.180672247,2.943880324
H,-0.4846041,-0.690303812,2.9381874676
H,-1.761012191,0.5382541307,2.9867191734
H,-1.5764640766,-2.859016233,0.3723563286
H,-1.0004482276,-2.0853044687,-1.1131952728
H,0.0921272338,-2.2509206496,0.2712707596
H,-3.2924885259,0.4205276551,-0.9231098121
H,-3.8474964565,-0.9499193487,0.0587092336
H,-3.7855524459,0.6718763011,0.7574601862
H,6.3261948222,0.9719865498,2.2771884107
H,6.6089181707,1.5191629684,0.5937508984
H,4.9462363948,1.0764291003,1.120731059
H,5.1901415233,-2.7466518782,1.574596657
H,5.5090401177,-1.5341831756,2.8551102936
H,4.1713163953,-1.2669571482,1.6756081586
C,-4.1483402331,3.6371919609,-2.1726912357
H,-4.5823810707,4.6240434693,-2.3694807868
H,-4.7325014107,2.8877695471,-2.7182977323
H,-4.2315293929,3.4294801817,-1.1003169391
---end---

TS2-S-t-Et-TMS

Electronic_Energy=-1853.83746230
Sum of electronic and thermal Free Energies = -1853.498348
Charge=0 Multiplicity=1
---Coordinates start---
C,0.0816709353,1.0072737111,-0.4546520505
C,-0.6046056193,0.9093347892,-1.9394012382
N,0.2154900974,-0.0166881651,-2.6812653005
C,1.3620710819,-0.306883654,-2.5070186052
Ag,3.2062472507,-0.7036513318,-1.7244152433
C,-0.5612095777,2.2578804654,-2.6546442308
O,0.4302012967,2.7510742917,-3.1531462753
O,-1.7609344732,2.8558131519,-2.5994647358
C,-1.8016306998,4.2547909832,-2.9872995862
O,1.4367991862,0.8867889813,-0.564649621
C,-0.3448939455,2.3361227497,0.1867125611
C,0.6378368016,3.2069771744,0.6791814793
C,-1.6944161575,2.6975925834,0.3560712283
C,0.2894314316,4.4041167137,1.3118042192
C,-2.0450759434,3.8901052165,0.9905724382
C,-1.0536143042,4.7522389361,1.4725539493
Si,-0.481594153,-0.4597658949,0.6956790008
C,0.3423316156,-0.1425658714,2.3696550272

C,0.1021881374,-2.1208570354,-0.0011730303
C,-2.3575133069,-0.6021076623,0.9533391108
O,5.0118505488,-0.8621664791,-0.5431872971
S,5.0197974579,-0.5222729079,0.9875001231
C,4.0918299172,1.0262893205,1.1847906511
C,3.8251865782,-1.6477791947,1.7611291872
H,-1.635731428,0.5577647311,-1.8934850695
H,-1.0531818253,4.7971212297,-2.4006616623
H,-1.5333117339,4.3360351857,-4.0455406829
H,1.6780693243,2.9267484707,0.5533360548
H,-2.4785638563,2.0544767906,-0.0290853963
H,1.0706515071,5.0636599155,1.6834757569
H,-3.0952963322,4.1479173068,1.1054742605
H,-1.3271398751,5.6798875802,1.9689804294
H,0.3023339433,-1.0344593582,3.0086679076
H,1.3933405786,0.1347872763,2.2387647132
H,-0.1555735209,0.6749419284,2.9061714366
H,-0.1144867363,-2.919523795,0.721666431
H,-0.4118550194,-2.372179405,-0.9371607136
H,1.1794121304,-2.1296841606,-0.1988309781
H,-2.9013893683,-0.6600507849,0.0013738987
H,-2.5866774835,-1.5182516486,1.5154052753
H,-2.7618030531,0.2431431916,1.5216275969
H,4.0080195693,1.2328213486,2.2571932238
H,4.6801049754,1.8143253219,0.7057518965
H,3.1015350973,0.9387325844,0.7142767799
H,4.2205031996,-2.6626129461,1.6656979255
H,3.7335097441,-1.3809368744,2.8187413014
H,2.8602372144,-1.5612061918,1.254821602
C,-3.2037705316,4.7562052819,-2.7139418201
H,-3.4454216262,4.666240812,-1.6496558372
H,-3.2769967752,5.81169016,-2.9990584633
H,-3.9426972044,4.1902097875,-3.2917065777
---end---

TS1-C-c-Et-TES

Electronic_Energy=-1971.77399716

Sum of electronic and thermal Free Energies = -1971.351776

Charge=0 Multiplicity=1

---Coordinates start---

C,0.253732215,1.0968801287,-0.569952079
C,-0.1124927168,1.1201087312,-2.2627429002
N,1.0235862602,0.5720906648,-2.9067712686
C,2.1119861642,0.1954116976,-2.6400206143
Ag,3.7700489434,-0.3931652226,-1.626773967
C,-1.3508512286,0.3559700098,-2.6900322004
O,-1.3718274987,-0.8163662696,-3.0134028238
O,-2.4318304318,1.1510627692,-2.6574713921
C,-3.6965439254,0.5691798497,-3.0771697662
O,1.5284379843,0.7144883441,-0.355641742
C,-0.03205823,2.5337613271,-0.1015397243
C,0.9588150824,3.2343917338,0.6018630219
C,-1.2674207213,3.1705869139,-0.3100088681
C,0.722215021,4.5216406664,1.0926385606
C,-1.508552538,4.4555030607,0.1800851285
C,-0.5152628797,5.1381472551,0.8900705595
Si,-0.73002051,-0.2475239036,0.4552525452
C,-0.53739988,0.1919978927,2.2997382415
C,0.0431370093,-1.9313085205,0.0119307094
C,-2.6120194084,-0.5353957546,0.2500652969
O,5.3350812391,-0.9053879574,-0.2424758905
S,5.0667395807,-0.9031720259,1.30320319
C,4.2083409273,0.6534289993,1.6700141749
C,3.6754042809,-2.0368188516,1.5714652486
H,-0.2197157818,2.1617901586,-2.5722708585
H,-3.5783159817,0.1922592092,-4.0979168972
H,-3.9350071361,-0.275463214,-2.4256214138
H,1.9170790878,2.7495676594,0.7537230107
H,-2.041791897,2.6640386902,-0.8756780432
H,1.5068311746,5.0432964757,1.6366616643
H,-2.4739595912,4.9247211058,0.0043154227
H,-0.7033119318,6.1369424858,1.2759791837
H,-1.0831555938,-0.5860347417,2.8553985426
H,-1.1039235933,1.1193197687,2.4696976377
H,-0.5106709137,-2.3309057319,-0.8493152714
H,1.062620609,-1.738162118,-0.3386714766
H,-2.8097667973,-0.8830968947,-0.7698724779
H,-2.7945229094,-1.4168060397,0.8872886659
H,3.9662916926,0.660977844,2.7376263248
H,4.9051425163,1.4653573734,1.4437237049
H,3.2986524663,0.7307433643,1.0608709589
H,3.9993207535,-3.0333173341,1.2595789593
H,3.4357032455,-2.0404904145,2.6391324992
H,2.819017143,-1.7026286913,0.9797381033
C,-4.7424755873,1.6602122928,-2.9918202338
H,-4.4804035505,2.505759484,-3.6370054375
H,-5.7093119427,1.2618814924,-3.319081182
H,-4.8487234484,2.0219368123,-1.9637826018
C,0.0540356539,-2.9674034416,1.1481489841
H,0.4842309748,-3.9244490143,0.8210775728

H,0.644642574,-2.6223327628,2.0052611746
H,-0.9581693127,-3.1799895365,1.5173670024
C,0.8737043017,0.3481509538,2.8797700806
H,1.4691327223,-0.5603245523,2.7422253585
H,1.4104530893,1.1627796082,2.3890980273
H,0.8449663221,0.5631626189,3.957745224
C,-3.6065850409,0.5668428984,0.64074121
H,-3.5298722281,1.4370806119,-0.017244773
H,-4.6446627475,0.2104079632,0.5852813018
H,-3.4390440605,0.918863188,1.6663650222
---end---

TS2-S-c-Et-TES

Electronic_Energy=-1971.77938089
Sum of electronic and thermal Free Energies = -1971.355251
Charge=0 Multiplicity=1
---Coordinates start---
C,0.1364736959,0.6699218764,-0.7206142087
C,-0.1286989585,0.5958907229,-2.2973244954
N,1.0396619955,-0.1183090968,-2.8280729512
C,2.1381217768,-0.1818170807,-2.3535068778
Ag,3.7783943603,-0.1868878695,-1.1409867336
C,-0.2686205987,1.929830108,-3.0263141719
O,-1.3507216929,2.3917180184,-3.3396656297
O,0.9015343716,2.52785644,-3.2610934476
C,0.8502198945,3.8202364815,-3.9218268554
O,1.4414001683,0.9850489769,-0.4829558622
C,-0.2763258504,-0.7151442752,-0.1696725199
C,-1.5737873543,-1.2368006582,-0.3079892453
C,0.6699564263,-1.4858874531,0.5163328877
C,-1.9080565031,-2.4836656452,0.225802714
C,0.3447397082,-2.7355260613,1.0492536595
C,-0.9504627449,-3.240680862,0.9093269289
Si,-0.7719948681,2.0868160867,0.2787644207
C,-2.6661719567,1.9157123324,0.4251793293
C,-0.3377610813,3.7760381191,-0.4822119478
C,-0.1151274475,2.0859776241,2.0656332929
O,5.3041088966,0.0114687113,0.3797201086
S,4.9665414549,0.0703246034,1.9086632508
C,3.5093192003,1.1415069884,2.0853480201
C,4.1919963791,-1.5191231442,2.3120301769
H,-1.0338738181,0.0360710479,-2.5275098441
H,0.3779866689,3.692192953,-4.9013486484
H,0.2285111848,4.4942355168,-3.325794067
H,-2.3342640541,-0.6697869125,-0.8382027555
H,1.6644621611,-1.0747576769,0.6326679811
H,-2.9197608505,-2.8644534015,0.1074381276
H,1.1017855451,-3.3090425077,1.580032095
H,-1.2127307123,-4.2093942186,1.3269793101
H,-0.9990434944,3.9506060282,-1.3387755503
H,0.679675275,3.7060140801,-0.8846382367
H,-0.6027880412,2.949816831,2.5421168842
H,0.9549547135,2.3271335462,2.0383229241
H,3.1346328767,1.036452218,3.1086328048
H,3.8439222777,2.1693116636,1.9183875214
H,2.7422051521,0.8723594377,1.3473737441
H,4.9561406124,-2.2931422438,2.2020932151
H,3.8429034757,-1.4821235146,3.3487738614
H,3.3591280023,-1.7041352256,1.6287055737
C,2.2746819916,4.3193893324,-4.0370288271
H,2.8874088321,3.6252413882,-4.6228157749
H,2.2814818149,5.2938793799,-4.5379432171
H,2.7273593696,4.4366770714,-3.046082074
C,-3.4954062913,2.0530953239,-0.860379931
H,-3.3427657,3.0296374166,-1.3340481074
H,-3.2222702601,1.3002490941,-1.6078593225
H,-4.5703200931,1.9468298371,-0.6582035799
H,-2.8892127779,0.9578100241,0.9141289259
H,-2.9807437928,2.6890234673,1.1438637463
C,-0.4394694673,4.9663119682,0.4876073383
H,-0.2364148284,5.9163625906,-0.0253763888
H,-1.4399531834,5.0474571059,0.9327032143
H,0.2787295025,4.8815888593,1.3116096235
C,-0.3504568011,0.8458090756,2.9428621861
H,0.2375113785,-0.0106339599,2.6008909664
H,-0.0734122391,1.0391916642,3.9885983596
H,-1.4038242814,0.5372391164,2.9381481686
---end---

TS1-C-t-Et-TES

Electronic_Energy=-1971.77382892
Sum of electronic and thermal Free Energies = -1971.357162
Charge=0 Multiplicity=1
---Coordinates start---
C,-0.0813524253,1.0674171932,0.4273423606
C,-0.4818448436,0.9942064749,-1.6317451474
N,0.7966545917,0.600628237,-2.0044205804
C,1.8341150111,0.3376296526,-1.4705713776
Ag,3.7371722153,-0.2502359458,-1.0759787359
C,-0.933140658,2.3217185728,-2.0844738824

O,-2.11089198,2.6518168031,-2.1475169172
O,0.0890045457,3.1694895762,-2.3200748777
C,-0.2655014496,4.5570247783,-2.5264548692
O,1.1545067764,0.6442493359,0.4931839677
C,-0.2917373117,2.531697678,0.7498004407
C,0.8263274677,3.3570146665,0.9535891398
C,-1.5691109172,3.1032969504,0.8733875464
C,0.6777863834,4.7083867314,1.26578044
C,-1.721872874,4.4544943266,1.1942412715
C,-0.6002256837,5.2655247,1.3898152638
Si,-1.2205224776,-0.3152720101,1.1241300111
C,-0.8632890288,-0.4211848031,2.9921365761
C,-0.6722141922,-1.9212039071,0.2715604662
C,-3.1104945583,-0.1366267855,0.9634504934
O,5.7057062008,-0.8930804185,-0.504908738
S,6.1862830732,-1.0203372706,0.9790260332
C,5.8299834839,0.5739366692,1.7675462486
C,4.9353630164,-2.0152112562,1.8367910157
C,1.025437352,5.3476267198,-2.5844598598
C,0.5873029217,-0.7619361046,3.3713218951
C,-3.6903776507,-0.0256530277,-0.4560605607
C,-1.2839285843,-3.1969842325,0.8741611977
H,-1.2282068222,0.2260525081,-1.8120180256
H,-0.8398895803,4.6458738245,-3.4552290544
H,-0.9024405874,4.8838975685,-1.6991168508
H,1.8123100894,2.9122156264,0.8630935193
H,-2.4504065819,2.4980102586,0.6941113764
H,1.5582991508,5.328708004,1.4182744568
H,-2.720616235,4.8751791352,1.2851217938
H,-0.7197393242,6.3170945139,1.6382399707
H,-0.9169130318,-1.8658186758,-0.7986143782
H,0.422903252,-1.9610425254,0.3277792122
H,-3.5264222906,-1.028849241,1.4572160587
H,-3.4462653646,0.7127460546,1.5746089307
H,6.0658442723,0.4927909068,2.83369437
H,6.4717664038,1.3246532595,1.2990858987
H,4.7735518697,0.8239062798,1.6207750687
H,4.9627560377,-3.0207397981,1.4086881956
H,5.1949680174,-2.0542394924,2.8998164533
H,3.9484933547,-1.5617801506,1.6931886263
H,0.8009152997,6.4087315688,-2.7418037351
H,1.5808247987,5.2466128347,-1.646000476
H,1.6613915062,5.0037389923,-3.4080285442
H,0.727834619,-0.7909606315,4.4608193866
H,0.8821629687,-1.7431052594,2.9771102576
H,1.2837534755,-0.0258786942,2.9556239446
H,-1.5475513012,-1.1659487377,3.4254575199
H,-1.147889325,0.5400357086,3.4462216002
H,-4.7891934885,-0.0220412501,-0.4421253107
H,-3.362709361,0.8905332005,-0.9592674952
H,-3.3784725557,-0.8728367688,-1.0812194325
H,-0.9301953811,-4.1001854885,0.3585560973
H,-1.0256469894,-3.3067191723,1.9352874213
H,-2.3793553004,-3.1930676632,0.8050543228
---end---

TS2-S-t-Et-TES

Electronic_Energy=-1971.77781415

Sum of electronic and thermal Free Energies = -1971.354751

Charge=0 Multiplicity=1

---Coordinates start---

C,0.1270100868,1.045764535,-0.4725834232
C,-0.5084996399,0.9801677939,-1.9941592003
N,0.3703827384,0.1271613907,-2.747569266
C,1.5152921023,-0.1544892064,-2.5636436464
Ag,3.3536796541,-0.5280543531,-1.7622045489
C,-0.5006808666,2.3563498032,-2.6562629719
O,0.489612194,2.9166346063,-3.0810428939
O,-1.731492325,2.8889638668,-2.6519312758
C,-1.8253411142,4.2937616365,-3.0091077022
O,1.4808931254,0.9030472808,-0.5258932652
C,-0.3056990708,2.3783002778,0.1570862406
C,0.6696894396,3.2464784841,0.6674459183
C,-1.656600185,2.7440943967,0.2988236323
C,0.3122890218,4.4405094251,1.3006554615
C,-2.0172613754,3.9340749576,0.9322659638
C,-1.0332795679,4.7899809077,1.4399609767
Si,-0.4788294558,-0.436914593,0.6458636594
C,0.3792557381,-0.2100180045,2.3311054938
C,0.09077585,-2.0937508353,-0.1047897845
C,-2.3626101445,-0.5499133676,0.928360176
O,5.1149088634,-0.6972456826,-0.5152932333
S,5.0186729286,-0.4869108715,1.036100173
C,4.081943328,1.0466997443,1.297766582
C,3.7711861253,-1.6663296849,1.6254689339
H,-1.5233095461,0.5816315237,-1.9953106541
H,-1.1364980968,4.8584861832,-2.3729095325
H,-1.5087987752,4.4145700116,-4.050097637
H,1.7113064376,2.9632890697,0.561782061
H,-2.4335110349,2.1036600258,-0.104556622

H,1.0876867201,5.09682107,1.6898592151
H,-3.0688951579,4.1938770508,1.0281285087
H,-1.3139348103,5.7147658292,1.9377133744
H,0.4761252684,-1.2026975318,2.7949207194
H,1.4018129218,0.1303073671,2.1309896811
H,0.1615599592,-2.8175171205,0.7209868504
H,1.1145904743,-1.9675697106,-0.4793741081
H,-2.8736369546,-0.6222190036,-0.0426168805
H,-2.7180716535,0.3812408262,1.3872101735
H,3.9333916156,1.1680122513,2.3762188781
H,4.6994324967,1.8663112887,0.918843645
H,3.1208320606,0.9989388697,0.7654721973
H,4.1788981342,-2.6713450246,1.4870346042
H,3.5902466097,-1.4794883112,2.6884830903
H,2.851191183,-1.5413382954,1.0472326701
C,-3.2637522202,4.715636774,-2.7976475094
H,-3.5539302676,4.5881678956,-1.7493818133
H,-3.3778458236,5.7724345652,-3.063736071
H,-3.9417055492,4.1261716721,-3.4246239227
C,-0.3035253436,0.7510355267,3.3208512205
H,-0.3546041954,1.7719996344,2.9262115593
H,-1.3293823794,0.4368773844,3.5491049014
H,0.241424655,0.7973720709,4.2740181948
C,-2.7711949677,-1.7398476558,1.8175941467
H,-3.8587332167,-1.7786551627,1.9690636443
H,-2.4699234208,-2.6995621732,1.380240382
H,-2.3079105935,-1.6765847309,2.8104376032
C,-0.8040160824,-2.6780340042,-1.2117192671
H,-0.4003140583,-3.6242404134,-1.5979596211
H,-1.8168215259,-2.8835246588,-0.845372848
H,-0.8989606635,-1.9960333615,-2.063971814
---end---

TS1-C-c-Et-TBS

Electronic_Energy=-1971.77980606
Sum of electronic and thermal Free Energies = -1971.358703
Charge=0 Multiplicity=1
---Coordinates start---
C,0.280042412,1.0178792862,-0.5107732942
C,-0.0739202388,0.9978804272,-2.2452461688
N,1.0737496145,0.430200459,-2.8426440222
C,2.1667466131,0.085729122,-2.5513897941
Ag,3.8802490572,-0.3294352676,-1.5418099382
C,-1.3123580612,0.2603759802,-2.7041472337
O,-1.3509643611,-0.9083663806,-3.0411773195
O,-2.3772011495,1.0785005725,-2.6871940366
C,-3.6511922532,0.525421275,-3.1121280724
O,1.5401351601,0.6116806593,-0.2937741661
C,0.0130121093,2.4771456935,-0.1183203771
C,1.0241655027,3.2174167818,0.5105386029
C,-1.2375524393,3.0912726162,-0.3097779206
C,0.7940434084,4.5251774386,0.9473162568
C,-1.4709882189,4.3964568078,0.1268391669
C,-0.4570639613,5.1202819895,0.7639731263
Si,-0.7661184889,-0.271443426,0.504263127
C,-0.5578765864,0.0198774876,2.4067767566
C,-0.0883163381,-1.9725944677,0.0254151108
C,-2.6450663242,-0.3044990726,0.1882018457
O,5.5045800594,-0.6019285351,-0.1496508527
S,5.2473252182,-0.5618475432,1.3971778597
C,4.1799649982,0.8737510547,1.704483712
C,4.0352724675,-1.8690112901,1.7317124497
H,-0.15261071,2.0398614724,-2.5609114076
H,-3.6061007477,0.3656453587,-4.1948204268
H,-3.804212603,-0.4433724345,-2.6310084452
H,1.9900077003,2.7453532885,0.6562830461
H,-2.0304513778,2.548084915,-0.8138108559
H,1.5928689534,5.0789354902,1.4360876863
H,-2.4471539753,4.8495309558,-0.0308183557
H,-0.640080468,6.1348396613,1.1089345574
H,-0.7362028722,-2.7781879065,0.3938007176
H,-0.0431613229,-2.0510178727,-1.0672130323
H,0.9210439706,-2.1310618663,0.418801106
H,-2.8754050232,-0.8468118891,-0.7337624806
H,-3.1499249918,-0.8358550988,1.0053578868
H,-3.0905527818,0.6931260454,0.1205063531
H,3.9379810643,0.8900725514,2.7720822575
H,4.758011387,1.7649318002,1.4437999218
H,3.2693238233,0.8013098416,1.0964125562
H,4.5136398313,-2.8251513347,1.5027597651
H,3.7660881585,-1.8303895959,2.7918137338
H,3.1542301307,-1.7163191836,1.1004312755
C,-4.7229044025,1.5232598423,-2.7280276649
H,-4.539223983,2.4967990968,-3.1953524303
H,-5.6997657914,1.1572076314,-3.0631235914
H,-4.7573081627,1.6563262664,-1.6412478234
C,-1.0438897932,-1.2536895916,3.1355116742
H,-0.9792315899,-1.1144570693,4.2259218665
H,-2.0880577553,-1.5002771655,2.9050375094
H,-0.4309171391,-2.1277861047,2.8822368163

C,0.9040203092,0.2745416125,2.8131186967
H,1.5597098162,-0.548721035,2.5121152203
H,1.295873522,1.1877122824,2.3597489399
H,0.9818620986,0.3775278737,3.9077504079
C,-1.4171535976,1.2127755849,2.8777699178
H,-1.0847708933,2.1585316025,2.4354693207
H,-2.477809975,1.0828683478,2.629612966
H,-1.3503437885,1.3210379186,3.9717202568
---end---

TS2-S-c-Et-TBS

Electronic_Energy=-1971.78415149
Sum of electronic and thermal Free Energies = -1971.359427
Charge=0 Multiplicity=1
---Coordinates start---
C,-0.0220862888,0.7295358262,-0.7368445927
C,-0.3487025207,0.6954887545,-2.2846404688
N,0.7296699045,-0.1296531704,-2.8566689349
C,1.8476991216,-0.1866957607,-2.4211164885
Ag,3.5834710313,-0.2662912986,-1.370677328
C,-0.2636288097,2.0481112804,-3.0018805845
O,0.7527592328,2.5583506673,-3.4233491606
O,-1.4846189679,2.5907565658,-3.1271250949
C,-1.5481567171,3.877629824,-3.8021490062
O,1.2996363831,1.0448146729,-0.5785019533
C,-0.3690224891,-0.6564467085,-0.1409185319
C,-1.5016621774,-1.4154016371,-0.4804859623
C,0.5045365042,-1.1892139153,0.819853927
C,-1.7452222896,-2.6564597556,0.1149470881
C,0.2630233282,-2.4245052577,1.4249534287
C,-0.8661386393,-3.1687357477,1.07387562
Si,-0.8648702028,2.1333562639,0.3441262005
C,-2.7777468755,2.0320330004,0.6451354784
C,-0.4338573207,3.8300743602,-0.3789223928
C,-0.0358923053,2.0154175786,2.0427083808
O,5.2543905847,-0.1307634178,-0.0096168463
S,5.0336376293,0.0482743691,1.532132274
C,3.71317377,1.2799871035,1.7330544349
C,4.1281408494,-1.4272448806,2.0758581993
H,-1.3176890659,0.2541729543,-2.5098276158
H,-0.8323945,4.5584977018,-3.3339883494
H,-1.2464541406,3.7291586245,-4.8443393383
H,-2.2115653579,-1.0495960105,-1.2154084064
H,1.3804992393,-0.6111148064,1.0829641293
H,-2.6268690908,-3.2237870877,-0.1738104327
H,0.9608968756,-2.8039948355,2.1684301932
H,-1.059482545,-4.1324859338,1.5379334289
H,-0.3239590416,4.5598464674,0.4333351617
H,0.5174491527,3.7791881692,-0.9177639049
H,-1.2018950229,4.2059291511,-1.0602740209
H,1.0104295242,2.3317225947,1.9787240565
H,-0.5443877016,2.6735747662,2.7592408104
H,-0.0571747062,0.9989955605,2.4498362585
H,3.4218825171,1.2932088038,2.7883113921
H,4.134048188,2.250493952,1.4547230835
H,2.8584139226,1.0408286255,1.0871314986
H,4.8163020991,-2.2744714345,2.0136521983
H,3.8077371575,-1.2812027604,3.1122408708
H,3.2679208833,-1.5862440109,1.4197031793
C,-2.9702334148,4.3844933642,-3.6911808829
H,-3.2440021154,4.5679220633,-2.6468946318
H,-3.0612192891,5.3277335656,-4.2414449907
H,-3.678022292,3.6658139384,-4.1182340866
C,-3.1179806423,0.9421605631,1.6838878999
H,-2.8304384125,-0.0589743838,1.3460714937
H,-2.623003396,1.1242785207,2.6457178092
H,-4.2026412944,0.9257803519,1.8741801973
C,-3.5712842529,1.7634534586,-0.6466114917
H,-3.371720129,2.5150240928,-1.4163051413
H,-3.3351957481,0.7844465752,-1.0772990093
H,-4.652951575,1.7763795901,-0.4392218357
C,-3.2312316214,3.3954862005,1.2174917911
H,-4.3024365652,3.3620762372,1.4705231569
H,-2.6918019902,3.6638496945,2.135381819
H,-3.0934903638,4.2123294197,0.498701264
---end---

TS1-C-t-Et-TBS

Electronic_Energy=-1971.77989528
Sum of electronic and thermal Free Energies = -1971.363382
Charge=0 Multiplicity=1
---Coordinates start---
C,-0.1361629138,0.9806214952,0.1043104397
C,-0.4693262472,0.8517266529,-1.9557031788
N,0.8226206296,0.4617758281,-2.2829803695
C,1.834469666,0.201937749,-1.6984250006
Ag,3.7321977832,-0.3613822349,-1.2464002193
C,-0.8763951532,2.1626086907,-2.4947575068
O,-0.1331891867,3.038820927,-2.9065310693
O,-2.2205578833,2.3018741824,-2.398418098

C,-2.754396142,3.6111039874,-2.701700615
O,1.0791024139,0.5159588554,0.2307967042
C,-0.2942401131,2.4688726702,0.3455237417
C,0.8533511763,3.2703934136,0.4540075533
C,-1.5481824185,3.0872073384,0.4846379801
C,0.7551112171,4.6435200479,0.6838344504
C,-1.6505812486,4.4600287351,0.7174698554
C,-0.4991600714,5.2476169714,0.8166362041
Si,-1.4066320961,-0.3354748422,0.6973807776
C,-1.2843488265,-0.4901705127,2.6153465342
C,-0.8537298636,-1.9677265116,-0.0848281043
C,-3.2105178536,-0.0039428197,0.2062436185
O,5.6982981524,-0.970708688,-0.6308437055
S,6.199890643,-0.9216839221,0.8510197152
C,5.8722248015,0.761766124,1.4404322457
C,4.9521729624,-1.7911406476,1.8398194209
H,-1.2035509766,0.0670418389,-2.1227035387
H,-2.1708747981,4.3655555795,-2.1665932758
H,-2.6481182691,3.796034554,-3.7766789749
H,1.8234706395,2.7918957994,0.3608815647
H,-2.4540164373,2.4997049391,0.396874043
H,1.6587665081,5.2441928572,0.7618917956
H,-2.6330635817,4.9144422132,0.8221437824
H,-0.5788597055,6.316259501,0.9995185276
H,-1.3278900364,-2.8244985972,0.410484814
H,-1.1132876284,-2.0203162619,-1.1494826572
H,0.2323055506,-2.0768822243,0.0029053397
H,-3.2798830823,0.4292408751,-0.7984055983
H,-3.7785344338,-0.9435083019,0.2073782555
H,-3.7122798515,0.6823364684,0.8989411149
H,6.1230966923,0.8110371792,2.5048797162
H,6.5150693852,1.4403663896,0.8735442068
H,4.816349583,1.0044953302,1.2774906896
H,4.9659208853,-2.8416312146,1.5376743071
H,5.2251126704,-1.7022565385,2.8964523214
H,3.9669602739,-1.3497405792,1.6539071079
C,-4.2065977346,3.6156028124,-2.2704462132
H,-4.6571466376,4.5878080361,-2.5002200145
H,-4.7747008855,2.8389705404,-2.794519736
H,-4.2913744251,3.4403529631,-1.1923884443
C,-2.3642988861,-1.4689838842,3.1209634999
H,-2.2889649866,-1.5933194734,4.212616227
H,-3.3781075882,-1.1090734533,2.9042828413
H,-2.2608332668,-2.4660713519,2.6737076642
C,-1.503104047,0.8803220251,3.2874152356
H,-0.7192043331,1.5969107538,3.0164389089
H,-2.4678751336,1.3263680678,3.0137834443
H,-1.4904196301,0.7756741987,4.3836039519
C,0.1066040088,-1.0221888545,3.0155900085
H,0.2864411489,-2.0299430201,2.6195176055
H,0.9051423884,-0.3716951759,2.6411138521
H,0.196244633,-1.080259361,4.1118661134
---end---

TS2-S-t-Et-TBS

Electronic_Energy=-1971.77889642
Sum of electronic and thermal Free Energies = -1971.355489
Charge=0 Multiplicity=1
---Coordinates start---
C,0.0430007712,1.0641389828,-0.4338117305
C,-0.5813580537,0.9786255158,-1.958780591
N,0.2728388924,0.0759044594,-2.6821476519
C,1.4178651258,-0.2083644247,-2.5076376489
Ag,3.2771209639,-0.5447819461,-1.7421623732
C,-0.5195623879,2.3308122934,-2.6710768031
O,0.4966840088,2.8567302342,-3.0772898221
O,-1.7404243559,2.8811462852,-2.7465152732
C,-1.7973231319,4.2696399341,-3.1693367849
O,1.393247935,0.8875407746,-0.4747015852
C,-0.3487438724,2.4202730556,0.1744802273
C,0.641547578,3.200862786,0.7899168604
C,-1.6689126259,2.9045154668,0.1878491312
C,0.33006516,4.4258838189,1.3871167638
C,-1.9834180325,4.1301599176,0.7774529648
C,-0.983862139,4.899624191,1.3825903453
Si,-0.5432556623,-0.4170338387,0.7142587008
C,0.3477054184,-0.1257258765,2.3606518495
C,0.0975852502,-2.0337170842,-0.0456121057
C,-2.4283573956,-0.6887465801,1.1119206909
O,5.0751594035,-0.6896724152,-0.5516801379
S,5.037421011,-0.4765918493,1.0014971867
C,4.0457890884,1.0148600171,1.2992953956
C,3.8720540681,-1.7066701199,1.6508502957
H,-1.6079266581,0.6183607855,-1.9636586712
H,-1.1189498011,4.8509328567,-2.5369312165
H,-1.446250302,4.3371375449,-4.2040097502
H,1.6604472166,2.8300280971,0.7857265901
H,-2.457882848,2.3313562989,-0.284284219
H,1.1178423115,5.0108597635,1.8568388917
H,-3.0119480469,4.4830530401,0.76375184

H,-1.2286159967,5.8524560403,1.8451785775
H,0.1535430455,-0.9429641699,3.0672251061
H,1.4278364635,-0.0643106609,2.2005835242
H,0.0276838984,0.8093967453,2.8354701229
H,0.055569841,-2.8441795605,0.6926273433
H,-0.4864783992,-2.3477616041,-0.9196510769
H,1.1382580865,-1.9192007268,-0.3618070569
H,3.9256625885,1.1264514355,2.3823043669
H,4.6153013912,1.8612917946,0.9045610984
H,3.0716740015,0.9299059522,0.7964262875
H,4.3121553247,-2.6939978101,1.4869112957
H,3.7429416712,-1.5290095698,2.723163165
H,2.9164579954,-1.619234991,1.125990068
C,-3.2340174631,4.7240426363,-3.0231685142
H,-3.5579231022,4.6538992213,-1.9793094317
H,-3.3220713918,5.7678462154,-3.3446052806
H,-3.9030498369,4.1147091551,-3.6406343452
C,-2.932485986,0.2969177822,2.1866702167
H,-2.8174876842,1.3434345257,1.8877163024
H,-4.0023240023,0.127485124,2.3864899468
H,-2.4011691463,0.1647297072,3.1372342867
C,-3.3116753787,-0.5692060483,-0.1459267113
H,-3.3458704613,0.4546212094,-0.5345166542
H,-2.9650578766,-1.2235424479,-0.9569101337
H,-4.348917072,-0.8598009986,0.0835942721
C,-2.5968094425,-2.1194145605,1.6751340161
H,-3.6365596484,-2.2756966004,2.0029431768
H,-2.3743644718,-2.8885418252,0.9262805291
H,-1.9528492771,-2.3026906549,2.5452321733

---end---

TS1-C-c-Et-TBS-CC

Electronic_Energy=-2454.40121754

Sum of electronic and thermal Free Energies = -2454.028741

Charge=0 Multiplicity=1

---Coordinates start---

C,0.1286061763,0.9386876666,0.5055882224
C,-0.1607043679,0.6187461095,-1.6175269489
N,1.0710744401,-0.0006561929,-1.7453096144
C,2.051280785,-0.187426377,-1.0831632519
Ag,3.9548562609,-0.8285108359,-0.6511826497
C,-0.3132542823,1.77721392,-2.5249708453
O,0.6034434754,2.3932154464,-3.0509965618
O,-1.6197390364,2.0918064226,-2.6939675471
C,-1.9187108292,3.2102971291,-3.5682710231
O,1.410873857,0.7399905981,0.6363803141
Si,-0.4862847243,2.707676721,0.9295448662
C,-0.2697573014,2.9737048181,2.8302282377
C,-2.319829548,2.8662288544,0.4995413696
C,0.600890876,3.9594384939,0.0226655122
C,-1.7589716445,4.550711665,-2.8695548182
C,-0.6113952898,4.4435024057,3.1602234055
C,1.182080881,2.6890090668,3.2659254822
C,-1.2131552146,2.053635851,3.6323963933
C,-0.7526054472,-0.1503024673,0.9067750087
C,-1.5279413953,-1.0192984482,1.2671216742
C,-2.4543276455,-2.0166454834,1.6931711324
C,-2.0326382416,-3.3416145059,1.9311017922
C,-3.8137345823,-1.6890132541,1.883781136
C,-2.947571378,-4.3073525306,2.3468431055
C,-4.7206134544,-2.6617154476,2.2999072751
C,-4.2928497181,-3.9729149484,2.5328312723
Cl,6.2997553947,-1.6379369361,-0.0408261236
C,7.3921983311,-0.4348483745,-0.8932875406
Cl,6.8783300305,-0.1381080603,-2.5693162317
H,-1.0064460855,-0.0628221501,-1.6231134448
H,-1.277242391,3.1466507584,-4.4519211767
H,-2.9555430153,3.0394368824,-3.8680072764
H,-2.4985566443,2.6263838074,-0.5519749918
H,-2.9167443525,2.1739900514,1.1050041827
H,-2.6915236966,3.8813564168,0.6876466542
H,0.8186727657,3.6480557294,-1.0022839135
H,0.1196721246,4.9441902017,-0.0131653905
H,1.5595063523,4.0747487583,0.5417545455
H,-2.0583451309,5.3529413111,-3.5548526727
H,-2.3902264331,4.6067410102,-1.9771452461
H,-0.7187934801,4.7152573252,-2.577838261
H,-0.507950766,4.6262859517,4.2409482454
H,0.0563761601,5.1468741266,2.6465878881
H,-1.6432607859,4.6988921037,2.8857936662
H,1.4739946173,1.6559379584,3.0471830563
H,1.9004995809,3.3489557783,2.7632935456
H,1.2931900414,2.852134531,4.3491862646
H,-2.2686365788,2.2375000879,3.3970623075
H,-1.009609183,0.9932883382,3.4437490349
H,-1.0859659776,2.2271277695,4.7122750005
H,-0.9876355254,-3.6006735893,1.7870100915
H,-4.1445755455,-0.6703611825,1.7033685195

H,-2.6095714333,-5.3246218355,2.5260098211
H,-5.7646405141,-2.3957540995,2.442953218
H,-5.0028563312,-4.7287454145,2.857416907
H,8.3861003837,-0.8791601341,-0.8843191418
H,7.3388054371,0.4918682018,-0.3252744764
---end---

TS2-S-c-Et-TBS-CC

Electronic_Energy=-2454.40778761
Sum of electronic and thermal Free Energies = -2454.037678
Charge=0 Multiplicity=1
---Coordinates start---
C,0.2538313052,0.9076628806,0.3252124504
C,-0.302952626,0.896810217,-1.6449423274
N,0.8828982909,0.3761025499,-2.1451849135
C,1.9431521296,0.0130361442,-1.744745649
Ag,3.8393981403,-0.6365831198,-1.2995493314
C,-0.5976223833,2.2820783171,-2.0789165288
O,0.2001297319,3.0697282392,-2.5593830805
O,-1.8786831175,2.5875903046,-1.7814426598
C,-2.2672108516,3.9748243559,-1.923213758
O,1.4570565201,0.3905345529,0.3413674045
Si,-1.1038844525,-0.2202028827,1.0863495162
C,-0.6987147355,-0.501476868,2.947083948
C,-1.0154710403,-1.8772936194,0.1754397277
C,-2.8101364092,0.5759595346,0.8990043877
C,-3.5690670503,4.1559707276,-1.1690267437
C,-1.8412049536,-1.307787435,3.6008562366
C,-0.5559345094,0.8453438988,3.6847050811
C,0.6211778446,-1.2887218378,3.0848765099
C,0.1496622563,2.3331080505,0.6302402175
C,0.013051259,3.5084561747,0.9169742233
C,-0.1675082734,4.8932228934,1.2142729383
C,-0.8402674578,5.2969773902,2.3857204972
C,0.3082237945,5.8798706409,0.3250819923
C,-1.0300555423,6.6512959637,2.6567623582
C,0.1135020689,7.231607121,0.6046101565
C,-0.5547842567,7.6224434154,1.7695987511
Cl,6.1265388593,-1.4173973273,-0.4849067235
C,5.8819402185,-1.4912247379,1.3351340016
Cl,4.4502601405,-2.4448938978,1.7775588062
H,-1.1441826155,0.217678015,-1.7589813741
H,-1.4751067254,4.6102672815,-1.5190264294
H,-2.376298528,4.2004702037,-2.9903688183
H,-1.4708341011,-2.6832916837,0.7637727855
H,-1.5320597273,-1.844831766,-0.7914206104
H,0.0318338212,-2.1440795524,-0.0097430041
H,-2.9775396405,0.9033653596,-0.1331253027
H,-3.6099845461,-0.1248194356,1.1694318359
H,-2.908392946,1.4606242834,1.5399409385
H,-3.9090963844,5.1933933555,-1.2646733964
H,-4.349529422,3.4970571974,-1.5655172163
H,-3.4305734742,3.9329809806,-0.1057729583
H,-1.6122923255,-1.5065474814,4.6593387106
H,-2.7950186147,-0.7657361111,3.5708317577
H,-1.9934672383,-2.2804424416,3.1150719125
H,0.2737862093,1.441790133,3.2887884564
H,-1.4667092355,1.4534431288,3.611203317
H,-0.3613437531,0.6758243173,4.7550667319
H,0.5550740611,-2.2806224745,2.6192490126
H,1.4529949514,-0.7554768516,2.612030265
H,0.868533292,-1.4412696139,4.1471563281
H,-1.2094646241,4.5413654941,3.073047006
H,0.8197189359,5.5699225865,-0.5813227438
H,-1.5510108027,6.9496136049,3.5627924019
H,0.4837078673,7.9818781566,-0.0890839976
H,-0.7051648409,8.677069121,1.9842354003
H,5.755445809,-0.4643502911,1.67271625
H,6.779649698,-1.9613171626,1.7328252529
---end---

TS1-C-t-Et-TBS-CC

Electronic_Energy=-2454.40923293
Sum of electronic and thermal Free Energies = -2454.034451
Charge=0 Multiplicity=1
---Coordinates start---
C,0.3511972522,1.3072228995,-0.5965291162
C,-0.2172673114,1.1417788502,-2.1301116845
N,0.8542798456,0.5265441784,-2.8705152122
C,2.0010769849,0.420505202,-2.5176460904
Ag,3.5123970573,-0.1115729454,-1.1012867978
C,-0.5612546597,2.4921984407,-2.7472000583
O,0.2292142827,3.2303948543,-3.2974180389
O,-1.8552389729,2.7752307482,-2.5375213298
C,-2.2782945574,4.1287374245,-2.8519212716
O,1.7333867432,1.387912485,-0.6386659895
Si,-0.1633099089,-0.2338414247,0.4952984374
C,0.9564444807,-0.2041655693,2.0170755866
C,0.2006070646,-1.8076988365,-0.4966934868
C,-2.0184315668,-0.2302401741,1.0395742372

H,-1.1013389512,0.5056021301,-2.1610100993
H,-1.5946782949,4.827896808,-2.3611455196
H,-2.2011794971,4.2746775115,-3.9344139068
H,0.656311379,-0.9683606062,2.7454513852
H,1.9955564337,-0.4045090944,1.7289197639
H,0.9286031521,0.7704321811,2.5181093083
H,0.042192626,-2.6912870864,0.1341320496
H,-0.439357802,-1.9099402123,-1.3816277556
H,1.2429055423,-1.832068134,-0.8367465106
C,-3.7002560424,4.2832770413,-2.3544474473
H,-3.7472272334,4.1537000517,-1.2681521528
H,-4.0648144948,5.2876926906,-2.5972784491
H,-4.3631182003,3.5500987476,-2.8268781211
C,-2.2256545748,0.696445413,2.2569763528
H,-1.950127596,1.7328915893,2.0394646693
H,-3.284327728,0.6907609091,2.5594099464
H,-1.6381917066,0.3689885541,3.1234182065
C,-2.9459971217,0.2305666092,-0.1042965003
H,-2.722322745,1.2509835127,-0.4345222647
H,-2.8769266793,-0.4278755192,-0.9803744196
H,-3.995598349,0.2130182677,0.227425167
C,-2.421017993,-1.6641735372,1.4515892128
H,-3.4537276379,-1.6716630861,1.8325971153
H,-2.3800178387,-2.3636202965,0.6080695605
H,-1.7797828158,-2.0625430452,2.2491132701
C,-0.2133228186,2.5319706008,-0.0225608541
C,-0.6680035315,3.5375463398,0.48868232
C,-1.2672067644,4.6961819805,1.0689895087
C,-2.6314832949,4.6825950889,1.4303404709
C,-0.5180870427,5.8719796562,1.278104358
C,-3.2246503213,5.8164984698,1.9832093252
H,-3.2130258512,3.7790467409,1.2742819425
C,-1.120194132,7.0002333183,1.8330530774
H,0.5316633825,5.8891595166,1.0001529253
C,-2.473179869,6.9782965903,2.1867480547
H,-4.276396831,5.7927218794,2.2560387191
H,-0.5313952443,7.9003652085,1.9887990949
H,-2.9385944516,7.8604951081,2.6179211555
Cl,5.4642476386,-1.0434922797,0.2930714102
C,6.3389947183,-2.1522084925,-0.8719653387
H,6.9471787823,-2.8161727615,-0.26005738
H,6.9351949068,-1.5165309053,-1.523510686
Cl,5.2065825883,-3.1109267214,-1.8546488494
---end---

TS2-S-t-Et-TBS-CC

Electronic_Energy=-2454.41342899
Sum of electronic and thermal Free Energies = -2454.035388
Charge=0 Multiplicity=1
---Coordinates start---
C,0.1233203254,1.2356503016,-0.9508343645
C,-0.2362999911,1.2418535987,-2.4925910452
N,0.946454335,0.6530871583,-3.1391019722
C,2.0429661251,0.6736786502,-2.6241213874
Ag,3.4271055967,0.1524617591,-1.1076833299
C,-0.4297805841,2.6325213736,-3.1059334195
O,0.4605420847,3.3538987514,-3.5013368076
O,-1.7340969971,2.944494313,-3.158187706
C,-2.072522592,4.2402098846,-3.7249905555
O,1.4481971233,1.6234612651,-0.8276816746
Si,-0.8580335659,2.4090338017,0.2701351234
C,-2.6934132112,1.8651433202,0.5645351321
C,-0.7551149706,4.1993508036,-0.3331796573
C,0.0992217484,2.2898652979,1.8951196969
H,-1.1197059659,0.6386318172,-2.7026948362
H,-1.4535148445,5.0069528418,-3.2515972606
H,-1.8300396362,4.2164794806,-4.792702083
H,-0.8031027975,4.8770558732,0.5285046715
H,0.1965030489,4.377296567,-0.8454145216
H,-1.5683320083,4.4697119047,-1.0113345604
H,1.0902559804,2.7404501003,1.7729236704
H,-0.4217633229,2.8228903948,2.7009059912
H,0.2378217534,1.2497428029,2.2116643992
C,-3.5497579352,4.4652581379,-3.4795758182
H,-3.7685225521,4.4917883624,-2.4064704233
H,-3.8509512605,5.423292797,-3.9177298946
H,-4.1486512414,3.6710600063,-3.9381104788
C,-2.7772058582,0.8162632743,1.6952953065
H,-2.2192858792,-0.0937687927,1.4501642571
H,-2.3914613886,1.2016507541,2.6466690109
H,-3.8260659464,0.5259213152,1.861349626
C,-3.3276313293,1.2632171575,-0.7053034033
H,-3.2891696068,1.9518238285,-1.5549426317
H,-2.8234432312,0.3354540073,-1.0023804346
H,-4.3845517155,1.0161878887,-0.5212554964
C,-3.5102960704,3.1054031881,0.9912552204
H,-4.5442096245,2.8141673357,1.2314371284
H,-3.0948939433,3.5896311675,1.8851440877
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9. References

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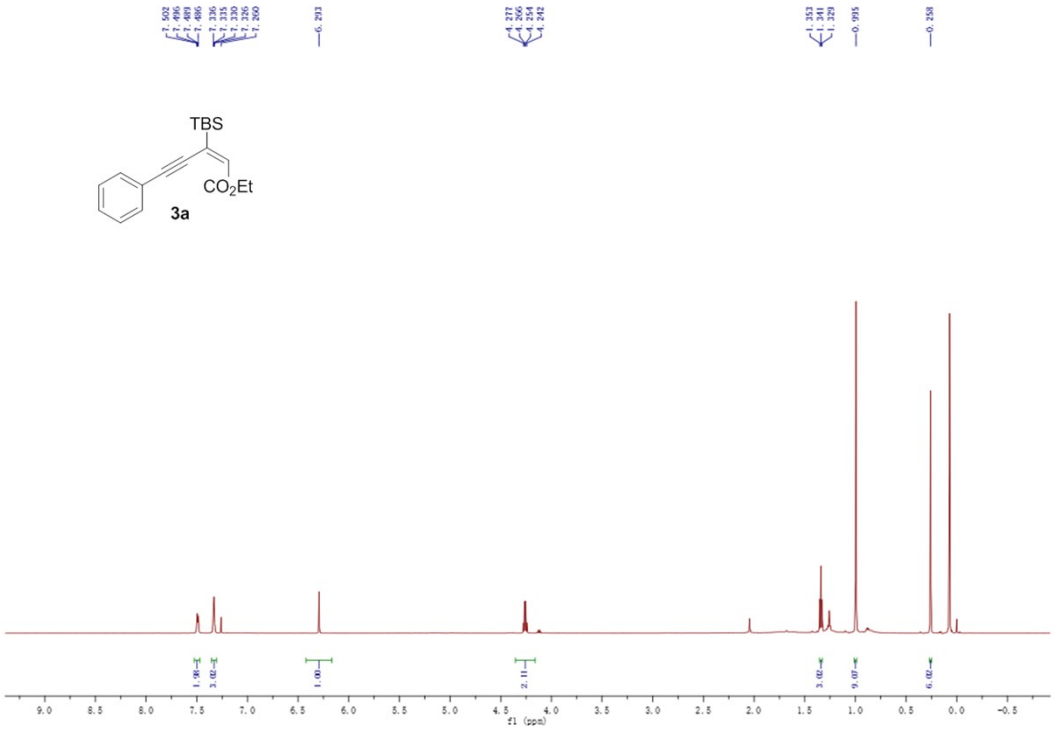
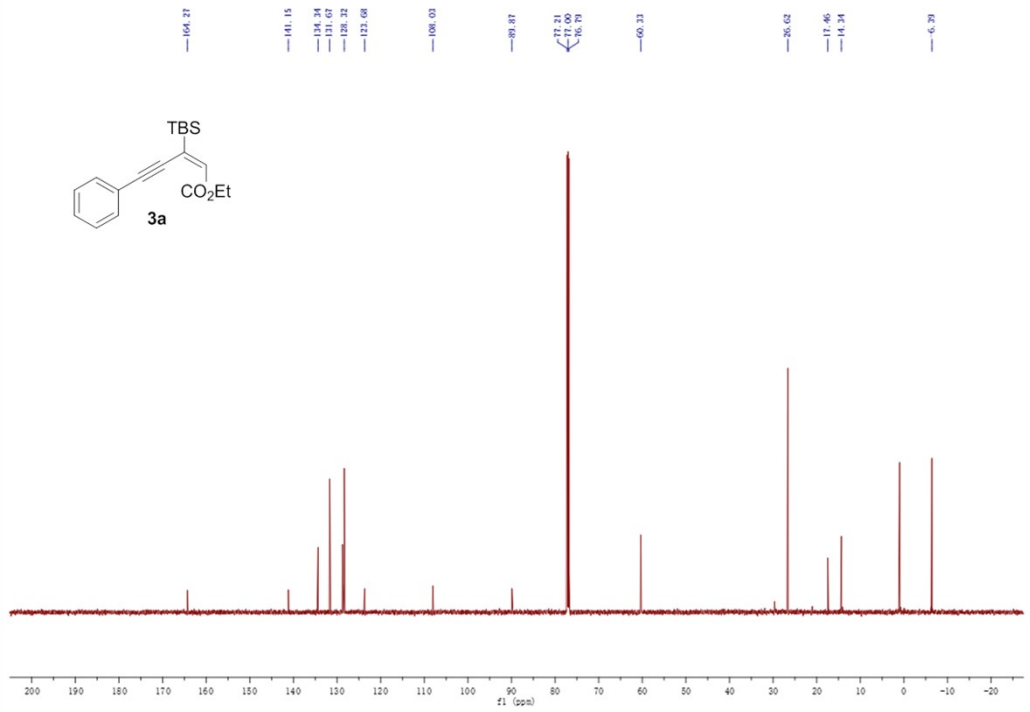
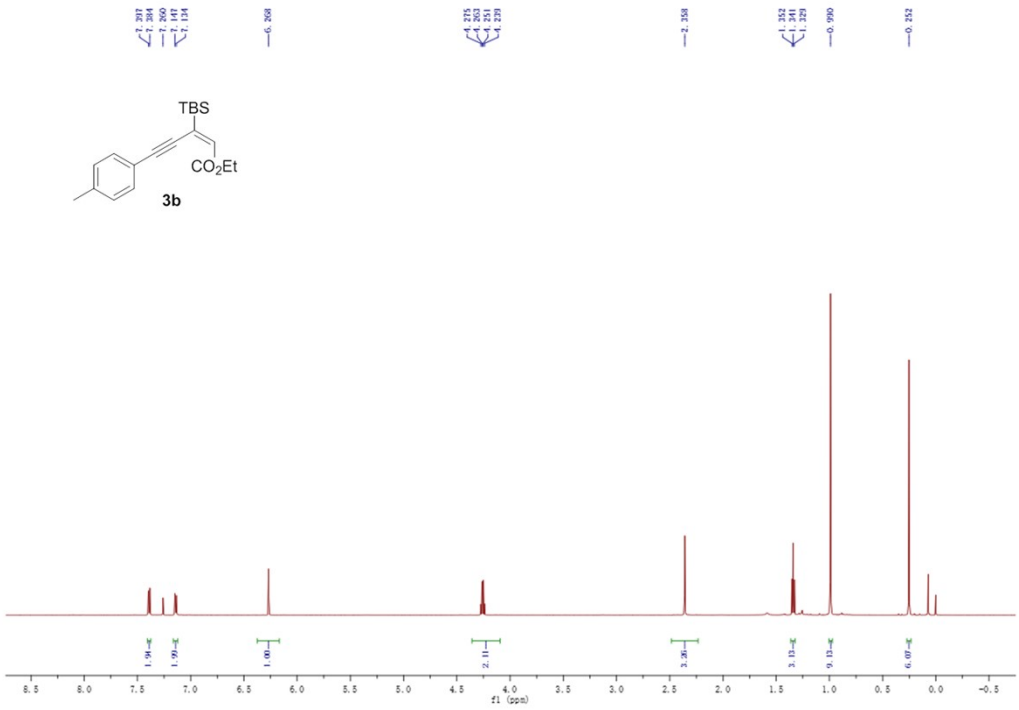
10. ^{1}H and ^{13}C NMR spectra of the products



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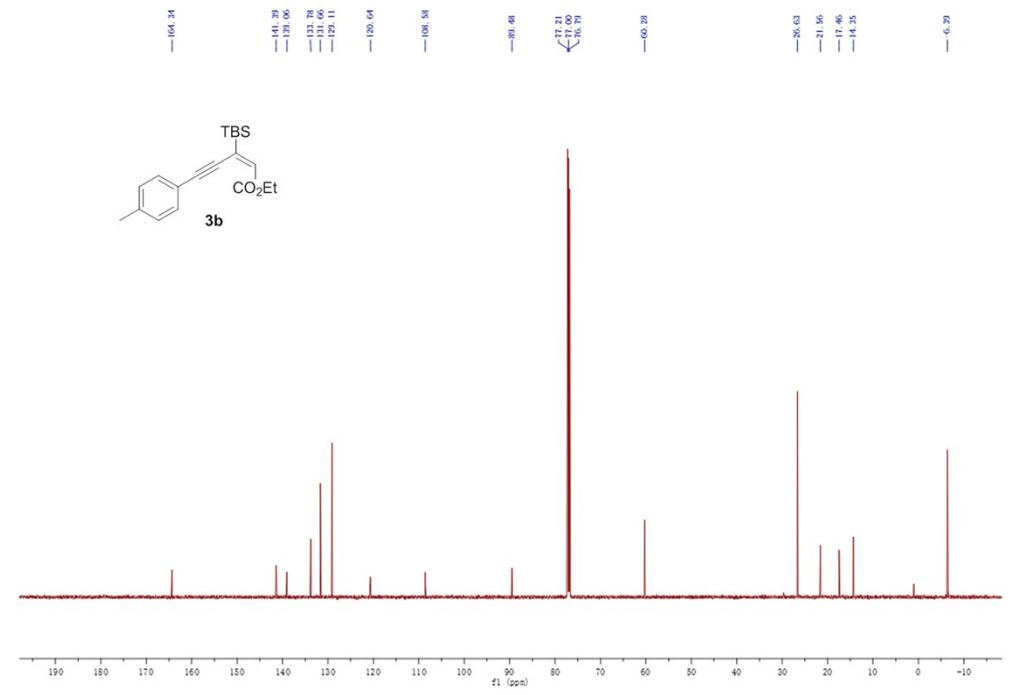
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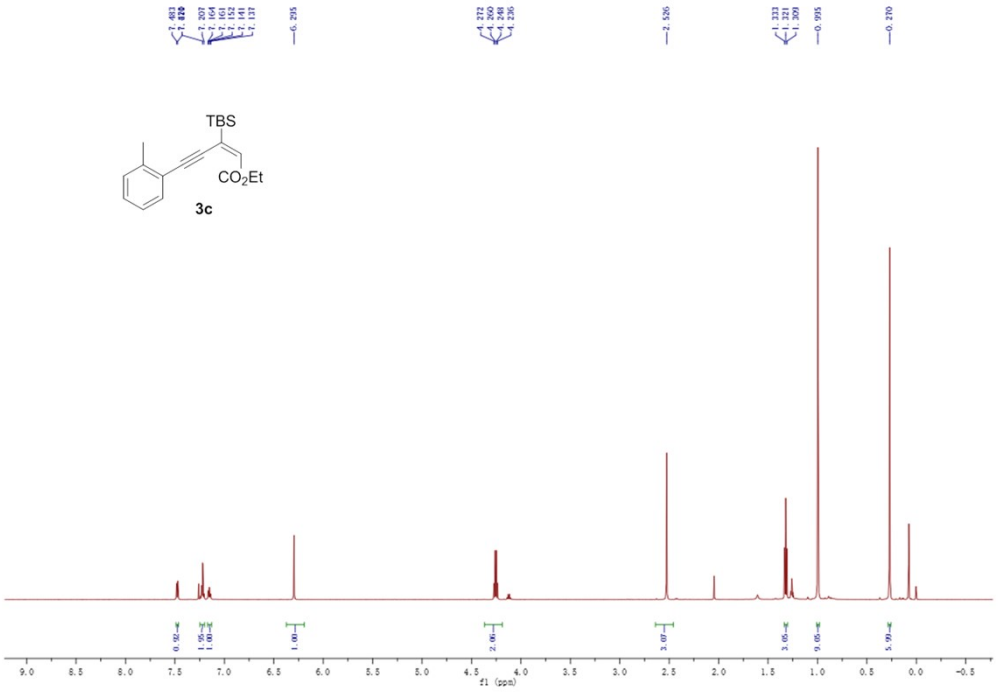
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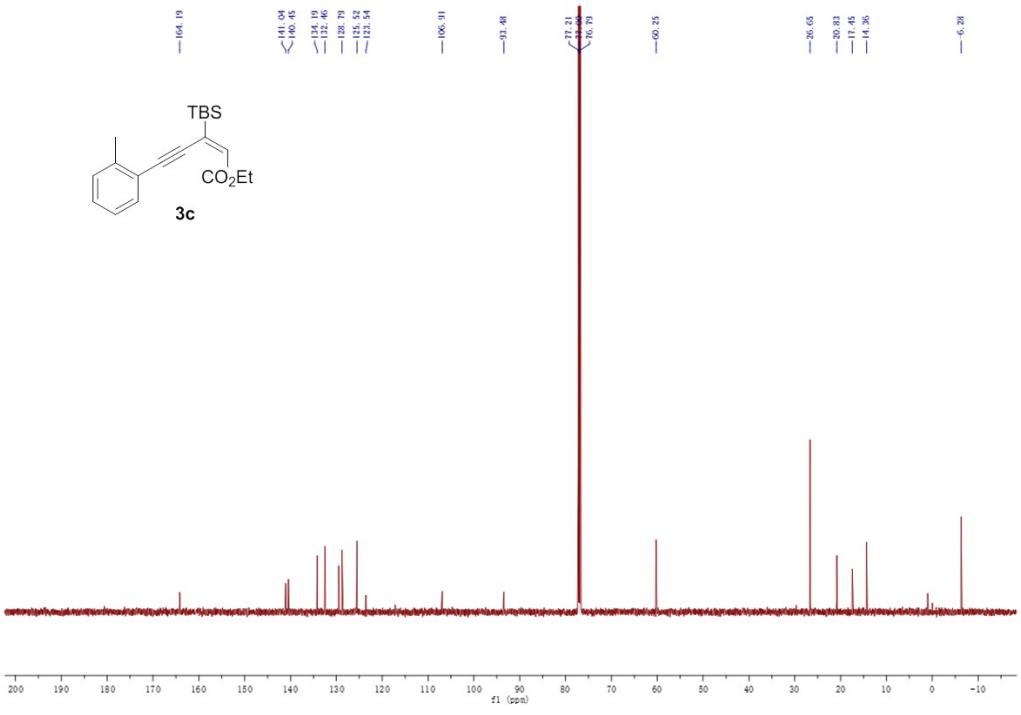
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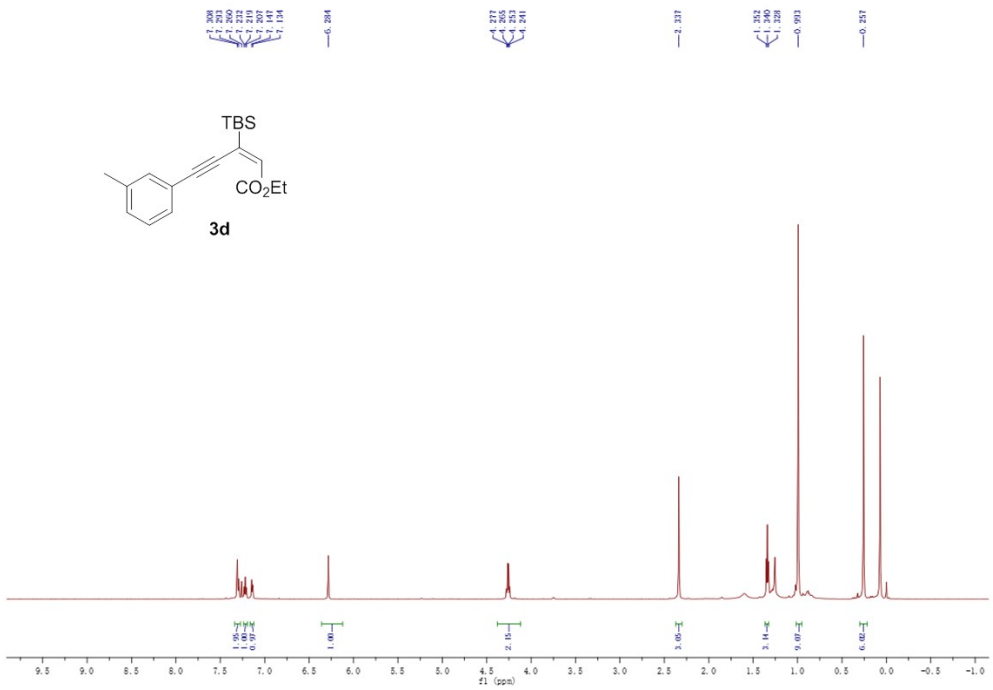
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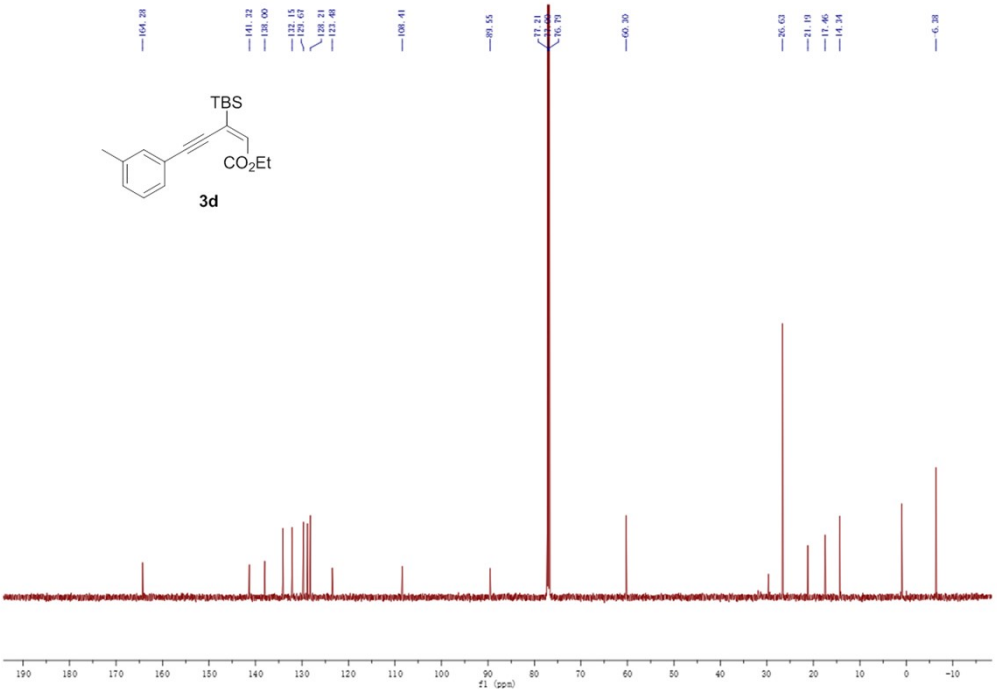
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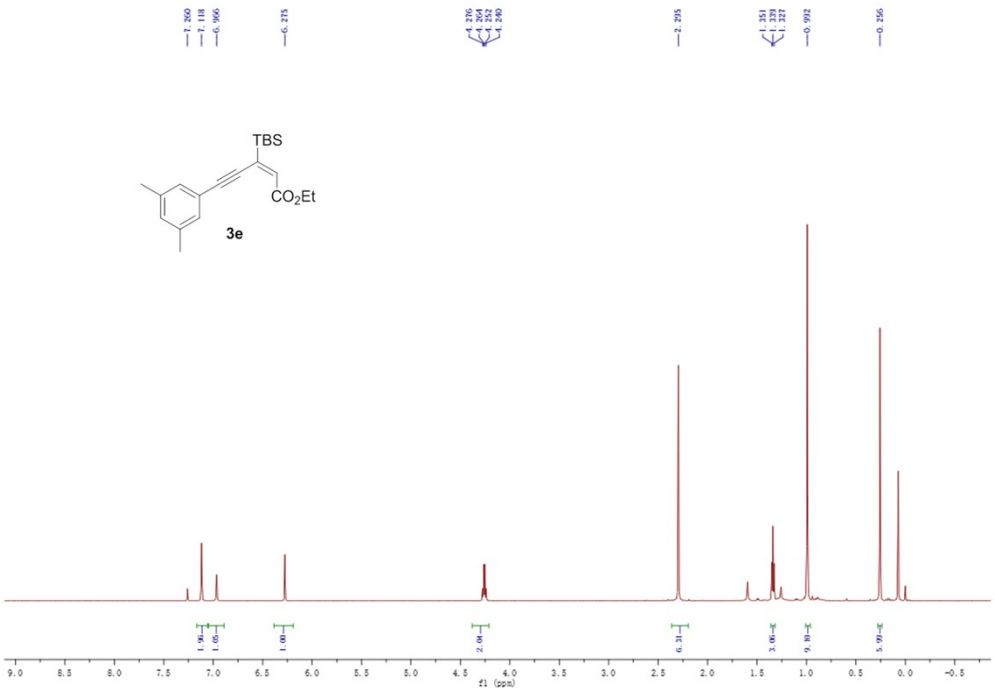
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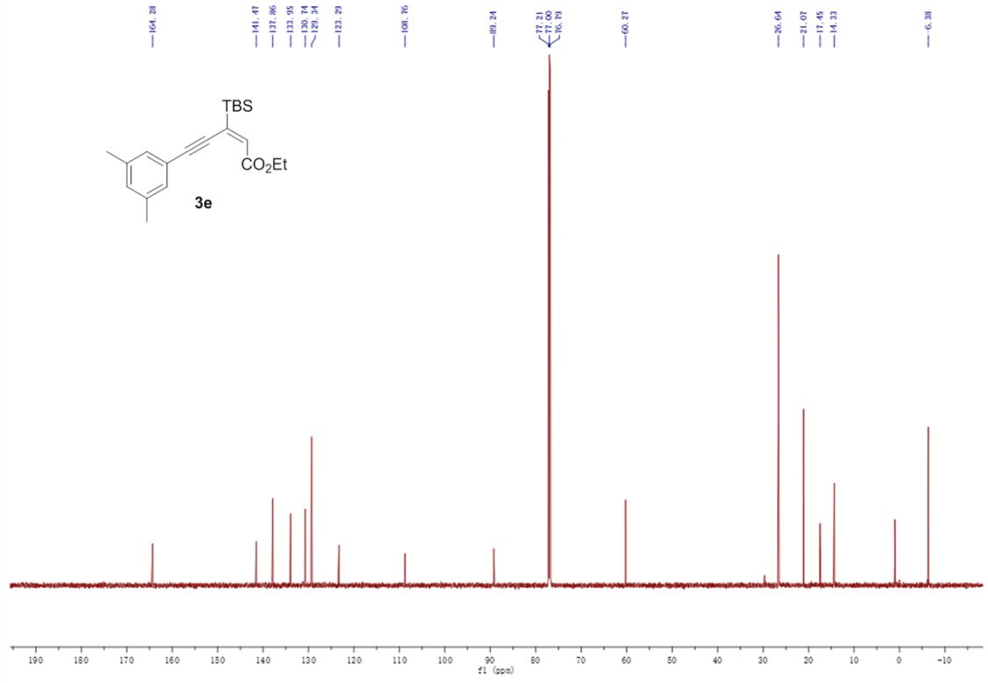
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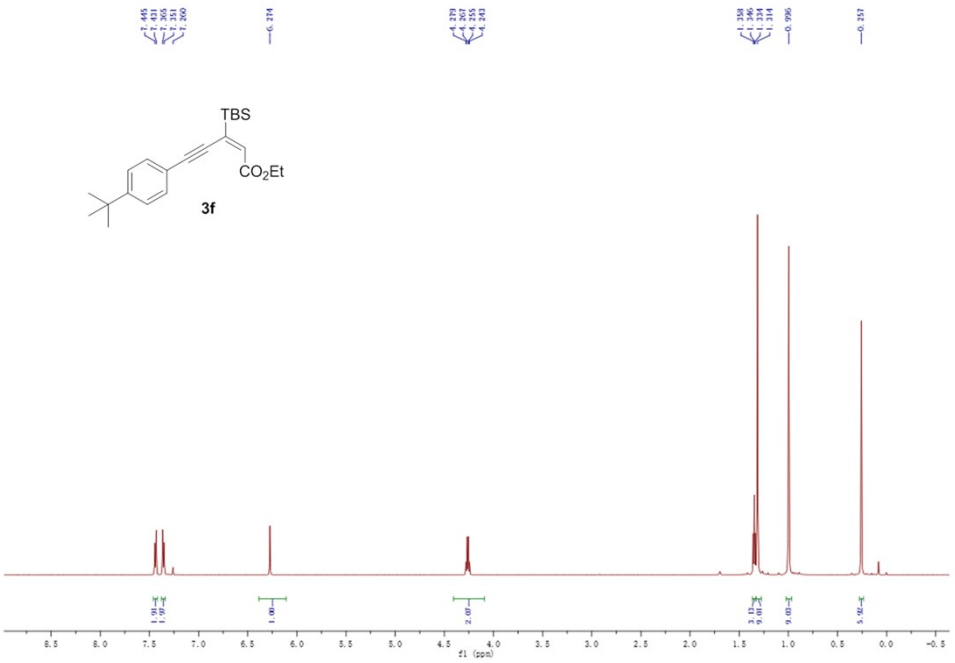
f1 (ppm)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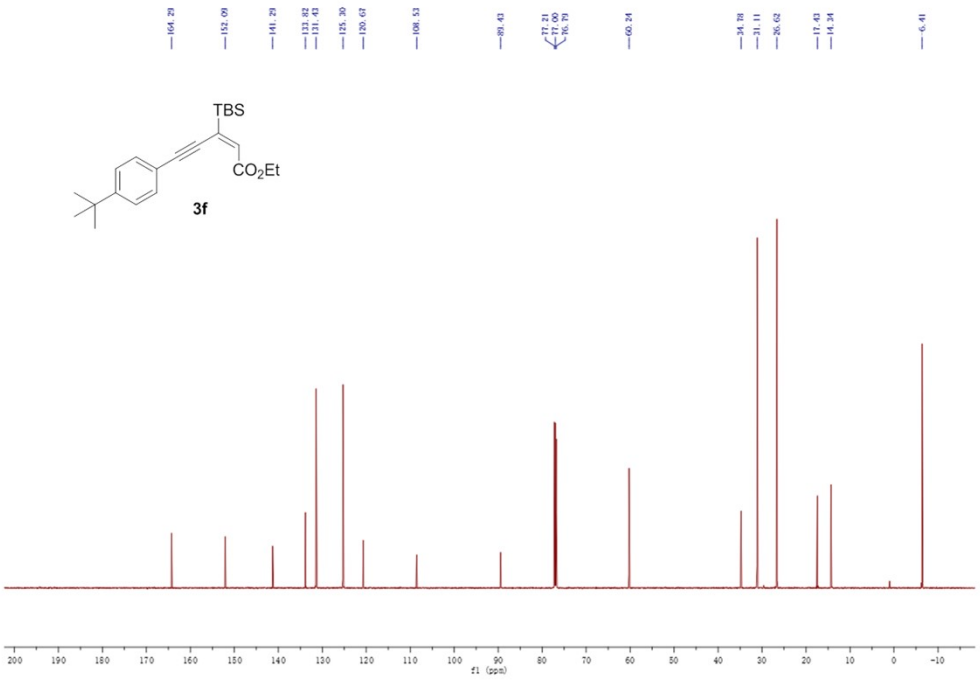
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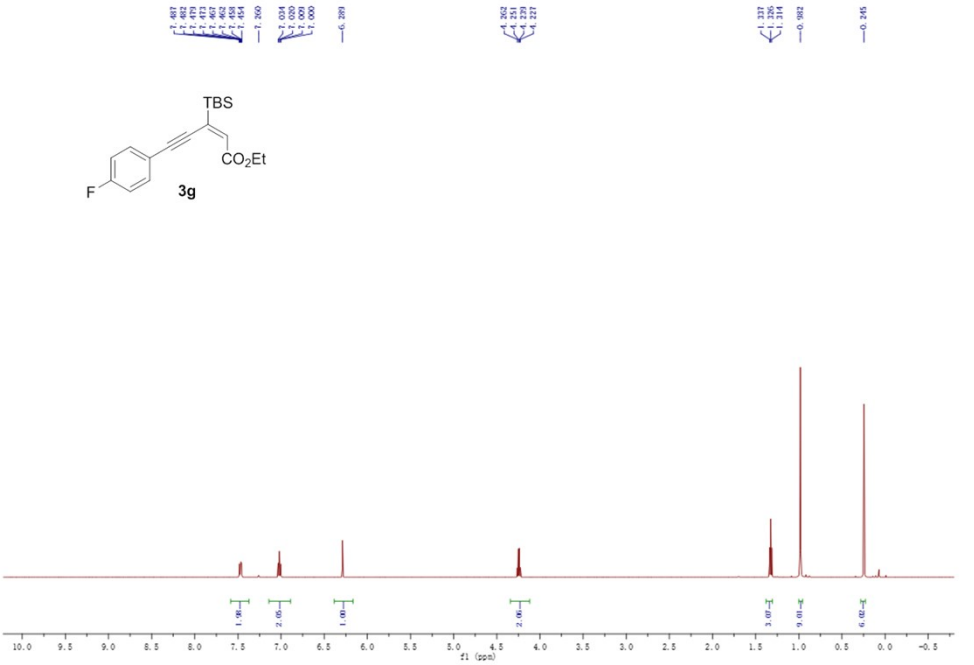
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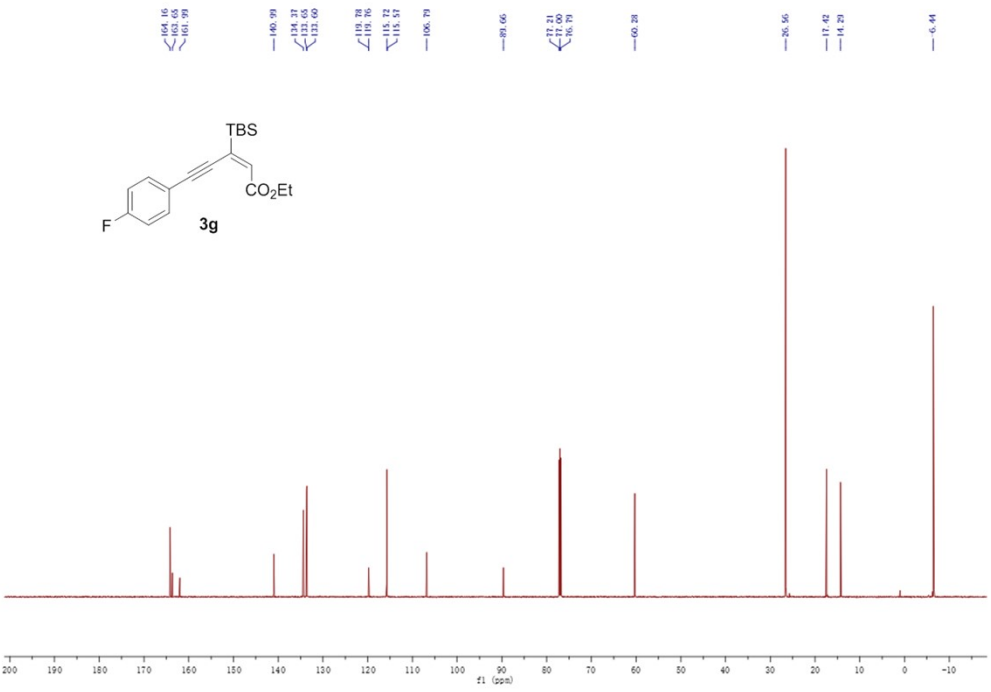
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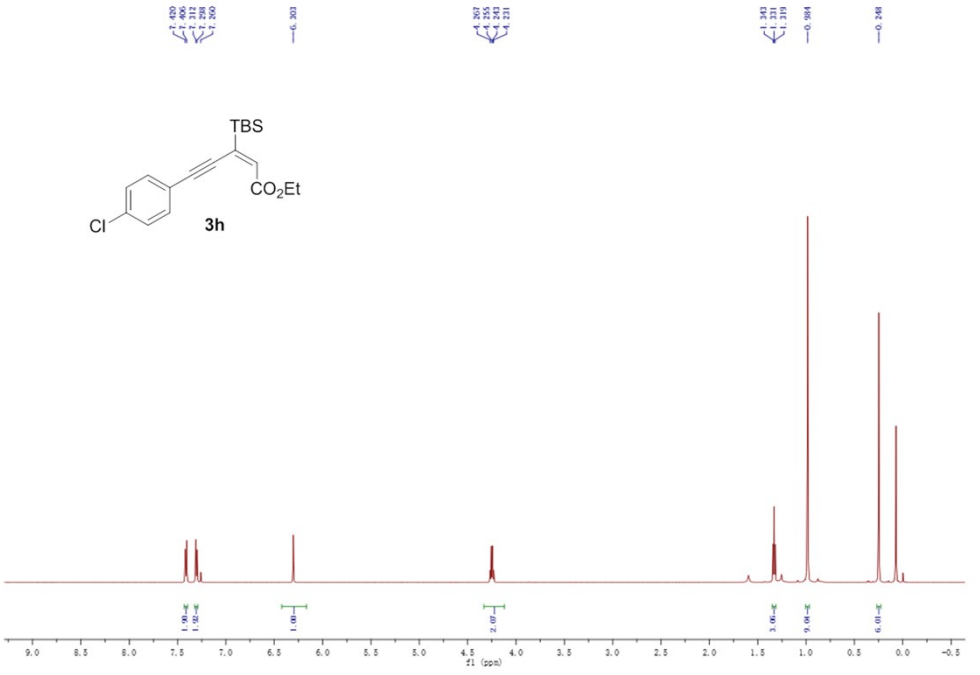
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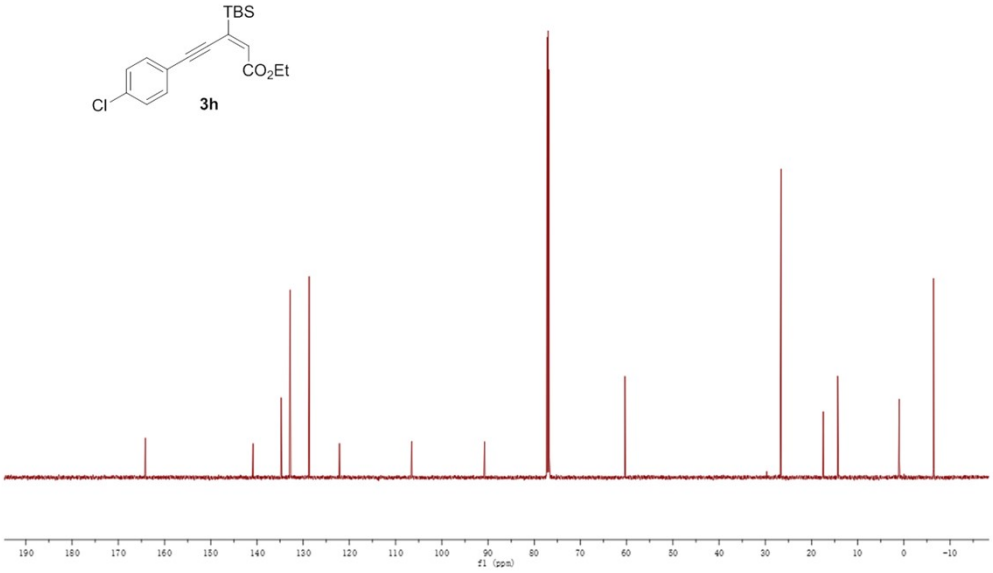
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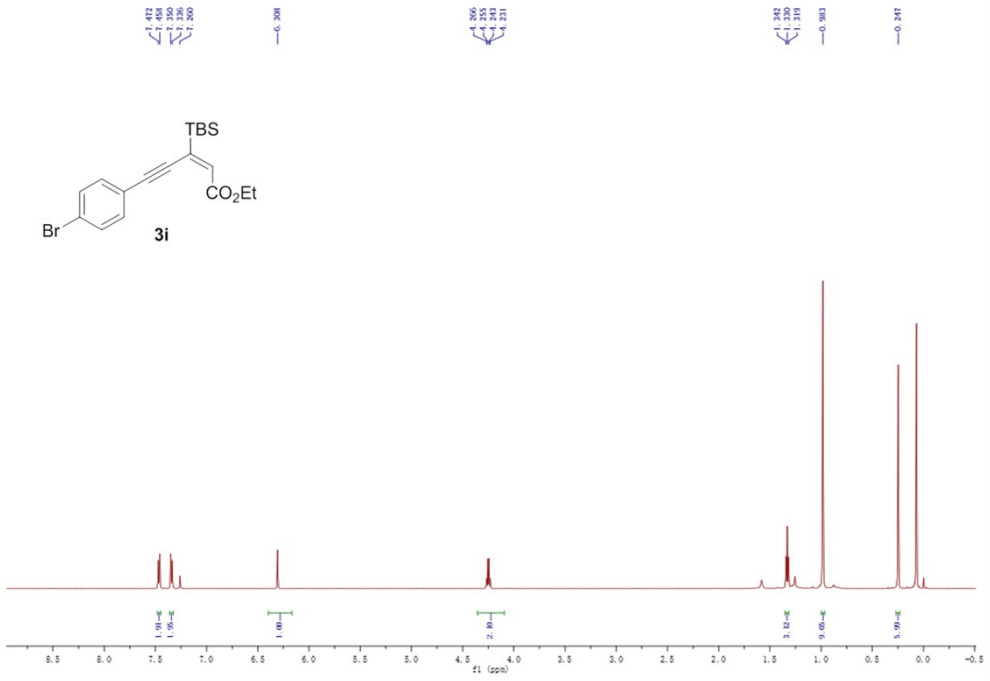
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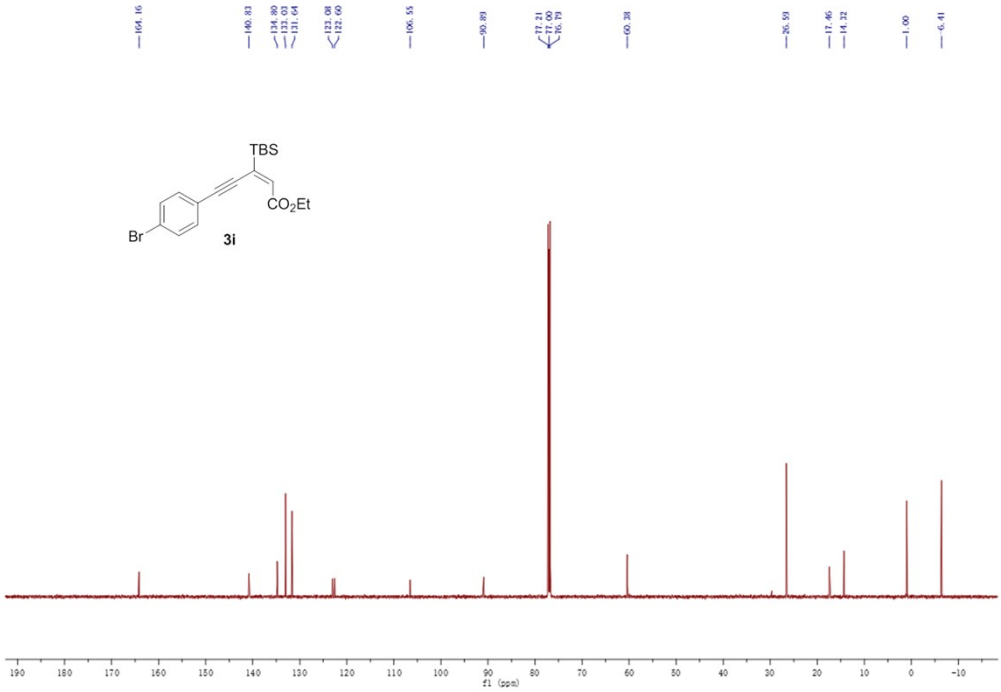
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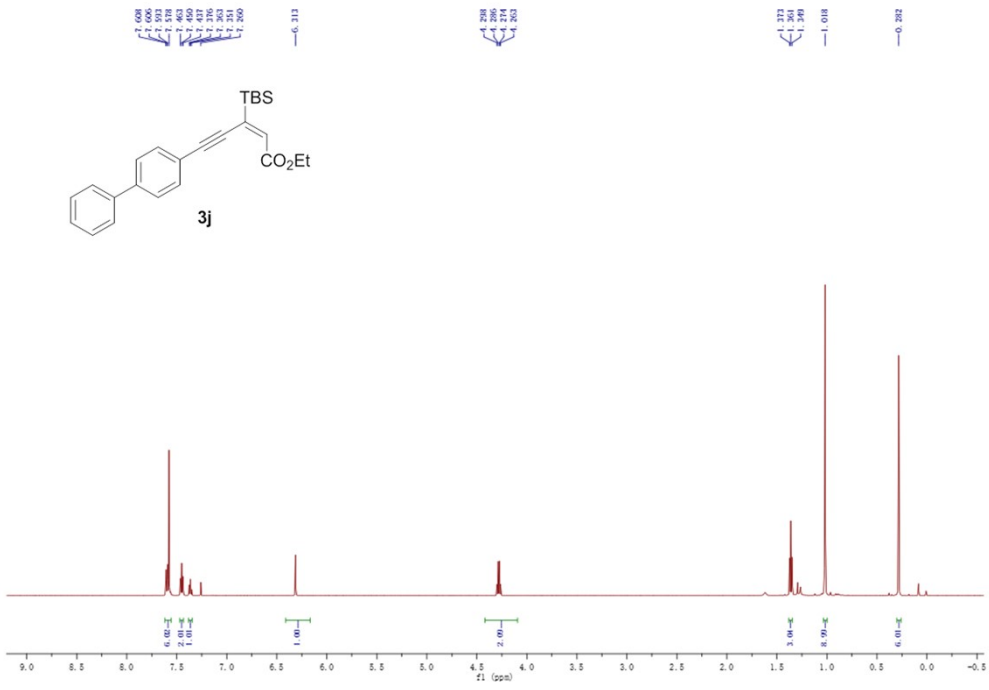
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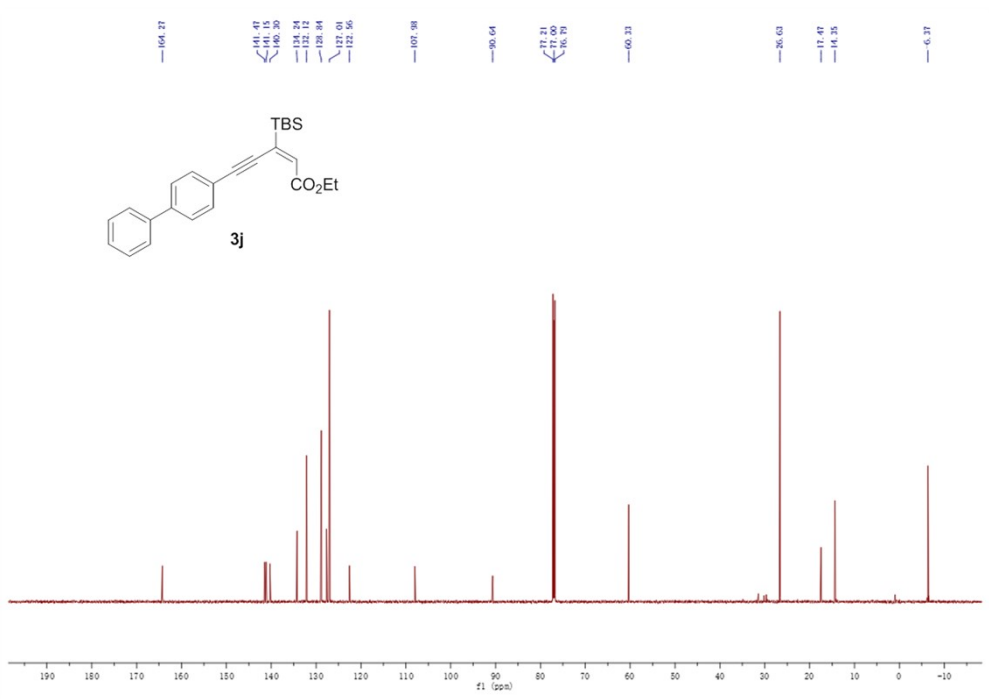
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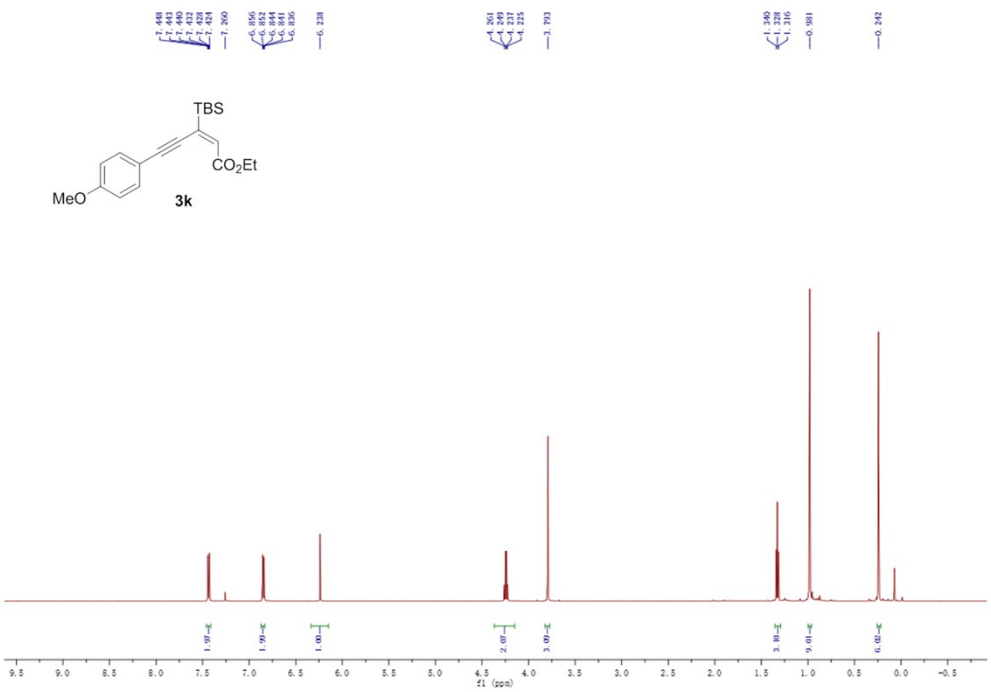
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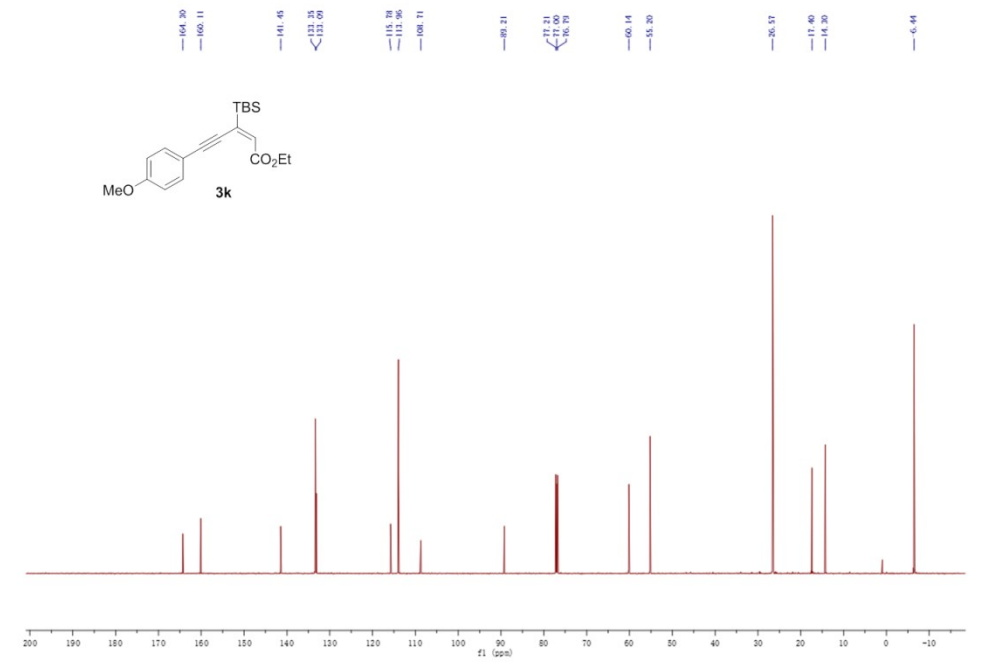
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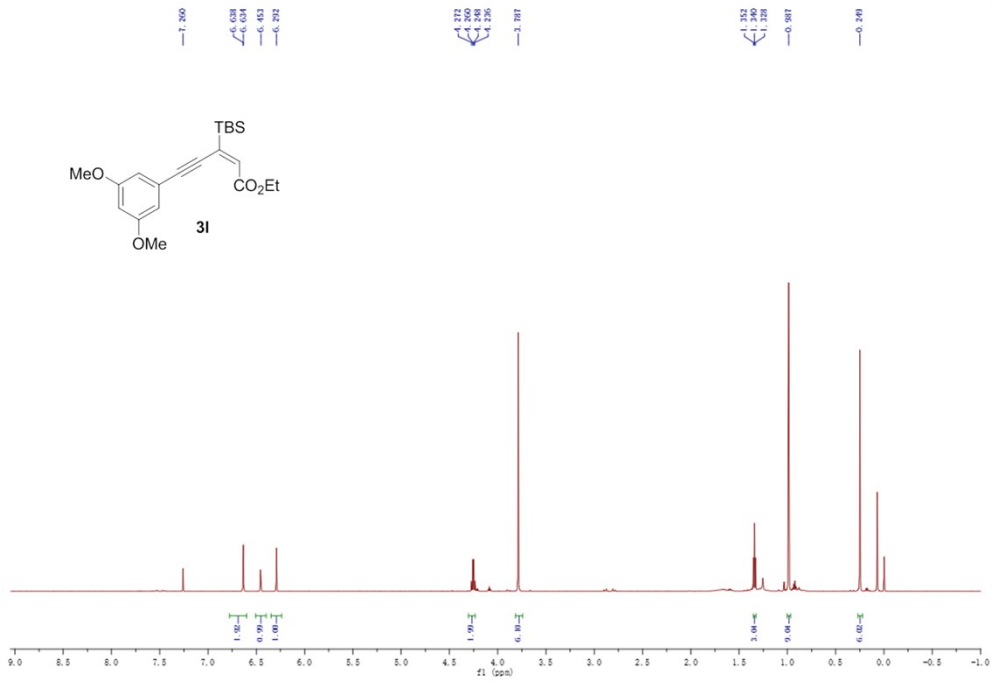
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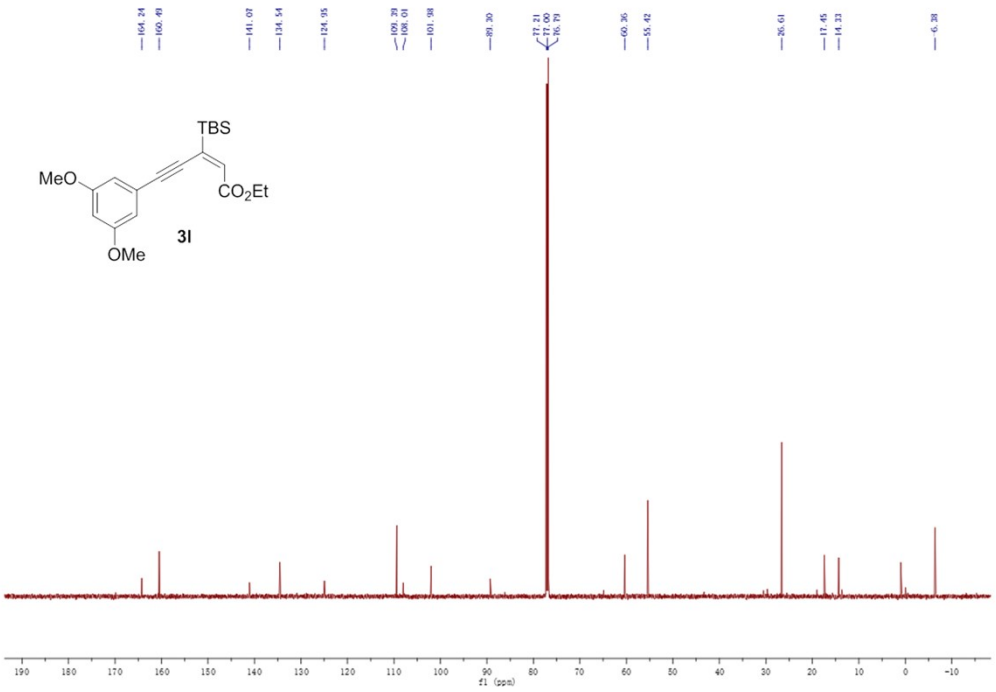
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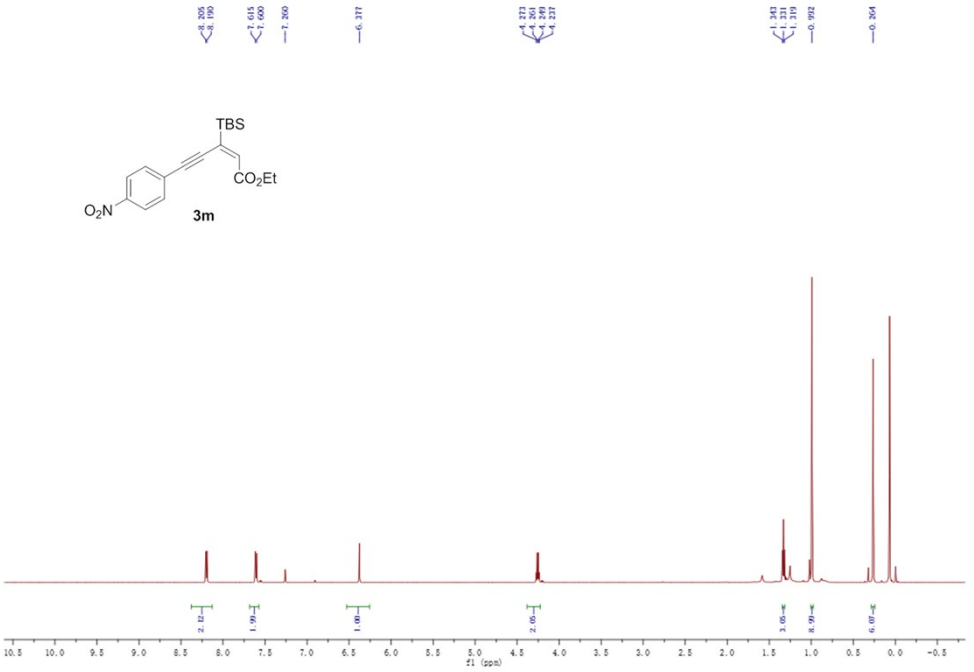
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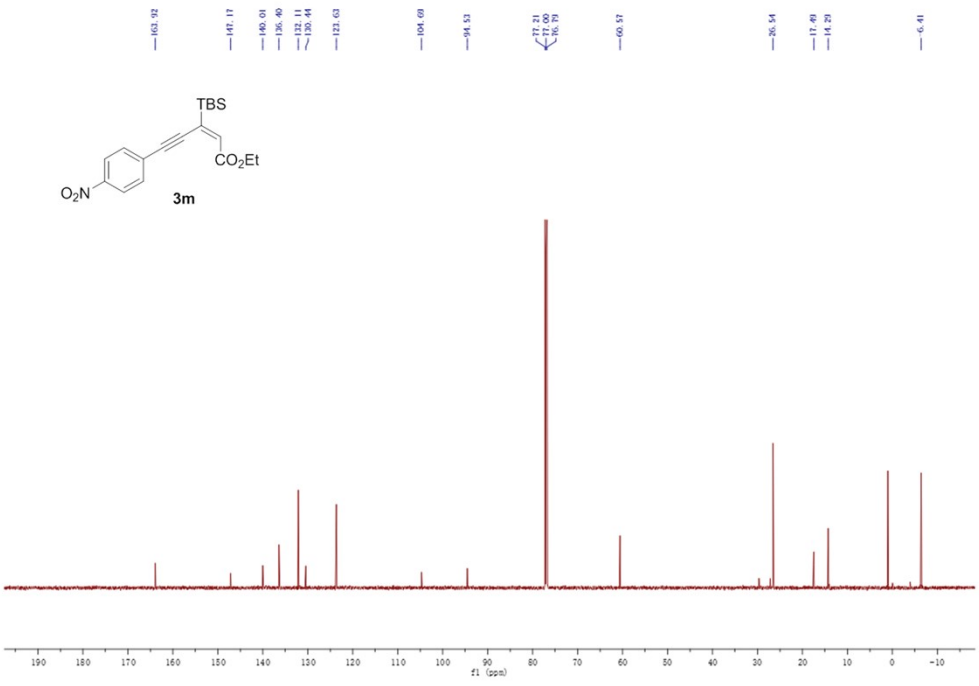
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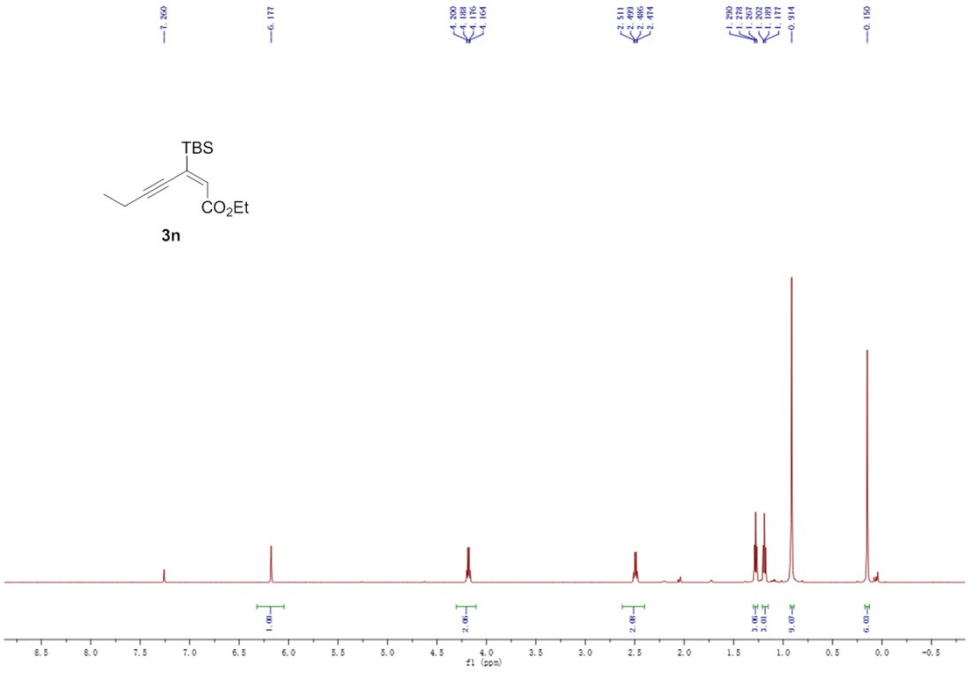
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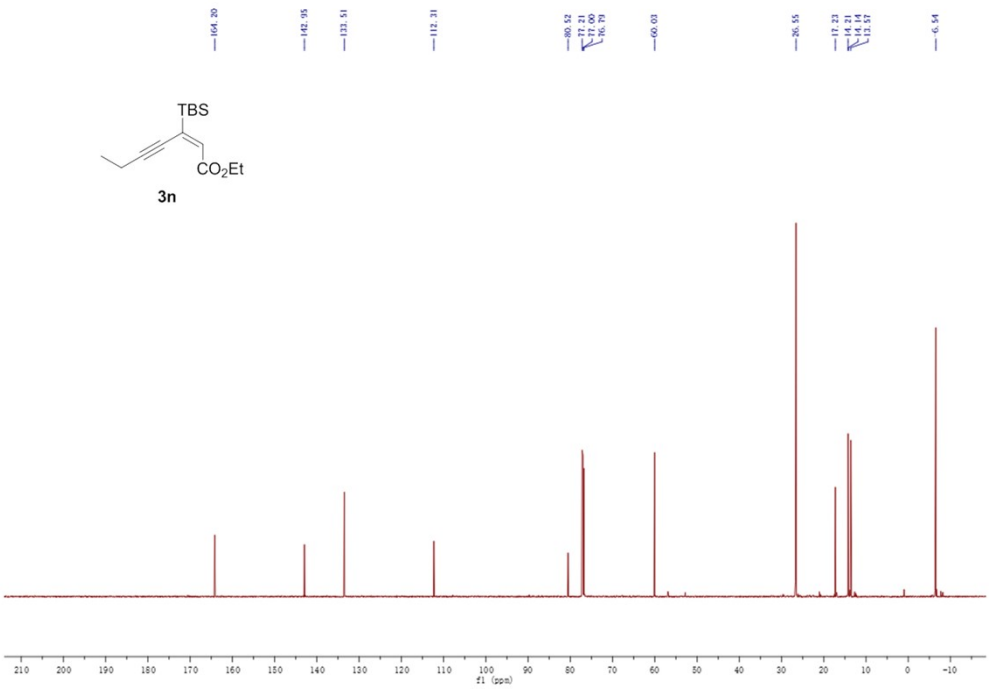
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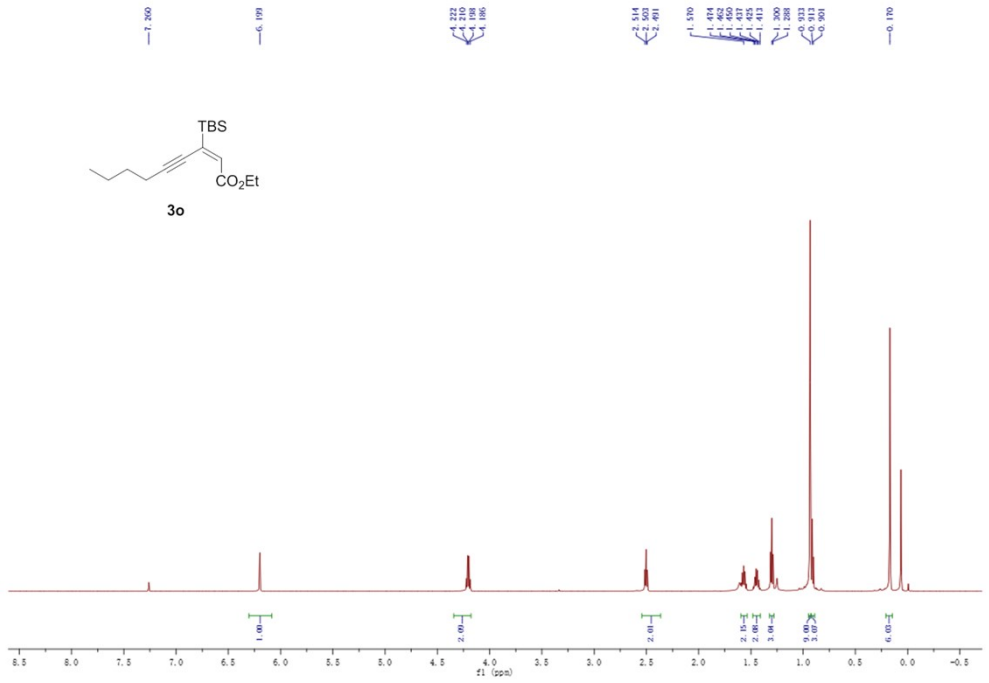
f1 (ppm)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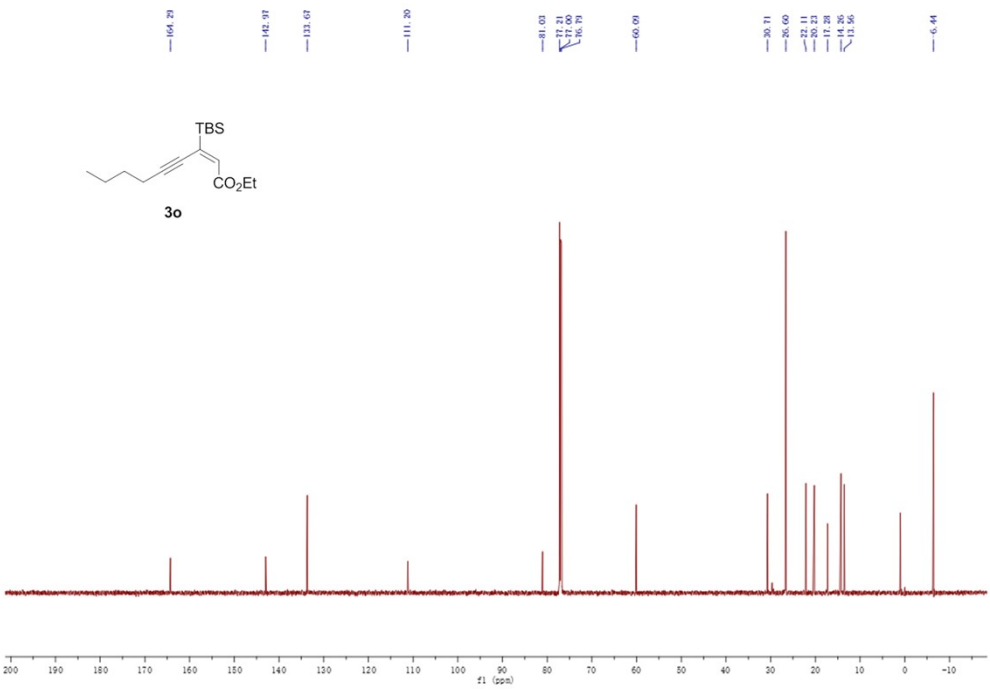
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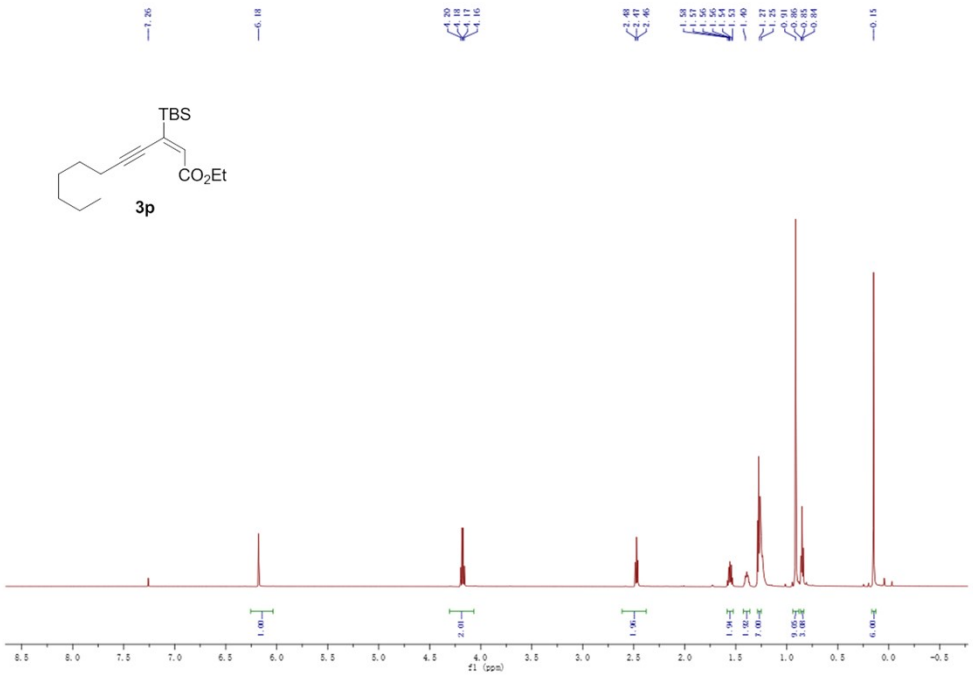
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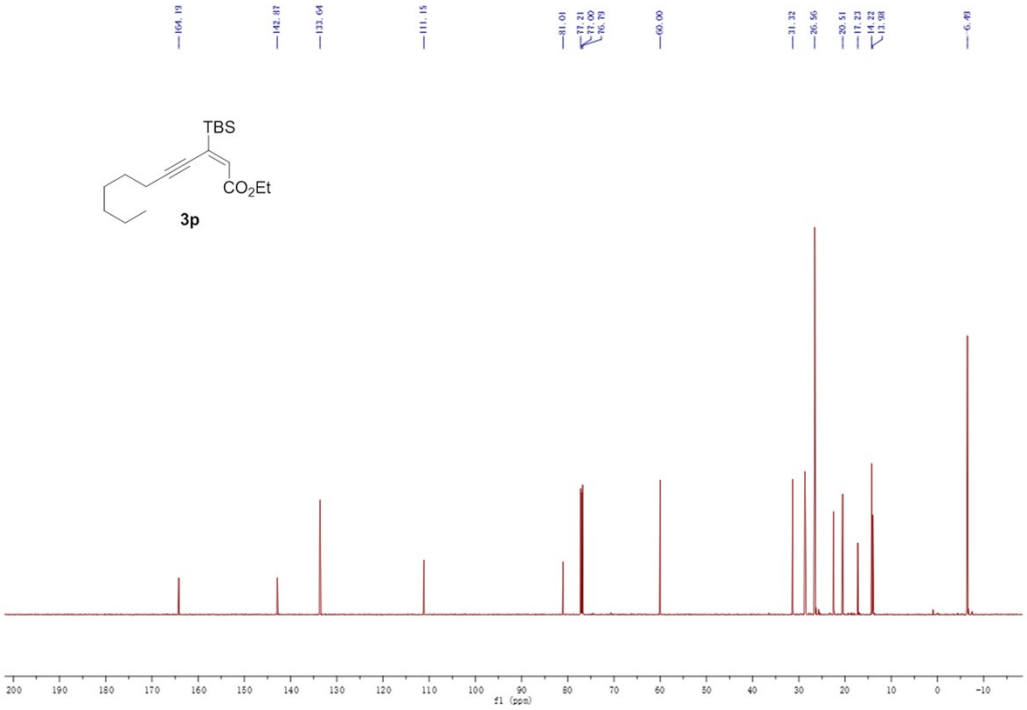
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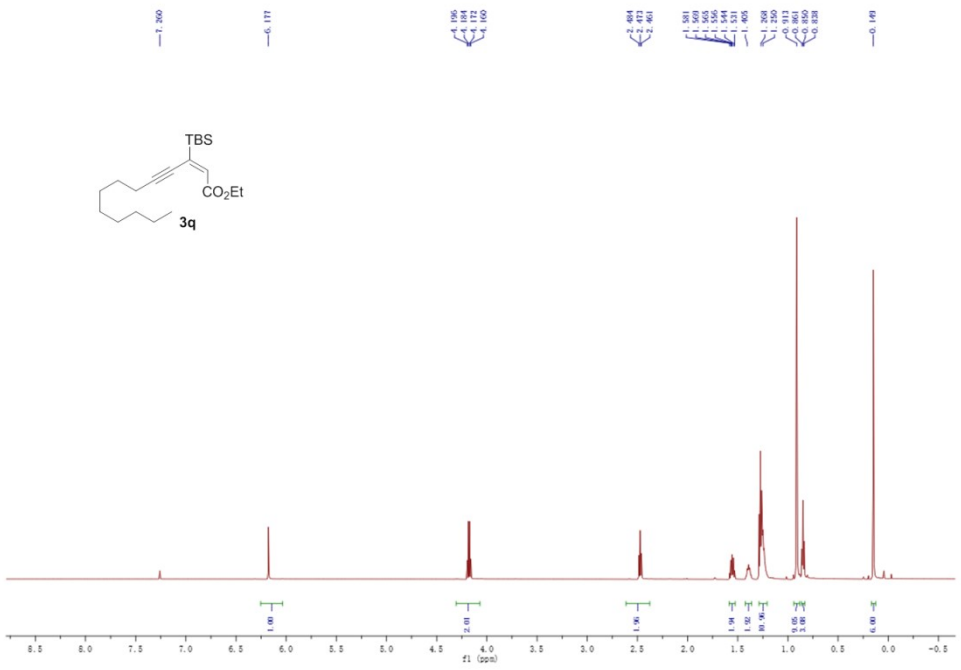
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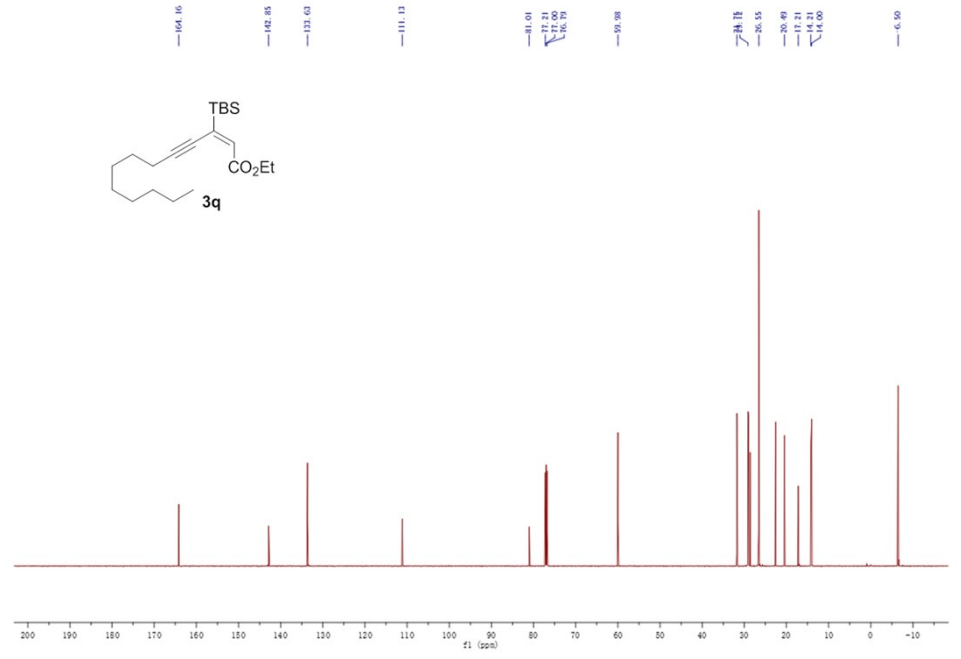
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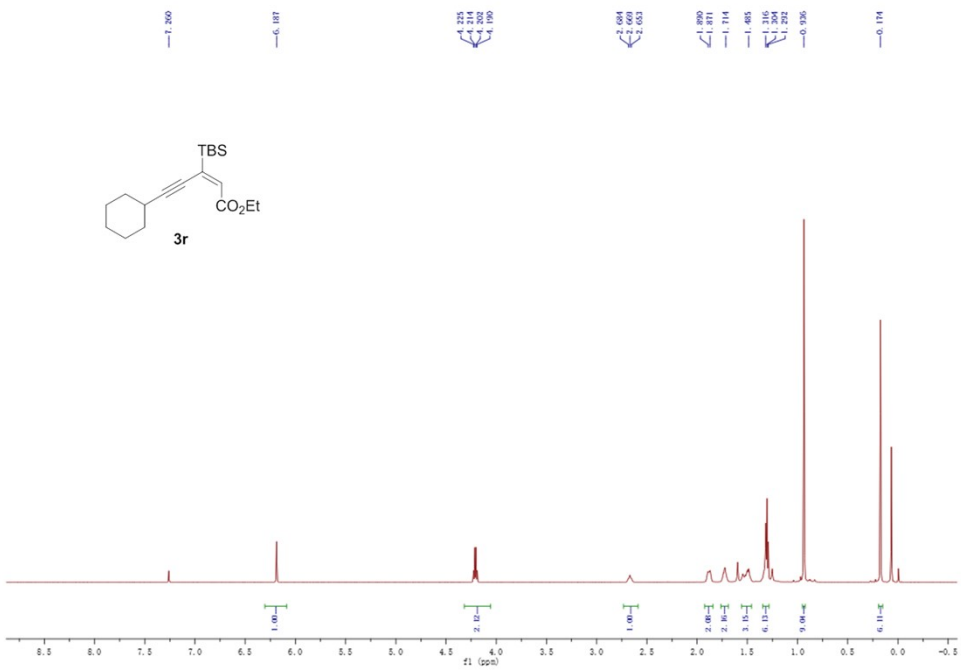
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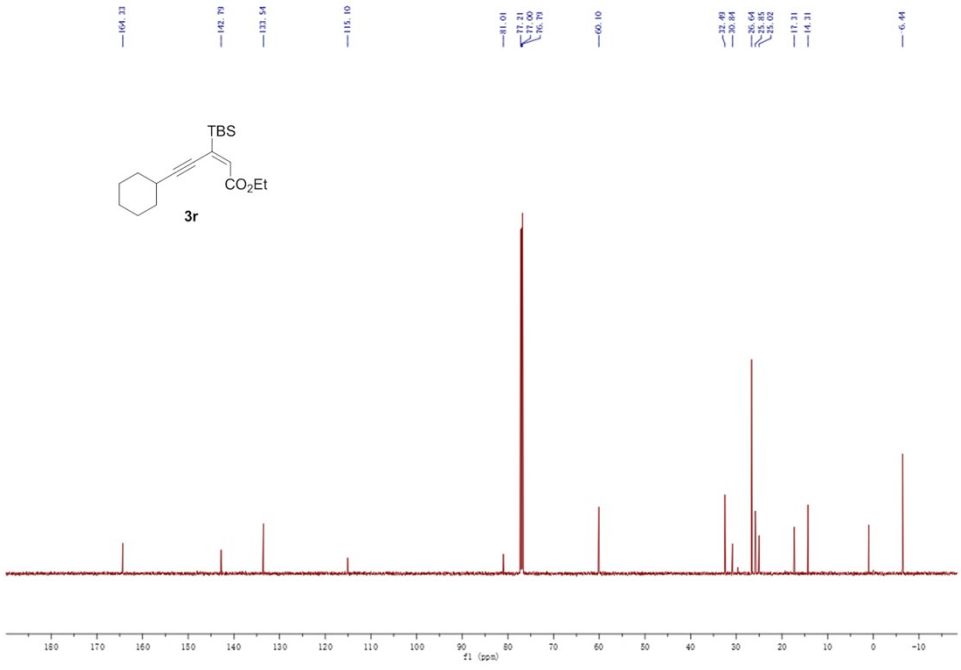
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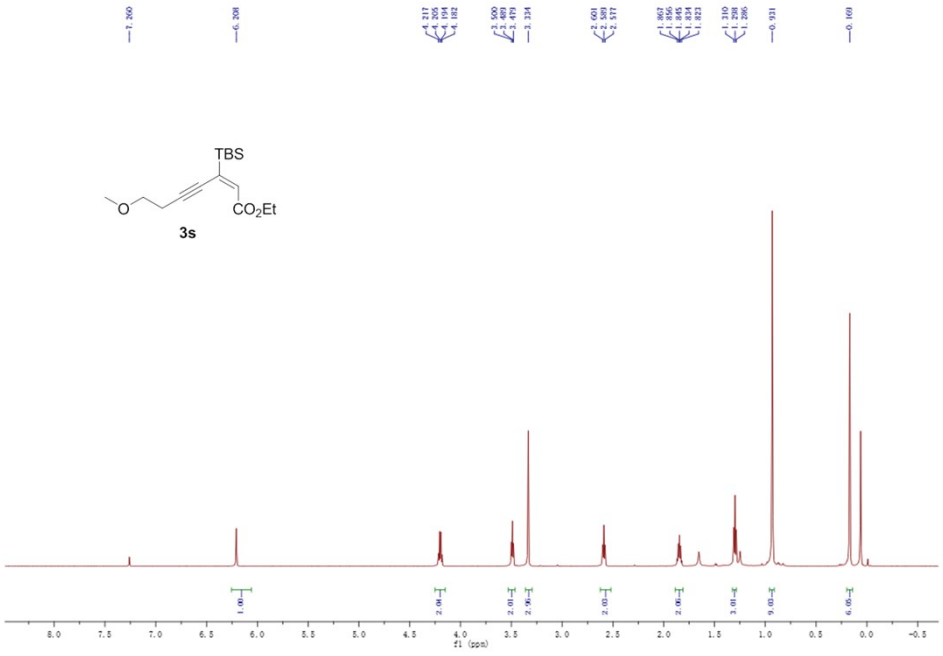
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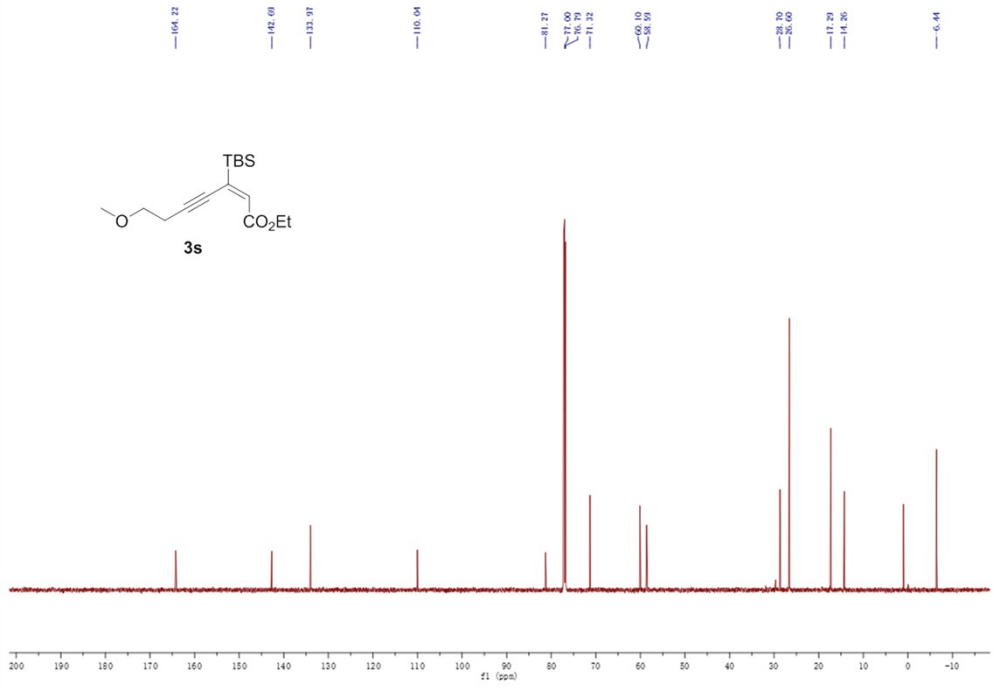
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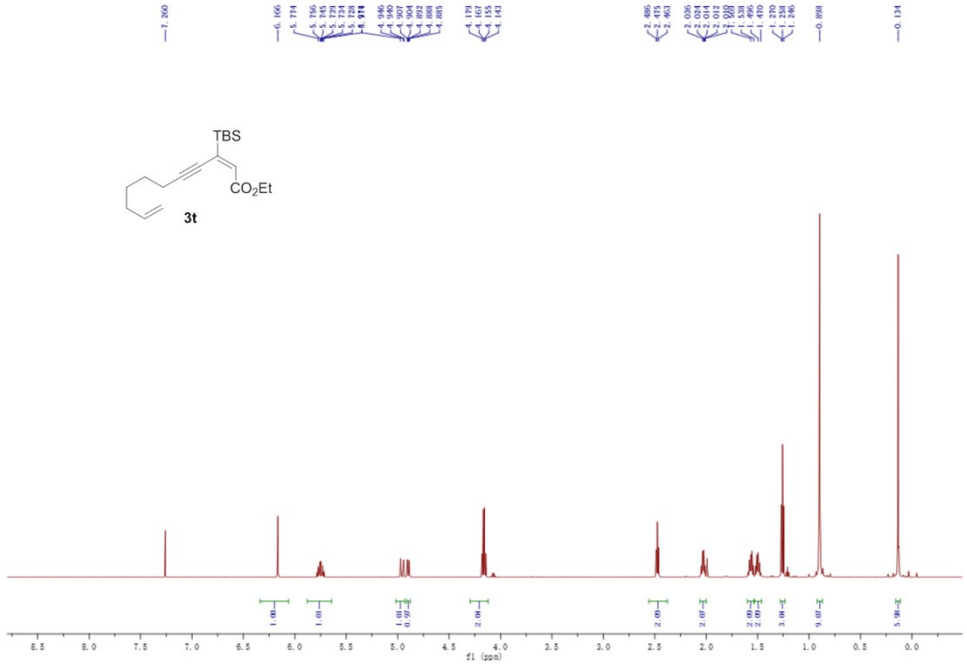
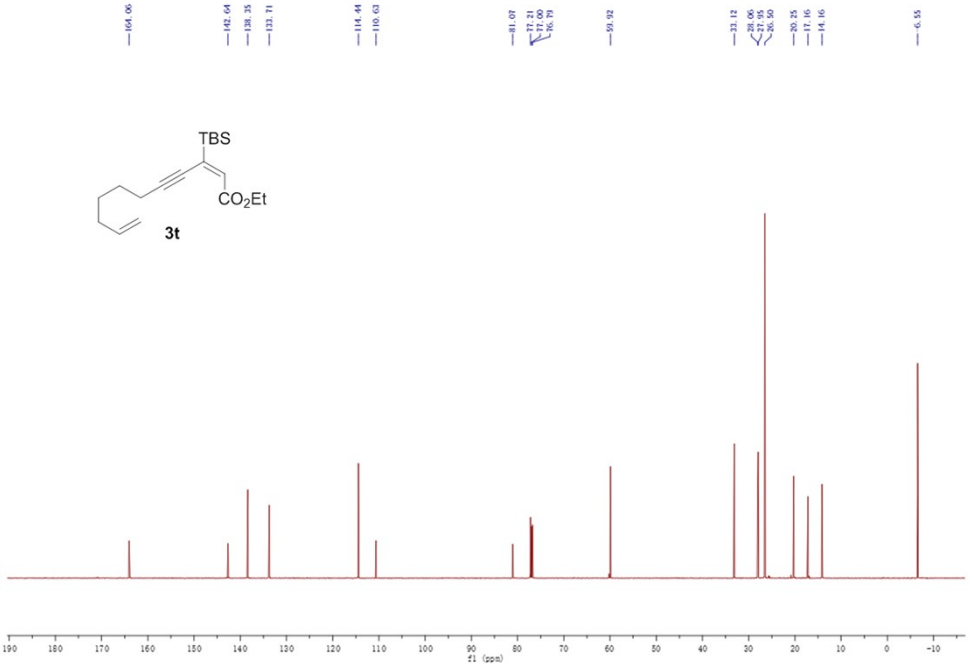
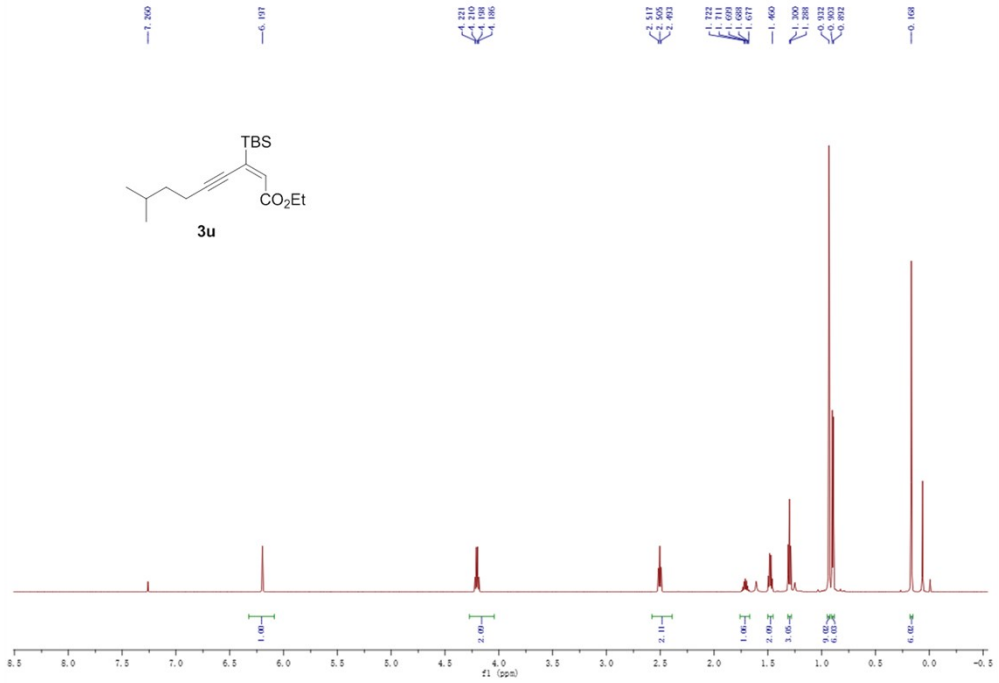
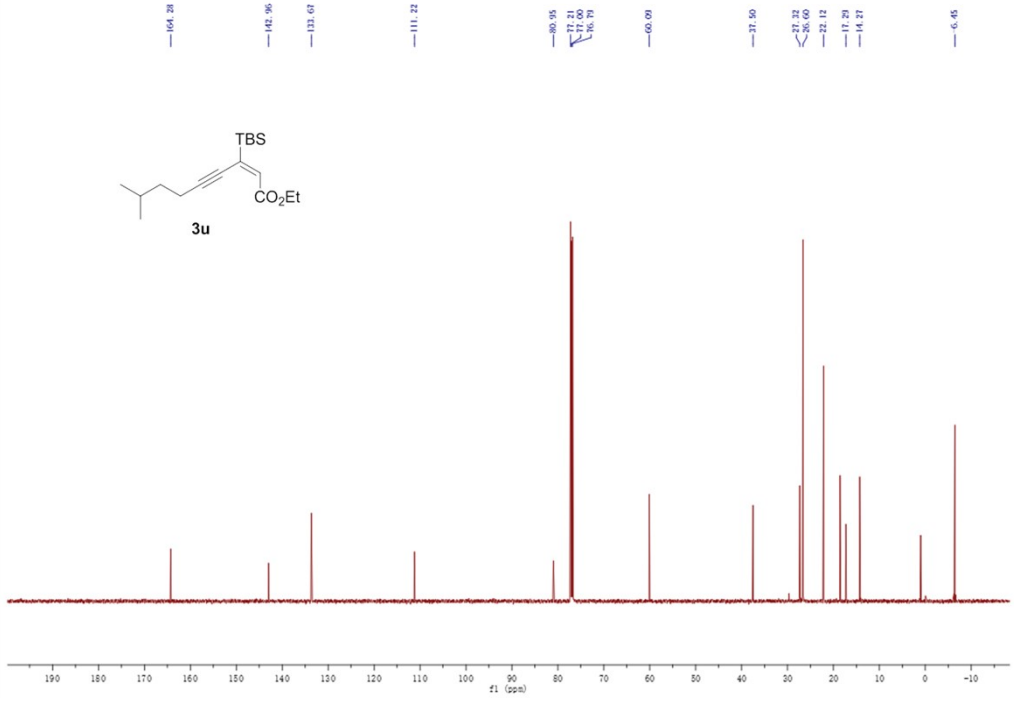
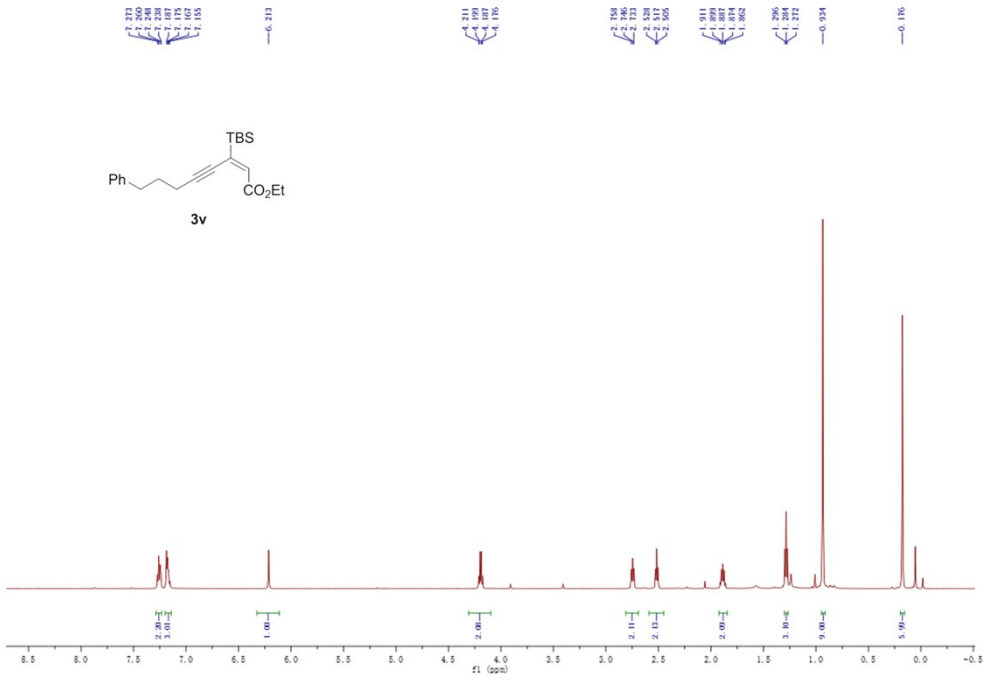
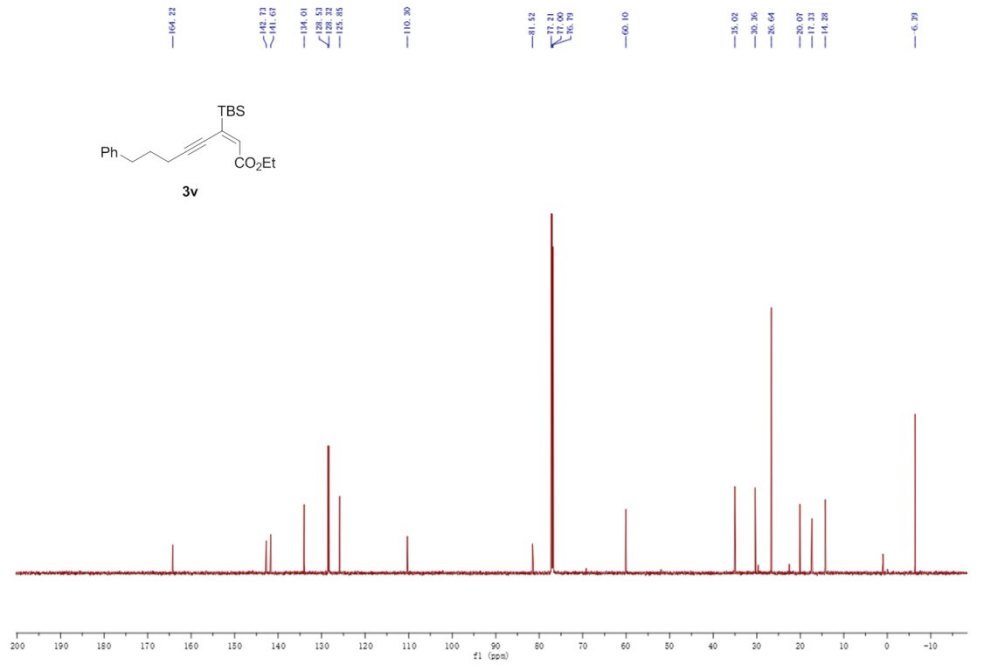

TBS
CO2Et
3t

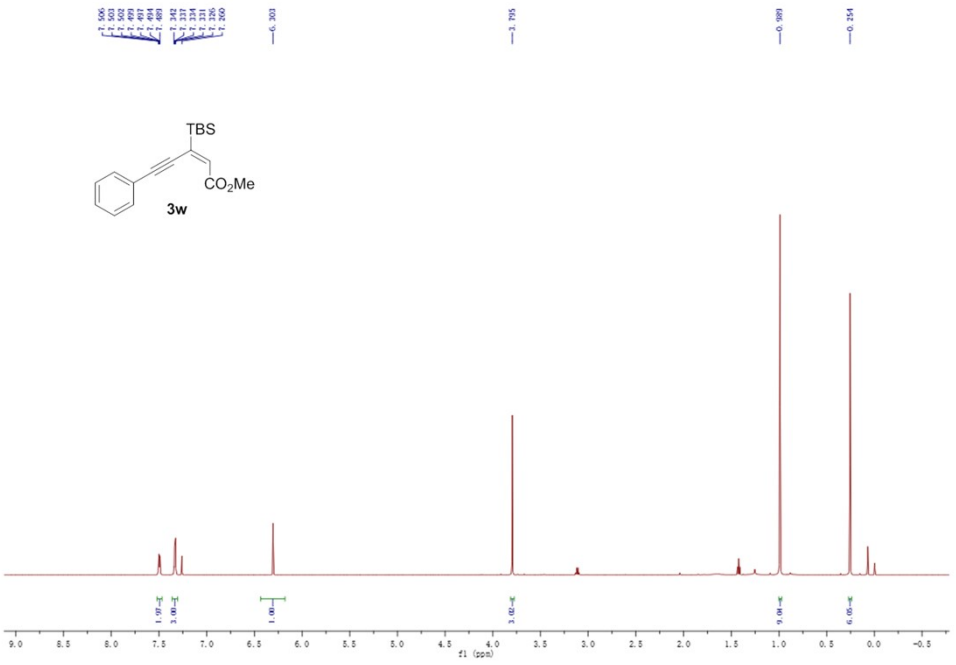

TBS
CO2Et
3t


TBS
CO2Et
3u


TBS
CO2Et
3u


TBS
Ph
CO2Et
3v
f1 (ppm)


TBS
Ph
CO2Et
3v
f1 (ppm)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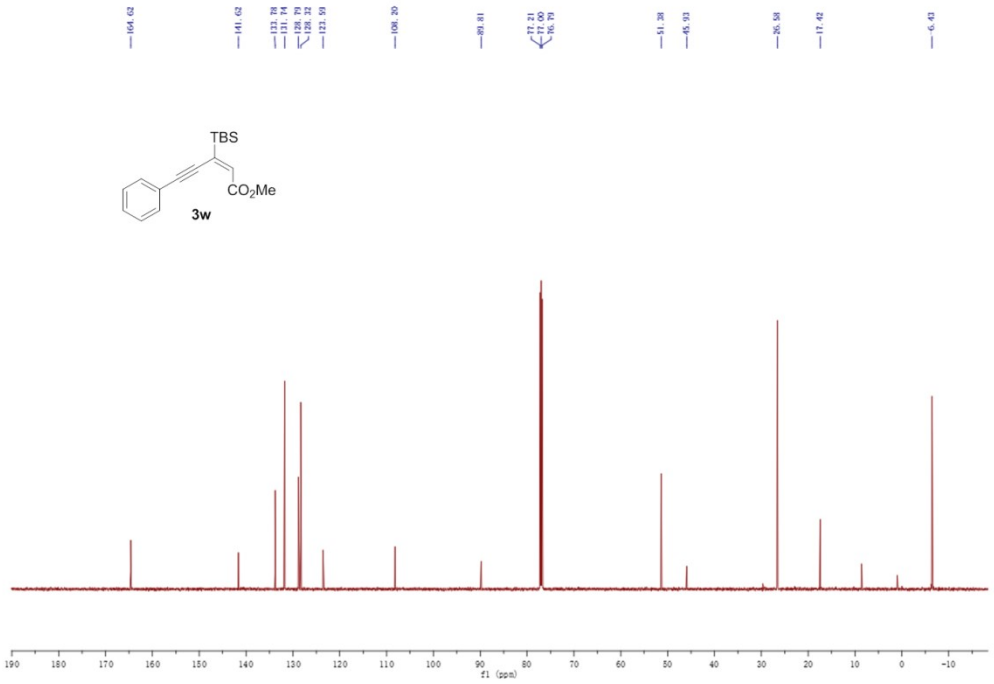
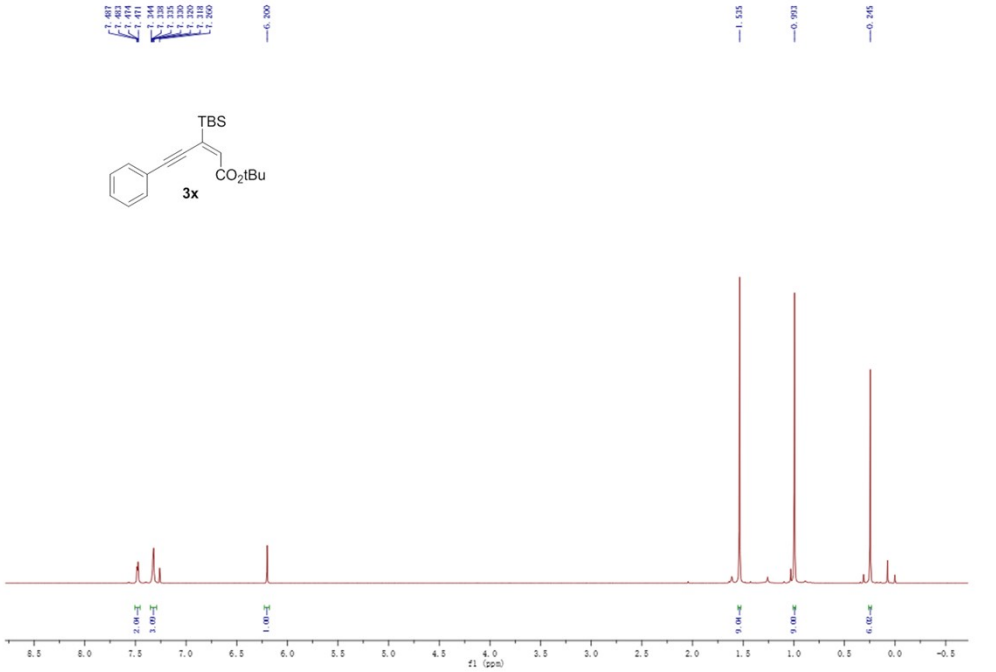
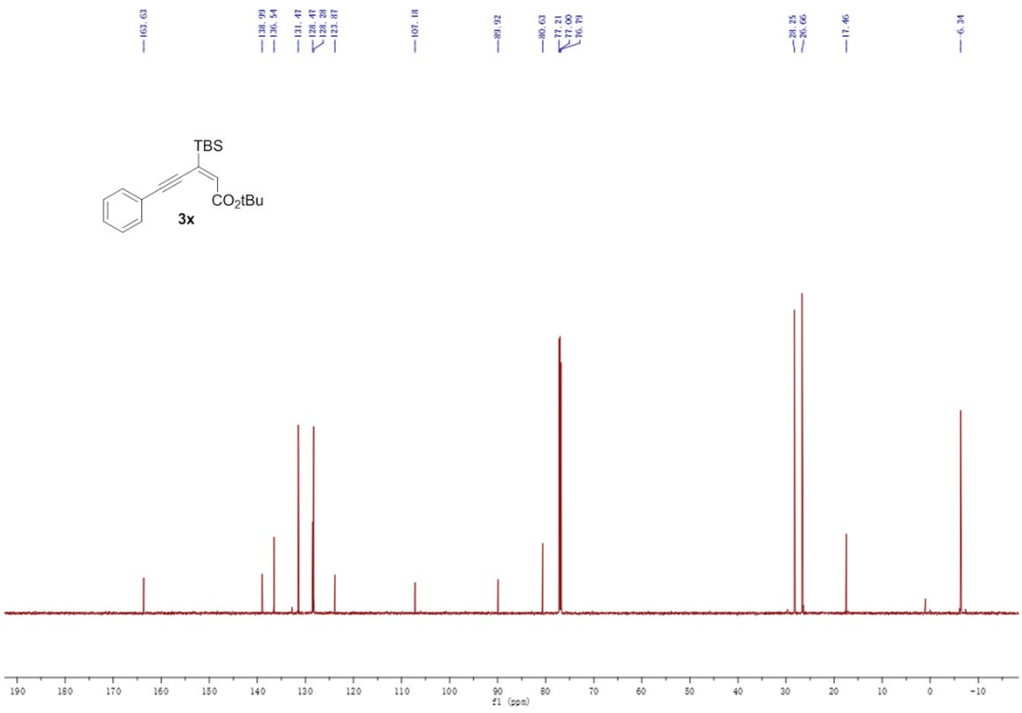
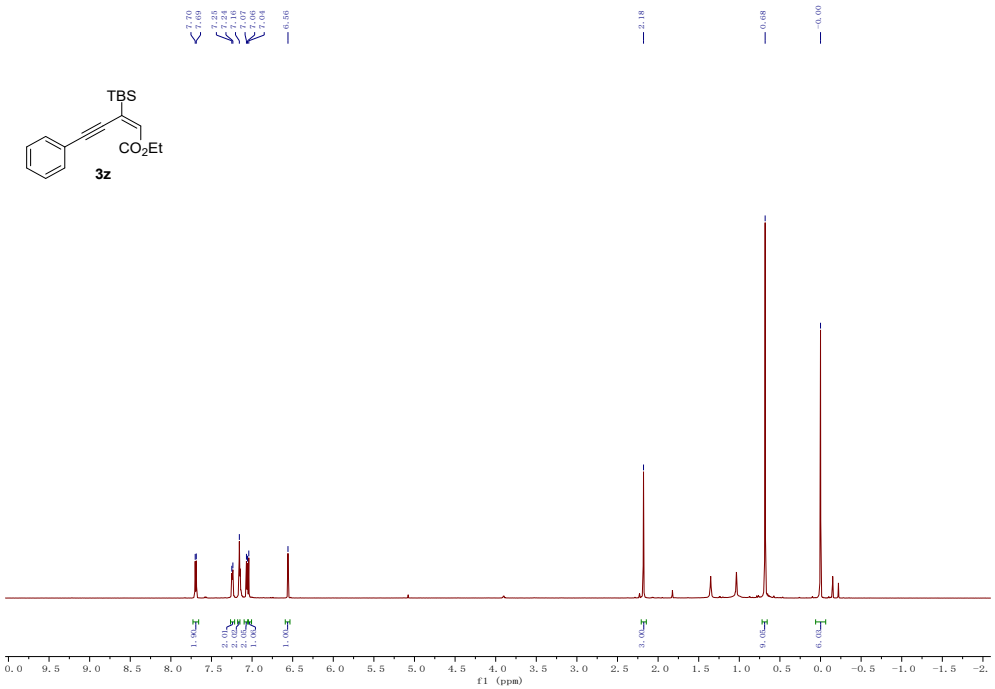
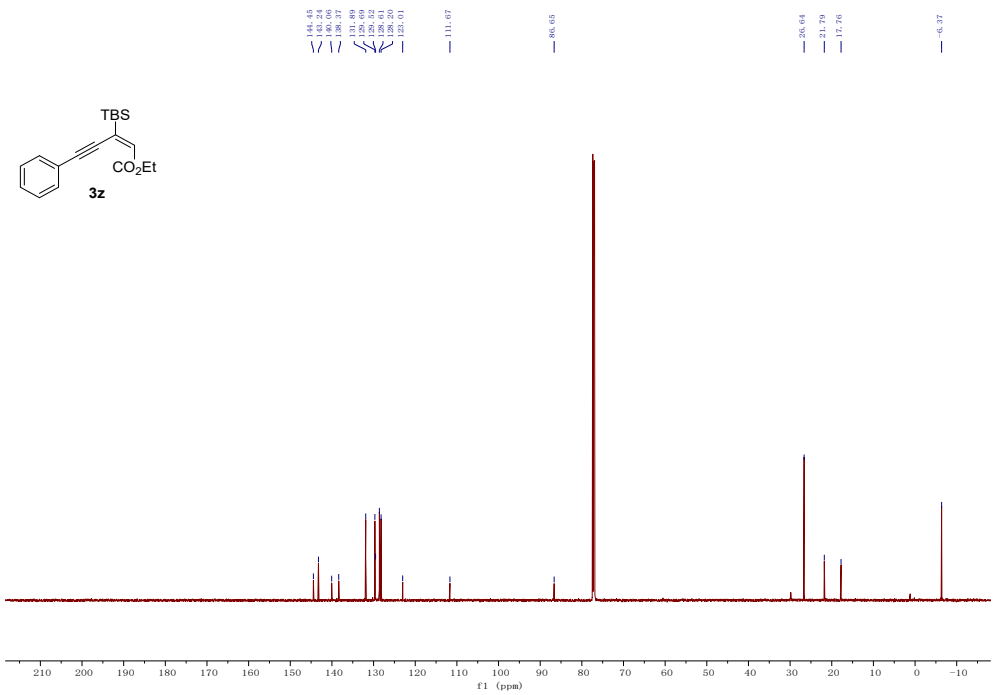
7.503
7.502
7.499
7.497
7.494
7.493
7.342
7.337
7.334
7.331
7.326
7.260
6.303
2.795
0.989
0.254
TBS
CO2Me
3w
1.97
3.00
1.00
3.02
9.04
6.05
f1 (ppm)

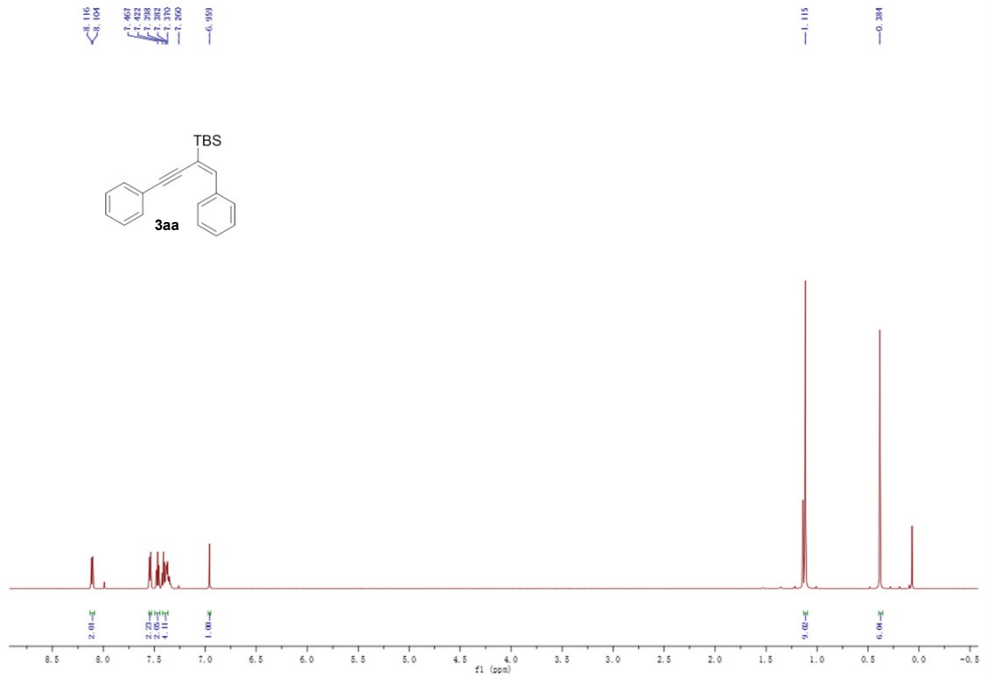

164.62
141.62
133.78
131.74
128.79
128.32
123.93
109.20
89.81
77.21
77.00
76.79
51.28
45.93
26.58
17.42
-6.43
TBS
CO2Me
3w
f1 (ppm)

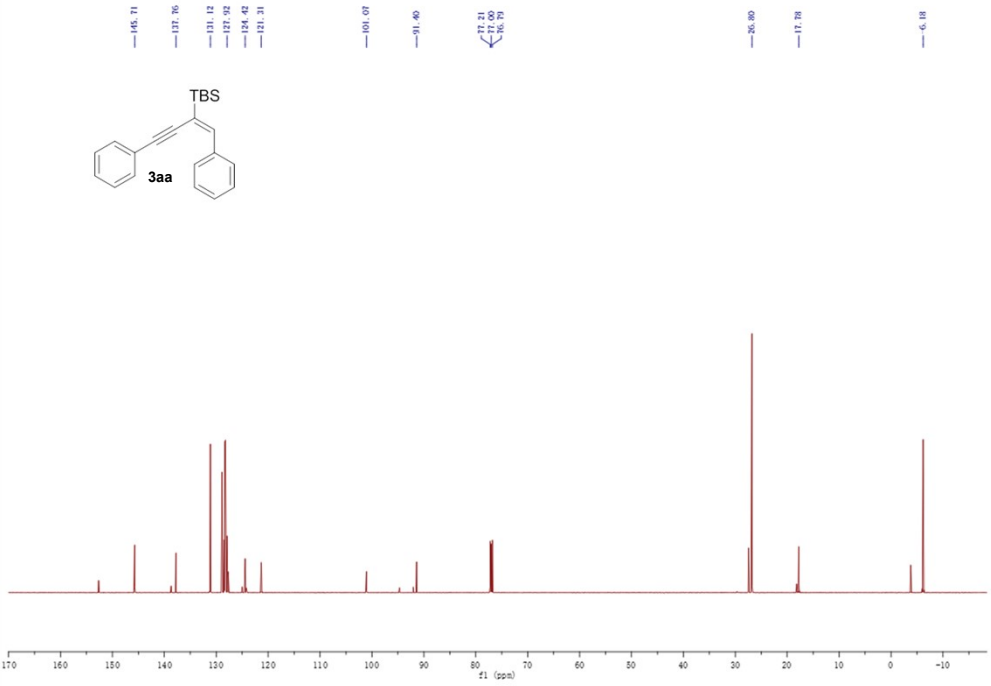

TBS
CO2tBu
3x

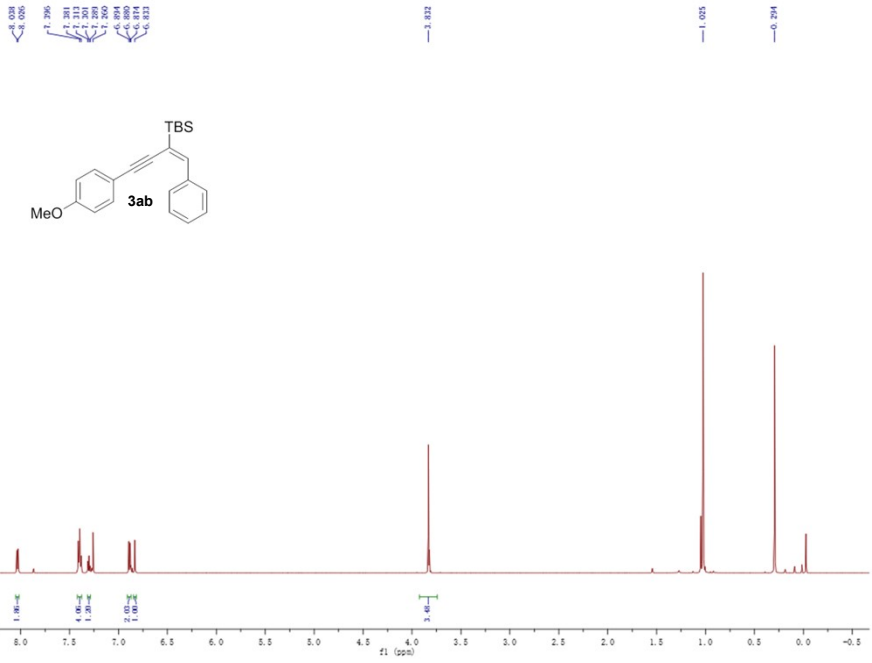

TBS
CO2tBu
3x

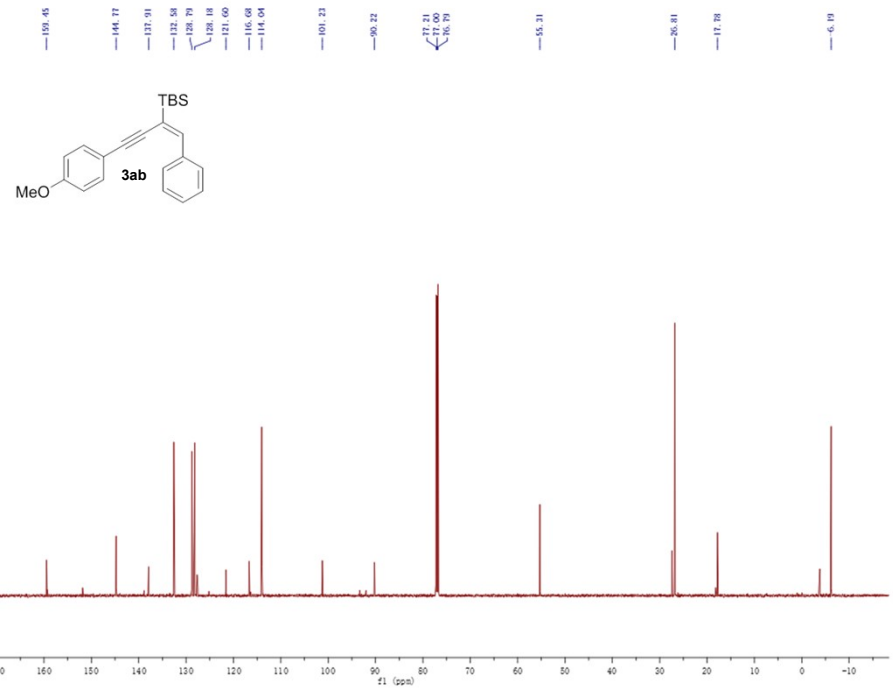

7.70
7.69
7.25
7.24
7.16
7.07
7.06
7.04
6.56
2.18
0.68
-0.00
TBS
CO2Et
3z
1.90
2.01
2.00
2.03
1.00
1.00
3.00
9.00
6.03
f1 (ppm)

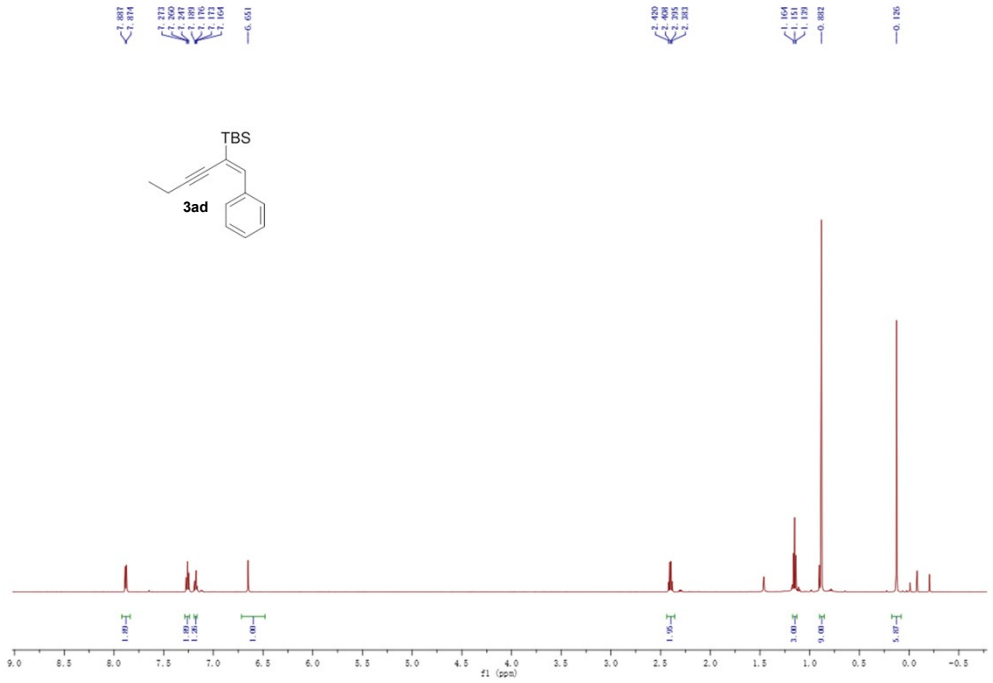

144.45
142.24
140.06
138.37
131.89
129.69
129.52
128.61
128.33
123.01
111.67
86.65
26.64
21.79
17.76
-6.37
TBS
CO2Et
3z
f1 (ppm)

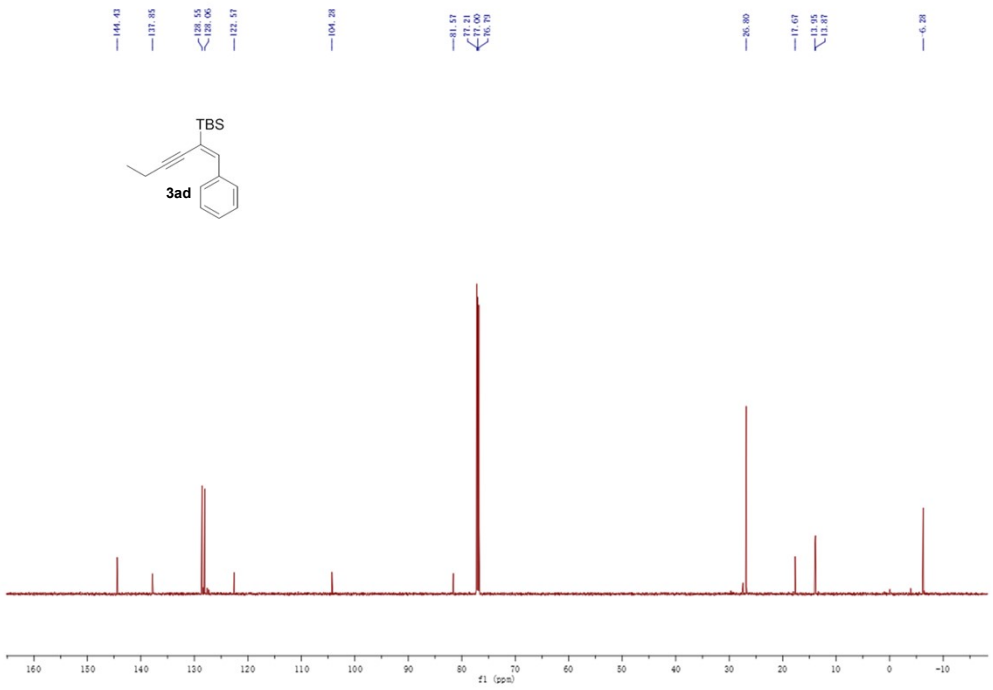

8.116
8.104
7.467
7.422
7.398
7.382
7.370
7.260
6.959
1.115
0.384
TBS
3aa
2.01
2.27
2.05
4.11
1.00
9.02
6.04
f1 (ppm)

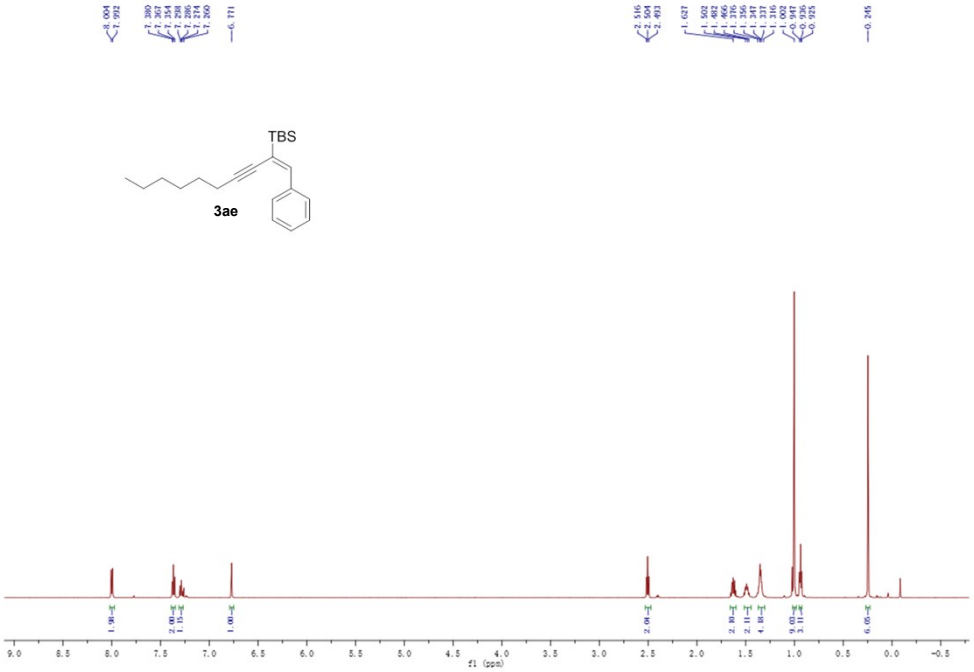

145.71
137.76
131.12
127.92
124.42
121.31
101.07
91.40
17.21
17.00
16.79
26.80
17.78
-5.18
TBS
3aa
f1 (ppm)

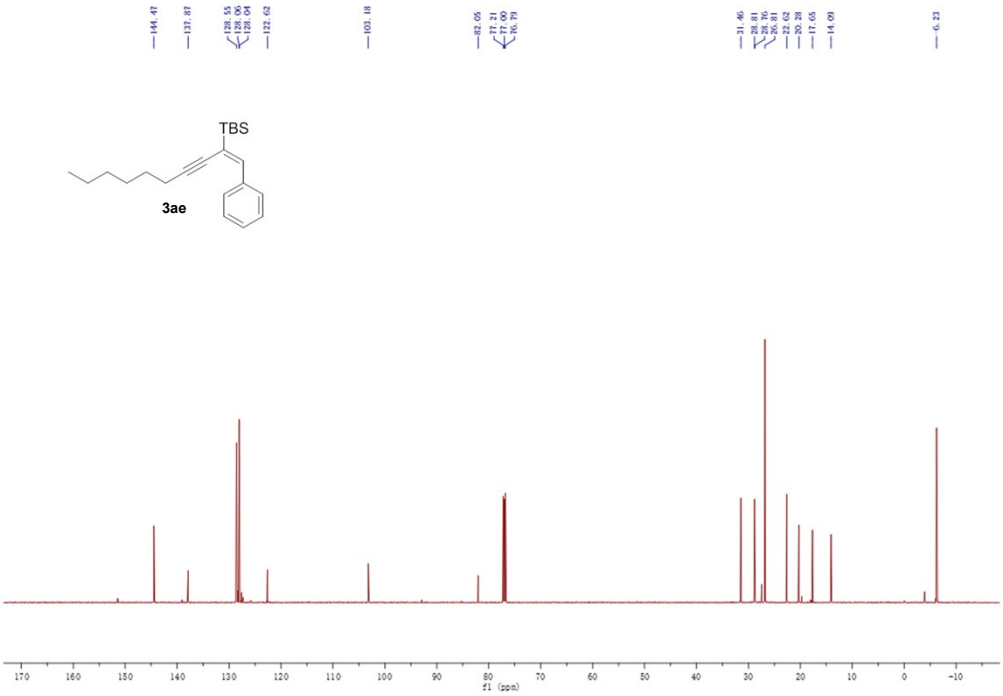

TBS
MeO
3ab

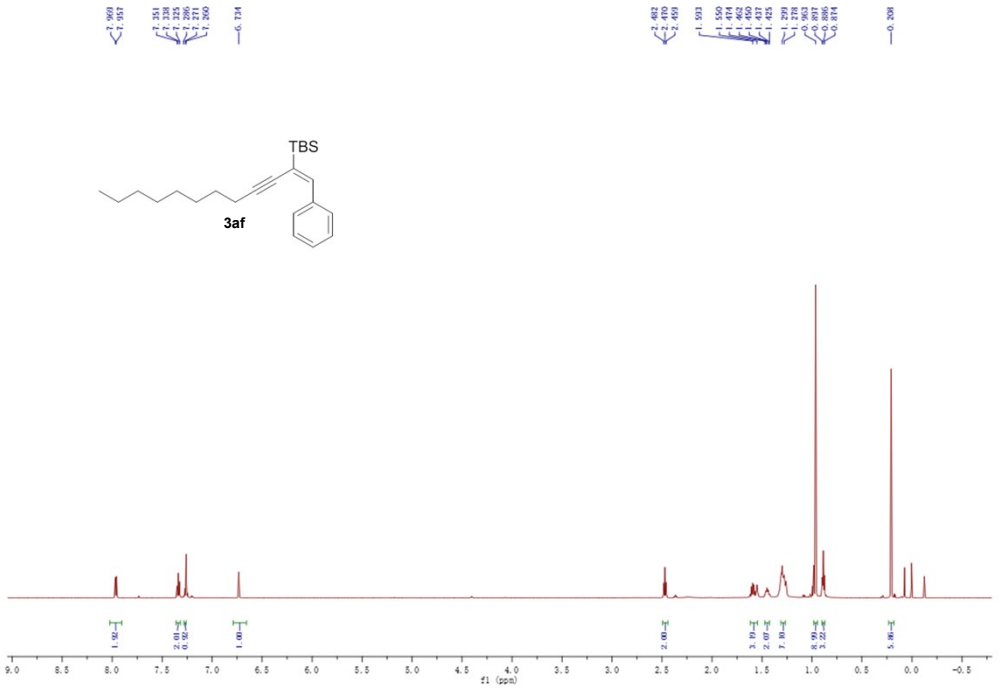

TBS
MeO
3ab

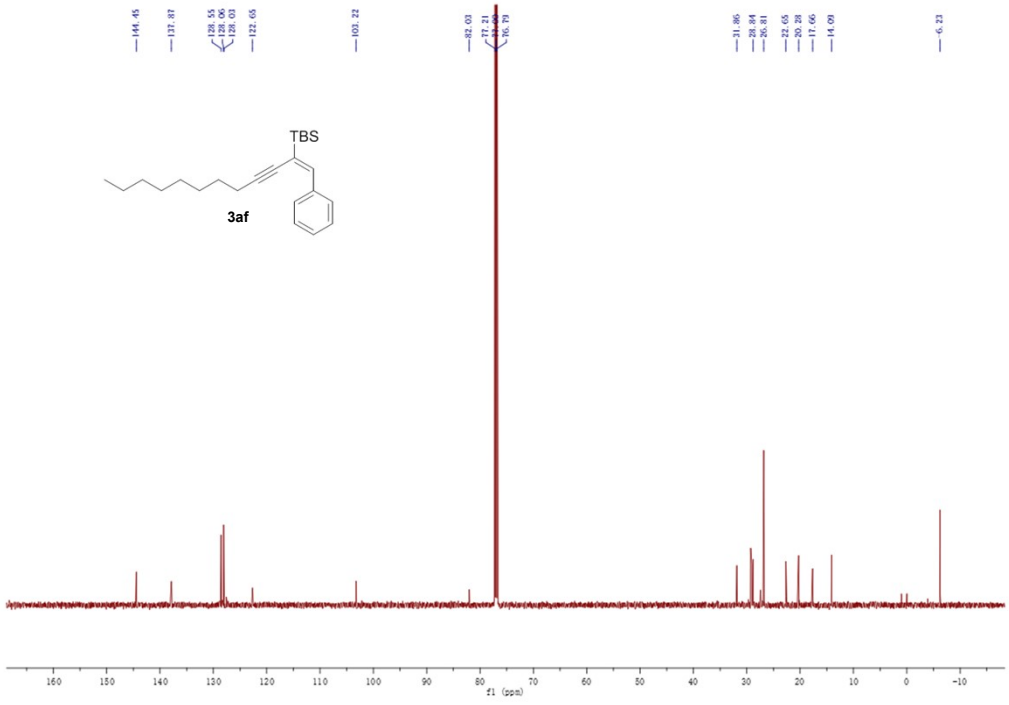

TBS
3ad

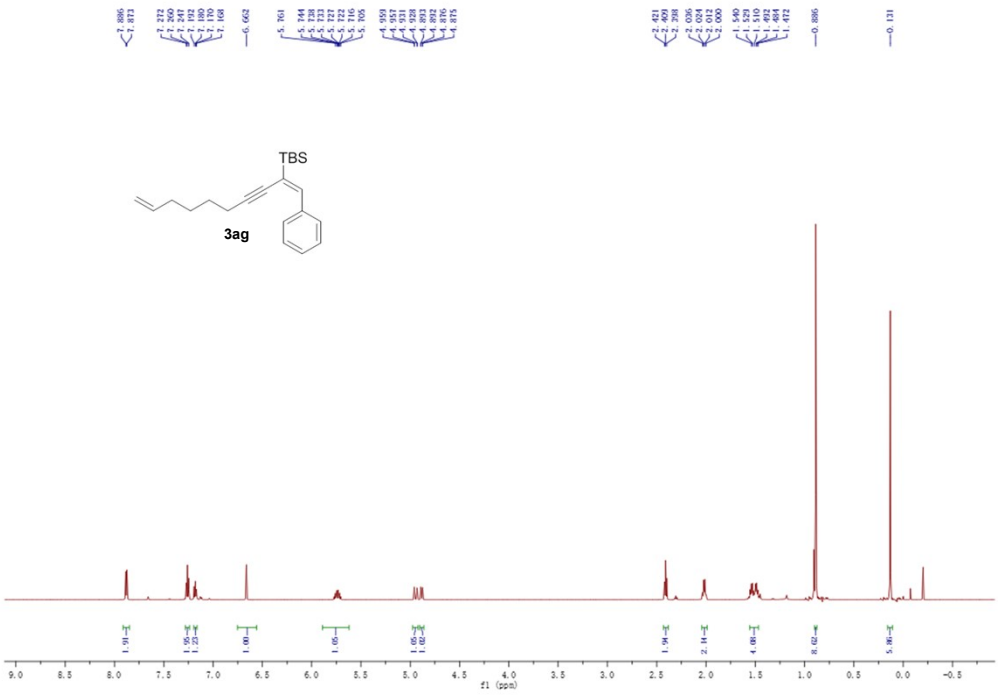

TBS
3ad

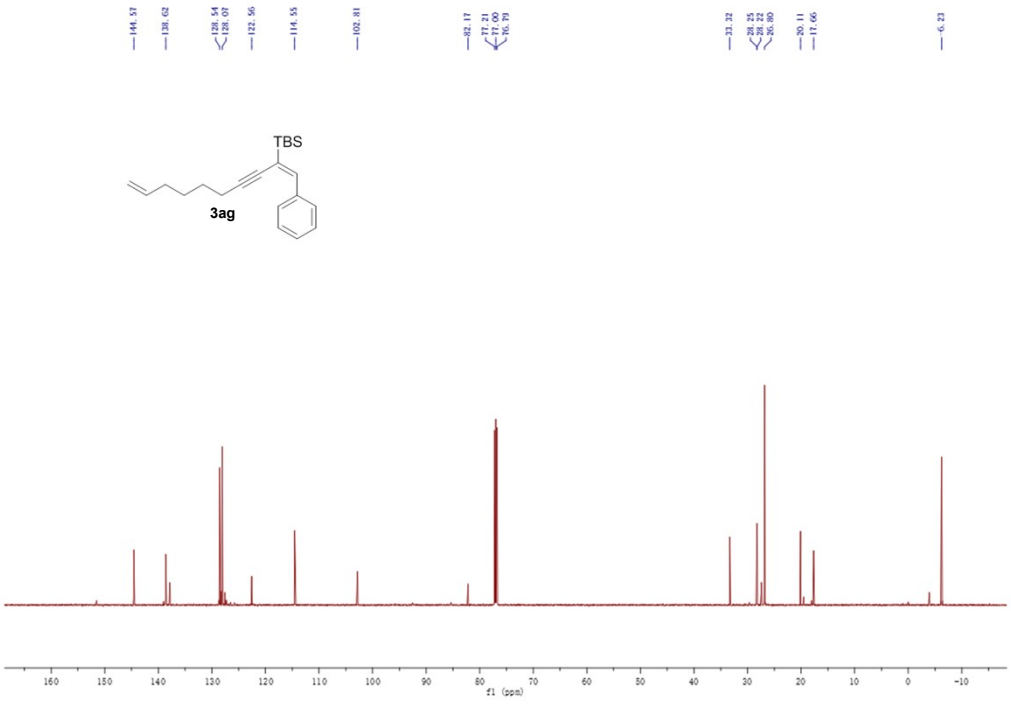

TBS
3ae

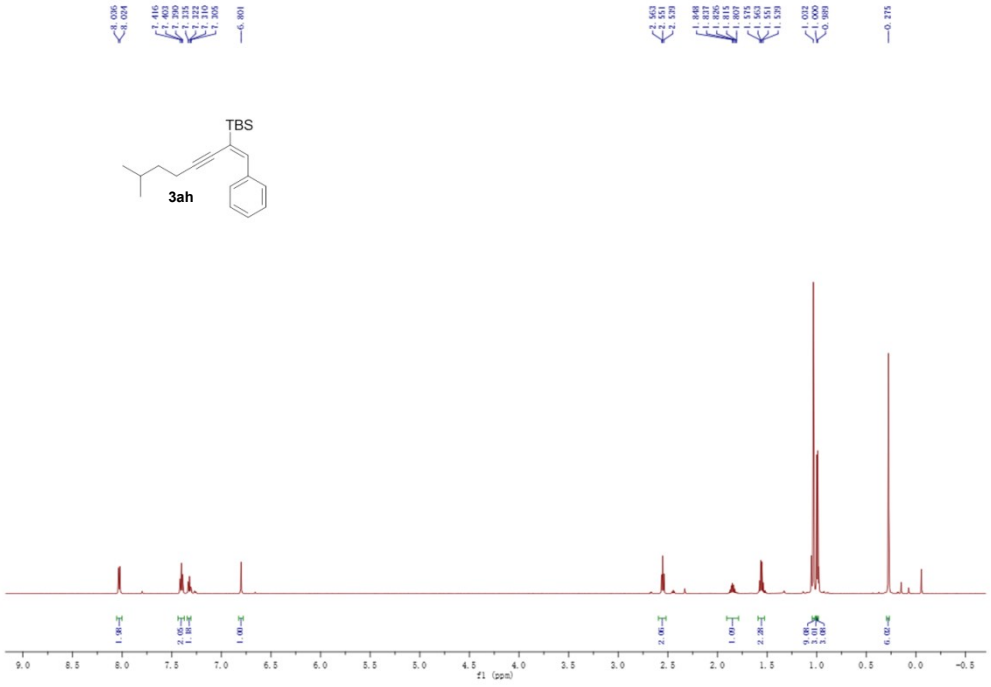

TBS
3ae

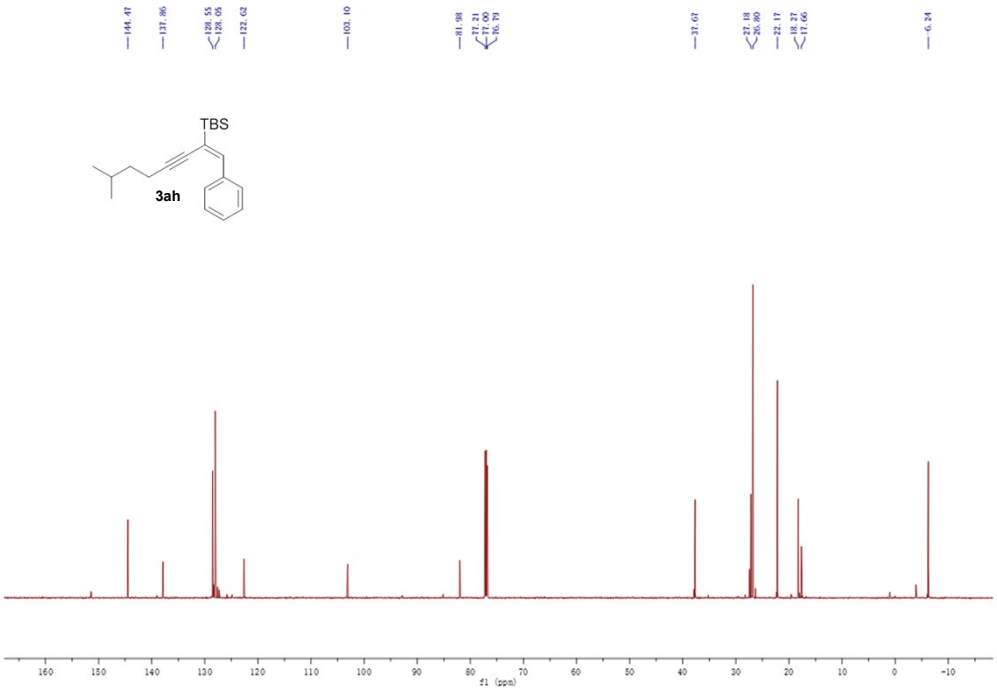

TBS
3af
f1 (ppm)

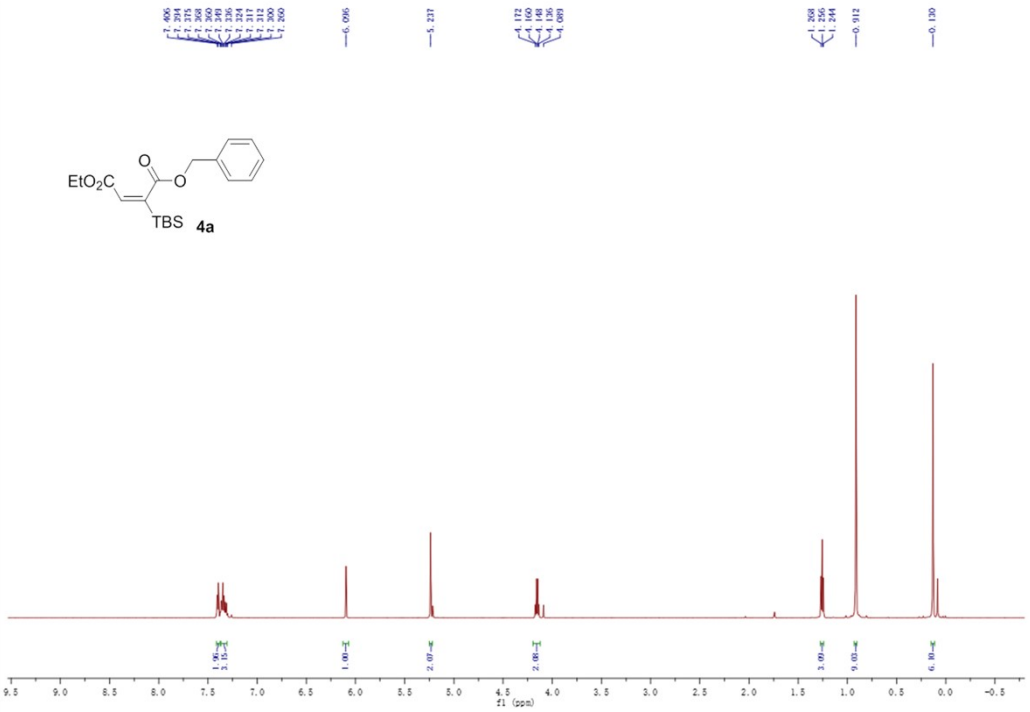

TBS
3af
f1 (ppm)

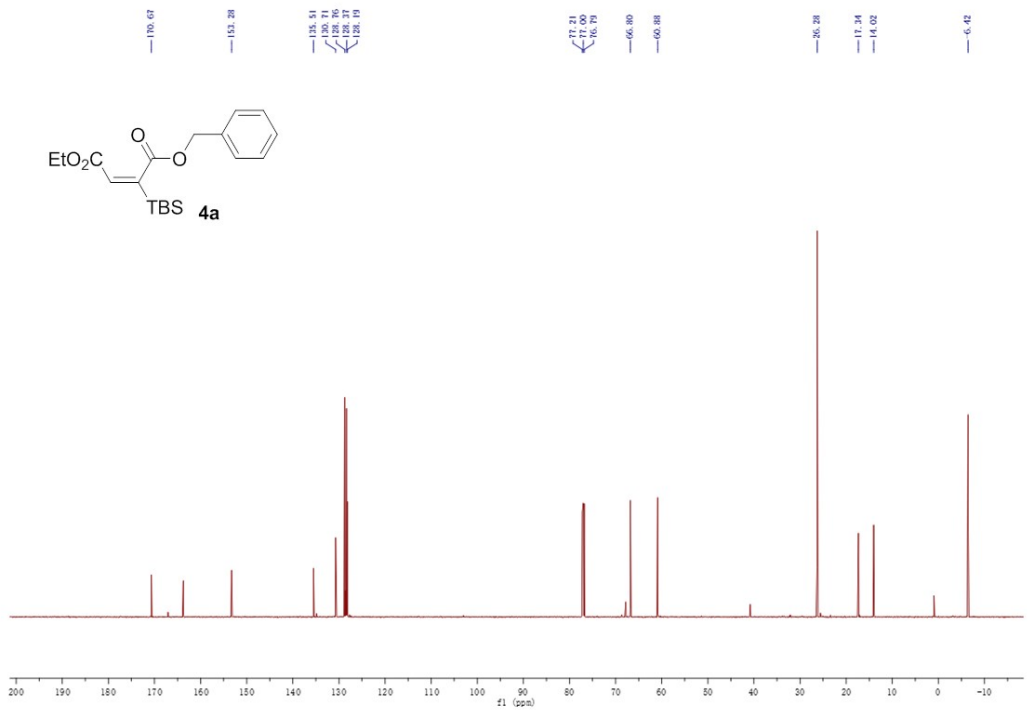

TBS
3ag
f1 (ppm)

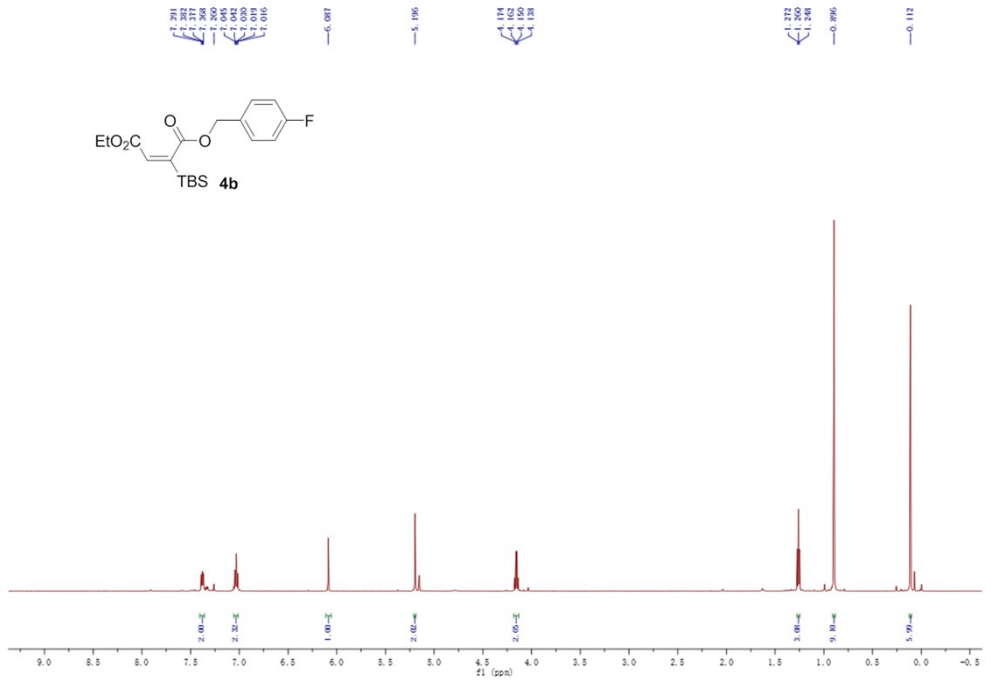

TBS
3ag
f1 (ppm)

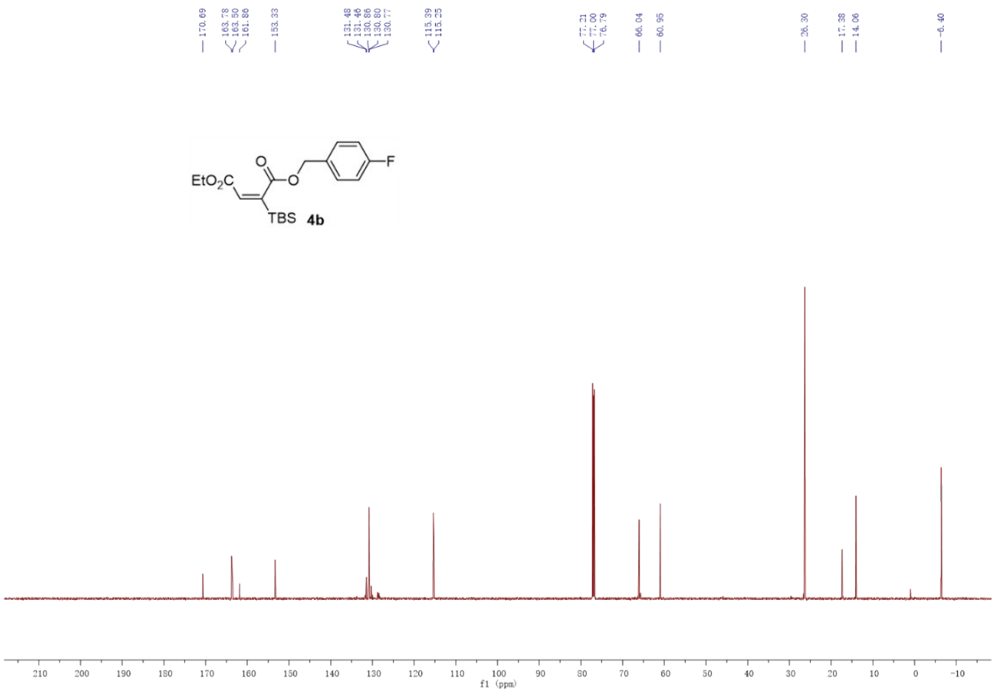

TBS
3ah
f1 (ppm)

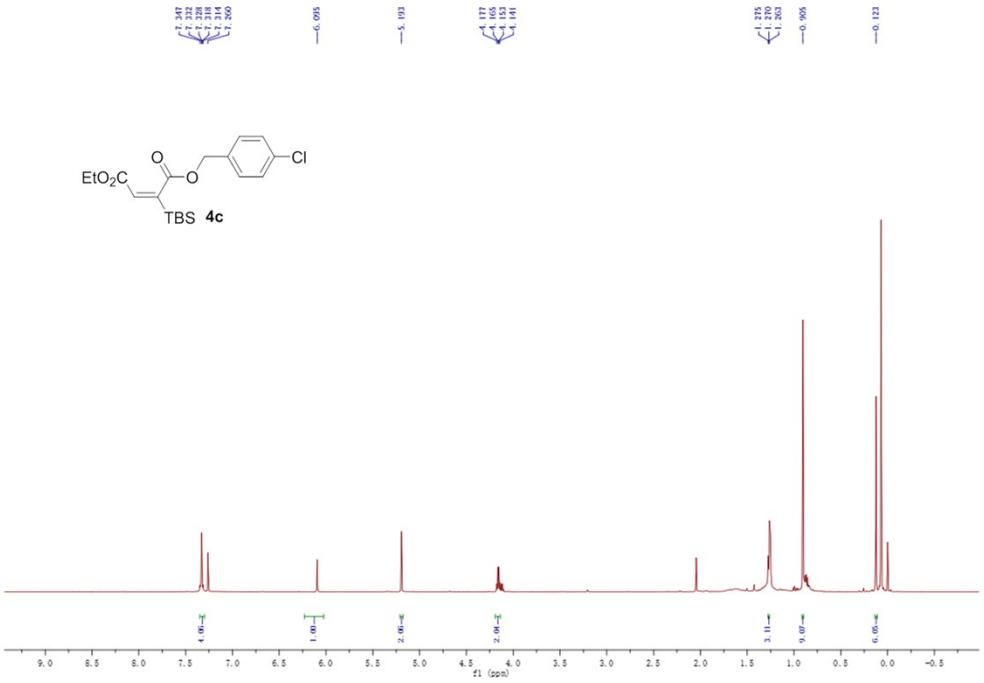

TBS
3ah
f1 (ppm)

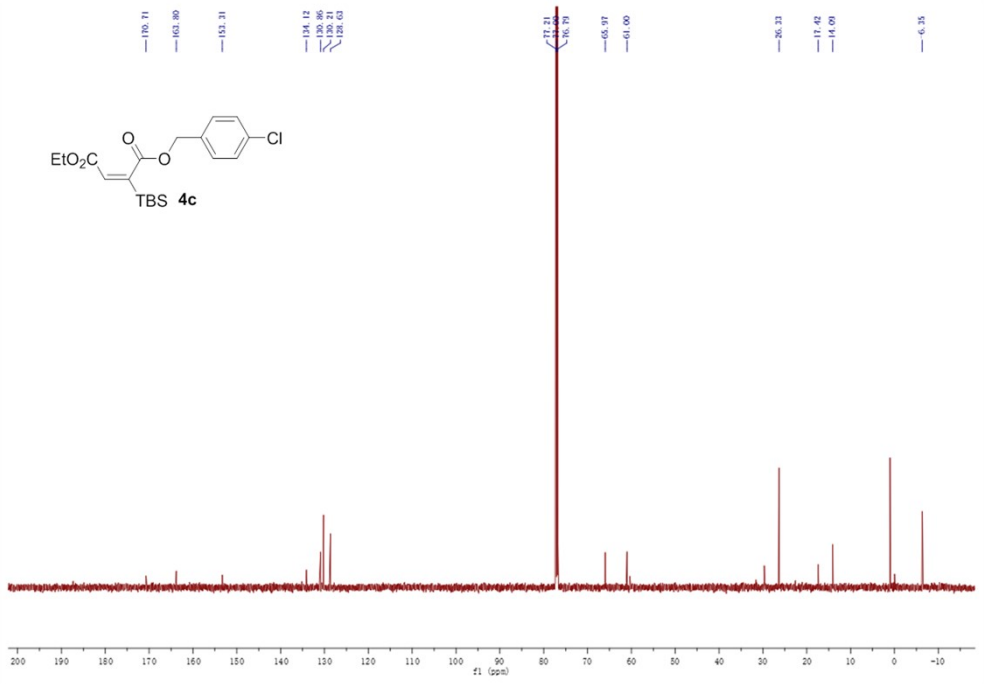

EtO2C
O
O
TBS
4a
f1 (ppm)

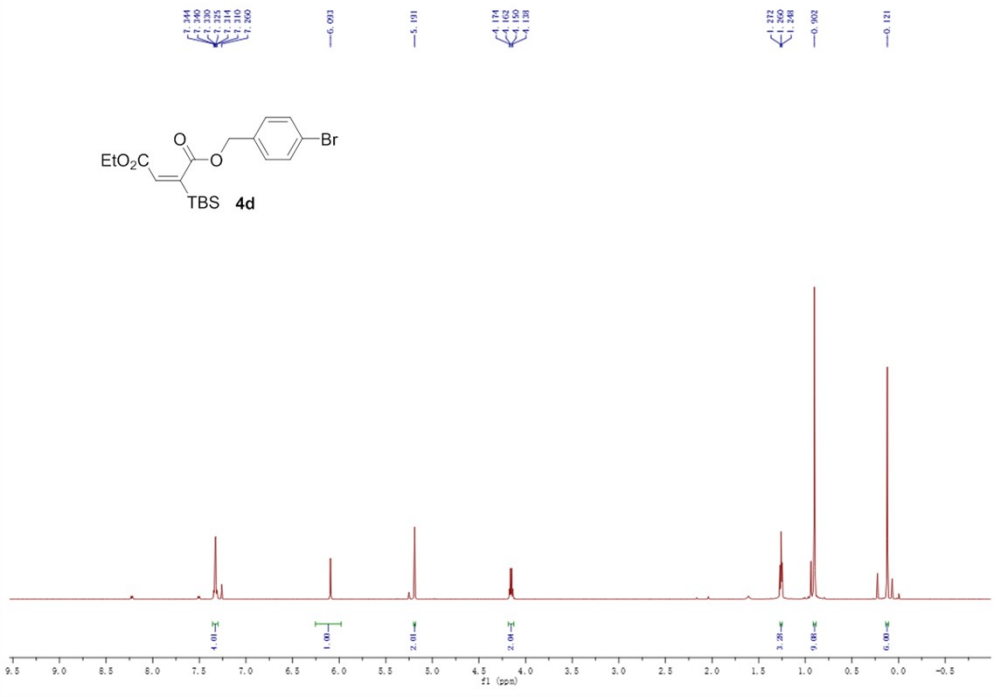

EtO2C
O
O
TBS
4a
f1 (ppm)

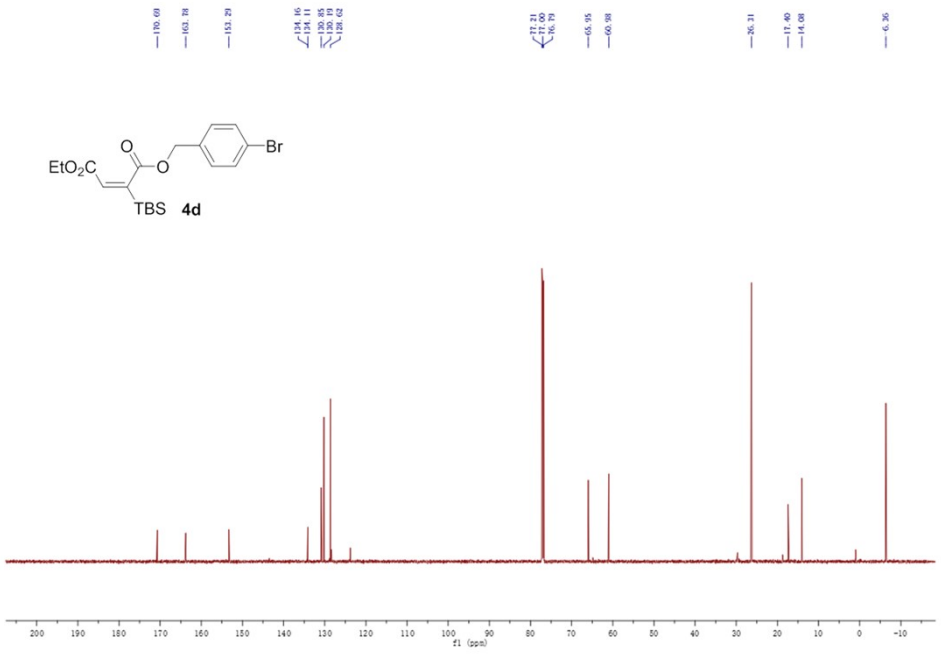

EtO2C
O
O
F
TBS
4b

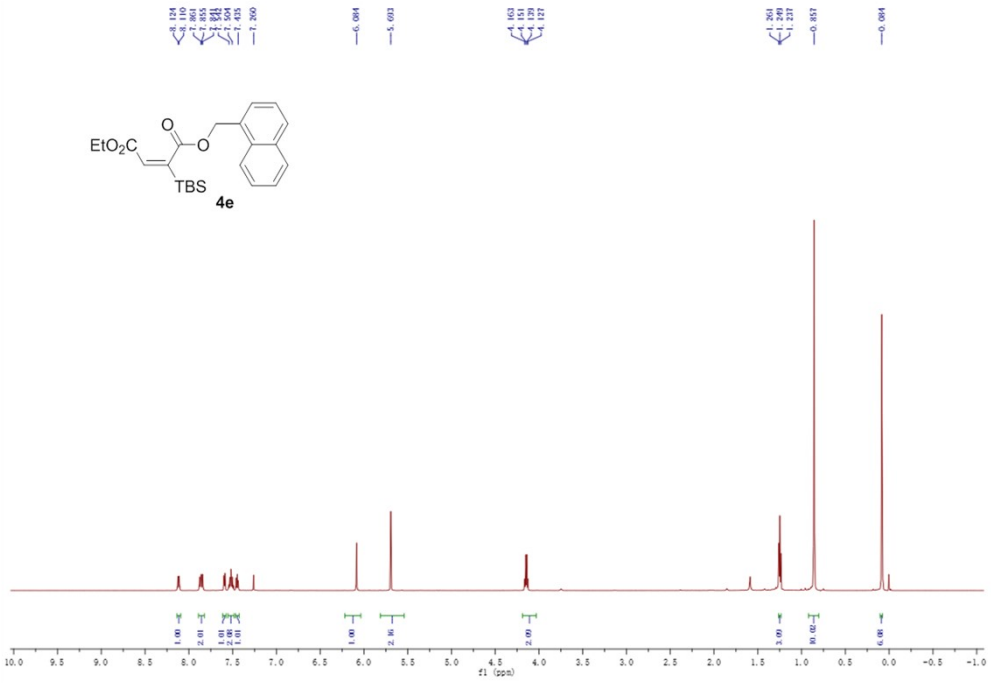

EtO2C
O
O
F
TBS
4b

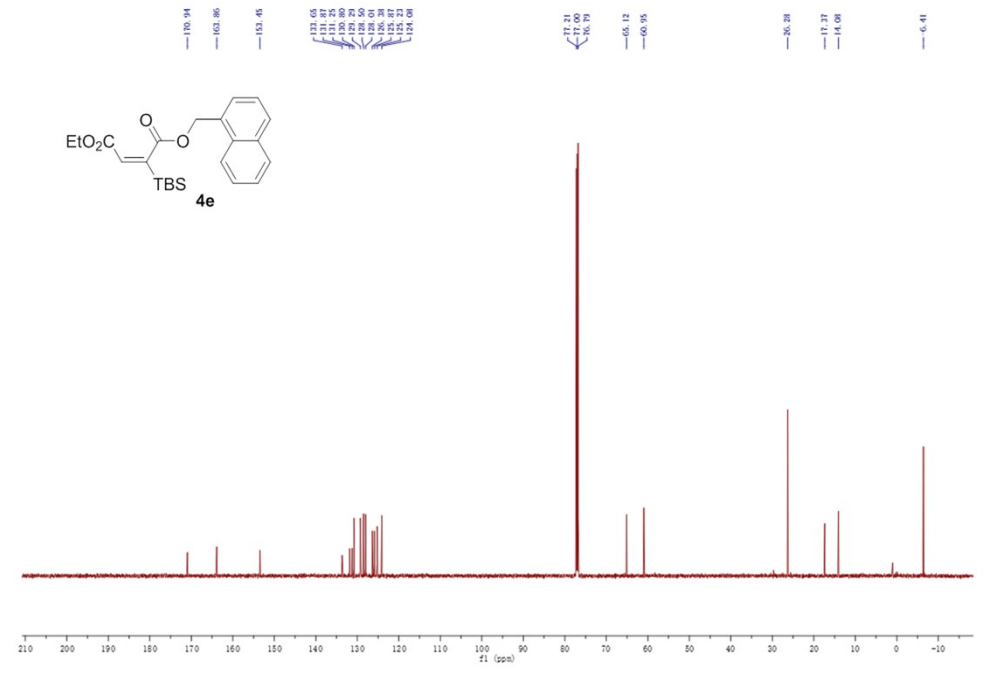

EtO2C
O
O
Cl
TBS 4c
f1 (ppm)

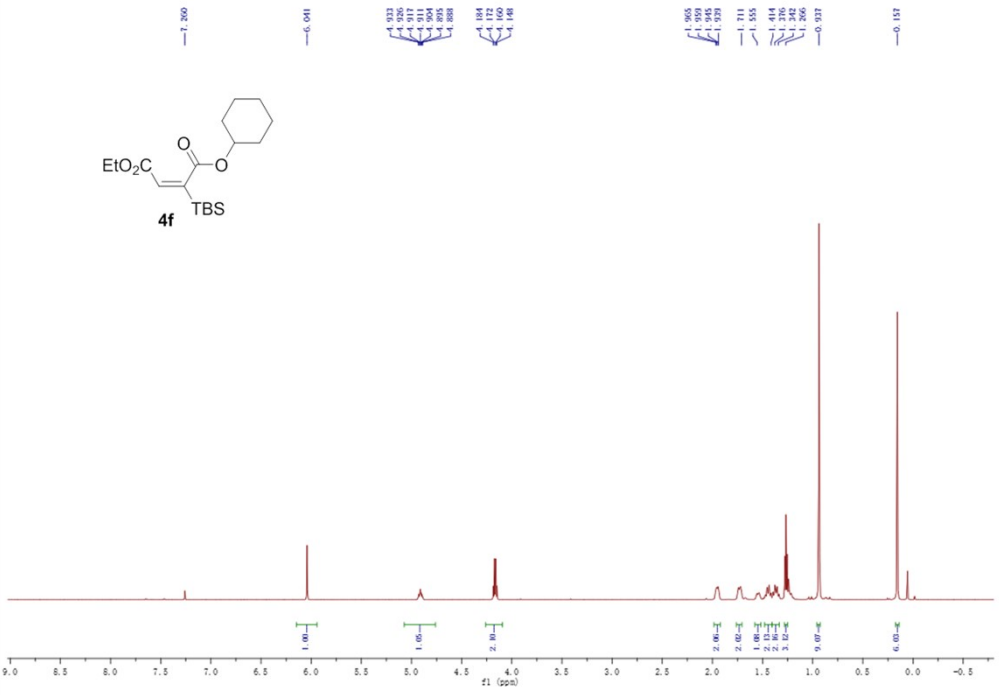

EtO2C
O
O
Cl
TBS 4c
f1 (ppm)

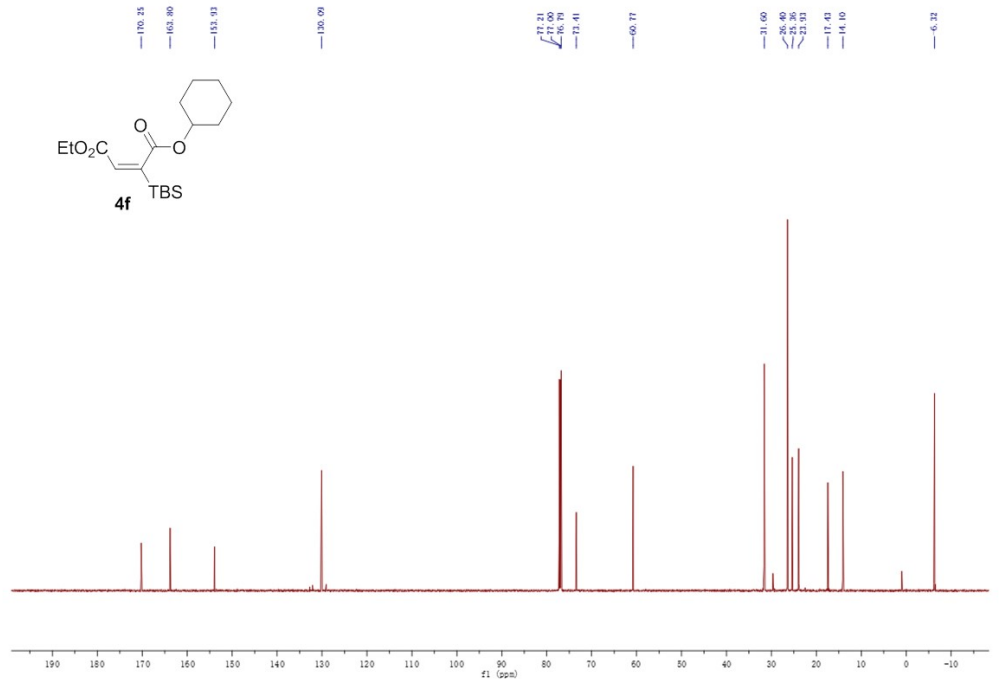

EtO2C
O
O
Br
TBS
4d

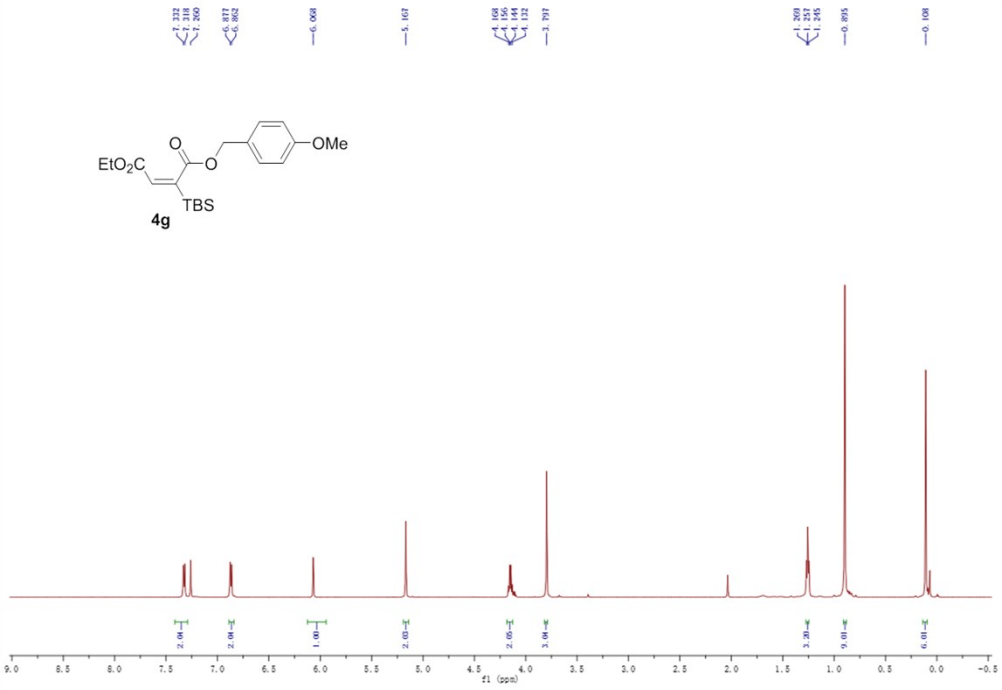

EtO2C
O
O
Br
TBS
4d

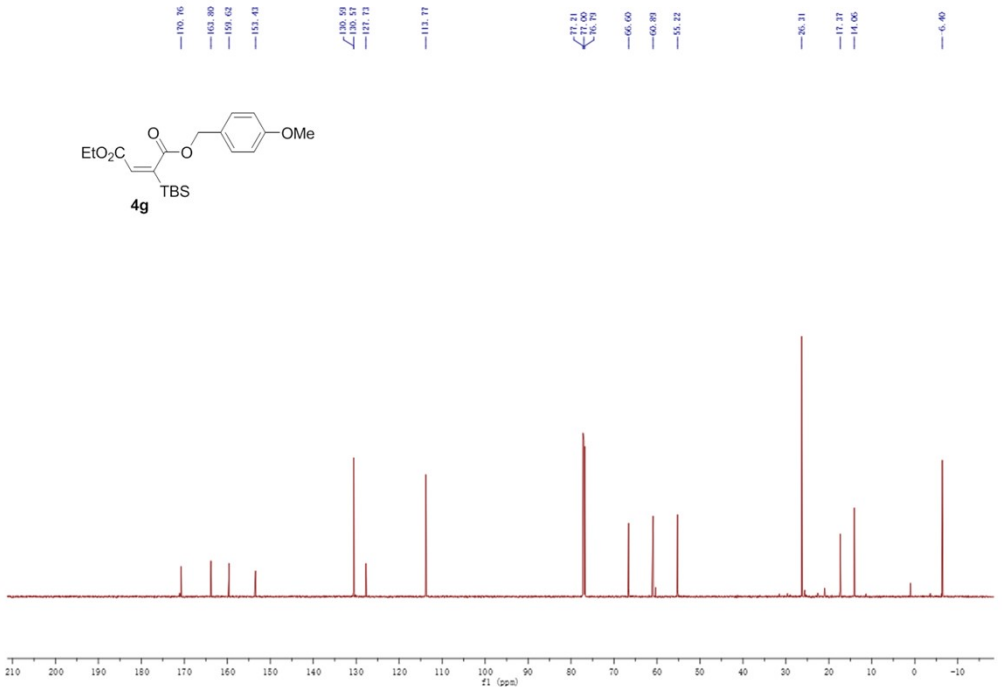

EtO2C
O
O
TBS
4e

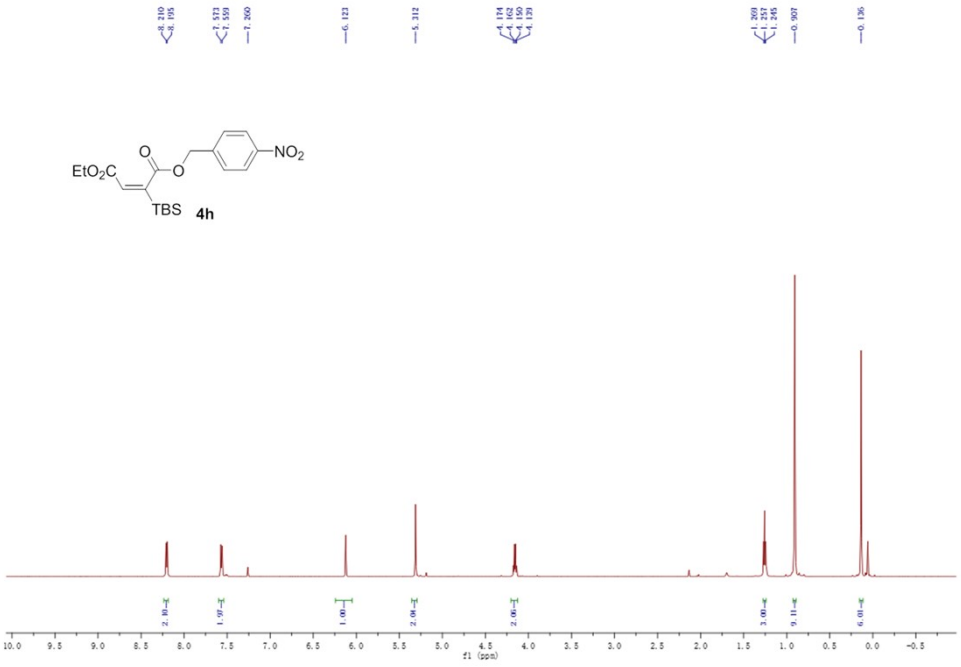

EtO2C
O
O
TBS
4e

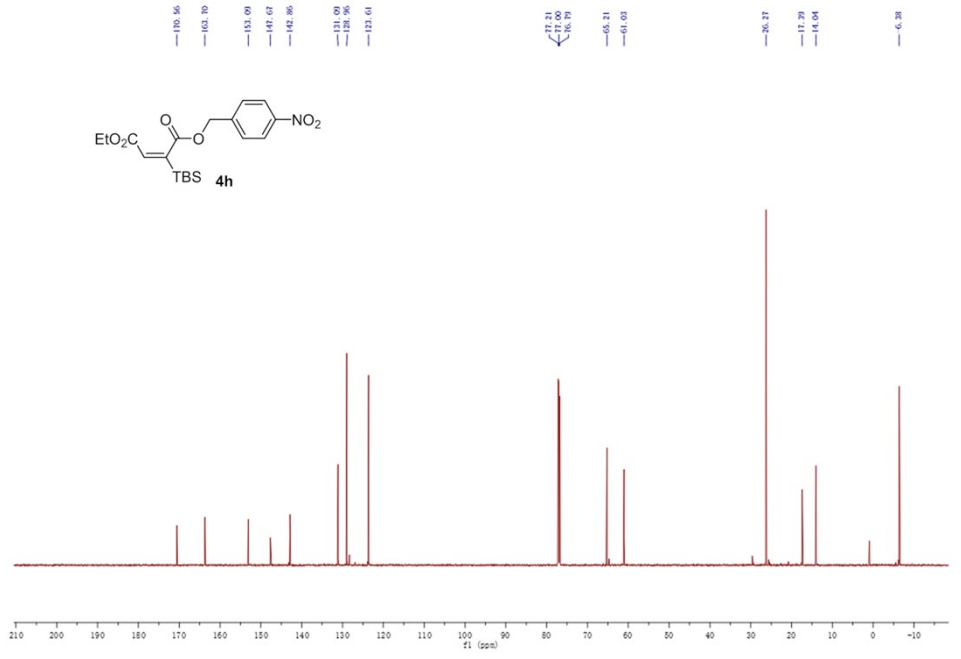

7.269
6.041
4.933
4.926
4.917
4.911
4.904
4.895
4.888
4.184
4.172
4.160
4.148
1.965
1.959
1.945
1.939
1.711
1.555
1.414
1.376
1.342
1.266
0.937
0.157
EtO2C
O
O
TBS
4f
1.00
1.05
2.10
2.00
2.02
1.08
2.15
2.10
3.12
9.07
6.03
f1 (ppm)

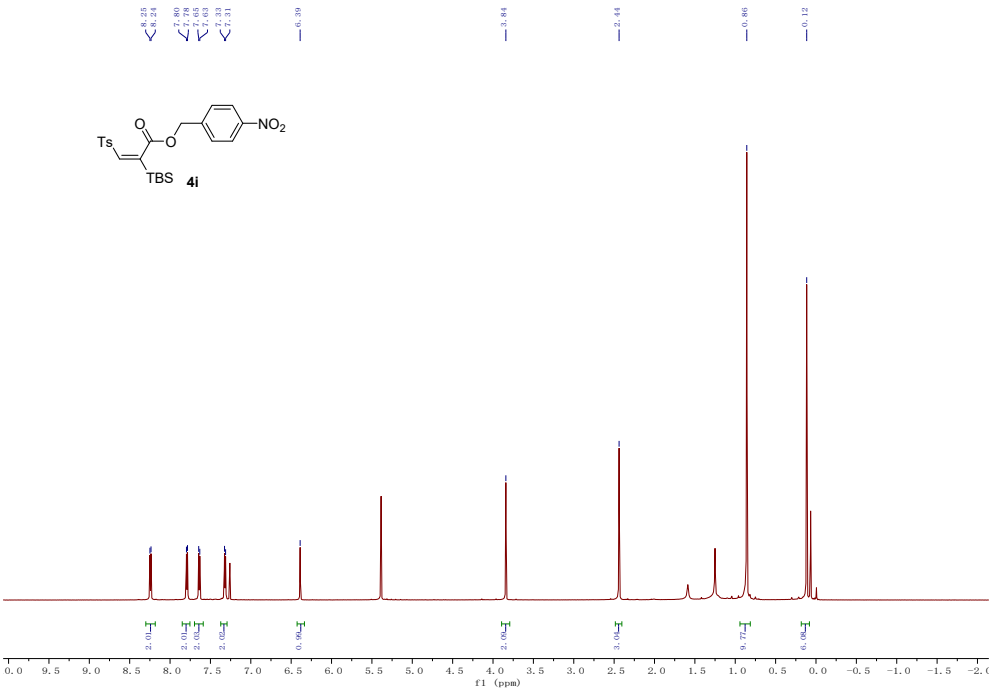

170.25
163.80
153.93
130.09
77.21
77.00
76.79
73.41
60.77
31.60
26.40
25.35
23.93
17.43
14.10
-6.32
EtO2C
O
O
TBS
4f
f1 (ppm)

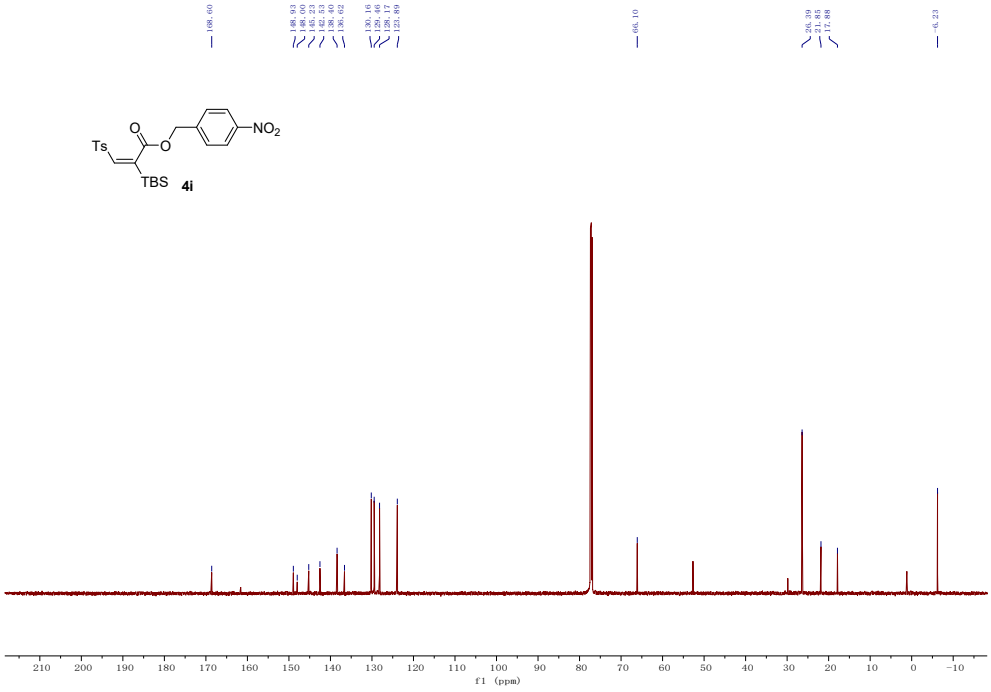

EtO2C
O
O
OMe
TBS
4g

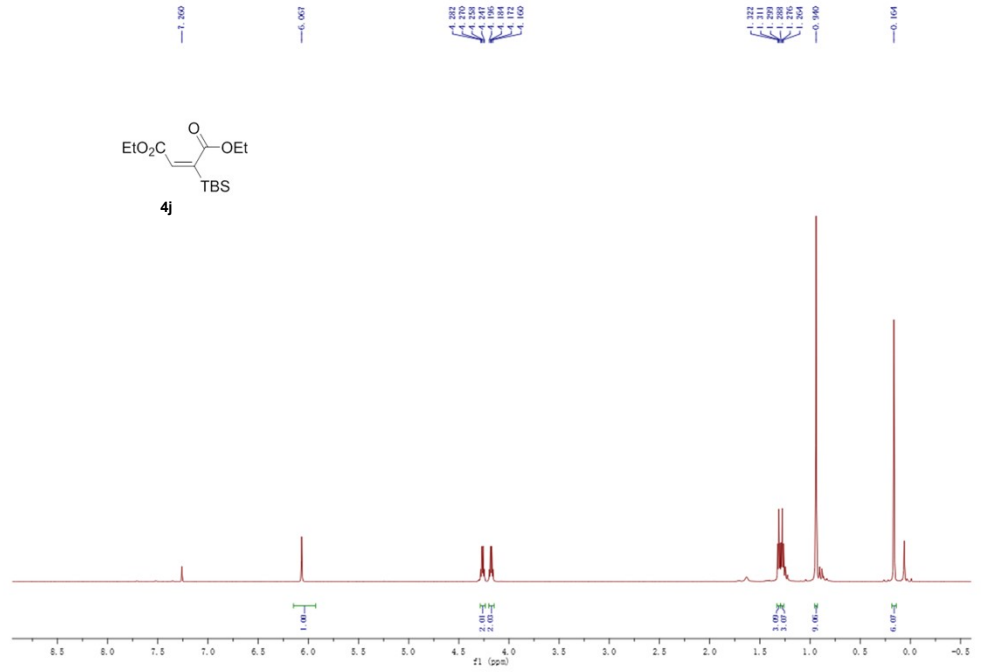

EtO2C
O
O
OMe
TBS
4g

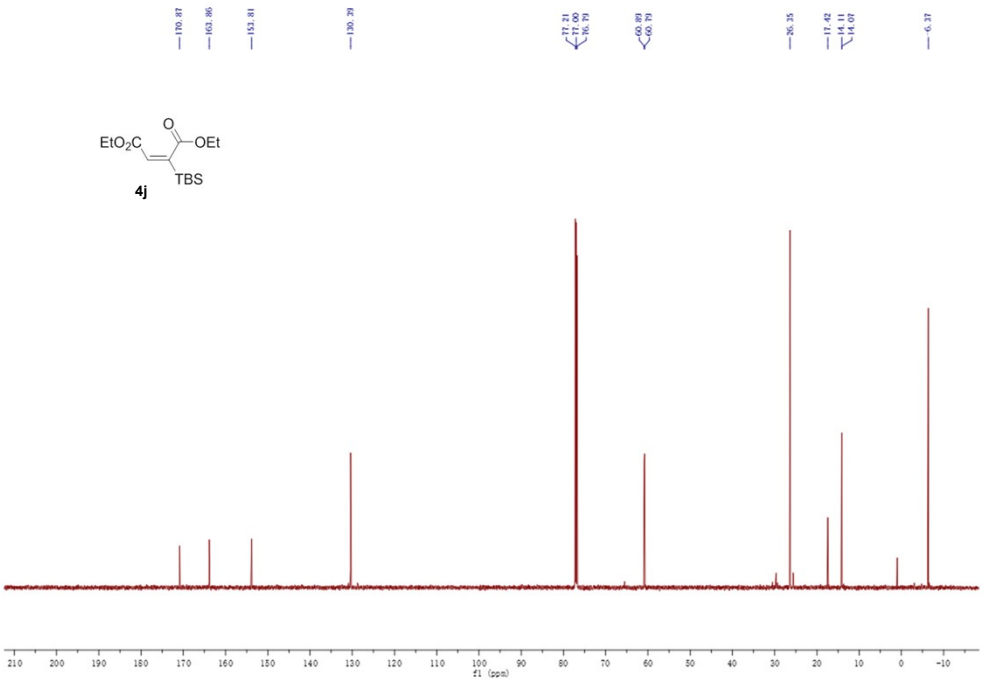

8.310
8.195
7.573
7.559
7.260
6.123
5.312
4.174
4.162
4.150
4.139
1.269
1.257
1.245
0.907
0.135
EtO2C
O
O
NO2
TBS
4h
2.10
1.97
1.00
2.04
2.06
3.00
9.11
6.01
f1 (ppm)


170.56
163.70
153.09
147.67
142.86
131.09
128.96
123.61
77.21
77.00
76.79
65.21
61.03
26.27
17.29
14.04
-6.38
EtO2C
O
O
NO2
TBS
4h
f1 (ppm)


8.25
8.24
7.80
7.78
7.65
7.63
7.33
7.31
6.39
3.84
2.44
0.86
0.12
Ts
O
O
NO2
TBS
4i
2.01
2.01
2.00
2.02
0.90
2.00
3.04
9.77
6.06
f1 (ppm)


168.60
148.93
146.60
145.23
142.53
138.40
136.62
130.16
129.46
128.17
125.89
66.10
26.39
21.85
17.88
-6.23
Ts
O
O
NO2
TBS
4i
f1 (ppm)


7.369
6.067
4.383
4.270
4.258
4.247
4.196
4.184
4.172
4.160
1.322
1.311
1.299
1.288
1.276
1.264
0.940
0.164
EtO2C
O
OEt
TBS
4j
1.00
2.01
3.07
3.07
9.06
6.07
f1 (ppm)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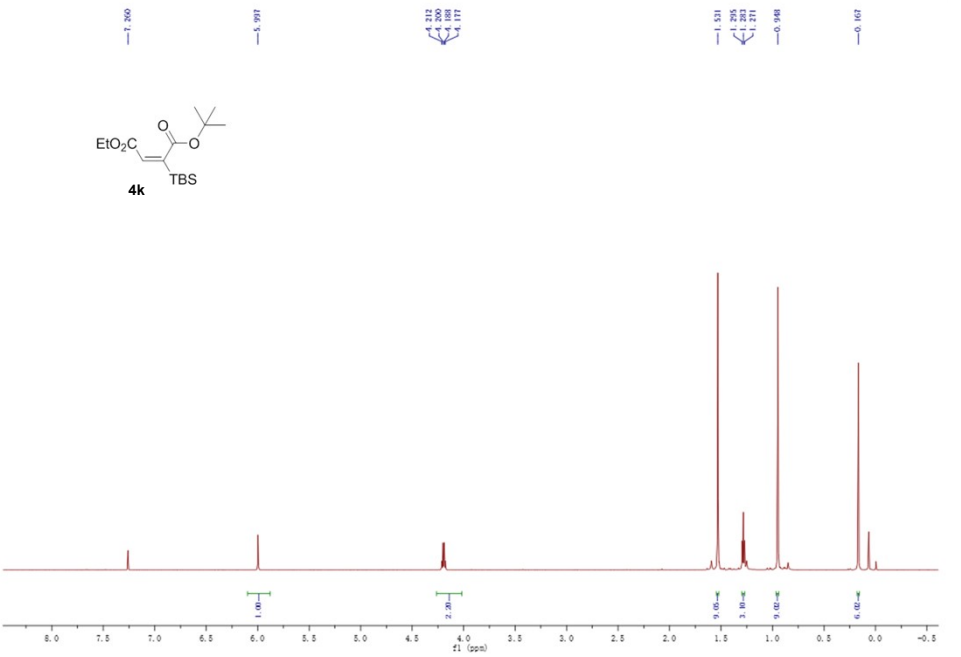
163.86
153.81
130.39
77.21
77.00
76.79
60.89
60.79
26.25
17.42
14.11
14.07
-6.17
EtO2C
O
OEt
TBS
4j
f1 (ppm)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4.212
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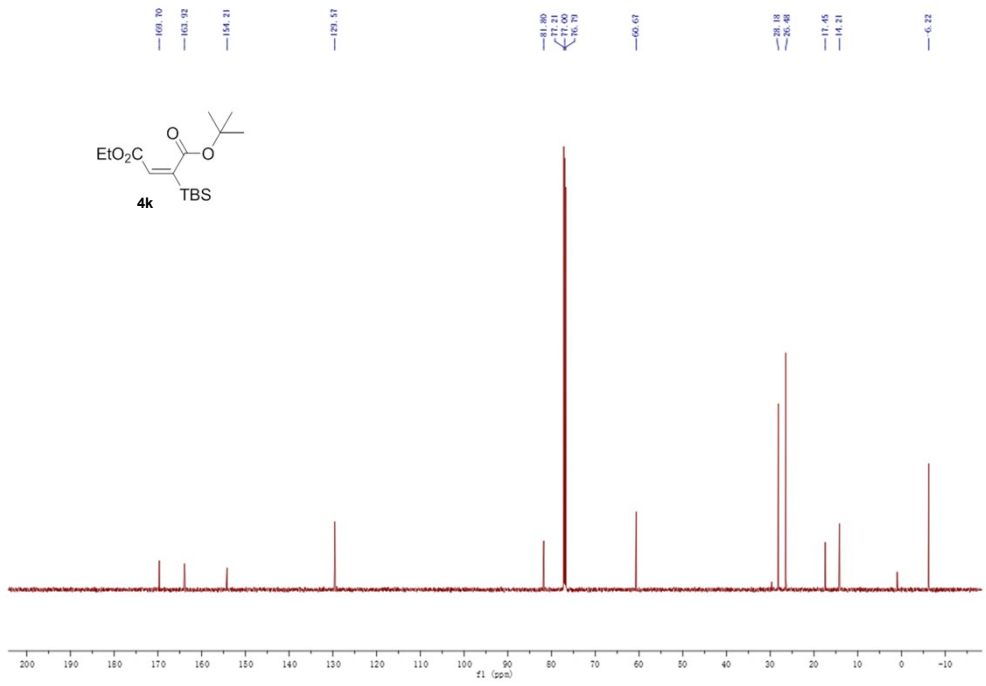
4.188
4.177
1.531
1.295
1.283
1.271
0.948
0.167
EtO2C
O
O
TBS
4k
1.00
2.20
9.05
3.10
9.02
6.02
f1 (ppm)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163.92
154.21
129.57
81.89
77.71
77.00
76.79
60.67
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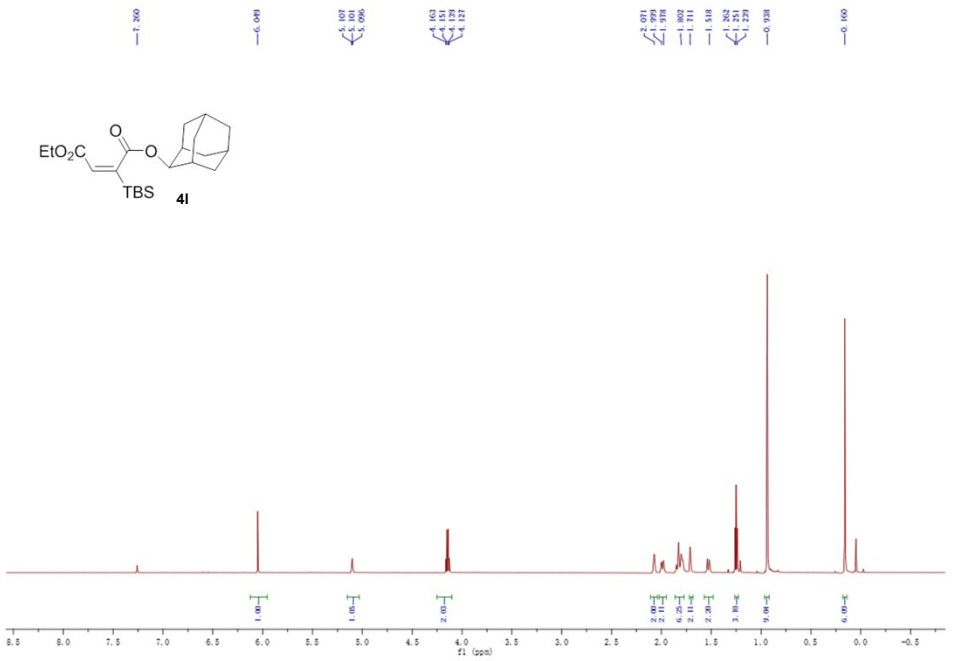
26.48
17.45
14.21
-6.22
EtO2C
O
O
TBS
4k
f1 (ppm)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6.049
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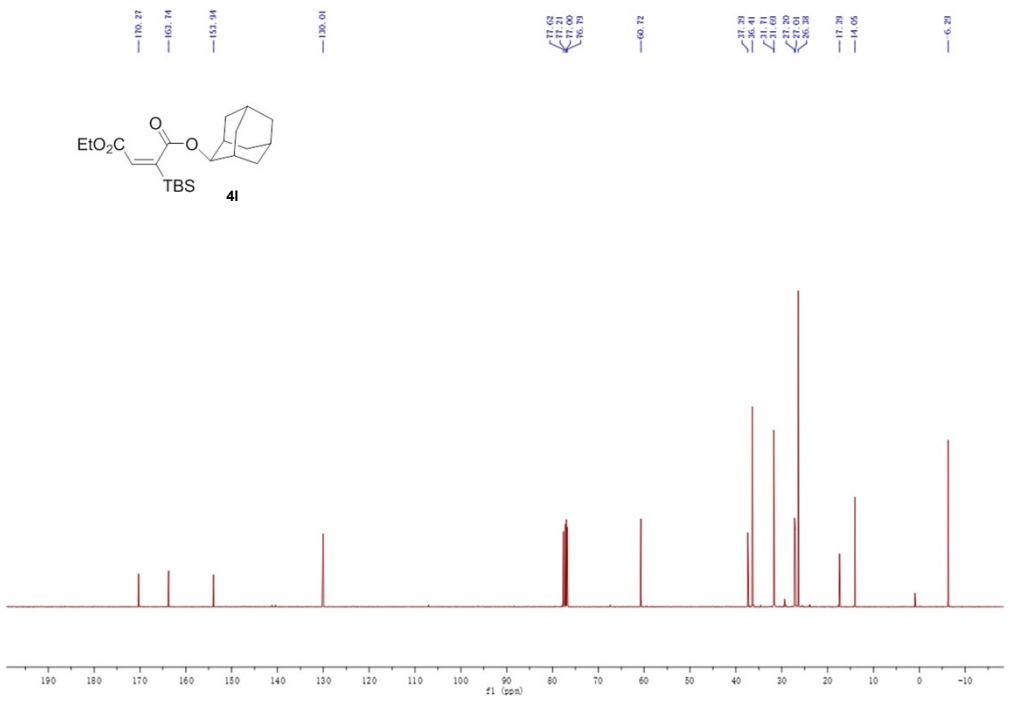
5.101
5.096
4.163
4.151
4.139
4.127
2.071
1.999
1.978
1.802
1.711
1.518
1.262
1.251
1.229
0.938
0.160
EtO2C
O
O
TBS
4l
1.00
1.05
2.03
2.00
2.11
6.25
2.11
2.20
3.10
9.04
6.09
f1 (ppm)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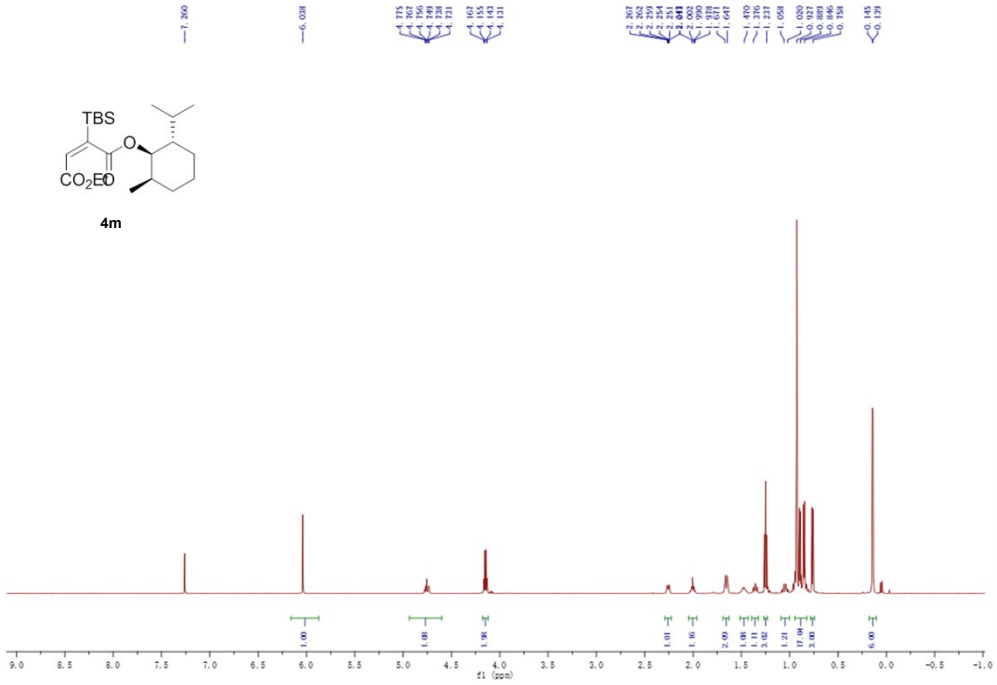
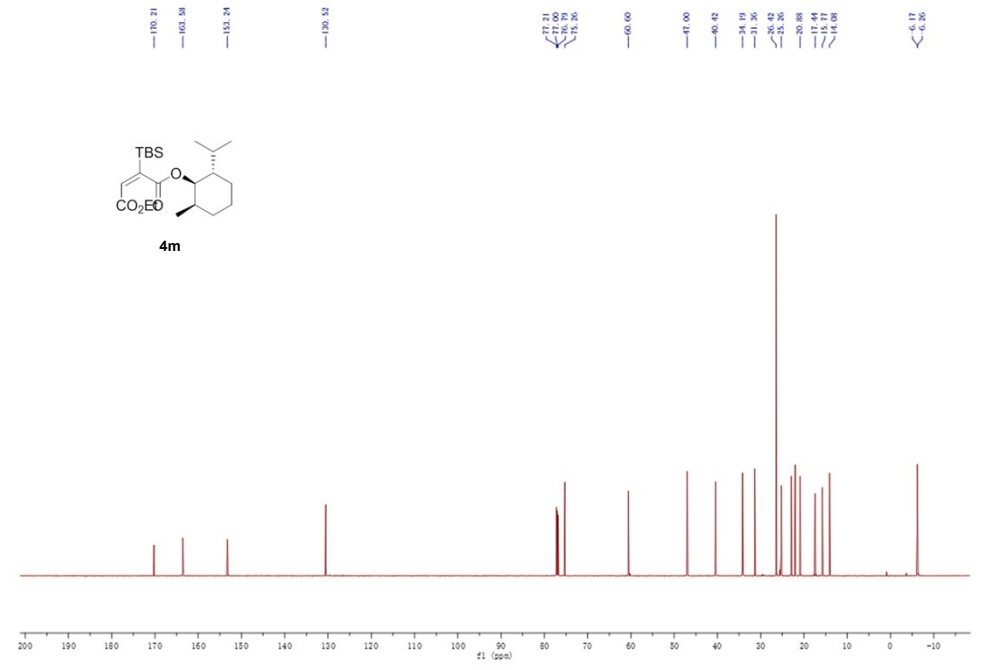
130.01
77.62
77.21
77.00
76.79
60.72
37.39
36.41
31.71
27.60
27.39
27.01
26.38
17.39
14.05
-6.29
EtO2C
O
O
TBS
4l
f1 (ppm)


TBS
O
CO2Et
4m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O
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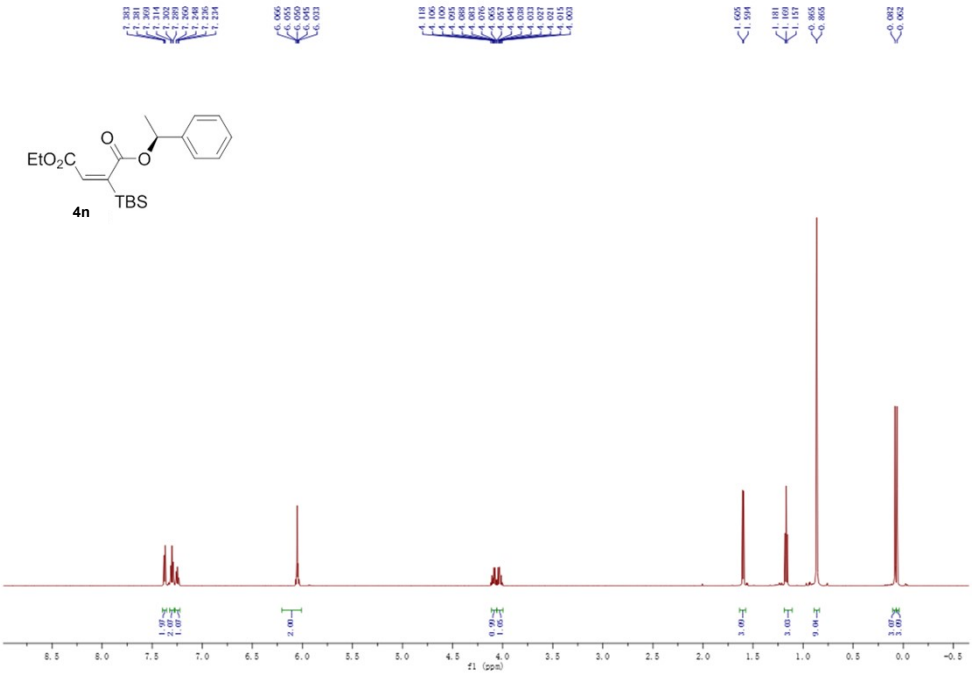
4m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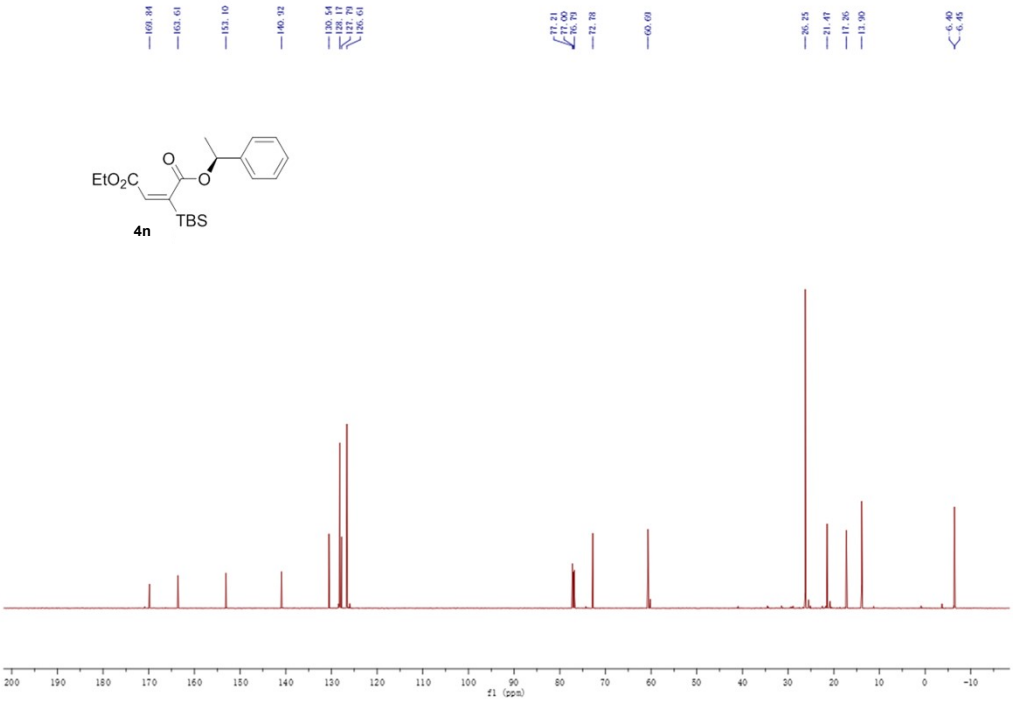
O
O
TBS
4n
f1 (ppm)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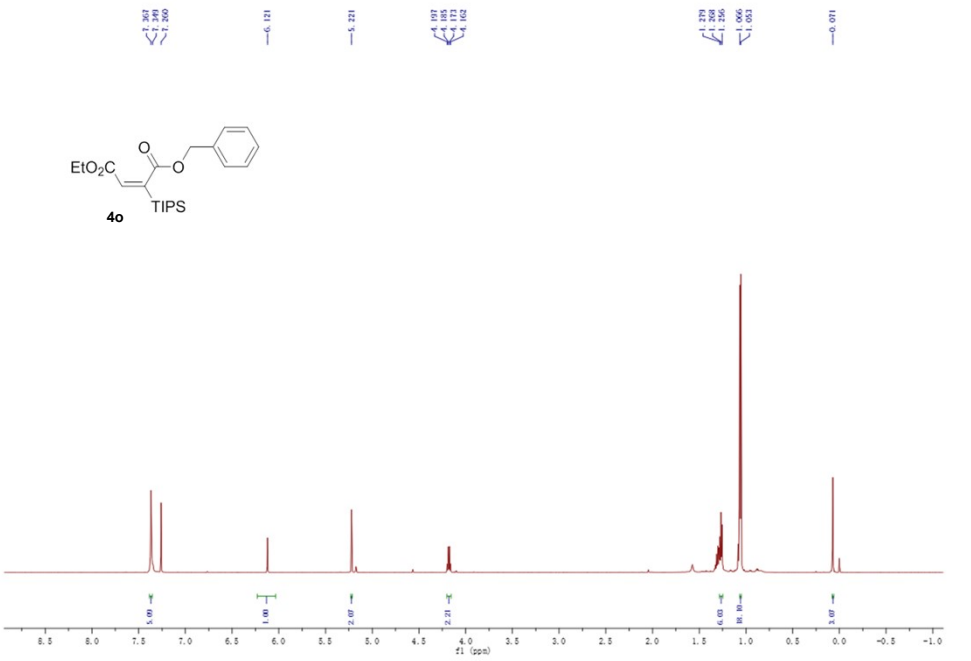
O
O
TBS
4n
f1 (ppm)



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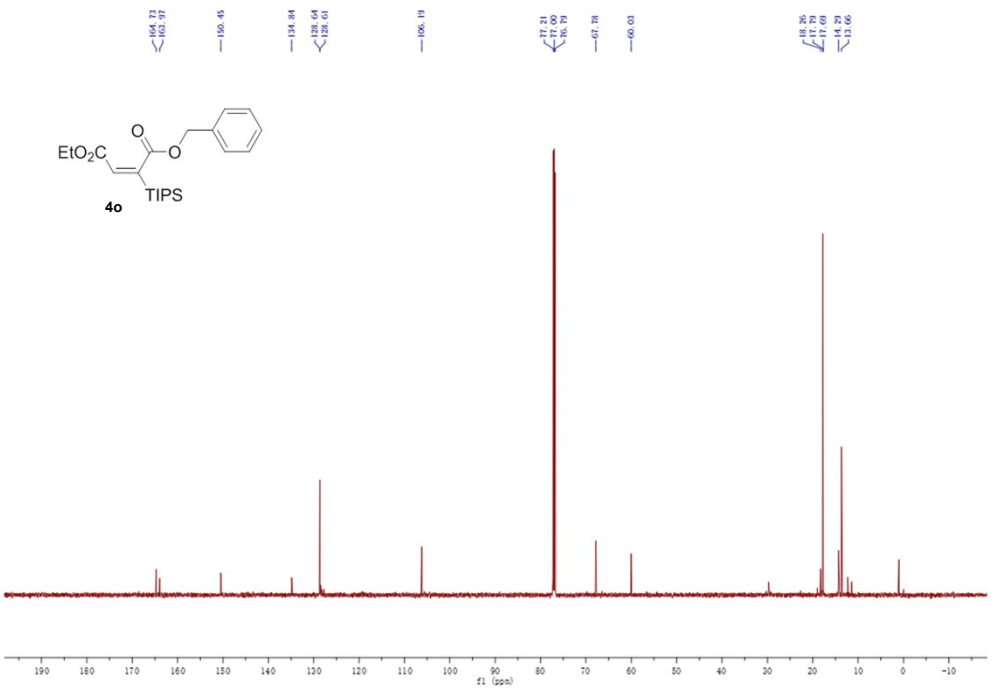

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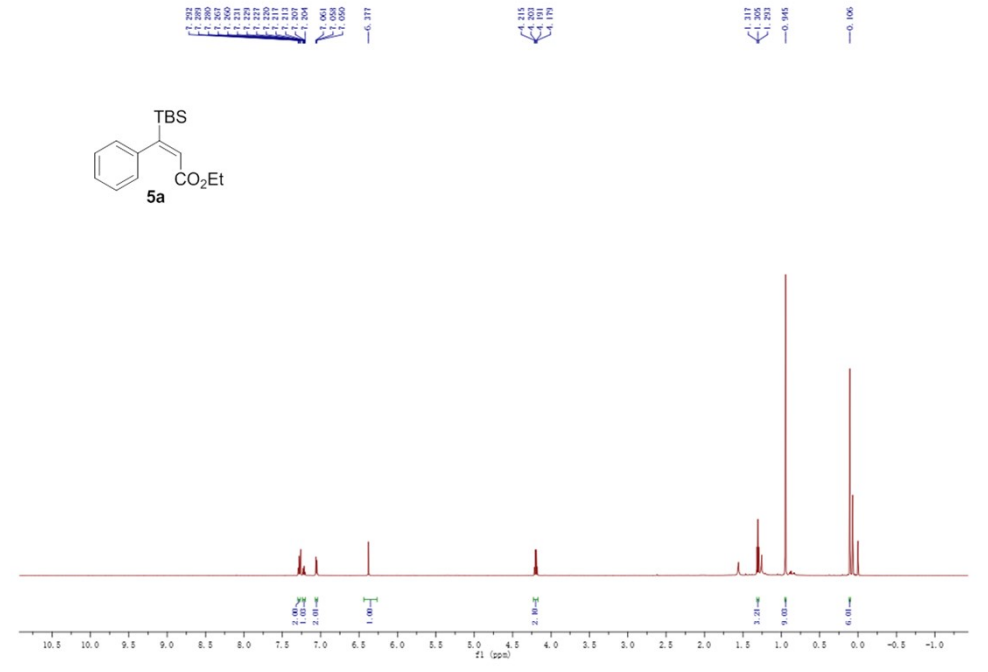
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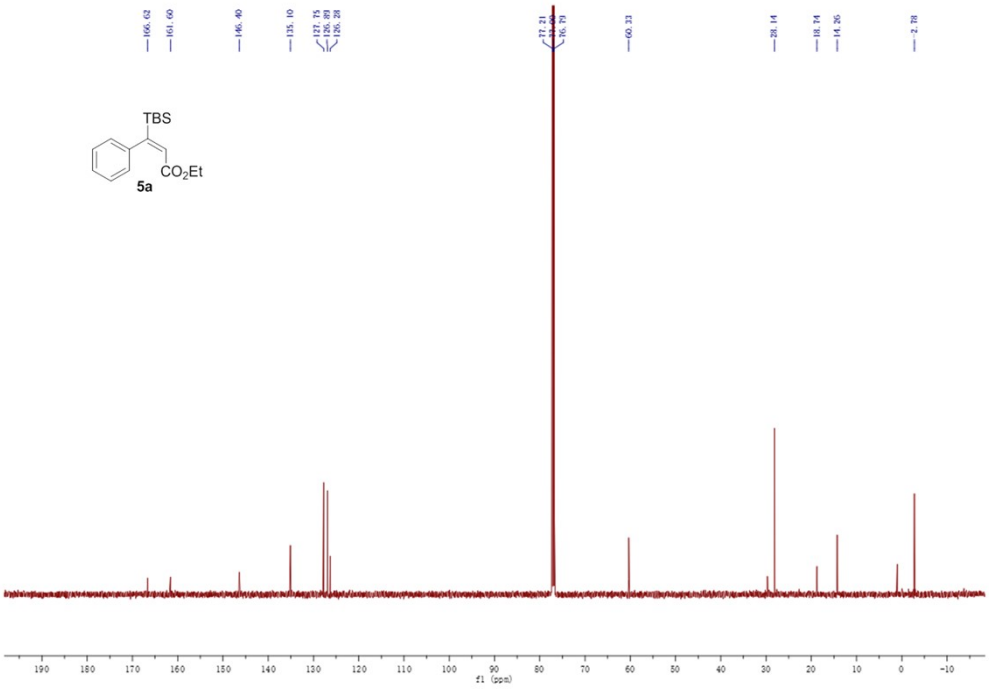
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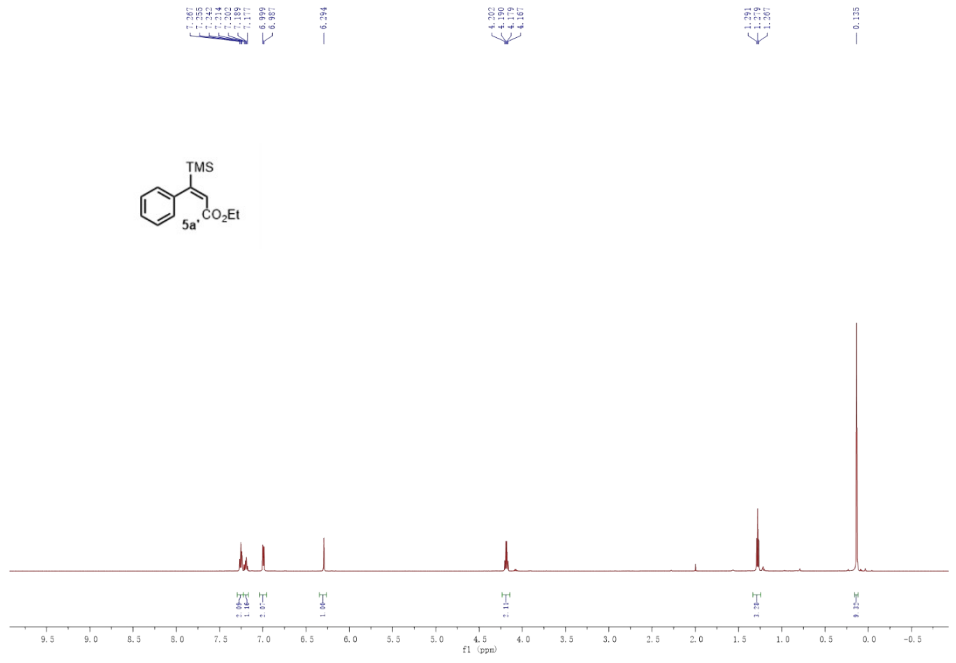
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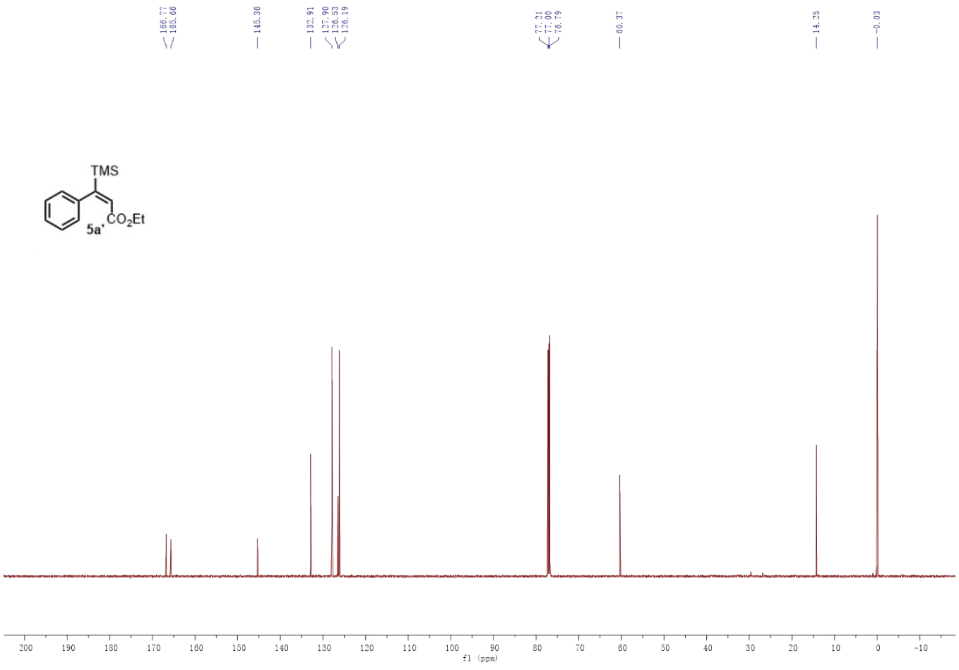
f1 (ppm)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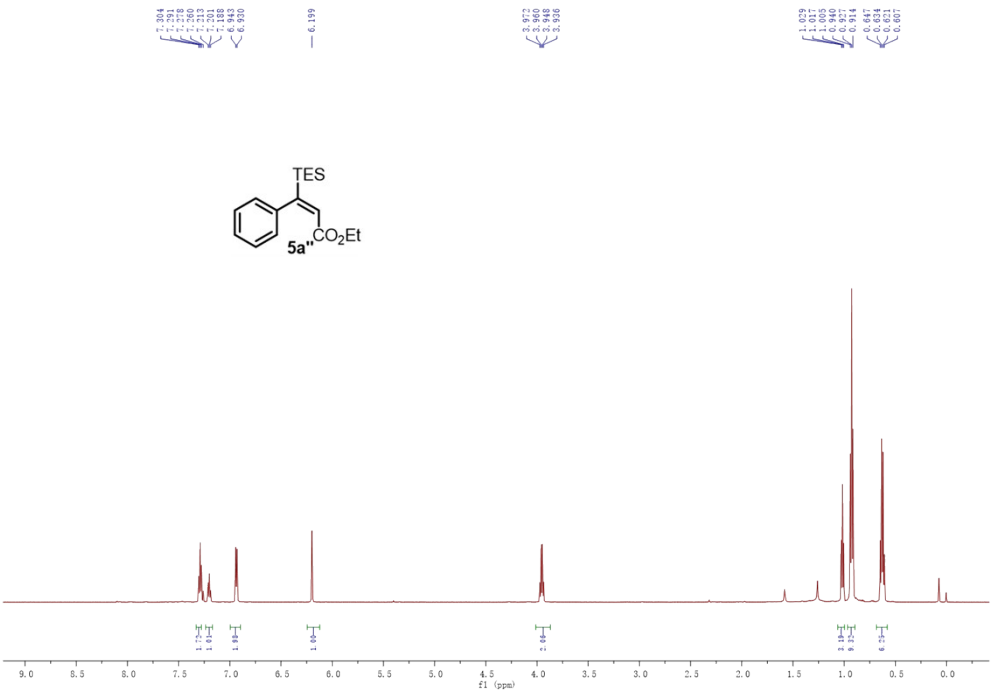
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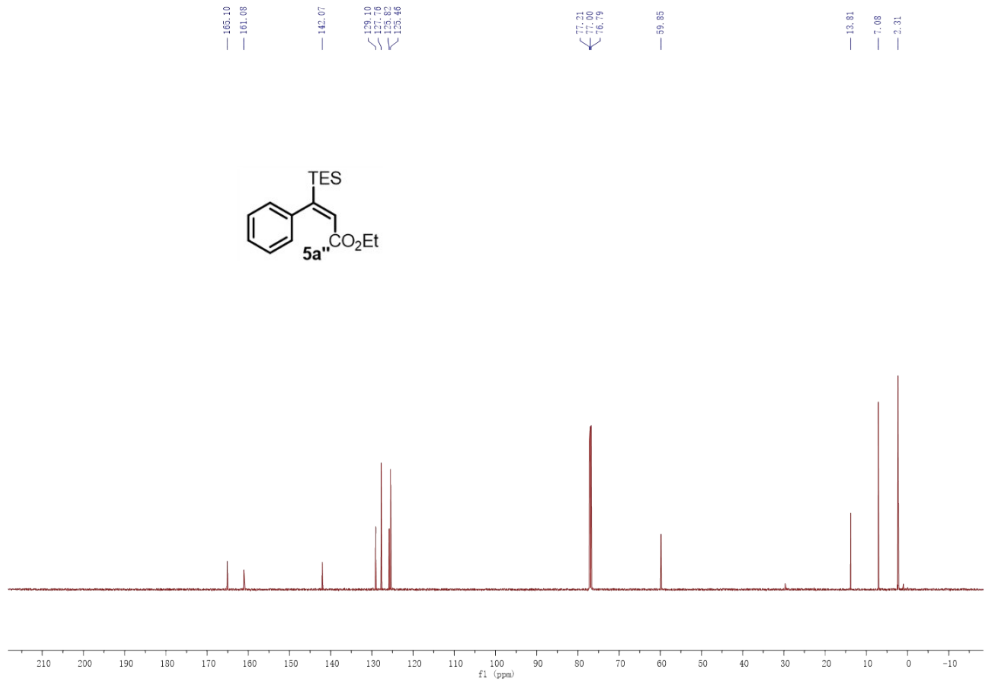
TES
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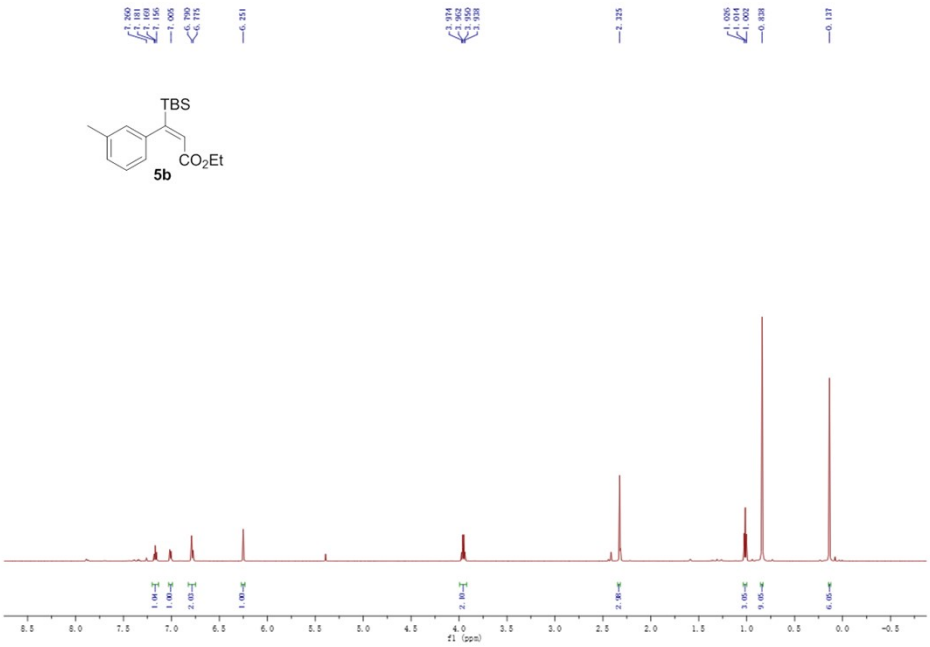
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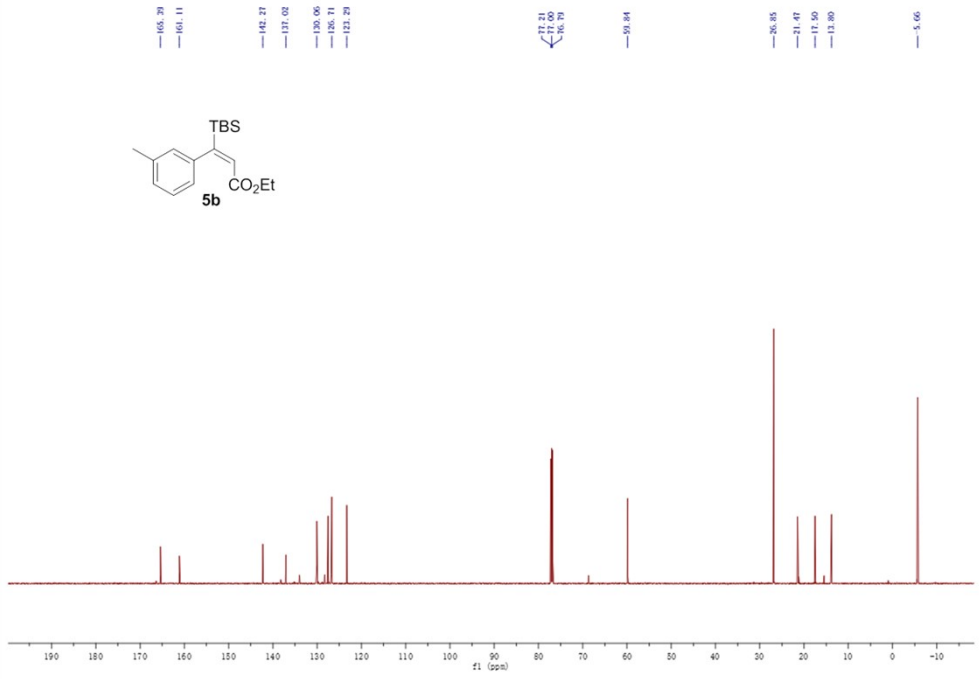
f1 (ppm)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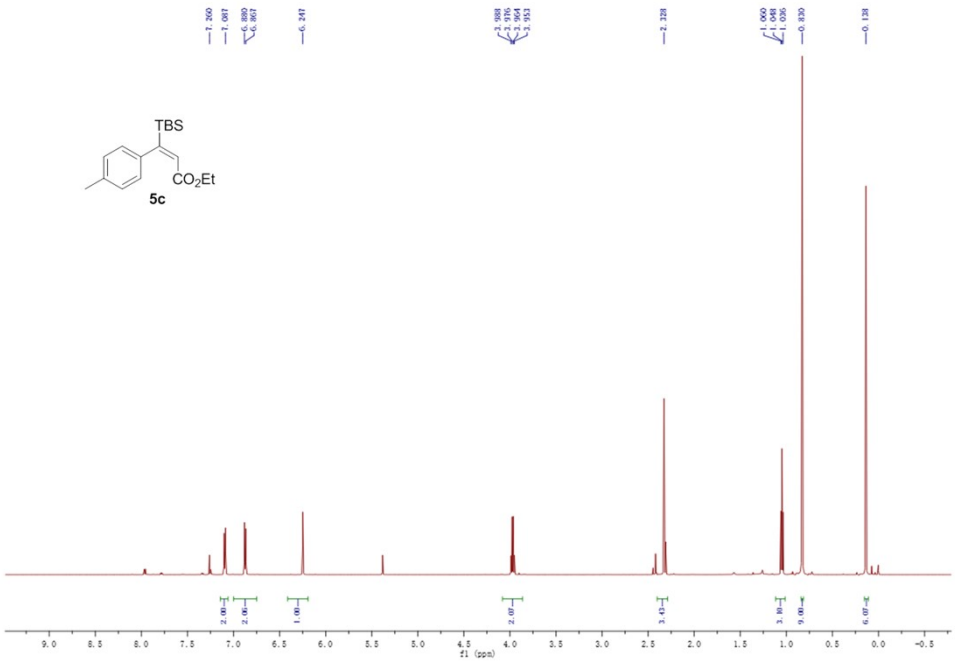
CO2Et
5b
f1 (ppm)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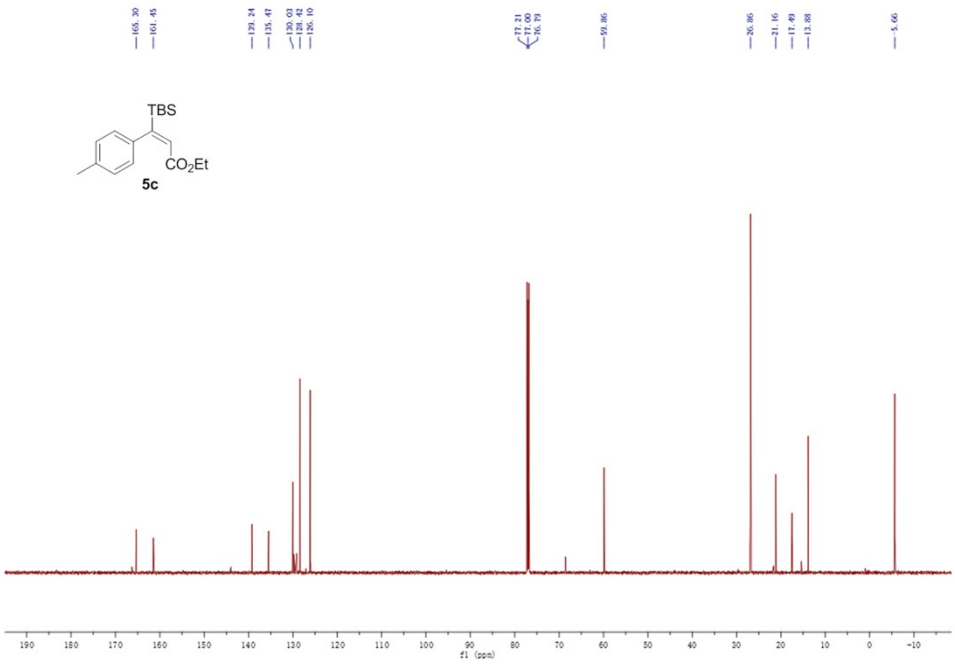
2.328
1.060
1.048
1.035
0.839
0.138
TBS
CO2Et
5c
2.00
2.00
1.00
2.07
3.43
3.10
9.00
6.07
f1 (ppm)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161.45
139.24
135.47
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128.42
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77.21
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76.79
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26.86
21.16
17.49
13.88
-5.66
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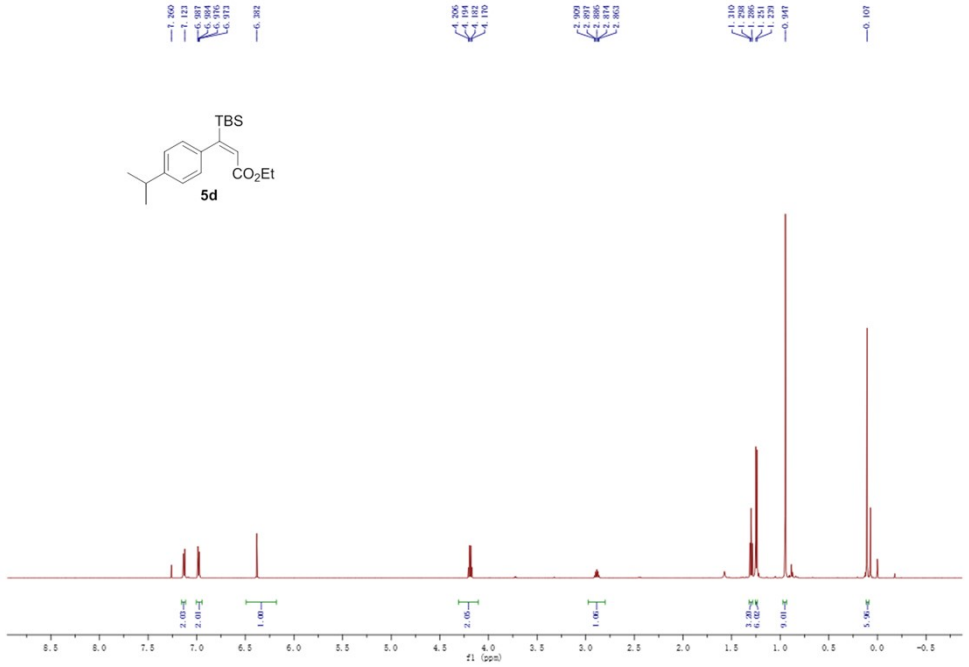
CO2Et
5c
f1 (ppm)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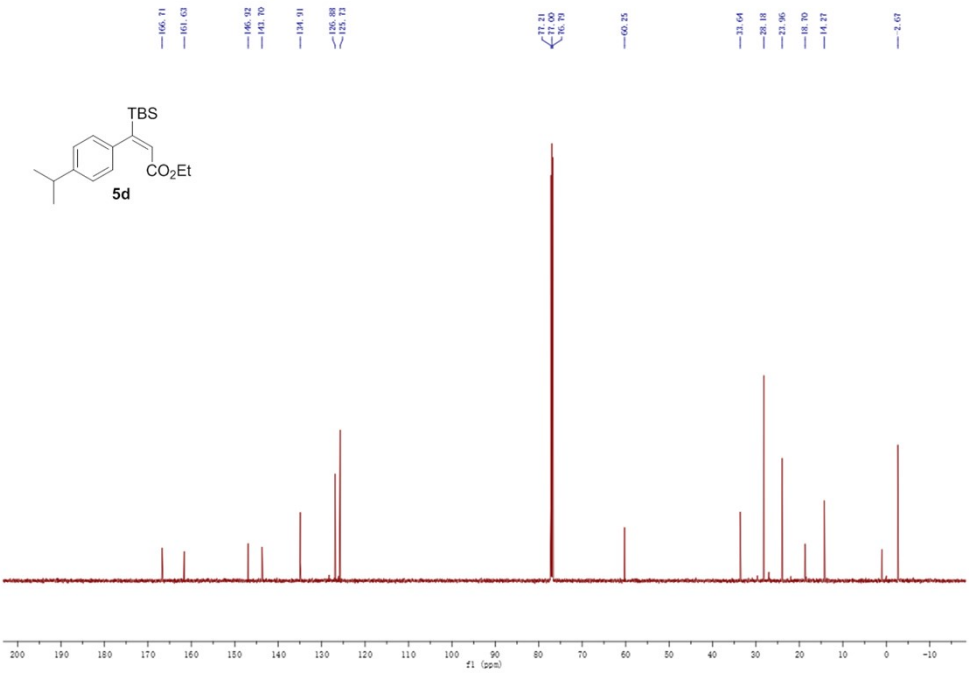
f1 (ppm)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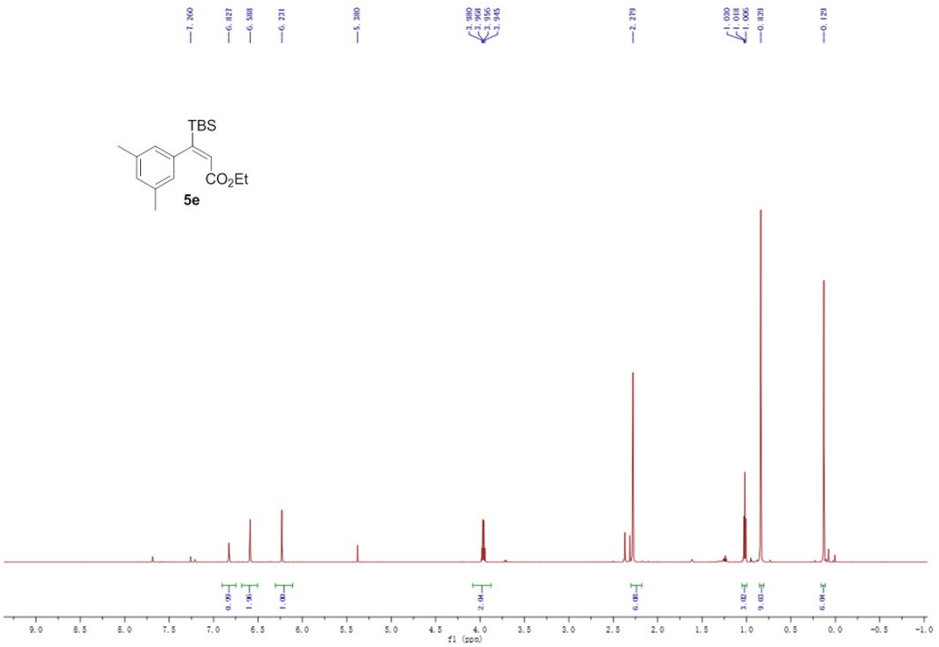
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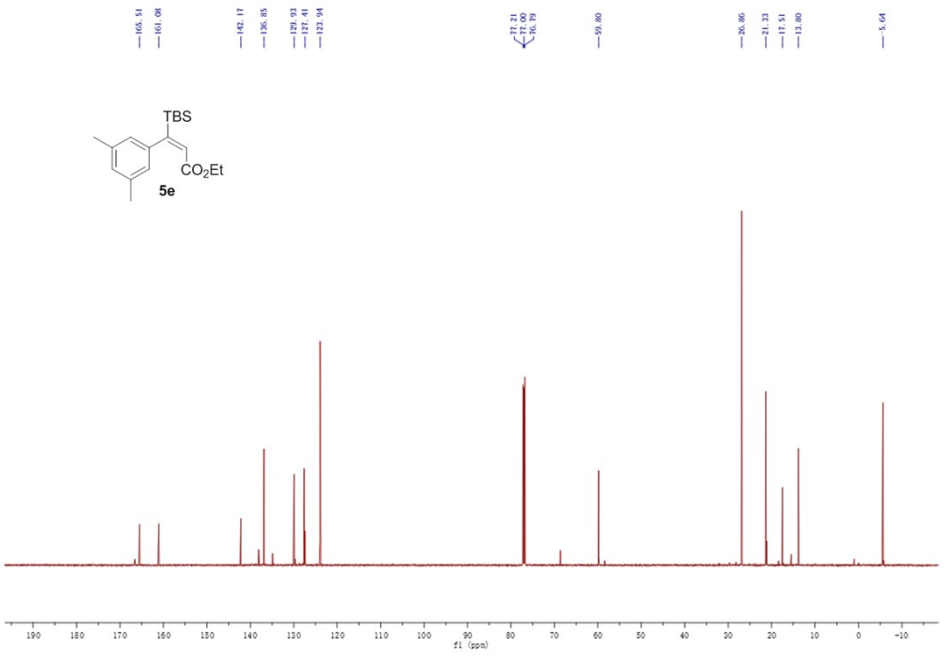
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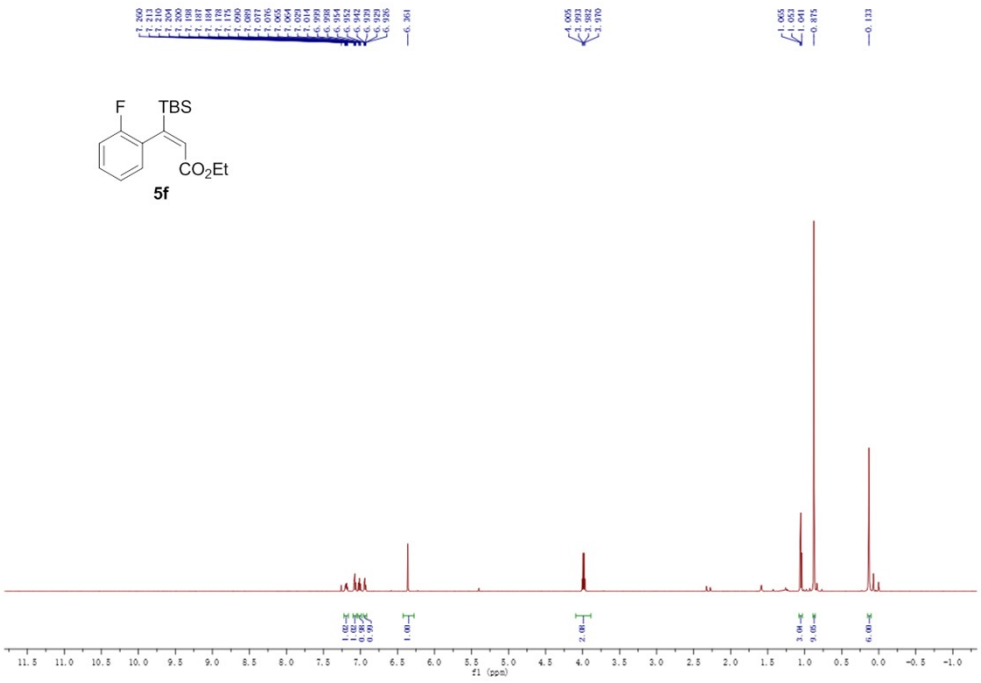
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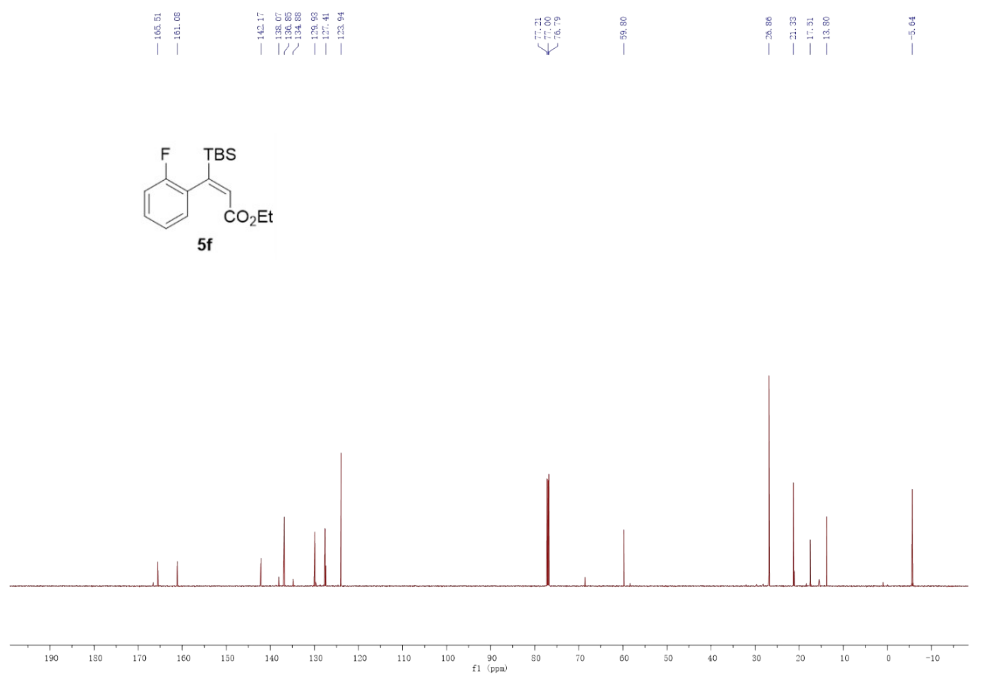
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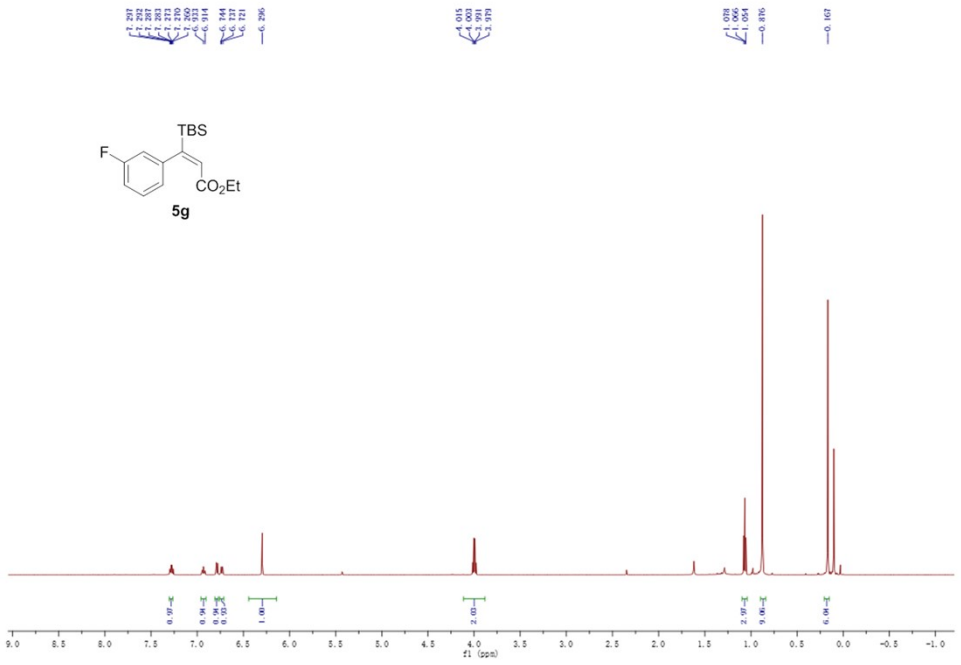
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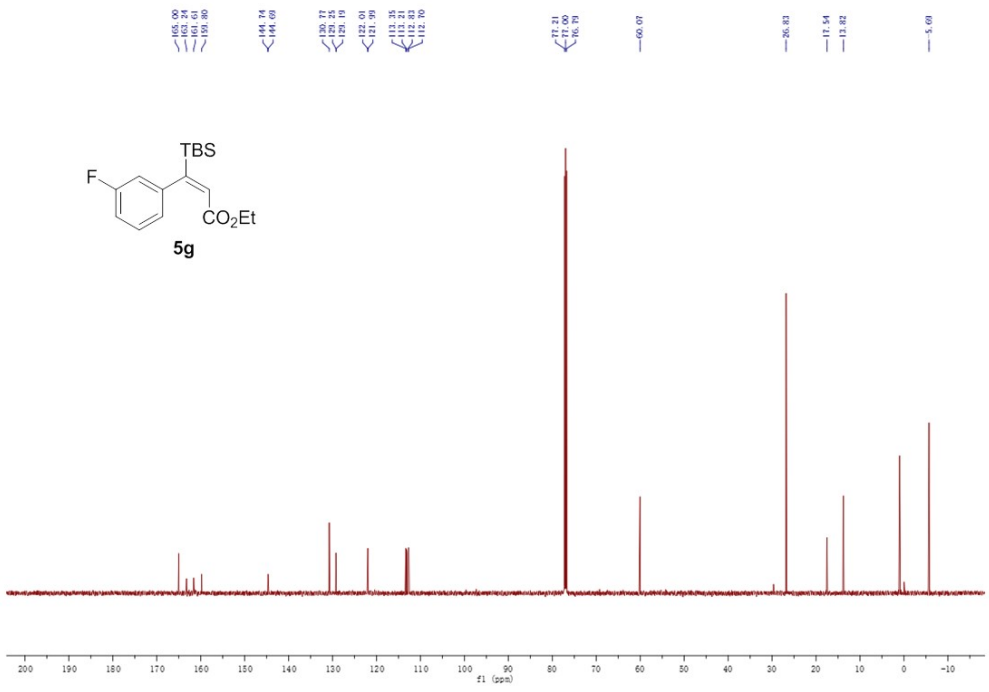
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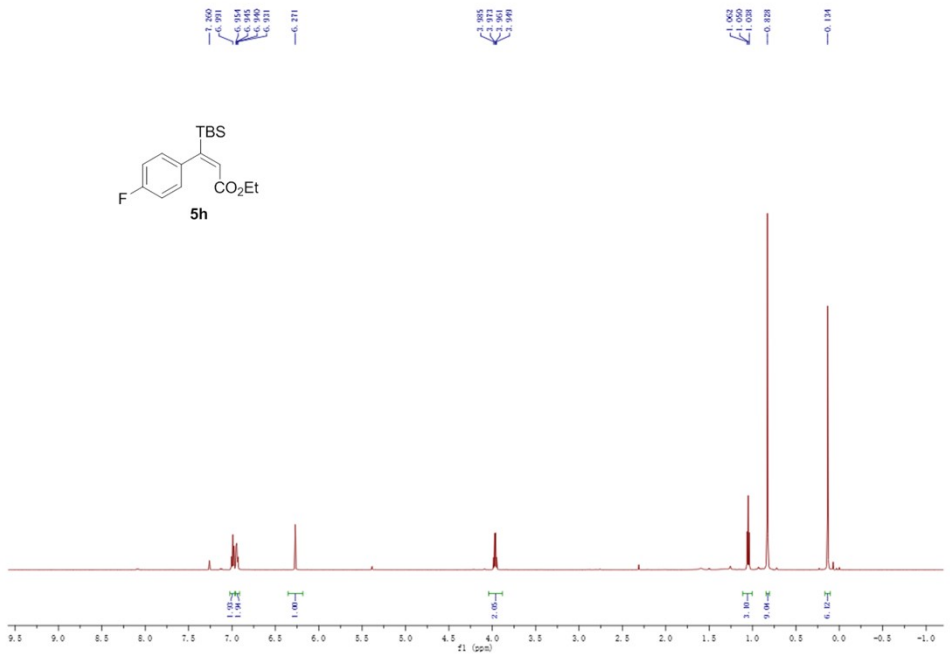
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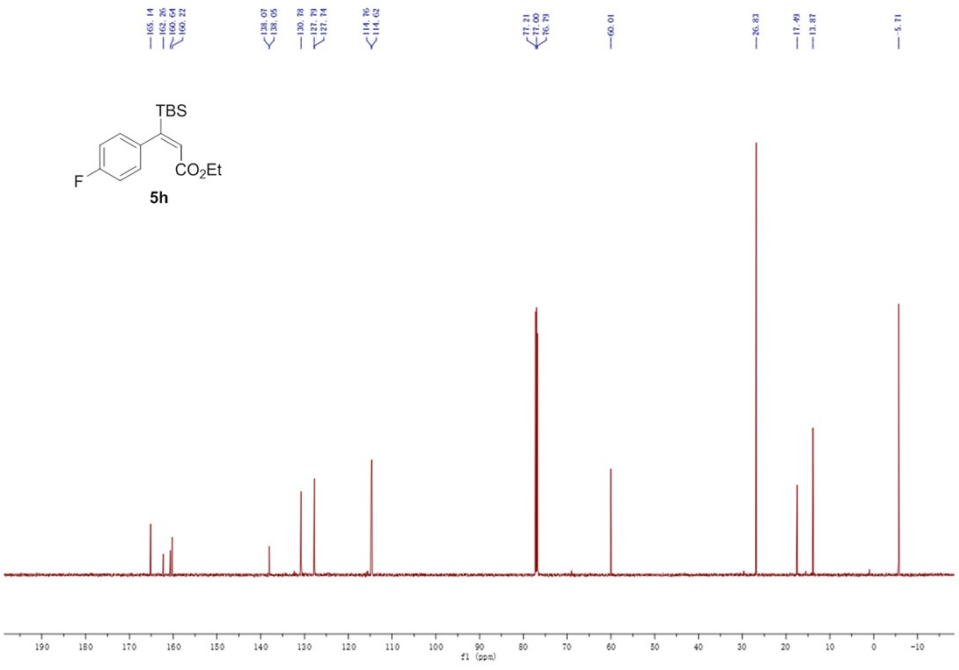
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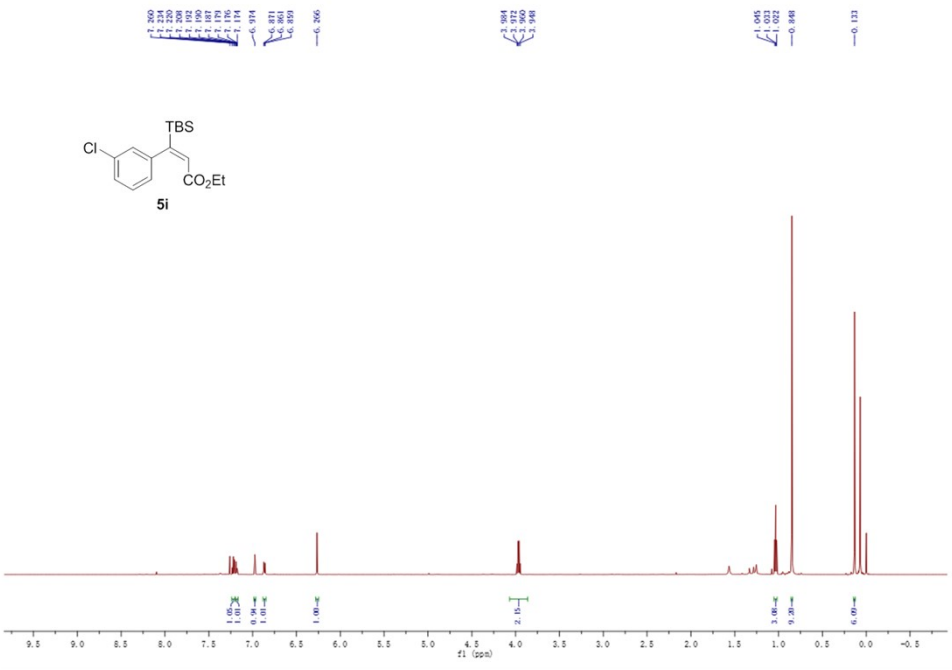
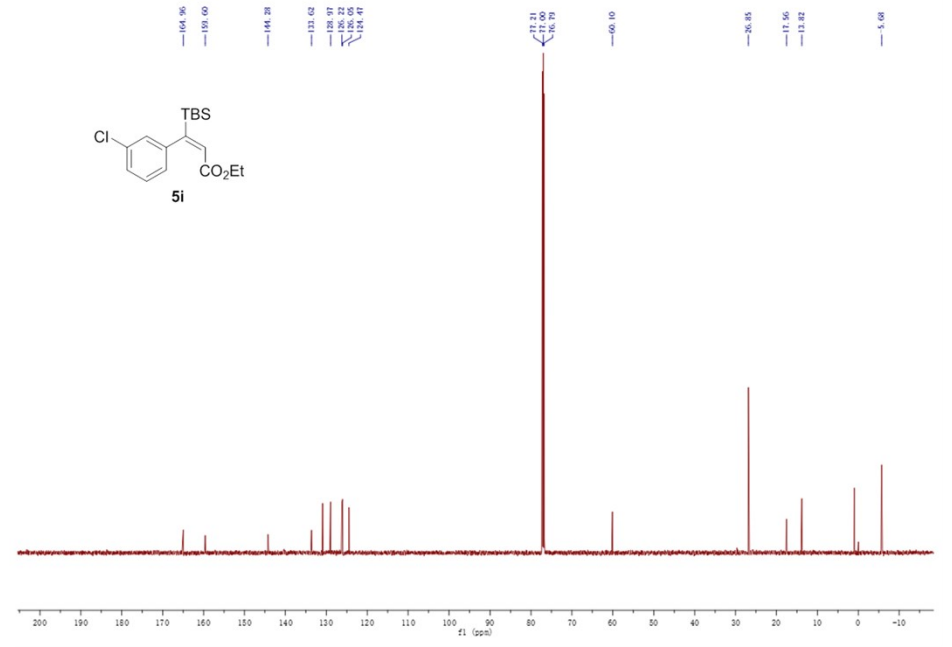
5h


TBS
Cl
CO2Et
5i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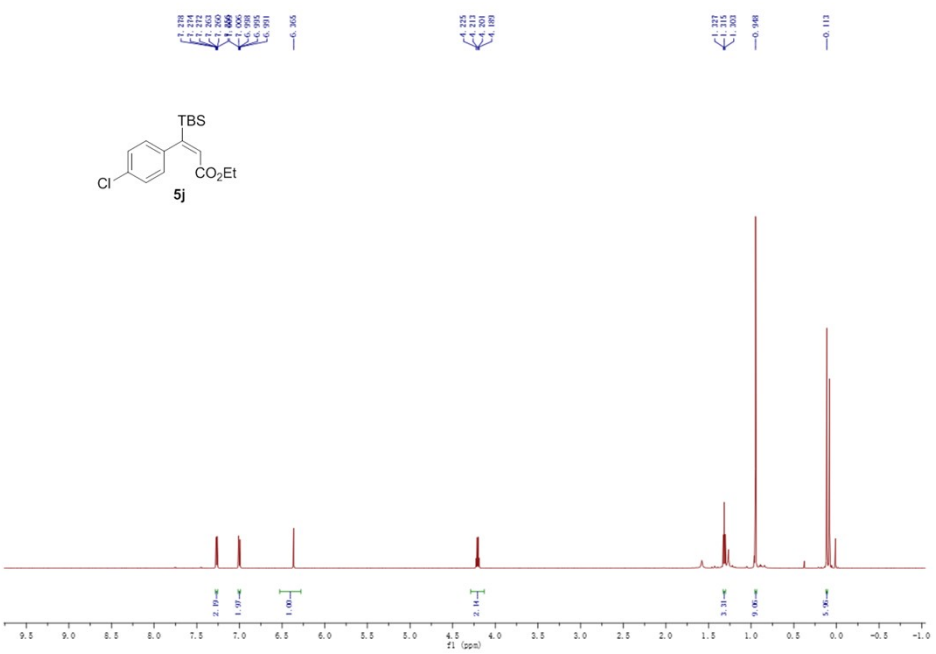
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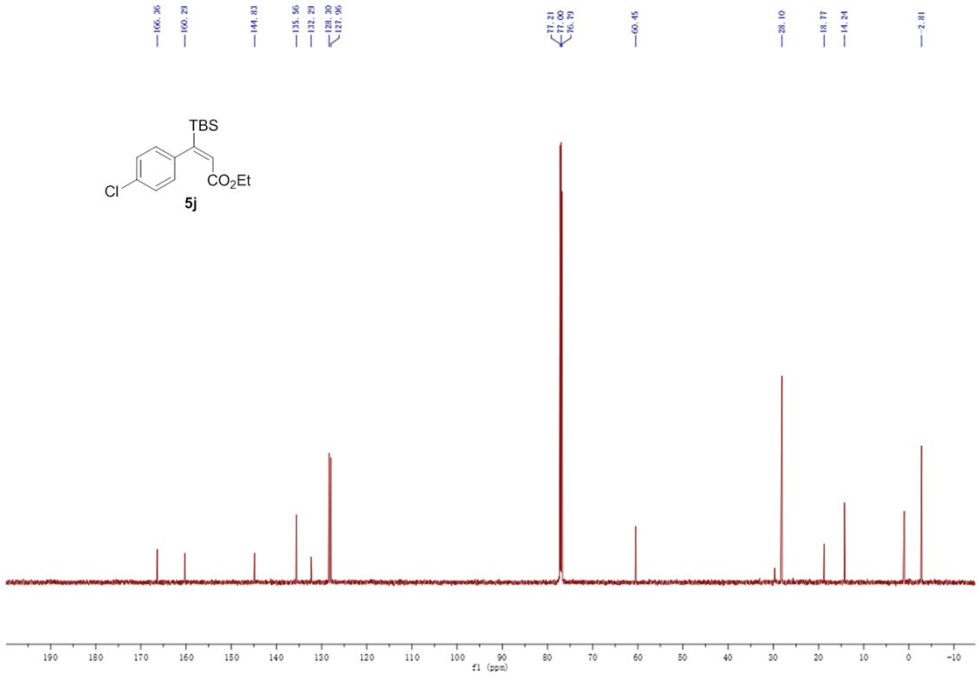
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Cl
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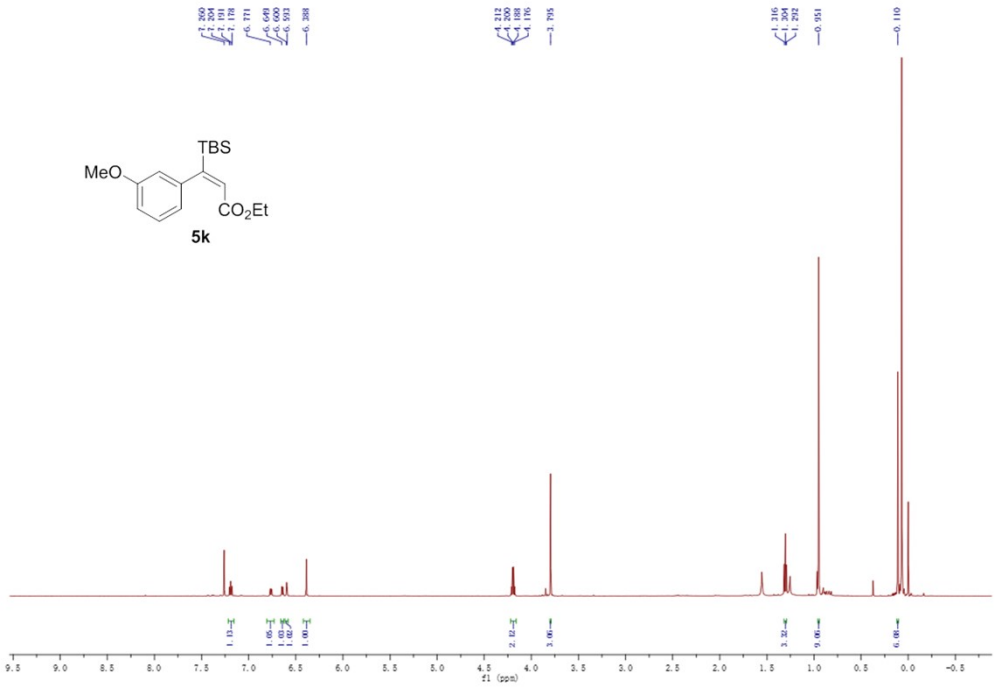
5j


TBS
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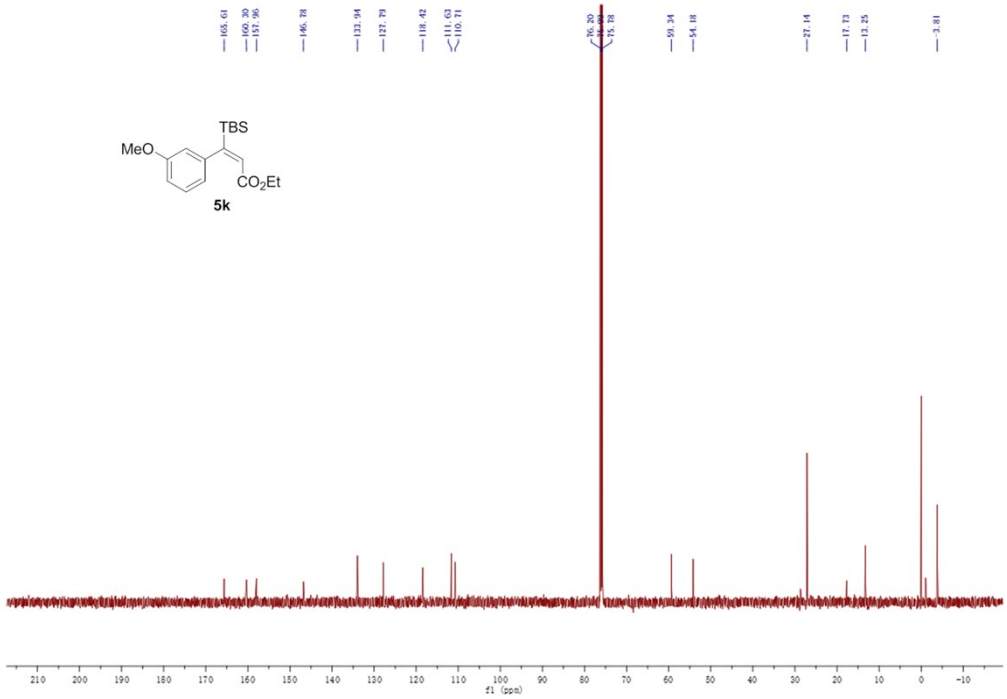
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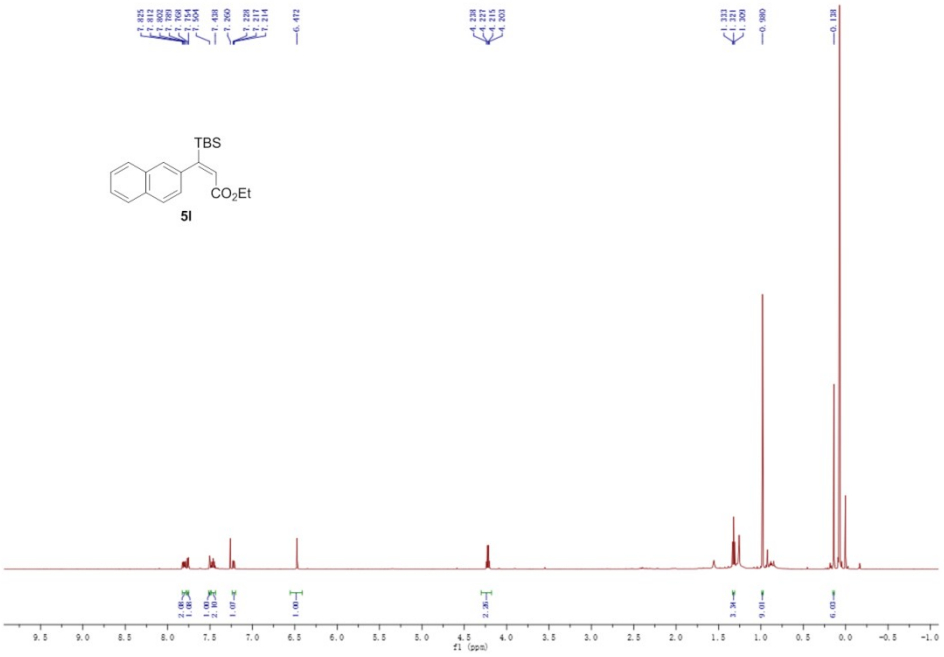
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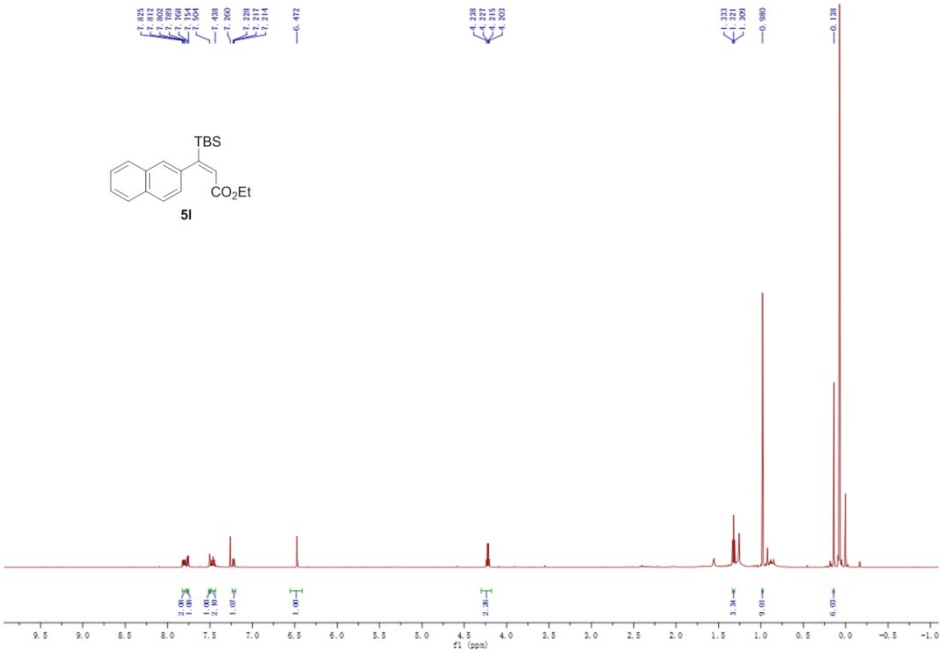
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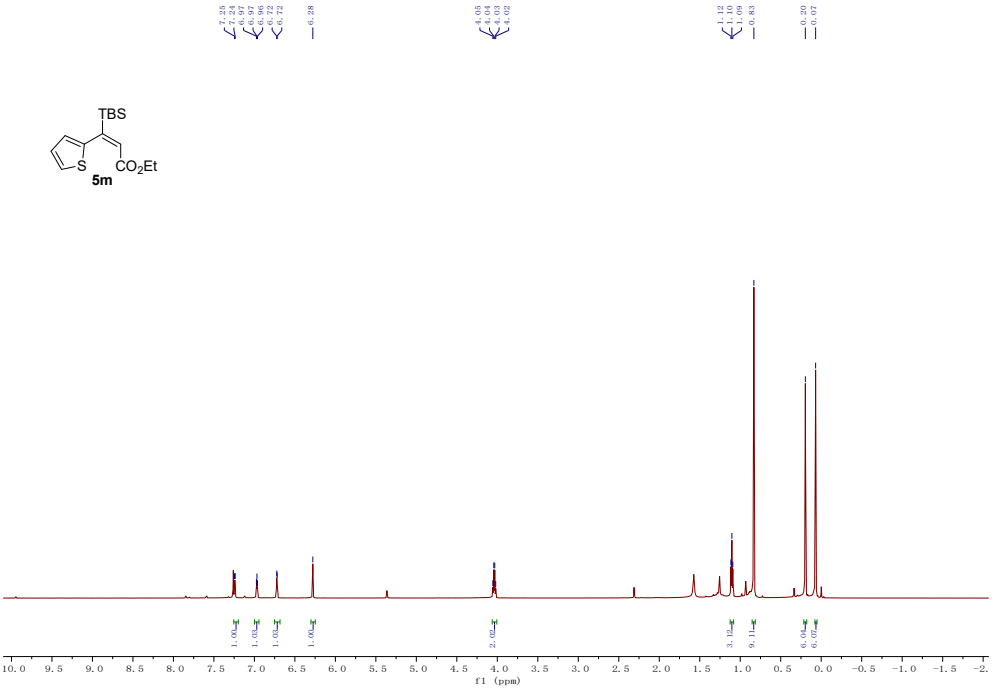
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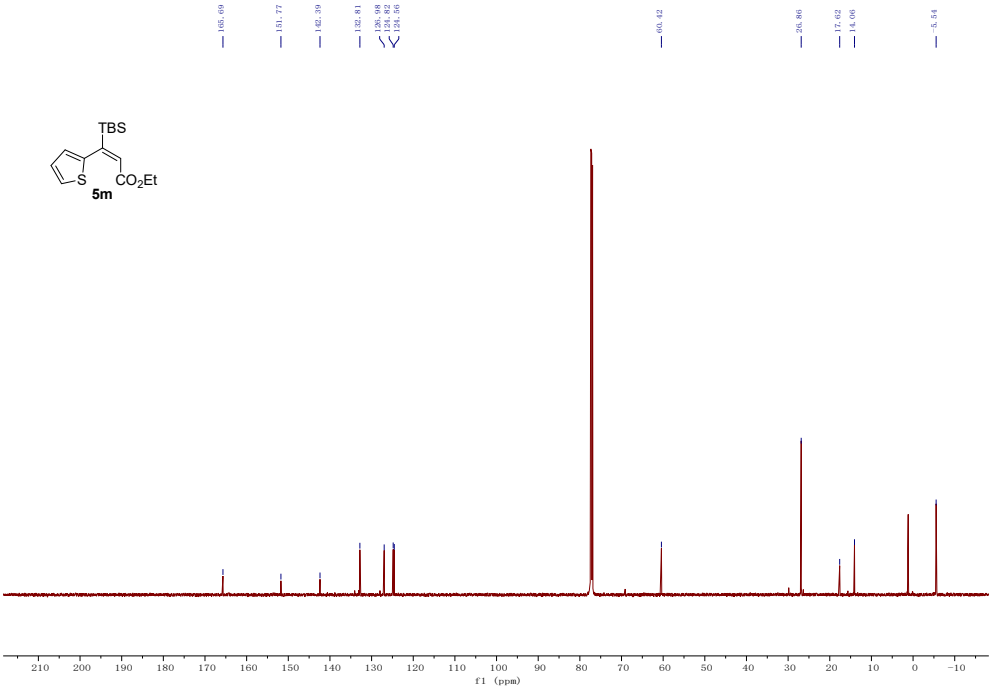
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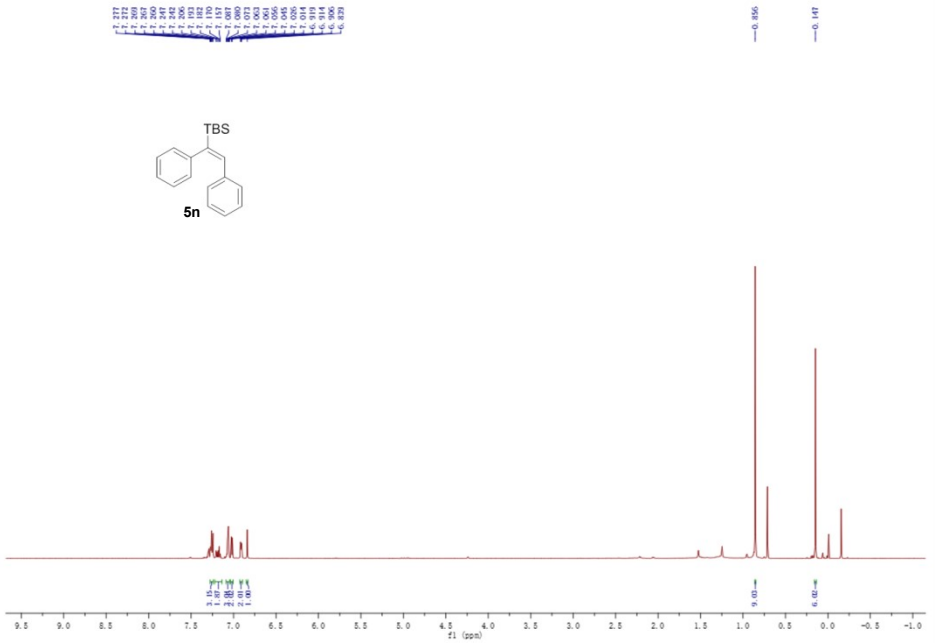
f1 (ppm)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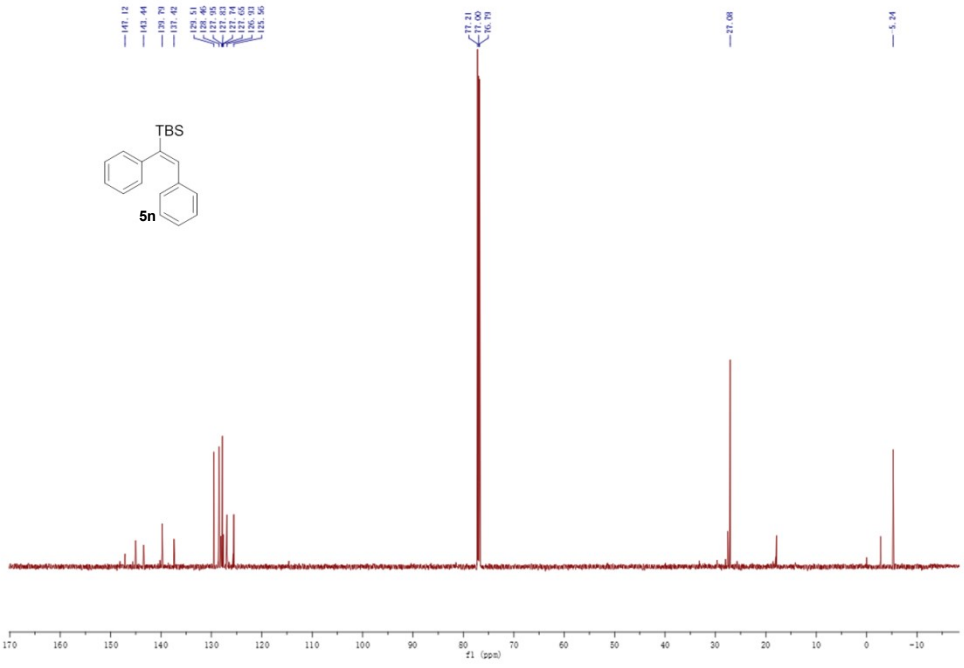
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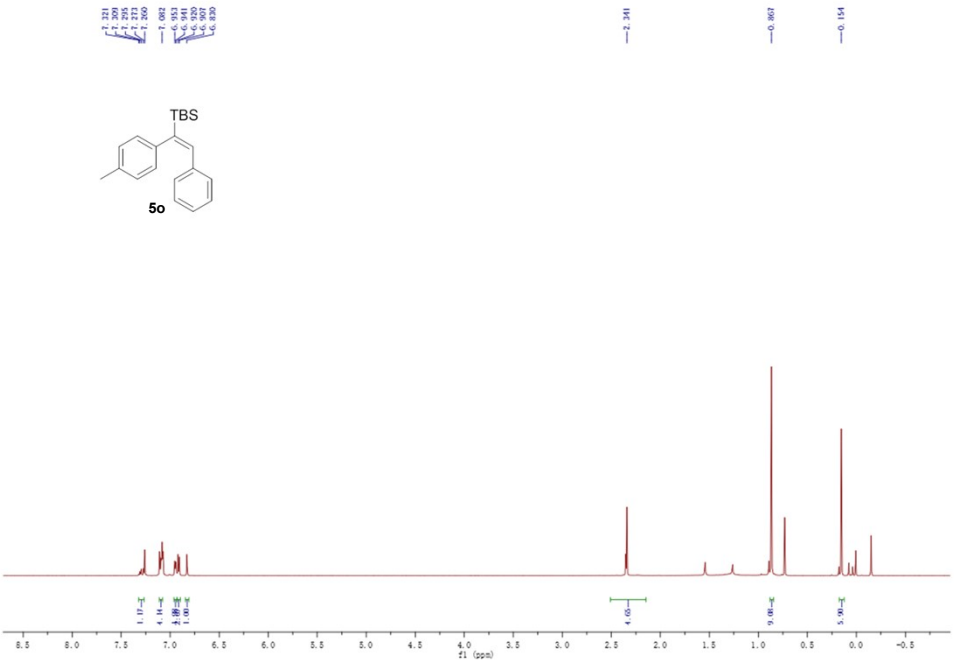
f1 (ppm)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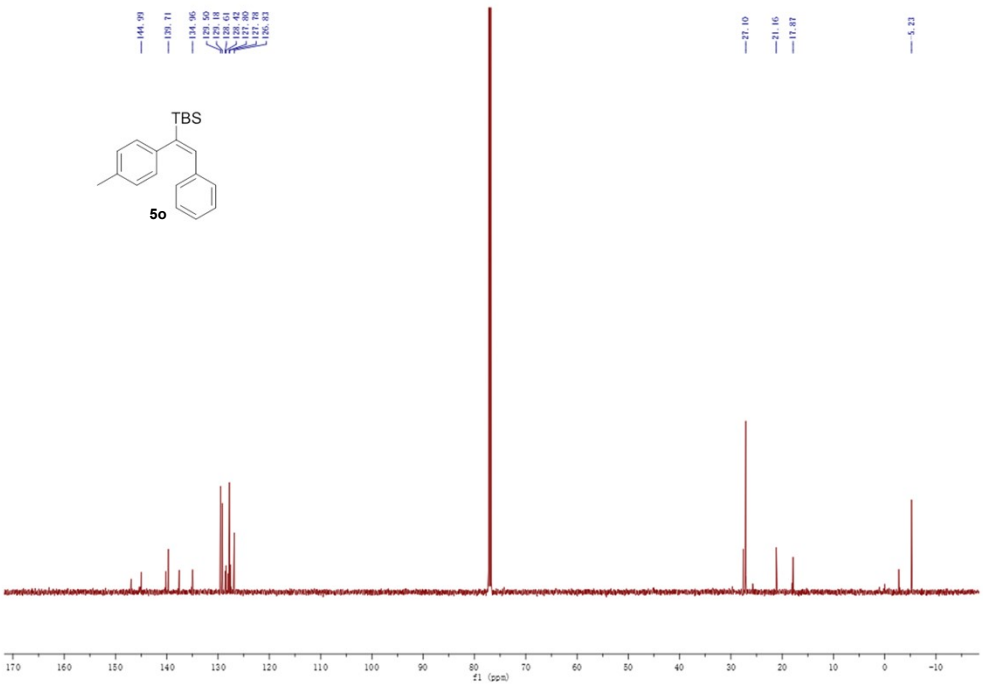
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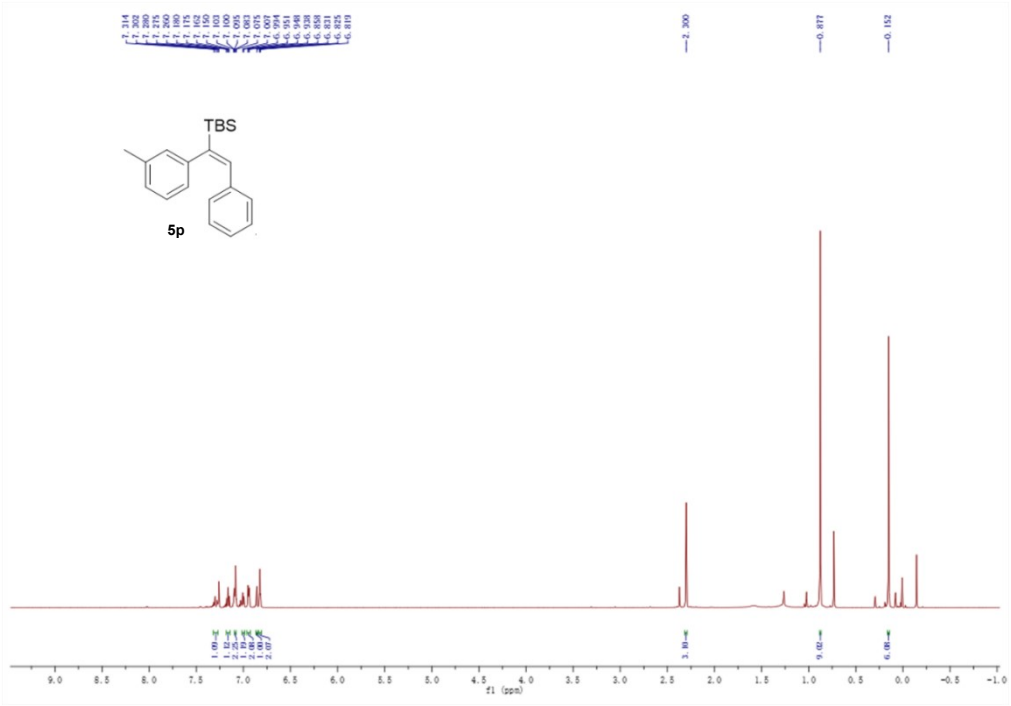
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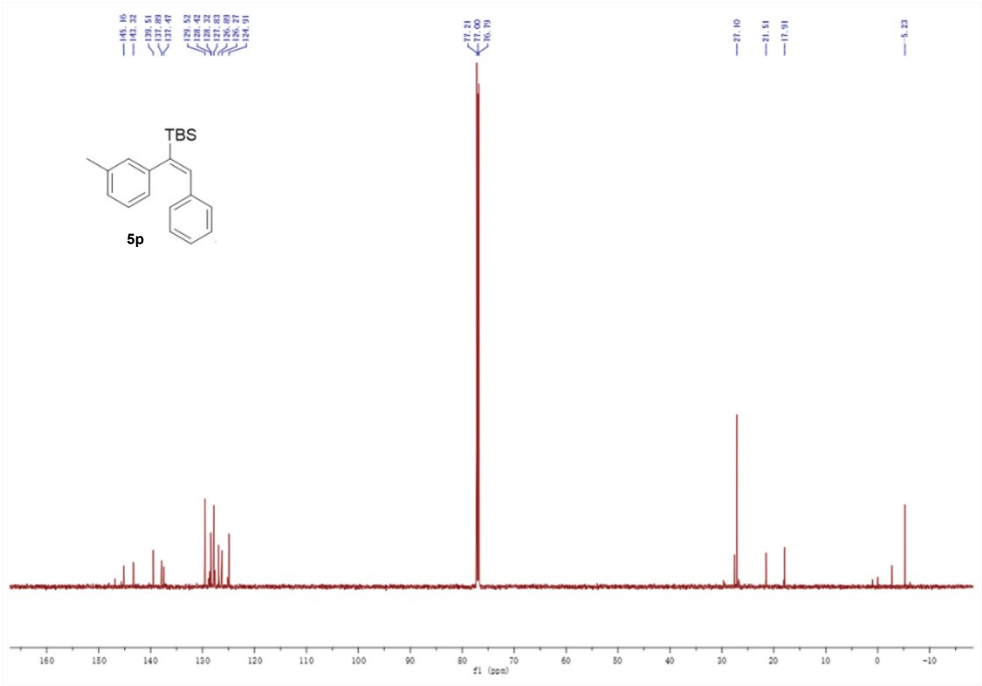
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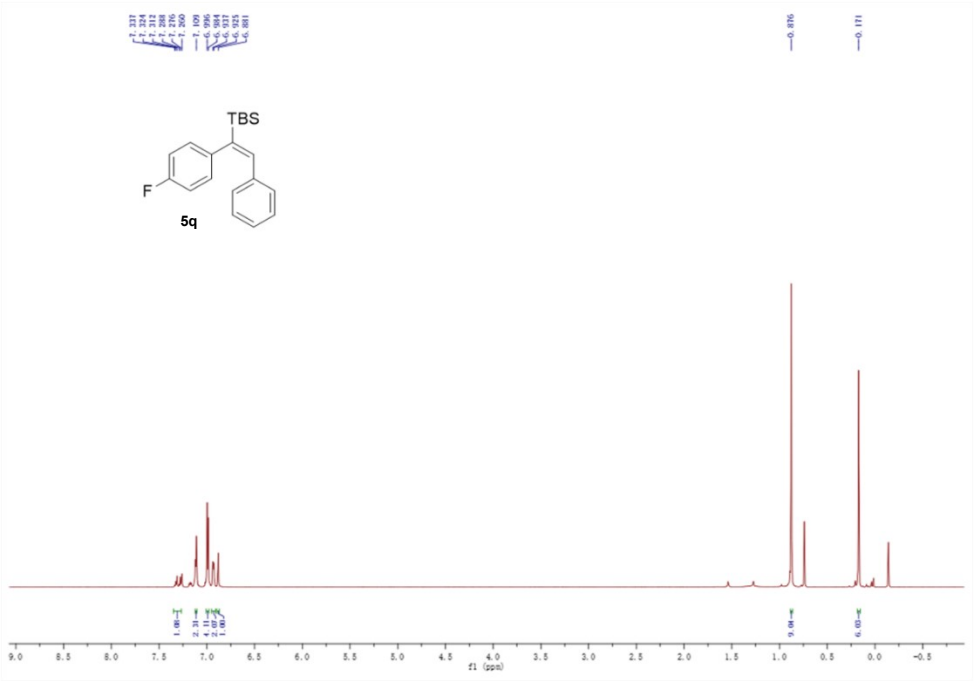
f1 (ppm)


TBS
F
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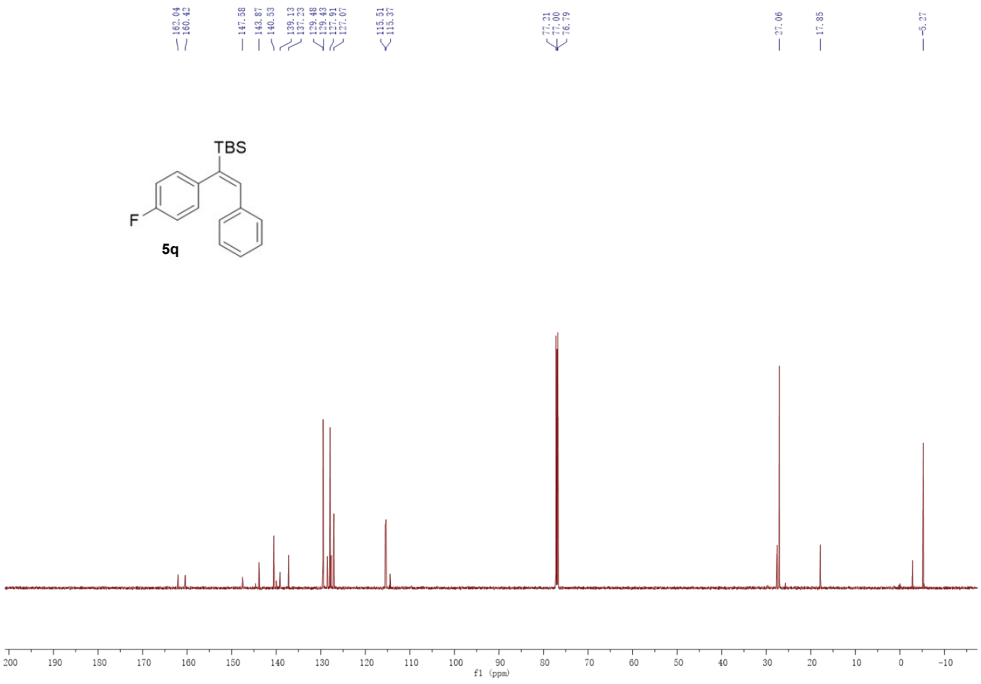
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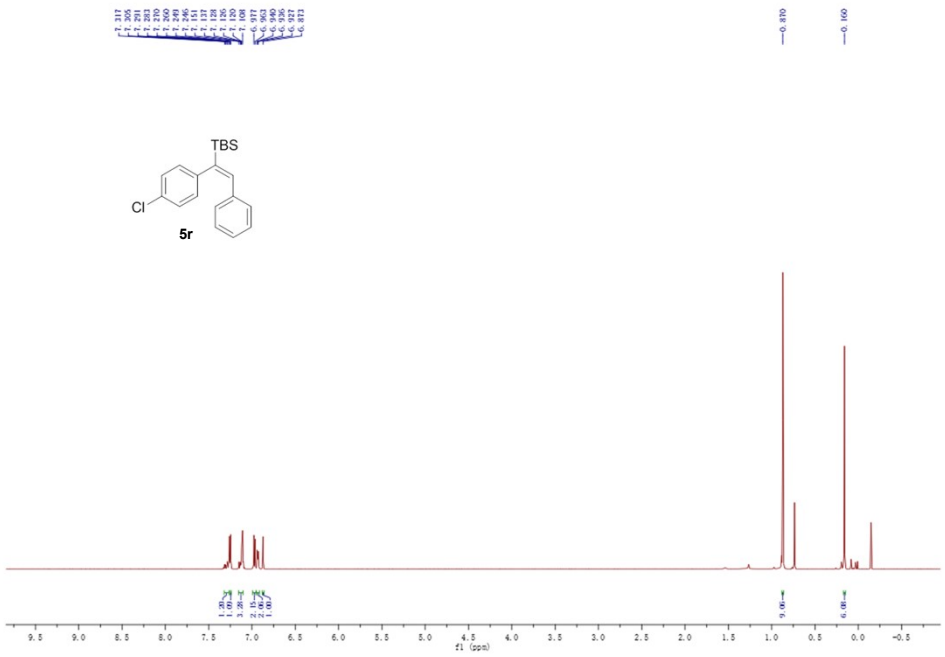
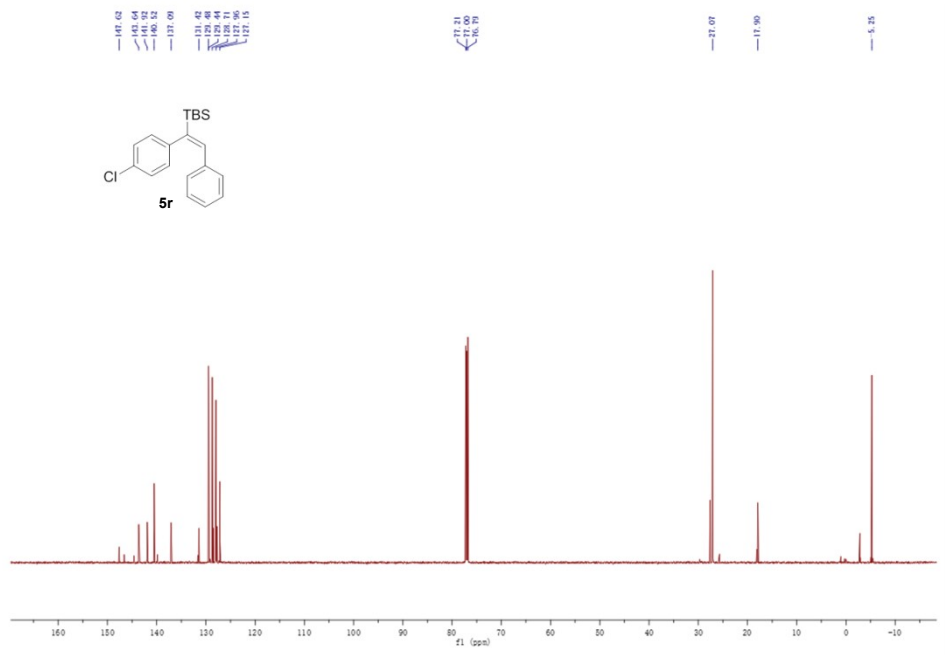
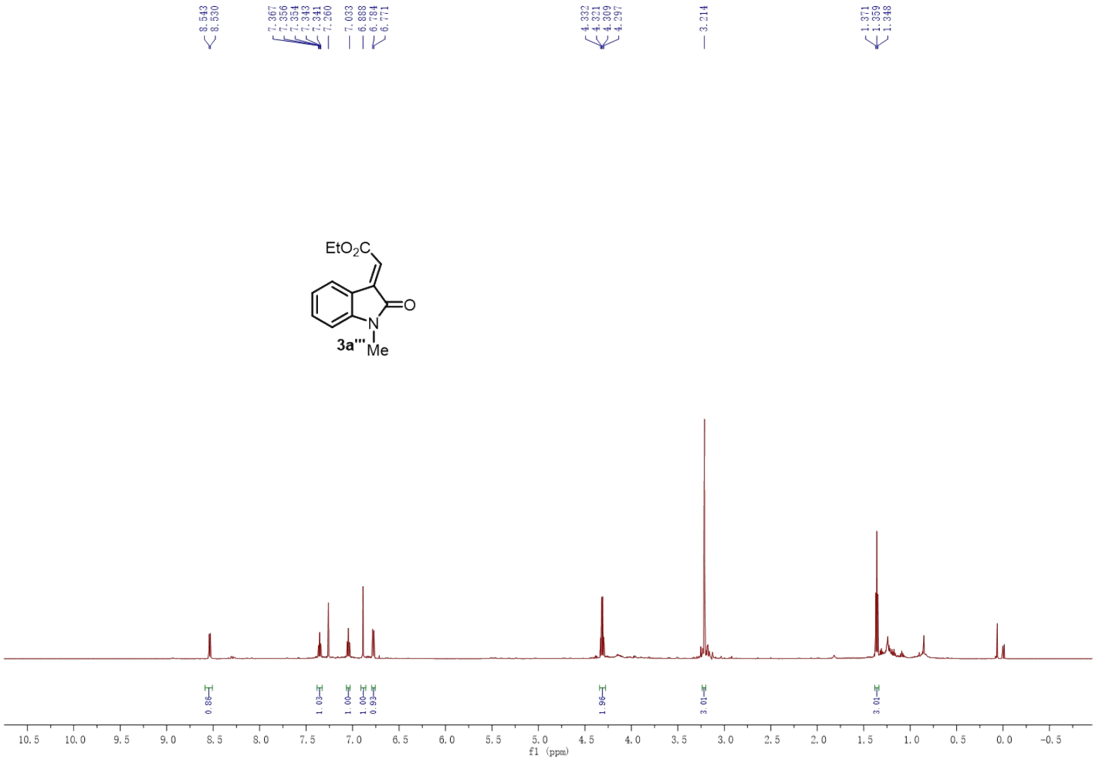
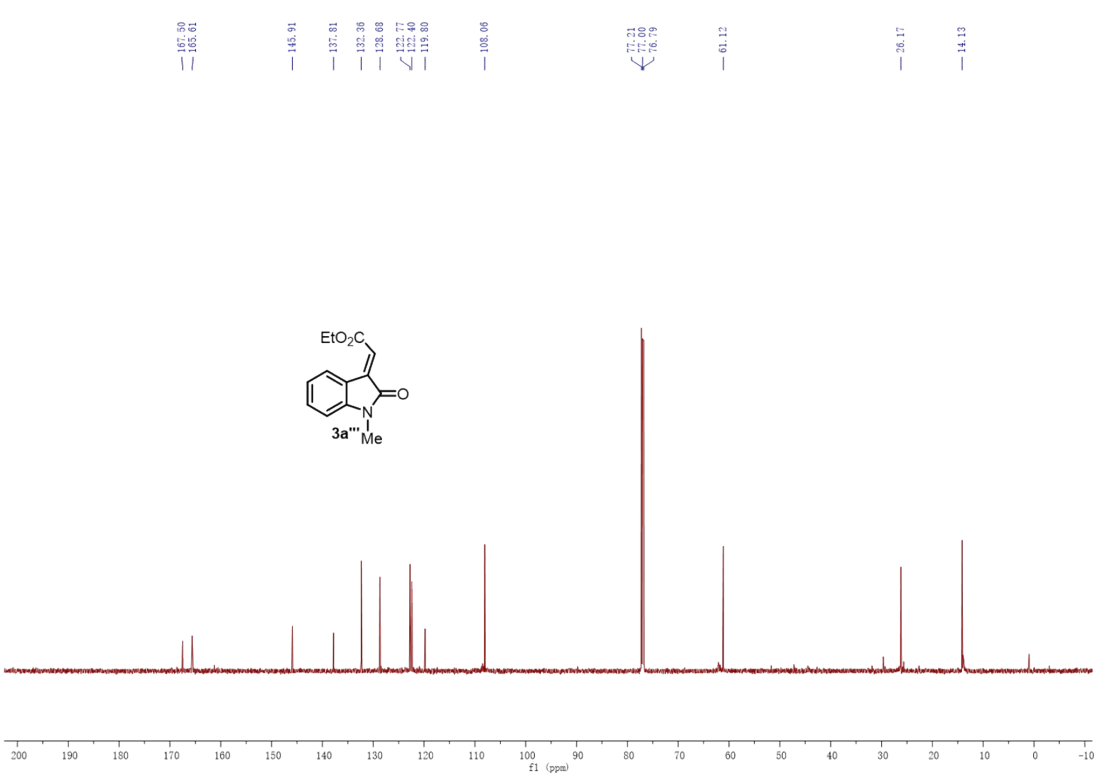
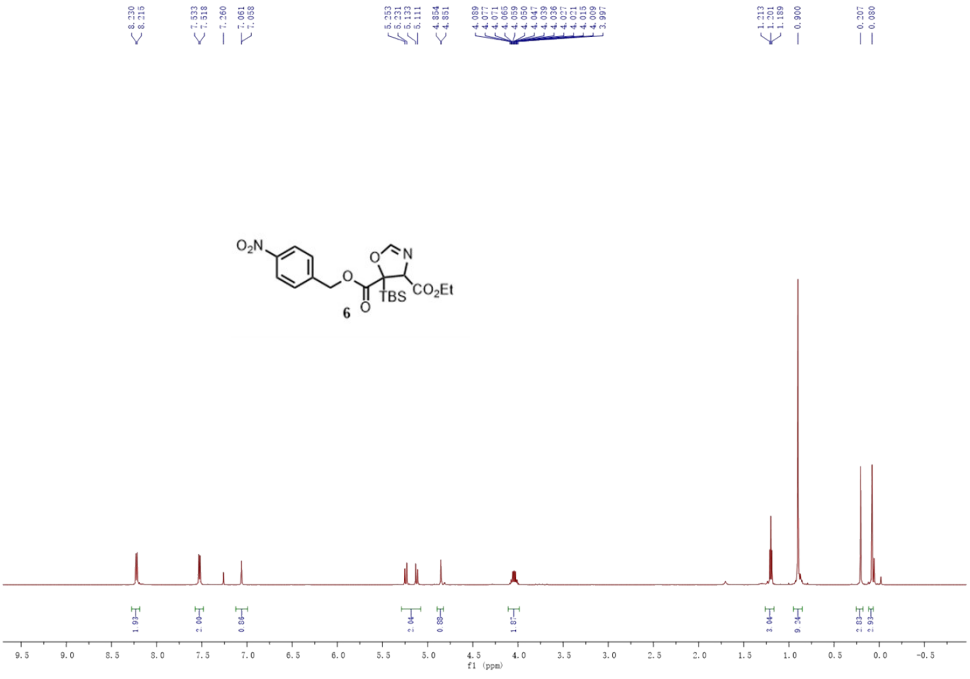
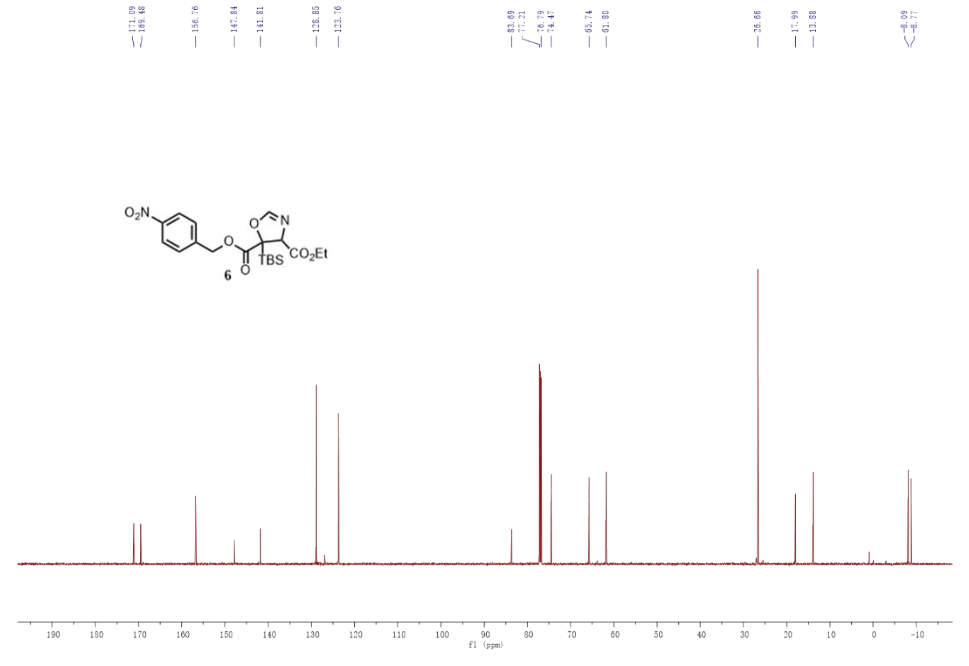

TBS
Cl
5r

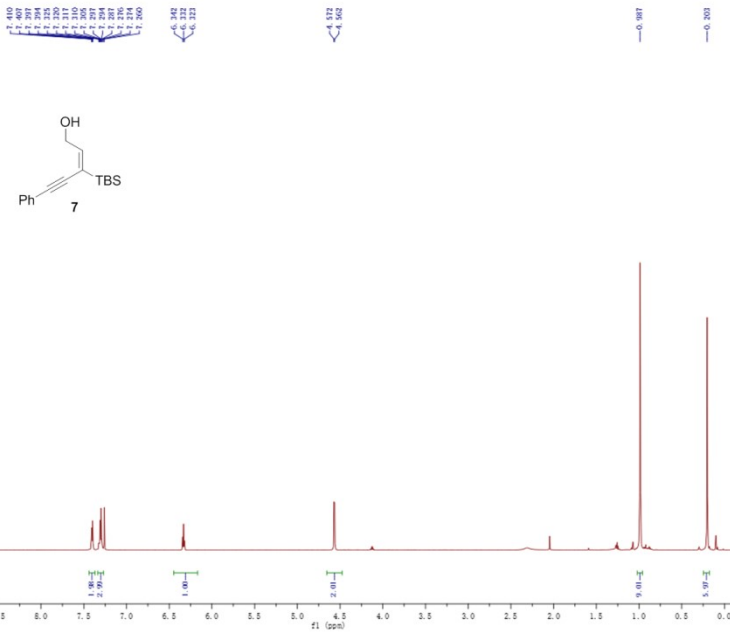

TBS
Cl
5r

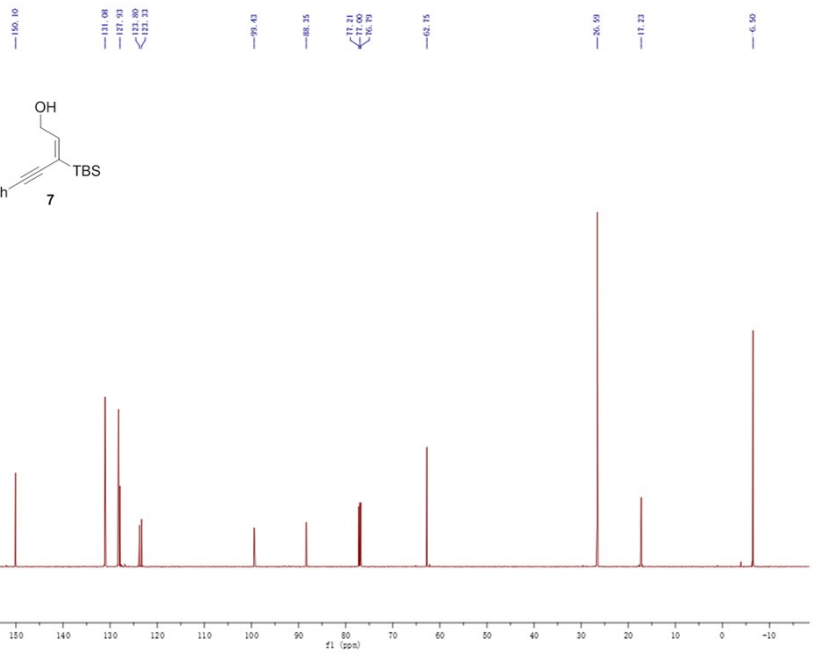

8.543
8.530
7.367
7.356
7.354
7.343
7.341
7.330
7.033
6.888
6.784
6.771
4.332
4.321
4.309
4.297
3.214
1.371
1.359
1.348
EtO2C
O
N
Me
3a'''
0.88
1.00
1.00
0.93
1.89
3.01
3.01
f1 (ppm)

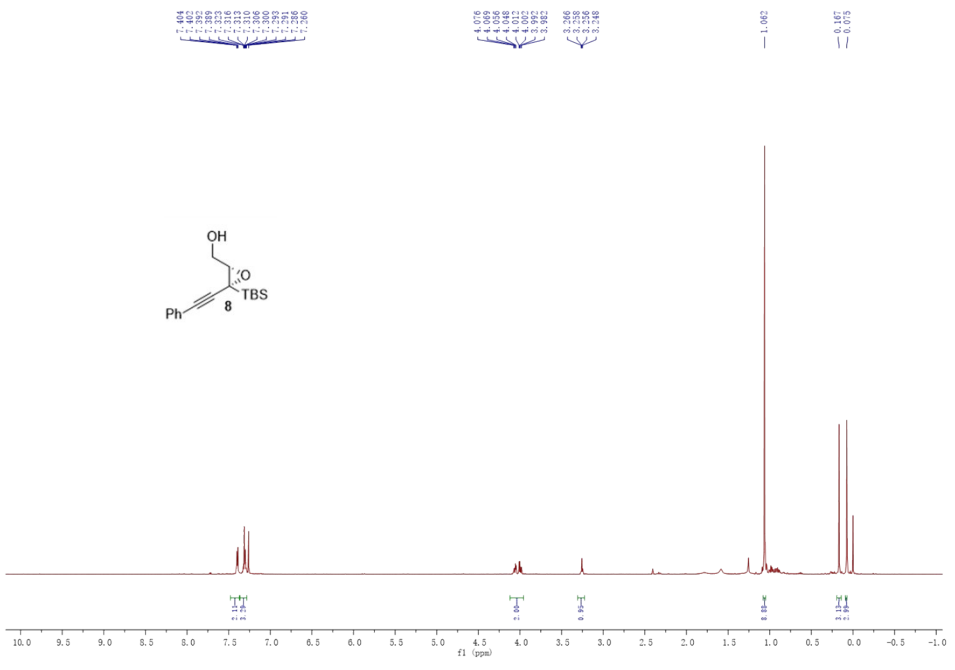

167.50
165.61
145.91
137.81
132.36
128.68
122.77
122.40
119.80
108.06
77.21
77.00
76.79
61.12
26.17
14.13
EtO2C
O
N
Me
3a'''
f1 (ppm)

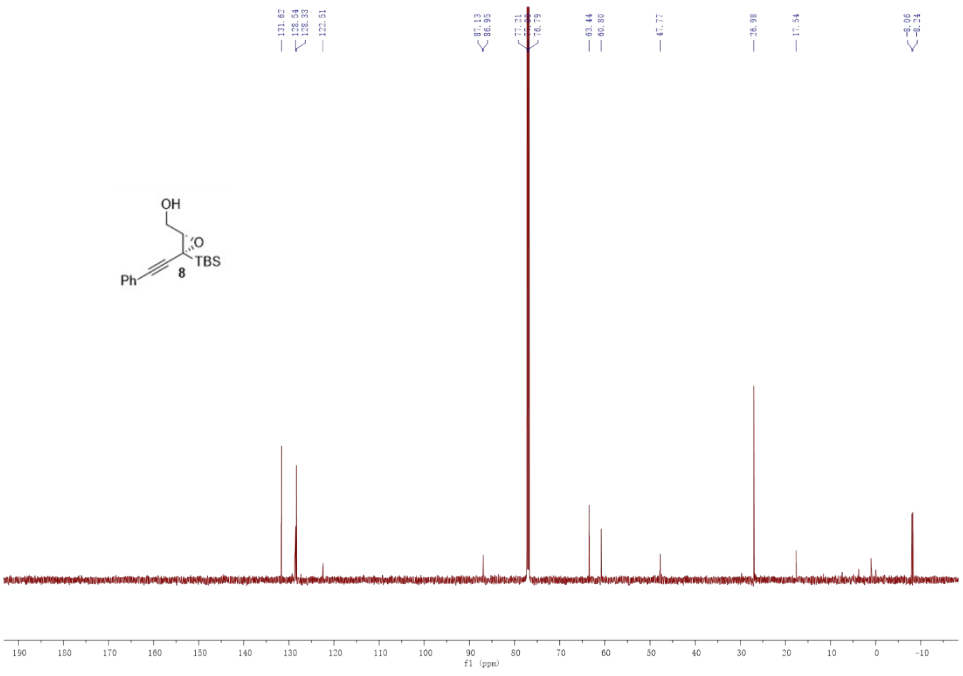

8.230
8.215
7.533
7.518
7.260
7.061
7.058
5.253
5.231
5.123
5.111
4.854
4.851
4.089
4.077
4.071
4.065
4.059
4.050
4.047
4.039
4.036
4.027
4.021
4.015
4.009
3.997
1.213
1.201
1.188
0.900
0.207
0.080
O2N
O
N
O
TBS
CO2Et
6
1.03
2.00
0.89
2.04
0.88
1.07
3.04
9.34
2.03
2.03
f1 (ppm)

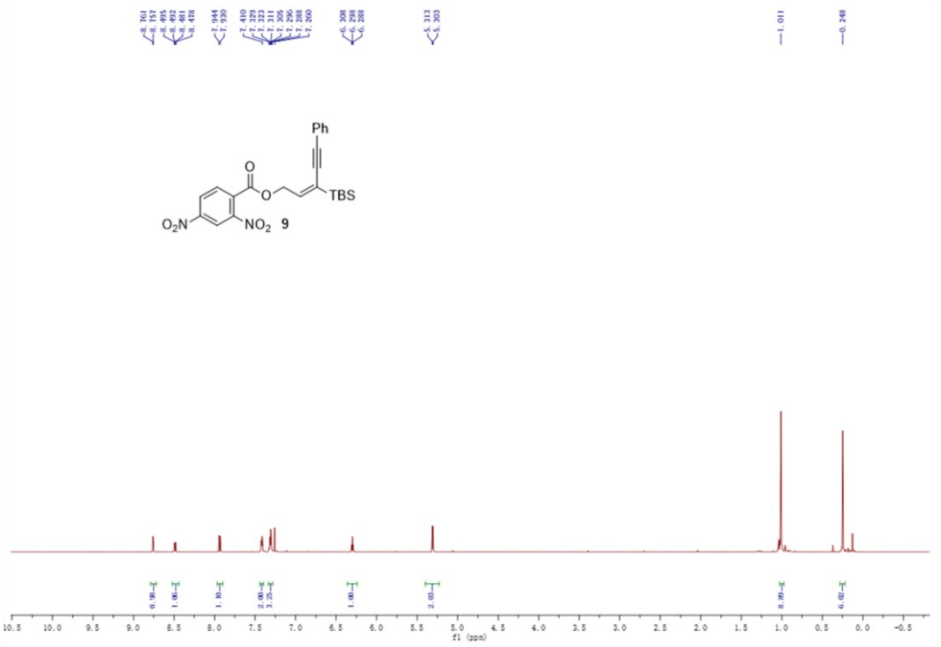

171.09
169.48
158.76
147.84
141.81
128.85
123.76
83.69
77.21
76.79
74.47
65.74
61.80
26.66
17.99
13.88
-0.09
-0.77
O2N
O
N
O
TBS
CO2Et
6
f1 (ppm)

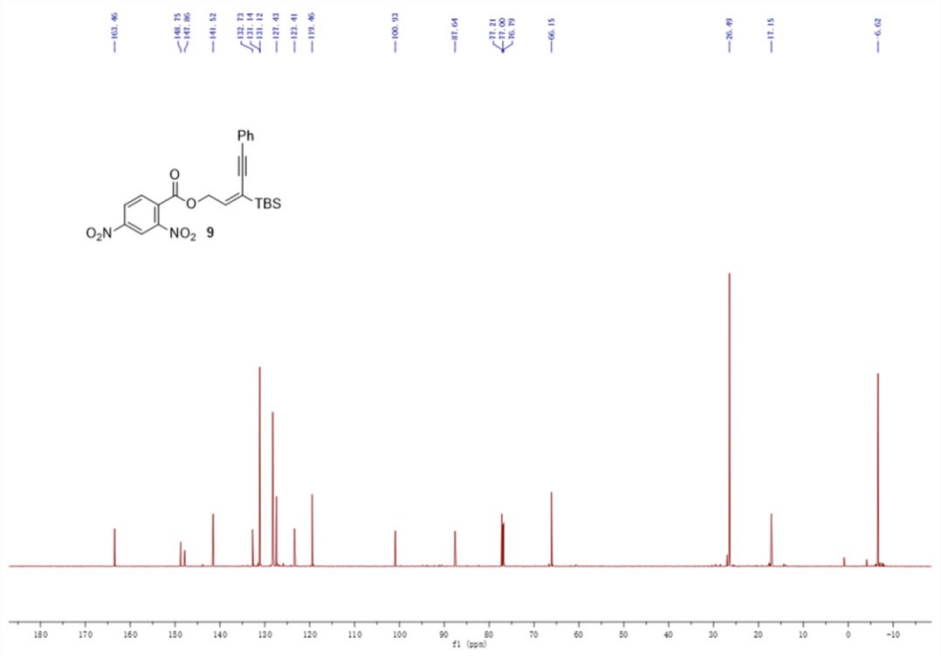

OH
TBS
Ph
7

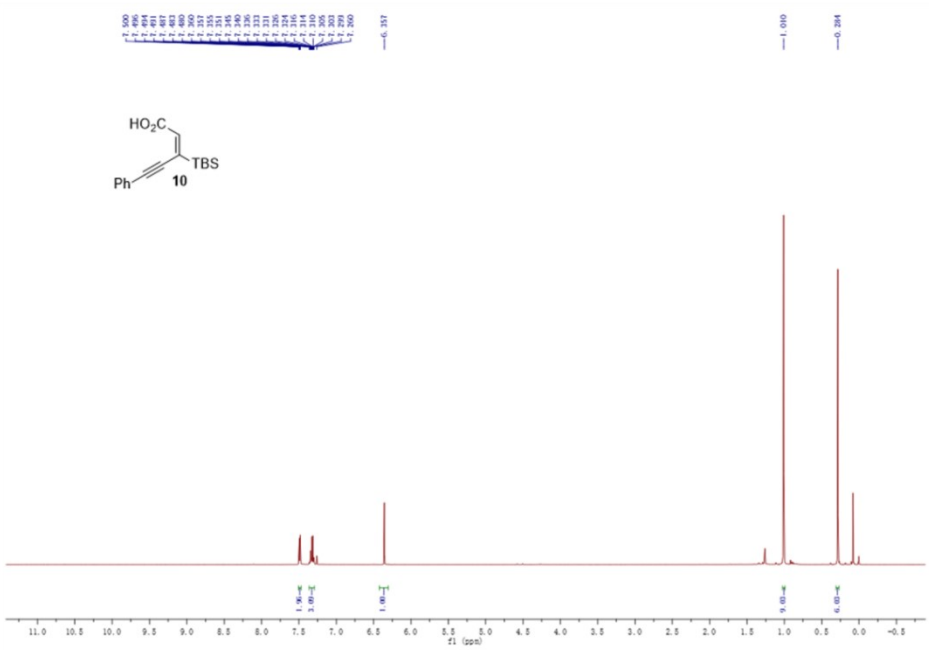

OH
TBS
Ph
7

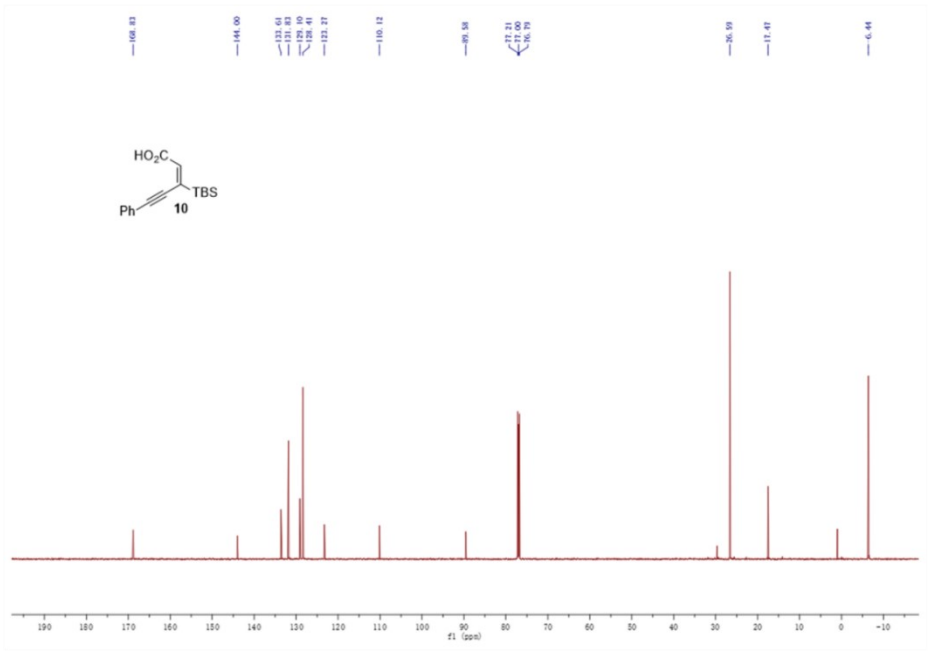

OH
O
TBS
Ph
8
f1 (ppm)


OH
O
TBS
Ph
8
f1 (ppm)


Ph
TBS
O_2N
NO_2
9


Ph
TBS
O_2N
NO_2
9


HO2C
TBS
Ph
10


HO2C
TBS
Ph
10