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Supporting Information

Co-Catalyzed Asymmetric Intramolecular [3+2] Cycloaddition of Yne-Alkylidenecyclopropanes and its Reaction Mechanism

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Content

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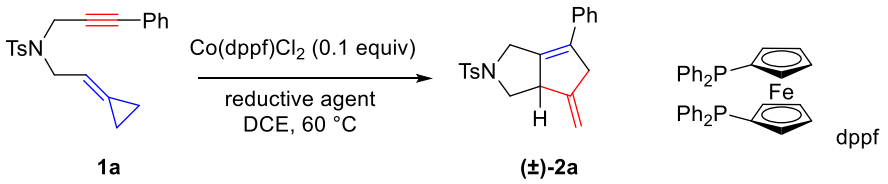
1. General Information

Air and moisture sensitive reactions were carried out in oven-dried glassware sealed with rubber septa under a positive pressure of dry argon, and sensitive liquids and solutions were transferred via syringe. Reactions were stirred using Teflon-coated magnetic stir bars. Elevated temperatures were maintained using Thermostat-controlled silicone oil baths. Organic solutions were concentrated using a Büchi rotary evaporator with a desktop vacuum pump. Tetrahydrofuran, diethyl ether, and toluene were distilled from sodium and benzophenone prior to use. Dichloromethane was distilled from CaH_2 prior to use. DCE was superdry (water ≤ 30 ppm), which could be purchased from J&K. Synthetic reagents were purchased from J&K and Acros Organics and used without further purification, unless otherwise indicated. Analytical TLC was performed with 0.25 mm silica gel G plates with a 254 nm fluorescent indicator. The TLC plates were visualized by ultraviolet light and treatment with phosphomolybdic acid stain followed by gentle heating. Purification of products was accomplished by flash chromatography on silica gel and the purified compounds showed a single spot by analytical TLC.

NMR spectra were measured on Bruker ARX 400 (^{1}H NMR at 400 MHz, ^{13}C NMR at 101 MHz) nuclear magnetic resonance spectrometers. Data for ^{1} H NMR spectra were reported as follows: chemical shift (ppm), referenced to residual solvent peak ($CDCl_3$ = δ 7.26 ppm, CD_2Cl_2 = δ 5.32 ppm; s = singlet, d = doublet, t = triplet, q = quartet, dd = doublet of doublets, dt = doublet of triplets, ddd = doublet of doublet of doublets, ddt = doublet of doublet of triplets, coupling constant (Hz), and integration. Data for ^{13}C{1H} NMR were reported in terms of chemical shift (ppm) relative to residual solvent peak ($CDCl_3$ = δ 77.16 ppm, CD_2Cl_2 = δ 53.84 ppm). High-resolution mass spectra (HRMS) were recorded on a Bruker Apex IV FTMS mass spectrometer [electrospray ionization (ESI) or electron ionization (EI)] with an FT-ICR analyzer. The enantiomer excesses (e.e.) of the products were determined by chiral HPLC analysis using UltiMate 3000 Pump. Optical rotations were measured on PerkinElmer model 341LC Polarimeter at 20 °C with visible light (λ = 589 nm) and 100 mm length cuvette.

2. Experimental procedures and characterization data

2.1 Table S1. Reaction optimization of racemic version.[a]

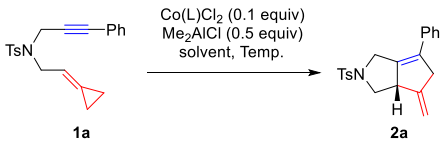


1a **(±)-2a**

Entry	reductant	solvent	time	yield (recovery)	Procedure
1	Zn (0.5 equiv), ZnI_2 (0.1 equiv)	DCE	24 h	15% (74%)	C
2	Et_2Zn (0.5 equiv)	DCE	1 h	32%	A
3	Me_3Al (1.0 equiv)	DCE	16 h	5%	A
4	Et_3Al (1.0 equiv)	DCE	16 h	6%	A
5	Et_2AlCl (1.0 equiv)	DCE	16 h	63%	A
6	Et_2AlCl (1.0 equiv)	THF	16 h	8%	A
7	Et_2AlCl (1.0 equiv)	1,4-dioxane	16 h	trace	A
8	Et_2AlCl (1.0 equiv)	Toluene	16 h	38%	A
9	Me_2AlCl (1.0 equiv)	DCE	10 h	94%	A
10	Me_2AlCl (0.5 equiv)	DCE	16 h	93%	A
11[b]	Me_2AlCl (0.5 equiv)	DCE	24 h	74%	A
12	Me_2AlCl (0.3 equiv)	DCE	30 h	82%	A

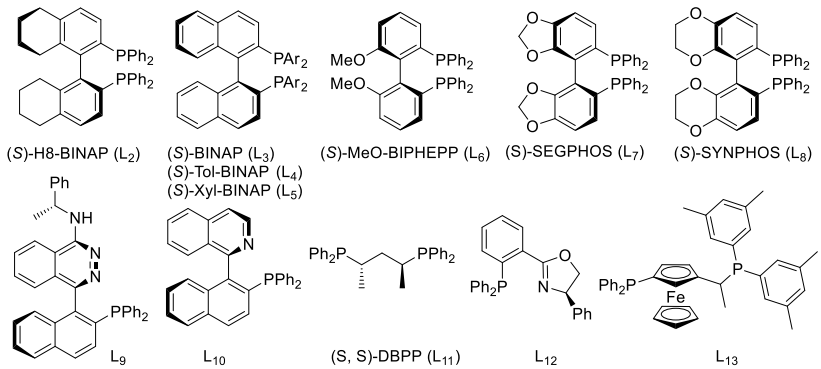
[a] Isolated yields in 30 mg scale of reactant and enantiomeric excess (e.e.) values were determined by high-performance liquid chromatography (HPLC). Either general procedure A or procedure C (described in the experimental description of [3+2] reaction) was used. [b] dppp was used instead of dppf.

2.2 Table S2. Reaction optimization of asymmetric version.[a]



1a **2a**

Entry	Ligand	Solvent	Temp.	Time	yield	ee
1	L_2	DCE	60 °C	18 h	90%	6%
2	L_3	DCE	60 °C	18 h	94%	87%
3	L_4	DCE	60 °C	18 h	86%	85%
4	L_5	DCE	60 °C	18 h	85%	89%
5	L_6	DCE	60 °C	18 h	12%	60%
6	L_7	DCE	60 °C	18 h	82%	33%
7	L_8	DCE	60 °C	18 h	73%	54%
8	L_9	DCE	60 °C	18 h	76%	-39%
9	L_{10}	DCE	60 °C	18 h	17%	22%
10	L_{11}	DCE	60 °C	18 h	85%	-16%
11	L_{12}	DCE	60 °C	18 h	82%	25%
12	L_{13}	DCE	60 °C	18 h	83%	21%
13	L_5	DCE	30 °C	18 h	98%	90%
14	L_5	DCE	0 °C	18 h	99%	90%
15	L_5	DCE	0 °C	18 h	99%	90%
16[b]	L_5	DCE	30 °C	18 h	95%	90%
17	L_5	benzene	30 °C	12 h	89%	86%
18	L_5	*p*-xyl-Ph	30 °C	18 h	40%	90%
19	L_5	$PhCF_3$	30 °C	18 h	18%	92%
19	L_5	$PhCF_3$: *n*-Heptane (1:1)	60 °C	8 h	90%	90%
20	L_5	DCE: *n*-Heptane (1:1)	30 °C	1.5 h	94%	91%



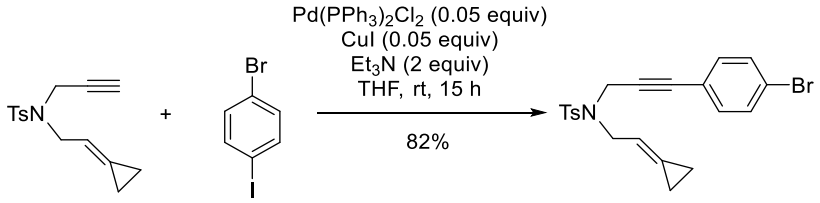
(*S*)-H8-BINAP (L_2) (*S*)-BINAP (L_3) (*S*)-Tol-BINAP (L_4) (*S*)-Xyl-BINAP (L_5) (*S*)-MeO-BIPHEPP (L_6) (S)-SEGPHOS (L_7) (*S*)-SYNPHOS (L_8)

L_9 L_{10} (S, S)-DBPP (L_{11}) L_{12} L_{13}

[a] Isolated yields in 0.08 mmol scale and enantiomeric excess (e.e.) values were determined by high-performance liquid chromatography (HPLC), *c* = 0.1 M; conditions: A solution of **1a** (1.0 equiv), $Co(L)Cl_2$ (0.1 equiv) was added Me_2AlCl (0.5 equiv). [b] *c* = 0.025 M.

2.3 Synthesis of Substrates

Substrates **1a**[1], **1b**[1], **1c**[1], **1i**[1], **1l**[1], **1m**[1], **1n**[2], **1o**[1], **1t**[1] **S1**[1], **S2**[1], **S3**[3], **S4**[3], **S5**[1], **S6**[4], **S7**[5], **S8**[6], **S9**[7], **S10**[8], **S12**[9] are known compounds and were synthesized according to the corresponding literature. The synthesis of the other new substrates are shown below.



S1 2.0 equiv **1d**

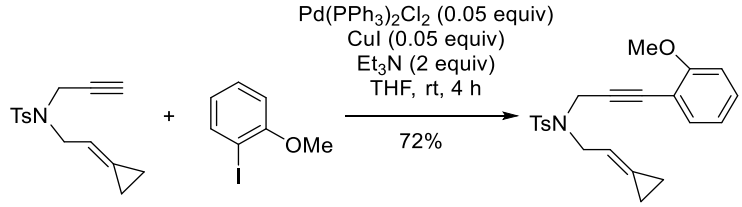
To a stirred mixture of **S1** (200.0 mg, 0.726 mmol), 1-bromo-4-iodobenzene (411.0 mg, 1.453 mmol), $Pd(PPh_3)_2Cl_2$ (25.4 mg, 0.036 mmol), CuI (6.9 mg, 0.036 mmol) in THF (1.5 mL) was added Et_3N (147.4 mg, 1.453 mmol), the reaction was stirred at rt for 15 h. Upon completion, the reaction mixture was concentrated and the crude product was purified by flash column chromatography on silica gel (eluted with PE/EA, 14:1) to afford **1d** (256.5 mg, 82%).

light yellow solid, m.p. = 85.7-86.8 °C, TLC R_f = 0.58 (PE/EA 8:1);

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.77 (d, J = 8.0 Hz, 2H), 7.40-7.35 (m, 2H), 7.26-7.23 (m, 2H), 6.93-6.89 (m, 2H), 5.79-5.72 (m, 1H), 4.26 (s, 2H), 4.02 (d, J = 7.2 Hz, 2H), 2.34 (s, 3H), 1.14-1.03 (s, 4H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 143.5, 136.2, 133.0, 131.5, 129.6, 129.0, 128.0, 122.7, 121.4, 112.1, 84.4, 83.5, 48.2, 36.7, 21.6, 2.8, 2.0.

HRMS (ESI) calcd for $C_{21}H_{21}BrNO_2S$ ([M + H]$^+$) 430.0471, found 430.0469.



S1 1.5 equiv **1e**

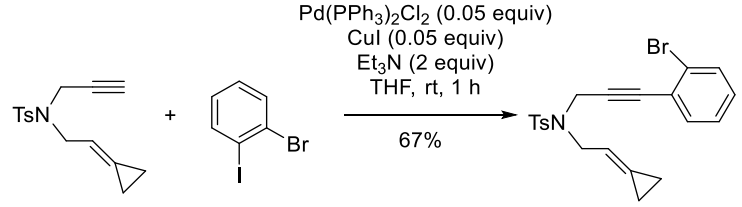
To a stirred mixture of **S1** (200.0 mg, 0.726 mmol), 2-Iodoanisole (255.0 mg, 1.089 mmol), $Pd(PPh_3)_2Cl_2$ (25.4 mg, 0.036 mmol), CuI (6.9 mg, 0.036 mmol) in THF (1.5 mL) was added Et_3N (147.4 mg, 1.453 mmol), the reaction was stirred at rt for 4 h. Upon completion, the reaction mixture was concentrated and the crude product was purified by flash column chromatography on silica gel (eluted with PE/EA, 8:1) to afford **1e** (200.3 mg, 72%).

light yellow solid, m.p. = 105.5-107.3 °C, TLC R_f = 0.34 (PE/EA 8:1).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.79 (d, J = 8.0 Hz, 2H), 7.27-7.20 (m, 3H), 6.91 (dd, J = 8.0, 2.0 Hz, 1H), 6.82 (m, 2H), 5.80-5.74 (m, 1H), 4.34 (s, 2H), 4.05 (d, J = 6.8 Hz, 2H), 3.80 (s, 3H), 2.30 (s, 3H), 1.09 (m, 4H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 160.1, 143.3, 136.3, 133.6, 129.9, 129.5, 129.0, 128.0, 120.3, 112.2, 111.7, 110.6, 86.2, 82.0, 55.7, 48.1, 37.1, 21.5, 2.8, 2.0.

HRMS (ESI) calcd for $C_{22}H_{24}NO_3S$ ([M + H]$^+$) 382.1471, found 382.1463.



S1 2.0 equiv **1f**

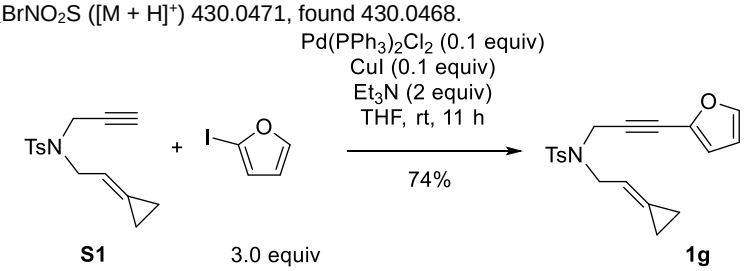
To a stirred mixture of **S1** (200.0 mg, 0.726 mmol), 2-Bromoiodobenzene (411.0 mg, 1.089 mmol), $Pd(PPh_3)_2Cl_2$ (25.4 mg, 0.036 mmol), CuI (6.9 mg, 0.036 mmol) in THF (1.5 mL) was added Et_3N (147.4 mg, 1.453 mmol), the reaction was stirred at rt for 1 h. Upon completion, the reaction mixture was concentrated and the crude product was purified by flash column chromatography on silica gel (eluted with PE/EA, 15:1) to afford **1f** (208.3 mg, 67%).

light yellow solid, m.p. = 97.8-98.8 °C, TLC R_f = 0.52 (PE/EA 8:1).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.77 (d, J = 8.0 Hz, 2H), 7.51 (dd, J = 8.0, 1.2 Hz, 1H), 7.21-7.17 (m, 3H), 7.16-7.11 (m, 1H), 7.08 (dd, J = 7.6, 1.6 Hz, 1H), 5.81-5.75 (m, 1H), 4.33 (s, 2H), 4.09 (d, J = 7.2 Hz, 2H), 2.24 (s, 3H), 1.10 (m, 4H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 143.6, 136.1, 133.5, 132.4, 129.6, 129.1, 127.9, 126.9, 125.2, 124.7, 112.1, 87.0, 83.9, 48.3, 36.7, 21.5, 2.8, 2.3.

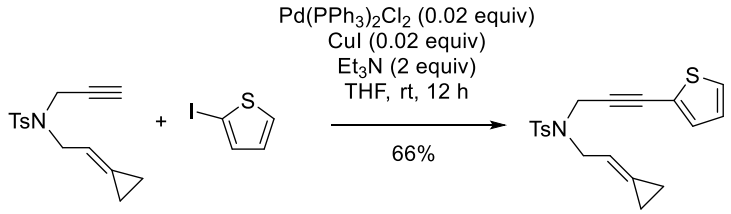
HRMS (ESI) calcd for $C_{21}H_{21}BrNO_2S$ ([M + H]$^+$) 430.0471, found 430.0468.



S1 3.0 equiv **1g**

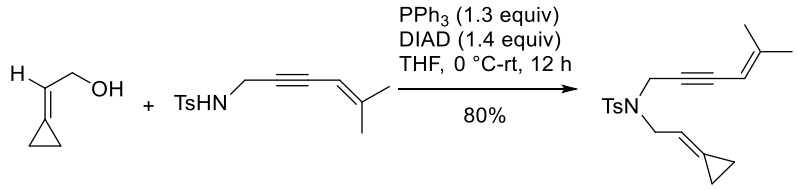
To a stirred mixture of **S1** (150.0 mg, 0.545 mmol), 2-Iodofuran (304.0 mg, 1.634 mmol), $Pd(PPh_3)_2Cl_2$ (38.2 mg, 0.055 mmol), CuI (10.4 mg, 0.055 mmol) in THF (1.8 mL) was added Et_3N (110.6 mg, 1.090 mmol), the reaction was stirred at rt for 11 h. Upon completion,

the reaction mixture was concentrated and the crude product was purified by flash column chromatography on silica gel (eluted with PE/EA, 12:1) to afford **1g** (138.0 mg, 74%).
light yellow solid, m.p. = 77.7-78.8 ºC, TLC R_f = 0.47 (PE/EA 8:1).
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.76 (d, J = 8.0 Hz, 2H), 7.31-7.27 (m, 3H), 6.33-6.29 (m, 2H), 5.77-5.70 (m, 1H), 4.29 (s, 2H), 4.00 (d, J = 7.2 Hz, 2H), 2.38 (s, 3H), 1.11 (m, 4H).
^{13}C NMR (101 MHz, $CDCl_3$) δ 143.6, 136.4, 135.9, 129.7, 129.3, 127.9, 115.3, 111.9, 110.8, 86.7, 75.8, 48.3, 36.7, 21.7, 2.8, 2.1.
HRMS (ESI) calcd for $C_{19}H_{20}NO_3S$ ([M + H]$^+$) 342.1158, found 342.1157.



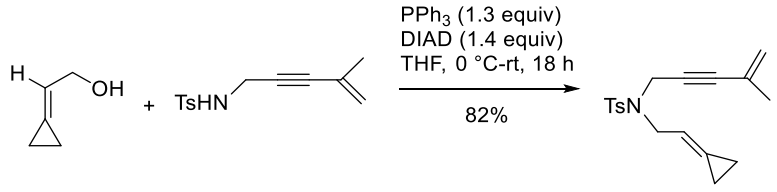
S1 1.3 equiv **1h**

To a stirred mixture of **S1** (275.4 mg, 1.0 mmol), 2-Iodothiophene (273.1 mg, 1.3 mmol), $Pd(PPh_3)_2Cl_2$ (14.0 mg, 0.020 mmol), CuI (3.8 mg, 0.020 mmol) in THF (1.8 mL) was added Et_3N (202.4 mg, 2.0 mmol), the reaction was stirred at rt for 12 h. Upon completion, the reaction mixture was concentrated and the crude product was purified by flash column chromatography on silica gel (eluted with PE/EA, 12:1) to afford **1h** (236.0 mg, 66%).
light yellow solid, m.p. = 76.9-77.4 ºC, TLC R_f = 0.52 (PE/EA 8:1).
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.77 (d, J = 8.0 Hz, 2H), 7.28 (d, J = 8.0 Hz, 2H), 7.19 (dd, J = 3.6, 2.4 Hz, 1H), 6.90 (m, 2H), 5.78-5.72 (m, 1H), 4.29 (s, 2H), 4.01 (d, J = 6.8 Hz, 2H), 2.36 (s, 3H), 1.10 (m, 4H).
^{13}C NMR (101 MHz, $CDCl_3$) δ 143.6, 135.9, 132.1, 129.7, 129.1, 127.8, 127.2, 126.9, 122.4, 112.0, 86.1, 78.7, 48.2, 36.9, 21.6, 2.8, 2.1.
HRMS (ESI) calcd for $C_{19}H_{20}NO_2S_2$ ([M + H]$^+$) 358.0930, found 358.0928.



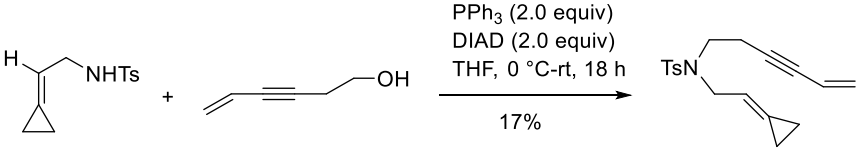
S2 **S3** (1.2 equiv) **1j**

To a stirred solution of **S2** (80.0 mg, 0.95 mmol), **S3** (300.0 mg, 1.14 mmol), and PPh_3 (324.0 mg, 1.24 mmol) in THF (3.2 mL) was added DIAD (269.0 mg, 1.33 mmol) at 0 °C. The reaction was gradually allowed to warm to rt, monitored by TLC, and stirred for 12 h. Upon completion, the reaction mixture was concentrated and the crude product was purified by flash column chromatography on silica gel (eluted with PE/EA, 12:1) to afford **1j** (250.0 mg, 80%)
light yellow solid, m.p. = 54.7-55.7 °C, TLC R_f = 0.43 (PE/EA, 8:1)
^{1}H NMR (400 MHz, CD_2Cl_2) δ 7.71 (d, J = 8.2 Hz, 2H), 7.30 (d, J = 8.2 Hz, 2H), 5.74-5.68 (m, 1H), 5.00 (m, 1H), 4.19 (d, J = 1.2 Hz, 2H), 3.96 (d, J = 6.8 Hz, 2H), 2.40 (s, 3H), 1.73 (s, 3H), 1.64 (s, 3H), 1.12-1.04 (m, 4H).
^{13}C NMR (101 MHz, CD_2Cl_2) δ 149.4, 143.9, 136.7, 129.8, 128.9, 128.0, 112.5, 104.6, 84.3, 83.6, 48.3, 37.2, 24.7, 21.6, 20.9, 2.8, 2.2.
HRMS (ESI) calcd for $C_{19}H_{24}NO_2S$ ([M + H]$^+$) 330.1522, found 330.1521.



S2 **S4** (1.0 equiv) **1k**

To a stirred solution of **S2** (100.0 mg, 1.19 mmol), **S4** (296.4 mg, 1.19 mmol), and PPh_3 (375.1 mg, 1.43 mmol) in THF (2.5 mL) was added DIAD (289.0 mg, 1.43 mmol) at 0 °C. The reaction was gradually allowed to warm to room temperature, monitored by TLC, and stirred for 18 h. Upon completion, the reaction mixture was concentrated and the crude product was purified by flash column chromatography on silica gel (eluted with PE/EA, 10:1) to afford **1k** (307.1 mg, 82%)
light yellow solid, m.p. = 66.7-68.0 °C, TLC R_f = 0.68 (PE/EA, 5:1)
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.75 (d, J = 8.2 Hz, 2H), 7.28 (d, J = 8.2 Hz, 2H), 5.76-5.69 (m, 1H), 5.11-5.08 (m, 1H), 4.96 (m, 1H), 4.18 (s, 2H), 3.97 (d, J = 6.8 Hz, 2H), 2.40 (s, 3H), 1.63 (dd, J = 1.0, 1.0 Hz, 3H), 1.13-1.04 (m, 4H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 143.4, 136.2, 129.6, 128.9, 127.9, 126.1, 122.0, 112.1, 86.7, 81.2, 48.0, 36.6, 23.2, 21.6, 2.8, 2.0.
HRMS (ESI) calcd for $C_{18}H_{22}NO_2S$ ([M + H]$^+$) 316.1366, found 316.1361.



S5 **S6** (2.0 equiv) **1p**

SUPPORTING INFORMATION

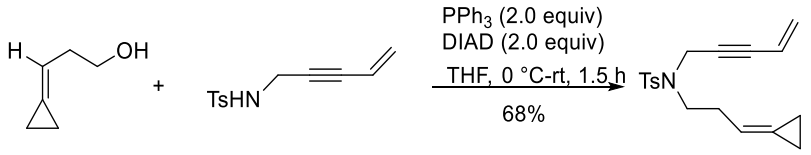
To a stirred solution of **S5** (200.0 mg, 0.84 mmol), **S6** (162.0 mg, 1.69 mmol), and PPh_3 (442.0 mg, 1.69 mmol) in THF (2.1 mL) was added DIAD (340.8 mg, 1.69 mmol) at 0 °C. The reaction was gradually allowed to warm to room temperature, monitored by TLC, and stirred for 18 h. Upon completion, the reaction mixture was concentrated and the crude product was purified by flash column chromatography on silica gel (eluted with PE/EA, 10:1) to afford **1p** (45.0 mg, 17%).

light yellow oil, TLC R_f = 0.68 (PE/EA, 5:1)

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.72 (d, J = 8.2 Hz, 2H), 7.30 (d, J = 8.2 Hz, 2H), 5.72 (ddt, J = 17.2, 11.2, 2.4 Hz, 1H), 5.66-5.60 (m, 1H), 5.54 (dd, J = 17.2, 2.4 Hz, 1H), 5.40 (dd, J = 11.2, 2.4 Hz, 1H), 3.98 (d, J = 6.8 Hz, 2H), 3.31-3.25 (m, 2H), 2.59-2.53 (m, 2H), 2.43 (s, 3H), 1.57 (s, 2H), 1.11-1.02 (m, 4H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 143.4, 137.4, 129.9, 128.0, 127.4, 126.5, 117.4, 113.0, 87.6, 81.0, 49.9, 46.1, 21.7, 20.3, 2.8, 2.0.

HRMS (ESI) calcd for $C_{18}H_{22}NO_2S$ ([M + H]$^+$) 316.1366, found 316.1360.



S7 **S8** (2.0 equiv) **1q**

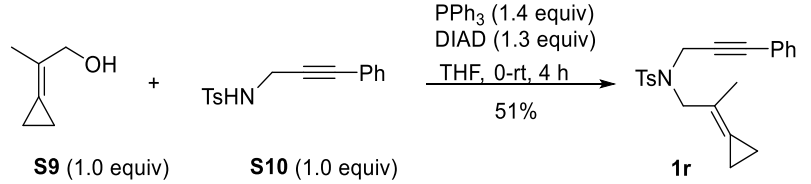
To a stirred solution of **S7** (37.5 mg, 0.38 mmol), **S8** (180.0 mg, 0.76 mmol), and PPh_3 (200.4 mg, 0.76 mmol) in THF (2.5 mL) was added DIAD (154.5 mg, 0.76 mmol) at 0 °C. The reaction was gradually allowed to warm to room temperature, monitored by TLC, and stirred for 1.5 h. Upon completion, the reaction mixture was concentrated and the crude product was purified by flash column chromatography on silica gel (eluted with PE/EA, 10:1) to afford **1q** (82.5 mg, 68%).

light yellow oil, TLC R_f = 0.54 (PE/EA, 8:1)

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.73 (d, J = 8.2 Hz, 2H), 7.28 (d, J = 8.2 Hz, 2H), 5.77-5.71 (m, 1H), 5.52 (ddt, J = 17.2, 11.2, 2.2 Hz, 1H), 5.37 (dd, J = 11.2, 2.2 Hz), 5.32 (dd, J =17.2, 2.2 Hz), 4.25 (d, J = 1.6 Hz, 2H), 3.34-3.27 (m, 2H), 2.49-2.42 (m, 2H), 2.40 (s, 3H), 1.07-0.98 (m, 4H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 143.4, 136.0, 129.5, 127.9, 127.4, 124.3, 116.4, 114.2, 84.2, 82.7, 46.1, 37.1, 30.4, 21.6, 2.6, 2.0.

HRMS (ESI) calcd for $C_{18}H_{22}NO_2S$ ([M + H]$^+$) 316.1366, found 316.1363.



S9 (1.0 equiv) **S10** (1.0 equiv) **1r**

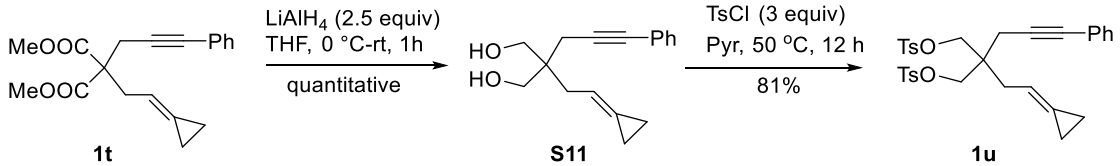
To a stirred solution of **S9** (60.0 mg, 0.60 mmol), **S10** (172.5 mg, 0.60 mmol), and PPh_3 (220.0 mg, 0.84 mmol) in THF (2.0 mL) was added DIAD (157.7 mg, 0.78 mmol) at 0 °C. The reaction was gradually allowed to warm to room temperature, monitored by TLC, and stirred for 4 h. Upon completion, the reaction mixture was concentrated and the crude product was purified by flash column chromatography on silica gel (eluted with PE/EA, 15:1) to afford **1r** (130.0 mg, 51%).

White solid, m.p. = 90.0-91.5 °C, TLC R_f = 0.65 (PE/EA, 8:1)

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.80 (d, J = 8.0 Hz, 2H), 7.32-7.20 (m, 5H), 7.07-7.00 (m, 2H), 4.20 (s, 2H), 3.99 (s, 2H), 2.32 (s, 3H), 1.90 (s, 3H), 1.07 (s, 4H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 143.4, 136.2, 131.5, 129.6, 128.4, 128.2, 127.9, 85.4, 82.1, 52.0, 36.3, 21.5, 18.3, 2.9, 2.4.

HRMS (ESI) calcd for C22H23NNaO2S ([M + Na]$^+$) 388.1342, found 388.1343.



1t **S11** **1u**

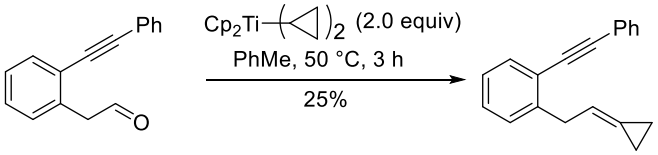
To a stirred mixture of $LiAlH_4$ (380 mg, 10.0 mmol) in THF (3 mL) at 0 °C was added the solution of **1t** (1.25 g, 4.0 mmol) in THF (5 mL) slowly, after completed, the reaction was stired at rt for 1 h. Then the reaction was quenched with H_2O (365 μL), 15% NaOH aqueous solution (365 μL), H_2O (1.1 mL) successively. After stirred for another 1 h, the mixture was filtered, concentrated and the crude product was purified by flash column chromatography on silica gel (eluted with PE/EA, 3:1) to afford **S11** (quantitative). Then, to a solution of **S11** (800 mg, 3.1 mmol) in pyrdine (46.8 mmol) was added TsCl (1.78 g, 9.4 mmol) at 0 °C, then the reaction was stirred at 50 °C for 12 h. After completed, the reaction was quenched with H_2O, diluted with EtOAc, the combined organic layer was washed with H_2O and brine. The organic layer was separated, dried over Na_2SO_4, filtered and concentrated in vacuo. The residue was purified by silica gel column chromatography to afford **1u** (1.41g, 81%).

White solid, m.p. = 107.4–108.5 °C, TLC R_f = 0.48 (PE/EA, 4:1).

^{1}H NMR (400 MHz, CD_2Cl_2) δ 7.74 (m, 4H), 7.35-7.25 (m, 7H), 7.20-7.15 (m, 2H), 5.59 (t, J = 7.2 Hz, 1H), 3.89 (s, 4H), 2.40-2.27 (m, 10H), 1.10-1.08 (m, 4H).

^{13}C NMR (101 MHz, CD_2Cl_2) δ 145.7, 132.5, 131.8, 130.3, 128.6, 128.40, 128.37, 128.3, 123.4, 110.8, 84.1, 83.9, 70.6, 42.4, 33.5, 22.6, 21.7, 3.2, 2.3.

HRMS (ESI) calcd for $C_{31}H_{32}NaO_6S_2$ ([M + Na]$^+$) 587.1532, found 587.1532.



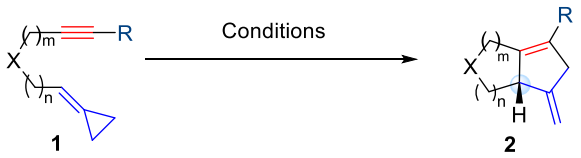
S12 **1v**

To a stirred solution of **S12** (500 mg, 2.27 mmol) in PhMe (11 mL) at 50 °C was added Ti regent (1.18 g, 4.54 mmol) in PhMe (11 mL) slowly, the reaction was stired at 50 °C for 3 h. Then, the reaction mixture was concentrated and the crude product was purified by flash column chromatography on silica gel (eluted with PE/EA, 100:1) to afford **1v** (140.0 mg, 25%).
light yellow oil, TLC R_f = 0.60 (PE/EA, 50:1).
^{1}H NMR (400 MHz, CD_2Cl_2) δ 7.58-7.47 (m, 3H), 7.40-7.32 (m, 3H), 7.30-7.25 (m, 2H), 7.23-7.15 (m, 1H), 6.05-5.96 (m, 1H), 3.78 (d, J = 6.8 Hz, 2H), 1.12-1.00 (m, 4H).
^{13}C NMR (101 MHz, CD_2Cl_2) δ 143.7, 132.4, 131.8, 129.3, 128.9, 128.8, 128.7, 126.3, 123.8, 123.6, 122.9, 116.5, 93.4, 88.6, 37.3, 2.8, 2.2.
HRMS (EI) calcd for $C_{19}H_{16}$ ([M]$^+$) 244.1252, found 244.1247.

2.4 Experimental Detail for Asymmetric Co-Catalyzed [3+2] Cycloaddition.

General procedure for preparation of $CoLCl_2$:

All cobalt(II) complexes were prepared following literature[10] with the following modifications: Anhydrous THF (0.1 M) was added to a mixture of $CoCl_2$ (1.05 equiv) and ligand (1.0 equiv) under argon. The mixture was stirred at room temperature for 24 h (the complex may be precipitated). Then, concentrated carefully, followed by adding cyclohexane, ultrasound. The resulting suspension was left to stand, then remove the supernatant, the remaining solid was dried under high vacuum to afford the desired complex without further purification.



1 **2**

m = 1 or 2
n = 1 or 2

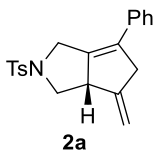
m = 1 or 2
n = 1 or 2

General procedure for the asymmetric [3+2] cycloaddition reaction:

General procedure A: A 10-mL Schlenk flask was charged with starting material (**1**) (1.0 equiv), Co[(*S*)-xyl-BINAP]Cl_2 (0.1 equiv) and a magnetic stirred bar. The flask was connected to a Schlenk line with argon and subjected to vacuum, and then was refilled three times by argon. DCE (0.2 M) and Heptane (0.2 M) were added. The glassware was then immersed into an oil bath at 30 °C, after 5 min, Dimethylaluminium chloride solution (0.9 M) in Heptane (0.5 equiv) was added dropwise. The reaction was monitored by TLC. Upon completion, the reaction was purified directly by flash column chromatography on silica gel to afford **2**.

General procedure B: A 10-mL Schlenk flask was charged with starting material (**1**) (1.0 equiv), Co[(*S*)-xyl-BINAP]Cl_2 (0.1 equiv) and a magnetic stirred bar. The flask was connected to a Schlenk line with argon and subjected to vacuum, and then was refilled three times by argon. DCE (0.2 M) and Heptane (0.2 M) were added. The glassware was then immersed into an oil bath at 60 °C, after 5 min, Dimethylaluminium chloride solution (0.9 M) in Heptane (1.0 equiv) was added dropwise. The reaction was monitored by TLC. Upon completion, the reaction was purified directly by flash column chromatography on silica gel to afford **2**.

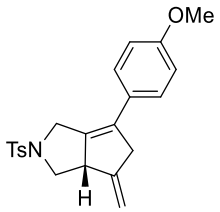
General procedure C: A 10-mL Reaction tube was charged with starting material (**1**) (1.0 equiv), Co[(*S*)-xyl-BINAP]Cl_2 (0.1 equiv), Zn (0.5 equiv), ZnI_2 (0.1 equiv) and a magnetic stirred bar in a glove box. then, DCE (0.1 M) was added. The glassware was then immersed into an oil bath at 80 °C. The reaction was monitored by TLC. Upon completion, the reaction was purified directly by flash column chromatography on silica gel to afford **2**.



2a

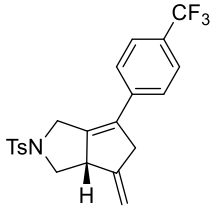
Following the **general procedure A**, 1.5 h, eluted with PE/EA 14:1
Run 1: 30.0 mg of **1a** was used, and 28.2 mg of **2a** was obtained in 94% yield and 91% ee as determined by HPLC analysis (chiral OD-H, hexane/*i*-PrOH = 95/5, 1.0 mL/min, 220 nm, 25 °C), t_r, 16.33 min (major), 20.83 min (minor); $[\alpha]^{20}_D$ = -114.8° (c = 0.127, $CHCl_3$).
Run 2: **1a** (140.0 mg) was converted into **2a** (137.2 mg, 98%).
The average yield of two runs was 96%.
2a: colorless oil, TLC, R_f = 0.47 (PE/EA, 8:1).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.71 (d, J = 8.4 Hz, 2H), 7.36 (m, 2H), 7.30-7.25 (m, 3H), 7.18 (m, 2H), 5.02 (dd, J = 3.6, 2.0 Hz, 1H), 4.87 (dd, J = 4.0, 2.0 Hz, 1H), 4.31-4.23 (m, 1H), 3.99-3.87 (m, 3H), 3.66 (m, 2H), 2.74-2.66 (m, 1H), 2.39 (s, 3H).
^{13}C NMR (101 MHz, $CDCl_3$) δ 147.5, 143.6, 138.1, 134.6, 134.2, 132.7, 129.9, 128.7, 127.8, 127.5, 127.0, 108.8, 54.9, 50.4, 47.6, 44.4, 21.6.
HRMS (ESI) calcd for $C_{21}H_{22}NO_2S$ ([M + H]$^+$) 352.1366, found 352.1359.



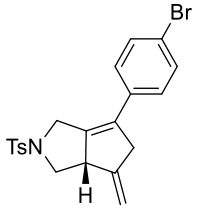
2b

Following the **general procedure A**, 3 h, eluted with PE/EA 8.5:1
Run 1: 30.5 mg of **1b** was used, and 27.5 mg of **2b** was obtained in 90% yield and 91% ee as determined by HPLC analysis (chiral OD-H, hexane/*i*-PrOH = 95/5, 1.0 mL/min, 220 nm, 25 ºC), t_r, 20.98 min (minor), 23.58 min (major), $[\alpha]^{20}_D$ = -116.2° (c = 0.143, $CHCl_3$).
Run 2: 30.5 mg of **1b** was used, and 28.4 mg of **2b** was obtained in 93% yield
The average yield of two runs was 92%
2b: colorless oil, TLC, R_f = 0.18 (PE/EA, 8:1).
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.71 (d, J = 8.2 Hz, 2H), 7.28 (d, J = 8.2 Hz, 2H), 7.12 (d, J = 8.8 Hz, 2H), 6.88 (d, J = 8.8 Hz, 2H), 5.00 (dd, J = 4.0, 2.0 Hz, 1H), 4.85 (dd, J = 4.0, 2.0 Hz, 1H), 4.24 (dm, J = 14.2, 1H), 3.94-3.86 (m, 3H), 3.82 (s, 3H), 3.65-3.59 (m, 2H), 2.67 (dd, J = 13.2, 12.0 Hz, 1H), 2.39 (s, 3H).
^{13}C NMR (101 MHz, $CDCl_3$) δ 159.2, 147.7, 143.6, 135.6, 134.2, 132.2, 129.9, 128.2, 127.5, 127.4, 114.1, 108.6, 55.4, 54.7, 50.5, 47.6, 44.5, 21.6.
HRMS (ESI) calcd for $C_{22}H_{24}NO_3S$ ([M + H]$^+$) 382.1471, found 382.1469.



2c

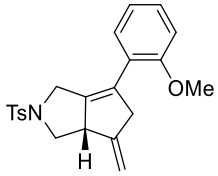
Following the **general procedure A**, 6 h, eluted with PE/EA 8.5:1
Run 1: 33.6 mg of **1c** was used, and 26.2 mg of **2c** was obtained in 78% yield and 92% ee as determined by HPLC analysis (chiral OD-H, hexane/*i*-PrOH = 95/5, 1.0 mL/min, 220 nm, 25 ºC), t_r, 14.20 min (minor), 15.67 min (major); $[\alpha]^{20}_D$ = -128.0° (c = 0.148, $CHCl_3$).
Run 2: 100.0 mg of **1c** was used, and 75.0 mg of **2c** was obtained in 75% yield.
The average yield of two runs was 77%.
2c: white solid, m.p. = 195.4-196.8 °C,TLC, R_f = 0.46 (PE/EA, 8:1).
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.72 (d, J = 8.4 Hz, 2H), 7.60 (d, J = 8.4 Hz, 2H), 7.29 (d, J = 8.4 Hz, 2H), 7.27 (d, J = 8.4 Hz, 2H), 5.04 (d, J = 4.0, 2.0 Hz, 1H), 4.89 (dd, J = 4.4, 2.0 Hz, 1H), 4.32-4.26 (dm, J = 14.4 Hz, 1H), 3.99-3.90 (m, 3H), 3.68 (m, 2H), 2.71 (dd, J = 8.4, 7.2 Hz, 1H), 2.40 (s, 3H).
^{13}C NMR (101 MHz, $CDCl_3$) δ 146.7, 143.7, 141.1, 137.9, 133.9, 131.5, 129.9, 129.6, 129.3, 127.4, 127.0, 125.62, 125.59, 125.55, 125.51, 125.4, 122.7, 109.2, 55.0, 50.1, 47.4, 44.3, 21.5.
HRMS (ESI) calcd for $C_{22}H_{21}F_3NO_2S$ ([M + H]$^+$) 420.1240, found 420.1241.



2d

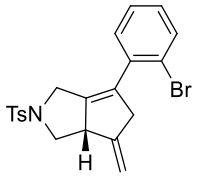
Following the **general procedure A**, 3 h, eluted with PE/EA 12:1
Run 1: 34.4 mg of **1d** was used, and 32.7 mg of **2d** was obtained in 95% yield and 89% ee as determined by HPLC analysis (chiral AD-H, hexane/*i*-PrOH = 95/5, 1.0 mL/min, 220 nm, 25 ºC), t_r, 30.60 min (major), 32.77 min (minor); $[\alpha]^{20}_D$ = -92.3° (c = 0.147, $CHCl_3$).
Run 2: 34.4 mg of **1d** was used, and 31.7 mg of **2d** was obtained in 92% yield.
The average yield of two runs was 94%.
2d: white solid, m.p. = 150.2-151.8 °C, TLC, R_f = 0.45 (PE/EA, 8:1).
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.71 (d, J = 8.4 Hz, 2H), 7.47 (d, J = 8.8 Hz, 2H), 7.29 (d, J = 8.0 Hz, 2H), 7.03 (d, J = 8.4 Hz, 2H), 5.01 (dd, J = 4.0, 2.0 Hz, 1H), 4.87 (dd, J = 4.0, 2.0 Hz, 1H), 4.28-4.19 (dm, J = 14.4 Hz, 1H), 3.94-3.86 (m, 3H), 3.62 (m, 2H), 2.69 (dd, J = 12.8, 12.0 Hz, 1H), 2.39 (s, 3H).
^{13}C NMR (101 MHz, $CDCl_3$) δ 147.1, 143.7, 139.1, 134.1, 133.5, 131.9, 131.8, 130.0, 128.5, 127.5, 121.8, 109.1, 55.0, 50.3, 47.5, 44.4, 21.6.

HRMS (ESI) calcd for $C_{21}H_{21}BrNO_2S$ ([M + H]$^+$) 430.0471, found 430.0471.



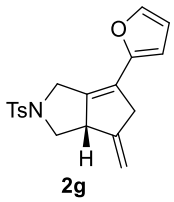
2e

Following the **general procedure A**, 3 h, eluted with PE/EA 7.5:1
Run 1: 30.5 mg of **1e** was used, and 27.5 mg of **2e** was obtained in 90% yield and 91% ee as determined by HPLC analysis (chiral AD-H, hexane/*i*-PrOH = 95/5, 1.0 mL/min, 220 nm, 25 °C), t_r, 22.12 min (major), 26.06 min (minor); $[\alpha]^{20}_D$ = -96.9° (c = 0.128, $CHCl_3$).
Run 2: 30.5 mg of **1e** was used, and 26.6 mg of **2e** was obtained in 87% yield
The average yield of two runs was 89%.
2e: colorless oil, TLC, R_f = 0.52 (PE/EA, 8:1).
^{1}H NMR (400 MHz, CD_2Cl_2) δ 7.66 (d, *J* = 8.0 Hz, 2H), 7.30 (d, *J* = 8.0 Hz, 2H), 7.28-7.22 (m, 1H), 7.10 (dd, *J* = 8.2, 1.8 Hz, 1H), 6.93-6.88 (m, 2H), 4.98 (dd, *J* = 3.6, 2.0 Hz, 1H), 4.85 (dd, *J* = 4.0, 2.0 Hz, 1H), 4.01-3.95 (dm, *J* = 14.4 Hz, 1H), 3.90-3.83 (m, 2H), 3.79 (s, 3H), 3.76-3.70 (m, 1H), 3.69 – 3.56 (m, 2H), 2.75 (dd, *J* = 13.2, 12.4 Hz, 1H), 2.40 (s, 3H).
^{13}C NMR (101 MHz, CD_2Cl_2) δ 157.1, 149.0, 144.0, 140.1, 134.7, 130.11, 130.09, 129.44, 129.40, 127.7, 124.4, 120.7, 111.5, 108.1, 55.6, 54.3, 51.6, 48.3, 46.6, 21.6.
HRMS (ESI) calcd for $C_{22}H_{24}NO_3S$ ([M + H]$^+$) 382.1471, found 382.1465.



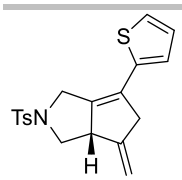
2f

Following the **general procedure B**, 0.5 h, eluted with PE/EA 9:1
Run 1: 34.4 mg of **1f** was used, and 27.2 mg of **2f** was obtained in 79% yield and 88% ee as determined by HPLC analysis (chiral AD-H, hexane/*i*-PrOH = 95/5, 1.0 mL/min, 220 nm, 25 °C), t_r, 15.07 min (major), 16.47 min (minor), $[\alpha]^{20}_D$ = -129.7° (c = 0.113, $CHCl_3$).
Run 2: 34.4 mg of **1f** was used, and 27.8 mg of **2f** was obtained in 81% yield.
The average yield of two runs was 80%.
2f: colorless oil, TLC, R_f = 0.52 (PE/EA, 8:1).
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.68 (d, *J* = 8.2 Hz, 2H), 7.54 (dd, *J* = 8.0, 1.0 Hz, 1H), 7.30 (d, *J* = 8.2 Hz, 2H), 7.24 (td, *J* = 7.2, 1.0 Hz, 1H), 7.13 (td, *J* = 8.0, 1.6 Hz, 1H), 7.05 (dd, *J* = 7.6, 1.6 Hz, 1H), 4.99 (dd, *J* = 3.6, 2.2 Hz, 1H), 4.87 (d, *J* = 4.4, 2.2 Hz, 1H), 3.92-3.82 (m, 3H), 3.75-3.66 (dm, *J* = 17.2 Hz, 1H), 3.62 (d, *J* = 14.0 Hz, 1H), 3.48 (d, *J* = 19.6 Hz, 1H), 2.85 (dd, *J* = 8.8, 8.0 Hz, 1H), 2.43 (s, 3H).
^{13}C NMR (101 MHz, $CDCl_3$) δ 148.3, 143.6, 140.8, 136.9, 134.3, 133.8, 133.2, 129.9, 129.8, 129.4, 127.6, 127.3, 122.3, 109.0, 53.5, 51.4, 47.4, 46.8, 21.7.
HRMS (ESI) calcd for $C_{21}H_{21}BrNO_2S$ ([M + H]$^+$) 430.0471, found 430.0470.



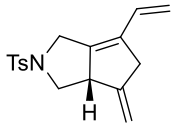
2g

Following the **general procedure B**, 0.5 h, eluted with PE/EA 9:1
Run 1: 27.3 mg of **1g** was used, and 20.5 mg of **2g** was obtained in 75% yield and 81% ee as determined by HPLC analysis (chiral OD-H, hexane/*i*-PrOH = 85/15, 1.0 mL/min, 220 nm, 25 °C), t_r, 8.02 min (major), 9.67 min (minor); $[\alpha]^{20}_D$ = -37.9° (c = 0.103, $CHCl_3$).
Run 2: 27.3 mg of **1g** was used, and 20.8 mg of **2g** was obtained in 76% yield.
The average yield of two runs was 76%.
2g: colorless oil, TLC, R_f = 0.35 (PE/EA, 8:1).
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.73 (d, *J* = 8.2 Hz, 2H), 7.41 (d, *J* = 1.2 Hz, 1H), 7.30 (d, *J* = 8.2 Hz, 2H), 6.38 (dd, *J* = 3.4, 2.0 Hz, 1H), 6.15 (d, *J* = 3.4 Hz, 1H), 4.97 (dd, *J* = 3.6, 2.4 Hz, 1H), 4.82 (dd, *J* = 4.4, 2.4 Hz, 1H), 4.19-4.08 (m, 2H), 3.89 (dd, *J* = 8.2, 8.2 Hz, 1H), 3.86-3.79 (m, 1H), 3.67-3.59 (m, 1H), 3.38 (d, *J* = 19.2 Hz, 1H), 2.70 (dd, *J* = 9.2, 8.4 Hz, 1H), 2.40 (s, 3H).
^{13}C NMR (101 MHz, $CDCl_3$) δ 150.7, 147.6, 143.6, 143.0, 136.7, 134.2, 129.9, 127.6, 122.6, 111.3, 108.8, 108.0, 53.9, 50.8, 47.4, 43.4, 21.7.
HRMS (ESI) calcd for $C_{19}H_{20}NO_3S$ ([M + H]$^+$) 342.1158, found 342.1156.



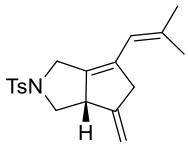
2h

Following the **general procedure B**, 0.5 h, eluted with PE/EA 10:1
Run 1: 28.6 mg of **1h** was used, and 25.7 mg of **2h** was obtained in 90% yield and 92% ee as determined by HPLC analysis (chiral OJ-H, hexane/*i*-PrOH = 85/15, 1.0 mL/min, 220 nm, 25 °C), t_r, 25.71 min (major), 33.23 min (minor); $[\alpha]^{20}_D$ = -67.5994° (c = 0.184, $CHCl_3$).
Run 2: 28.6 mg of **1h** was used, and 26.6 mg of **2h** was obtained in 93% yield.
The average yield of two runs was 92%.
2h: colorless oil, TLC, R_f = 0.44 (PE/EA, 8:1).
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.73 (d, *J* = 8.4 Hz, 2H), 7.33-7.27 (m, 3H), 7.02 (dd, *J* = 4.8, 3.4 Hz, 1H), 6.85 (d, *J* = 3.4 Hz, 1H), 4.99 (d, *J* = 3.6, 2.4 Hz, 1H), 4.84 (d, *J* = 3.6, 2.4 Hz, 1H), 4.17-4.10 (dm, *J* = 14.8 Hz, 1H), 4.00 (d, *J* = 14.4 Hz, 1H), 3.92-3.86 (m, 2H), 3.78-3.69 (m, 1H), 3.52 (dm, *J* = 18.8 Hz, 1H), 2.68 (m, 1H), 2.40 (s, 3H).
^{13}C NMR (101 MHz, $CDCl_3$) δ 147.3, 143.7, 138.4, 136.7, 134.0, 129.9, 127.7, 127.6, 126.8, 126.0, 124.9, 108.8, 54.3, 50.6, 47.1, 45.6, 21.6.
HRMS (ESI) calcd for $C_{19}H_{20}NO_2S_2$ ($[M + H]^+$) 358.0930, found 358.0926.



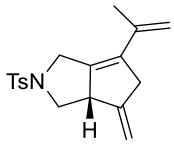
2i

Following the **general procedure B**, 0.5 h, eluted with PE/EA 9:1
Run 1: 24.1 mg of **1i** was used, and 22.9 mg of **2i** was obtained in 95% yield and 83% ee as determined by HPLC analysis (chiral AS-H, hexane/*i*-PrOH = 92/8, 1.0 mL/min, 220 nm, 25 °C), t_r, 25.03 min (major), 29.15 min (minor); $[\alpha]^{20}_D$ = -170.5° (c = 0.120, $CHCl_3$).
Run 2: 24.1 mg of **1i** was used, and 23.4 mg of **2h** was obtained in 97% yield.
The average yield of two runs was 96%.
2i: colorless oil, TLC, R_f = 0.44 (PE/EA, 8:1).
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.72 (d, *J* = 8.2 Hz, 2H), 7.32 (d, *J* = 8.2 Hz, 2H), 6.31 (dd, *J* = 17.2, 10.8 Hz, 1H), 5.16 (d, *J* = 10.8 Hz, 1H), 5.07 (d, *J* = 17.2 Hz, 1H), 4.95 (dd, *J* = 4.0, 2.4 Hz, 1H), 4.80 (dd, *J* = 4.4, 2.4 Hz, 1H), 3.97-3.82 (m, 3H), 3.75-3.69 (m, 1H), 3.44 (m, 1H), 3.20 (d, *J* = 19.2 Hz, 1H), 2.70 (dd, *J* = 9.6, 8.8 Hz, 1H), 2.42 (s, 3H).
^{13}C NMR (101 MHz, $CDCl_3$) δ 148.1, 143.7, 140.5, 134.2, 132.4, 130.1, 129.9, 127.5, 116.6, 108.7, 53.6, 50.9, 45.8, 42.4, 21.7. HRMS (ESI) calcd for $C_{17}H_{20}NO_2S$ ($[M + H]^+$) 302.1209, found 302.1206.



2j

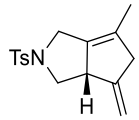
Following the **general procedure B**, 0.5 h, eluted with PE/EA 14:1
Run 1: 26.4 mg of **1j** was used, and 24.8 mg of **2j** was obtained in 94% yield and 81% ee as determined by HPLC analysis (chiral OJ-H, hexane/*i*-PrOH = 95/5, 1.0 mL/min, 220 nm, 25 °C), t_r, 15.32 min (minor), 18.59 min (major); $[\alpha]^{20}_D$ = -62.8° (c = 0.112, $CHCl_3$).
Run 2: 26.4 mg of **1j** was used, and 23.8 mg of **2j** was obtained in 90% yield.
The average yield of two runs was 92%.
2j: colorless oil, TLC, R_f = 0.34 (PE/EA, 8:1).
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.71 (d, *J* = 8.0 Hz, 2H), 7.31 (d, *J* = 8.0 Hz, 2H), 5.55 (s, 1H), 4.90 (dd, *J* = 3.6, 2.2 Hz, 1H), 4.76 (dd, *J* = 4.0, 2.2 Hz, 1H), 3.84-3.76 (m, 2H), 3.72-3.64 (m, 2H), 3.55 (dm, *J* = 19.2 Hz, 1H), 3.17 (d, *J* = 19.2 Hz, 1H), 2.67 (dd, *J* = 9.0, 9.0 Hz, 1H), 2.42 (s, 3H), 1.78 (s, 3H), 1.69 (s, 3H).
^{13}C NMR (101 MHz, $CDCl_3$) δ 149.5, 143.5, 137.7, 137.3, 134.5, 132.5, 129.9, 127.6, 119.6, 108.2, 52.7, 51.3, 47.0, 46.6, 27.0, 21.7, 20.0.
HRMS (ESI) calcd for $C_{19}H_{24}NO_2S$ ($[M + H]^+$) 330.1522, found 330.1522.



2k

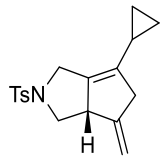
Following the **general procedure B**, 1 h, eluted with PE/EA 10:1
Run 1: 25.3 mg of **1k** was used, and 21.5 mg of **2k** was obtained in 85% yield and 91% ee as determined by HPLC analysis (chiral AS-H, hexane/*i*-PrOH = 92/8, 1.0 mL/min, 220 nm, 25 °C), t_r, 19.45 min (minor), 25.13 min (major); $[\alpha]^{20}_D$ = -202.4° (c = 0.110, $CHCl_3$).
Run 2: 25.3 mg of **1k** was used, and 22.3 mg of **2k** was obtained in 88% yield.

The average yield of two runs was 87%.
2k: colorless oil, TLC, R_f = 0.42 (PE/EA, 8:1).
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.72 (d, J = 8.0 Hz, 2H), 7.32 (d, J = 8.0 Hz, 2H), 4.94 (s, 1H), 4.90 (dd, J = 3.6, 2.4 Hz, 1H), 4.80 (s, 1H), 4.75 (dd, J = 4.0, 2.4 Hz, 1H), 4.10 (dm, J = 14.8 Hz, 1H), 3.98 (dm, J = 14.8 Hz, 1H), 3.84 (dd, J = 8.2, 8.2 Hz, 1H), 3.80-3.72 (m, 1H), 3.50-3.42 (dm, J = 19.2 Hz, 1H), 3.25 (dm, J = 19.2 Hz, 1H), 2.67 (dd, J = 10.0, 8.4 Hz, 1H), 2.43 (s, 3H), 1.86 (s, 3H).
^{13}C NMR (101 MHz, $CDCl_3$) δ 147.8, 143.7, 138.9, 138.7, 134.0, 133.7, 129.9, 127.6, 115.3, 107.9, 55.0, 50.3, 47.5, 44.7, 21.8, 21.7.
HRMS (ESI) calcd for $C_{18}H_{22}NO_2S$ ([M + H]$^+$) 316.1366, found 316.1357.



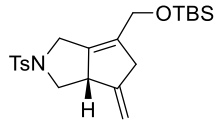
2l

Following the **general procedure B**, 1 h, eluted with PE/EA 10:1
Run 1: 23.2 mg of **1l** was used, and 18.7 mg of **2l** was obtained in 81% yield and 85% ee as determined by HPLC analysis (chiral OJ-H, hexane/*i*-PrOH = 95/5, 1.0 mL/min, 220 nm, 25 °C), t_r, 17.94 min (minor), 21.29 min (major). $[\alpha]^{20}_D$ = -109.0° (c = 0.081, $CHCl_3$).
Run 2: 23.2 mg of **1l** was used, and 19.5 mg of **2l** was obtained in 84% yield.
The average yield of two runs was 83%.
2l: colorless oil, TLC, R_f = 0.43 (PE/EA, 8:1).
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.71 (d, J = 8.2 Hz, 2H), 7.31 (d, J = 8.2 Hz, 2H), 4.87 (d, J = 3.6, 2.4 Hz, 1H), 4.75 (dd, J = 4.4, 2.4 Hz, 1H), 3.79-3.75 (m, 3H), 3.62-3.53 (m, 1H), 3.36 (dm, J = 19.6 Hz, 1H), 2.89 (d, J = 19.6 Hz, 1H), 2.68 (dd, J = 9.4, 9.4 Hz, 1H), 2.42 (s, 3H), 1.59 (s, 3H).
^{13}C NMR (101 MHz, $CDCl_3$) δ 149.4, 143.5, 135.6, 134.6, 130.9, 129.8, 127.5, 108.1, 53.1, 51.3, 47.9, 45.6, 21.7, 14.6.
HRMS (ESI) calcd for $C_{16}H_{20}NO_2S$ ([M + H]$^+$) 290.1209, found 290.1209.



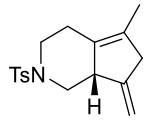
2m

Following the **general procedure B**, 1 h, eluted with PE/EA 10:1
Run 1: 25.2 mg of **1m** was used, and 22.7 mg of **2m** was obtained in 90% yield and 87% ee as determined by HPLC analysis (chiral OJ-H, hexane/*i*-PrOH = 95/5, 1.0 mL/min, 220 nm, 25 °C), t_r, 21.32 min (minor), 30.81 min (major); $[\alpha]^{20}_D$ = -106.2° (c = 0.073, $CHCl_3$).
Run 2: 25.2 mg of **1m** was used, and 22.4 mg of **2m** was obtained in 89% yield.
The average yield of two runs was 90%.
2m: colorless oil, TLC, R_f = 0.52 (PE/EA, 8:1).
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.72 (d, J = 8.0 Hz, 2H), 7.32 (d, J = 8.0 Hz, 2H), 4.85 (dd, J = 3.2, 2.4 Hz, 1H), 4.74 (d, J = 4.2, 2.4 Hz, 1H), 3.91-3.81 (m, 2H), 3.76 (dd, J = 8.4, 8.4 Hz, 1H), 3.62-3.54 (m, 1H), 3.16-3.07 (dm, J = 19.2 Hz, 1H,), 2.73 (d, J = 19.2 Hz, 1H), 2.69 (t, J = 9.6 Hz, 1H), 2.43 (s, 3H), 1.38-1.30 (m, 1H), 0.70-0.57 (m, 2H), 0.48-0.41 (m, 2H).
^{13}C NMR (101 MHz, $CDCl_3$) δ 148.6, 143.5, 135.6, 134.7, 134.6, 129.8, 127.5, 108.2, 53.3, 51.1, 45.8, 42.7, 21.7, 10.8, 4.9, 4.8. HRMS (ESI) calcd for $C_{18}H_{22}NO_2S$ ([M + H]$^+$) 316.1366, found 316.1357.



2n

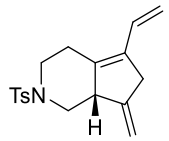
Following the **general procedure B**, 1 h, eluted with PE/EA 14:1
Run 1: 33.6 mg of **1n** was used, and 24.9 mg of **2n** was obtained in 74% yield and 71% ee as determined by HPLC analysis (chiral AS-H, hexane/*i*-PrOH = 95/5, 1.0 mL/min, 220 nm, 25 °C), t_r, 9.54 min (minor), 12.41 min (major); $[\alpha]^{20}_D$ = -71.8° (c = 0.10, $CHCl_3$).
Run 2: 33.6 mg of **1n** was used, and 23.5 mg of **2n** was obtained in 70% yield.
The average yield of two runs was 72%.
2n: colorless oil, TLC, R_f = 0.45 (PE/EA, 8:1).
^{1}H NMR (400 MHz, CD_2Cl_2) δ 7.68 (d, J = 8.0 Hz, 2H), 7.33 (d, J = 8.0 Hz, 2H), 4.89 (dd, J = 3.6, 2.4 Hz, 1H), 4.79 (d, J = 4.0, 2.4 Hz, 1H), 4.15-4.07 (m, 2H), 3.91-3.83 (m, 2H), 3.80 (dd, J = 8.4, 8.4 Hz, 1H), 3.70-3.65 (m, 1H), 3.36-3.26 (dm, J = 19.6 Hz, 1H), 2.97 (d, J = 19.6 Hz, 1H), 2.59 (dd, J = 9.6, 8.4 Hz, 1H), 2.42 (s, 3H), 0.88 (s, 9H), 0.018 (s, 3H), -0.002 (s, 3H).
^{13}C NMR (101 MHz, CD_2Cl_2) δ 149.2, 144.0, 136.4, 134.3, 133.7, 130.1, 127.8, 108.2, 61.4, 53.7, 51.1, 46.4, 43.8, 26.0, 21.6, 18.5, -5.4, -5.5.
HRMS (ESI) calcd for $C_{22}H_{34}NO_3SSi$ ([M + H]$^+$) 420.2023, found 420.2016.



2o

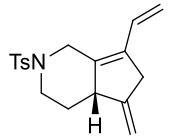
Following the **general procedure B**, 2 h, eluted with PE/EA 10:1

Run 1: 24.3 mg of **1o** was used, and 20.4 mg of **2o** was obtained in 84% yield and 74% ee as determined by HPLC analysis (chiral OD-H, hexane/*i*-PrOH = 95/5, 1.0 mL/min, 220 nm, 25 °C), t_r, 10.28 min (major), 11.46 min (minor), $[\alpha]^{20}_D$ = -43.0° (c = 0.046, $CHCl_3$).
Run 2: 24.3 mg of **1o** was used, and 19.7 mg of **2o** was obtained in 81% yield.
The average yield of two runs was 83%.
2o: colorless oil, TLC, R_f = 0.56 (PE/EA, 8:1).
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.64 (d, *J* = 8.2 Hz, 2H), 7.29 (d, *J* = 8.2 Hz, 2H), 4.98 (dd, *J* = 4.0, 2.2 Hz, 1H), 4.92 (dd, *J* = 4.4, 2.2 Hz, 1H), 4.04 (ddd, *J* = 10.8, 6.0, 1.6 Hz, 1H), 3.93-3.87 (m, 1H), 3.31-3.23 (m, 1H), 3.07 (dm, *J* = 20.6 Hz, 1H), 2.86 (dm, *J* = 20.6 Hz, 1H), 2.45 (dm, *J* = 13.6 Hz, 1H), 2.40 (s, 3H), 2.24-2.13 (m, 1H), 2.03 (ddd, *J* = 12.4, 10.8, 3.2 Hz, 1H), 1.91 (dd, *J* = 11.2, 10.8 Hz, 1H), 1.58 (m, 3H).
^{13}C NMR (101 MHz, $CDCl_3$) δ 148.9, 143.5, 133.9, 131.7, 129.8, 127.7, 107.6, 52.3, 48.7, 46.8, 44.1, 25.6, 21.6, 13.3.
HRMS (ESI) calcd for $C_{17}H_{22}NO_2S$ ([M + H]$^+$) 304.1366, found 304.1360.



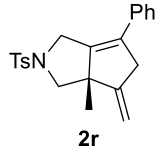
2p

Following the **general procedure B**, 5 h, eluted with PE/EA 10:1
Run 1: 20.0 mg of **1p** was used, and 13.4 mg of **2o** was obtained in 67% yield and 55% ee as determined by HPLC analysis (chiral OJ-H, hexane/*i*-PrOH = 95/5, 1.0 mL/min, 220 nm, 25 °C), t_r, 15.04 min (major), 17.18 min (minor)
Run 2: 25.2 mg of **1o** was used, and 17.2 mg of **2o** was obtained in 68% yield.
The average yield of two runs was 68%.
2p: colorless oil, TLC, R_f = 0.58 (PE/EA, 8:1).
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.64 (d, *J* = 8.0 Hz, 2H), 7.30 (d, *J* = 8.0 Hz, 2H), 6.52 (dd, *J* = 17.2, 10.6 Hz, 1H), 5.10 (d, *J* = 10.6 Hz, 1H), 5.07 (dd, *J* = 4.0, 2.0 Hz, 1H), 5.05 (d, *J* = 17.2 Hz, 1H), 4.97 (dd, *J* = 4.4, 2.0 Hz, 1H), 4.10 (ddd, *J* = 11.2, 6.4, 2.0 Hz, 1H), 3.97-3.90 (m, 1H), 3.46-3.37 (m, 1H), 3.27-3.21 (dm, *J* = 20.0 Hz, 1H), 3.16-3.08 (dm, *J* = 20.0 Hz, 1H), 2.67 (dm, *J* = 13.6, 1H), 2.41 (s, 3H), 2.34-2.26 (m, 1H), 2.14-2.06 (m, 1H), 1.99 (dd, *J* = 10.8, 10.8 Hz, 1H).
^{13}C NMR (101 MHz, $CDCl_3$) δ 147.7, 143.7, 137.8, 133.8, 132.4, 129.8, 129.5, 127.6, 115.3, 108.3, 52.0, 49.5, 46.6, 38.6, 25.9, 21.6.
HRMS (ESI) calcd for $C_{18}H_{22}NO_2S$ ([M + H]$^+$) 316.1366, found 316.1358.



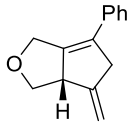
2q

Following the **general procedure B**, 0.5 h, eluted with PE/EA 10:1
Run 1: 25.2. mg of **1q** was used, and 24.2 mg of **2q** was obtained in 96% yield and 59% ee as determined by HPLC analysis (chiral AD-H, hexane/*i*-PrOH = 92/8, 1.0 mL/min, 220 nm, 25 °C), t_r, 12.03 min (minor), 18.27 min (major); $[\alpha]^{20}_D$ = -117.4° (c = 0.092, $CHCl_3$).
Run 2: 25.2 mg of **1q** was used, and 23.7 mg of **2q** was obtained in 94% yield.
The average yield of two runs was 95%.
2q: colorless oil, TLC, R_f = 0.58 (PE/EA, 8:1).
^{1}H NMR (400 MHz, CD_2Cl_2) δ 7.65 (d, *J* = 8.2 Hz, 2H), 7.34 (d, *J* = 8.2 Hz, 2H), 6.68 (dd, *J* = 17.2, 10.8 Hz, 1H), 5.22 (d, *J* = 10.8 Hz, 1H), 5.17 (d, *J* = 17.2 Hz, 1H), 5.02 (dd, *J* = 4.4, 2.2 Hz, 1H), 4.90 (dd, *J* = 4.8, 2.2 Hz, 1H), 4.66 (d, *J* = 13.2 Hz, 1H), 3.88 (dm, *J* = 12.0 Hz, 1H), 3.30-3.15 (m, 2H), 3.04-2.95 (m, 1H), 2.92 (dm, *J* = 13.2 Hz, 1H), 2.47 (dd, *J* =12.4, 2.4 Hz, 1H), 2.43 (s, 3H), 2.08-2.00 (m, 1H), 1.38 (m, 1H).
^{13}C NMR (101 MHz, CD_2Cl_2) δ 150.6, 144.2, 134.4, 133.9, 133.8, 130.0, 129.5, 128.1, 116.3, 107.1, 48.8, 46.4, 45.2, 38.9, 31.7, 21.6.
HRMS (ESI) calcd for $C_{18}H_{22}NO_2S$ ([M + H]$^+$) 316.1366, found 316.1361.



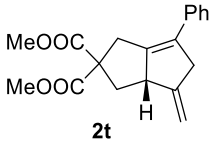
2r

Following the **general procedure B**, Co[(s)-xyl-BINAP]Cl_2 (0.15 equiv) was used. 4 h, eluted with PE/EA 15:1.
Run 1: 29.2 mg of **1r** was used, and 4.0 mg of **2r** was obtained in 14% yield and 0% ee as determined by HPLC analysis (chiral AD-H, hexane/*i*-PrOH = 96/4, 1.2 mL/min, 220 nm, 25 °C), t_r, 16.55 min, 17.44 min;
2r: colorless oil, TLC, R_f = 0.65 (PE/EA, 8:1).
Run 2: 22.0 mg of **1r** was used, and 2.6 mg of **2r** was obtained in 12% yield.
The average yield of two runs was 13%.
^{1}H NMR (400 MHz, CD_2Cl_2) δ 7.78-7.55 (m, 2H), 7.37-7.33 (m, 2H), 7.30-7.25 (m, 2H), 7.20-7.18 (2H, m), 4.98 (m, 1H), 4.85 (m, 1H), 4.24 (dm, *J* = 14.2 Hz, 1H), 3.95 (d, *J* = 14.0 Hz, 1H), 3.74 – 3.60 (m, 2H), 3.50 (d, *J* = 8.6 Hz, 1H), 2.85 (d, *J* = 8.6 Hz, 1H), 2.38 (s, 3H), 1.21 (s, 3H).
^{13}C NMR (101 MHz, CD_2Cl_2) δ 153.7, 144.0, 142.1, 135.0, 131.7, 130.1, 128.9, 128.0, 127.7, 127.4, 107.2, 59.1, 56.5, 47.0, 42.8, 25.1, 21.6.
HRMS (ESI) calcd for $C_{22}H_{23}NNaO_2S$ ([M + Na]$^+$) 388.1342, found 388.1340.



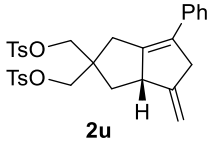
2s

Following the **general procedure B**, 4 h, eluted with PE/EA 50:1.
Run 1: 30 mg of **1s** was used, and 27.0 mg of **2s** was obtained in 90% yield and 87% ee as determined by HPLC analysis (chiral AD-H, hexane/*i*-PrOH = 98/2, 1.0 mL/min, 220 nm, 25 °C), t_r, 7.48 min (major), 9.85 min (minor); $[\alpha]^{20}_D$ = -200.7° (c = 0.215, $CHCl_3$).
Run 2: 30 mg of **1s** was used, and 27.2 mg of **2s** was obtained in 91% yield.
The average yield of two runs was 90%.
2s: colorless oil, TLC, R_f = 0.32 (PE/EA, 50:1).
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.42-7.30 (m, 2H), 7.27-7.22 (m, 1H), 7.21-7.14 (m, 2H), 5.04 (m, 1H), 4.86 (m, 1H), 4.57 (d, *J* = 12.8 Hz, 1H), 4.48 (d, *J* = 13.2 Hz, 1H), 4.23-4.04 (m, 2H), 3.91-3.77 (m, 2H), 3.31 (dd, *J* = 8.8, 7.2 Hz, 1H).
^{13}C NMR (101 MHz, $CDCl_3$) δ 147.6, 143.5, 135.2, 131.3, 128.7, 127.5, 126.9, 108.4, 69.3, 65.6, 57.2, 45.8.
HRMS (ESI) calcd for $C_{14}H_{14}NaO$ ([M + Na]$^+$) 221.0937, found 211.0939.



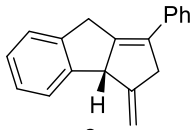
2t

Following the **general procedure C**, 12 h, eluted with PE/EA 15:1.
Run 1: 40 mg of **1t** was used, and 32.8 mg of **2t** was obtained in 82% yield and 88% ee as determined by HPLC analysis (chiral AD-H, hexane/*i*-PrOH = 95/5, 1.0 mL/min, 220 nm, 25 °C), t_r, 7.23 min (major), 7.67 min (minor); $[\alpha]^{20}_D$ = -155.0° (c = 0.204, $CHCl_3$).
Run 2: 40 mg of **1t** was used, and 31.6 mg of **2t** was obtained in 79% yield.
The average yield of two runs was 81%.
2t: colorless oil, TLC, R_f = 0.60 (PE/EA, 8:1).
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.35 (m, 4H), 7.26-7.21 (m, 1H), 4.99 (s, 1H), 4.90 (s, 1H), 3.90-3.78 (m, 1H), 3.80 (s, 3H), 3.76-3.66 (2H, m), 3.70 (s, 3H), 3.29 (d, *J* = 17.8 Hz, 1H), 3.14 (d, *J* = 17.8 Hz, 1H), 2.69 (dd, *J* = 12.0, 7.2 Hz, 1H), 1.86 (dd, *J* = 12.0, 12.0 Hz, 1H).
^{13}C NMR (101 MHz, $CDCl_3$) δ 172.8, 172.0, 150.6, 143.4, 135.8, 130.1, 128.5, 127.0, 107.1, 64.0, 56.1, 53.2, 53.0, 44.9, 37.3, 34.6.
HRMS (ESI) calcd for $C_{19}H_{20}NaO_4$ ([M + Na]$^+$) 335.1254, found 335.1253.



2u

Following the **general procedure C**, 8 h, eluted with PE/EA 5.5:1.
Run 1: 45.2 mg of **1u** was used, and 42.3 mg of **2u** was obtained in 94% yield and 88% ee as determined by HPLC analysis (chiral OD-H, hexane/*i*-PrOH = 92/8, 1.2 mL/min, 220 nm, 25 °C), t_r, 27.86 min (major), 33.10 min (minor); $[\alpha]^{20}_D$ = -23.9° (c = 0.082, $CHCl_3$).
Run 2: 40.0 mg of **1u** was used, and 31.6 mg of **2u** was obtained in 90% yield.
The average yield of two runs was 92%.
2u: colorless oil, TLC, R_f = 0.34 (PE/EA, 8:1).
^{1}H NMR (400 MHz, CD_2Cl_2) δ 7.77 (d, *J* = 8.0 Hz, 2H), 7.63 (d, *J* = 8.0 Hz, 2H), 7.39-7.24 (m, 9H), 4.93 (s, 1H), 4.77 (s, 1H), 3.98 (s, 2H), 3.78 (d, *J* = 9.2 Hz, 1H), 3.72 (d, *J* = 9.2 Hz, 1H), 3.70-3.55 (m, 2H), 2.46 (s, 3H), 2.40 (s, 3H), 2.45-2.36 (m, 1H), 2.30 (s, 2H), 1.89 (dd, *J* = 12.8, 8.4 Hz, 1H), 1.07 (dd, *J* = 12.0 11.6 Hz, 1H).
^{13}C NMR (101 MHz, CD_2Cl_2) δ 151.5, 145.8, 145.6, 143.2, 135.9, 132.7, 132.6, 131.2, 130.5, 130.3, 128.7, 128.3, 128.2, 127.3, 127.2, 106.9, 72.8, 71.6, 55.0, 51.1, 44.7, 34.6, 33.0, 21.8, 21.8.
HRMS (ESI) calcd for $C_{31}H_{32}NaO_6S_2$ ([M + Na]$^+$) 587.1532, found 587.1535.



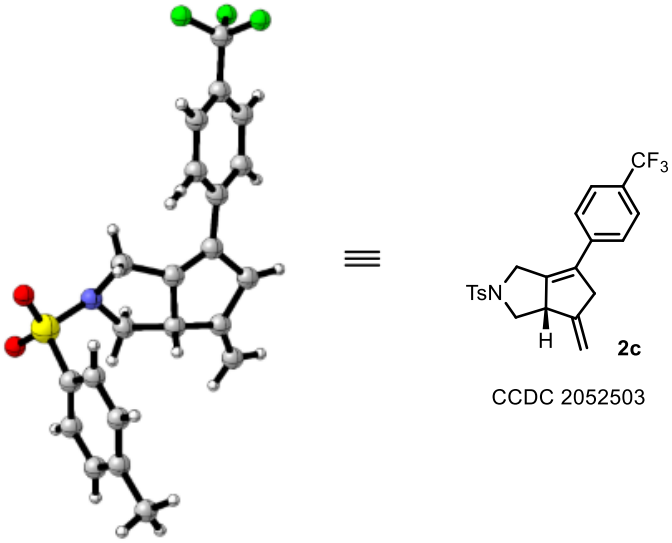
2v

Following the **general procedure B**, 1.5 h, eluted with PE/EA 50:1.
Run 1：19.5 mg of **1v** was used, and 16.7 mg of **2v** was obtained in 86% yield and 7% ee as determined by HPLC analysis (chiral OJ-H, hexane/*i*-PrOH = 100/0, 0.5 mL/min, 220 nm, 25 °C), t_r, 21.50 min (minor), 17.44 min (major)
Run 2：19.5 mg of **1v** was used, and 16.4 mg of **2v** was obtained in 84% yield.
The average yield of two runs was 85%.
2v: colorless oil, TLC, R_f = 0.60 (PE/EA, 100:1).
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.62 (d, *J* = 7.2 Hz, 1H), 7.52 (m, 2H), 7.36 (m, 2H), 7.26-7.7.20 (m, 2H), 7.18-7.13 (m, 1H), 7.12-7.05 (m, 1H), 4.96 (s, 1H), 4.93 (s, 1H), 4.23-4.12 (m, 1H), 4.01 (d, *J* = 19.4 Hz, 1H), 3.54 (d, *J* = 19.4 Hz, 1H), 3.12 (dd, *J* = 14.8, 8.6 Hz, 1H), 2.82 (dd, *J* = 14.8, 8.6 Hz, 1H).
^{13}C NMR (101 MHz, $CDCl_3$) δ 152.6, 150.2, 145.2, 137.4, 136.7, 131.0, 128.3, 128.1, 127.4, 127.3, 126.5, 125.9, 122.8, 105.5, 58.1, 48.4, 34.3.
HRMS (EI) calcd for $C_{19}H_{16}$ ([M]$^+$) 244.1252, found 244.1248.

2.5 X-ray crystal analysis

Crystal compound **2c** was obtained by ethyl acetate solution and then stilling at -20 °C for weeks.

Crystallographic Data of Compound 2c



CCDC 2052503

2.5.1. Table S3. Crystal data and structure refinement for 2c

Identification code	TX4070A
Empirical formula	$C_{22}H_{19.5}F_3NO_2S$
Formula weight	418.94
Temperature/K	169.99(12)
Crystal system	monoclinic
Space group	P21
a/Å	8.29306(5)
b/Å	25.38724(17)
c/Å	9.49206(6)
α /°	90
β /°	91.3809(6)
γ /°	90
Volume/Å3	1997.86(2)
Z	4
ρ calcg/cm3	1.393
μ /mm-1	1.849
F(000)	870.0
Crystal size/mm3	0.28 × 0.22 × 0.16
Radiation	Cu Kα (λ = 1.54184)
2Θ range for data collection/°	6.964 to 151.006
Index ranges	-10 ⩽ h ⩽ 10, -31 ⩽ k ⩽ 31, -11 ⩽ l ⩽ 11
Reflections collected	27024
Independent reflections	7944 [Rint = 0.0231, Rsigma = 0.0203]
Data/restraints/parameters	7944/1/525
Goodness-of-fit on F^2	1.021
Final R indexes [I>=2σ (I)]	R_1 = 0.0314, wR_2 = 0.0851
Final R indexes [all data]	R_1 = 0.0318, wR_2 = 0.0855
Largest diff. peak/hole / e $Å^{-3}$	0.34/-0.34
Flack parameter	0.007(4)

3. DFT Calculations

3.1 The computed energy surface for the model complex 1NT1-dmpp with more details.

Here we show the relative energies of all stationary points computed by DFT method.

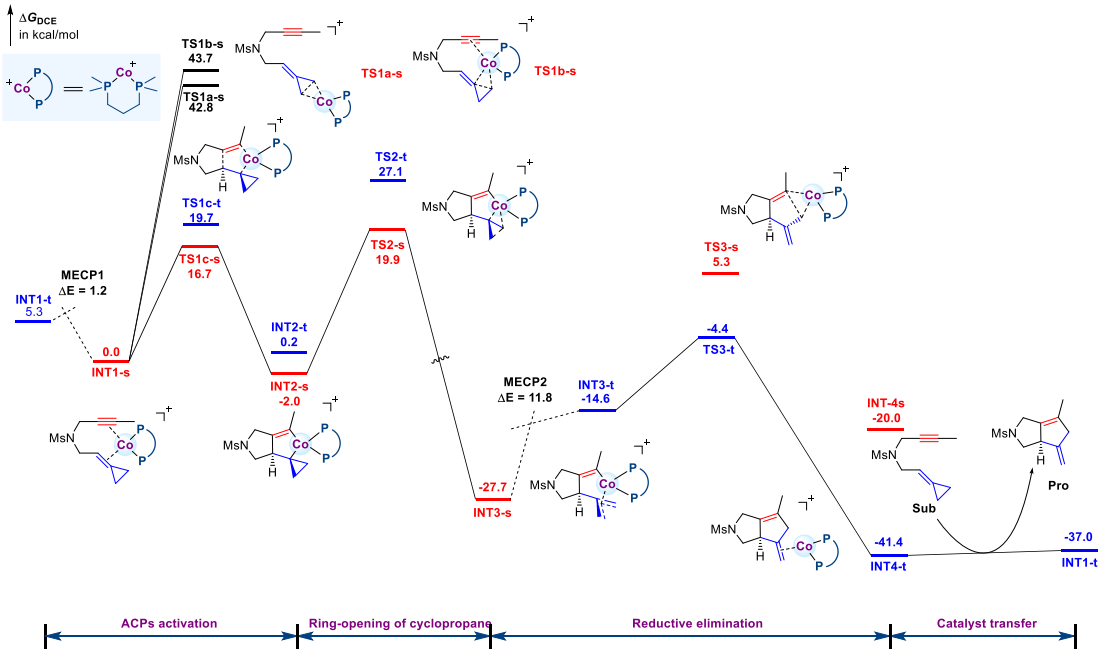


Figure S1. Computed energy surface for the [3+2] cycloaddition catalyzed by a model cobalt(I)-diphospine species at the SMD(DCE)/M06L/6-311+G(2d,p) (SDD for Co)//B3LYP/6-31G(d) (LANL2DZ for Co) level. Note that the suffixes s and t on the structure numberings refer to the singlet and triplet state

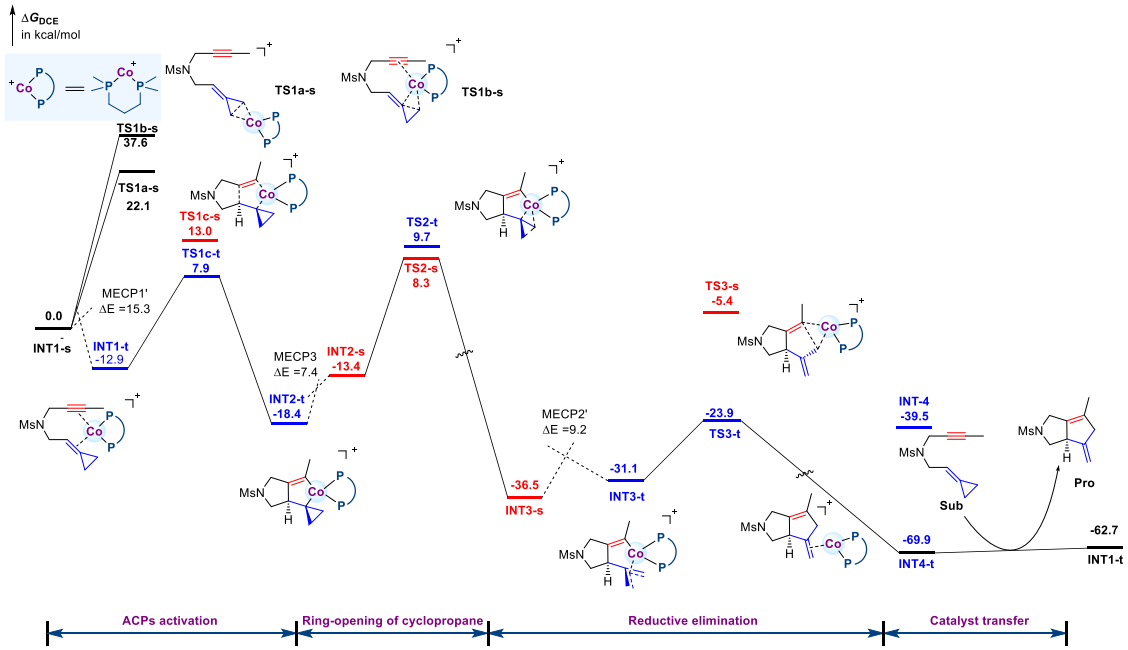


Figure S2. Computed energy surface for the [3+2] cycloaddition catalyzed by a model cobalt(I)-diphospine species at the SMD(DCE)/B3LYP/6-31G(d) (LANL2DZ for Co)//B3LYP/6-31G(d) (LANL2DZ for Co) level compared to **Figure S1**. Note that the suffixes s and t on the structure numberings refer to the singlet and triplet state

Discussion: Figure S2 is the energy surface computed at the SMD(DCE)/B3LYP/6-31G(d) (LANL2DZ for Co)//B3LYP/6-31G(d) (LANL2DZ for Co) level (note that the suffixes s and t on the structure numberings refer to the singlet and triplet state). The mechanism is similar to that discussed in the main text. The major difference is the relative energies of some singlet and triplet species. It was reported that B3LYP overestimate the stability of triplet state with respect to its singlet,[11] while M06L gives reasonable results.[12,13]

Consequently we used energies of **Figures 1** and **S1** for discussion of the mechanism of Co-catalyzed [3+2] reaction at the SMD(DCE)/M06L/6-311+G(2d,p) (SDD for Co)//B3LYP/6-31G(d) (LANL2DZ for Co) level.

Single-point energies (SPEs) of MECP

	SPE[a] (a.u.)	SPE[b] (a.u.)
INT1-t	-2098.523973	-2099.547191
MECP1	-2098.499620	-2099.545282
INT3-s	-2098.564225	-2099.602238
MECP2	-2098.549601	-2099.583356
INT2-t	-2098.517700	
MECP3	-2098.505826	

[a] The geometries of MECPs were optimized at the B3LYP/6-31G(d) (LANL2DZ for Co) level. [b] The geometries of MECPs were optimized at the M06L/6-311+G(2d,p) (SDD for Co) level.

3.2 The computed energy surface for the model complex 1NT1-dppp

We have also computed the energy surface with the key stationary points using dppp ligand (Figure S3) and our conclusion here is that, both calculation models supported the same mechanistic pathways. Here we did not search for all possible conformations for each stationary point, but just by replacing the Me group in the ligand for every structure in Figure S1 by a Ph group and then full optimizing the corresponding structure to get the one shown in the potential energy surface below. The MECP were not computed here.

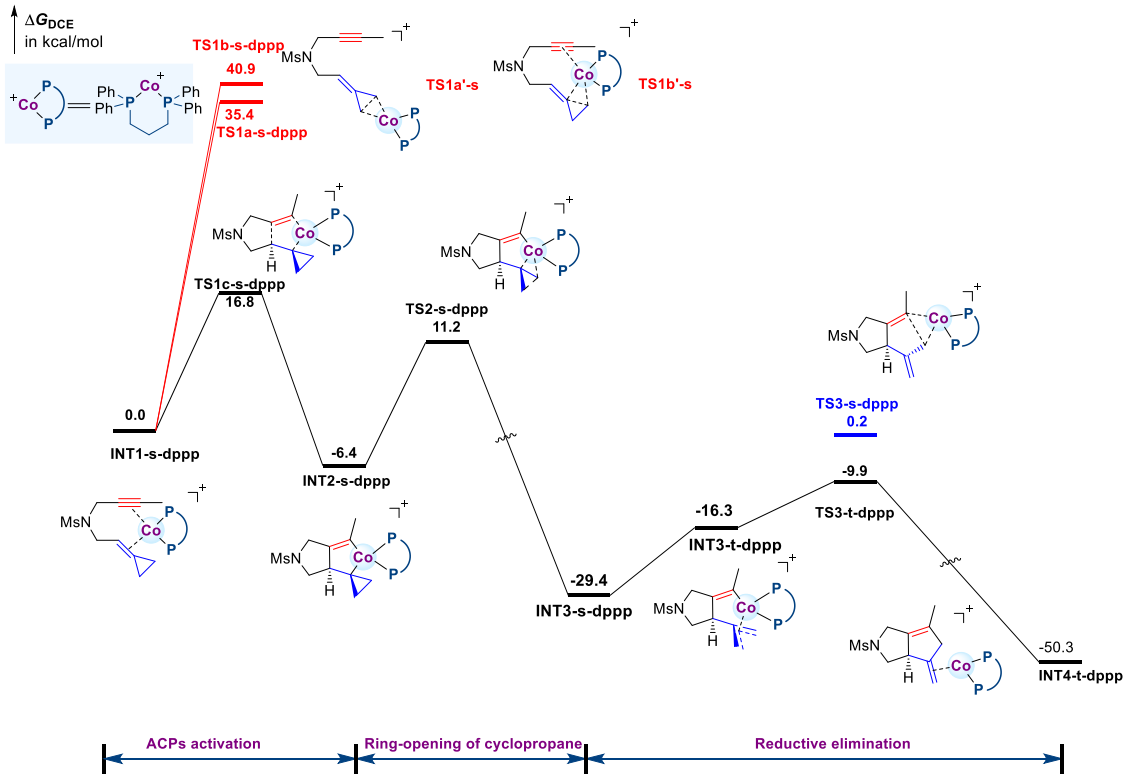


Figure S3. Computed energy surface for the [3+2] cycloaddition catalyzed by a cobalt(I)-dppp species at the (SMD(DCE)/M06L/6-311+G(2d,p) (SDD for Co)//B3LYP/6-31G(d) (LANL2DZ for Co) level. Note that the suffixes s and t on the structure numberings refer to the singlet and triplet state

3.3 Table S4. Thermal corrections to Gibbs energies (TCGs) and single-point energies (SPEs)

	TCG [a, b] (a.u.)	SPE[a] (a.u.)	SPE[c] (a.u.)	SPE[d] (a.u.)
INT1-s	0.420417	-2098.503400	-2098.589104	-2099.555469
INT1-t	0.414992	-2098.523973	-2098.604160	-2099.547191
TS1a-s	0.407871	-2098.447585	-2098.541330	-2099.466740
TS1b-s	0.418339	-2098.443106	-2098.527156	-2099.485380
TS1c-s	0.421789	-2098.489271	-2098.569689	-2099.535470
TS1c-t	0.414557	-2098.492364	-2098.571930	-2099.524392
INT2-s	0.420947	-2098.518233	-2098.611045	-2099.552090
INT2-t	0.412587	-2098.517700	-2098.610693	-2099.540024
TS2-s	0.420522	-2098.492611	-2098.576060	-2099.526102
TS2-t	0.413242	-2098.481193	-2098.566486	-2099.505474
INT3-s	0.423218	-2098.564225	-2098.650106	-2099.602238
INT3-t	0.417129	-2098.552754	-2098.635407	-2099.578517
TS3-s	0.424701	-2098.523564	-2098.602002	-2099.558649

TS3-t	0.417158	-2098.541253	-2098.624048	-2099.562173
INT4-s	0.422450	-2098.570103	-2098.654063	-2099.591120
INT4-t	0.417900	-2098.606390	-2098.697546	-2099.613542
Sub	0.190107	-993.270418	-993.291662	-993.419027
Pro	0.198894	-993.362291	-993.379414	-993.499336
INT1-s-dppp	0.617768	-2865.414411	-2865.508255	-2866.580592
TS1a-s-dppp	0.603632	-2865.370063	-2865.473889	-2866.500023
TS1b-s dppp	0.614357	-2865.356641	-2865.450119	-2866.512403
TS1c-s dppp	0.618703	-2865.40023	-2865.488223	-2866.560617
INT2-s dppp	0.617194	-2865.434661	-2865.536462	-2866.582297
TS2-s dppp	0.615843	-2865.410262	-2865.506079	-2866.558795
INT3-s dppp	0.620695	-2865.47947	-2865.575607	-2866.628089
INT3-t dppp	0.615071	-2865.470275	-2865.563458	-2866.604514
TS3-s dppp	0.621087	-2865.434845	-2865.526153	-2866.586067
TS3-t dppp	0.611258	-2865.458842	-2865.55986	-2866.582655
INT4-t dppp	0.612208	-2865.528710	-2865.631549	-2866.136839

[a] Computed at the B3LYP/6-31G(d)&LANL2DZ level. [b] A standard state at 1atm and 298 K was used. [c] Computed at the SMD(DCE)/6-31G(d)&LANL2DZ level. [d] Computed at the M06L/6-311+G(2d, p)&SDD level.

3.4 Cartesian coordinates of all stationary points

INT1-s

N	2.88734100	-0.04869300	0.03276700
C	2.27872600	-0.90543200	1.06819600
C	0.79943000	-0.82903200	1.05498800
C	-0.29977300	-1.21146200	1.61673200
C	-0.84020100	-2.11338100	2.66988500
C	2.21422600	1.25353200	-0.12006600
C	0.92566900	1.10326100	-0.88486400
C	-0.17831600	1.91020800	-0.69242900
C	-0.95684400	2.87746800	-1.50284700
C	-0.39969800	3.26759400	-0.12722900
S	4.60928400	0.03682400	0.15696800
O	5.01306800	1.28026200	-0.50097600
O	5.00660700	-0.26209100	1.53618400
C	5.11781400	-1.34315900	-0.88113500
H	2.59183900	-1.94402900	0.90256900
H	2.63149600	-0.62553900	2.07314500
H	-0.90713400	-3.13974400	2.28490300
H	-0.16654100	-2.13810100	3.53520700
H	-1.83635500	-1.83138400	3.02116400
H	2.04027200	1.74970200	0.84561600
H	2.88655600	1.89261800	-0.70180800
H	1.03709600	0.58193500	-1.83559100
H	-0.47904500	3.29804500	-2.38593300
H	-2.03390200	2.78537100	-1.58918300
H	-1.12230800	3.41674200	0.67196200
H	0.44296900	3.95495700	-0.08272700
H	4.69338400	-2.27147600	-0.49346600
H	4.79165500	-1.15281200	-1.90421500
H	6.20847100	-1.38379200	-0.82644700
Co	-0.64516200	0.07433700	0.24101700
P	-2.77217500	0.61343500	0.91293300
P	-1.39979600	-1.07213500	-1.46514400
C	-0.14989500	-2.26998600	-2.09715300
H	0.09867000	-2.98989100	-1.31241300
H	-0.53909000	-2.80743000	-2.96878100
H	0.76500700	-1.74300800	-2.37994100
C	-1.92046500	-0.15497500	-2.97394400
H	-2.21050100	-0.85744000	-3.76285500
H	-2.76526700	0.50325200	-2.75657300
H	-1.09543500	0.46487500	-3.33427800
C	-2.83888500	-2.16815200	-1.05693800
H	-3.09154100	-2.71692900	-1.97337600
H	-2.46927900	-2.90774300	-0.33589500
C	-3.84109000	1.92229200	0.14982400
H	-4.02982400	1.71993200	-0.90807000
H	-4.80355900	1.95795700	0.67196000
H	-3.36930000	2.90442200	0.23264200
C	-3.92577200	-0.84191400	0.88839600
H	-4.90101500	-0.51368000	1.26825700

H	-3.54379900	-1.58984000	1.59221100
C	-2.76940200	1.15327100	2.68019700
H	-3.79236500	1.30188000	3.04271700
H	-2.26834600	0.41407300	3.30900200
H	-2.22467000	2.09825900	2.77107400
C	-4.09857500	-1.47926600	-0.50260800
H	-4.88569200	-2.23911100	-0.43174100
H	-4.47255500	-0.73756500	-1.21998000

INT1-t

N	3.05878800	0.98964200	0.57976600
C	2.24883400	0.97659700	1.79650900
C	0.94364600	0.26510000	1.73516200
C	0.03782500	-0.47812300	2.11101500
C	-0.74368600	-1.47914700	2.85093800
C	2.53566000	1.81537200	-0.51889100
C	1.28605000	1.32235800	-1.21362100
C	0.13542100	2.03801700	-1.26736000
C	-0.95570800	2.42368900	-2.19331800
C	-0.38009800	3.41999100	-1.16906200
S	3.83876100	-0.47134700	0.15926700
O	3.68031300	-1.37647400	1.29857600
O	3.40707800	-0.86786100	-1.18980600
C	5.56403300	0.02945300	0.05036900
H	2.83259700	0.50745200	2.59233300
H	2.08927700	2.02445700	2.07636000
H	-0.94651000	-2.36415500	2.23953800
H	-0.16885800	-1.80441500	3.72644900
H	-1.70036400	-1.08526800	3.20667200
H	2.36795600	2.81503900	-0.10404500
H	3.32275900	1.90952000	-1.27601600
H	1.40640200	0.42819700	-1.81846100
H	-0.69643200	2.54285900	-3.24372100
H	-1.97513400	2.08979300	-2.02704800
H	-1.03585200	3.69318300	-0.34479200
H	0.24561700	4.23597400	-1.52574600
H	5.66561000	0.81547500	-0.70040900
H	5.88863500	0.37873400	1.03153500
H	6.13042200	-0.85470600	-0.25220100
Co	-0.61848500	0.47603300	0.10800000
P	-2.97831400	0.65234100	0.72382700
P	-0.84026000	-1.61978500	-1.11112900
C	0.50641600	-2.87193800	-0.93323800
H	0.64591900	-3.12015300	0.12351300
H	0.27517100	-3.78772200	-1.48849900
H	1.44938100	-2.45351600	-1.29738200
C	-1.00899500	-1.48471000	-2.95271700
H	-1.12775600	-2.47122300	-3.41441500
H	-1.87415100	-0.86698400	-3.21406900
H	-0.11650600	-1.01041400	-3.37359100
C	-2.35339500	-2.62023400	-0.66100600
H	-2.45598500	-3.41817700	-1.40749000
H	-2.14263600	-3.12100600	0.29296600
C	-4.08069900	1.66224200	-0.37595300
H	-4.07972400	1.26835800	-1.39688900
H	-5.11047600	1.64849900	-0.00235100
H	-3.73795000	2.70115000	-0.40809600
C	-3.86514600	-0.98985900	0.71548300
H	-4.93201100	-0.78146200	0.86702700
H	-3.53057000	-1.55504900	1.59363400
C	-3.41870200	1.35090900	2.38142700
H	-4.49517500	1.27687600	2.57093300
H	-2.88178500	0.83032300	3.17888600
H	-3.12867200	2.40609700	2.41703400
C	-3.68422500	-1.84938700	-0.55432700
H	-4.49299900	-2.59012000	-0.55843300
H	-3.84670600	-1.24209400	-1.45498300

TS1a-s

N	-4.10501000	-0.36336200	-0.36308200
C	-3.77457400	1.00383600	-0.79098900
C	-3.64411200	1.97387300	0.30850400
C	-3.54923900	2.76928400	1.21682500
C	-3.46106900	3.74485200	2.30204600
C	-3.12251000	-1.07542500	0.45893000
C	-2.01572000	-1.62598500	-0.40489000
C	-0.72810500	-1.34089000	-0.25693900
C	0.20293200	-0.53498200	0.53990800
C	0.59027200	-1.62738200	-0.83185600
S	-5.73012700	-0.82964800	-0.30587800
O	-6.37326000	-0.18849100	-1.45161600
O	-5.71934700	-2.28180900	-0.12475500
C	-6.42781900	-0.09441700	1.18994100
H	-2.83567300	0.94807800	-1.35784400
H	-4.54587700	1.31815300	-1.49998100
H	-4.15576400	4.57716300	2.13975200
H	-3.71114100	3.28769900	3.26678600
H	-2.45170800	4.16525500	2.38456900
H	-2.72267600	-0.41283400	1.23879400
H	-3.63373000	-1.91237700	0.94372600
H	-2.32801100	-2.30432500	-1.19729800
H	0.15739300	0.55128700	0.45134100
H	0.44232200	-0.90181100	1.54938600
H	1.03589400	-2.60338600	-0.59566500
H	0.79413600	-1.26898800	-1.84171400
H	-5.92775100	-0.51657000	2.06411500

H	-6.29482400	0.98823400	1.14887700
H	-7.48994100	-0.35058700	1.20464300
Co	2.22888500	-0.68821000	0.08065000
P	4.27002900	-0.84661100	0.97468500
P	2.81028100	0.95225700	-1.22510800
C	3.99370700	2.19804900	-0.51967500
H	4.19966600	2.93606400	-1.30538700
H	3.46020200	2.72698700	0.28073200
C	1.41667000	2.01620900	-1.80787500
H	1.77733900	2.78499800	-2.49969100
H	0.66619800	1.40911800	-2.32377900
H	0.93681900	2.51006700	-0.95716000
C	3.60565000	0.41866800	-2.80516300
H	2.90869100	-0.20297400	-3.37553200
H	3.88341000	1.28591900	-3.41423600
H	4.50003700	-0.17775000	-2.60662600
C	5.50874600	-1.90995600	0.10566300
H	5.73349500	-1.51027400	-0.88733200
H	6.43976000	-1.97370700	0.67965400
H	5.10332100	-2.91828800	-0.02239100
C	5.18036400	0.74300000	1.26910100
H	6.17296900	0.50692300	1.67212700
H	4.63648400	1.28434900	2.05384000
C	4.18862500	-1.61143500	2.65736000
H	5.18892700	-1.70099700	3.09484500
H	3.56653100	-1.00094000	3.31891100
H	3.74774700	-2.61171100	2.59373300
C	5.31988000	1.63351200	0.02115400
H	5.85589500	1.09642400	-0.77179900
H	5.96106900	2.48322800	0.28373300

TS1b-s

N	2.86958700	0.40614100	-0.08577400
C	2.46531600	0.02658600	1.28256900
C	1.12496400	0.50414200	1.65800400
C	0.09363700	0.80365200	2.24806200
C	-0.90686200	1.28756900	3.21243100
C	1.86143400	0.07972800	-1.12576600
C	1.30213300	-1.32211300	-1.05057800
C	0.25768400	-1.75338300	-0.31363400
C	-0.25918900	-2.14104200	1.33224700
C	-0.06586400	-3.10288400	0.16373200
S	4.48276500	-0.11021600	-0.44962700
O	4.86900600	-1.15910400	0.49990800
O	4.53347100	-0.33471100	-1.89510500
C	5.43014400	1.37271300	-0.06940800
H	2.50064600	-1.06254800	1.42047400
H	3.18115300	0.45141900	1.99520000
H	-1.78515700	1.71810400	2.72162800
H	-1.25336900	0.46498200	3.84796800
H	-0.46414500	2.05392500	3.85985300
H	1.06931100	0.81867800	-1.00523700
H	2.33375800	0.24920900	-2.09355700
H	1.80559500	-2.07045700	-1.66645700
H	0.56903700	-2.06228400	2.02906500
H	-1.23369800	-2.13078500	1.82836300
H	-0.98534600	-3.56313400	-0.19997100
H	0.74537600	-3.82992700	0.22637600
H	5.10838800	2.17315600	-0.73661300
H	5.27884200	1.64500800	0.97701800
H	6.48010200	1.12374000	-0.24214000
Co	-0.86407500	-0.29023800	0.50876700
P	-1.46182800	1.79200900	-0.38862000
P	-2.85116700	-1.14024200	-0.28465500
C	-4.32377900	-0.00170100	-0.15140200
H	-5.18332300	-0.56190800	-0.54023600
H	-4.50527900	0.14100600	0.92240900
C	-3.56208100	-2.58474900	0.63836600
H	-4.52547600	-2.86252800	0.19788400
H	-2.90526400	-3.45609700	0.60640000
H	-3.72622800	-2.31394900	1.68618400
C	-2.90162100	-1.72543700	-2.03602300
H	-2.14266900	-2.49841000	-2.18555100
H	-3.88651800	-2.13636900	-2.28189900
H	-2.67935900	-0.90650700	-2.72467800
C	-1.20092200	1.91062900	-2.22180700
H	-1.67736400	1.08083600	-2.74833000
H	-1.61084100	2.85375800	-2.59970100
H	-0.13325800	1.88038100	-2.45229800
C	-3.23227900	2.33923100	-0.22977500
H	-3.32728400	3.32486700	-0.70164700
H	-3.44707300	2.47591600	0.83842900
C	-0.54378100	3.28889300	0.19305200
H	-0.83276600	4.16388000	-0.39860000
H	-0.75916300	3.49211300	1.24551800
H	0.53284500	3.12833800	0.09191400
C	-4.24807000	1.36504900	-0.84648500
H	-4.05155600	1.23958800	-1.91844200
H	-5.24130700	1.82560900	-0.78239000

TS1c-s

N	-3.23237500	0.85804800	0.47353300
C	-2.34575800	1.69579300	-0.33693200
C	-0.92163800	1.19408000	-0.31347500
C	0.19793300	1.70737800	-0.78998600
C	0.46748500	2.95720700	-1.56456800

C	-2.40780900	0.17504100	1.47448500
C	-1.20531100	-0.46682000	0.79133400
C	-0.03408500	-0.87582700	1.54267300
C	0.17731600	-2.14257700	2.30788700
C	0.12666300	-0.80546900	3.03517200
S	-4.33203700	-0.15281900	-0.39992400
O	-4.26524800	0.23889300	-1.81156900
O	-4.10310200	-1.54567100	0.00547300
C	-5.91552000	0.37382200	0.26704900
H	-2.71568700	1.74887500	-1.36465600
H	-2.34595000	2.71622600	0.07241200
H	0.14793400	2.81818400	-2.60618900
H	-0.09629700	3.81274400	-1.16840000
H	1.52736100	3.22872400	-1.58847100
H	-2.09520300	0.90884400	2.22472200
H	-2.99032500	-0.60452200	1.97133600
H	-1.54022100	-1.18247600	0.04032400
H	-0.66305200	-2.82248200	2.44032500
H	1.14210300	-2.64226500	2.27178300
H	1.05498400	-0.43354400	3.46143500
H	-0.74404400	-0.59633600	3.65434600
H	-5.92182600	0.19888500	1.34426000
H	-6.05547900	1.43178600	0.04051700
H	-6.68255600	-0.23093800	-0.22274800
Co	0.79783600	0.21613200	0.15632200
P	2.79472800	0.92797500	0.66713500
P	1.57212500	-1.43725600	-1.03864000
C	0.24349000	-2.06102300	-2.15371800
H	-0.22769300	-1.22563700	-2.67809900
H	0.66446800	-2.75789500	-2.88691300
H	-0.52223000	-2.58578200	-1.57529500
C	2.29519400	-2.98920100	-0.35797800
H	2.63892100	-3.62617200	-1.18011800
H	3.13965300	-2.78267700	0.30438200
H	1.53608400	-3.52924900	0.21203200
C	2.86209000	-0.81421400	-2.21677700
H	3.13106100	-1.64403800	-2.88257900
H	2.37308600	-0.05024700	-2.83354800
C	3.77292000	-0.03975500	1.89919400
H	3.93149200	-1.06605200	1.55902400
H	4.74813600	0.42993500	2.06910700
H	3.23373300	-0.07846700	2.84970900
C	3.93331900	1.07184500	-0.78550200
H	4.90300300	1.44493100	-0.43326400
H	3.51195000	1.83992900	-1.44533700
C	2.78090700	2.61413900	1.41130000
H	3.79689600	2.93127100	1.67022500
H	2.34619500	3.33242400	0.71202300
H	2.17076700	2.60537100	2.31950800
C	4.13565300	-0.23802400	-1.57077000
H	4.85648700	-0.03861500	-2.37231100
H	4.61081400	-0.99248900	-0.93117000

TS1c-t

N	3.33424400	-1.00146900	-0.47865800
C	2.43081500	-0.87172000	-1.61584500
C	1.04365600	-0.43725900	-1.16772200
C	-0.04274300	-0.09103500	-1.77384300
C	-0.48178600	0.25228700	-3.15658400
C	2.53092500	-1.51308100	0.63115800
C	1.25979200	-0.67181300	0.79239000
C	0.11510100	-1.23798700	1.46354200
C	-0.32025000	-1.20502000	2.89131700
C	-0.05510900	-2.53321800	2.18085700
S	4.30037500	0.39411300	-0.12429500
O	4.22650900	1.27880400	-1.29007100
O	3.95072600	0.88504200	1.21599800
C	5.94421900	-0.32829300	-0.04786400
H	2.82709600	-0.15869400	-2.34145600
H	2.35177000	-1.85474900	-2.09705200
H	-0.94716600	1.24457600	-3.18942200
H	0.35894700	0.25622100	-3.86154000
H	-1.22804600	-0.46179700	-3.52475400
H	2.28213300	-2.55791600	0.41787100
H	3.09705200	-1.47251400	1.56499700
H	1.50453700	0.34857300	1.08639600
H	0.39616800	-0.87528100	3.64272200
H	-1.35372500	-0.97269200	3.13957700
H	-0.91698200	-3.16163900	1.96486500
H	0.83001100	-3.09682000	2.47163400
H	5.96473200	-1.08483400	0.73849400
H	6.17769700	-0.76560200	-1.01954900
H	6.63546200	0.48462100	0.18732300
Co	-0.86490700	-0.41326000	-0.02757900
P	-3.06324800	-1.07840000	-0.45205700
P	-1.30238400	1.87298800	0.61172400
C	-0.00982800	3.13636300	0.23947500
H	0.26684700	3.08649500	-0.81743500
H	-0.36356000	4.14655400	0.47235900
H	0.88844300	2.93233100	0.83098400
C	-1.72824400	2.22449900	2.37659900
H	-1.96330700	3.28447500	2.52267800
H	-2.58864300	1.62572400	2.69073200
H	-0.88114600	1.95885800	3.01586900
C	-2.79133800	2.50497200	-0.31618700

H	-3.01620900	3.51021200	0.06283400
H	-2.49058500	2.62853200	-1.36458400
C	-4.02638600	-1.68717100	1.00285900
H	-4.02495600	-0.94445300	1.80602200
H	-5.06363000	-1.90157700	0.72270000
H	-3.56970000	-2.60435100	1.38718300
C	-4.07597700	0.34941200	-1.08703400
H	-5.10896300	-0.00725200	-1.19151200
H	-3.71788300	0.57069600	-2.10034100
C	-3.34212800	-2.39432600	-1.71486600
H	-4.41207000	-2.56394100	-1.87695100
H	-2.87913800	-2.10720500	-2.66331500
H	-2.88238100	-3.32915600	-1.37973700
C	-4.06619800	1.63831700	-0.23697300
H	-4.89851000	2.25744200	-0.59276000
H	-4.30806000	1.40851400	0.80904600

INT2-s

N	-3.53551700	-0.31165700	-0.28213600
C	-2.58160600	0.25604200	-1.27418000
C	-1.23413600	-0.10878400	-0.68398700
C	-0.01900500	0.41743000	-0.89550700
C	0.34268900	1.36652500	-2.00333600
C	-2.82718900	-0.63405800	0.98464300
C	-1.44618600	-1.07091000	0.45383000
C	-0.21506900	-1.00526200	1.32161200
C	-0.03366000	-1.69073000	2.62484300
C	-0.09338600	-0.16263800	2.59338300
S	-5.02401700	0.51069000	-0.09086800
O	-5.45929800	0.24064900	1.28059700
O	-4.88832600	1.88511600	-0.58772800
C	-6.09504600	-0.38466100	-1.22583000
H	-2.74917700	-0.20696100	-2.25634700
H	-2.71228600	1.33859000	-1.38249100
H	-0.54821100	1.63630400	-2.58543800
H	0.77922000	2.30008800	-1.63345500
H	1.06101700	0.92853100	-2.70806600
H	-2.73746100	0.24205500	1.63950300
H	-3.36334400	-1.41671500	1.52297600
H	-1.55632400	-2.09387400	0.06046400
H	-0.88425700	-2.22346700	3.04811300
H	0.92667400	-2.12625800	2.89798200
H	0.85795800	0.33910000	2.82414400
H	-0.95131600	0.37708600	2.98456000
H	-5.69178200	-0.30896200	-2.23781500
H	-6.15778000	-1.42453100	-0.90268500
H	-7.07618500	0.09402300	-1.17754200
Co	1.18226900	-0.00419300	0.52462200
P	2.93770500	1.58861900	0.39142300
P	2.15373000	-1.56460200	-0.60577100
C	1.11319000	-2.76014400	-1.53651000
H	0.51949100	-2.23140100	-2.28618800
H	1.74080100	-3.50879400	-2.03163900
H	0.43084700	-3.26596800	-0.84812500
C	3.13636300	-2.63822300	0.53184800
H	3.67430300	-3.40385500	-0.03832200
H	3.86278200	-2.05194400	1.10187100
H	2.46344600	-3.13518100	1.23623700
C	3.38326600	-0.99805800	-1.87666000
H	3.84824300	-1.90713800	-2.27921100
H	2.81846200	-0.54855000	-2.70244400
C	4.12123700	1.39158100	1.80487800
H	4.50239100	0.36745800	1.86005400
H	4.97074200	2.07572400	1.70196900
H	3.61044100	1.61367400	2.74745600
C	4.02778400	1.41055600	-1.10239300
H	4.90540400	2.05479100	-0.96609900
H	3.47241900	1.80990300	-1.95964400
C	2.57838700	3.39994100	0.45444100
H	3.50723200	3.98004500	0.42944300
H	1.95089700	3.70148200	-0.38854900
H	2.04026200	3.63268500	1.37847700
C	4.48539900	-0.03036900	-1.40101000
H	5.23614400	0.02115900	-2.19838300
H	5.01185700	-0.45111900	-0.53487100

INT2-t

N	-3.77063400	-0.40648500	0.27653800
C	-2.90839600	-1.18970900	-0.65407800
C	-1.51902200	-0.78518500	-0.21617100
C	-0.34673100	-0.77696600	-0.87553900
C	-0.06020500	-1.27826700	-2.26207100
C	-2.96665800	0.62720200	0.98140800
C	-1.60467600	-0.08453100	1.10569800
C	-0.32662900	0.74779500	1.22381600
C	0.31086500	1.19147600	2.52109300
C	-0.30902500	2.20327700	1.57865900
S	-5.28036300	0.12156200	-0.32501900
O	-5.59256400	1.35858000	0.39334800
O	-5.25849100	0.07831200	-1.79184000
C	-6.39047500	-1.17302300	0.24821000
H	-3.09914300	-2.26315200	-0.52285300
H	-3.10703200	-0.93389000	-1.70086100
H	-0.98764900	-1.57831500	-2.76972500
H	0.41079400	-0.50655300	-2.88565700
H	0.60790600	-2.14959300	-2.26221500

H	-2.86417100	1.54792400	0.39233700
H	-3.43435900	0.87462700	1.93582300
H	-1.66633100	-0.81127000	1.93040100
H	-0.19081700	0.92215700	3.44921300
H	1.39949300	1.20946200	2.60753800
H	0.36711600	2.88314400	1.06604000
H	-1.25536300	2.66409200	1.85306100
H	-6.07294600	-2.13037700	-0.17014400
H	-6.37201900	-1.19371400	1.33866400
H	-7.38882000	-0.91778200	-0.11547500
Co	1.10971400	-0.02777600	0.15269300
P	2.73877500	1.66932300	-0.58298300
P	2.85698100	-1.72318100	0.49467900
C	2.34810400	-3.49472100	0.41729400
H	1.86570800	-3.70496300	-0.54186400
H	3.21038100	-4.15950200	0.53621300
H	1.62658700	-3.70321400	1.21315100
C	3.78025700	-1.62180400	2.09331300
H	4.58588500	-2.36336000	2.12752900
H	4.21012400	-0.62527900	2.22930100
H	3.09333300	-1.81021500	2.92420100
C	4.18998400	-1.61099400	-0.80243300
H	4.94122200	-2.37440600	-0.56278300
H	3.73482500	-1.91022900	-1.75566400
C	3.69378800	2.63427000	0.67258700
H	4.24086100	1.96122200	1.33963700
H	4.40892400	3.30996100	0.19055800
H	3.00715600	3.22998200	1.28242400
C	4.05901100	0.87365600	-1.62844100
H	4.73302200	1.67222400	-1.96324100
H	3.56421700	0.48711300	-2.52921500
C	2.06478000	2.97285200	-1.70321000
H	2.86033400	3.62601300	-2.07772700
H	1.55879900	2.50460900	-2.55298900
H	1.32989600	3.58173100	-1.16780900
C	4.88777000	-0.24522600	-0.96414600
H	5.76669900	-0.41170900	-1.59823900
H	5.28899900	0.09571300	-0.00123900

TS2-s

N	3.53734600	-0.86621300	-0.48878400
C	2.47986100	-0.61311200	-1.50710200
C	1.20356800	-0.42351200	-0.69075000
C	-0.07902500	-0.42503300	-1.05609100
C	-0.57657200	-0.48555600	-2.47034800
C	2.86172300	-1.30956200	0.75268700
C	1.57497400	-0.44538400	0.77104800
C	0.36099900	-0.79186400	1.59923000
C	0.47511200	-1.28838700	2.88337500
C	-0.49552700	-2.09203100	1.22848300
S	4.68343200	0.40695200	-0.26736500
O	4.56943400	1.30921000	-1.41671700
O	4.56347400	0.92330700	1.10424500
C	6.23985500	-0.48387100	-0.39344300
H	2.75610700	0.25028100	-2.11670000
H	2.41006300	-1.48678800	-2.16656600
H	0.26170800	-0.44346900	-3.17837300
H	-1.12547100	-1.41237400	-2.67513800
H	-1.24320500	0.34910100	-2.71845400
H	2.62947400	-2.37743100	0.65440200
H	3.50908000	-1.16126700	1.61669500
H	1.89251200	0.55663200	1.09891200
H	1.44412400	-1.55092100	3.31382000
H	-0.37374200	-1.40638500	3.55014600
H	-1.21348200	-2.50236700	1.93982200
H	0.08243300	-2.86683100	0.72627000
H	6.27588200	-1.24946400	0.38362900
H	6.30568500	-0.93029100	-1.38656500
H	7.03764600	0.24767400	-0.24400700
Co	-1.23172900	-0.45324500	0.49672500
P	-3.23125200	-1.03577200	-0.41862300
P	-1.57231400	1.79245900	0.44423300
C	-0.11516300	2.88775100	0.17649100
H	0.41012800	2.59367700	-0.73577400
H	-0.42424000	3.93516000	0.09662100
H	0.57834600	2.78822900	1.01656300
C	-2.28482800	2.44795200	2.02438100
H	-2.46167300	3.52702800	1.95580600
H	-3.23216600	1.95559400	2.26529600
H	-1.58576900	2.25952900	2.84512900
C	-2.77768600	2.39552200	-0.83881700
H	-2.94712000	3.46447100	-0.65719800
H	-2.28024200	2.32133600	-1.81402900
C	-4.38308600	-1.26096700	1.01856900
H	-4.38457100	-0.38070500	1.66860600
H	-5.40703200	-1.43744500	0.67108300
H	-4.06708800	-2.12411300	1.61319100
C	-4.10362700	0.23266000	-1.46085500
H	-5.13101800	-0.11769300	-1.62335400
H	-3.61579400	0.23897900	-2.44325800
C	-3.49806400	-2.60359800	-1.35694600
H	-4.56491400	-2.76927300	-1.54237400
H	-2.97716900	-2.57246000	-2.31738400
H	-3.10147100	-3.44481800	-0.78060000
C	-4.13300400	1.66166200	-0.88245900

H	-4.80910800	2.25317500	-1.51124600
H	-4.59438200	1.65664000	0.11369400

TS2t

N	-3.74768400	-0.49209400	0.60617800
C	-2.80134200	0.29786500	1.45045000
C	-1.46371800	0.14567700	0.74497200
C	-0.19387300	0.23577000	1.17952600
C	0.19068300	0.61878000	2.58552000
C	-2.95855400	-1.31789200	-0.33806700
C	-1.72723000	-0.43374200	-0.62507400
C	-0.42478400	-1.07824700	-1.08654600
C	0.41772600	-0.38966300	-2.18185700
C	-0.40528500	-2.26516300	-1.79354500
S	-5.06613400	0.37154400	-0.08326600
O	-5.03521100	1.74172200	0.43713100
O	-5.07517800	0.11659500	-1.53010900
C	-6.48345200	-0.46754200	0.63866000
H	-3.14649100	1.33336200	1.51556500
H	-2.77765200	-0.11786900	2.46469000
H	-0.68021800	0.76451700	3.23929300
H	0.81863600	-0.15398200	3.05062100
H	0.77269000	1.55030900	2.61562200
H	-2.66606000	-2.24564900	0.17162100
H	-3.55723300	-1.55989700	-1.21586700
H	-2.03894400	0.33466700	-1.35070100
H	-0.14604000	0.27912600	-2.83099400
H	1.24978500	-0.89139300	-2.66773900
H	0.51382900	-2.78489400	-2.04248000
H	-1.32723000	-2.74357400	-2.12851100
H	-6.45955000	-1.51846200	0.34554000
H	-6.43666400	-0.36267700	1.72374400
H	-7.37842900	0.01954800	0.24401200
Co	1.08947000	0.00666700	-0.31424200
P	2.85827100	-1.60655700	0.31045600
P	2.52625900	1.85659200	-0.47495700
C	1.70546200	3.48845400	-0.22335800
H	1.13534100	3.47632900	0.70988400
H	2.44115600	4.29921700	-0.18723300
H	1.00760700	3.67917400	-1.04437700
C	3.50103500	2.10125100	-2.02449000
H	4.16006300	2.97219800	-1.93885200
H	4.10825700	1.21744500	-2.24046800
H	2.81790600	2.25792200	-2.86478400
C	3.81800800	1.81197400	0.86358600
H	4.45362600	2.69677100	0.72883000
H	3.29413700	1.94474900	1.81846600
C	4.00482200	-2.38541100	-0.92148900
H	4.48181300	-1.62064400	-1.54176200
H	4.78460800	-2.97148100	-0.42269500
H	3.44360200	-3.05244600	-1.58434300
C	4.03334800	-0.72937200	1.46478300
H	4.80947200	-1.44988800	1.75282300
H	3.46906500	-0.49668800	2.37702500
C	2.33239100	-3.05679000	1.32926200
H	3.19321700	-3.61782900	1.70949000
H	1.72720200	-2.71296900	2.17341000
H	1.71383800	-3.72771700	0.72475200
C	4.70510000	0.55105500	0.92639900
H	5.53980900	0.78409700	1.59837900
H	5.16819900	0.35948300	-0.05047500

INT3-s

N	-3.60391200	-0.82565100	0.34039300
C	-2.54449300	-0.54256300	1.34349100
C	-1.28851900	-0.26795700	0.51239600
C	-0.00907700	-0.24568600	0.88854000
C	0.44538300	-0.32806500	2.31889400
C	-2.93777000	-1.14009000	-0.94706600
C	-1.71815700	-0.19731100	-0.94009000
C	-0.51091300	-0.44976200	-1.81135500
C	0.17092500	0.67490900	-2.29896500
C	0.23914000	-1.65107700	-1.69692500
S	-4.86676700	0.34748300	0.23991100
O	-4.82863400	1.12902300	1.47935300
O	-4.80765000	1.01334600	-1.06877300
C	-6.32827000	-0.69885100	0.26827900
H	-2.85047100	0.29149200	1.97984100
H	-2.40788000	-1.42499800	1.98024500
H	1.04061900	-1.22431100	2.52943300
H	1.05138000	0.53511900	2.61786500
H	-0.41918600	-0.35367400	2.99435200
H	-2.63915500	-2.19498900	-0.93536200
H	-3.61207200	-0.96942400	-1.78605100
H	-2.10637500	0.80726100	-1.15707500
H	-0.30290000	1.65150300	-2.31166700
H	0.99504900	0.54015000	-3.00522000
H	0.94962400	-1.89196600	-2.48904500
H	-0.18348700	-2.50663100	-1.17905100
H	-6.29616900	-1.38075300	-0.58352400
H	-6.34419800	-1.24819300	1.21044800
H	-7.19374300	-0.03630800	0.19102700
Co	1.20216000	-0.15205200	-0.64137700
P	2.79969900	-1.48766800	0.18558100
P	2.15613200	1.82889600	-0.06085100
C	3.41756200	1.76884700	1.30473200
H	3.92679200	2.74062800	1.32063900
H	2.88023000	1.68651200	2.25680800
C	0.99557000	3.14898200	0.48878800
H	1.54076100	4.04455000	0.80502000
H	0.32625100	3.41184000	-0.33530100
H	0.38325700	2.78599900	1.31817300
C	3.09558500	2.63228400	-1.43791400
H	2.42812200	2.82702000	-2.28223100
H	3.52828500	3.58230800	-1.10594000

H	3.90617500	1.98446800	-1.78641700
C	3.93569900	-1.81131000	-1.24143500
H	4.28419300	-0.87411000	-1.68624200
H	4.80854000	-2.38699300	-0.91435900
H	3.41073500	-2.38214100	-2.01296200
C	3.93744400	-0.78139000	1.47426000
H	4.78555800	-1.47146300	1.56906700
H	3.40982000	-0.80236700	2.43474300
C	2.43722300	-3.18448500	0.80718300
H	3.36334200	-3.70381600	1.07605800
H	1.78622900	-3.14603600	1.68459500
H	1.92467200	-3.75360800	0.02636900
C	4.46312800	0.64128700	1.19516700
H	4.96304500	0.67683800	0.21820500
H	5.25034500	0.84738400	1.92995700

INT3-t

N	-3.77714200	-0.80809500	0.47591700
C	-2.81539800	-0.33943100	1.50771200
C	-1.45037800	-0.39973300	0.82815500
C	-0.21766300	-0.38362900	1.34711800
C	0.17033000	-0.29075400	2.79232400
C	-3.00383600	-1.51604200	-0.57229600
C	-1.69366400	-0.70097300	-0.65030700
C	-0.44633600	-1.30975700	-1.26026000
C	0.28048800	-2.27215800	-0.48595100
C	0.20802400	-0.66451900	-2.29640300
S	-4.86848400	0.39145600	-0.11661500
O	-4.91068400	1.46357400	0.88211400
O	-4.54969700	0.69065500	-1.52053700
C	-6.43070000	-0.49680400	-0.07583300
H	-3.10161300	0.65565000	1.85653500
H	-2.84860600	-1.02043500	2.36751800
H	0.66928100	-1.21228300	3.12231900
H	0.87193300	0.53198100	2.98365300
H	-0.69996900	-0.13681500	3.44483000
H	-2.81946600	-2.54267500	-0.23373200
H	-3.55415900	-1.54273500	-1.51251500
H	-1.94040700	0.22208500	-1.19274200
H	1.08065500	-2.82119200	-0.97657700
H	-0.20459700	-2.79821200	0.32725700
H	1.06932900	-1.11498900	-2.78329500
H	-0.25064400	0.18133400	-2.79986800
H	-6.35551800	-1.38010100	-0.71276900
H	-6.64583100	-0.77474700	0.95668500
H	-7.19274500	0.18473200	-0.46146700
Co	1.10054000	-0.33257900	-0.12327000
P	3.41132300	-1.19677800	0.01818400
P	1.76884900	1.92968600	-0.23826500
C	3.27843500	2.28398400	0.78898400
H	3.51303500	3.34855200	0.66140900
H	2.99422300	2.15102600	1.84096400
C	0.51991800	3.11970300	0.40958200
H	0.90917800	4.14331300	0.39536400
H	-0.38431900	3.07412600	-0.20464100
H	0.24640700	2.85066700	1.43355400
C	2.19595200	2.61695300	-1.89824000
H	1.31532300	2.57763200	-2.54582100
H	2.52700000	3.65780500	-1.81371500
H	2.98886400	2.02872200	-2.36880700
C	4.33803400	-1.47536900	-1.55875700
H	4.35713200	-0.56161200	-2.15999400
H	5.36820200	-1.79078000	-1.36029100
H	3.84230400	-2.25496300	-2.14601500
C	4.50583900	-0.01958800	0.96271800
H	5.52415400	-0.42813100	0.93934300
H	4.18140900	-0.05340600	2.01119900
C	3.67029100	-2.78143100	0.93101800
H	4.73535800	-3.02210000	1.01784900
H	3.23897800	-2.70576400	1.93384300
H	3.16766900	-3.59990900	0.40677600
C	4.53309300	1.44296600	0.47527800
H	4.76519600	1.48603900	-0.59677800
H	5.37930600	1.93222300	0.97217900

TS3-s

N	-3.27850400	-0.80257300	-0.00493300
C	-2.44674100	-1.47249500	-1.04936600
C	-1.16087700	-1.73758900	-0.31875000
C	0.13704600	-1.78610000	-0.70720700
C	0.58809000	-2.13715300	-2.09866400
C	-2.63600700	-0.84275500	1.34643300
C	-1.49212100	-1.84545500	1.15250700
C	-0.12816200	-1.68532700	1.78073200
C	0.82961500	-2.49478400	1.00700800
C	0.29755400	-0.67118800	2.60503800
S	-4.04648300	0.65511600	-0.42904500
O	-4.11929800	1.45989100	0.79402300
O	-3.40945800	1.19610900	-1.64045900
C	-5.70637400	0.12763800	-0.87233000
H	-2.93587100	-2.40730000	-1.36149800
H	-2.33361400	-0.82951900	-1.92480500
H	1.28433600	-1.41189700	-2.52712700
H	1.08156100	-3.11748700	-2.10540600
H	-0.27576200	-2.21484400	-2.76977300
H	-2.26987700	0.14459800	1.63490900

H	-3.36089400	-1.16718800	2.09678200
H	-1.87025900	-2.86062000	1.36461300
H	0.55881700	-3.51023400	0.72483300
H	1.87072400	-2.46313600	1.34497800
H	1.28270500	-0.69631400	3.06065100
H	-0.41169700	0.03092200	3.03223000
H	-5.64593100	-0.57683900	-1.70426000
H	-6.17049800	-0.33338000	0.00078900
H	-6.25571400	1.02293900	-1.17364300
Co	1.11105900	-0.49089700	0.47071900
P	0.96674500	1.74423900	0.41933200
P	3.16424200	-0.41451500	-0.39269500
C	3.53051200	0.82659700	-1.72394500
H	4.59631900	0.75175500	-1.97360800
H	2.97186200	0.51983900	-2.61796600
C	3.89038300	-1.96785100	-1.09109800
H	4.95246500	-1.81729700	-1.31182500
H	3.79966700	-2.78402200	-0.36745600
H	3.38237100	-2.26460100	-2.01066200
C	4.41976300	-0.02266900	0.91200800
H	4.40794700	-0.80677000	1.67583900
H	5.42545800	0.02751100	0.47947000
H	4.20026100	0.92688600	1.40477000
C	1.70597900	2.72531200	1.80300400
H	2.77589000	2.52907800	1.90989000
H	1.56036100	3.79784300	1.63410200
H	1.21793000	2.44970100	2.74254700
C	1.68464100	2.53254100	-1.10360400
H	1.50215800	3.61161700	-1.02745100
H	1.08918300	2.17216800	-1.95260900
C	-0.75685600	2.39344300	0.37285300
H	-0.73534400	3.48641000	0.29634800
H	-1.30435300	1.99597500	-0.48588800
H	-1.30154600	2.12678200	1.28147800
C	3.17811800	2.28024200	-1.36448800
H	3.77632700	2.61310100	-0.50692800
H	3.48755800	2.91637600	-2.20234000

TS3-t

N	3.36475300	0.46636100	0.07445500
C	2.64041600	0.04516200	1.30899700
C	1.44286200	-0.72643000	0.78755700
C	0.24707000	-0.98638000	1.34370300
C	-0.15433700	-0.99317300	2.78616800
C	2.51821700	0.17444900	-1.11339500
C	1.71918600	-1.05984400	-0.67262900
C	0.39450700	-1.47087100	-1.26870700
C	-0.29917400	-2.39541700	-0.37420700
C	-0.23794800	-0.84829300	-2.30428700
S	5.01003200	-0.04933000	-0.03851300
O	5.38717700	-0.57256000	1.27711600
O	5.16437000	-0.86118700	-1.25079200
C	5.87131600	1.50772500	-0.29599400
H	3.29703800	-0.56248000	1.94023200
H	2.33615000	0.92402400	1.88856500
H	-1.13121400	-0.52758000	2.96296600
H	-0.21721000	-2.02476400	3.15605300
H	0.59045900	-0.47279500	3.40423200
H	1.86071800	1.03390300	-1.29725700
H	3.14229100	0.00433300	-1.99008400
H	2.40974000	-1.91878000	-0.71373300
H	0.29920400	-3.10412900	0.18904300
H	-1.23488400	-2.82956900	-0.72029300
H	-1.17669700	-1.22624500	-2.69760100
H	0.24720900	-0.06143400	-2.87288700
H	5.50557900	1.96880700	-1.21525200
H	5.69504700	2.15256500	0.56608000
H	6.93389400	1.26978800	-0.38789700
Co	-1.10981800	-0.43438300	0.03871500
P	-1.60265000	1.92147700	-0.05739200
P	-3.51346900	-1.03171400	-0.08101100
C	-4.58950400	0.19625200	0.82125500
H	-5.63179600	-0.12144700	0.69063800
H	-4.36600700	0.09498000	1.89187400
C	-4.06864600	-2.62994400	0.66977200
H	-5.15588200	-2.74678200	0.60418400
H	-3.59625500	-3.47139300	0.15274300
H	-3.77147800	-2.67035700	1.72252700
C	-4.29155400	-1.10343300	-1.76072900
H	-3.83790000	-1.91251500	-2.34267600
H	-5.36948700	-1.28747000	-1.69261400
H	-4.12636100	-0.16731900	-2.30250800
C	-1.85949800	2.66016000	-1.73417400
H	-2.63440100	2.11288200	-2.27832900
H	-2.15119100	3.71393800	-1.66339100
H	-0.93243900	2.58989900	-2.31146900
C	-3.16277300	2.38818700	0.84824700
H	-3.29391800	3.47241600	0.73969600
H	-2.98514600	2.20109300	1.91574300
C	-0.36854200	3.07435800	0.69707600
H	-0.70449800	4.11482500	0.62964000
H	-0.21628200	2.82023600	1.75070800
H	0.59252000	2.98119300	0.18172000
C	-4.45340600	1.67326700	0.40203300
H	-4.59130800	1.77713400	-0.68187500

H	-5.29395000	2.21502700	0.85227900

INT4-s

N	-3.12490800	0.00694400	0.62975300
C	-3.12844000	1.48586300	0.38443400
C	-1.93239700	1.67103800	-0.50293000
C	-0.97373300	2.59775400	-0.63469500
C	-0.92095700	3.97933700	-0.05847900
C	-1.95347500	-0.62133700	-0.04197000
C	-1.62731200	0.36151900	-1.18593800
C	-0.23539100	0.59048600	-1.74189200
C	0.14771600	2.03604900	-1.49183500
C	0.55309800	-0.21366300	-2.54286700
S	-4.63103200	-0.79520400	0.43721800
O	-5.52987100	0.03393100	-0.37297100
O	-4.32277800	-2.17513300	0.04859100
C	-5.26200000	-0.80604300	2.12127900
H	-4.06367200	1.77816000	-0.10650900
H	-3.04512900	2.03396800	1.32982700
H	0.00744000	4.15033200	0.50241400
H	-0.95622500	4.73959200	-0.85015600
H	-1.76296100	4.16712300	0.61404800
H	-1.11732500	-0.66711600	0.66758100
H	-2.21217700	-1.62967000	-0.36255800
H	-2.32725700	0.16753400	-2.01382800
H	0.37769700	2.59614500	-2.40941800
H	1.13979700	2.10484000	-0.91905600
H	1.31551900	0.21111600	-3.19575800
H	0.23297300	-1.21995200	-2.79501400
H	-4.57340700	-1.37058600	2.75113700
H	-5.36350600	0.22311600	2.47162800
H	-6.24161200	-1.28913000	2.08886900
Co	1.47005300	0.25817500	-0.70495200
P	1.98668900	-1.86465800	-0.37601800
P	2.98684600	1.01214800	0.81263100
C	3.44307700	-0.09422500	2.22965300
H	4.27484800	0.37789100	2.76720100
H	2.58758700	-0.10869400	2.91747500
C	2.55602400	2.58548500	1.68395200
H	3.34388100	2.86420000	2.39212300
H	2.43633800	3.39688700	0.95950800
H	1.61509800	2.46690700	2.22970500
C	4.61729300	1.41590000	0.03663500
H	4.47631000	2.16053600	-0.75277600
H	5.31580600	1.81617300	0.77973300
H	5.05809900	0.52447200	-0.41880700
C	3.31116300	-2.40803800	-1.54571900
H	4.21529900	-1.80696500	-1.41501000
H	3.56106100	-3.46260300	-1.38616200
H	2.96713400	-2.27873700	-2.57583500
C	2.64372800	-2.36166400	1.29147500
H	2.93714000	-3.41638900	1.21892300
H	1.80094100	-2.31807700	1.99380200
C	0.67992100	-3.14897200	-0.61488500
H	1.10663600	-4.14720800	-0.46890200
H	-0.12822800	-3.00570600	0.10726700
H	0.25709400	-3.09731100	-1.62107900
C	3.81703500	-1.53187300	1.83513800
H	4.64818500	-1.52827100	1.11843900
H	4.20212300	-2.03706600	2.72883500

INT4-t

N	-2.71316600	-0.39476200	0.33660700
C	-3.19396100	1.02038700	0.18577500
C	-2.15815700	1.61255700	-0.71950000
C	-1.51411900	2.78203500	-0.82405800
C	-1.81021200	4.07747000	-0.13321600
C	-1.54635600	-0.66000100	-0.54663500
C	-1.55681700	0.50863700	-1.55139200
C	-0.26086300	1.13265500	-2.05407900
C	-0.36093700	2.64809300	-1.81247600
C	0.70310200	0.49702500	-2.78486300
S	-3.92609400	-1.60971700	0.36882600
O	-5.12789000	-1.12737200	-0.31799900
O	-3.26781300	-2.85392600	-0.04036300
C	-4.30216200	-1.71255800	2.12502700
H	-4.19469400	1.02499600	-0.26340100
H	-3.24925700	1.51482000	1.16179000
H	-0.91579800	4.48462000	0.35767400
H	-2.14260000	4.83865200	-0.85172100
H	-2.59811900	3.96919600	0.61823200
H	-0.62482900	-0.63907100	0.06940800
H	-1.62369600	-1.65224300	-0.99074700
H	-2.20742100	0.23983200	-2.39886700
H	-0.56892300	3.16752600	-2.76173700
H	0.56938400	3.09522600	-1.43070700
H	1.50779900	1.05647500	-3.26034300
H	0.57858500	-0.53371300	-3.10373600
H	-3.40447300	-2.02228800	2.66145200
H	-4.65830600	-0.74129500	2.47459700
H	-5.09249400	-2.45945300	2.23291200
Co	1.31304600	0.44922000	-0.62825900
P	2.81659800	-1.38598000	-0.85344600
P	1.80554700	0.96882200	1.62317300
C	2.43530800	-0.50050200	2.57650600
H	2.73370800	-0.13965600	3.56917600

H	1.58084600	-1.17226200	2.73182500
C	0.40656500	1.55357100	2.68048800
H	0.72718200	1.70260500	3.71730600
H	0.01796900	2.49866400	2.28962500
H	-0.40390700	0.81825600	2.65854100
C	3.10414300	2.25539400	1.90658500
H	2.78241800	3.20787600	1.47400800
H	3.28801500	2.39934200	2.97678800
H	4.04191800	1.96521200	1.42326300
C	4.48144000	-0.89972900	-1.50452500
H	4.92163000	-0.11214300	-0.88490100
H	5.16502600	-1.75556400	-1.52374700
H	4.38052600	-0.51001500	-2.52252900
C	3.22684200	-2.21123400	0.76739200
H	4.05071000	-2.91216600	0.58195200
H	2.35704200	-2.82108400	1.04545200
C	2.38618500	-2.83821900	-1.91423600
H	3.17176100	-3.60106300	-1.88265600
H	1.44680500	-3.28669000	-1.57541800
H	2.25654600	-2.51521300	-2.95199800
C	3.60230900	-1.28244100	1.93907900
H	4.40891900	-0.59793400	1.64430300
H	4.03474000	-1.91268100	2.72548800

Sub

N	0.52017900	-0.62071400	0.39303200
C	0.20338300	0.47365700	1.32716500
C	0.02666900	1.79667200	0.70471300
C	-0.12734700	2.88647200	0.20016600
C	-0.31375100	4.20715800	-0.39746200
C	-0.51251200	-0.96412100	-0.60568500
C	-1.71840500	-1.57397800	0.06135700
C	-2.94375500	-1.07966300	-0.04159300
C	-4.37143200	-1.18824200	0.28316100
C	-3.83109500	-0.04206900	-0.59057800
S	2.13812000	-0.85265800	-0.01739100
O	2.91628600	-0.58621300	1.19473900
O	2.21677400	-2.13987800	-0.71130600
C	2.56749600	0.42822200	-1.22121800
H	-0.72066300	0.18395900	1.84119000
H	0.99663500	0.50155700	2.07861100
H	-1.30266800	4.61593100	-0.15734600
H	0.43786300	4.91861400	-0.03478300
H	-0.23027200	4.16392800	-1.49021000
H	-0.80974000	-0.07650000	-1.18176800
H	-0.06137300	-1.69207900	-1.28630300
H	-1.53638000	-2.47471900	0.64680700
H	-4.96470900	-1.96285500	-0.20104100
H	-4.70275800	-0.94671900	1.29232800
H	-3.80134200	0.95791200	-0.15995200
H	-4.06905600	-0.05699800	-1.65346500
H	1.96355400	0.29038200	-2.12068100
H	2.38292500	1.40787300	-0.77720100
H	3.62682100	0.30132400	-1.45677600

Pro

N	0.91120100	-0.08872200	0.30861900
C	0.11754000	-1.27282400	-0.14710800
C	-1.25648500	-0.68663700	-0.26898300
C	-2.50257700	-1.10694100	-0.02196500
C	-2.96995400	-2.49611800	0.28724200
C	0.07204900	1.14014300	0.41429000
C	-1.15032500	0.80578000	-0.46440400
C	-2.54051500	1.29511400	-0.09418000
C	-3.46347400	0.07425600	-0.06320100
C	-2.88595900	2.54906000	0.19600700
S	2.52024800	0.03093500	-0.16096200
O	2.81524100	-1.08443800	-1.06797400
O	2.80071500	1.41822400	-0.54973000
C	3.41740300	-0.27841700	1.37262900
H	0.51824100	-1.64533800	-1.09605200
H	0.17283700	-2.08658100	0.58611100
H	-3.53814000	-2.52152600	1.22709700
H	-3.64351800	-2.87250000	-0.49529300
H	-2.13536400	-3.19963300	0.37219200
H	-0.23489000	1.29016500	1.45665300
H	0.64403800	2.00577000	0.07971400
H	-0.90239100	1.05542100	-1.50916500
H	-4.11540200	0.03742700	-0.95137800
H	-4.13827100	0.08362500	0.80480200
H	-3.90334000	2.81256900	0.47590200
H	-2.16723100	3.36420400	0.16161800
H	3.14221500	0.48621400	2.10150700
H	3.16075700	-1.27469000	1.73755600
H	4.48422000	-0.21982200	1.14346700

MECP1

N	2.91425400	0.76564000	0.80442900
C	2.17189600	0.27873300	1.95669700
C	0.76779100	-0.08193100	1.68273100
C	-0.34220900	-0.59932400	2.03515500
C	-1.07528000	-1.41781700	3.01271300
C	2.19752400	1.78128300	0.03112100
C	1.01210600	1.28669200	-0.74554200
C	-0.18689800	1.97695000	-0.86772000
C	-0.93477500	2.60162300	-1.97359200
C	-0.62745500	3.37782900	-0.70463900
S	3.81928100	-0.35785600	-0.06742400
O	3.70361600	-1.62482900	0.61089300

O	3.48364400	-0.22267900	-1.46711400
C	5.47173800	0.25084800	0.13422600
H	2.69325300	-0.58527100	2.37245000
H	2.18575300	1.06382800	2.72312700
H	-1.35989000	-2.38184300	2.58064800
H	-0.46108800	-1.62097900	3.89354300
H	-1.99760400	-0.94124700	3.35230000
H	1.90276700	2.57067500	0.73041000
H	2.90696400	2.23028600	-0.67180300
H	1.27995100	0.58439600	-1.53287100
H	-0.37145500	2.84327800	-2.86984600
H	-1.97005000	2.35309000	-2.16279900
H	-1.47074000	3.60054700	-0.05757500
H	0.11634600	4.16828700	-0.73760000
H	5.51462600	1.27238000	-0.23871500
H	5.73952100	0.21025000	1.18747400
H	6.13099100	-0.38772500	-0.45216100
Co	-0.53511600	0.36864600	0.34154100
P	-2.81917600	0.51785700	0.51690200
P	-0.72903800	-1.41178800	-1.15760700
C	0.75685800	-2.45015200	-1.23822500
H	0.97138400	-2.86363400	-0.25114300
H	0.62168800	-3.26825800	-1.94995200
H	1.61727300	-1.85009600	-1.54095600
C	-1.02751500	-0.93256700	-2.88908600
H	-1.07839100	-1.81445700	-3.53223200
H	-1.95645900	-0.36956300	-2.98656500
H	-0.21218800	-0.29463600	-3.23465400
C	-2.06829300	-2.60613800	-0.78464300
H	-2.06608700	-3.36020600	-1.57889500
H	-1.77845200	-3.12764700	0.13464100
C	-3.85003600	1.35155100	-0.74370500
H	-3.68839700	0.93062600	-1.73684900
H	-4.90689000	1.23708500	-0.49058500
H	-3.62097700	2.41641700	-0.78257700
C	-3.65413900	-1.11953000	0.59210600
H	-4.72127400	-0.92706800	0.74482100
H	-3.30327600	-1.63542500	1.49032200
C	-3.40867400	1.34925000	2.03173600
H	-4.49021000	1.23881600	2.13941100
H	-2.91999500	0.94855300	2.91936200
H	-3.17160700	2.41285000	1.97493400
C	-3.46145800	-2.00720100	-0.63459100
H	-4.17993700	-2.82950600	-0.57234600
H	-3.73763600	-1.46261800	-1.54524400

MECP1'

N	2.91758421	0.01070789	0.03229136
C	2.33694842	-0.78010444	1.13299343
C	0.85336928	-0.79586568	1.09537657
C	-0.23622781	-1.23758374	1.60311081
C	-0.85666027	-2.18377785	2.56794686
C	2.27013796	1.32396504	-0.13673388
C	0.97651099	1.18846922	-0.89231671
C	-0.12175133	1.99115609	-0.69858217
C	-0.96600855	2.91328188	-1.49284889
C	-0.38250235	3.34277412	-0.13965289
S	4.64604839	0.07470309	0.09253500
O	5.04176938	1.22627967	-0.71950127
O	5.09001666	-0.06635261	1.48254173
C	5.09538365	-1.42544833	-0.79608963
H	2.70241449	-1.81132291	1.06308983
H	2.66048001	-0.39242496	2.11175883
H	-1.34272864	-3.01255992	2.03806042
H	-0.09932709	-2.61226645	3.23428554
H	-1.62300355	-1.70735164	3.18785228
H	2.11422779	1.83508560	0.82412572
H	2.95027601	1.94160427	-0.73365699
H	1.06435394	0.62815647	-1.82290519
H	-0.53286882	3.34073968	-2.39541591
H	-2.04032487	2.77397446	-1.54222109
H	-1.08582847	3.46620620	0.68014392
H	0.43248272	4.06437947	-0.12704557
H	4.67202189	-2.29692221	-0.29244856
H	4.73883085	-1.34433400	-1.82336242
H	6.18661946	-1.47873842	-0.76975177
Co	-0.62009246	0.13054528	0.26119316
P	-2.79209645	0.62229231	0.97392791
P	-1.40992752	-1.11397509	-1.51322193
C	-0.16159593	-2.33710017	-2.10096045
H	0.12645553	-2.98927894	-1.27180138
H	-0.56145551	-2.94470669	-2.91987163
H	0.73411794	-1.81383921	-2.44836801
C	-1.90128652	-0.22845020	-3.05520589
H	-2.20022754	-0.94004389	-3.83260129
H	-2.73064405	0.45679324	-2.86108138
H	-1.05668282	0.36189204	-3.42167352
C	-2.87181512	-2.18297754	-1.09912749
H	-3.16253422	-2.71376469	-2.01482665
H	-2.51371041	-2.94454159	-0.39448943
C	-3.87917524	1.92237896	0.22128386
H	-4.04733127	1.73433960	-0.84295530
H	-4.85056171	1.93344702	0.72842863
H	-3.42491297	2.91152734	0.32638285
C	-3.90709700	-0.86446617	0.89779726
H	-4.88297856	-0.56987755	1.30304032
H	-3.49785061	-1.62407056	1.57342522
C	-2.84443294	1.12160102	2.75482265
H	-3.87643673	1.17044419	3.11939761
H	-2.27782573	0.42084711	3.37263746
H	-2.38838350	2.11091344	2.86526421
C	-4.10031713	-1.46414727	-0.50984252
H	-4.91036242	-2.20083265	-0.44717220
H	-4.45707553	-0.69406654	-1.20607181

MECP2

N	-3.65915118	0.77801710	-0.45143524
C	-2.63701204	0.42504306	-1.45429202
C	-1.36355438	0.23874558	-0.66881682
C	-0.08537624	0.19944181	-1.07896368
C	0.31292366	0.22696815	-2.51536167
C	-2.95637298	1.15567002	0.78554840

C	-1.73959858	0.22877444	0.79122419
C	-0.54083978	0.54502884	1.63915333
C	0.16984060	-0.49662798	2.27140234
C	0.16815967	1.74570519	1.43868185
S	-4.88221822	-0.39058958	-0.22550720
O	-5.01650633	-1.08366314	-1.47936956
O	-4.65018034	-1.10989757	1.00560351
C	-6.28929137	0.66173345	0.00905936
H	-2.95370617	-0.45631939	-2.01723977
H	-2.52832969	1.24433430	-2.17515626
H	1.03902790	1.02019353	-2.72441678
H	0.79287437	-0.70877811	-2.82407149
H	-0.53211153	0.38298488	-3.19567413
H	-2.65352724	2.20692259	0.71442351
H	-3.60857239	1.03769932	1.64982468
H	-2.10638935	-0.77247635	1.05931329
H	-0.27517865	-1.48337276	2.35806773
H	0.92237118	-0.25485869	3.02097925
H	0.87080180	2.07939990	2.19860144
H	-0.24957639	2.52834422	0.81351086
H	-6.11303998	1.30471335	0.86987778
H	-6.43972269	1.24963091	-0.89309899
H	-7.14470295	0.01493042	0.19746485
Co	1.09559308	0.11900008	0.50438001
P	2.95084380	1.42657282	0.04180114
P	2.14275704	-1.78242611	0.02946788
C	3.40124745	-1.72067694	-1.30657160
H	3.85728134	-2.71496927	-1.36296696
H	2.86907216	-1.57270977	-2.25236777
C	1.01985984	-3.10591600	-0.50899251
H	1.56416909	-4.03312081	-0.70113983
H	0.27055743	-3.28912620	0.26214819
H	0.49716753	-2.80099948	-1.41602177
C	3.05366173	-2.51982980	1.42617676
H	2.35412099	-2.79356668	2.21696328
H	3.59795709	-3.41440947	1.11468793
H	3.76336464	-1.80444564	1.84415212
C	4.14828941	1.73512487	1.38243763
H	4.62185802	0.80629756	1.70240644
H	4.92555241	2.42789622	1.05079431
H	3.64283088	2.16780672	2.24663943
C	3.99207180	0.77586858	-1.31990830
H	4.84074840	1.45913375	-1.43027067
H	3.40613104	0.86103061	-2.24135275
C	2.53241832	3.10080623	-0.53320066
H	3.41439196	3.61599874	-0.91985302
H	1.77543107	3.04698714	-1.31625706
H	2.12223421	3.68141806	0.29367283
C	4.48251685	-0.65696706	-1.14150689
H	4.98453576	-0.77028032	-0.17298744
H	5.26117172	-0.84462511	-1.88627795

MECP2'

N	-3.69807800	-0.91383200	0.42532500
C	-2.65814800	-0.63783200	1.45035500
C	-1.35224300	-0.49901800	0.66754200
C	-0.08247200	-0.46461300	1.08719300
C	0.38176900	-0.52964600	2.51283200
C	-2.99881500	-1.40191600	-0.78798000
C	-1.71826000	-0.54105000	-0.81385600
C	-0.51323300	-0.94641800	-1.63280600
C	0.28366700	-2.05123500	-1.21570600
C	0.08978500	0.00969400	-2.45186200
S	-4.80223500	0.38495700	0.13957500
O	-4.81333600	1.20757500	1.35229600
O	-4.52443200	0.99352500	-1.17085500
C	-6.36188400	-0.49973900	0.02024900
H	-2.93241100	0.24631600	2.03079600
H	-2.60539200	-1.49125500	2.13787200
H	0.95712000	-1.44585000	2.70150300
H	1.03616300	0.31162900	2.77679800
H	-0.45572000	-0.52302400	3.22344000
H	-2.77246000	-2.46681600	-0.65428400
H	-3.61985900	-1.27858100	-1.67534900
H	-2.03837000	0.45728900	-1.14049700
H	1.03612700	-2.43455900	-1.90446900
H	-0.10619400	-2.77012900	-0.50342700
H	0.91755000	-0.26139500	-3.10568100
H	-0.41983600	0.94093800	-2.68090900
H	-6.30039600	-1.22631500	-0.79242900
H	-6.55690800	-0.99095400	0.97436700
H	-7.12947000	0.24677200	-0.19698500
Co	1.12859300	-0.27742000	-0.47356700
P	3.23837400	-1.26730300	0.13146000
P	1.82474600	1.91886100	-0.17140700
C	3.19265900	2.13212500	1.06912600
H	3.47561600	3.19213300	1.06057900
H	2.77028200	1.93201200	2.06167100
C	0.48890800	3.01911200	0.46320000
H	0.87072000	4.02856300	0.65060700
H	-0.32002500	3.07595000	-0.27138700
H	0.07637800	2.60895300	1.38868300
C	2.44887200	2.82390600	-1.65581100
H	1.66834100	2.85293600	-2.42169700
H	2.72587800	3.85102600	-1.39420800
H	3.32182200	2.31798600	-2.07894200
C	4.34477300	-1.59738500	-1.31622600
H	4.52937200	-0.67625900	-1.87729400
H	5.30549100	-2.01090800	-0.98967900
H	3.86867700	-2.31416900	-1.99249600
C	4.29254800	-0.22012000	1.24917800
H	5.28222500	-0.69136800	1.30226600
H	3.85958100	-0.28553100	2.25505200
C	3.20829300	-2.88875900	1.01093000
H	4.22362900	-3.24372000	1.21846300
H	2.66970600	-2.79021500	1.95760000
H	2.68901000	-3.63314800	0.40045700
C	4.44356500	1.25883500	0.84490400
H	4.78718400	1.33904300	-0.19498600
H	5.25309300	1.68269300	1.45053000

MECP3

N	3.67268697	0.14474533	-0.27626798
C	2.75132032	-0.51206009	-1.24349095
C	1.38979718	-0.07356556	-0.74357740
C	0.15572443	-0.55028872	-0.98491733
C	-0.19475260	-1.52956045	-2.07502028
C	2.92871553	0.54069260	0.94653750
C	1.57762952	0.95755637	0.32894990
C	0.30374988	0.99216356	1.13704306
C	0.07006805	1.87439926	2.31071556
C	0.10235892	0.36315518	2.51183255
S	5.18895370	-0.59908623	-0.01519282
O	5.56019363	-0.28933419	1.36705541
O	5.13363655	-1.98258586	-0.49927376
C	6.25998896	0.33322283	-1.12036780
H	2.96181044	-0.15887174	-2.26186973
H	2.86549684	-1.60242338	-1.23420892
H	0.66325250	-1.70968687	-2.73666718
H	-0.50864394	-2.50277189	-1.67990569
H	-1.00925395	-1.15817352	-2.71089388
H	2.80060021	-0.29810255	1.64384025
H	3.45589857	1.34552467	1.46015094
H	1.72651155	1.94380388	-0.13882463
H	0.91260596	2.46094629	2.67474276
H	-0.89280918	2.35566998	2.47330921
H	-0.86664993	-0.08400197	2.77217128
H	0.93472007	-0.13175818	3.00454745
H	5.89728125	0.22981312	-2.14508507
H	6.26144918	1.37780028	-0.80616577
H	7.26054658	-0.09677959	-1.03154388
Co	-1.12814742	-0.05205884	0.38335050
P	-2.95129191	-1.61441726	0.33692677
P	-2.37802682	1.71773300	-0.43906735
C	-1.35118560	2.98723217	-1.28541387
H	-0.71013004	2.50521664	-2.02876638
H	-1.97486282	3.74111396	-1.77711678
H	-0.70955123	3.47735912	-0.54745666
C	-3.45205790	2.70975871	0.69192460
H	-3.98744590	3.48352977	0.13021182
H	-4.18110751	2.07242117	1.19979362
H	-2.83494668	3.19597849	1.45256541
C	-3.53799409	1.12668240	-1.76797594
H	-4.04575083	2.01346147	-2.16902110
H	-2.91656653	0.72720795	-2.57955190
C	-4.09009834	-1.43533885	1.78646006
H	-4.42219836	-0.39986481	1.90360166
H	-4.96990522	-2.07777426	1.67054520
H	-3.56458956	-1.72727271	2.70132956
C	-4.06457555	-1.35556316	-1.13217852
H	-4.91589910	-2.04053581	-1.02958711
H	-3.50482843	-1.68063622	-2.01856522
C	-2.64621201	-3.43497079	0.31328756
H	-3.59403190	-3.98401740	0.30982376
H	-2.07193875	-3.71556427	-0.57324902
H	-2.07256074	-3.72471045	1.19888839
C	-4.58793984	0.07906321	-1.34441191
H	-5.33869378	0.03392652	-2.14251386
H	-5.13283890	0.42075668	-0.45531697

INT1-s-dppp

N	-3.21825900	-1.49634400	-0.89196900
C	-2.79369300	-2.02989600	0.41372000
C	-1.41727000	-1.61132000	0.75840000
C	-0.43157000	-1.71866500	1.58371300
C	0.02484300	-2.35224000	2.84921700
C	-2.15750600	-1.48863000	-1.91116900
C	-1.19996700	-0.34229900	-1.70369100
C	0.14349800	-0.42315300	-2.00936100
C	1.10732800	0.18806000	-2.95820600
C	0.97043700	-1.33235900	-2.85057900
S	-4.75577100	-2.06923500	-1.40069300
O	-4.78048600	-1.98447900	-2.86244500
O	-5.05200200	-3.32508600	-0.70371100
C	-5.85336100	-0.80090600	-0.74653800
H	-3.47958000	-1.66561300	1.18834700
H	-2.84528500	-3.12968400	0.43119600
H	-0.13571800	-1.67317100	3.69753100
H	-0.54533700	-3.26653900	3.05312900
H	1.08802200	-2.60665300	2.82694600
H	-1.61512400	-2.44465500	-1.94784400
H	-2.64852000	-1.35498800	-2.88064400
H	-1.68052600	0.63380800	-1.64791200
H	0.69688300	0.67839300	-3.83990200
H	2.03715000	0.61677100	-2.59986400
H	1.81867400	-1.85538800	-2.41677700
H	0.48317200	-1.87641900	-3.65786400
H	-5.73316800	-0.73649200	0.33647900
H	-5.60996700	0.14977900	-1.22194500
H	-6.87142500	-1.11086400	-0.99468300
Co	0.01249800	-0.56439200	0.11207700
P	2.30387300	-0.48941700	0.56439300
P	-0.37097800	1.47551600	0.92731800
C	0.43447400	1.57791200	2.60201900
H	0.06213000	2.48076700	3.09746400
H	0.05612500	0.72886100	3.17967700
C	2.64172800	0.23333300	2.25886700
H	3.72514800	0.33818800	2.37856400
H	2.31217400	-0.52968900	2.97296400
C	1.97282700	1.57506900	2.60603700
H	2.29475700	1.83893200	3.62136400
H	2.35213300	2.37574800	1.96325500
C	-2.15651500	1.74656300	1.29659400
C	-2.91997700	2.64616900	0.53651300
C	-2.77356800	1.05422200	2.35250100
C	-4.26992800	2.85151600	0.83060500
H	-2.46405500	3.20270400	-0.27572800
C	-4.11824600	1.27196900	2.65186700
H	-2.21024400	0.34302500	2.94905400
C	-4.87079600	2.17045000	1.88979400
H	-4.84570500	3.55596300	0.23723000
H	-4.57604000	0.74508100	3.48443600
H	-5.91674000	2.34267400	2.12662100

C	0.13131700	3.02575600	0.07363400
C	0.31437400	4.21558300	0.80363600
C	0.26602700	3.06146600	-1.32211800
C	0.63851600	5.40342600	0.14928100
H	0.19554700	4.23085700	1.88203900
C	0.58122400	4.25542100	-1.97494500
H	0.13593000	2.15666200	-1.90041000
C	0.77235300	5.42651600	-1.24148200
H	0.77941600	6.31242900	0.72670200
H	0.67999300	4.26555900	-3.05651700
H	1.02029500	6.35431700	-1.74867400
C	3.56515900	0.32755900	-0.51513700
C	4.47899600	-0.43006800	-1.26713300
C	3.60568500	1.72923300	-0.62498500
C	5.41436800	0.19779000	-2.09248000
H	4.47273800	-1.51265100	-1.20597300
C	4.54831000	2.35308300	-1.44268700
H	2.89479000	2.34741200	-0.08889200
C	5.45582400	1.58943000	-2.17974500
H	6.11343400	-0.40635900	-2.66357500
H	4.56778300	3.43731800	-1.50615800
H	6.18708400	2.07577200	-2.81865500
C	2.95668700	-2.20664400	0.73987600
C	4.14950800	-2.46381900	1.43900500
C	2.27292400	-3.28325000	0.15334800
C	4.63593200	-3.76589100	1.55639300
H	4.71235100	-1.65006500	1.88591300
C	2.76568800	-4.58542300	0.26486400
H	1.34567500	-3.10972500	-0.38317900
C	3.94552800	-4.82910200	0.96897400
H	5.55627200	-3.94847900	2.10354000
H	2.22486400	-5.40708600	-0.19587500
H	4.32710200	-5.84188100	1.05937500

TS1a-s-dppp

N	5.21541300	0.38021300	-1.05952000
C	5.14299200	-0.54676900	0.07819900
C	5.31698800	0.08858000	1.39538400
C	5.47491400	0.61807000	2.47319400
C	5.68907300	1.24680000	3.77563000
C	4.14282300	1.37198600	-1.20479600
C	2.94274400	0.75657200	-1.87920200
C	1.73104600	0.67669900	-1.34432300
C	0.98027200	0.97963700	-0.12000600
C	0.38452400	0.17079900	-1.63293700
S	6.70295200	0.64256400	-1.80912000
O	7.40190700	-0.64242400	-1.78762800
O	6.40335700	1.34828700	-3.05604400
C	7.62660400	1.77588700	-0.74693200
H	4.16863400	-1.04933400	0.02912700
H	5.90112900	-1.31846600	-0.08330100
H	6.00469500	2.29087300	3.66334300
H	4.77561700	1.24023200	4.38237600
H	6.46953500	0.72509100	4.34194700
H	3.87864400	1.78372100	-0.22158800
H	4.51737400	2.18795000	-1.82955200
H	3.11786700	0.35413200	-2.87565200
H	1.24039200	0.43608800	0.78878200
H	0.67698100	2.02606700	0.02690500
H	-0.23057700	0.76794800	-2.31913400
H	0.26120500	-0.90876400	-1.72135500
H	7.10045700	2.73153000	-0.69842800
H	7.72147000	1.33214200	0.24582900
H	8.61014000	1.91135000	-1.20324100
Co	-1.02299800	0.44121400	-0.11213000
P	-3.04827000	1.14103900	0.52987900
P	-1.23265400	-1.52125600	0.83231300
C	-2.10869000	-1.49962900	2.47825000
H	-2.13542400	-2.52894800	2.85243200
H	-1.49115500	-0.92362200	3.17709800
C	-3.59579700	0.60314100	2.22042400
H	-4.60143700	0.98684900	2.42272200
H	-2.92713300	1.11336700	2.92443800
C	-3.53360000	-0.91813400	2.44533800
H	-4.13728900	-1.44316900	1.69512000
H	-4.00113600	-1.13287100	3.41400100
C	-2.92493500	2.97418700	0.65835500
C	-3.81990900	3.84527400	0.01877500
C	-1.87214900	3.51364300	1.42074400
C	-3.66649000	5.22716000	0.14663900
H	-4.63778000	3.45009000	-0.57474900
C	-1.72704200	4.89453000	1.55093400
H	-1.16816100	2.85266400	1.92238100
C	-2.62337400	5.75381100	0.91060000
H	-4.36679600	5.89224500	-0.35030600
H	-0.91532500	5.29877600	2.14900100
H	-2.50875600	6.82943600	1.00711800
C	-4.45177000	0.81533700	-0.60791100
C	-5.74956600	0.51456000	-0.16756900
C	-4.20659200	0.89205200	-1.99053400
C	-6.77525800	0.29211900	-1.08931000
H	-5.97740300	0.45228200	0.89137800
C	-5.23412600	0.68308000	-2.90914300
H	-3.20650400	1.12391400	-2.34987600
C	-6.52130600	0.37801600	-2.45862500
H	-7.77399400	0.05644800	-0.73359000
H	-5.03041300	0.75541100	-3.97364800
H	-7.32215300	0.20894800	-3.17243700
C	0.38923700	-2.30642000	1.21193200
C	0.94029400	-3.27030100	0.35175200
C	1.13736400	-1.88404600	2.32536100
C	2.20246600	-3.80956100	0.60881200
H	0.37993300	-3.61693600	-0.51094500
C	2.39766000	-2.42575200	2.57999100
H	0.74206400	-1.13430600	3.00572800
C	2.93233000	-3.39110200	1.72283500
H	2.61119600	-4.56087500	-0.06065800
H	2.96217700	-2.09334600	3.44587500
H	3.91158000	-3.81514600	1.92448500
C	-2.15387200	-2.78353100	-0.13255500
C	-2.36088100	-4.07605900	0.38359700

C	-2.66251700	-2.46572100	-1.40019200
C	-3.06768400	-5.02333400	-0.35458100
H	-1.95650100	-4.35210600	1.35358800
C	-3.36993800	-3.41762000	-2.13826000
H	-2.51212000	-1.47027200	-1.80546000
C	-3.57383400	-4.69488400	-1.61622000
H	-3.22062300	-6.01886500	0.05182700
H	-3.76146800	-3.15805300	-3.11745500
H	-4.12335400	-5.43590500	-2.18946100

TS1b-s-dppp

N	-3.07302600	-1.81936600	0.60144900
C	-2.68814400	-2.32171600	-0.73228900
C	-1.88870900	-1.37281200	-1.52523300
C	-1.27347800	-0.84035800	-2.44154300
C	-0.80248700	-0.31580000	-3.73007400
C	-1.94093100	-1.26708700	1.38963700
C	-0.69468200	-2.12034100	1.38875200
C	0.31219900	-2.09659500	0.49097400
C	0.81545900	-2.56870200	-1.13751700
C	1.33298800	-3.10821200	0.18627000
S	-4.06675200	-2.95007700	1.45153200
O	-3.85872800	-4.29193600	0.89569600
O	-3.88014500	-2.68351200	2.87880200
C	-5.71661300	-2.40000200	0.98357600
H	-2.12930200	-3.26431700	-0.65424500
H	-3.59691700	-2.54469100	-1.30285200
H	-0.35173800	0.67588400	-3.63212200
H	-0.05408900	-0.98648000	-4.16711400
H	-1.64387900	-0.23366000	-4.42788400
H	-1.73514200	-0.28298400	0.96867500
H	-2.30326600	-1.11880800	2.40691900
H	-0.59610600	-2.82863000	2.21484200
H	0.03810900	-3.14918800	-1.62357000
H	1.55576900	-2.16220100	-1.82788200
H	2.37533300	-2.85173800	0.38113000
H	1.11285400	-4.14610800	0.44195600
H	-5.86403400	-1.38478300	1.35350200
H	-5.82542100	-2.44598800	-0.10182900
H	-6.41938600	-3.08995600	1.45704700
Co	0.24535900	-0.55418500	-0.80438900
P	-0.50034900	1.75021100	-0.72607800
P	2.45850700	0.15357000	-0.36681300
C	2.86967400	1.72231700	-1.29615900
H	3.94158800	1.90044000	-1.16282800
H	2.74042600	1.48598900	-2.35919000
C	0.64345700	2.99441600	-1.51771100
H	0.19718100	3.98726900	-1.39521500
H	0.68833600	2.79025200	-2.59452300
C	2.06607200	2.98242400	-0.94395000
H	2.03994600	3.14041000	0.14031100
H	2.59992000	3.84440900	-1.36294200
C	3.77844100	-0.94036400	-1.07336700
C	4.76420500	-1.53740200	-0.27318100
C	3.80836600	-1.16343300	-2.46207800
C	5.75266900	-2.33944400	-0.84931100
H	4.77045800	-1.37453800	0.79939300
C	4.79966000	-1.95995900	-3.03466700
H	3.06011600	-0.71084300	-3.10905600
C	5.77366700	-2.55276000	-2.22766500
H	6.50928000	-2.79315600	-0.21572900
H	4.81138800	-2.11622100	-4.10954700
H	6.54492200	-3.17456200	-2.67240300
C	3.03676000	0.47346000	1.35546600
C	3.95502800	1.49446800	1.65546200
C	2.59921900	-0.36348300	2.39658500
C	4.41358900	1.67768200	2.96071600
H	4.32819000	2.15441600	0.88027100
C	3.06834800	-0.18496100	3.69918600
H	1.88187400	-1.15058100	2.19388700
C	3.97384300	0.83819300	3.98542400
H	5.11956300	2.47524300	3.17319300
H	2.72332300	-0.84626800	4.48901200
H	4.33607200	0.97966200	4.99951000
C	-0.69931400	2.46363400	0.96400200
C	-1.29700600	3.72643000	1.13149400
C	-0.22555300	1.78134100	2.09213500
C	-1.41091300	4.28898900	2.40112500
H	-1.68705200	4.26598400	0.27301600
C	-0.33976100	2.34812500	3.36420900
H	0.23386300	0.80662100	1.98086500
C	-0.93181200	3.60067700	3.52039200
H	-1.87690000	5.26313900	2.51836100
H	0.03626700	1.80748000	4.22786500
H	-1.02440000	4.04077900	4.50910500
C	-2.12557600	2.14626700	-1.51127100
C	-2.22484600	2.80923400	-2.74440800
C	-3.30942200	1.75457700	-0.86139500
C	-3.47412000	3.07463000	-3.31271300
H	-1.33665700	3.14068000	-3.27227200
C	-4.55366500	2.02369300	-1.42817100
H	-3.26478000	1.24804500	0.09786700
C	-4.64054900	2.68282400	-2.65746800
H	-3.53014200	3.59716000	-4.26342500
H	-5.45776500	1.72391000	-0.90582800
H	-5.61105400	2.89488500	-3.09643300

TS1c-s-dppp

N	-3.29854900	-2.40857800	-1.11509400
C	-2.64592000	-2.66327200	0.17134000
C	-1.50306900	-1.70599400	0.42136100
C	-0.68400200	-1.56047800	1.44670100
C	-0.57750200	-2.24956100	2.76591500
C	-2.28227700	-1.83815700	-2.00794300
C	-1.58238600	-0.67255800	-1.32128000
C	-0.29194700	-0.18456300	-1.76209800
C	-0.03226200	0.74629200	-2.89960200
C	0.47733400	-0.68716700	-2.95413600
S	-4.79100100	-1.54077000	-1.04333900
O	-5.05944500	-1.18908600	0.35905100
O	-4.75644700	-0.50565400	-2.08146000

C	-5.96981400	-2.80479900	-1.53815900
H	-3.37186900	-2.60702600	0.98588500
H	-2.23395600	-3.68173600	0.15364100
H	-0.47447600	-1.52366700	3.58096300
H	-1.44519000	-2.88446500	2.98489900
H	0.31697800	-2.88449400	2.78672000
H	-1.57381800	-2.63247600	-2.26398300
H	-2.75408000	-1.48029100	-2.92566400
H	-2.29863800	0.11445700	-1.07892400
H	-0.86539200	1.00950200	-3.55046900
H	0.70382900	1.53850200	-2.80251100
H	1.55277500	-0.82430300	-2.86999300
H	0.00057200	-1.37203600	-3.65392600
H	-5.71888900	-3.14041700	-2.54548800
H	-5.92214100	-3.63086900	-0.82669400
H	-6.95896800	-2.34088600	-1.52143100
Co	0.04594900	-0.41540800	0.17023300
P	2.15789000	-0.79895500	0.65133400
P	0.05181300	1.70910200	0.85811800
C	1.03515500	1.86028500	2.43883800
H	1.01622300	2.91758500	2.72659200
H	0.43360000	1.32644000	3.18417800
C	2.62393600	-0.18955800	2.33799300
H	3.66192800	-0.47726500	2.53986200
H	1.98362100	-0.69698300	3.06790500
C	2.48145800	1.33409500	2.47535100
H	2.90556600	1.62219100	3.44509400
H	3.10353600	1.82429900	1.71880800
C	-1.62446900	2.25612400	1.41732800
C	-1.79643500	3.60370700	1.79017000
C	-2.71704900	1.38450000	1.51244500
C	-3.03093000	4.05468300	2.25281100
H	-0.97272000	4.30635200	1.70892000
C	-3.95852000	1.84409500	1.95863700
H	-2.61379200	0.34381300	1.23892700
C	-4.11641800	3.17749500	2.33290100
H	-3.14685200	5.09552500	2.54110800
H	-4.79427100	1.15221200	1.99314800
H	-5.08109400	3.53678000	2.67941200
C	0.56857700	3.13173300	-0.19071600
C	1.74611800	3.86132500	0.03562900
C	-0.28185500	3.52846000	-1.23849800
C	2.06787500	4.95702800	-0.76892500
H	2.41778600	3.59694100	0.84420100
C	0.04121300	4.62276200	-2.03923600
H	-1.20915700	2.99315100	-1.41722000
C	1.21869700	5.33863800	-1.80800500
H	2.97897900	5.51533900	-0.57409400
H	-0.63116200	4.92048500	-2.83852200
H	1.46729300	6.19412300	-2.42921100
C	3.51658800	-0.16727300	-0.41761900
C	3.30708300	0.90689600	-1.29254400
C	4.79910600	-0.73855000	-0.32905800
C	4.36036900	1.40965700	-2.06082200
H	2.32298800	1.35132600	-1.37544200
C	5.84718100	-0.23498200	-1.09746500
H	4.97860000	-1.58414900	0.32866700
C	5.62980300	0.83996700	-1.96455500
H	4.18339800	2.24284900	-2.73472100
H	6.83288000	-0.68518800	-1.02344500
H	6.44792500	1.22704400	-2.56502900
C	2.44262100	-2.61319700	0.67107600
C	2.91111200	-3.30030800	1.80184100
C	2.17848000	-3.33479600	-0.50636500
C	3.11263700	-4.68279600	1.75283100
H	3.13280100	-2.77035500	2.72270100
C	2.38367500	-4.71264800	-0.55107600
H	1.81842200	-2.81641400	-1.39081800
C	2.84903000	-5.39009300	0.57974400
H	3.48040700	-5.20245300	2.63288500
H	2.18446000	-5.25770200	-1.46936100
H	3.00954000	-6.46358100	0.54385500

INT2-s-dppp

N	-4.44063300	0.48590600	0.59764900
C	-3.68490500	0.73904900	-0.66127900
C	-2.27658900	0.32339200	-0.29479900
C	-1.09863400	0.63934200	-0.84342700
C	-0.90071800	1.41755000	-2.11300400
C	-3.51697200	0.22164200	1.73163900
C	-2.31155400	-0.41774400	1.01180600
C	-0.92458400	-0.34594100	1.59550900
C	-0.60243300	-0.47653600	3.03580600
C	-0.41910000	0.89050200	2.36409900
S	-5.75676600	1.51533600	0.93621600
O	-5.82816600	1.63107000	2.39485200
O	-5.67022300	2.70611400	0.08248200
C	-7.16166600	0.54115400	0.37389800
H	-4.10033000	0.12278200	-1.47092800
H	-3.75410600	1.78923900	-0.96291400
H	-1.87042200	1.66386000	-2.56567600
H	-0.37086300	2.35961400	-1.94018600
H	-0.33030200	0.86008900	-2.86657800
H	-3.23165700	1.14607300	2.24891500
H	-3.99447700	-0.44017100	2.45662400
H	-2.54830300	-1.47885600	0.83022700
H	-1.43000600	-0.58943000	3.73525900
H	0.31519700	-0.95449200	3.37305400
H	0.62942700	1.20692400	2.28798400
H	-1.09497100	1.71582200	2.57201900
H	-7.04580500	0.32834600	-0.69072500
H	-7.20583100	-0.38005300	0.95664500
H	-8.05626300	1.14583300	0.54168100
Co	0.36694900	0.09505600	0.28377200
P	2.18726600	1.33833700	-0.61257600
P	0.65632700	-1.78451000	-0.84266700
C	1.58179700	-1.53355900	-2.43797000
H	1.70704200	-2.52268100	-2.89233700
H	0.91622700	-0.98216000	-3.11057500
C	2.87473500	0.72150400	-2.23069900
H	3.88042000	1.13495900	-2.36527500

H	2.24577300	1.13010000	-3.03051500
C	2.94310800	-0.81236400	-2.34032100
H	3.50013200	-1.04832500	-3.25522200
H	3.54080400	-1.21886100	-1.51607900
C	-0.82173100	-2.75565800	-1.35251800
C	-1.20306400	-3.91090800	-0.65250700
C	-1.59170400	-2.34166800	-2.45345400
C	-2.32835400	-4.63726700	-1.04787300
H	-0.62013800	-4.25834000	0.19337500
C	-2.70949700	-3.07519700	-2.84930500
H	-1.32781000	-1.44871700	-3.01035100
C	-3.08223700	-4.22337400	-2.14605300
H	-2.60753100	-5.53189400	-0.49897600
H	-3.28757800	-2.74994300	-3.70948700
H	-3.95299100	-4.79341800	-2.45637300
C	1.68878400	-2.95733100	0.13043900
C	2.72084300	-3.71506300	-0.44924400
C	1.41365100	-3.12445300	1.49946200
C	3.46197300	-4.60840300	0.32540700
H	2.95316900	-3.62670900	-1.50469900
C	2.15301800	-4.02426600	2.26947900
H	0.60602100	-2.56316800	1.95543400
C	3.18296300	-4.76340300	1.68486500
H	4.25541900	-5.18754000	-0.13773900
H	1.92148400	-4.14832100	3.32349800
H	3.76135200	-5.46126300	2.28303800
C	3.59389700	1.18396800	0.56679000
C	4.59001700	2.16701700	0.68594600
C	3.66511800	0.04208500	1.38212700
C	5.63625100	2.00140100	1.59337500
H	4.54359200	3.06771500	0.08164200
C	4.71460800	-0.12234700	2.28818400
H	2.90855900	-0.73521900	1.30576200
C	5.70161500	0.85817500	2.39455100
H	6.39957000	2.76945200	1.67834400
H	4.75712400	-1.01318200	2.90821300
H	6.51675400	0.73612500	3.10178200
C	1.96532400	3.14336200	-0.85939100
C	2.66887300	3.86820800	-1.83582200
C	1.06458600	3.82575100	-0.02392700
C	2.47770400	5.24519200	-1.96645700
H	3.36905900	3.37021300	-2.49953400
C	0.87944900	5.20195400	-0.15365300
H	0.49504200	3.27705700	0.72134400
C	1.58592200	5.91371800	-1.12588300
H	3.02630300	5.79362400	-2.72669000
H	0.17835100	5.71556600	0.49762700
H	1.43788500	6.98437000	-1.23126900

TS2-s-dppp

N	4.08348700	-2.02590000	0.73650300
C	3.23644300	-2.13019600	-0.48617800
C	1.97380800	-1.35364200	-0.13456200
C	0.76799100	-1.33503400	-0.70509700
C	0.42170400	-2.03673600	-1.98789400
C	3.23187700	-1.57529100	1.86196700
C	2.21129400	-0.63966300	1.17053400
C	0.88842200	-0.27084700	1.79427100
C	0.76660800	0.01193200	3.14091900
C	-0.23278100	-1.38945400	1.97672300
S	5.58691200	-1.21171700	0.56307300
O	5.81181000	-0.97706600	-0.86731500
O	5.63894000	-0.10109200	1.52332300
C	6.75228100	-2.46833000	1.11046400
H	3.77761900	-1.71785400	-1.34134500
H	3.02429900	-3.18654400	-0.69208100
H	1.28363300	-2.60775200	-2.35883900
H	-0.41044100	-2.73896400	-1.87776700
H	0.14474800	-1.33385500	-2.78312900
H	2.73970700	-2.45387100	2.29901500
H	3.83906300	-1.08775100	2.62433500
H	2.73190600	0.31206700	0.98215200
H	1.59808200	-0.12868800	3.83532500
H	-0.13660300	0.42673700	3.57751800
H	-1.09204200	-1.20824900	2.62139200
H	0.17148900	-2.39494800	2.08759700
H	6.52449000	-2.73695600	2.14352100
H	6.66670800	-3.33481300	0.45310300
H	7.75087700	-2.02997000	1.04235500
Co	-0.47223800	-0.30347900	0.37493800
P	-2.46280000	-0.86541600	-0.59163900
P	-0.07460900	1.60043100	-0.83945200
C	-0.80583100	1.54965100	-2.55513800
H	-0.60765000	2.51612200	-3.03200900
H	-0.26909000	0.79509800	-3.13948200
C	-2.76585100	-0.18340500	-2.29933900
H	-3.83318200	-0.27999400	-2.52910700
H	-2.24504700	-0.86846700	-2.97841200
C	-2.31944700	1.26850900	-2.58381300
H	-2.67667000	1.51150800	-3.59232600
H	-2.82753600	1.97000100	-1.91348500
C	1.68368800	2.05813900	-1.10315800
C	2.33415700	2.90403700	-0.18833500
C	2.42791000	1.49363400	-2.15199000
C	3.69495100	3.18114200	-0.32523700
H	1.77818800	3.35488700	0.62829200
C	3.78916300	1.77235100	-2.28412100
H	1.95758300	0.82922700	-2.87006000
C	4.42604200	2.61336900	-1.37022500
H	4.18393900	3.83730700	0.38883900
H	4.35422700	1.32329900	-3.09513600
H	5.48750400	2.81818000	-1.46821700
C	-0.84912000	3.10190900	-0.11290500
C	-0.66659800	4.37418000	-0.68309800
C	-1.66241500	2.97864900	1.02320800
C	-1.28609700	5.49201700	-0.12644000
H	-0.02653800	4.49629600	-1.55258000
C	-2.28276300	4.09903800	1.58116400
H	-1.82504000	2.00170700	1.47192900
C	-2.09462200	5.35606600	1.00626700
H	-1.13570600	6.47020900	-0.57398100

H	-2.91173500	3.98752400	2.45958800
H	-2.57398700	6.22953100	1.43877300
C	-3.76928200	-0.13152300	0.48945200
C	-4.63215800	0.89815200	0.08405500
C	-3.89868800	-0.64303500	1.79433100
C	-5.58998200	1.40873600	0.96361500
H	-4.57946200	1.30451600	-0.91945100
C	-4.85635900	-0.13365900	2.67008200
H	-3.27604000	-1.47471500	2.11307200
C	-5.70116000	0.90035500	2.25810400
H	-6.25395400	2.20103800	0.63000600
H	-4.95147400	-0.55175000	3.66826100
H	-6.44927800	1.29738800	2.93793600
C	-2.98935200	-2.62454500	-0.71899000
C	-4.20632200	-2.97952800	-1.32552700
C	-2.18623200	-3.62993600	-0.16090100
C	-4.60083900	-4.31546900	-1.38180100
H	-4.85841500	-2.21741200	-1.74314900
C	-2.58587200	-4.96719700	-0.21471800
H	-1.24455000	-3.35928900	0.30739000
C	-3.79116800	-5.31104200	-0.82771400
H	-5.54271400	-4.57953800	-1.85387300
H	-1.95467900	-5.73777000	0.21878100
H	-4.10208500	-6.35074700	-0.87230600

INT3-s-dppp

N	-4.54407900	-1.18656800	-0.61105200
C	-3.75876700	-0.99427100	0.63938900
C	-2.39340800	-0.49781600	0.16213300
C	-1.23217700	-0.43108600	0.81729600
C	-1.10369800	-0.65215900	2.29794400
C	-3.58769500	-1.22845200	-1.74720700
C	-2.50889000	-0.21601200	-1.32028700
C	-1.12060000	-0.22306600	-1.91254600
C	-0.46010400	1.00984700	-2.01347700
C	-0.30931700	-1.38254100	-1.85201400
S	-5.87958100	-0.11900800	-0.82226000
O	-6.19558700	0.44737600	0.49296500
O	-5.62829500	0.75997000	-1.97312300
C	-7.18682500	-1.26700600	-1.27669400
H	-4.28258800	-0.30062900	1.30195100
H	-3.66935300	-1.95692000	1.15633800
H	-0.57240900	-1.57811600	2.54089800
H	-0.58499600	0.17476500	2.79708500
H	-2.09660400	-0.72316400	2.76046100
H	-3.18714000	-2.24606000	-1.82324300
H	-4.08423800	-0.96836500	-2.68191100
H	-2.94932700	0.78000100	-1.46892900
H	-1.01259400	1.93979700	-1.92918000
H	0.49717700	1.07552200	-2.53341900
H	0.58833200	-1.42850300	-2.46903900
H	-0.74939700	-2.33990200	-1.59420800
H	-6.89814100	-1.79283200	-2.18863500
H	-7.33865200	-1.96538700	-0.45275600
H	-8.08621400	-0.67156200	-1.45123400
Co	0.29023900	-0.07646300	-0.35013300
P	1.66309400	-1.62796600	0.63470600
P	1.14637600	1.82107200	0.70141700
C	2.16617800	1.48544400	2.23217500
H	2.74820200	2.39015000	2.44108800
H	1.44160900	1.39510900	3.05006800
C	2.40966600	-1.11253800	2.26295200
H	3.13679100	-1.88376900	2.54177500
H	1.62432000	-1.11554700	3.02468200
C	3.10247300	0.26041400	2.24180500
H	3.81681200	0.29605900	1.41277600
H	3.70628800	0.33106700	3.15504900
C	-0.00349100	3.13363100	1.28087700
C	0.51209600	4.32347200	1.82693000
C	-1.39235600	2.96951600	1.18494300
C	-0.35043600	5.32072100	2.27715200
H	1.58524400	4.48319300	1.88570000
C	-2.25346200	3.97389000	1.63527300
H	-1.79964000	2.05522000	0.76867800
C	-1.73474700	5.14705900	2.18252300
H	0.05725600	6.23615100	2.69612700
H	-3.32789900	3.83587100	1.55490100
H	-2.40455000	5.92778100	2.53112700
C	2.28148100	2.74541200	-0.42852200
C	3.68042900	2.66034500	-0.34477400
C	1.71729500	3.56369400	-1.42504200
C	4.49155000	3.36648600	-1.23720500
H	4.15663400	2.05810900	0.42004700
C	2.52854600	4.26661100	-2.31407900
H	0.63964100	3.67852700	-1.48923900
C	3.91954800	4.16613800	-2.22622300
H	5.57187700	3.29427200	-1.14949300
H	2.07343700	4.90173800	-3.06857300
H	4.55133500	4.71647700	-2.91714800
C	1.09448900	-3.35315400	0.92658900
C	0.87375900	-4.19554800	-0.17817900
C	0.85922000	-3.85756500	2.21537600
C	0.42073200	-5.50114300	0.00336500
H	1.08226700	-3.84241800	-1.18317900
C	0.40163200	-5.16575500	2.39368800
H	1.03872800	-3.24726800	3.09413100
C	0.17758200	-5.98833400	1.29031600
H	0.26367600	-6.14019400	-0.86078700
H	0.22800700	-5.53940200	3.39856900
H	-0.17574500	-7.00554600	1.43073400
C	3.13777300	-1.81758600	-0.45074300
C	4.00702800	-2.91469800	-0.32387900
C	3.42660600	-0.83000800	-1.40588900
C	5.13476700	-3.01705800	-1.13775300
H	3.79721400	-3.69575600	0.40076000
C	4.55602400	-0.93413600	-2.22054100
H	2.78192800	0.03896600	-1.51319200
C	5.40989800	-2.02962400	-2.08805500
H	5.79790200	-3.87070000	-1.03193600
H	4.76545700	-0.16036100	-2.95327700
H	6.28696400	-2.11587300	-2.72274000

INT3-t-dppp

N	-4.56108700	-2.09735300	-0.58324500
C	-3.83537200	-1.94673900	0.70487200
C	-2.44380400	-1.45229000	0.31646700
C	-1.32427900	-1.34089500	1.03859900
C	-1.15356300	-1.69620600	2.48569600
C	-3.53628100	-2.21120800	-1.65076600
C	-2.44953700	-1.21395200	-1.19182500
C	-1.03178900	-1.30883300	-1.72157200
C	-0.46793100	-0.24421200	-2.39859000
C	-0.16134500	-2.29434800	-1.15194000
S	-5.79660500	-0.92916900	-0.88108700
O	-5.82395100	0.03002800	0.23411700
O	-5.64850200	-0.45545200	-2.26133000
C	-7.28250500	-1.93582100	-0.78062600
H	-4.37473000	-1.26283200	1.36339500
H	-3.77793300	-2.92566100	1.19774300
H	-0.39450500	-2.48067600	2.60594000
H	-0.82519200	-0.83763800	3.08575000
H	-2.08491400	-2.06809900	2.93434200
H	-3.16173500	-3.24178200	-1.65390800
H	-3.96779600	-1.98048000	-2.62310500
H	-2.83677000	-0.21037400	-1.42221800
H	-1.07738000	0.60078500	-2.70395300
H	0.52920400	-0.31402700	-2.82527700
H	0.81030400	-2.45098100	-1.61292400
H	-0.56654300	-3.15501800	-0.63549200
H	-7.23309200	-2.70720900	-1.55059200
H	-7.34133300	-2.37971400	0.21460700
H	-8.13166000	-1.27058900	-0.95465200
Co	0.09859900	-0.47062300	-0.05815500
P	2.45529900	-1.05980700	0.48854100
P	0.30814500	1.79739200	0.75123300
C	1.22603400	1.72366000	2.37379600
H	1.27468000	2.74252700	2.77483800
H	0.56621400	1.16965000	3.05275500
C	2.72207000	-0.42951000	2.22954200
H	3.70899200	-0.77426800	2.55851800
H	1.98366500	-0.90958300	2.88213000
C	2.63897800	1.10116500	2.38313800
H	3.27823800	1.58181900	1.63466100
H	3.08209700	1.34679200	3.35627700
C	-1.23510100	2.70300500	1.17519600
C	-1.17550500	4.02716900	1.64443700
C	-2.48474700	2.09015000	1.01116000
C	-2.34889700	4.71165200	1.95501700
H	-0.21948200	4.53296600	1.74906600
C	-3.66040300	2.78101700	1.31420100
H	-2.54403400	1.06886300	0.65649300
C	-3.59129700	4.09058000	1.78950500
H	-2.29474900	5.73424300	2.31738100
H	-4.61735300	2.28846300	1.16773100
H	-4.50263500	4.63258500	2.02527100
C	1.24144500	2.99425600	-0.29197700
C	2.25923000	3.82084100	0.20926800
C	0.86964200	3.12461100	-1.64070500
C	2.89495700	4.74615200	-0.62234100
H	2.56463500	3.76165100	1.24850500
C	1.49902500	4.05436100	-2.46710600
H	0.07307300	2.50608500	-2.04277800
C	2.51857800	4.86453000	-1.96030000
H	3.68138300	5.37709100	-0.21835300
H	1.19116400	4.14893500	-3.50456700
H	3.01131800	5.58769600	-2.60352000
C	2.81502600	-2.85917100	0.59906500
C	3.34724500	-3.52966800	-0.51598800
C	2.47965800	-3.60543100	1.74070400
C	3.54487000	-4.91067700	-0.48446400
H	3.62856300	-2.97256400	-1.40527700
C	2.68259800	-4.98638200	1.76943400
H	2.06817200	-3.11939000	2.62000200
C	3.21342000	-5.64251100	0.65752700
H	3.96448700	-5.41249400	-1.35163700
H	2.42949600	-5.54729600	2.66458500
H	3.37167900	-6.71660300	0.68229700
C	3.86984400	-0.36273700	-0.45037500
C	5.19854200	-0.67141300	-0.10651200
C	3.62576900	0.50388500	-1.52535500
C	6.25626700	-0.11707900	-0.82468500
H	5.40830300	-1.35543300	0.71132200
C	4.68806600	1.05798400	-2.24380700
H	2.60507000	0.75861700	-1.79333300
C	6.00219100	0.74793200	-1.89419000
H	7.27911400	-0.36203900	-0.55346000
H	4.48504100	1.73160700	-3.07103800
H	6.82943600	1.17578500	-2.45313600

TS3-s-dppp

N	4.19708500	-1.45922400	-0.71032500
C	3.27049400	-2.21878300	0.17335700
C	1.94305200	-1.98406800	-0.50344400
C	0.66194000	-2.15935500	-0.10468600
C	0.24280300	-3.13354600	0.96066100
C	3.45770200	-0.50270200	-1.58262000
C	2.20418300	-1.34239500	-1.84597800
C	0.83474500	-0.83575200	-2.21523100
C	-0.13809900	-1.89717200	-1.89905200
C	0.43910800	0.46368600	-2.40242500
S	5.70652300	-1.00687000	-0.09492800
O	6.08651200	0.23499800	-0.77252700
O	5.66841100	-1.09660500	1.37090600
C	6.78265600	-2.32425000	-0.68526600
H	3.55481000	-3.28070200	0.19130500
H	3.29413600	-1.84928700	1.20417800
H	-0.22465000	-2.64932300	1.82269700
H	-0.48493400	-3.84961400	0.56494900
H	1.10614600	-3.70733000	1.31935900
H	3.23035800	0.43847400	-1.07076400
H	4.04388800	-0.29024200	-2.47763600
H	2.48606700	-2.13098700	-2.56602200
H	0.08046400	-2.92556200	-2.17877800

H	-1.18690800	-1.66857200	-2.11704300
H	-0.55531900	0.69954600	-2.76662400
H	1.16644600	1.26870600	-2.42757600
H	6.42676200	-3.28007500	-0.29529200
H	6.77915700	-2.31811600	-1.77628500
H	7.78439600	-2.11274500	-0.30332900
Co	-0.36823100	-0.43766300	-0.43233500
P	-0.08906800	1.51528800	0.66818000
P	-2.35550000	-0.84370800	0.58463400
C	-2.43592600	-0.38219700	2.38309200
H	-3.43778500	-0.60152900	2.76689800
H	-1.74750600	-1.05694900	2.90624000
C	-0.56621100	1.39451200	2.46688500
H	-0.30894200	2.34498500	2.94545300
H	0.06106400	0.62622600	2.93310000
C	-2.04863700	1.07117000	2.70372600
H	-2.68399200	1.77164500	2.14926900
H	-2.26487200	1.24071100	3.76557900
C	-3.01697900	-2.57352300	0.55597200
C	-3.38278900	-3.13974500	-0.67735800
C	-3.16202600	-3.34806800	1.71755100
C	-3.87183300	-4.44350200	-0.74842000
H	-3.31627800	-2.55550500	-1.59046500
C	-3.65363000	-4.65363600	1.64511100
H	-2.89692400	-2.94862300	2.69035800
C	-4.00588800	-5.20643100	0.41393700
H	-4.15654900	-4.85930900	-1.71070700
H	-3.76292600	-5.23522800	2.55596500
H	-4.38904700	-6.22111500	0.36007900
C	-3.74260000	0.08418200	-0.21213800
C	-4.85553400	0.53792600	0.51346400
C	-3.73251500	0.26551400	-1.60466500
C	-5.91989400	1.16472700	-0.13660200
H	-4.91111200	0.40196800	1.58845500
C	-4.80372800	0.87681900	-2.25733600
H	-2.87803200	-0.06933200	-2.18648000
C	-5.89899500	1.33330700	-1.52209200
H	-6.76999700	1.51401800	0.44219200
H	-4.78023600	0.99893100	-3.33666300
H	-6.73225900	1.81456400	-2.02555700
C	-0.93104800	3.06966700	0.14945700
C	-0.74907100	4.25747400	0.88270300
C	-1.76213500	3.09237300	-0.97710500
C	-1.39258600	5.43145300	0.49669300
H	-0.08849400	4.27609500	1.74489500
C	-2.40628800	4.27014000	-1.36440400
H	-1.91868900	2.18395700	-1.54527100
C	-2.22394200	5.43971800	-0.62775700
H	-1.24188500	6.34146900	1.07022900
H	-3.05134200	4.26863300	-2.23825700
H	-2.72345300	6.35664100	-0.92695000
C	1.68528000	1.99320700	0.75242500
C	2.55516900	1.34094500	1.64287400
C	2.20134000	2.98912300	-0.09386400
C	3.90515000	1.68896400	1.69839400
H	2.18833600	0.55739000	2.29967000
C	3.55481300	3.32750800	-0.04227100
H	1.54616200	3.51524600	-0.78129200
C	4.40838600	2.67881600	0.85134900
H	4.56871500	1.16466900	2.37733900
H	3.94038700	4.09974900	-0.70172000
H	5.46345300	2.93044600	0.87978500

TS3-t-dppp

N	-4.88585700	-0.30721000	0.36395200
C	-3.99454100	-0.87318100	-0.69002400
C	-2.64994300	-1.02070100	-0.00190300
C	-1.42432300	-1.16016800	-0.51717500
C	-1.07323000	-1.60147500	-1.91991600
C	-4.04886700	0.12505200	1.51718900
C	-2.87814000	-0.86747500	1.48044400
C	-1.54529800	-0.62227100	2.12280100
C	-0.48390500	-1.40816400	1.43856500
C	-1.31733700	0.20335100	3.15501800
S	-6.25437200	-1.27210900	0.76813100
O	-6.46706700	-2.19276400	-0.35231700
O	-6.11091900	-1.77573500	2.14018900
C	-7.57230200	-0.04869400	0.76126000
H	-4.40346500	-1.81795800	-1.06141900
H	-3.93745000	-0.17911200	-1.53700900
H	-0.26519300	-1.01759900	-2.38725000
H	-0.75653800	-2.65055800	-1.92867100
H	-1.95017100	-1.49909200	-2.57252000
H	-3.70728100	1.15228900	1.34067700
H	-4.62638500	0.08990400	2.44071600
H	-3.27431800	-1.83030400	1.85136000
H	-0.66113900	-2.48149700	1.37697600
H	0.52288300	-1.24062400	1.85292400
H	-0.32615400	0.31412600	3.58737500
H	-2.12037300	0.75952600	3.63015200
H	-7.34699800	0.72303700	1.49972600
H	-7.64880300	0.37636700	-0.24026600
H	-8.49228900	-0.57271300	1.03137200
Co	0.25041300	-0.20352800	-0.11957300
P	0.96010000	1.97459300	-0.84402200
P	2.39678200	-1.29512700	-0.60423300
C	3.27612900	-0.49945200	-2.04705600
H	4.24080500	-1.00327200	-2.17714200
H	2.68520000	-0.69484300	-2.95069200
C	2.26624800	1.90478600	-2.17347700
H	2.58179600	2.93101300	-2.39450500
H	1.74363800	1.55657800	-3.07364600
C	3.50099600	1.01934500	-1.90600100
H	3.93893300	1.24949900	-0.92757100
H	4.26166100	1.30060000	-2.64462000
C	3.64722300	-1.22990900	0.74312300
C	3.51969200	-0.25711400	1.74737600
C	4.74456100	-2.10725600	0.77778200
C	4.47323300	-0.15734900	2.76330800
H	2.68103600	0.43427400	1.73377800
C	5.69202600	-2.00857700	1.79580900

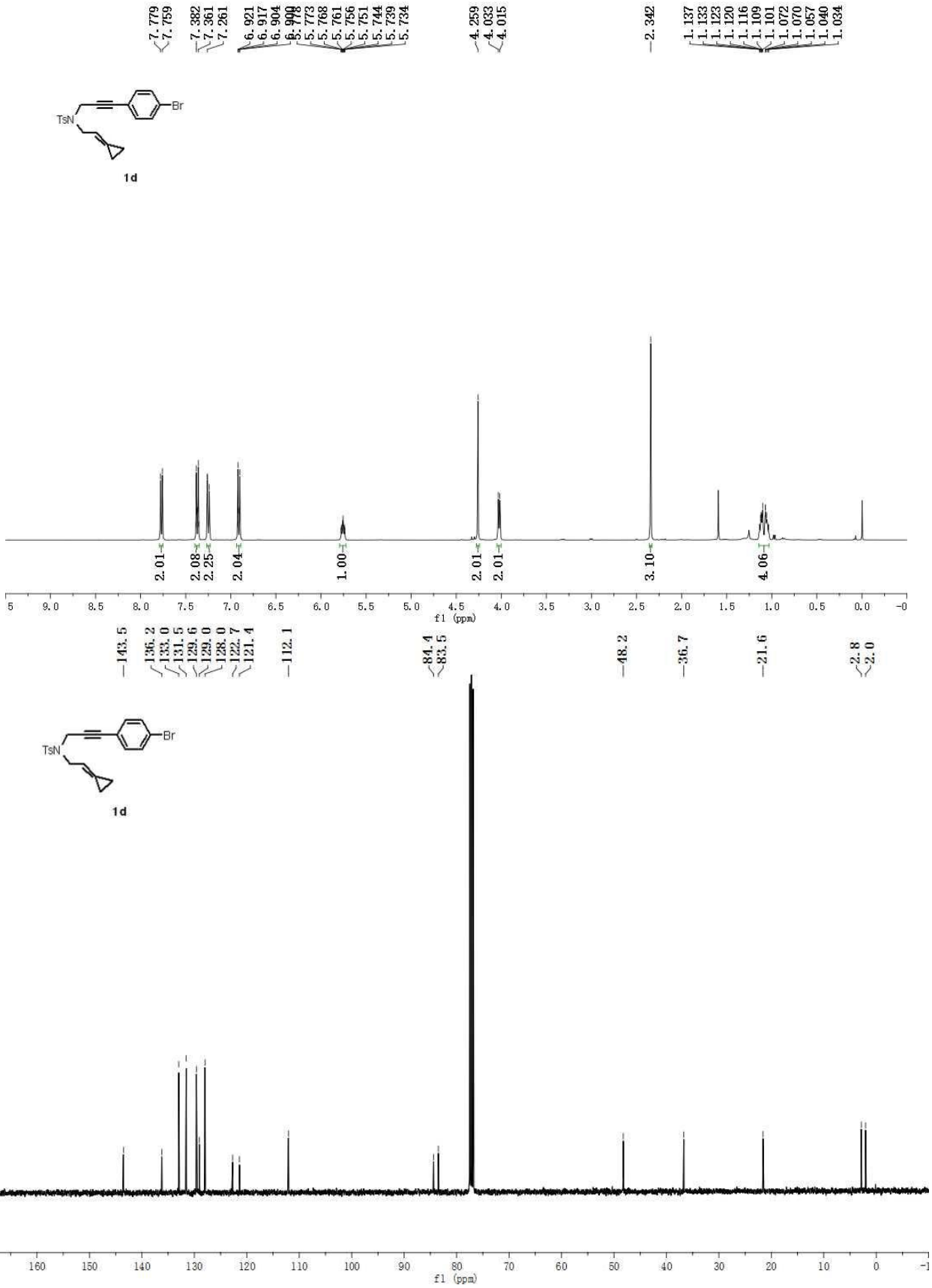
H	4.85194000	-2.87459200	0.01656700
C	5.55813400	-1.03413400	2.78932900
H	4.36431500	0.60210500	3.53219400
H	6.53459400	-2.69382200	1.81544900
H	6.29716000	-0.96228300	3.58207200
C	2.29804200	-3.07755200	-1.05242800
C	1.90695400	-3.99122100	-0.05567000
C	2.52155100	-3.55515800	-2.35307100
C	1.74963200	-5.34379100	-0.35229600
H	1.74309100	-3.64862700	0.96292400
C	2.35791500	-4.91167200	-2.64860400
H	2.83323400	-2.88400200	-3.14653600
C	1.97138100	-5.80751300	-1.65231200
H	1.45691700	-6.03660500	0.43148600
H	2.53964900	-5.26496900	-3.65959600
H	1.84703100	-6.86116500	-1.88402800
C	1.69391700	2.96235600	0.52368000
C	1.01878000	2.96129800	1.75716800
C	2.87170400	3.71573400	0.39738000
C	1.50341200	3.70431700	2.83341700
H	0.10499700	2.38255900	1.87437500
C	3.35932400	4.45269900	1.47947800
H	3.41963200	3.73798900	-0.53923900
C	2.67711600	4.45000800	2.69693100
H	0.96594600	3.70120500	3.77749800
H	4.27236900	5.03027900	1.36735300
H	3.05755500	5.02606800	3.53536700
C	-0.29926600	3.07925100	-1.60453500
C	-1.49205000	2.52125900	-2.08819300
C	-0.07875900	4.45838500	-1.75208200
C	-2.44271900	3.32423400	-2.72175100
H	-1.68040800	1.45815400	-1.96307400
C	-1.03199100	5.25875700	-2.38071100
H	0.83025900	4.91120300	-1.36614300
C	-2.21312700	4.69289800	-2.86857300
H	-3.36234300	2.88271000	-3.09538100
H	-0.85425600	6.32493800	-2.48774700
H	-2.95364900	5.31927100	-3.35739600

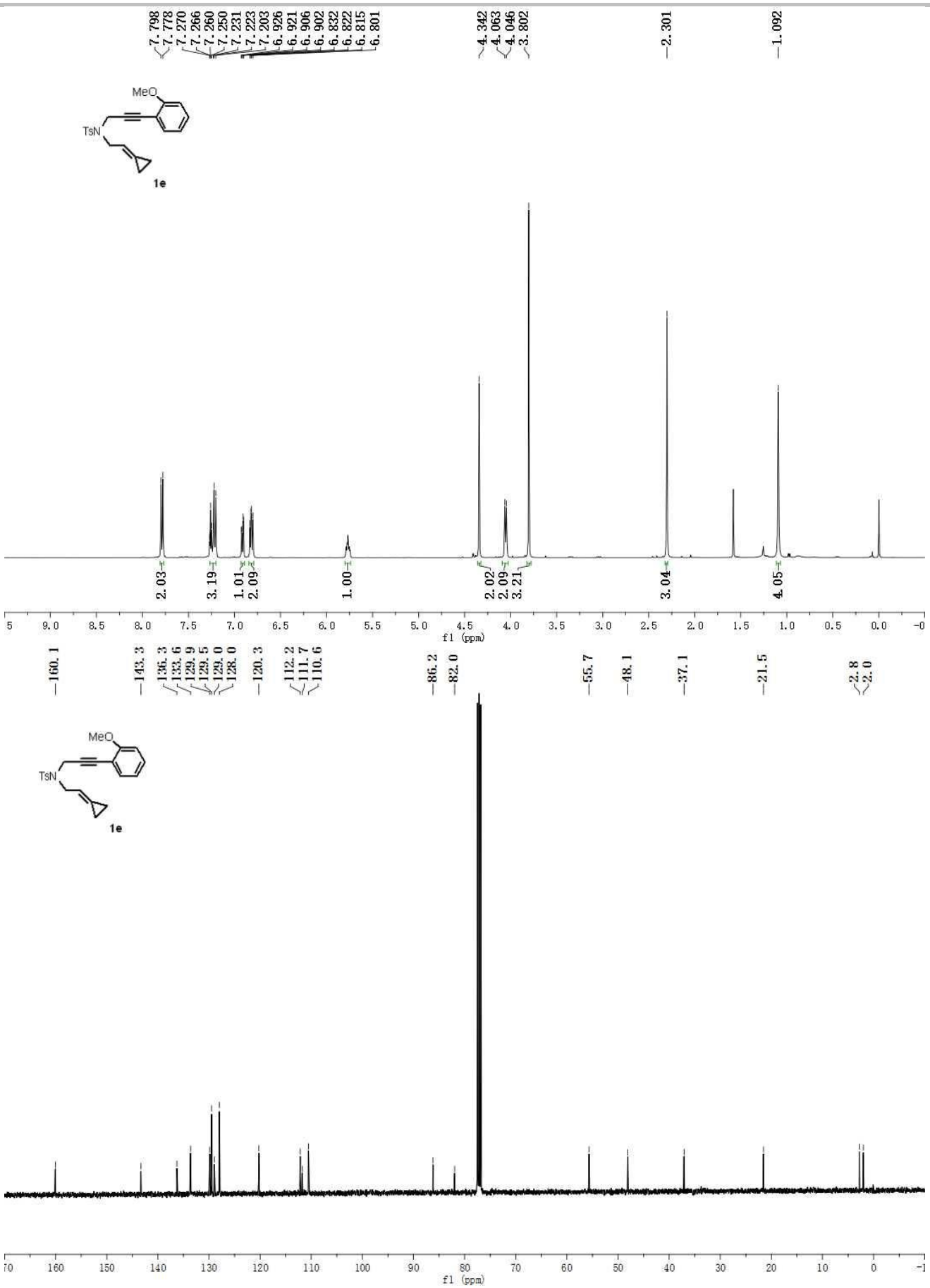
INT4-t-dppp

N	3.86909600	0.37379700	-0.13404600
C	4.30645200	1.30591600	0.95903900
C	3.14058300	1.23273900	1.89675400
C	2.38800200	2.11105400	2.57104200
C	2.64682400	3.56465200	2.82044400
C	2.64840700	-0.38215000	0.26034100
C	2.52339100	-0.13568200	1.77656500
C	1.15642500	0.03748900	2.42777300
C	1.11997400	1.43382000	3.07428400
C	0.24956400	-0.96385800	2.62966700
S	5.08982500	-0.52641200	-0.91681100
O	6.20138700	-0.78683400	0.00373300
O	4.40450600	-1.63213700	-1.59758600
C	5.66614100	0.63908000	-2.16033500
H	5.23569600	0.93961500	1.41378200
H	4.48300800	2.31057700	0.56059900
H	1.82048900	4.18301100	2.44556200
H	2.73530900	3.77042200	3.89537000
H	3.57242900	3.90064800	2.34335900
H	1.78008500	0.04535700	-0.27842800
H	2.72883000	-1.43059700	-0.02124000
H	3.10961100	-0.90167900	2.30678100
H	1.09965400	1.34376700	4.17142000
H	0.22635000	2.01901200	2.80851100
H	-0.61660900	-0.81587000	3.27483300
H	0.46470800	-1.98713700	2.33548200
H	4.83980900	0.87672100	-2.83126000
H	6.04463300	1.53614600	-1.66587700
H	6.47589000	0.14508000	-2.70281300
Co	-0.37408700	0.06000700	0.75344000
P	-1.03210300	-1.91852900	-0.45232200
P	-1.40204400	1.61249400	-0.70403300
C	-1.50024400	0.99531500	-2.46156000
H	-2.07938600	1.72263000	-3.04263800
H	-0.47354600	1.05771500	-2.84457100
C	-1.12921500	-1.58688700	-2.28935700
H	-1.46406500	-2.50781000	-2.77975500
H	-0.11439700	-1.38661700	-2.65283100
C	-2.06131800	-0.42391000	-2.68260600
H	-3.03346100	-0.53518400	-2.18756300
H	-2.26221600	-0.52092900	-3.75678400
C	-0.67928000	3.28986800	-0.92307400
C	0.68937900	3.47476700	-0.67412800
C	-1.44744800	4.37602400	-1.37237700
C	1.28327700	4.72071400	-0.88609800
H	1.29362700	2.64740400	-0.30978400
C	-0.85218200	5.62083400	-1.57637700
H	-2.51177300	4.25521400	-1.55265800
C	0.51344200	5.79431900	-1.33683500
H	2.34416900	4.85371800	-0.69398600
H	-1.45506700	6.45609600	-1.92081200
H	0.97380200	6.76501200	-1.49657000
C	-3.13666900	1.89846100	-0.16692100
C	-3.36700500	2.07828800	1.20857400
C	-4.22926500	1.95099600	-1.04629300
C	-4.65322900	2.31522500	1.69238400
H	-2.53173800	2.04632100	1.90602500
C	-5.51873400	2.17977700	-0.55975700
H	-4.08865000	1.81520800	-2.11400300
C	-5.73301200	2.36344600	0.80702000
H	-4.81259400	2.46147600	2.75690400
H	-6.35476100	2.21647100	-1.25217000
H	-6.73637300	2.54408700	1.18130400
C	0.10613500	-3.36037500	-0.32271300
C	1.28225800	-3.41688400	-1.09042800
C	-0.11795300	-4.35638900	0.64407600
C	2.20650300	-4.44636300	-0.90209500
H	1.50139400	-2.65972000	-1.83703100
C	0.80549200	-5.38790000	0.82496100
H	-1.02273000	-4.33983400	1.24470700
C	1.96910700	-5.43518100	0.05440800

H	3.11385600	-4.46087300	-1.49792200	H	-3.18817800	-0.98944400	1.29648600
H	0.61173100	-6.15593000	1.56848800	C	-4.45400700	-4.23914300	-0.39796900
H	2.68765300	-6.23635900	0.20005400	H	-2.53785600	-4.32185600	-1.36425500
C	-2.69882400	-2.59095800	-0.07058200	C	-5.27767100	-3.54590700	0.49445800
C	-3.53381500	-1.90461200	0.82305500	H	-5.45370900	-1.83583000	1.79701800
C	-3.17361600	-3.76624900	-0.68017900	H	-4.80898400	-5.14969100	-0.87200400
C	-4.81750100	-2.37871900	1.10401900	H	-6.27433100	-3.91791900	0.71374800

4. ^{1}H and ^{13}C-NMR spectra for new compounds

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7.250
7.231
7.223
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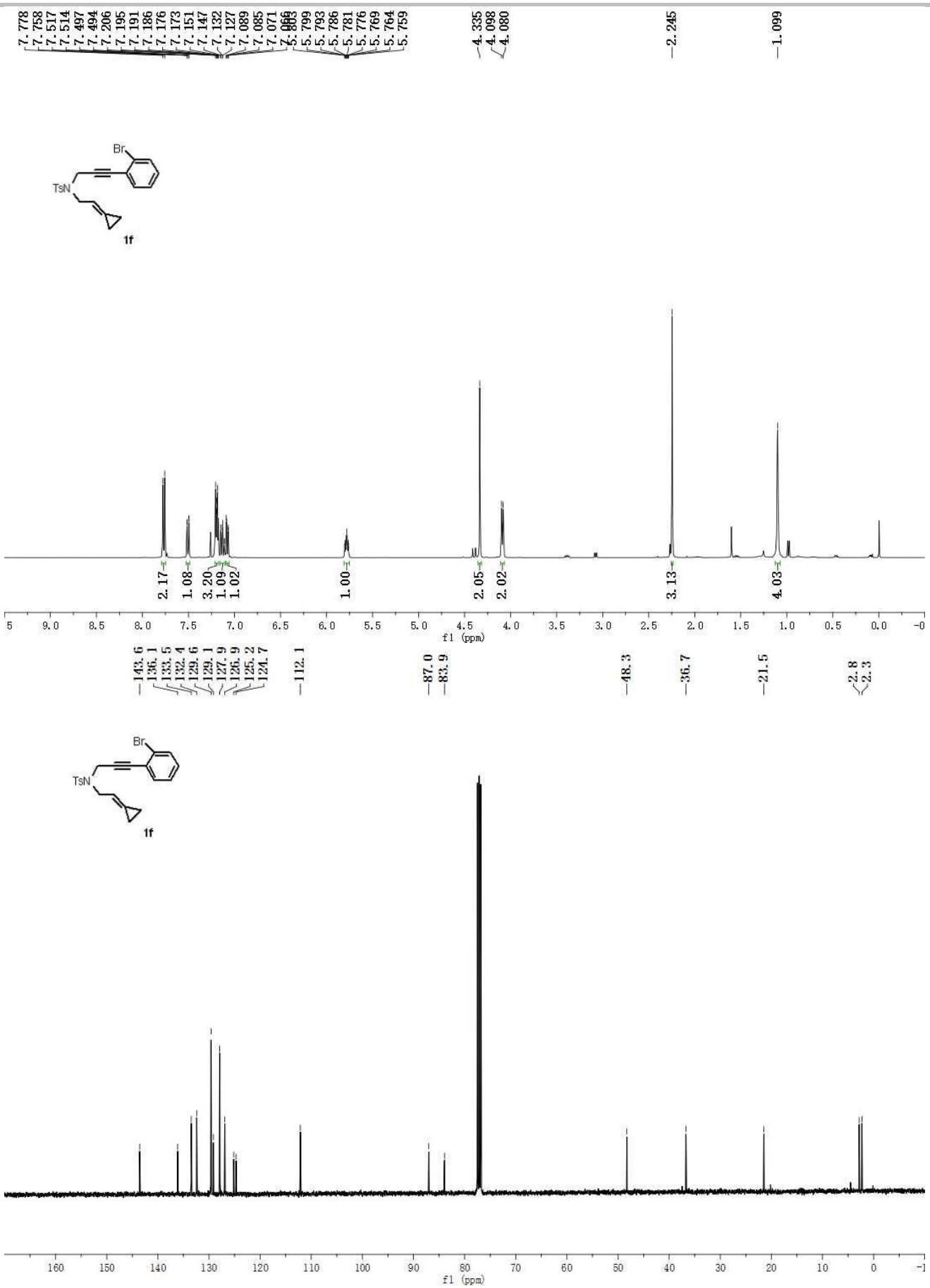
6.926
6.921
6.906
6.902
6.832
6.822
6.815
6.801
4.342
4.063
4.046
3.802
2.301
1.092
MeO
TsN
1e
2.03
3.19
1.01
2.09
1.00
2.02
2.09
3.21
3.04
4.05
f1 (ppm)
160.1
143.3
136.3
133.6
129.9
129.5
129.0
128.0
120.3
112.2
111.7
110.6
86.2
82.0
55.7
48.1
37.1
21.5
2.8
2.0
MeO
TsN
1e
f1 (ppm)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7.195
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7.186
7.176
7.173
7.151
7.147
7.132
7.127
7.089
7.085
7.071
5.803
5.799
5.793
5.786
5.781
5.776
5.769
5.764
5.759
4.335
4.098
4.080
2.245
1.099
Br
TsN
1f
2.17
1.08
3.20
1.09
1.02
1.00
2.05
2.02
3.13
4.03
f1 (ppm)
143.6
136.1
133.5
132.4
129.6
129.1
127.9
126.9
125.2
124.7
112.1
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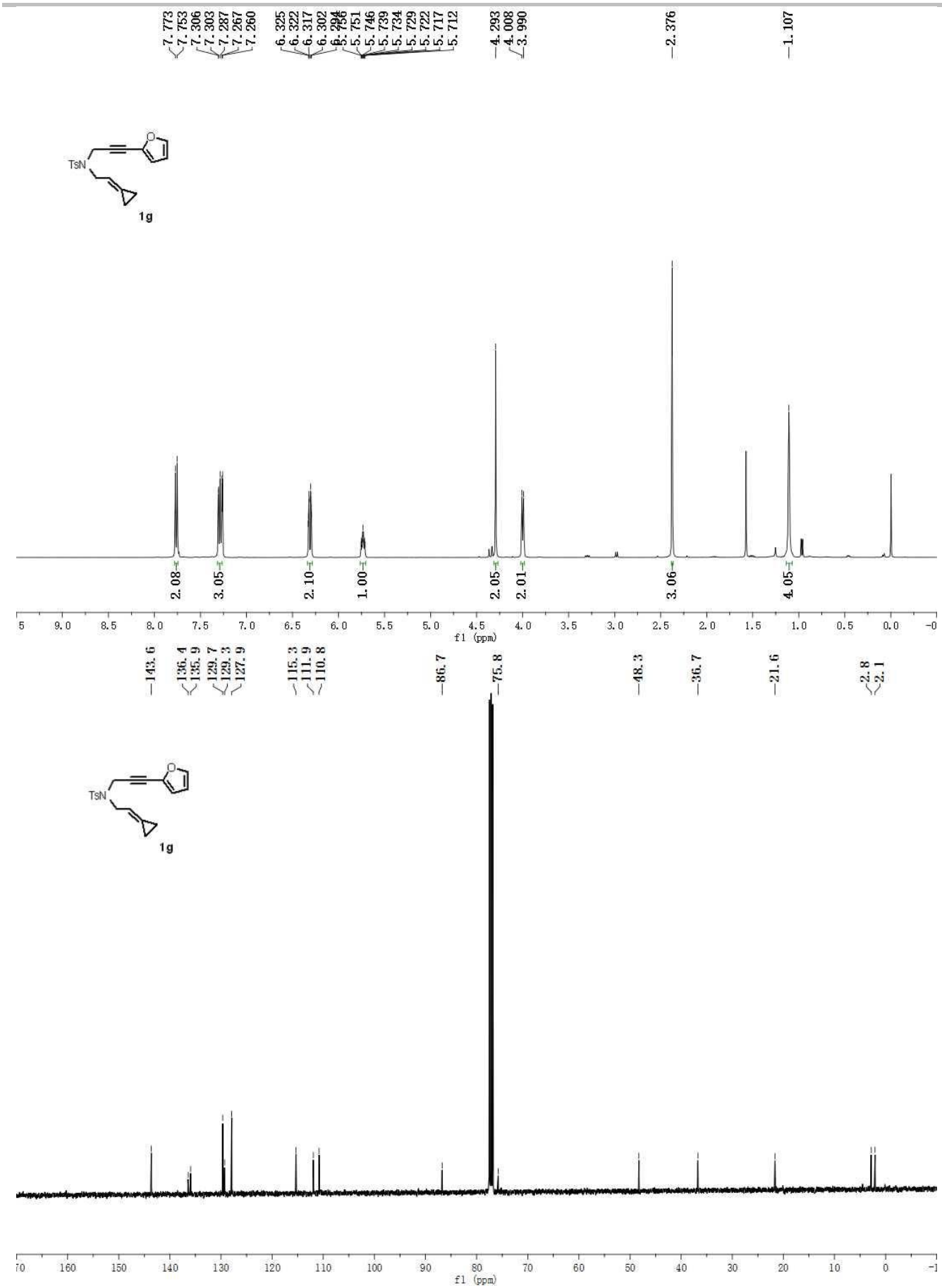
83.9
48.3
36.7
21.5
2.8
2.3
Br
TsN
1f
f1 (ppm)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7.260
6.325
6.322
6.317
6.302
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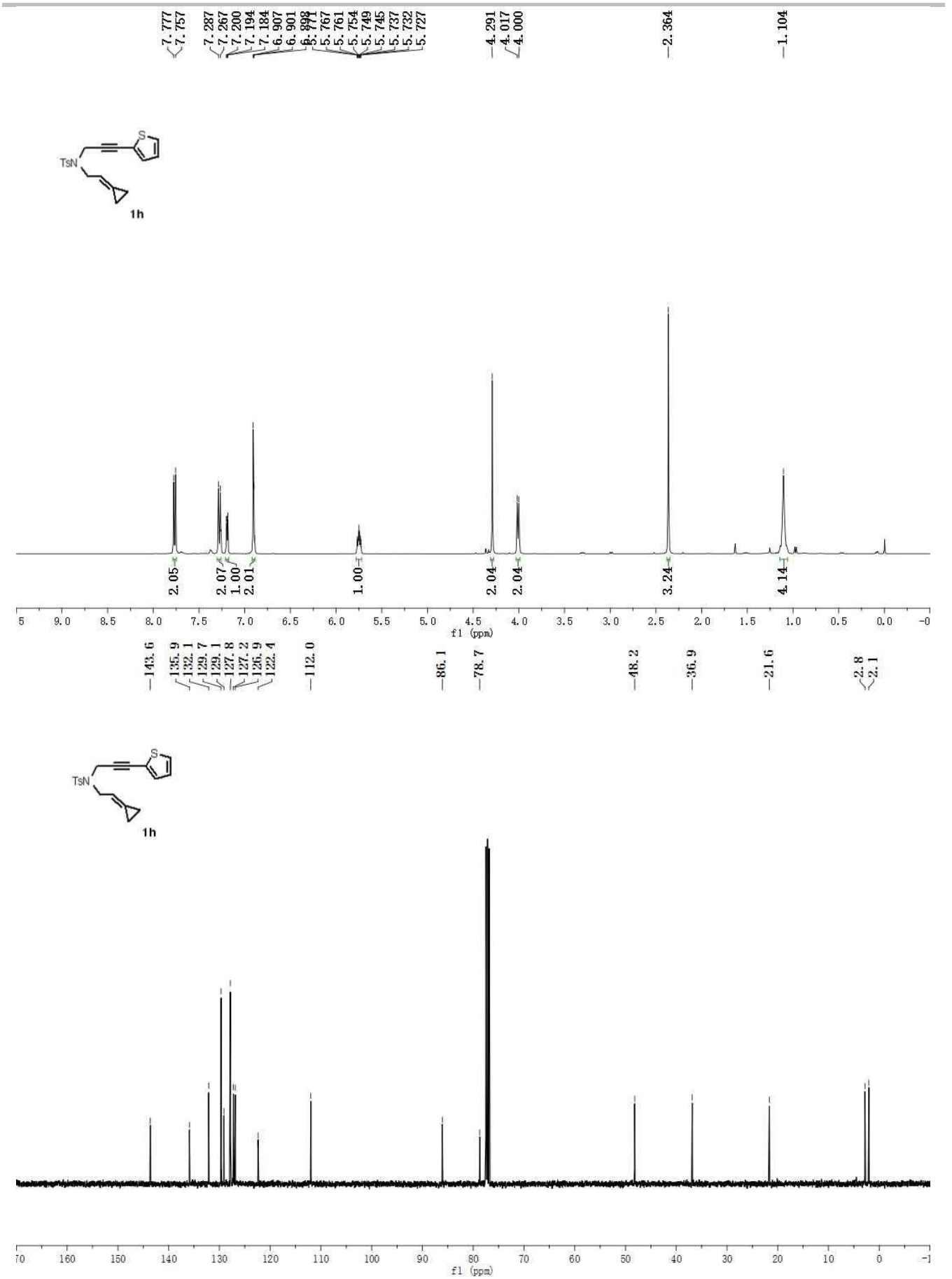
5.746
5.739
5.734
5.729
5.722
5.717
5.712
4.293
4.008
3.990
2.376
1.107
TsN
1g
2.08
3.05
2.10
1.00
2.05
2.01
3.06
4.05
f1 (ppm)
143.6
136.4
135.9
129.7
129.3
127.9
115.3
111.9
110.8
86.7
75.8
48.3
36.7
21.6
2.8
2.1
TsN
1g
f1 (ppm)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7.267
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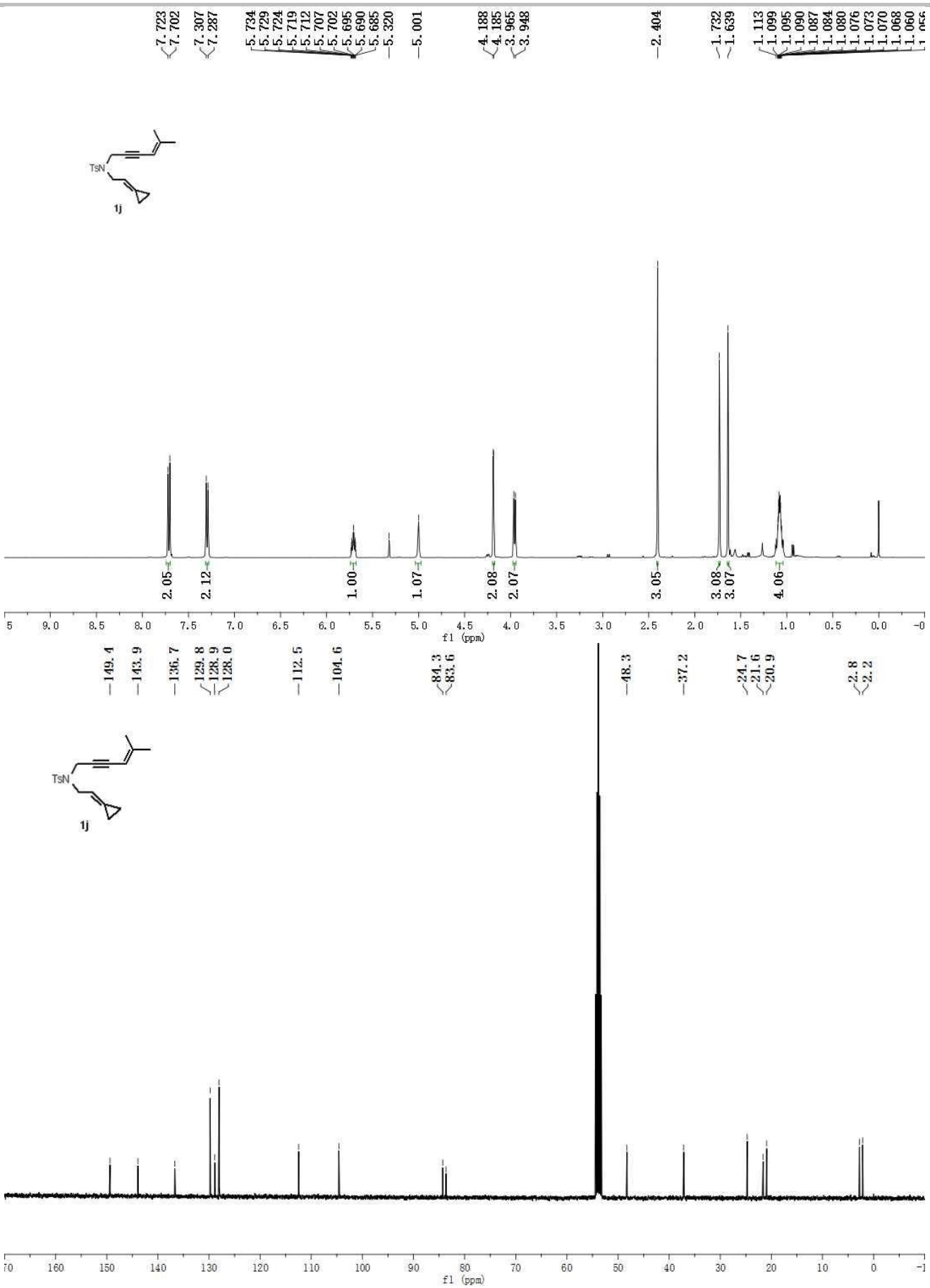
6.901
5.767
5.761
5.754
5.749
5.745
5.737
5.732
5.727
4.291
4.017
4.000
2.364
1.104
TsN
S
1h
2.05
2.07
1.00
2.01
1.00
2.04
2.04
3.24
4.14
f1 (ppm)
143.6
135.9
132.1
129.7
129.1
127.8
127.2
126.9
122.4
112.0
86.1
78.7
48.2
36.9
21.6
2.8
2.1
TsN
S
1h
f1 (ppm)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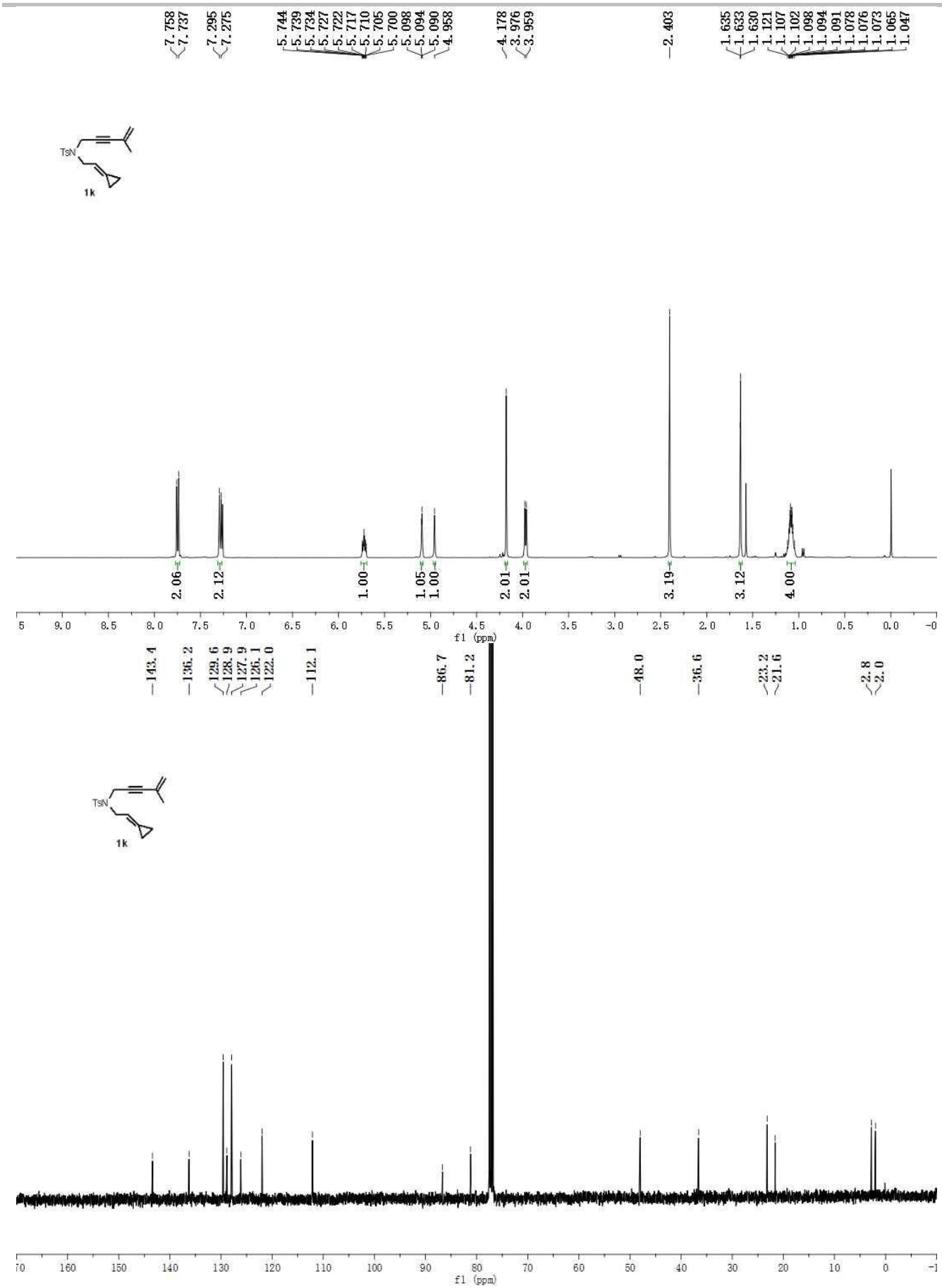
7.307
7.287
5.734
5.729
5.724
5.719
5.712
5.707
5.702
5.695
5.690
5.685
5.320
5.001
4.188
4.185
3.965
3.948
2.404
1.732
1.639
1.113
1.099
1.095
1.090
1.087
1.084
1.080
1.076
1.073
1.070
1.068
1.060
TsN
1j
2.05
2.12
1.00
1.07
2.08
2.07
3.05
3.08
3.07
4.06
f1 (ppm)
149.4
143.9
136.7
129.8
128.9
128.0
112.5
104.6
84.3
83.6
48.3
37.2
24.7
21.6
20.9
2.8
2.2
TsN
1j
f1 (ppm)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5.717
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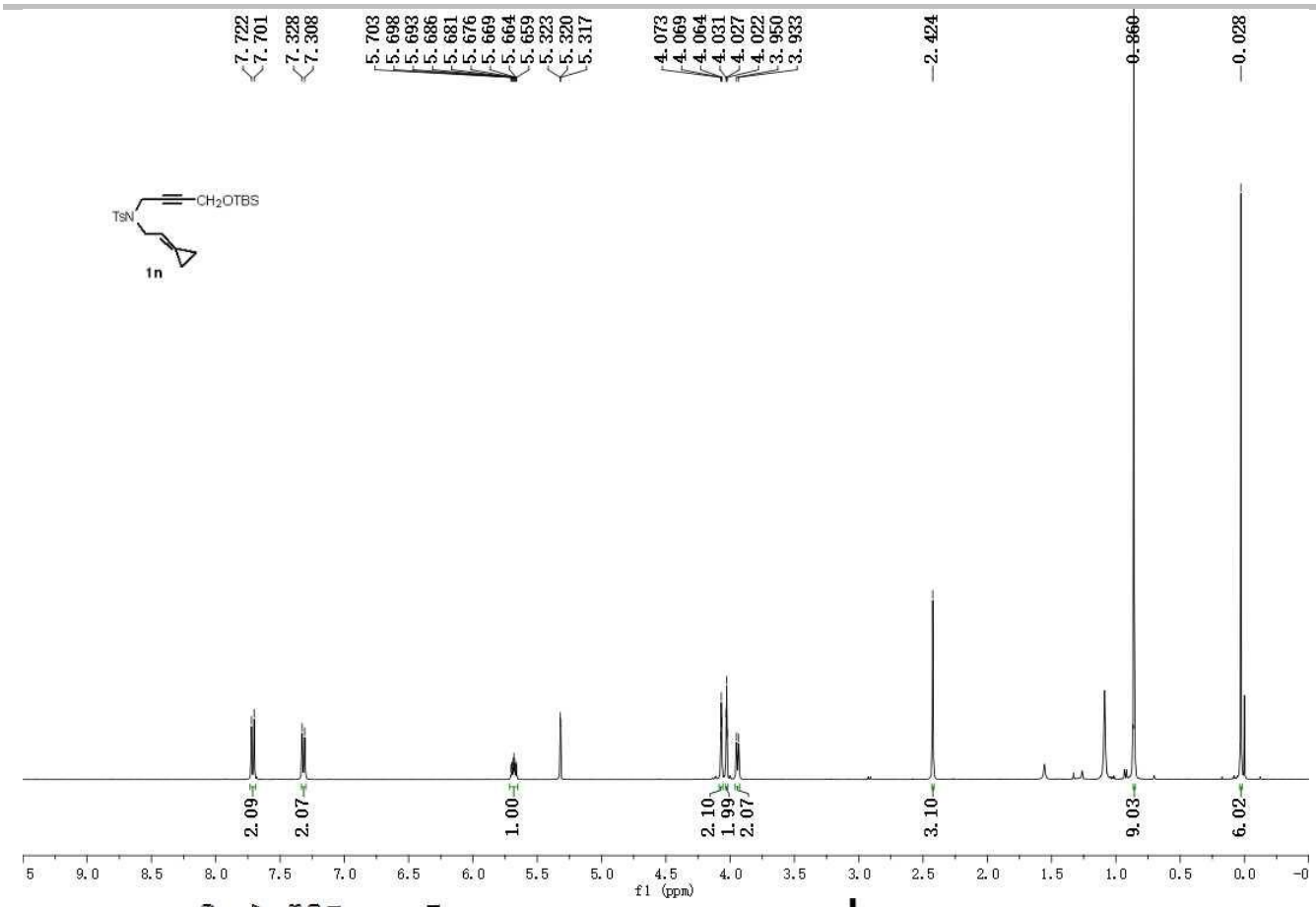
5.705
5.700
5.098
5.094
5.090
4.958
4.178
3.976
3.959
2.403
1.635
1.633
1.630
1.121
1.107
1.102
1.098
1.094
1.091
1.078
1.076
1.073
1.065
1.047
TsN
1k
2.06
2.12
1.00
1.05
1.00
2.01
2.01
3.19
3.12
4.00
f1 (ppm)
143.4
136.2
129.6
128.9
127.9
126.1
122.0
112.1
86.7
81.2
48.0
36.6
23.2
21.6
2.8
2.0
TsN
1k
f1 (ppm)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5.693
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5.681
5.676
5.669
5.664
5.659
5.323
5.320
5.317
4.073
4.069
4.064
4.031
4.027
4.022
3.950
3.933
2.424
0.960
0.028
CH2OTBS
TsN
1n
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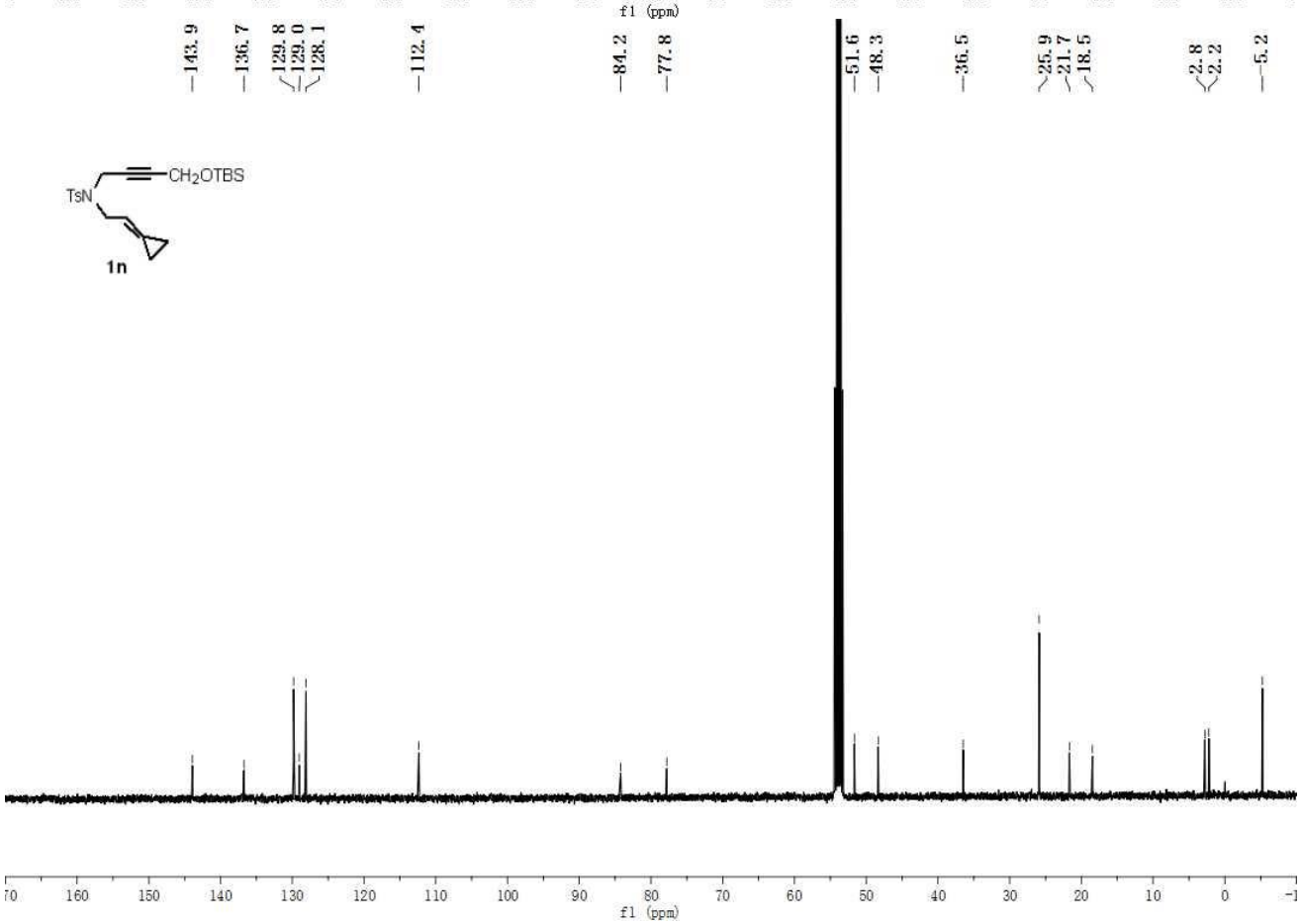
2.07
1.00
2.10
1.99
2.07
3.10
9.03
6.02
f1 (ppm)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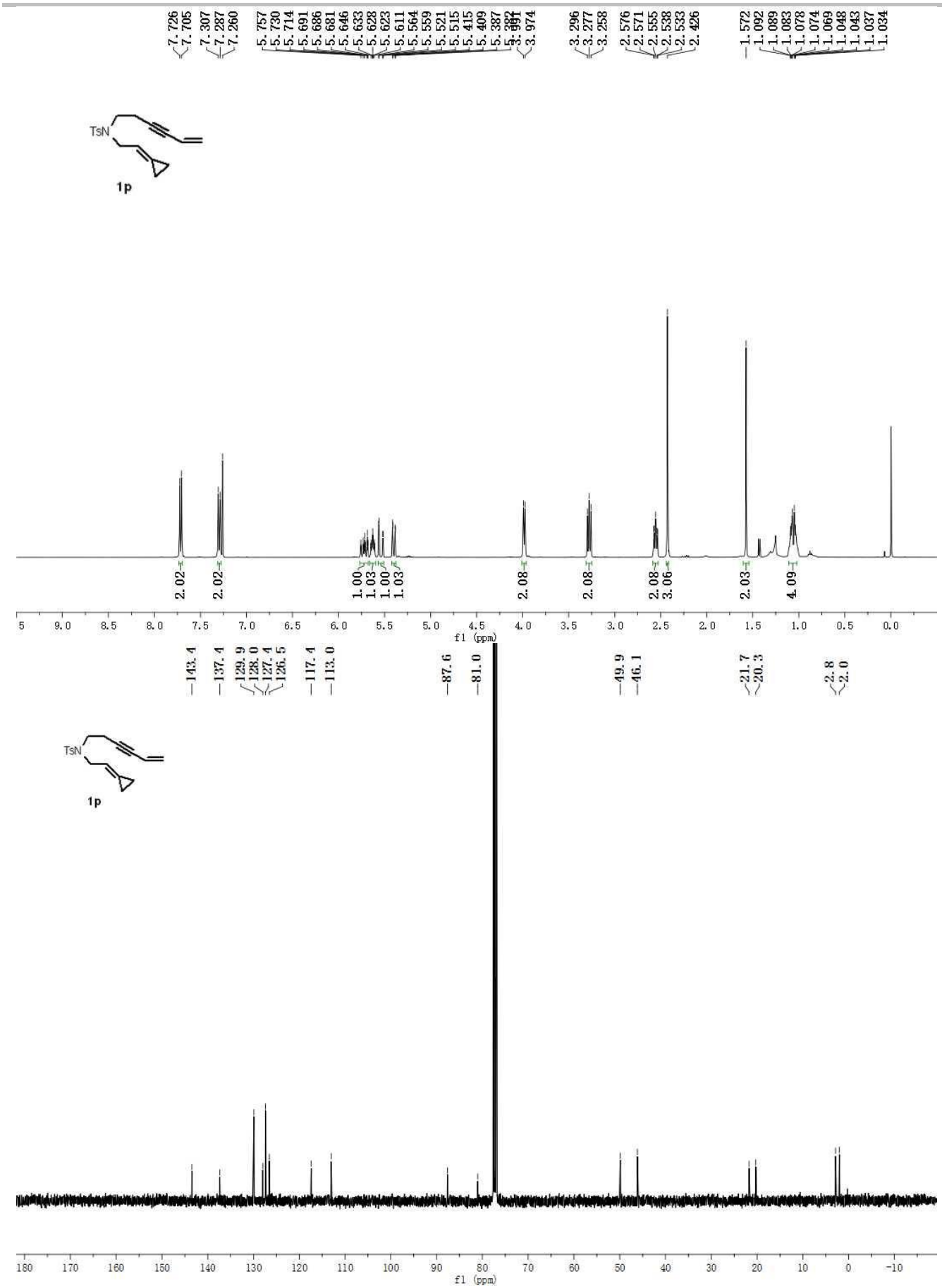
136.7
129.8
129.0
128.1
112.4
84.2
77.8
51.6
48.3
36.5
25.9
21.7
18.5
2.8
2.2
5.2
CH2OTBS
TsN
1n
f1 (ppm)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5.686
5.681
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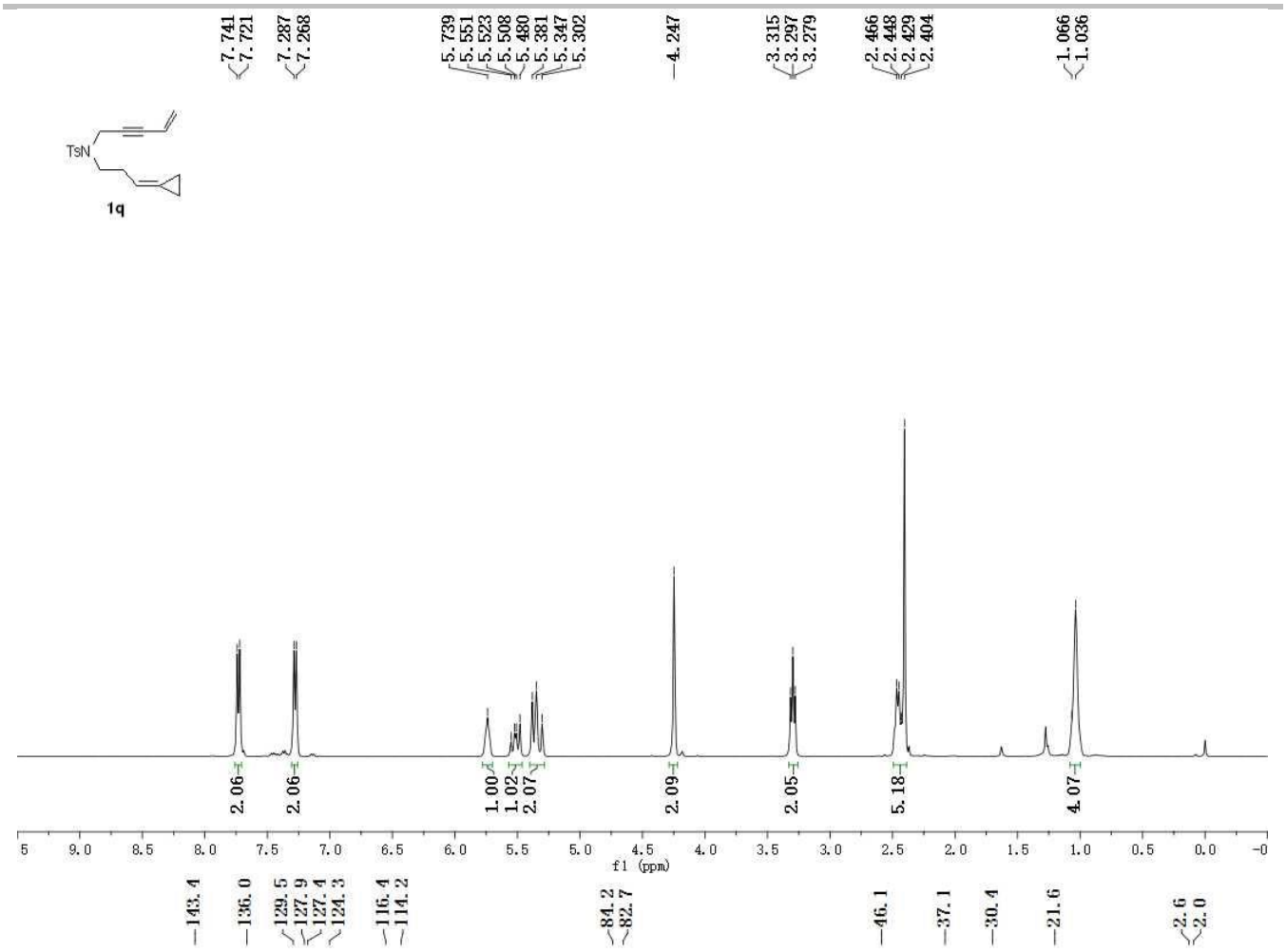
5.633
5.628
5.623
5.611
5.564
5.559
5.521
5.515
5.415
5.409
5.387
3.974
3.296
3.277
3.258
2.576
2.571
2.555
2.538
2.533
2.426
1.572
1.092
1.089
1.083
1.078
1.074
1.069
1.048
1.043
1.037
1.034
TsN
1p
2.02
2.02
1.00
1.03
1.00
1.03
2.08
2.08
2.08
3.06
2.03
4.09
f1 (ppm)
143.4
137.4
129.9
128.0
127.4
126.5
117.4
113.0
87.6
81.0
49.9
46.1
21.7
20.3
2.8
2.0
TsN
1p
f1 (ppm)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5.480
5.381
5.347
5.302
4.247
3.315
3.297
3.279
2.466
2.448
2.429
2.404
1.066
1.036
TsN
1q
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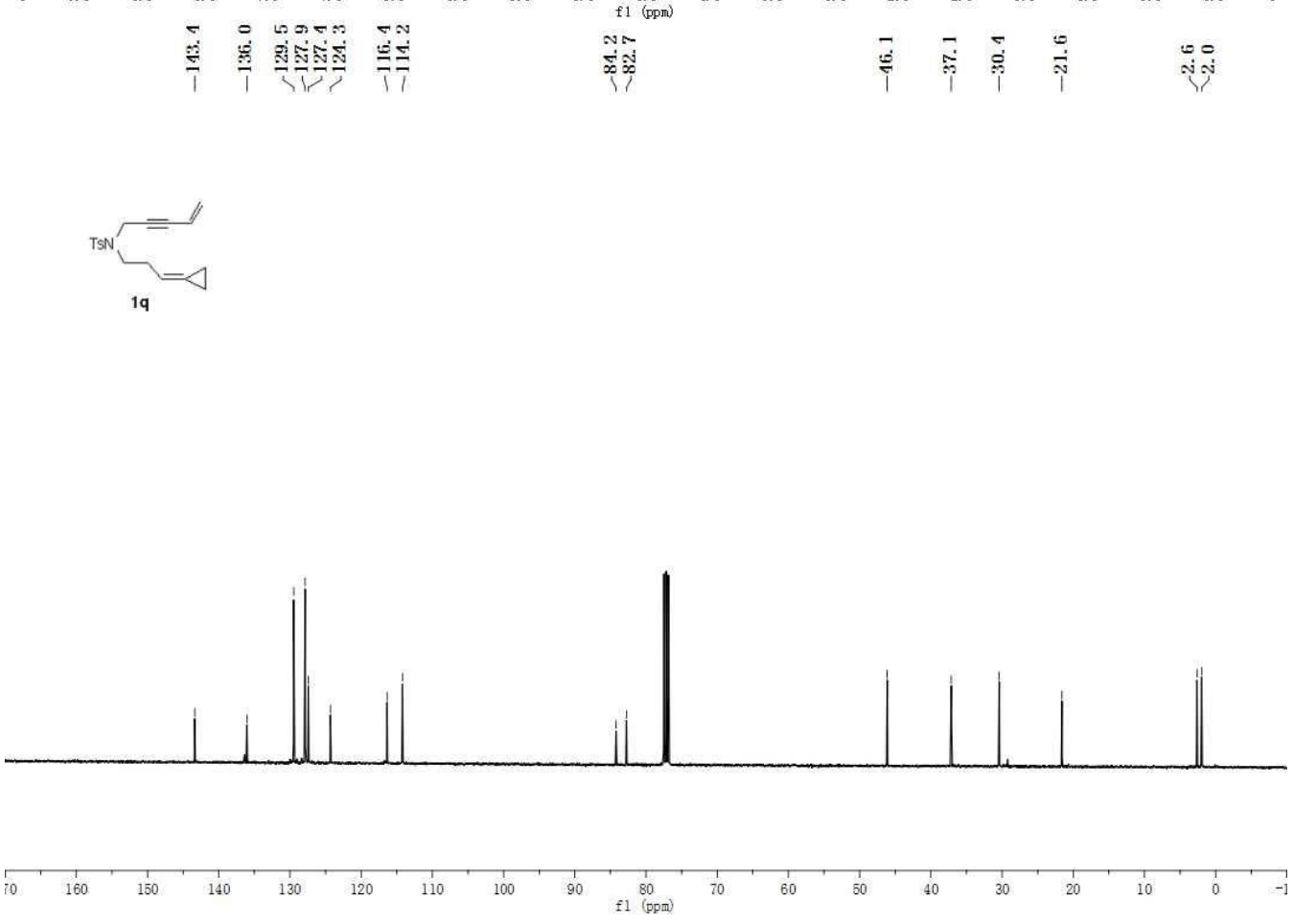
2.06
1.00
1.02
2.07
2.09
2.05
5.18
4.07
f1 (ppm)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129.5
127.9
127.4
124.3
116.4
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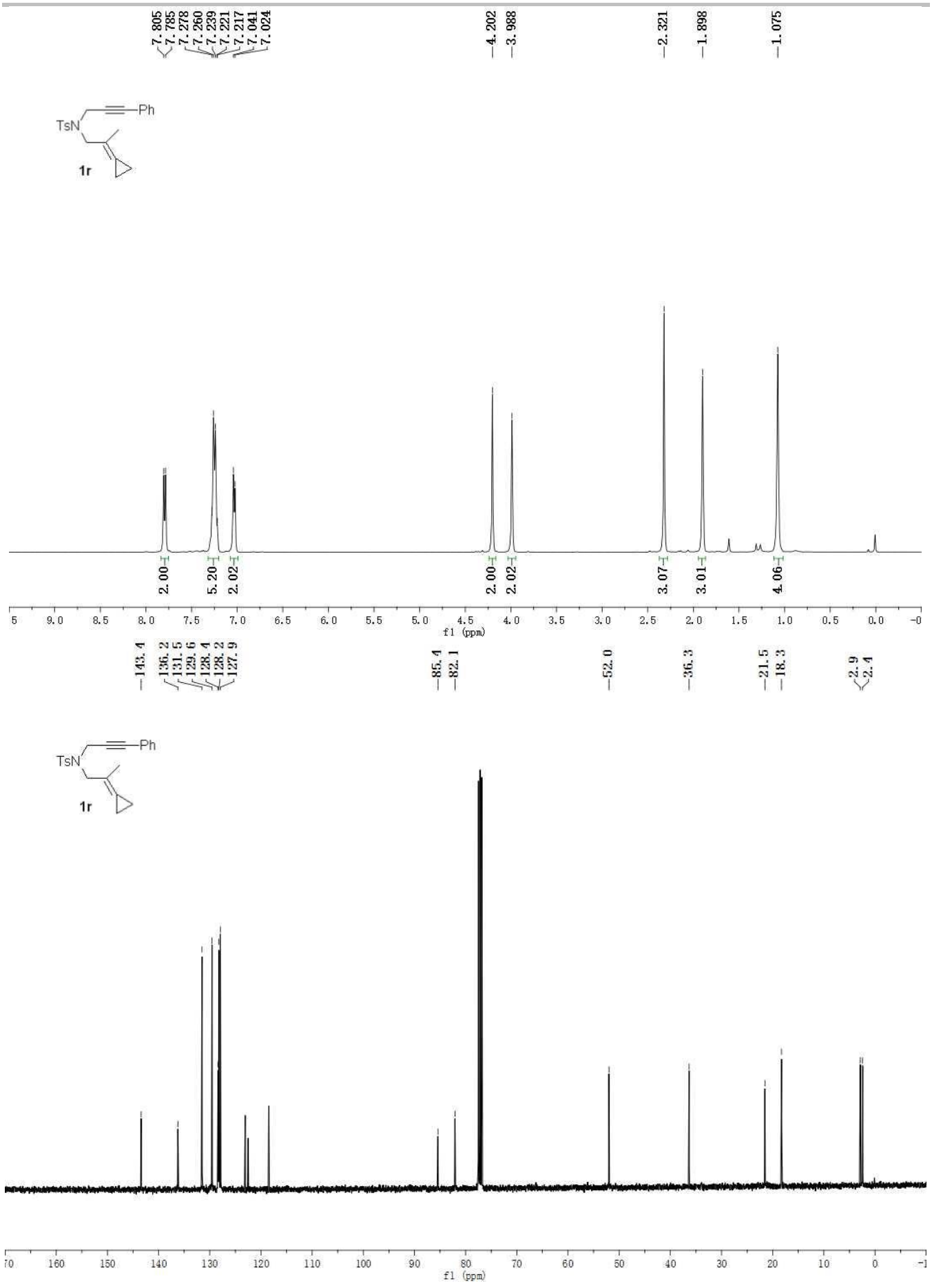
84.2
82.7
46.1
37.1
30.4
21.6
2.6
2.0
TsN
1q
f1 (ppm)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7.221
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7.041
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4.202
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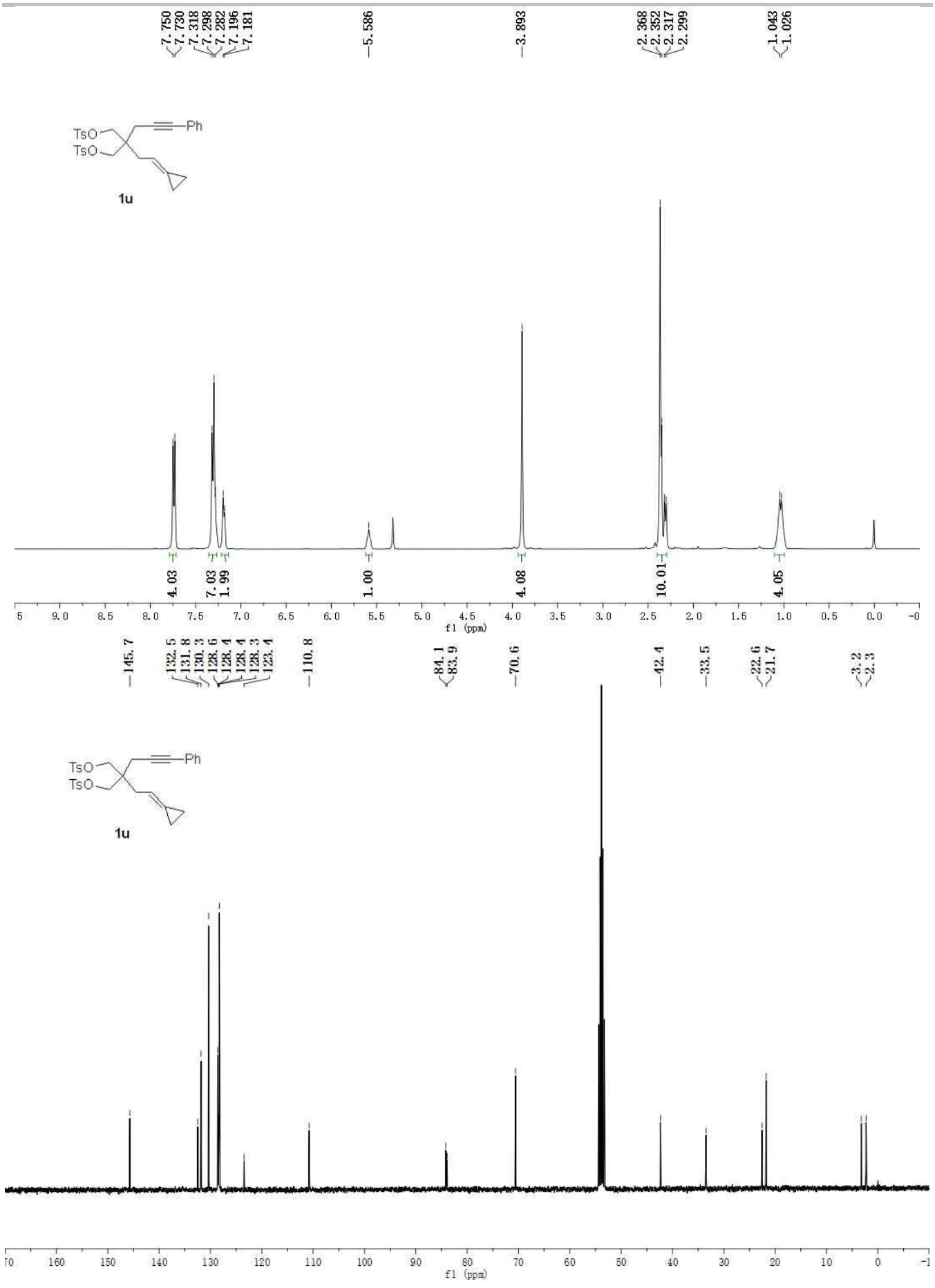
1.898
1.075
TsN
Ph
1r
2.00
5.20
2.02
2.00
2.02
3.07
3.01
4.06
f1 (ppm)
143.4
136.2
131.5
129.6
128.4
128.2
127.9
85.4
82.1
52.0
36.3
21.5
18.3
2.9
2.4
TsN
Ph
1r
f1 (ppm)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2.299
1.043
1.026
TsO
TsO
Ph
1u
4.03
7.03
1.99
1.00
4.08
10.01
4.05
f1 (ppm)
145.7
132.5
131.8
130.3
128.6
128.4
128.4
128.3
123.4
110.8
84.1
83.9
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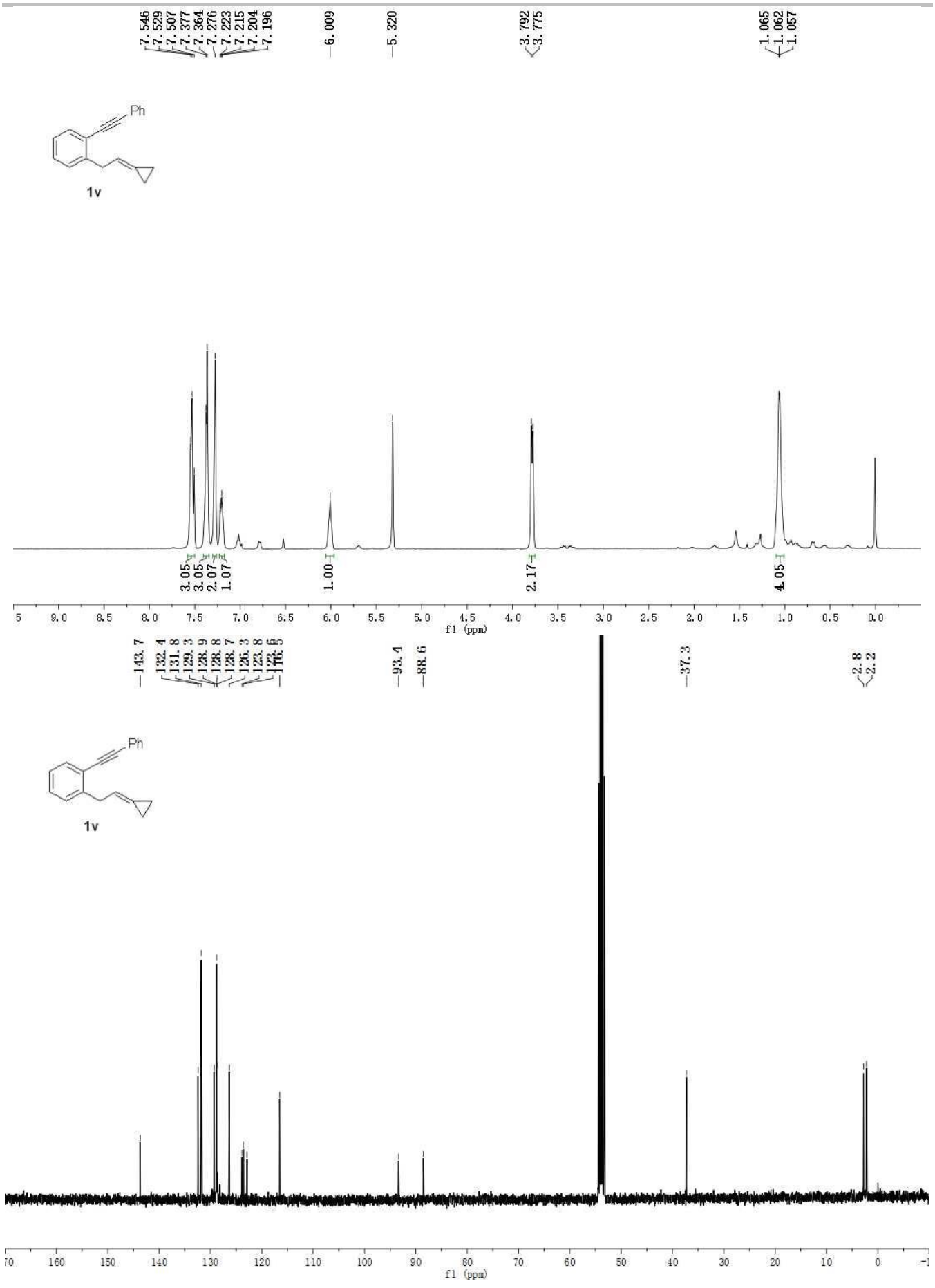
33.5
22.6
21.7
3.2
2.3
TsO
TsO
Ph
1u
f1 (ppm)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6.009
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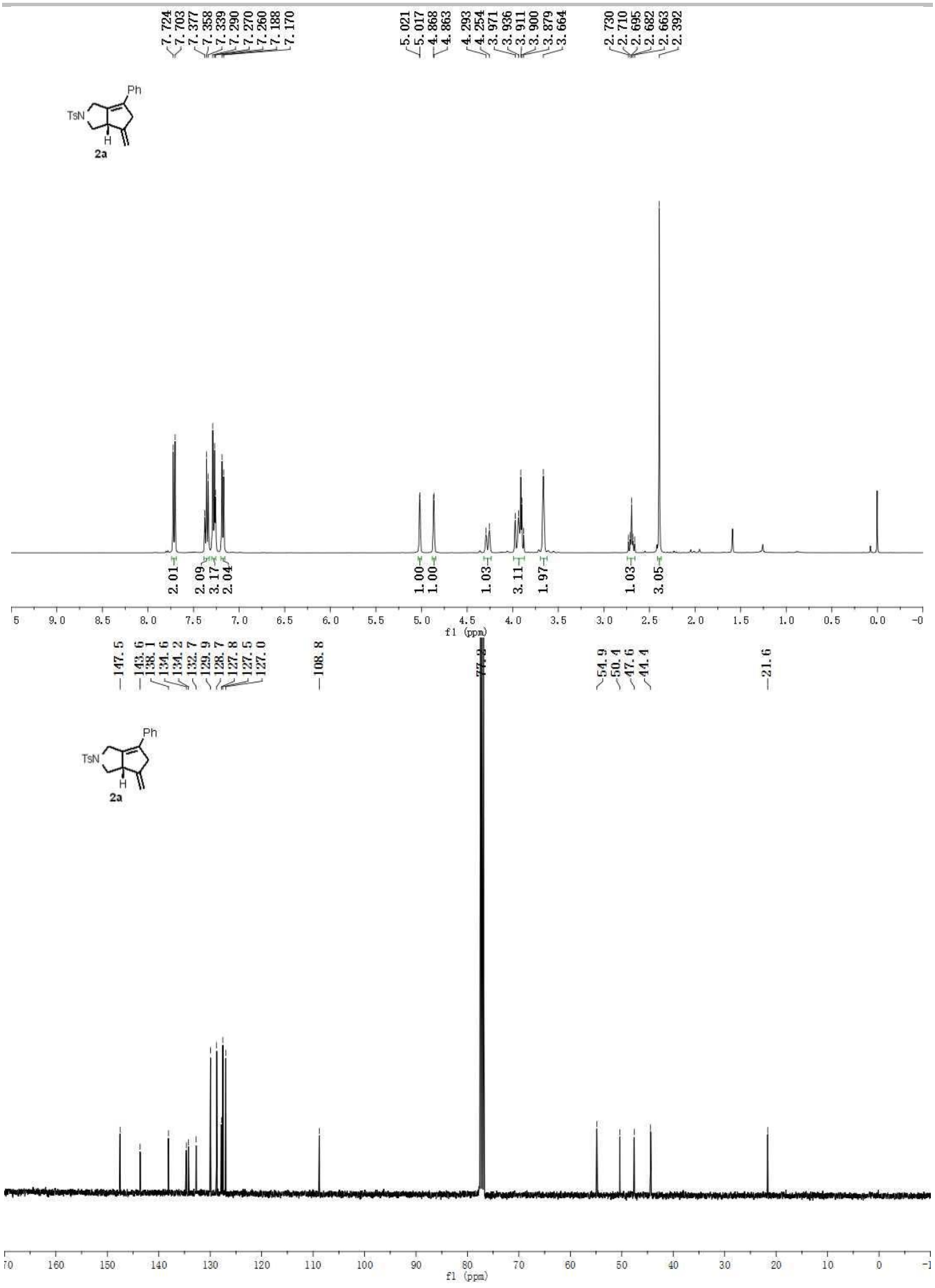
3.792
3.775
1.065
1.062
1.057
Ph
1v
3.05
3.05
2.07
1.07
1.00
2.17
4.05
f1 (ppm)
143.7
132.4
131.8
129.3
128.9
128.8
128.7
126.3
123.8
93.4
88.6
37.3
2.8
2.2
Ph
1v
f1 (ppm)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4.868
4.863
4.293
4.254
3.971
3.936
3.911
3.900
3.879
3.664
2.730
2.710
2.695
2.682
2.663
2.392
Ph
TsN
H
2a
2.01
2.09
3.17
2.04
1.00
1.00
1.03
3.11
1.97
1.03
3.05
f1 (ppm)
147.5
143.6
138.1
134.6
134.2
132.7
129.9
128.7
127.8
127.5
127.0
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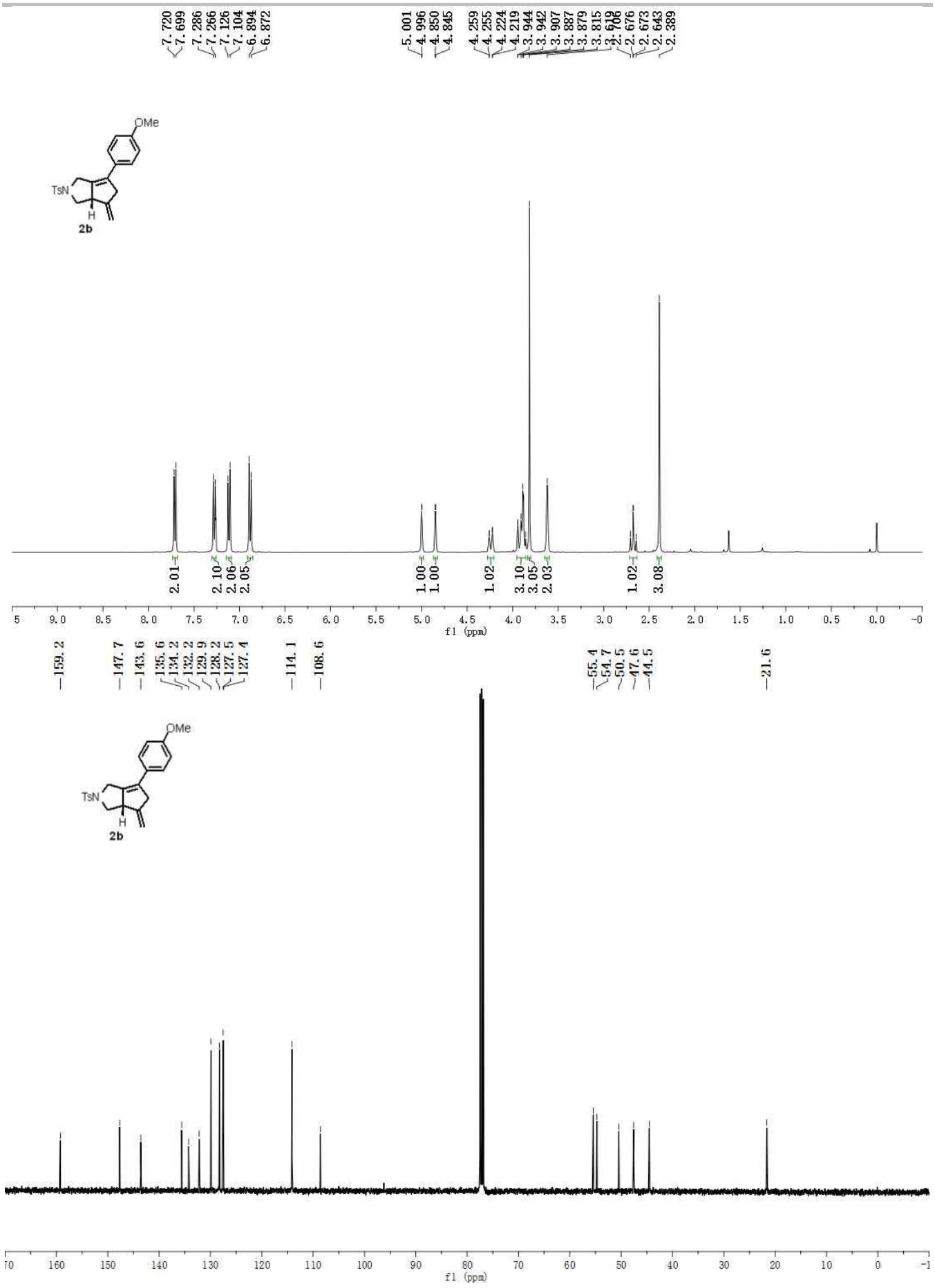
54.9
50.4
47.6
44.4
21.6
Ph
TsN
H
2a
f1 (ppm)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4.259
4.255
4.224
4.219
3.944
3.942
3.907
3.887
3.879
3.815
2.676
2.673
2.643
2.389
OMe
TsN
H
2b
2.01
2.10
2.06
2.05
1.00
1.00
1.02
3.10
3.05
2.03
1.02
3.08
f1 (ppm)
159.2
147.7
143.6
135.6
134.2
132.2
129.9
128.2
127.5
127.4
114.1
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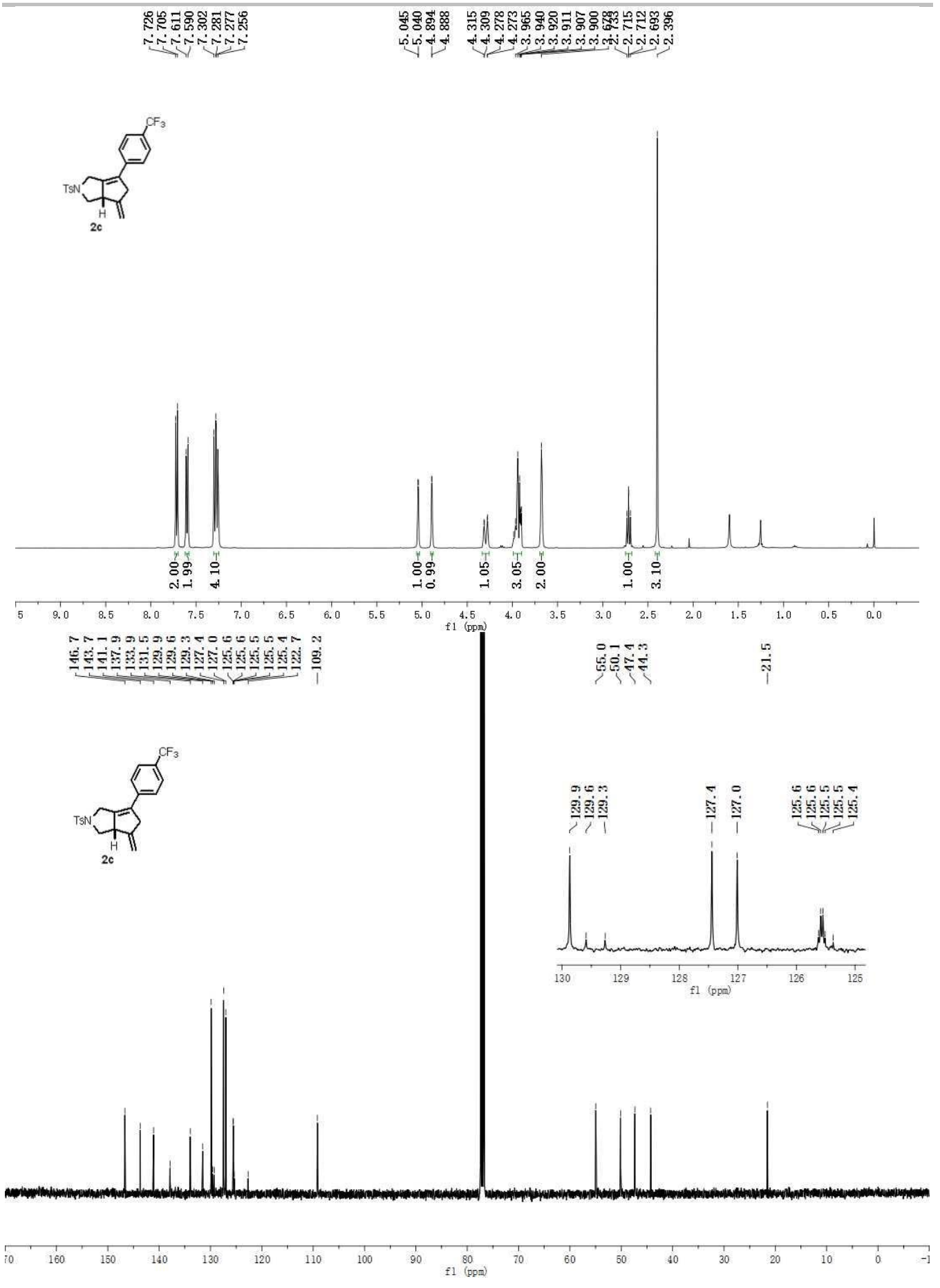
50.5
47.6
44.5
21.6
OMe
TsN
H
2b
f1 (ppm)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4.309
4.278
4.273
3.965
3.940
3.920
3.911
3.907
3.900
2.715
2.712
2.693
2.396
CF3
TsN
H
2c
2.00
1.99
4.10
1.00
0.99
1.05
3.05
2.00
1.00
3.10
f1 (ppm)
146.7
143.7
141.1
137.9
133.9
131.5
129.9
129.6
129.3
127.4
127.0
125.6
125.6
125.5
125.5
125.4
122.7
109.2
55.0
50.1
47.4
44.3
21.5
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129.6
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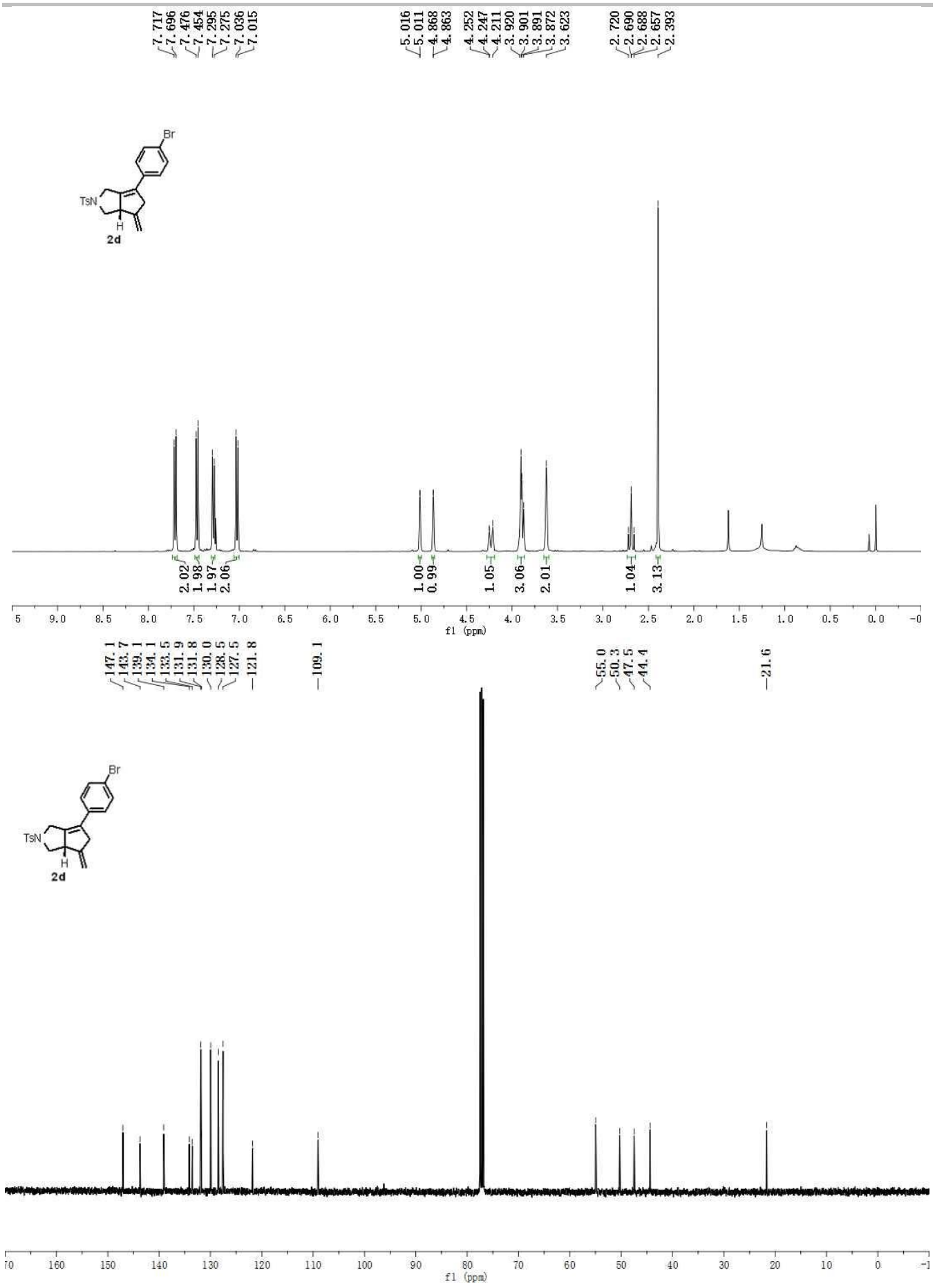
125.6
125.6
125.5
125.5
125.4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7.036
7.015
5.016
5.011
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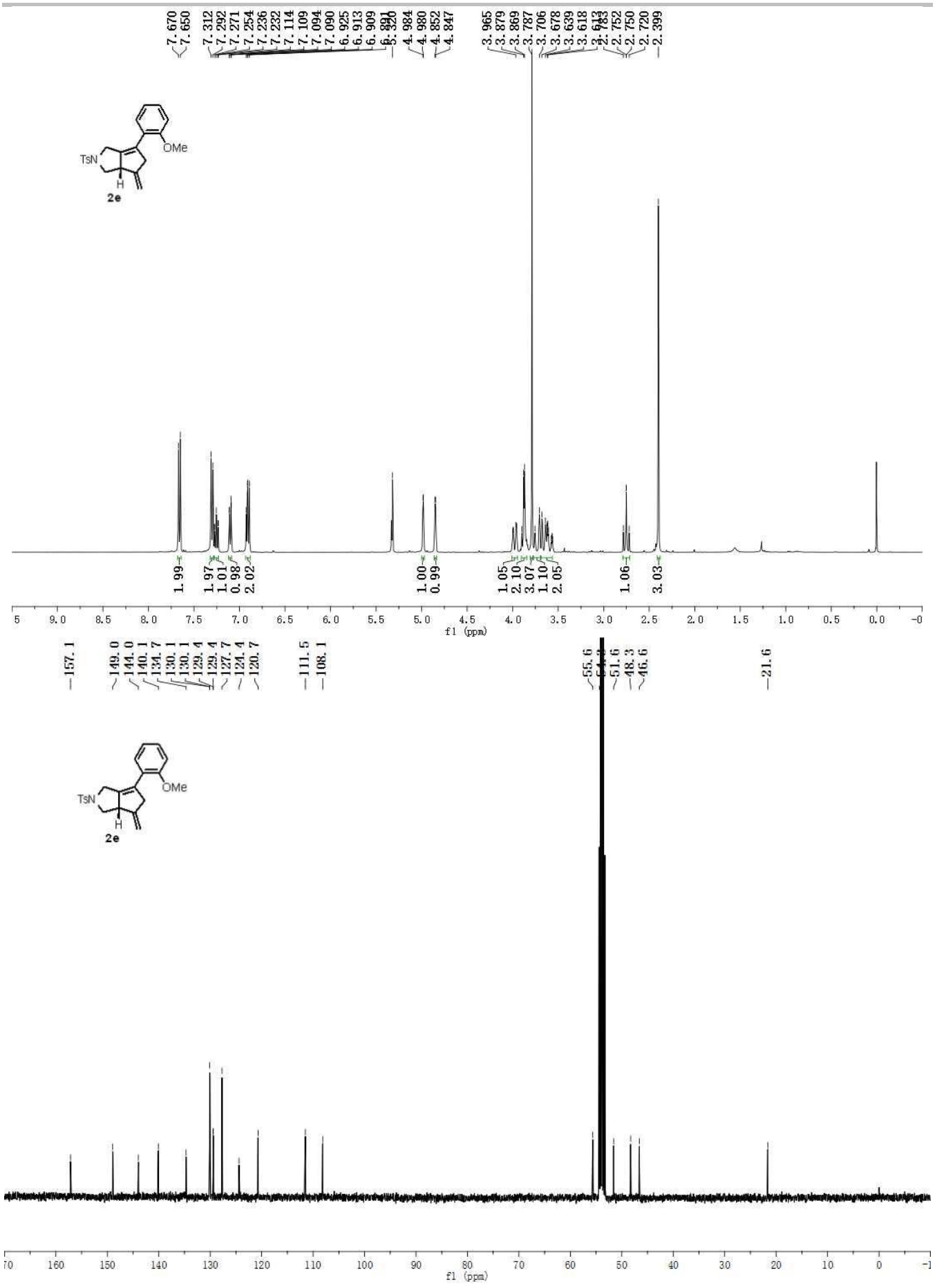
4.863
4.252
4.247
4.211
3.920
3.901
3.891
3.872
3.623
2.720
2.690
2.688
2.657
2.393
Br
TsN
H
2d
2.02
1.98
1.97
2.06
1.00
0.99
1.05
3.06
2.01
1.04
3.13
f1 (ppm)
147.1
143.7
139.1
134.1
133.5
131.9
131.8
130.0
128.5
127.5
121.8
109.1
55.0
50.3
47.5
44.4
21.6
Br
TsN
H
2d
f1 (ppm)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7.236
7.232
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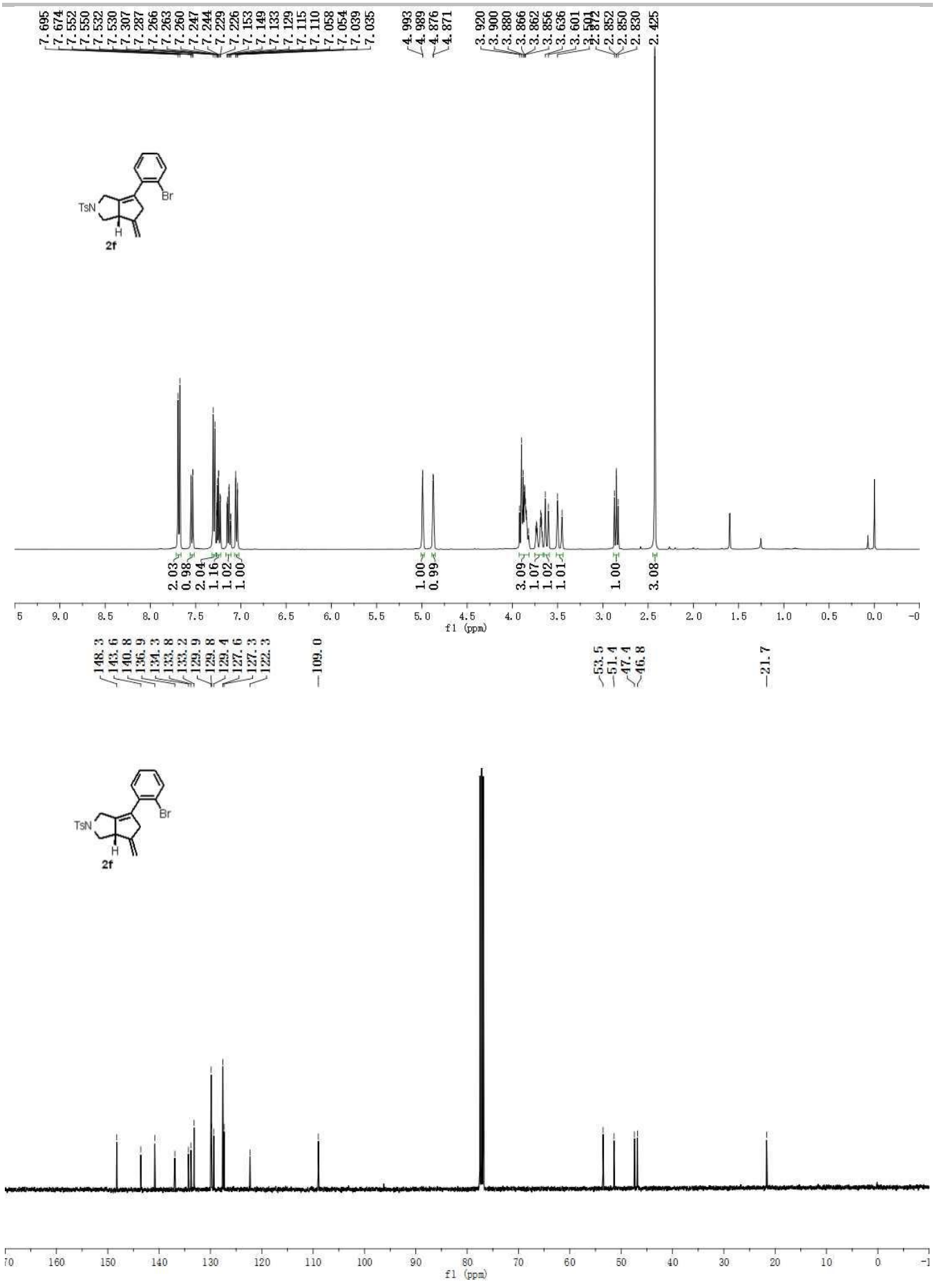
7.109
7.094
7.090
6.925
6.913
6.909
5.320
4.984
4.980
4.852
4.847
3.965
3.879
3.869
3.787
3.706
3.678
3.639
3.618
2.752
2.750
2.720
2.399
TsN
OMe
H
2e
1.99
1.97
1.01
0.98
2.02
1.00
0.99
1.05
2.10
3.07
1.10
2.05
1.06
3.03
f1 (ppm)
157.1
149.0
144.0
140.1
134.7
130.1
130.1
129.4
129.4
127.7
124.4
120.7
111.5
108.1
55.6
51.6
48.3
46.6
21.6
TsN
OMe
H
2e
f1 (ppm)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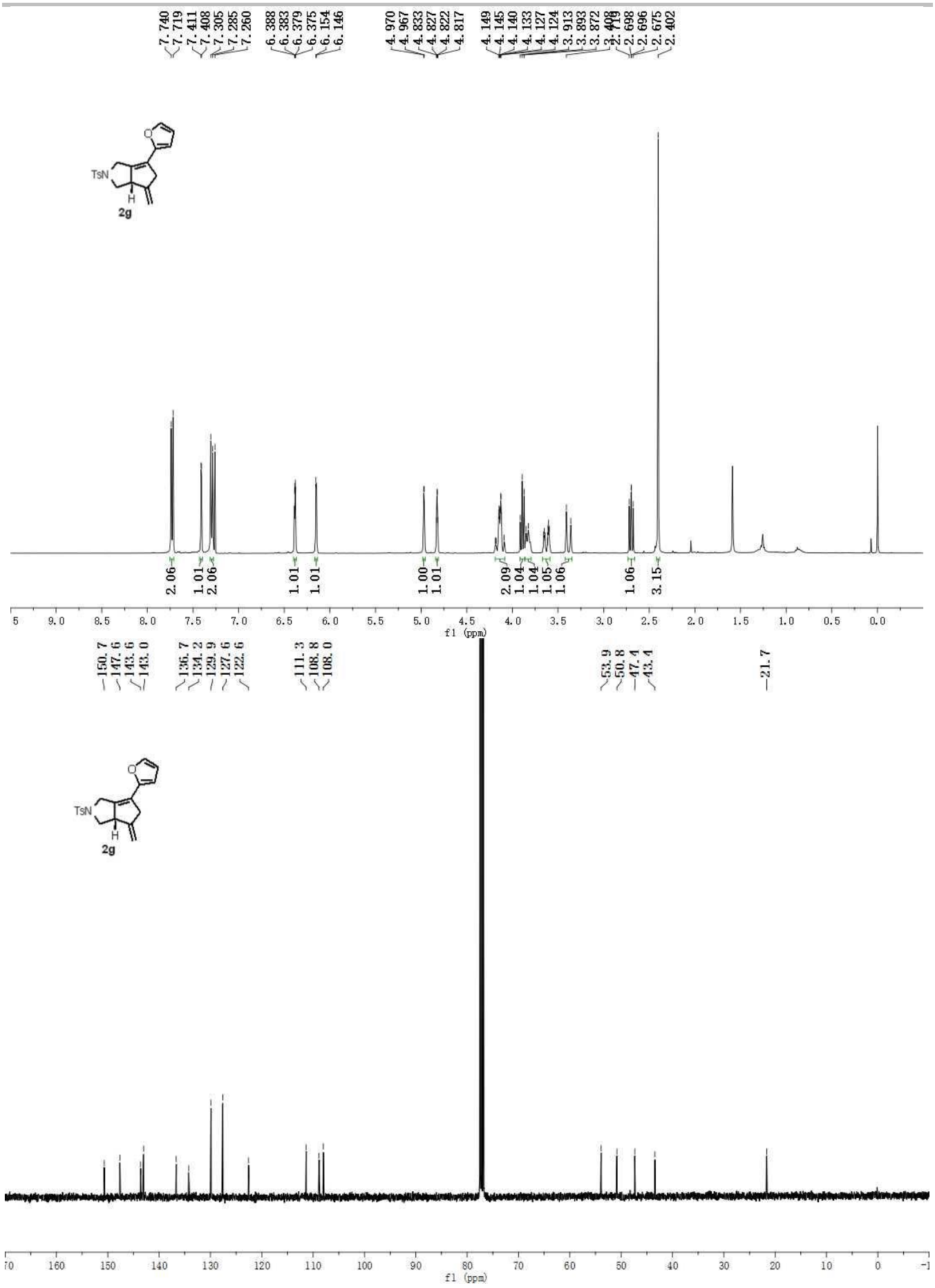
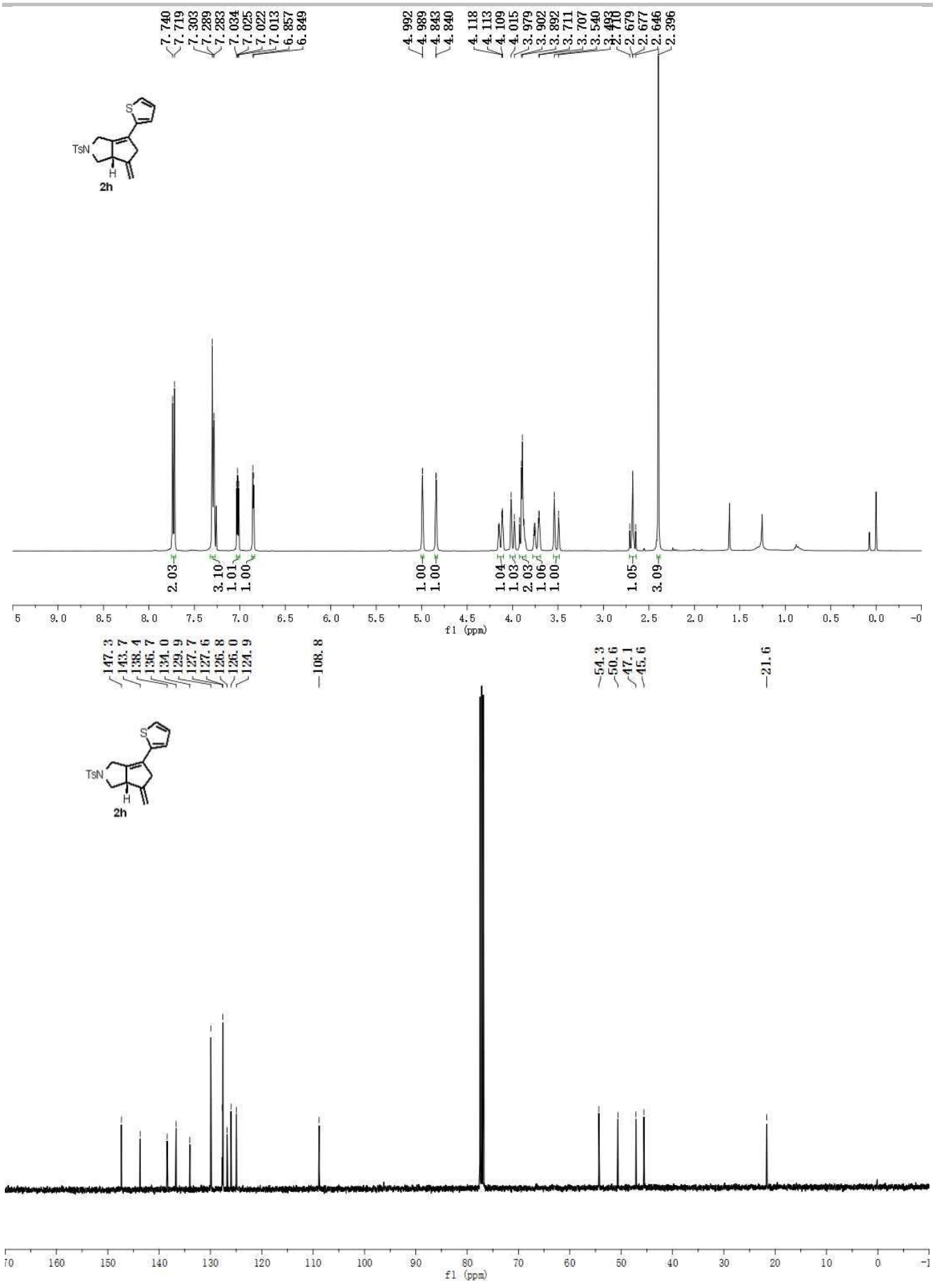
7.674
7.552
7.550
7.532
7.530
7.307
7.287
7.266
7.263
7.260
7.247
7.244
7.229
7.226
7.153
7.149
7.133
7.129
7.115
7.110
7.058
7.054
7.039
7.035
4.993
4.989
4.876
4.871
3.920
3.900
3.880
3.866
3.862
3.856
3.636
3.601
2.852
2.850
2.830
2.425
TsN
Br
H
2f
2.03
0.98
2.04
1.16
1.02
1.00
1.00
0.99
3.09
1.07
1.02
1.01
1.00
3.08
f1 (ppm)
148.3
143.6
140.8
136.9
134.3
133.8
133.2
129.9
129.8
129.4
127.6
127.3
122.3
109.0
53.5
51.4
47.4
46.8
21.7
TsN
Br
H
2f
f1 (ppm)


7.740
7.719
7.411
7.408
7.305
7.285
7.260
6.388
6.383
6.379
6.375
6.154
6.146
4.970
4.967
4.833
4.827
4.822
4.817
4.149
4.145
4.140
4.133
4.127
4.124
3.913
3.893
3.872
2.698
2.696
2.675
2.402
TsN
H
2g
2.06
1.01
2.06
1.01
1.01
1.00
1.01
2.09
1.04
1.04
1.05
1.06
1.06
3.15
f1 (ppm)
150.7
147.6
143.6
143.0
136.7
134.2
129.9
127.6
122.6
111.3
108.8
108.0
53.9
50.8
47.4
43.4
21.7
TsN
H
2g
f1 (ppm)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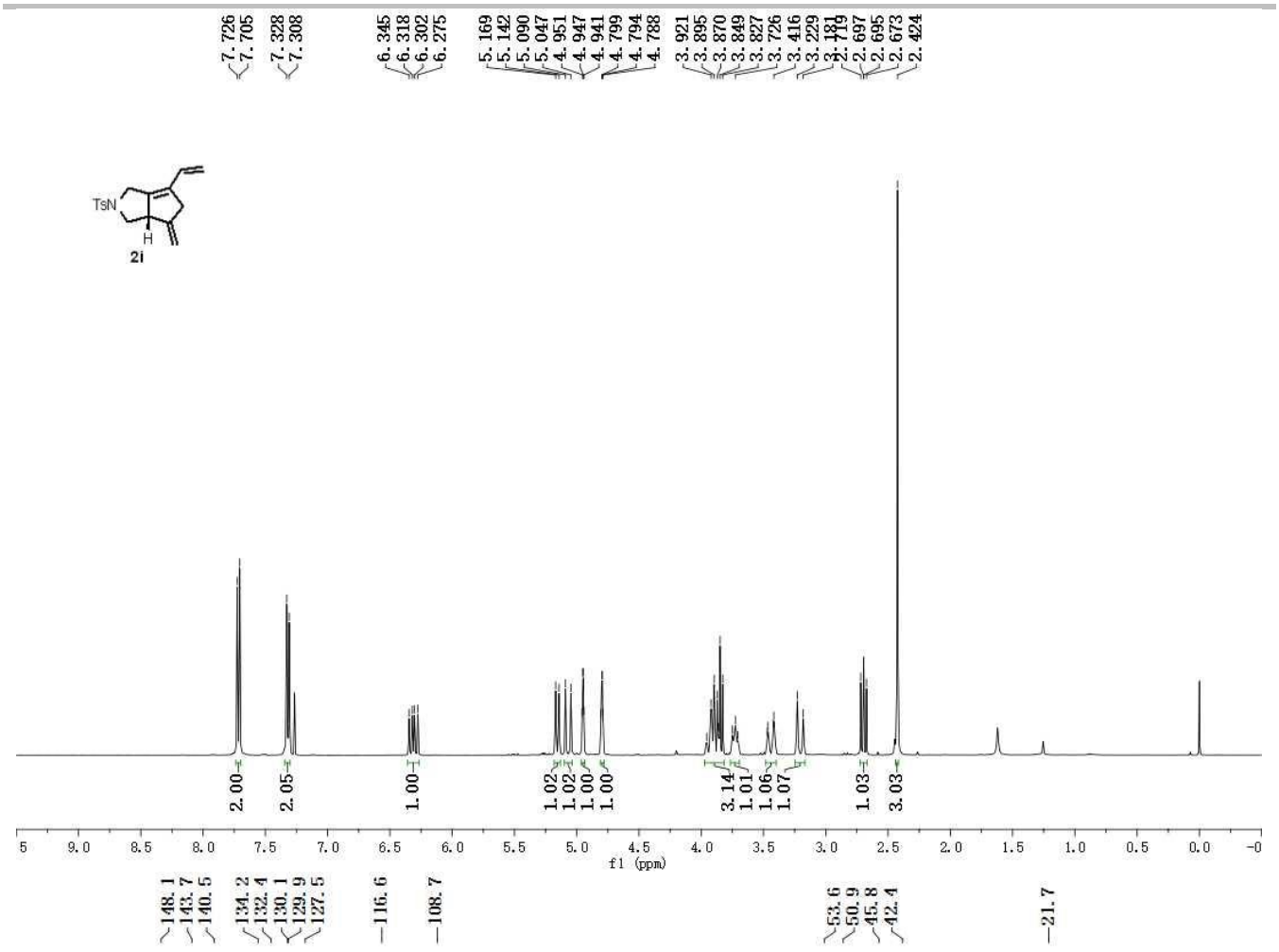
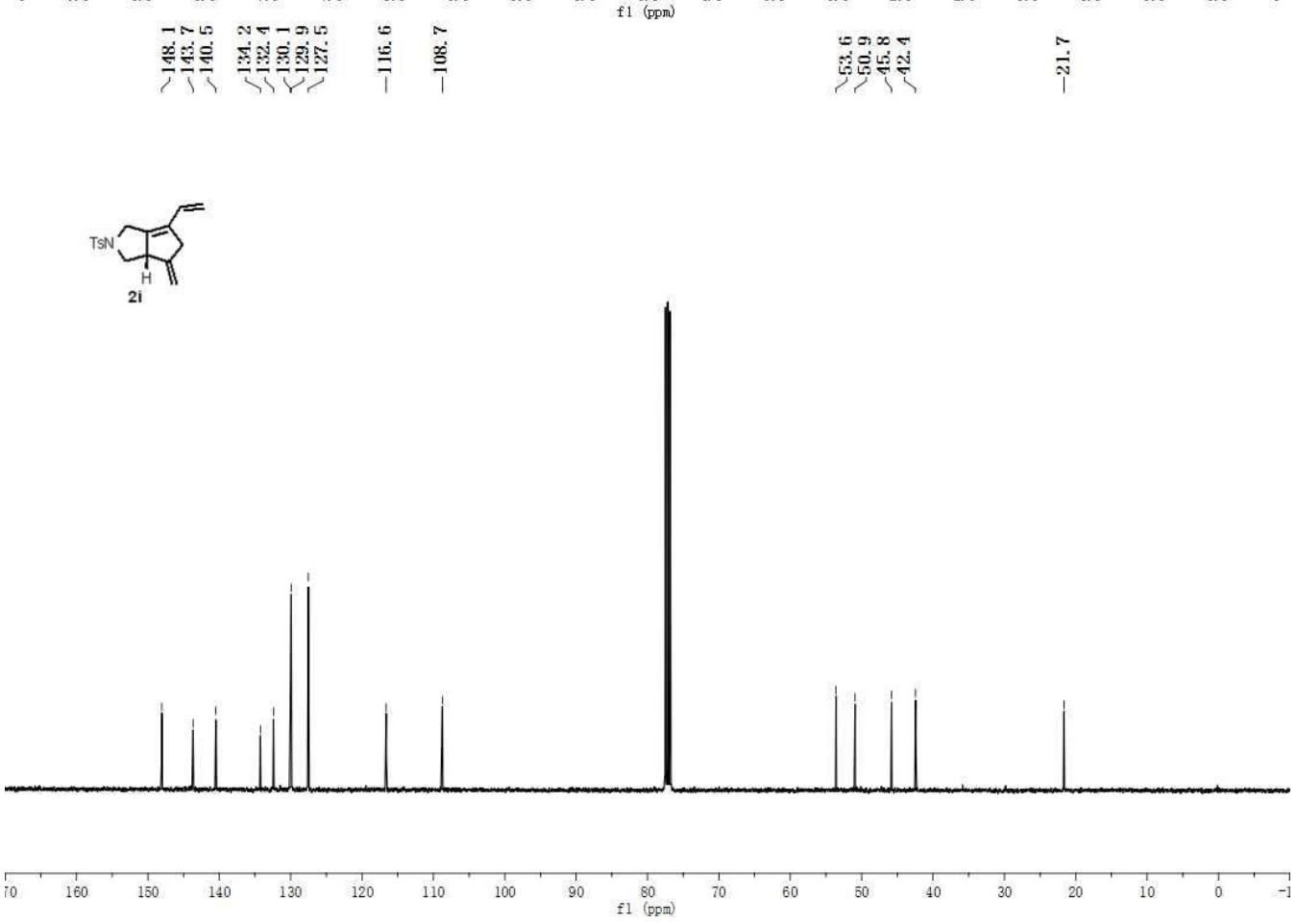
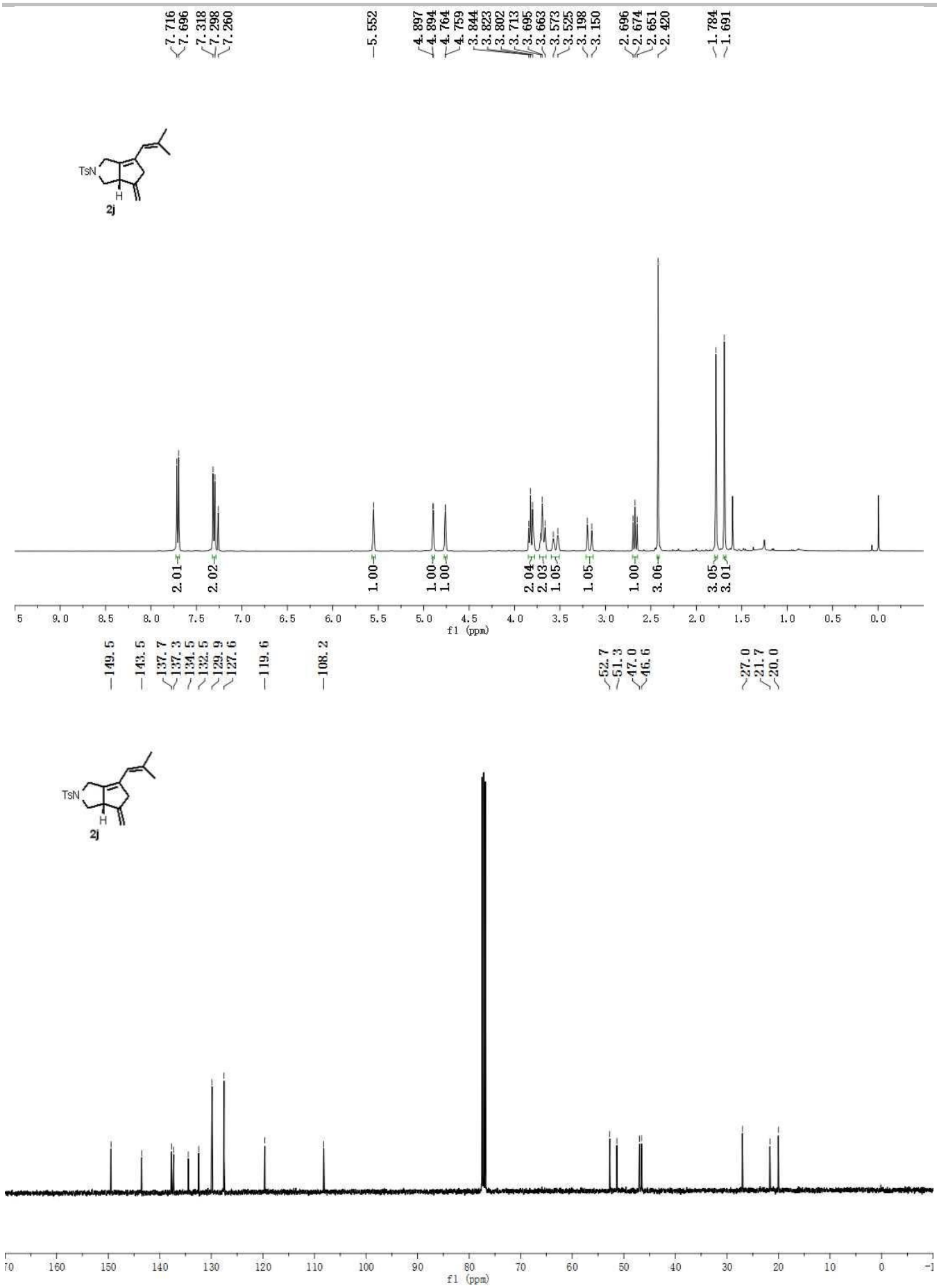
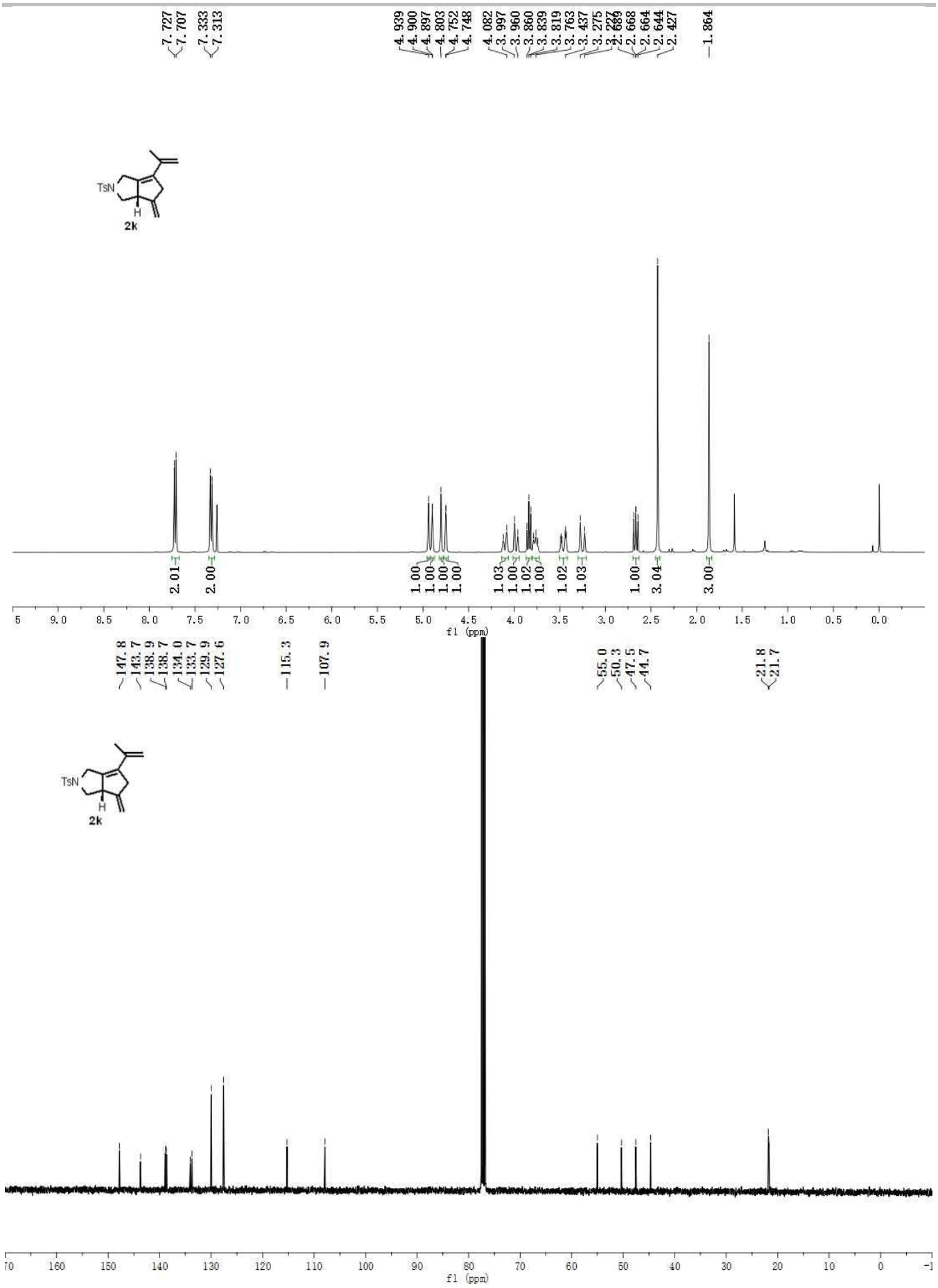
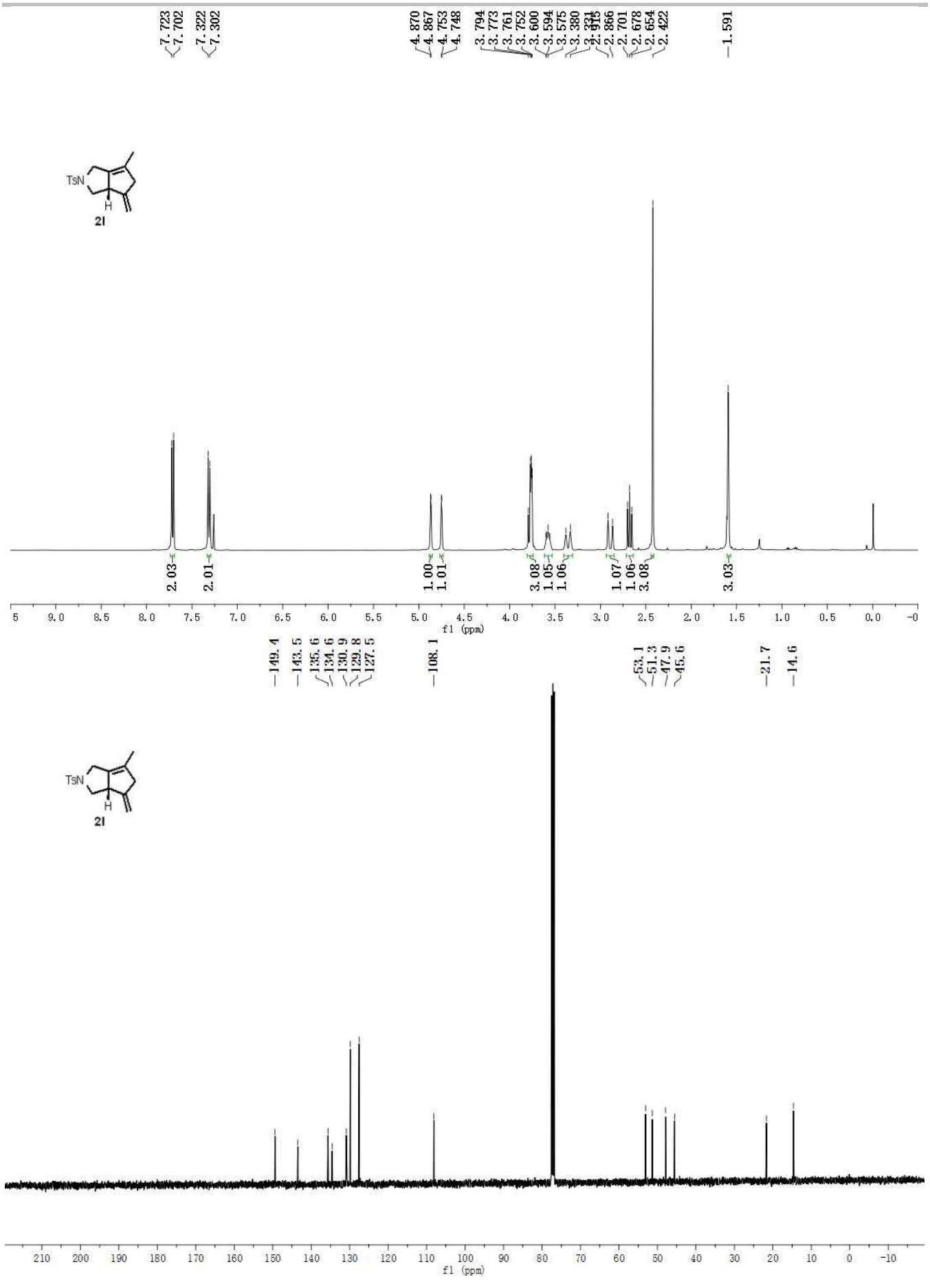
7.719
7.303
7.289
7.283
7.034
7.025
7.022
7.013
6.857
6.849
4.992
4.989
4.843
4.840
4.118
4.113
4.109
4.015
3.979
3.902
3.892
3.711
3.707
3.540
3.493
3.710
2.679
2.677
2.646
2.396
TsN
H
2h
2.03
3.10
1.01
1.00
1.00
1.00
1.04
1.03
2.03
1.06
1.00
1.05
3.09
f1 (ppm)
147.3
143.7
138.4
136.7
134.0
129.9
127.7
127.6
126.8
126.0
124.9
108.8
54.3
50.6
47.1
45.6
21.6
TsN
H
2h
f1 (ppm)


7.726
7.705
7.328
7.308
6.345
6.318
6.302
6.275
5.169
5.142
5.090
5.047
4.951
4.947
4.941
4.799
4.794
4.788
3.921
3.895
3.870
3.849
3.827
3.726
3.416
3.229
2.697
2.695
2.673
2.424
TsN
H
2i
2.00
2.05
1.00
1.02
1.02
1.00
1.00
3.14
1.01
1.06
1.07
1.03
3.03
f1 (ppm)

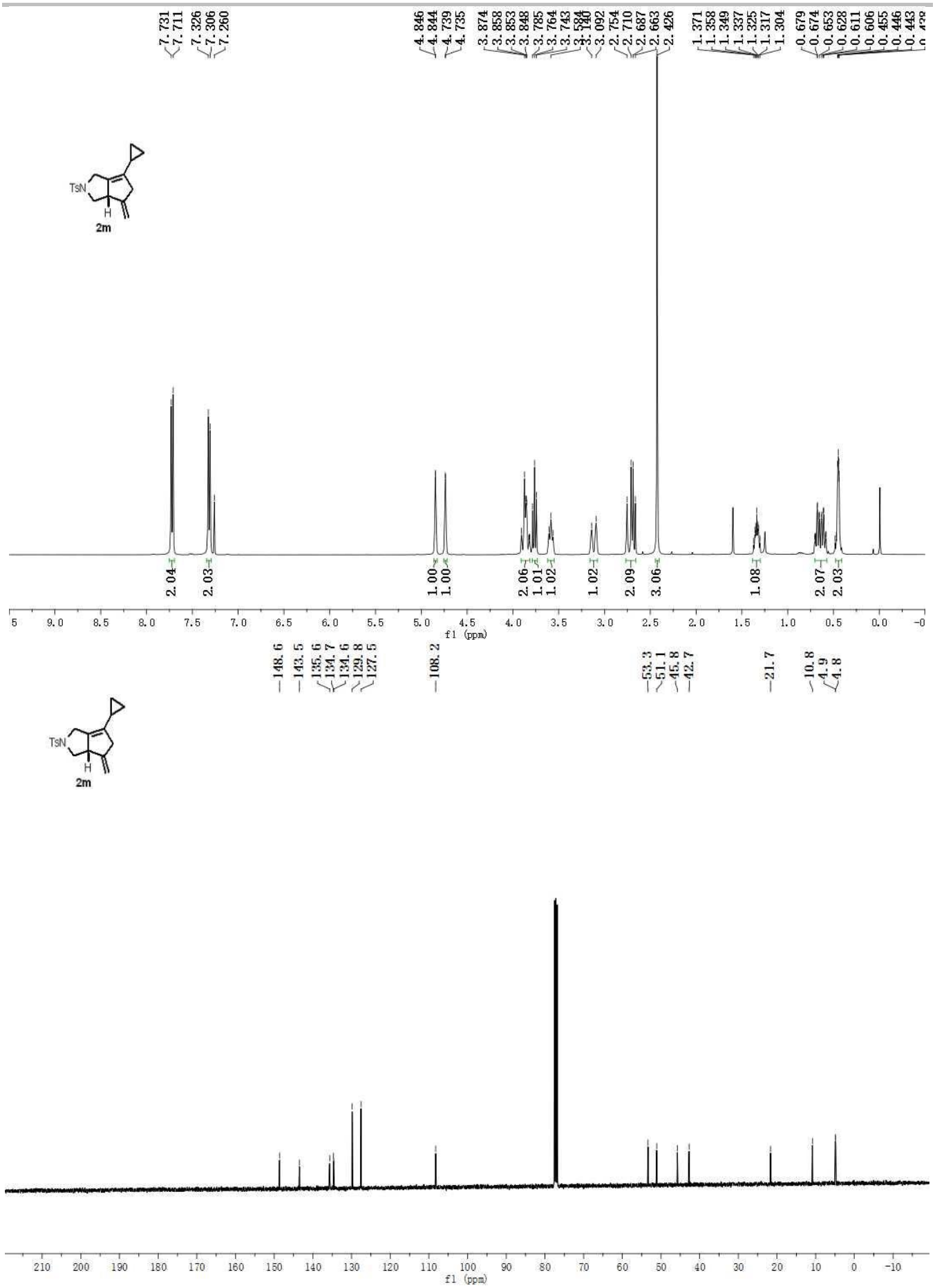

148.1
143.7
140.5
134.2
132.4
130.1
129.9
127.5
116.6
108.7
53.6
50.9
45.8
42.4
21.7
TsN
H
2i
f1 (ppm)

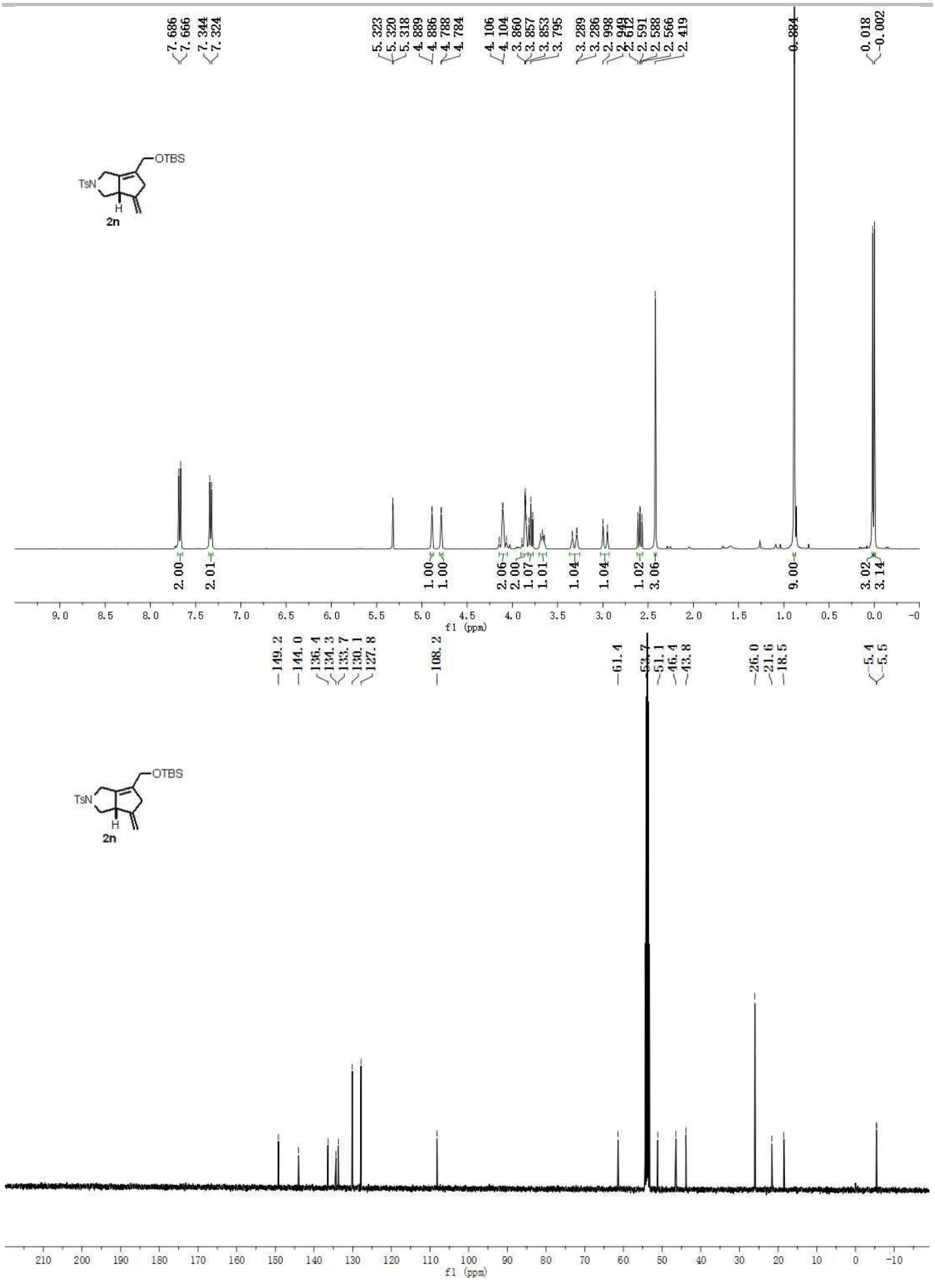

7.716
7.696
7.318
7.298
7.260
5.552
4.897
4.894
4.764
4.759
3.844
3.823
3.802
3.713
3.695
3.663
3.573
3.525
3.198
3.150
2.696
2.674
2.651
2.420
1.784
1.691
TsN
H
2j
2.01
2.02
1.00
1.00
1.00
2.04
2.03
1.05
1.05
1.00
3.06
3.05
3.01
f1 (ppm)
149.5
143.5
137.7
137.3
134.5
132.5
129.9
127.6
119.6
108.2
52.7
51.3
47.0
46.6
27.0
21.7
20.0
TsN
H
2j
f1 (ppm)


7.727
7.707
7.333
7.313
4.939
4.900
4.897
4.803
4.752
4.748
4.082
3.997
3.960
3.860
3.839
3.819
3.763
3.437
3.275
2.668
2.664
2.644
2.427
1.864
TsN
H
2k
2.01
2.00
1.00
1.00
1.00
1.00
1.03
1.00
1.02
1.00
1.02
1.03
1.00
3.04
3.00
f1 (ppm)
147.8
143.7
138.9
138.7
134.0
133.7
129.9
127.6
115.3
107.9
55.0
50.3
47.5
44.7
21.8
21.7
TsN
H
2k
f1 (ppm)


7.723
7.702
7.322
7.302
4.870
4.867
4.753
4.748
3.794
3.773
3.761
3.752
3.600
3.594
3.575
3.380
2.866
2.701
2.678
2.654
2.422
1.591
TsN
H
2l
2.03
2.01
1.00
1.01
3.08
1.05
1.06
1.07
1.06
3.08
3.03
f1 (ppm)
149.4
143.5
135.6
134.6
130.9
129.8
127.5
108.1
53.1
51.3
47.9
45.6
21.7
14.6
TsN
H
2l
f1 (ppm)

SUPPORTING INFORMATION

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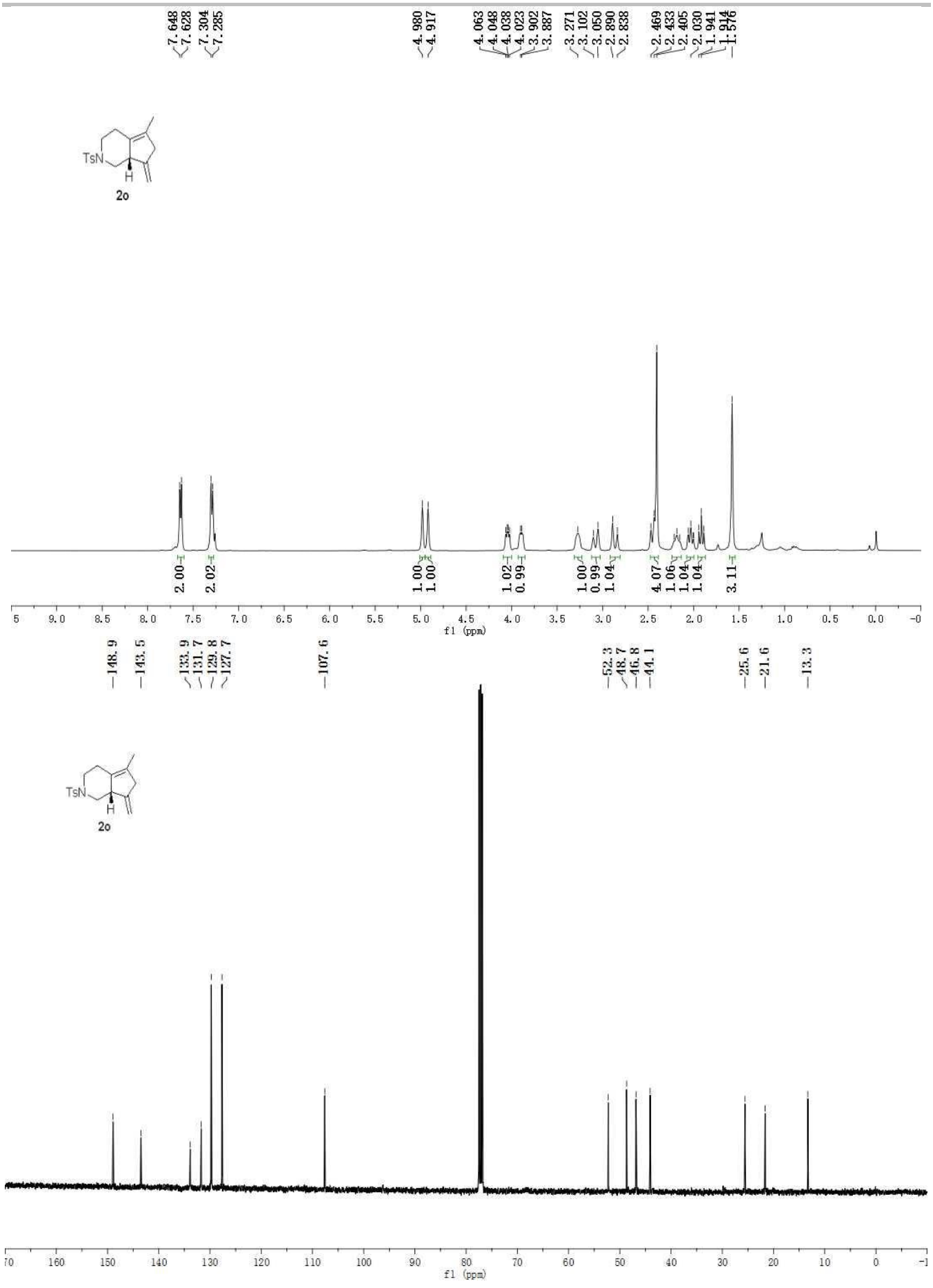
7.666
7.344
7.324
5.323
5.320
5.318
4.889
4.886
4.788
4.784
4.106
4.104
3.860
3.857
3.853
3.795
3.289
3.286
2.998
2.949
2.612
2.591
2.588
2.566
2.419
0.884
0.018
-0.002
OTBS
TsN
H
2n
2.00
2.01
1.00
1.00
2.06
2.00
1.07
1.01
1.04
1.04
1.02
3.06
9.00
3.02
3.14
f1 (ppm)
149.2
144.0
136.4
134.3
133.7
130.1
127.8
108.2
61.4
58.7
51.1
46.4
43.8
26.0
21.6
18.5
5.4
-5.5
OTBS
TsN
H
2n
f1 (ppm)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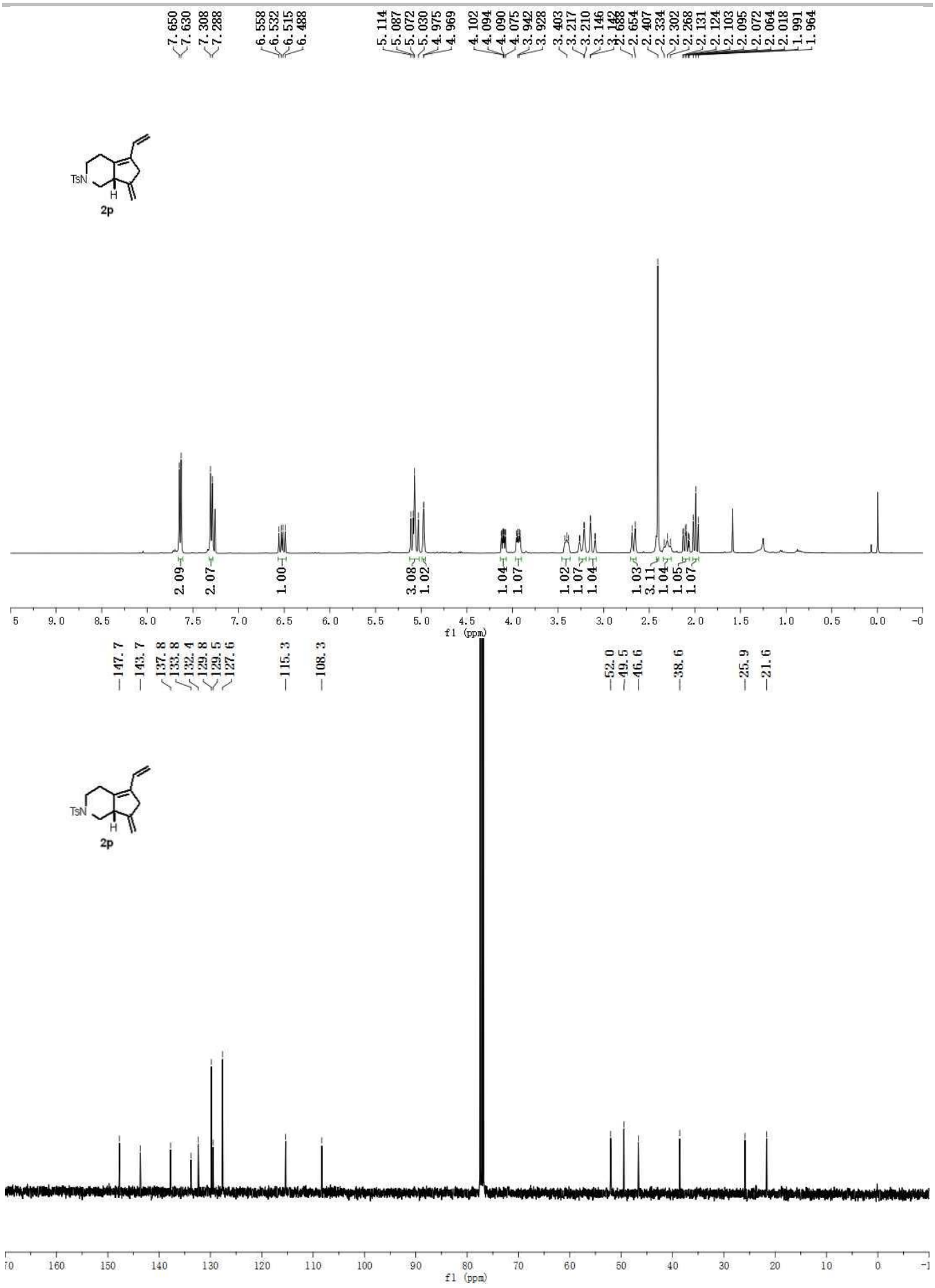
7.628
7.304
7.285
4.980
4.917
4.063
4.048
4.038
4.023
3.902
3.887
3.271
3.102
3.050
2.890
2.838
2.469
2.433
2.405
2.030
1.941
1.914
1.576
TsN
H
2o
2.00
2.02
1.00
1.00
1.02
0.99
1.00
0.99
1.04
4.07
1.06
1.04
1.04
3.11
f1 (ppm)
148.9
143.5
133.9
131.7
129.8
127.7
107.6
52.3
48.7
46.8
44.1
25.6
21.6
13.3
TsN
H
2o
f1 (ppm)


7.650
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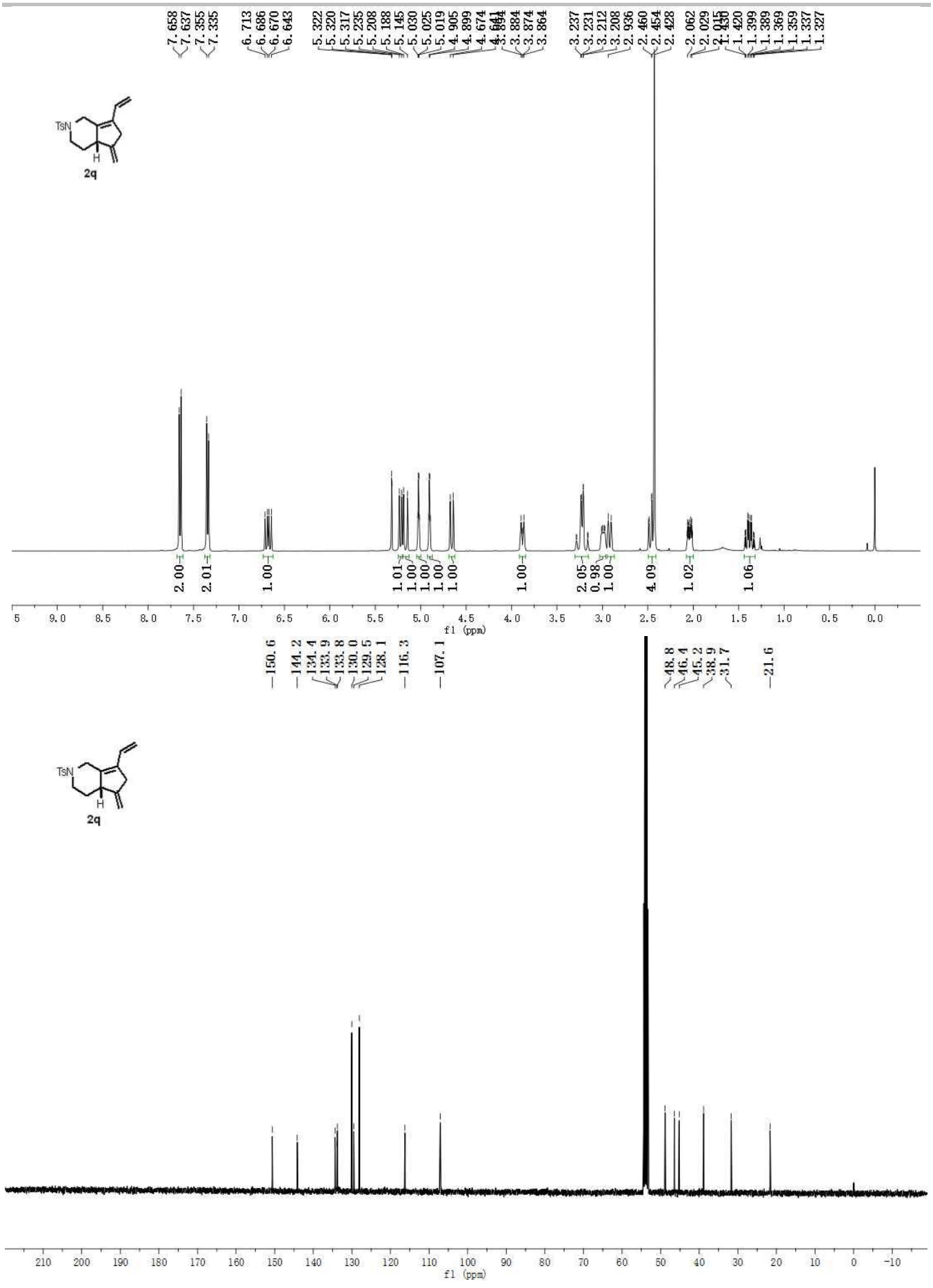
7.308
7.288
6.558
6.532
6.515
6.488
5.114
5.087
5.072
5.030
4.975
4.969
4.102
4.094
4.090
4.075
3.942
3.928
3.403
3.217
3.210
3.146
3.142
2.688
2.654
2.407
2.334
2.302
2.268
2.131
2.124
2.103
2.095
2.072
2.064
2.018
1.991
1.964
TsN
H
2p
2.09
2.07
1.00
3.08
1.02
1.04
1.07
1.02
1.07
1.04
1.03
3.11
1.04
1.05
1.07
f1 (ppm)
147.7
143.7
137.8
133.8
132.4
129.8
129.5
127.6
115.3
108.3
52.0
49.5
46.6
38.6
25.9
21.6
TsN
H
2p
f1 (ppm)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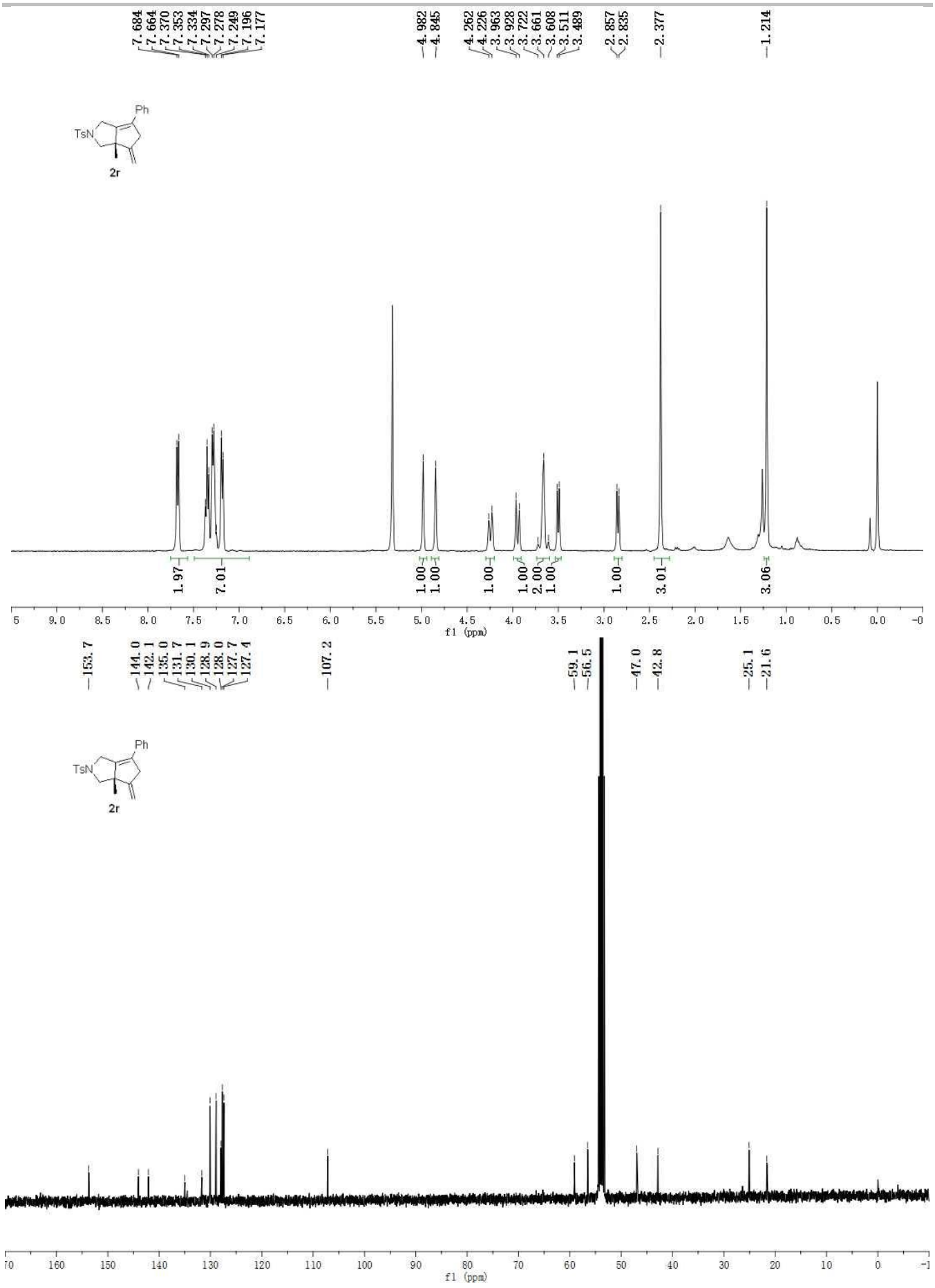
7.335
6.713
6.686
6.670
6.643
5.322
5.320
5.317
5.235
5.208
5.188
5.145
5.030
5.025
5.019
4.905
4.899
4.674
3.884
3.874
3.864
3.237
3.231
3.212
3.208
2.936
2.460
2.454
2.428
2.062
2.029
1.420
1.399
1.389
1.369
1.359
1.337
1.327
TsN
H
2q
2.00
2.01
1.00
1.01
1.00
1.00
1.00
1.00
2.05
0.98
1.00
4.09
1.02
1.06
f1 (ppm)
150.6
144.2
134.4
133.9
133.8
130.0
129.5
128.1
116.3
107.1
48.8
46.4
45.2
38.9
31.7
21.6
TsN
H
2q
f1 (ppm)


7.684
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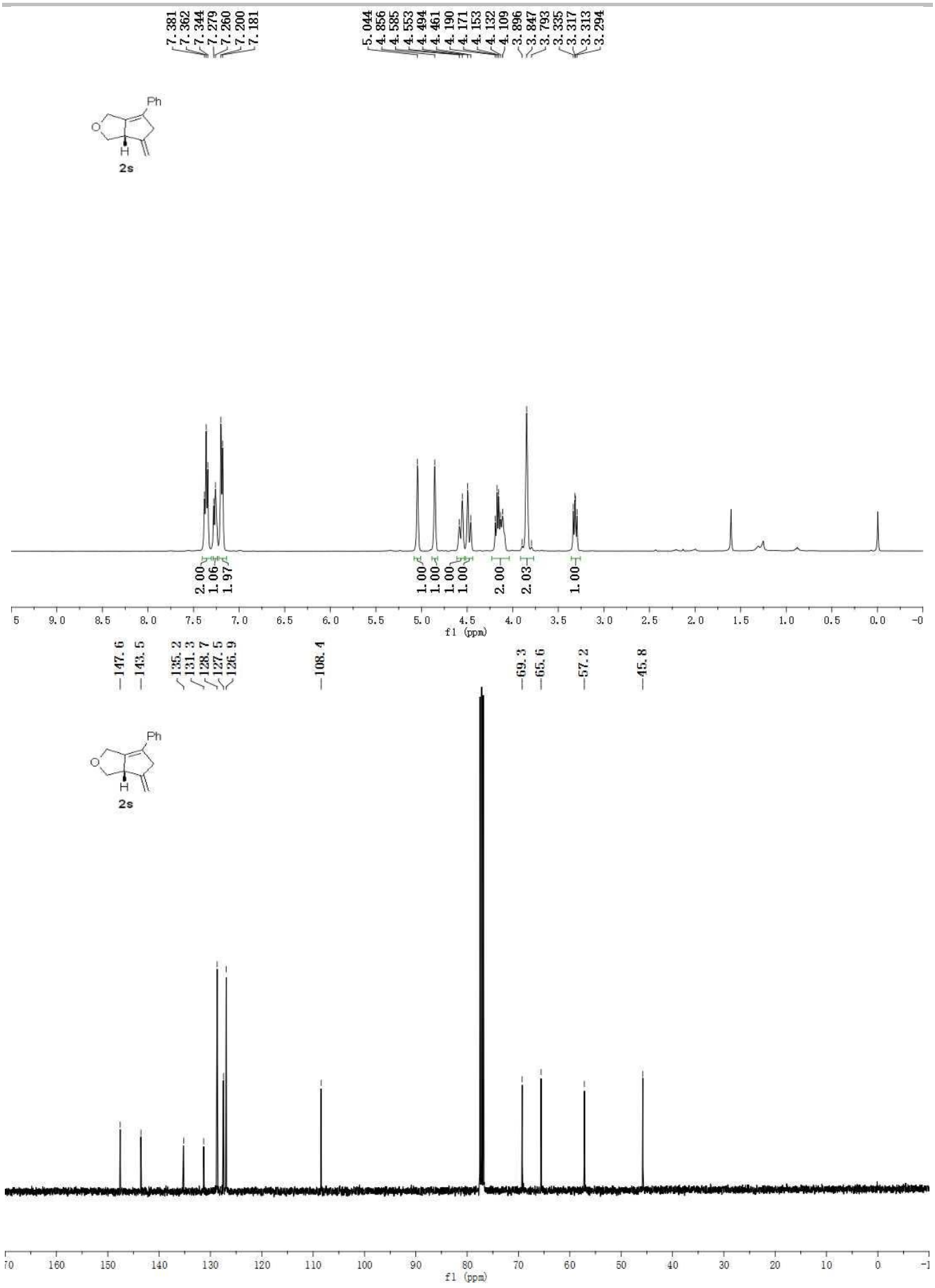
7.370
7.353
7.334
7.297
7.278
7.249
7.196
7.177
4.982
4.845
4.262
4.226
3.963
3.928
3.722
3.661
3.608
3.511
3.489
2.857
2.835
2.377
1.214
Ph
TsN
2r
1.97
7.01
1.00
1.00
1.00
1.00
2.00
1.00
1.00
3.01
3.06
f1 (ppm)
153.7
144.0
142.1
135.0
131.7
130.1
128.9
128.0
127.7
127.4
107.2
59.1
56.5
47.0
42.8
25.1
21.6
Ph
TsN
2r
f1 (ppm)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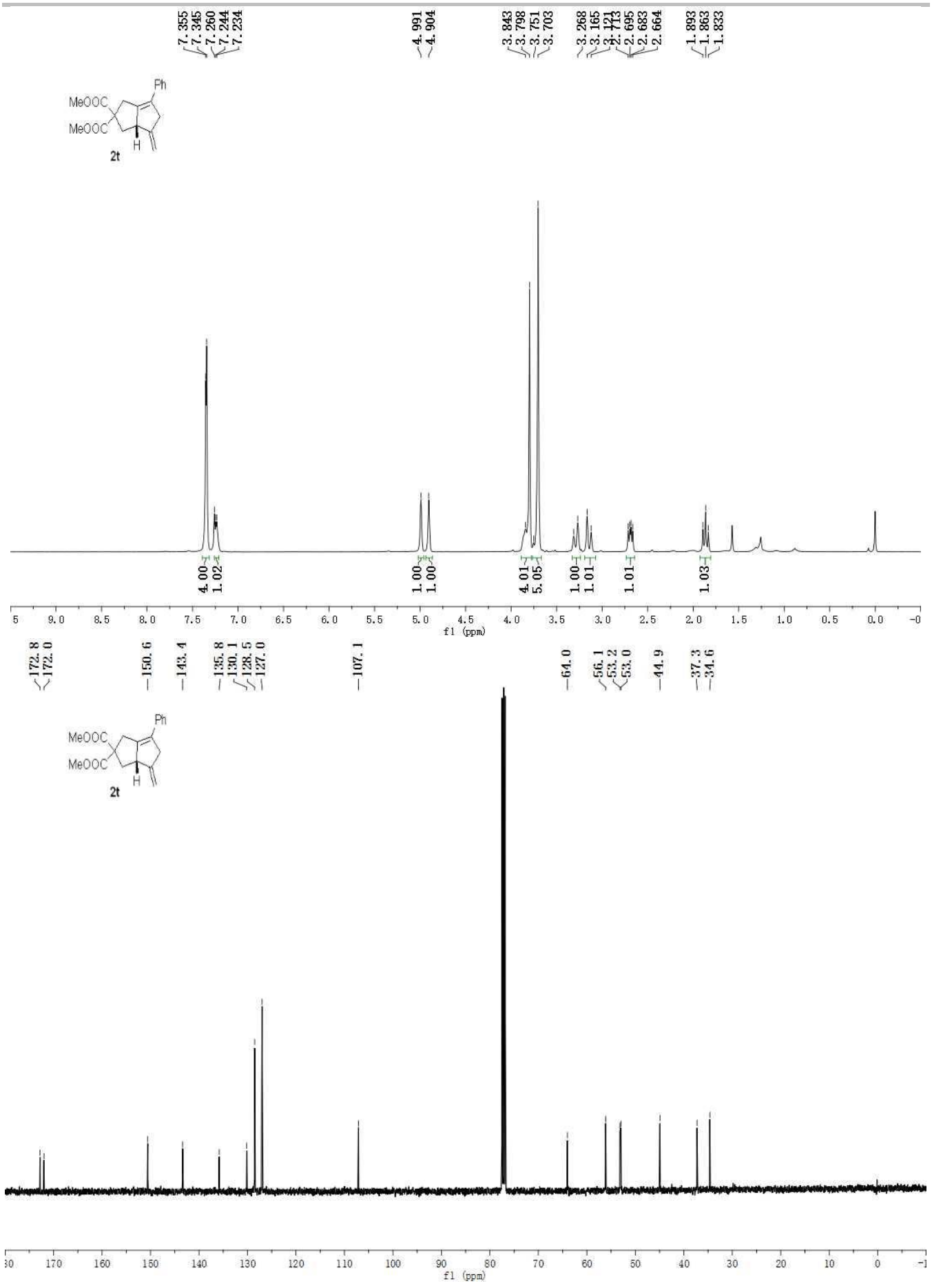
7.344
7.279
7.260
7.200
7.181
5.044
4.856
4.585
4.553
4.494
4.461
4.190
4.171
4.153
4.132
4.109
3.896
3.847
3.793
3.335
3.317
3.313
3.294
Ph
O
H
2s
2.00
1.06
1.97
1.00
1.00
1.00
1.00
2.00
2.03
1.00
f1 (ppm)
147.6
143.5
135.2
131.3
128.7
127.5
126.9
108.4
69.3
65.6
57.2
45.8
Ph
O
H
2s
f1 (ppm)


7.355
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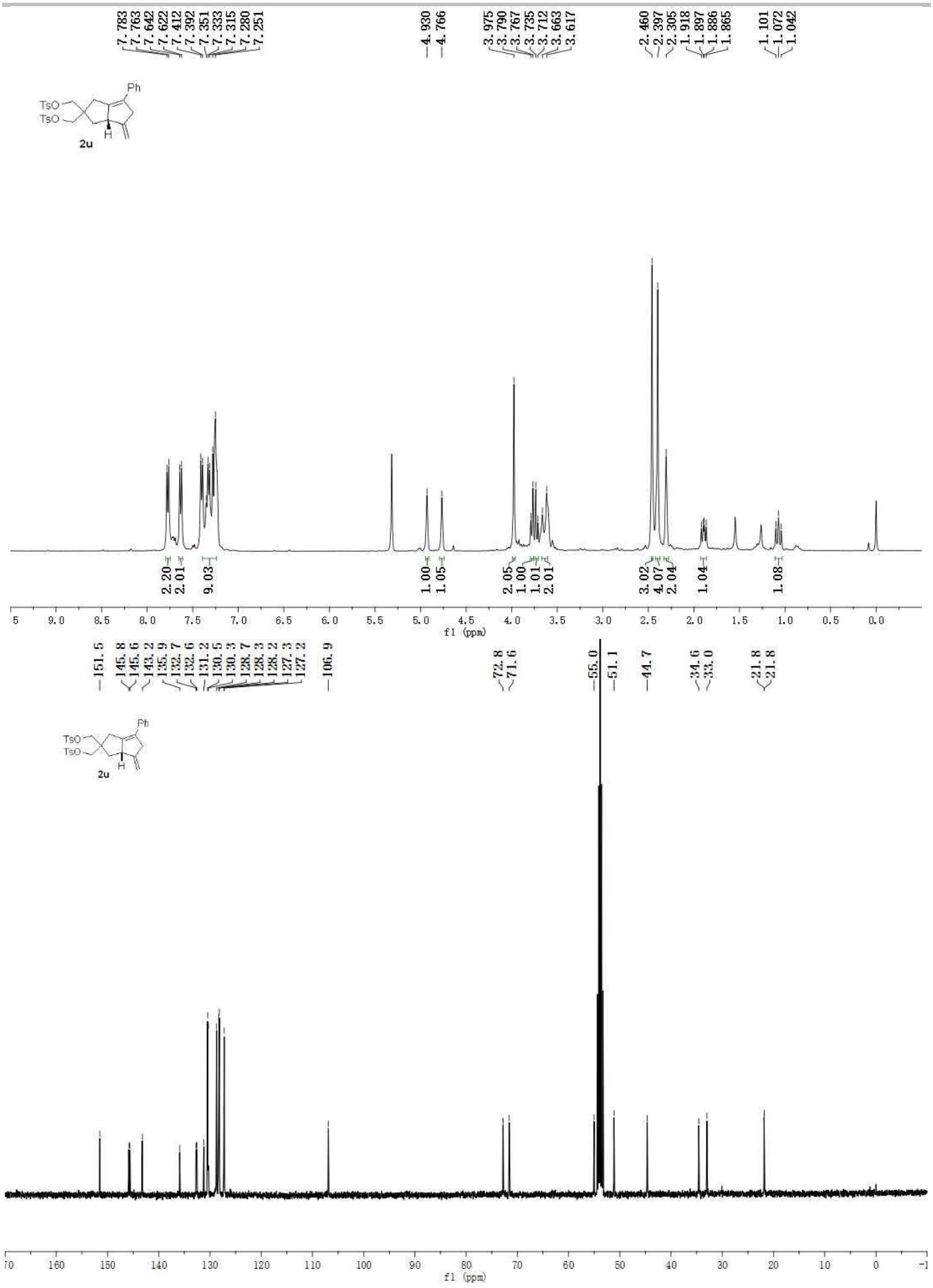
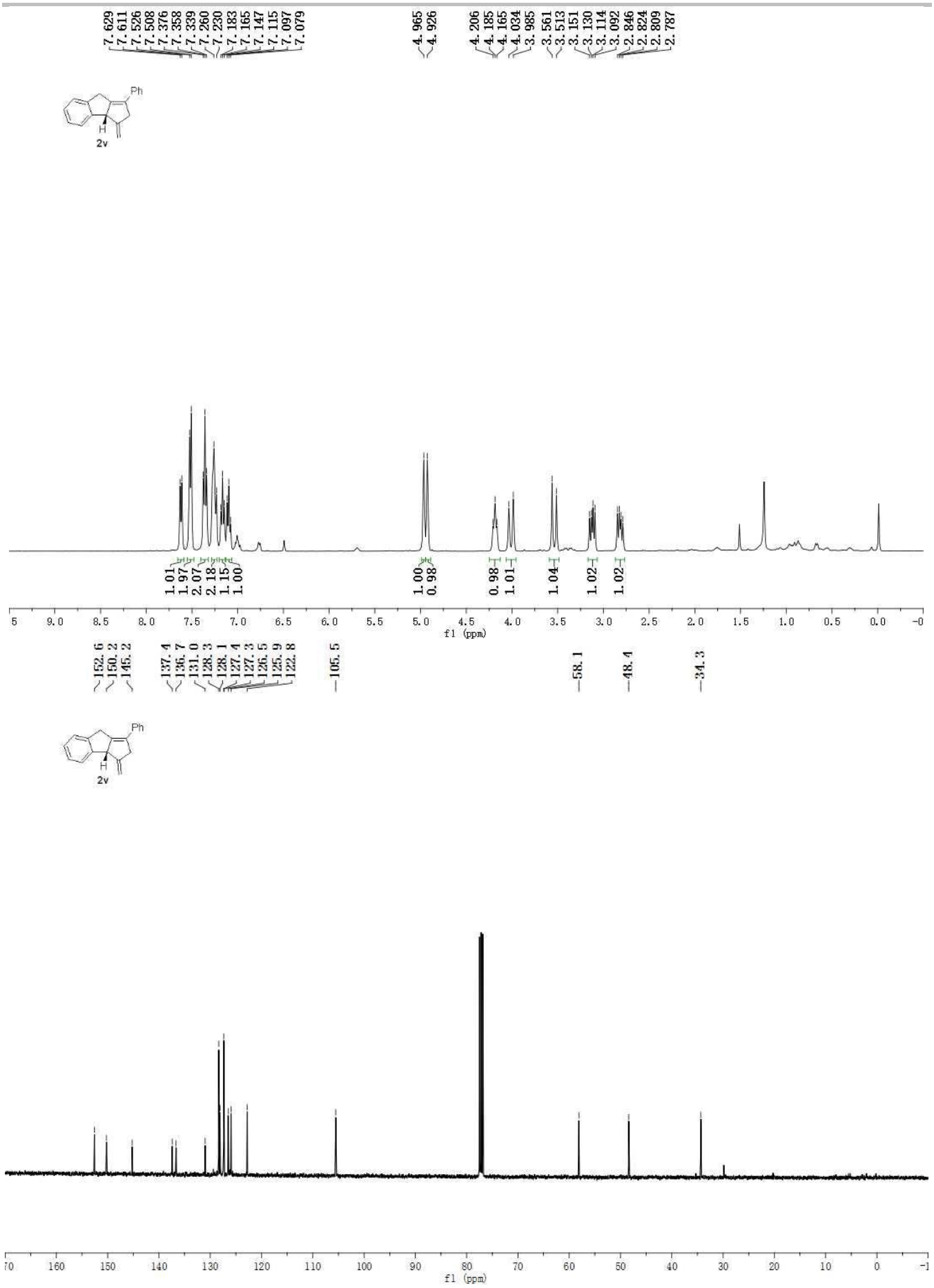
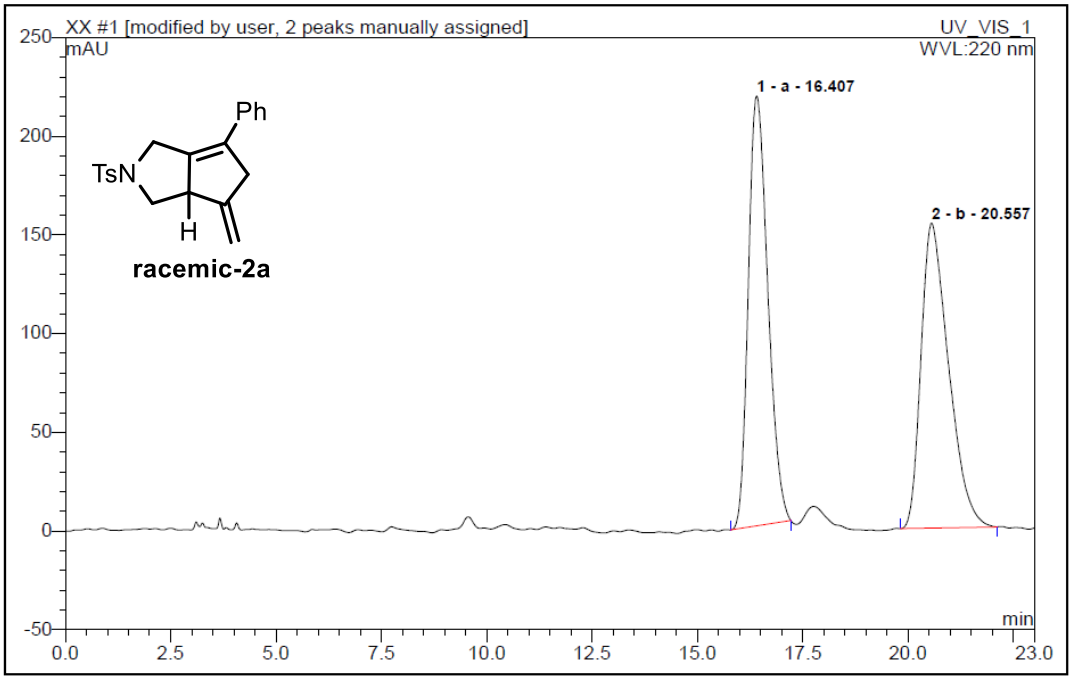
7.260
7.244
7.234
4.991
4.904
3.843
3.798
3.751
3.703
3.268
3.165
3.121
2.713
2.695
2.683
2.664
1.893
1.863
1.833
Ph
MeOOC
MeOOC
H
2t
4.00
1.02
1.00
1.00
4.01
5.05
1.00
1.01
1.01
1.03
f1 (ppm)
172.8
172.0
150.6
143.4
135.8
130.1
128.5
127.0
107.1
64.0
56.1
53.2
53.0
44.9
37.3
34.6
Ph
MeOOC
MeOOC
H
2t
f1 (ppm)


7.783
7.763
7.642
7.622
7.412
7.392
7.351
7.333
7.315
7.280
7.251
4.930
4.766
3.975
3.790
3.767
3.735
3.712
3.663
3.617
2.460
2.397
2.305
1.918
1.897
1.886
1.865
1.101
1.072
1.042
Ph
TsO
TsO
H
2u
2.20
2.01
9.03
1.00
1.05
2.05
1.00
1.01
2.01
3.02
4.07
2.04
1.04
1.08
f1 (ppm)
151.5
145.8
145.6
143.2
135.9
132.7
132.6
131.2
130.5
130.3
128.7
128.3
128.2
127.3
127.2
106.9
72.8
71.6
55.0
51.1
44.7
34.6
33.0
21.8
21.8
f1 (ppm)

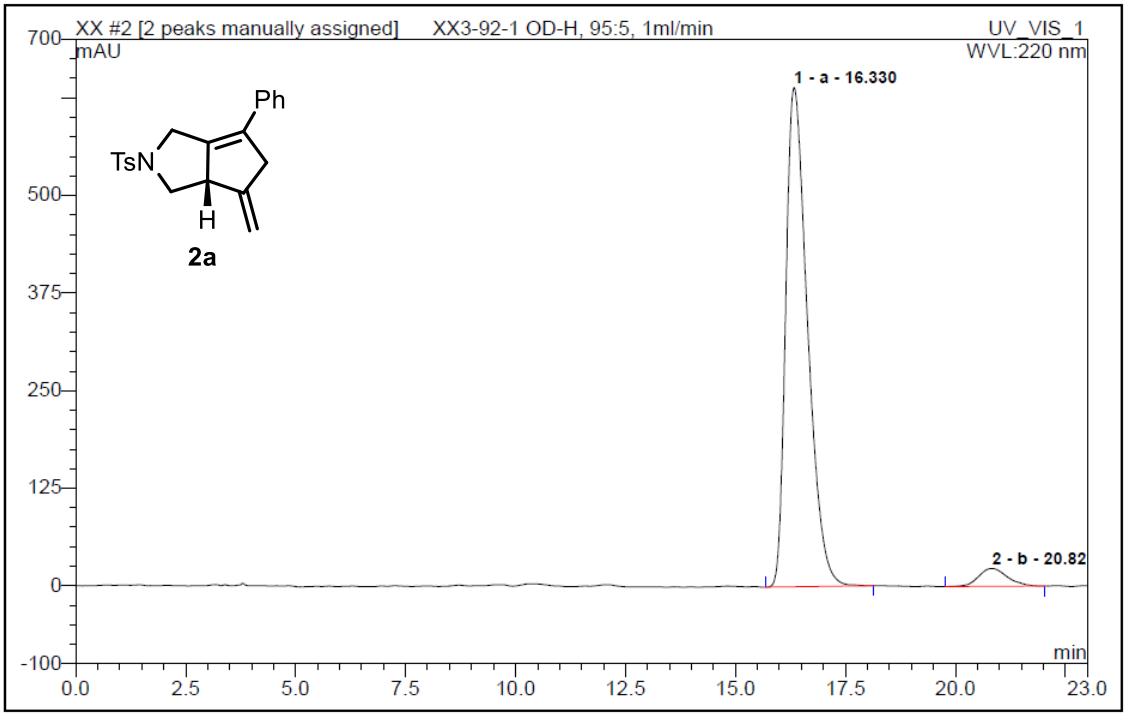
SUPPORTING INFORMATION



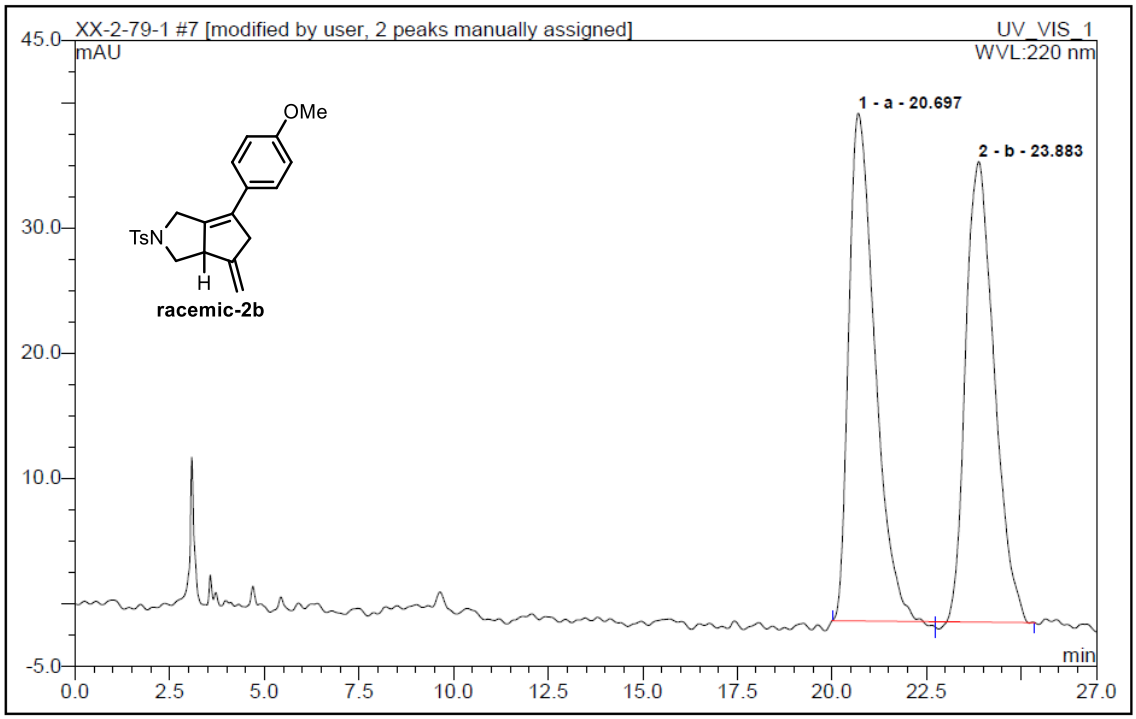
5. HPLC data for the asymmetric [3+2] cycloadducts



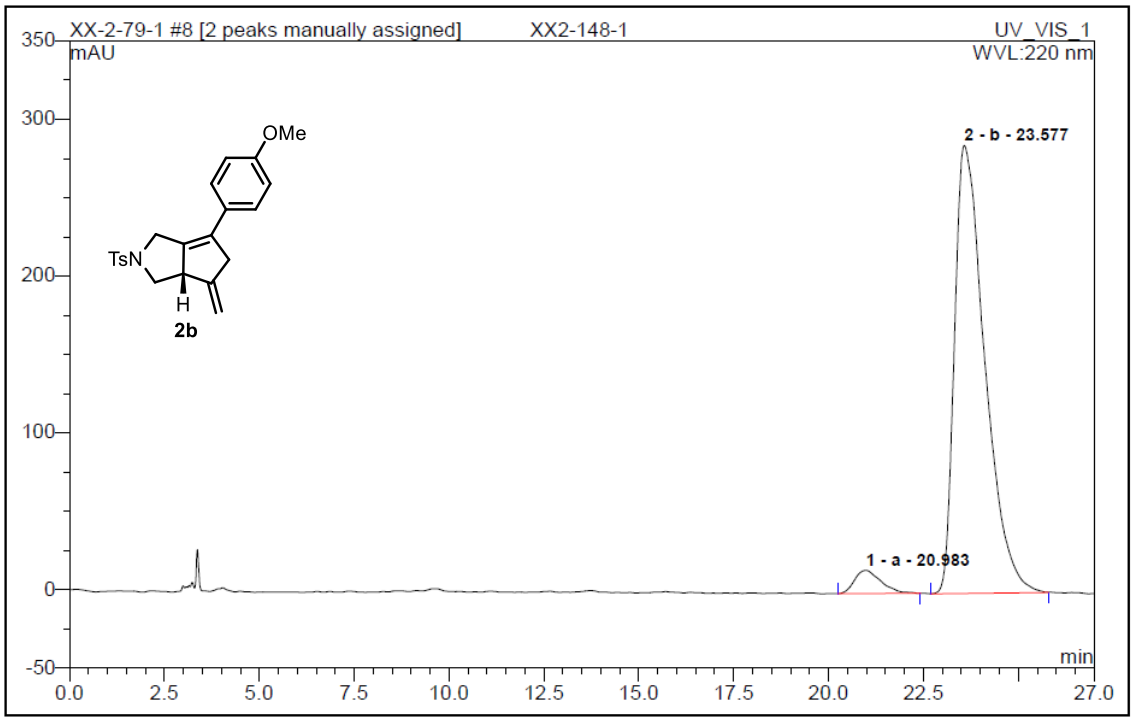
No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area(ident.) %	Amount mg/l	Type
2	16.41	a	217.782	116.959	49.97	n.a.	BMB*^
2	20.56	b	154.441	117.080	50.03	n.a.	BMB^
Total:			372.223	234.039	100.00	0.000	



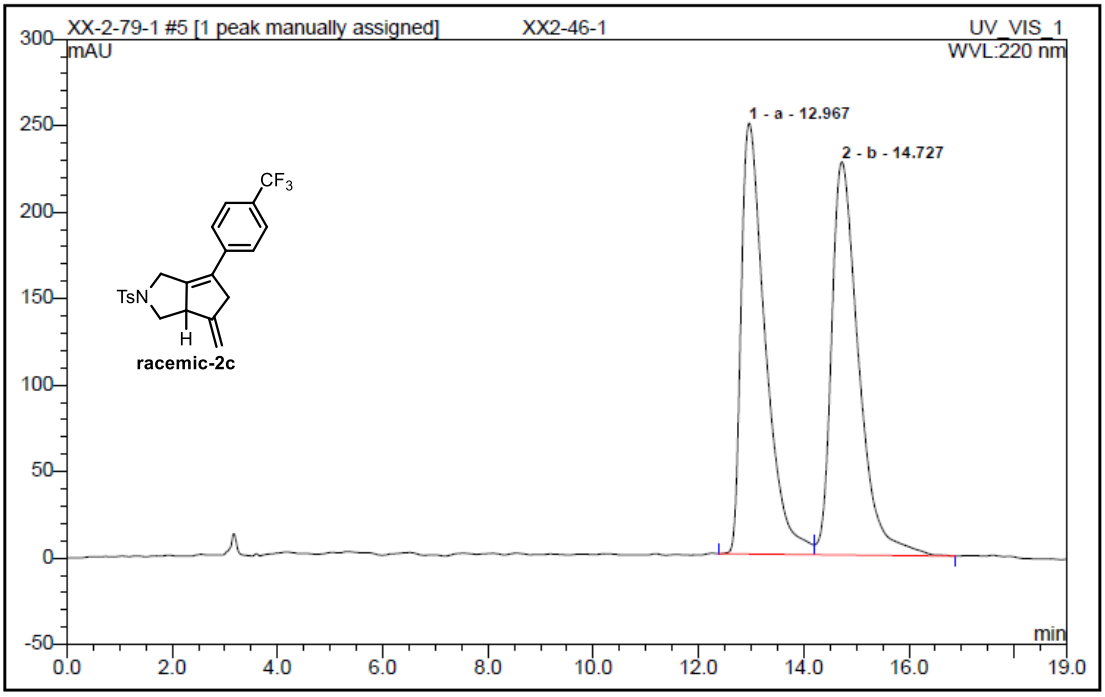
No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area(ident.) %	Amount mg/l	Type
2	16.33	a	639.544	366.515	95.48	n.a.	BMB^
2	20.83	b	22.731	17.334	4.52	n.a.	BMB^
Total:			662.274	383.849	100.00	0.000	



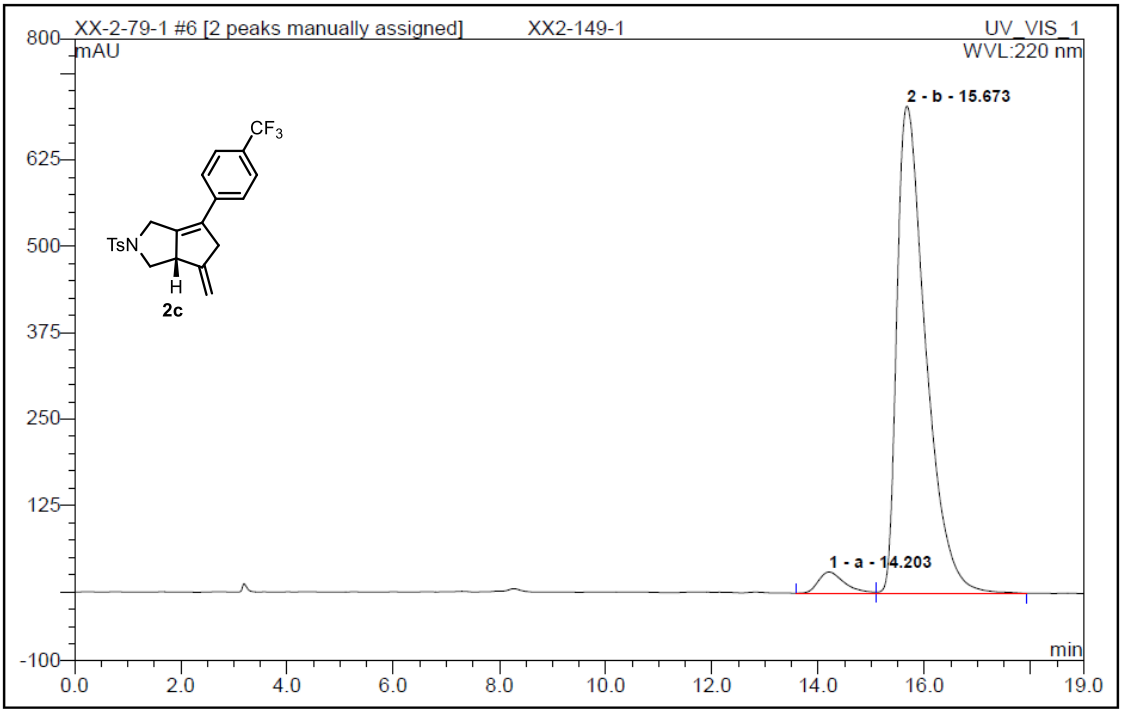
No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area(ident.) %	Amount mg/l	Type
2	20.70	a	40.533	32.486	50.20	n.a.	BM *^
2	23.88	b	36.764	32.227	49.80	n.a.	MB*^
Total:			77.297	64.714	100.00	0.000	



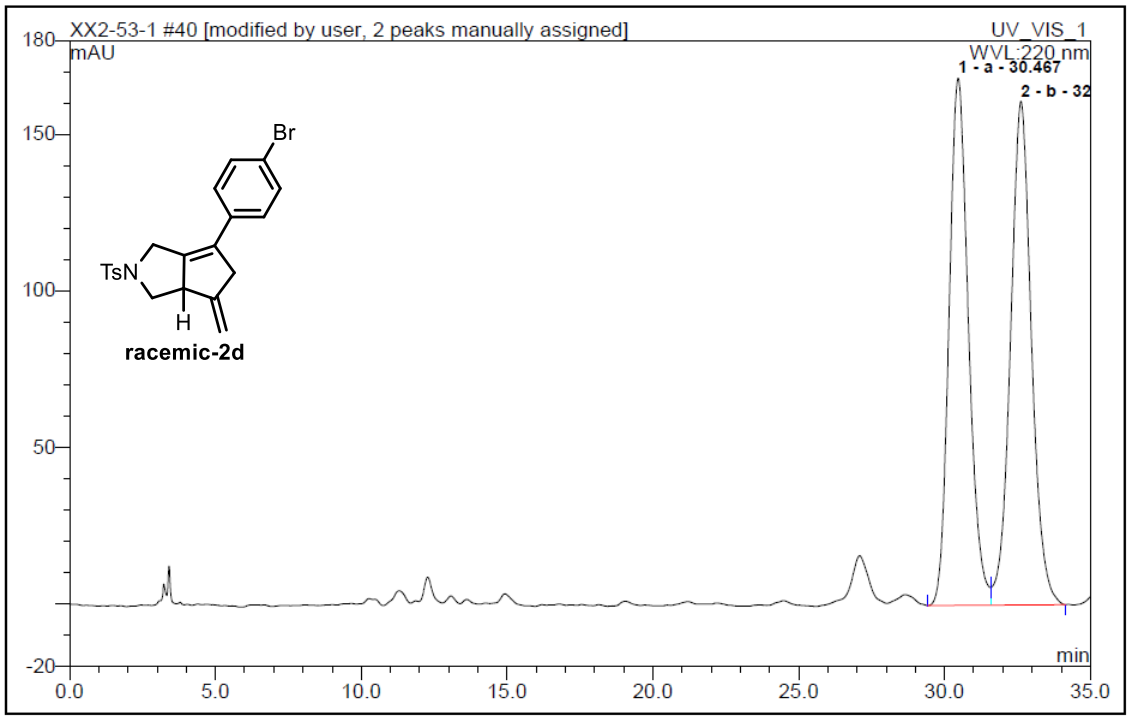
No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area(ident.) %	Amount mg/l	Type
2	20.98	a	14.789	11.997	4.35	n.a.	BMB^
2	23.58	b	285.636	264.041	95.65	n.a.	BMB^
Total:			300.425	276.038	100.00	0.000	



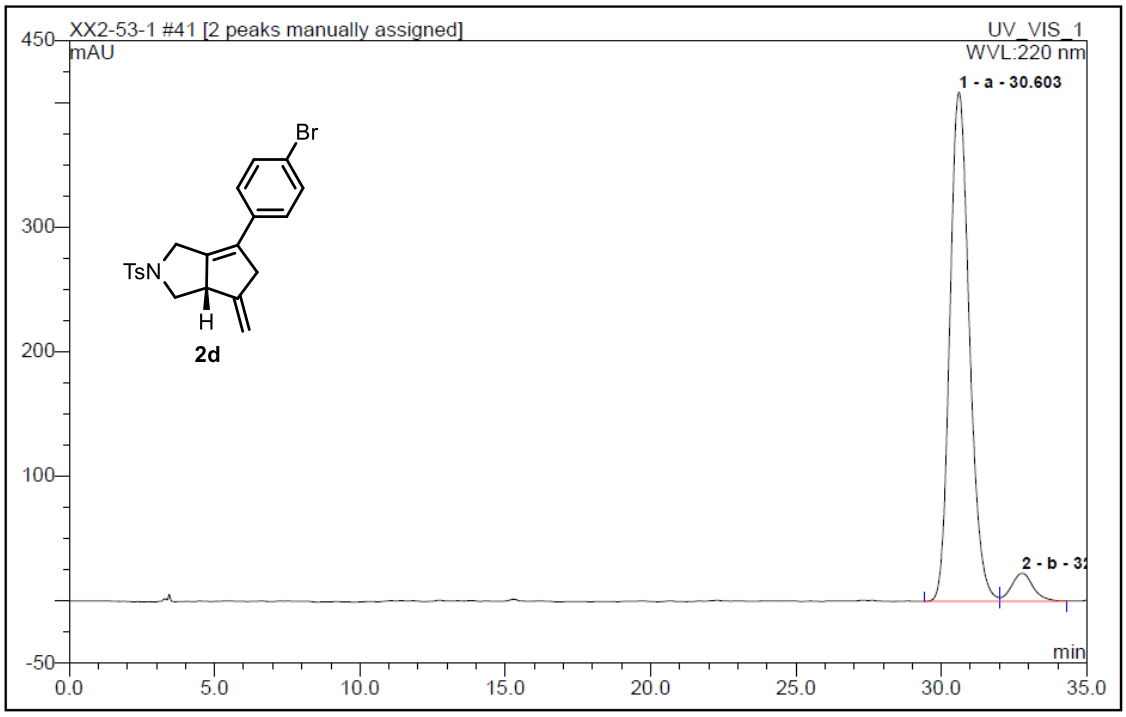
No.	Ret.Time min		Peak Name	Height mAU	Area mAU*min	Rel.Area(ident.) %	Amount mg/l	Type
2	12.97	a		249.191	132.478	49.38	n.a.	BM ^
2	14.73	b		227.334	135.796	50.62	n.a.	MB
Total:				476.525	268.273	100.00	0.000	



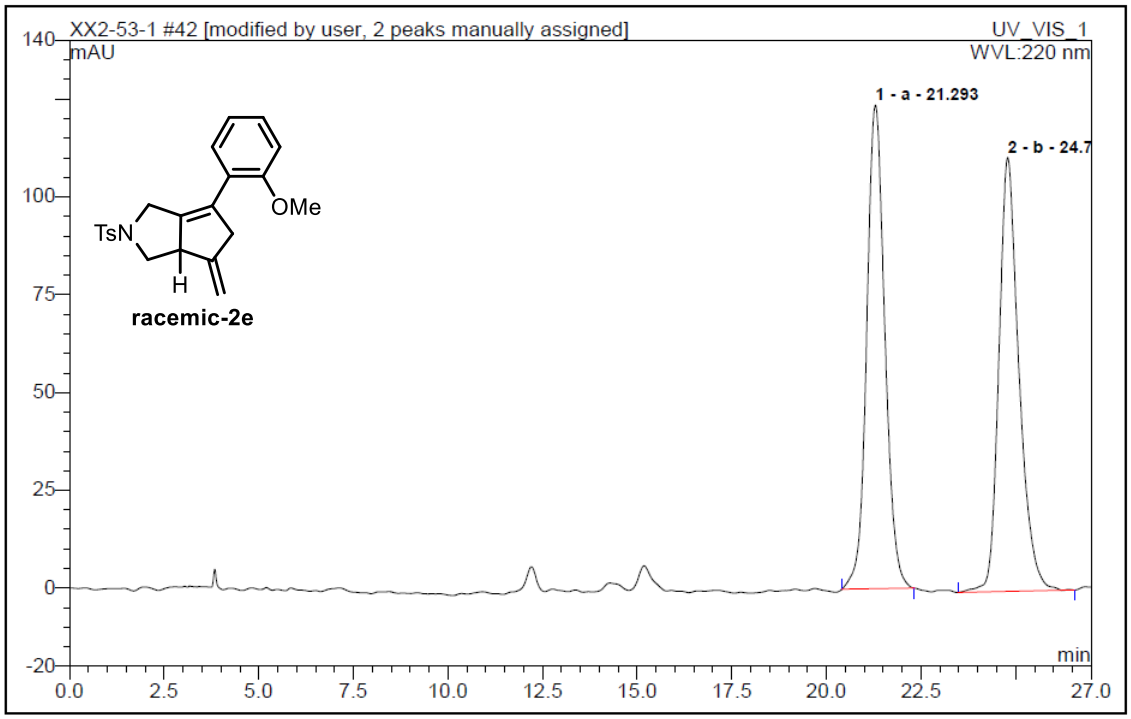
No.	Ret.Time min		Peak Name	Height mAU	Area mAU*min	Rel.Area(ident.) %	Amount mg/l	Type
2	14.20	a		30.833	17.572	3.81	n.a.	BM ^
2	15.67	b		704.892	443.664	96.19	n.a.	MB^
Total:				735.725	461.236	100.00	0.000	



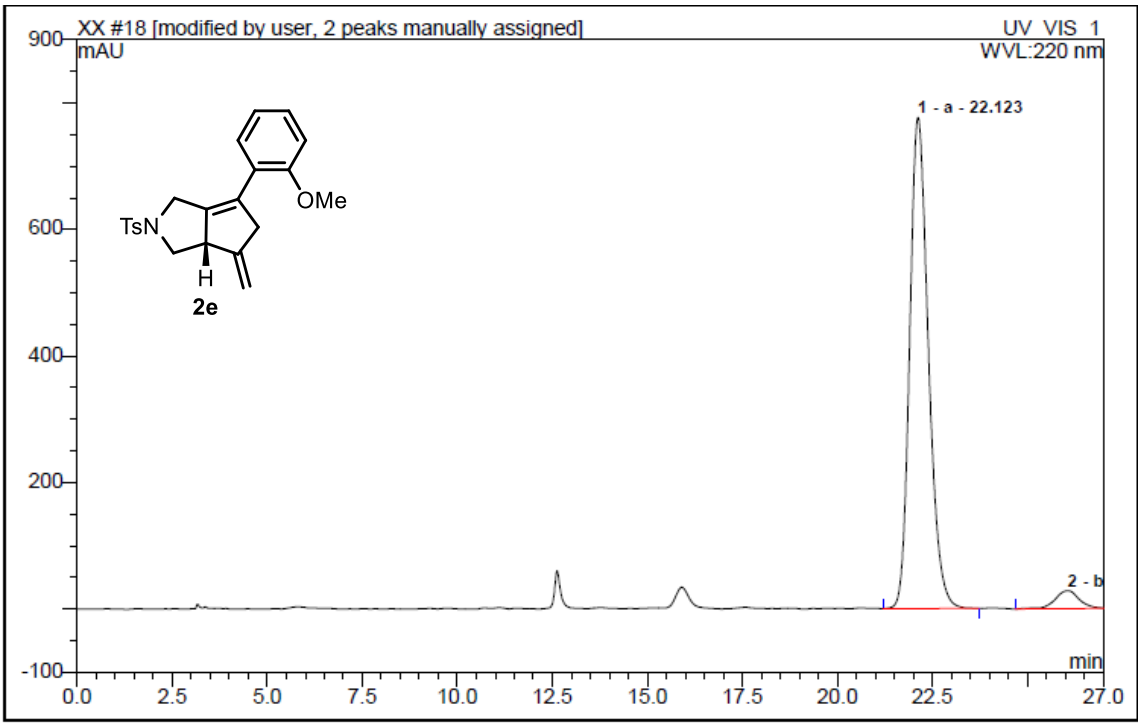
No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area(ident.) %	Amount mg/l	Type
2	30.47	a	168.508	130.131	49.20	n.a.	BM ^
2	32.62	b	160.978	134.378	50.80	n.a.	MB^
Total:			329.485	264.509	100.00	0.000	



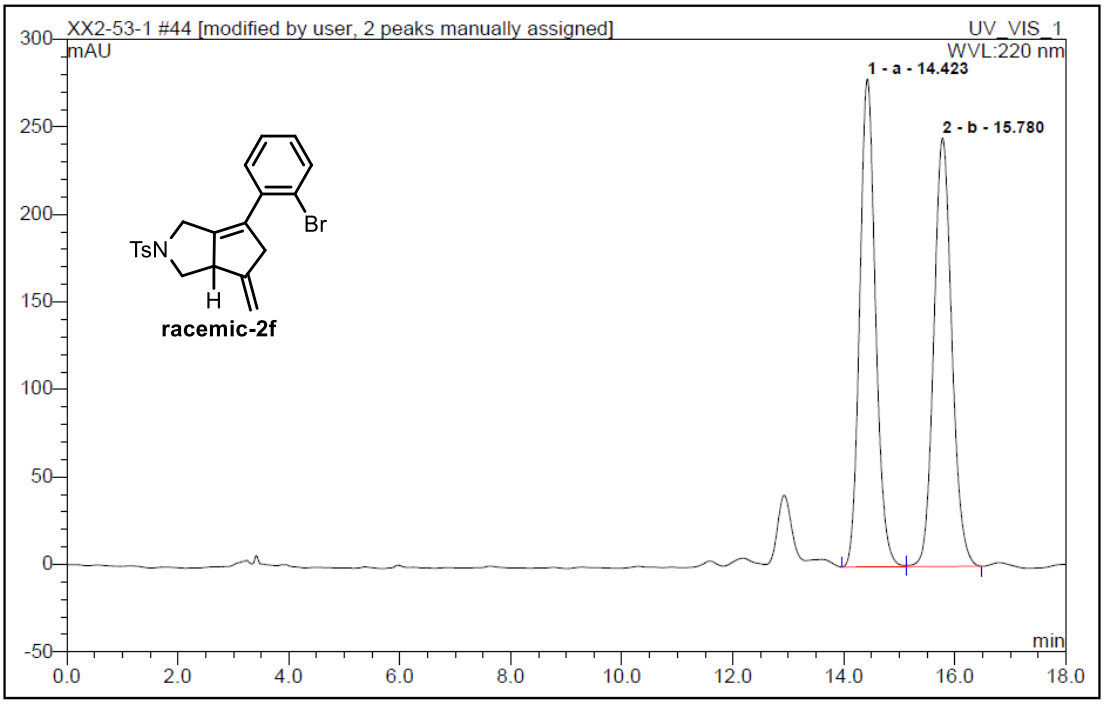
No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area(ident.) %	Amount mg/l	Type
2	30.60	a	408.587	319.517	94.27	n.a.	BM ^
2	32.77	b	22.356	19.409	5.73	n.a.	MB^
Total:			430.943	338.926	100.00	0.000	



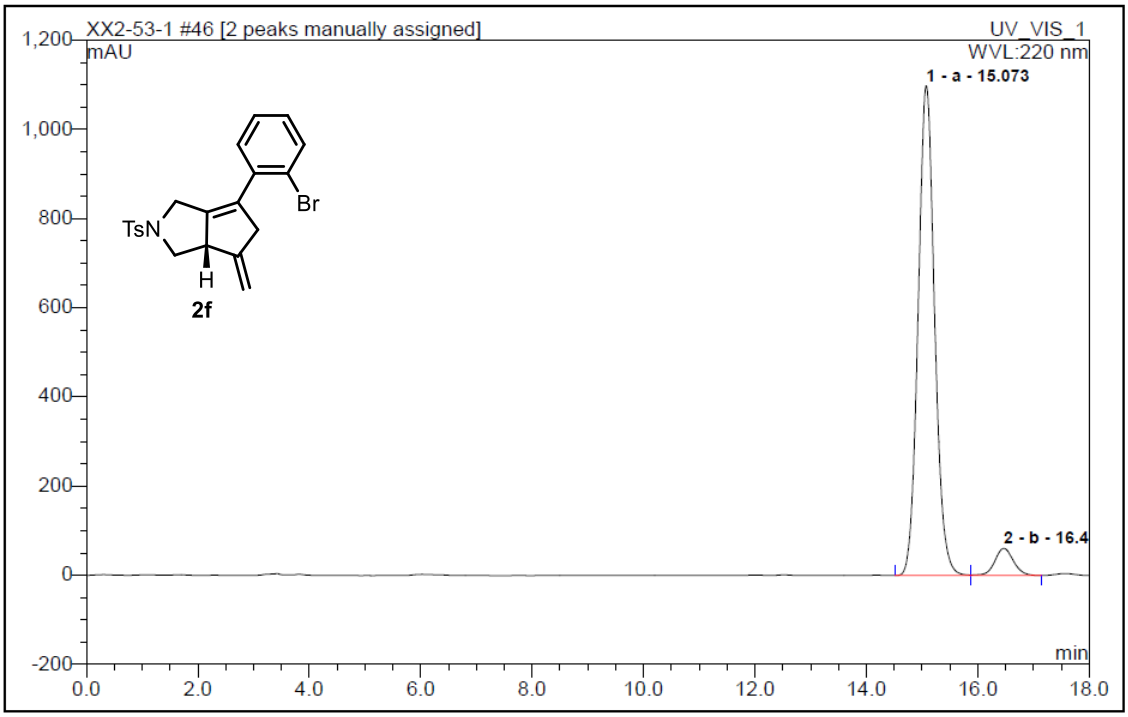
No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area(ident.) %	Amount mg/l	Type
2	21.29	a	123.613	68.744	50.14	n.a.	BMB*^
2	24.79	b	110.931	68.358	49.86	n.a.	BMB*^
Total:			234.544	137.102	100.00	0.000	



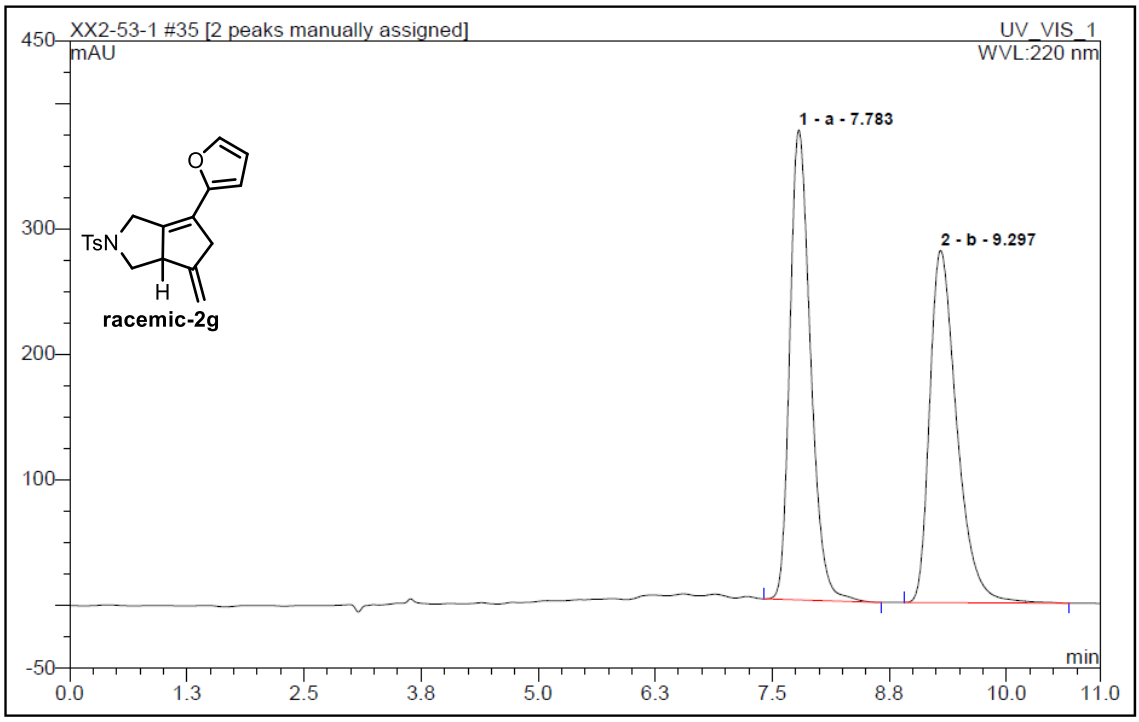
No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area(ident.) %	Amount mg/l	Type
2	22.12	a	776.219	441.874	95.53	n.a.	BMB^
2	26.06	b	28.105	20.658	4.47	n.a.	BMB^
Total:			804.324	462.532	100.00	0.000	



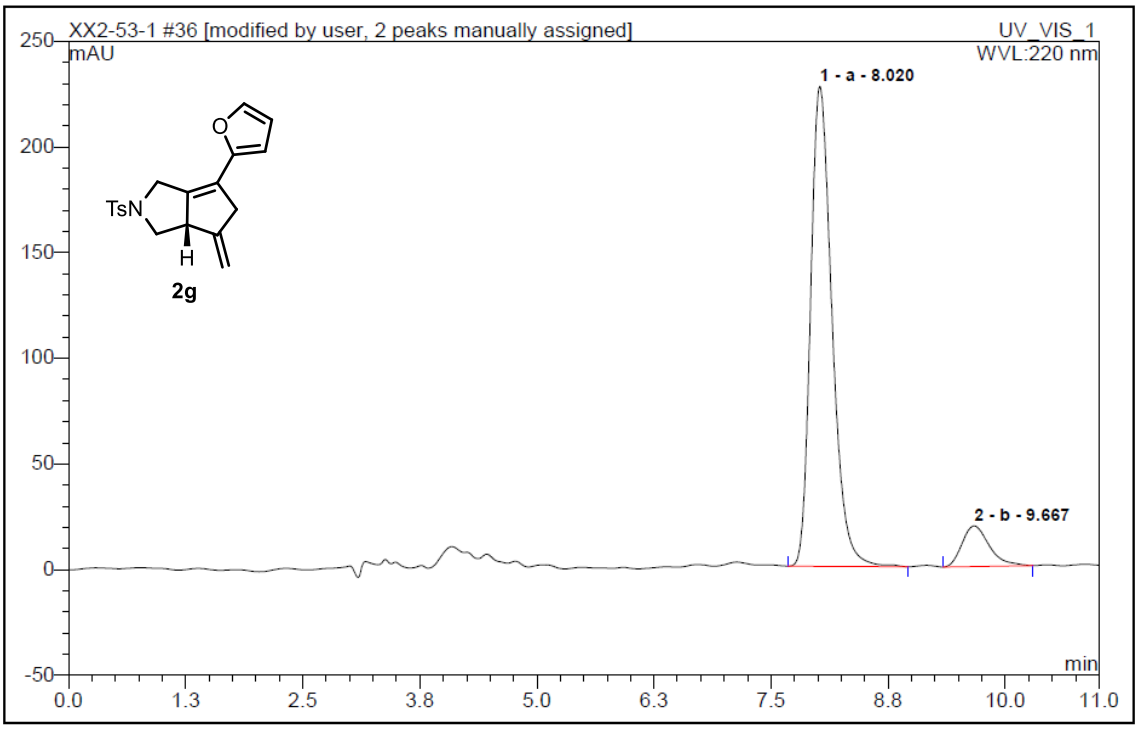
No.	Ret.Time min		Peak Name	Height mAU	Area mAU*min	Rel.Area(ident.) %	Amount mg/l	Type
2	14.42	a		278.733	92.041	49.93	n.a.	BM ^
2	15.78	b		244.720	92.283	50.07	n.a.	MB^
Total:				523.453	184.324	100.00	0.000	



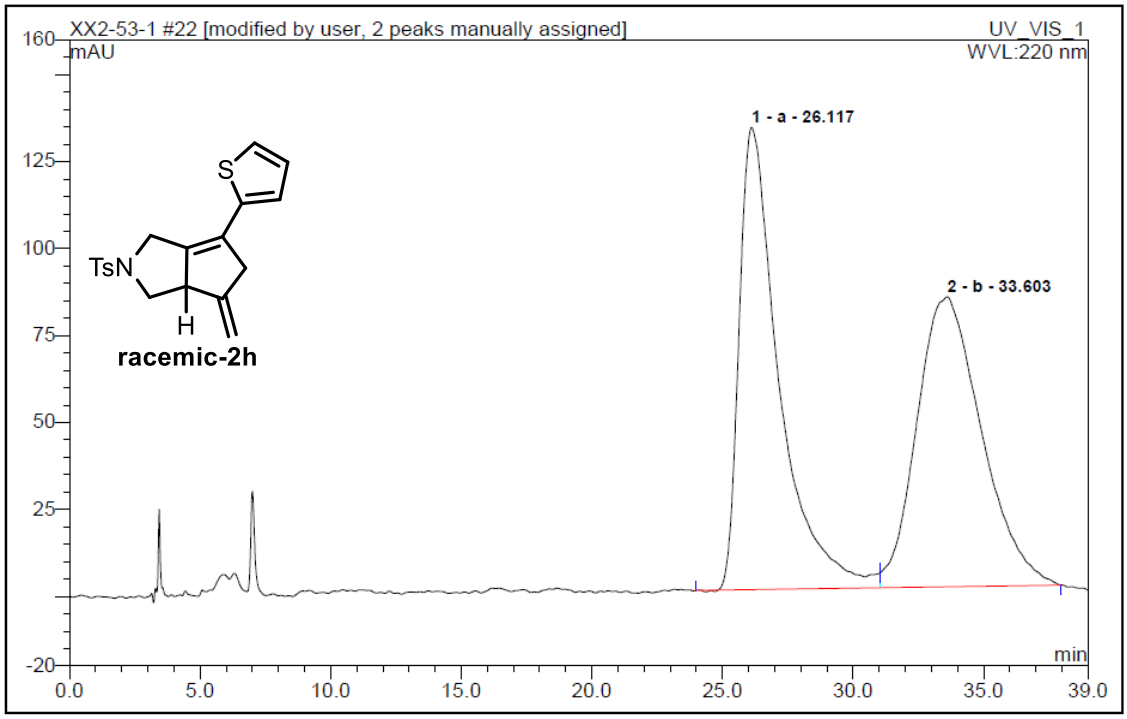
No.	Ret.Time min		Peak Name	Height mAU	Area mAU*min	Rel.Area(ident.) %	Amount mg/l	Type
2	15.07	a		1098.703	376.597	94.12	n.a.	BM ^
2	16.47	b		60.729	23.521	5.88	n.a.	MB^
Total:				1159.432	400.118	100.00	0.000	



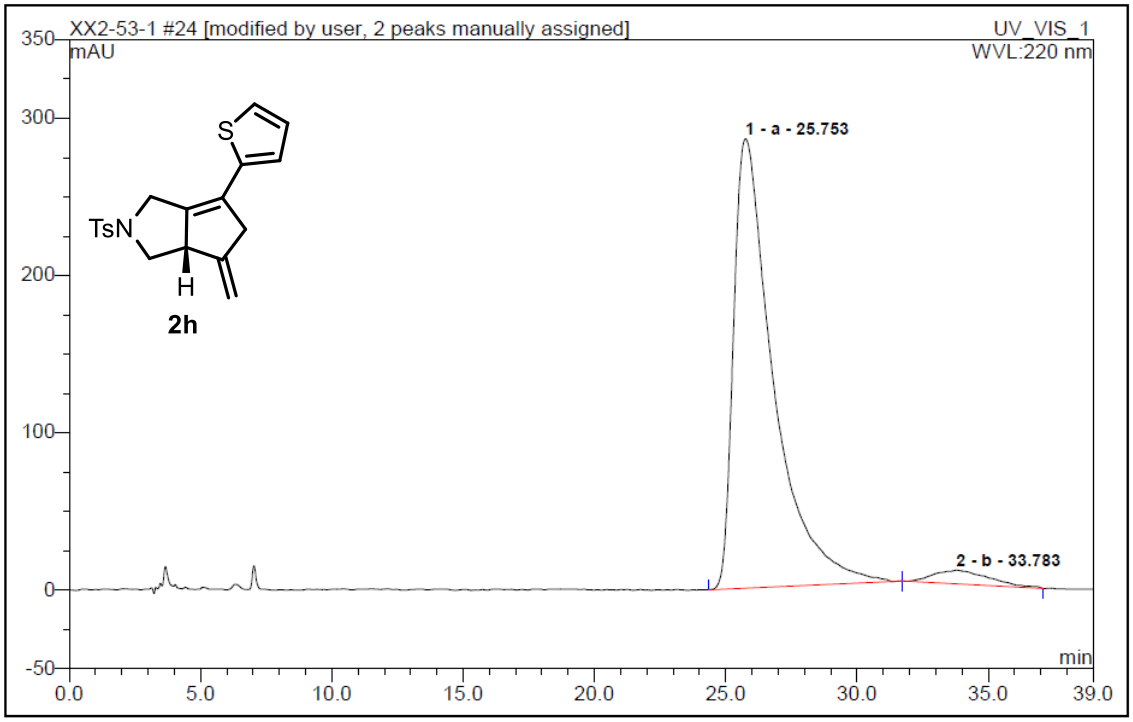
No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area(ident.) %	Amount mg/l	Type
2	7.78	a	374.457	96.009	50.41	n.a.	BMB^
2	9.30	b	280.544	94.464	49.59	n.a.	BMB^
Total:			655.001	190.473	100.00	0.000	



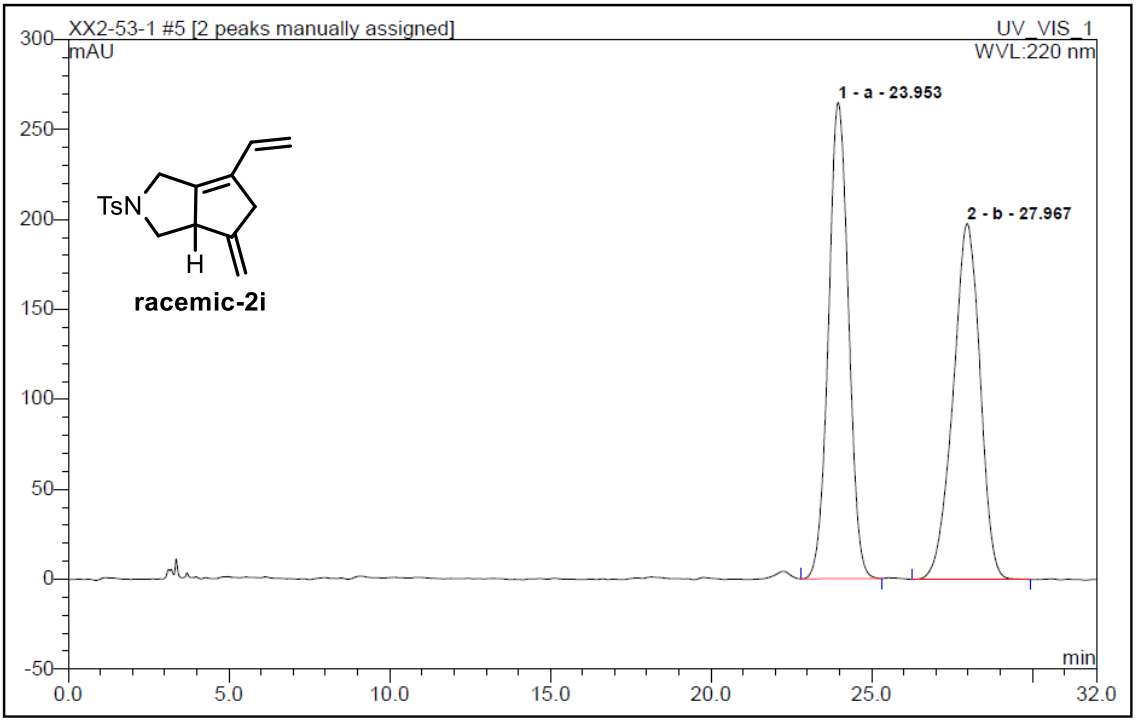
No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area(ident.) %	Amount mg/l	Type
2	8.02	a	227.136	60.212	90.26	n.a.	BMB^
2	9.67	b	19.231	6.496	9.74	n.a.	BMB^
Total:			246.367	66.709	100.00	0.000	



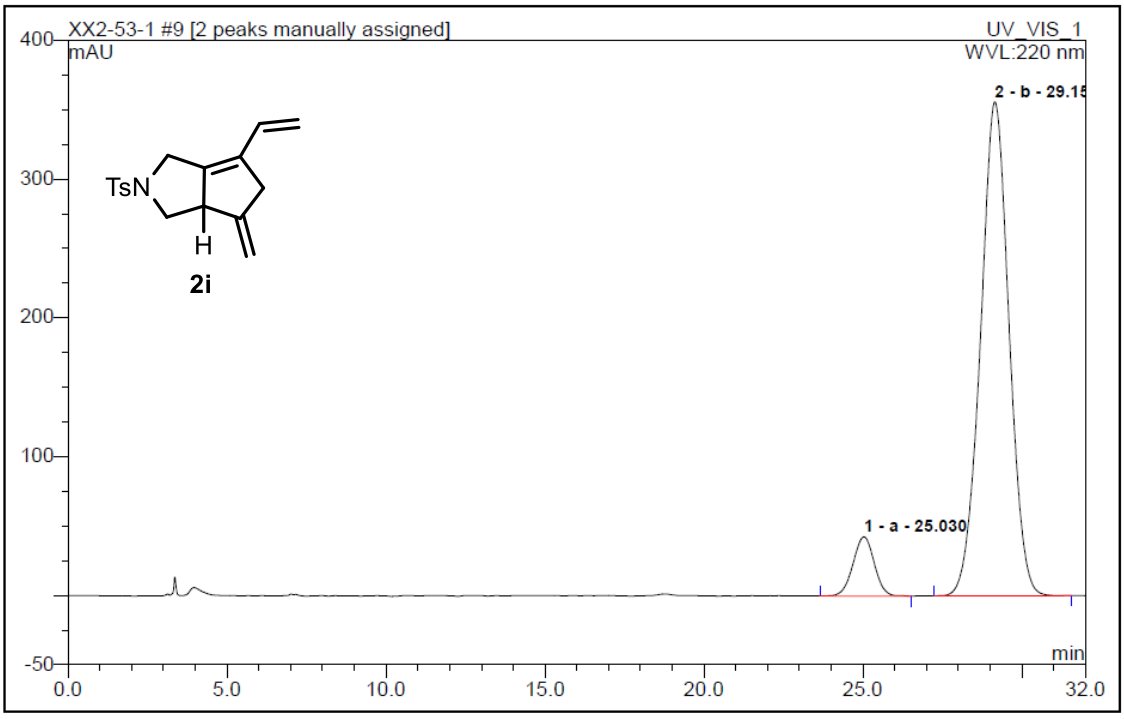
No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area(ident.) %	Amount mg/l	Type
2	26.12	a	132.953	235.190	49.60	n.a.	BM *^
2	33.60	b	83.392	238.993	50.40	n.a.	MB*^
Total:			216.345	474.183	100.00	0.000	



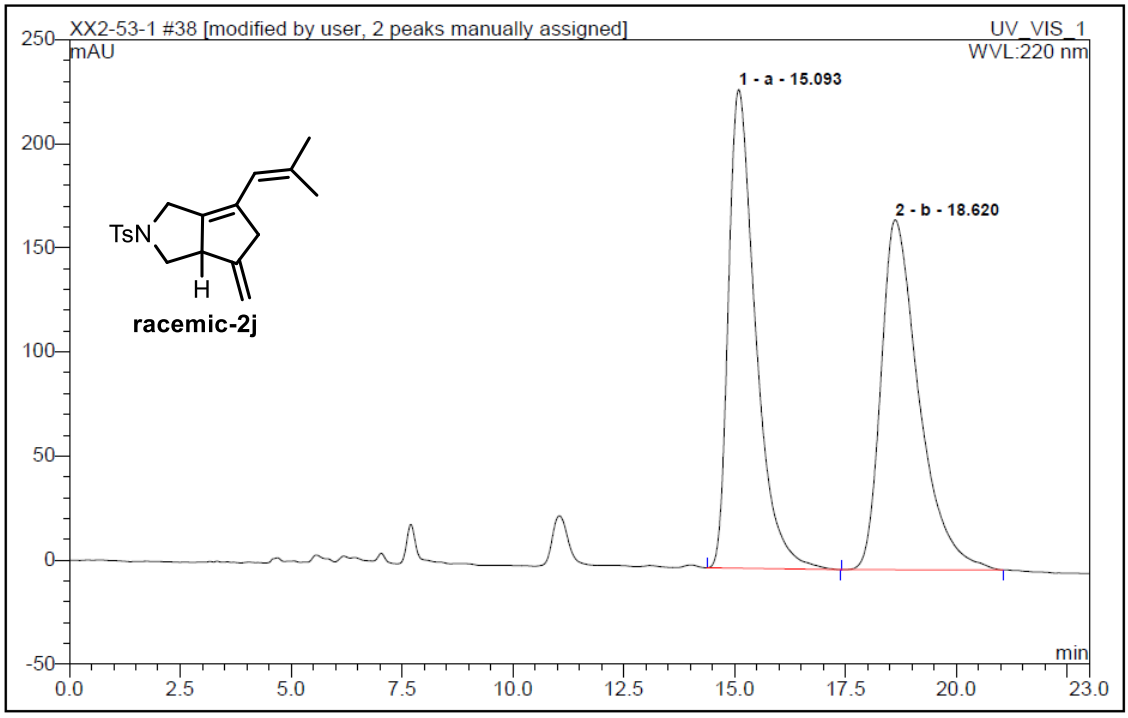
No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area(ident.) %	Amount mg/l	Type
2	25.75	a	285.714	502.215	95.93	n.a.	BMb*^
2	33.78	b	8.638	21.323	4.07	n.a.	bMB*^
Total:			294.352	523.538	100.00	0.000	



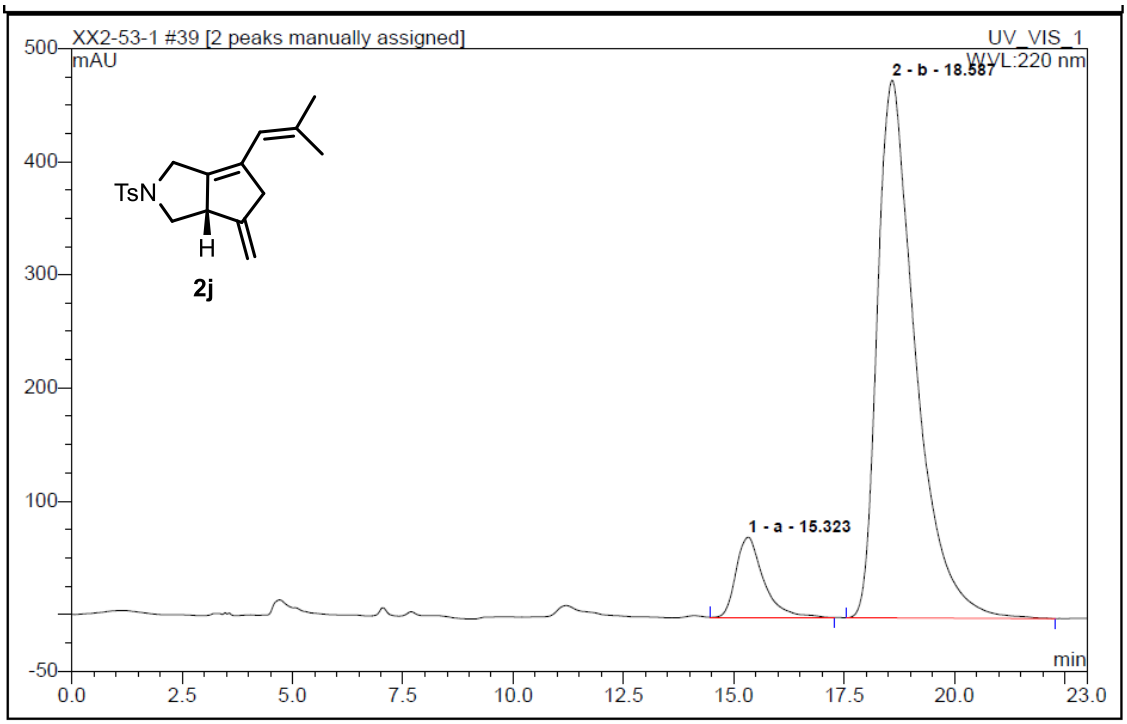
No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area(ident.) %	Amount mg/l	Type
2	23.95	a	264.649	191.841	49.90	n.a.	BMB^
2	27.97	b	197.716	192.599	50.10	n.a.	BMB^
Total:			462.366	384.440	100.00	0.000	



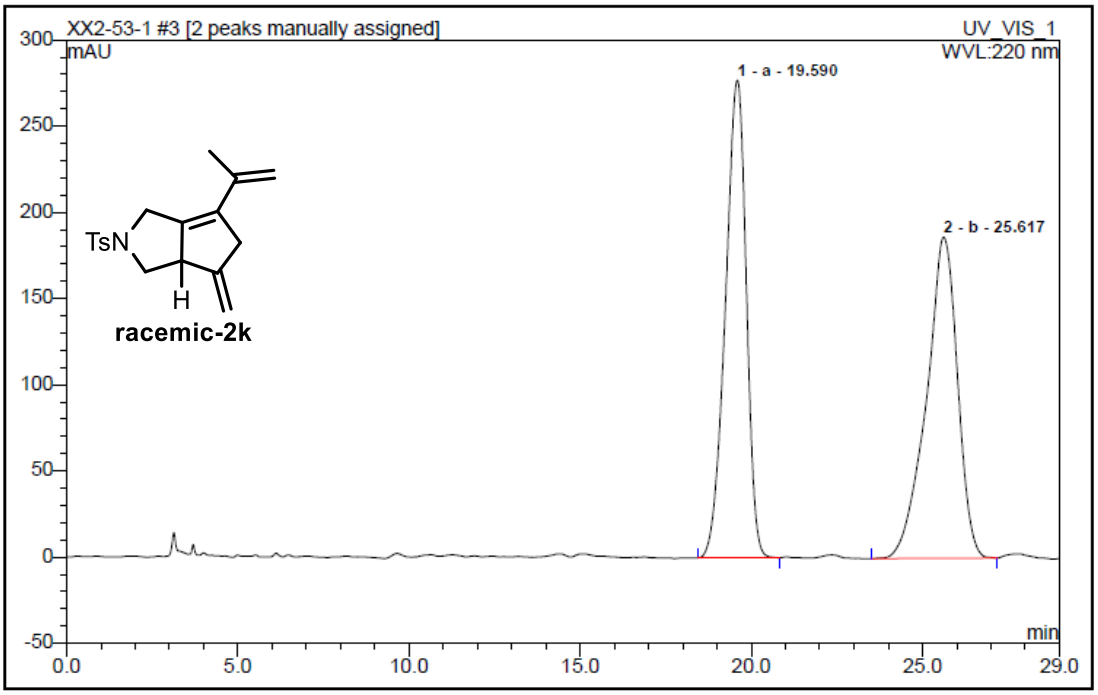
No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area(ident.) %	Amount mg/l	Type
2	25.03	a	42.704	33.366	8.28	n.a.	BMB^
2	29.15	b	356.004	369.361	91.72	n.a.	BMB^
Total:			398.707	402.727	100.00	0.000	



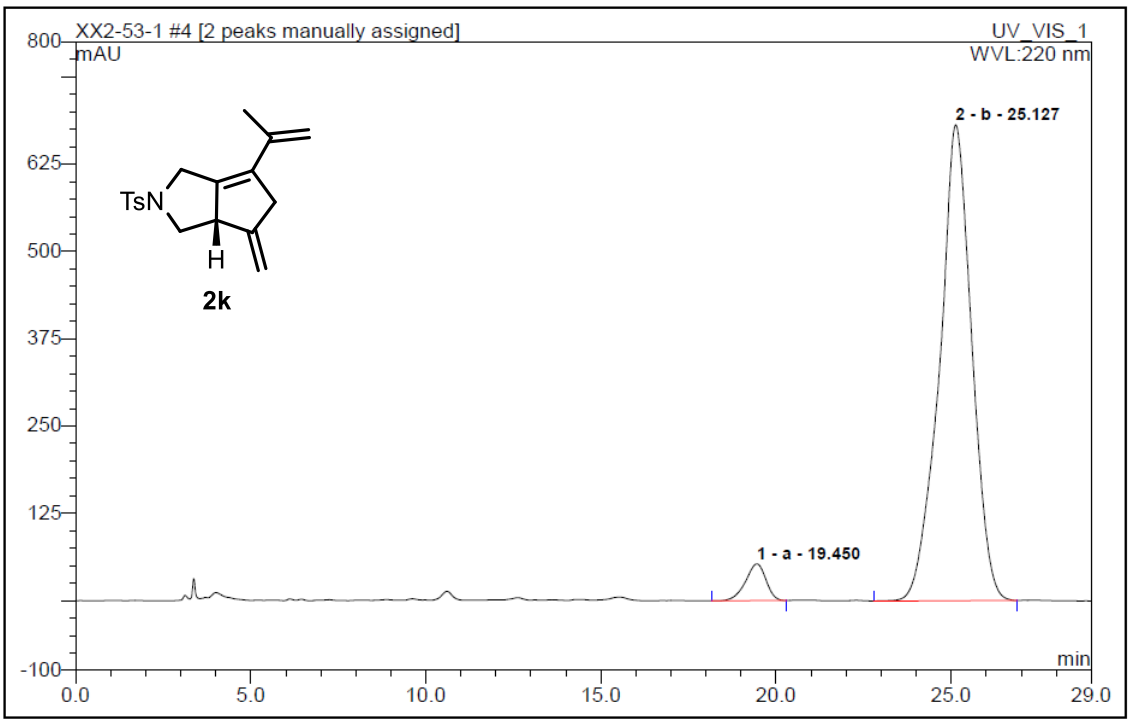
No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area(ident.) %	Amount mg/l	Type
2	15.09	a	229.997	163.662	49.51	n.a.	BMB^
2	18.62	b	168.114	166.919	50.49	n.a.	BMB^
Total:			398.110	330.581	100.00	0.000	



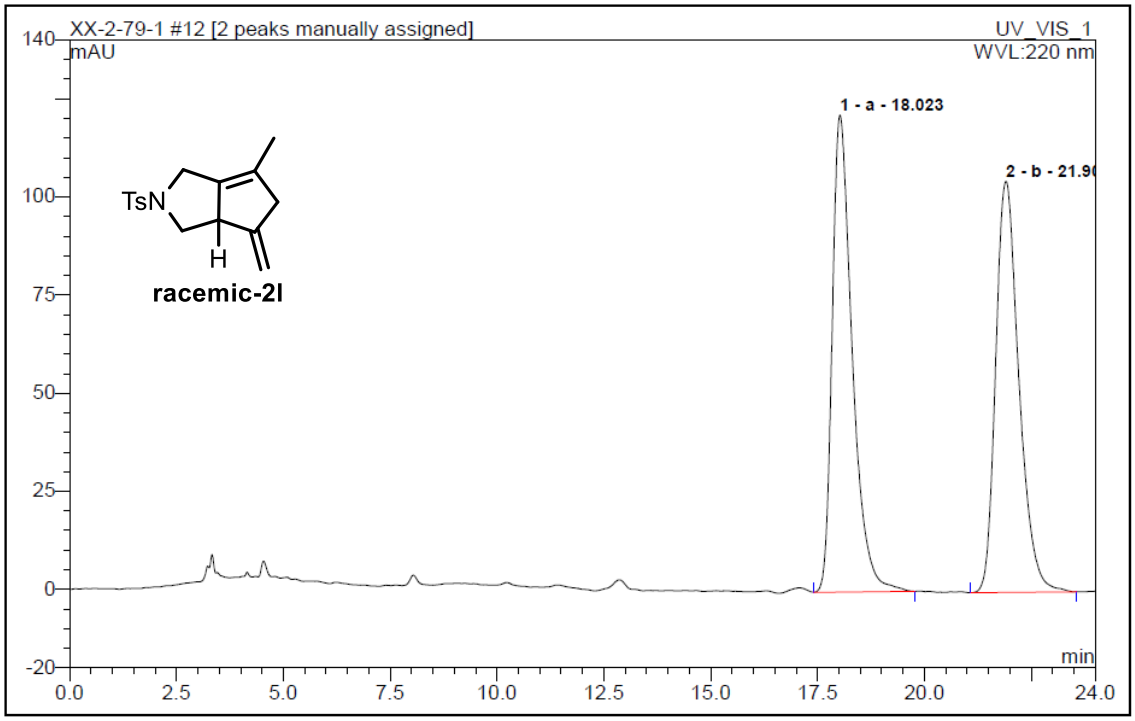
No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area(ident.) %	Amount mg/l	Type
2	15.32	a	70.710	51.145	9.67	n.a.	BMB^
2	18.59	b	474.806	477.848	90.33	n.a.	BMB^
Total:			545.516	528.994	100.00	0.000	



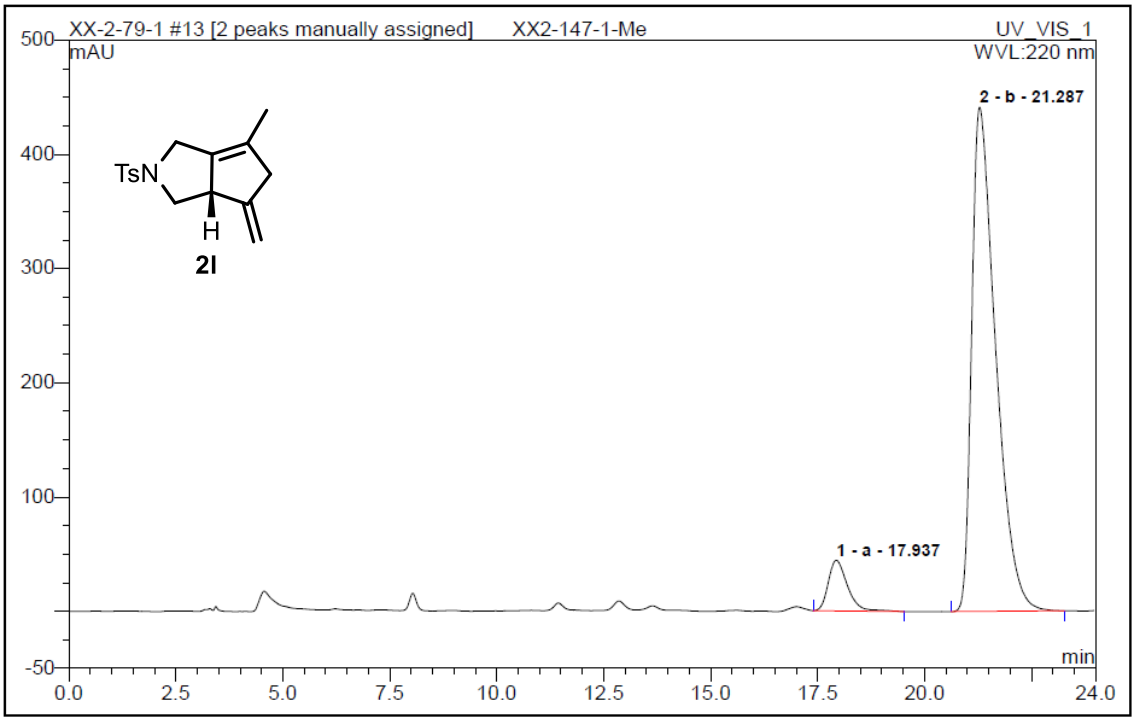
No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area(ident.) %	Amount mg/l	Type
2	19.59	a	277.108	195.557	49.88	n.a.	BMB^
2	25.62	b	186.347	196.472	50.12	n.a.	BMB^
Total:			463.455	392.028	100.00	0.000	



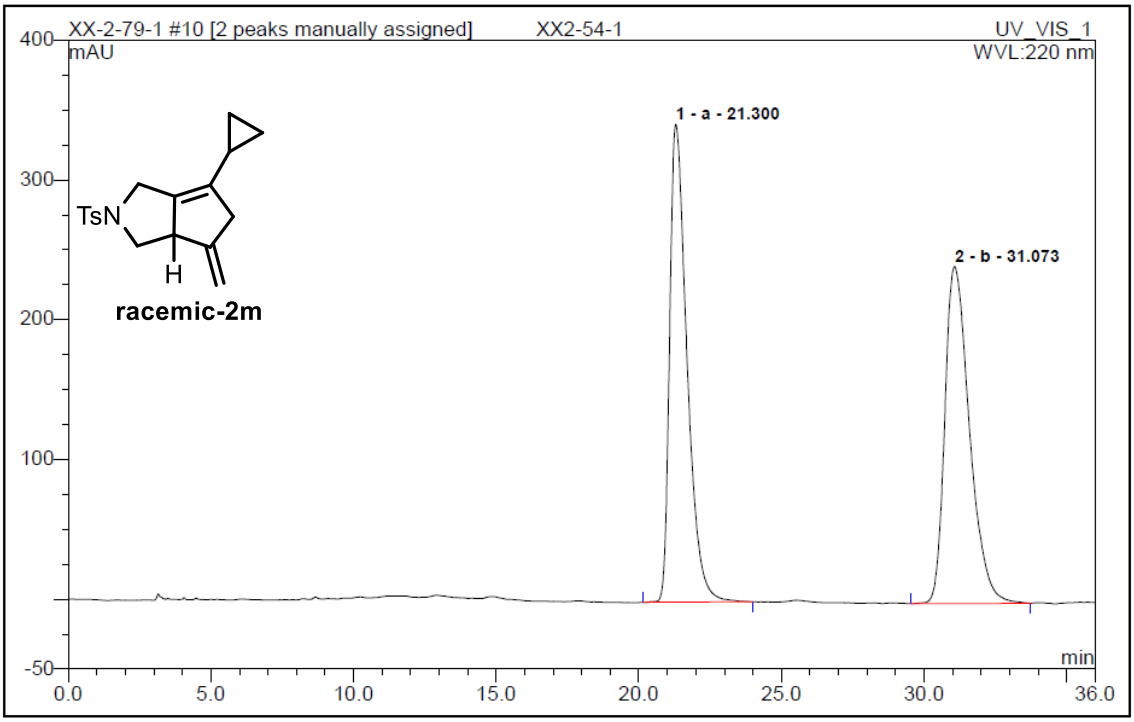
No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area(ident.) %	Amount mg/l	Type
2	19.45	a	52.549	35.544	4.65	n.a.	BMB^
2	25.13	b	681.860	728.719	95.35	n.a.	BMB^
Total:			734.409	764.263	100.00	0.000	



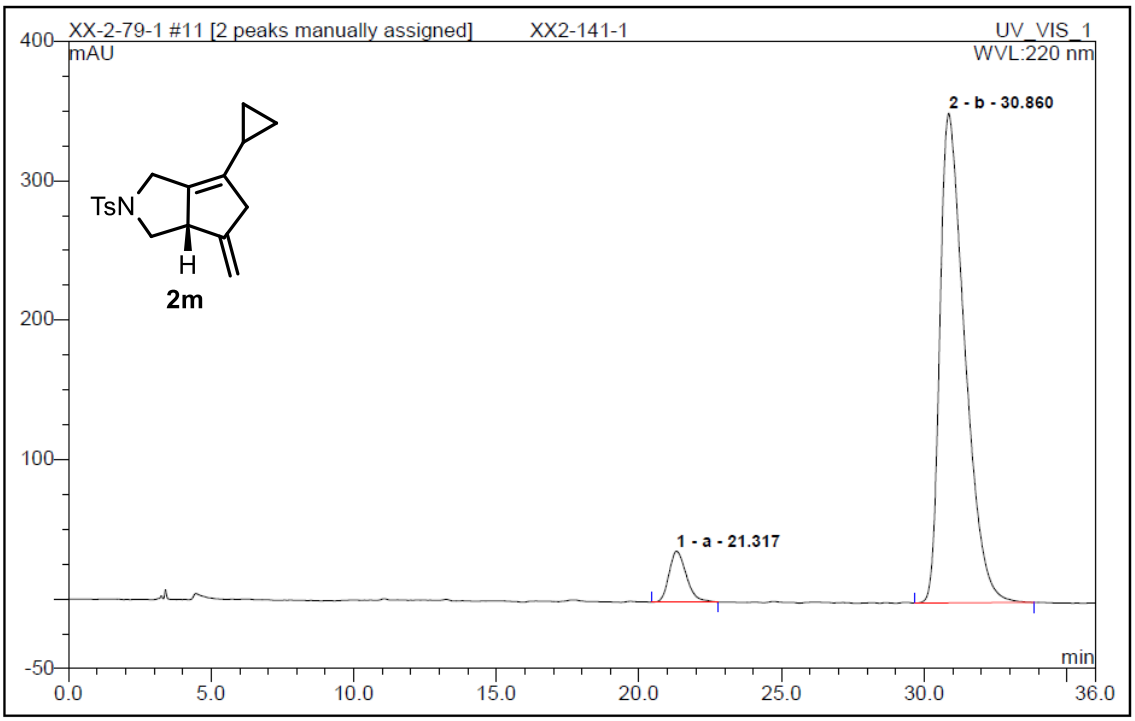
No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area(ident.) %	Amount mg/l	Type
2	18.02	a	121.498	66.090	50.00	n.a.	BMB^
2	21.91	b	104.716	66.092	50.00	n.a.	BMB^
Total:			226.214	132.182	100.00	0.000	



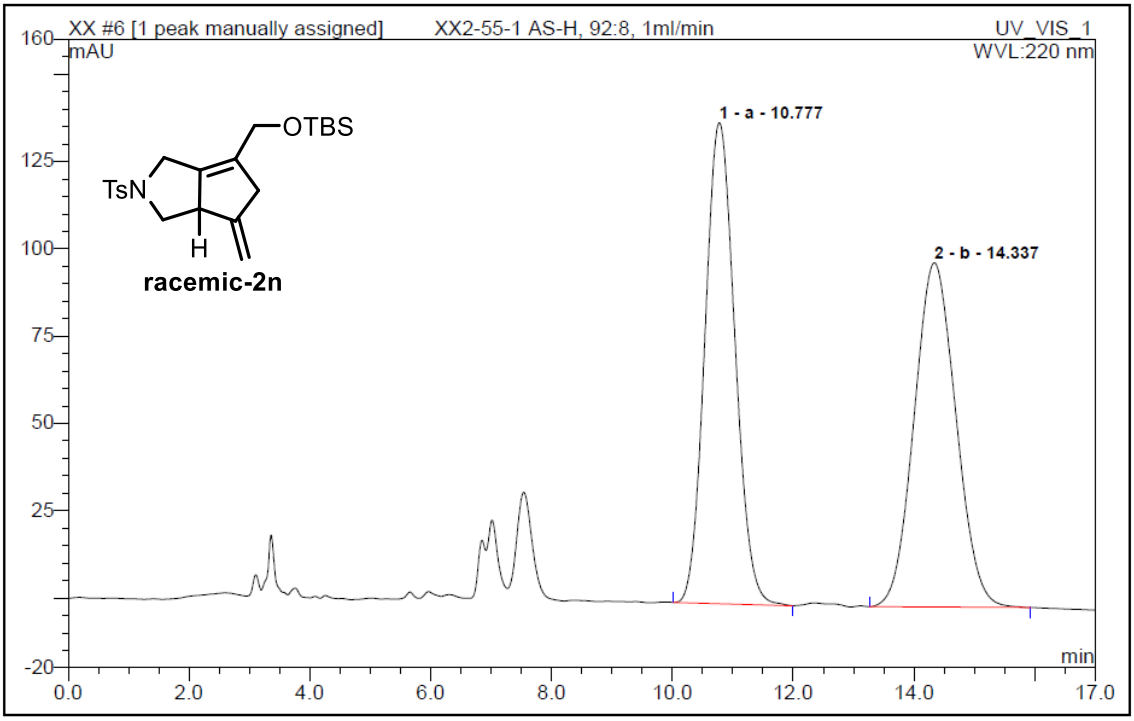
No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area(ident.) %	Amount mg/l	Type
2	17.94	a	44.237	22.876	7.41	n.a.	BMB^
2	21.29	b	441.484	285.888	92.59	n.a.	BMB^
Total:			485.721	308.764	100.00	0.000	



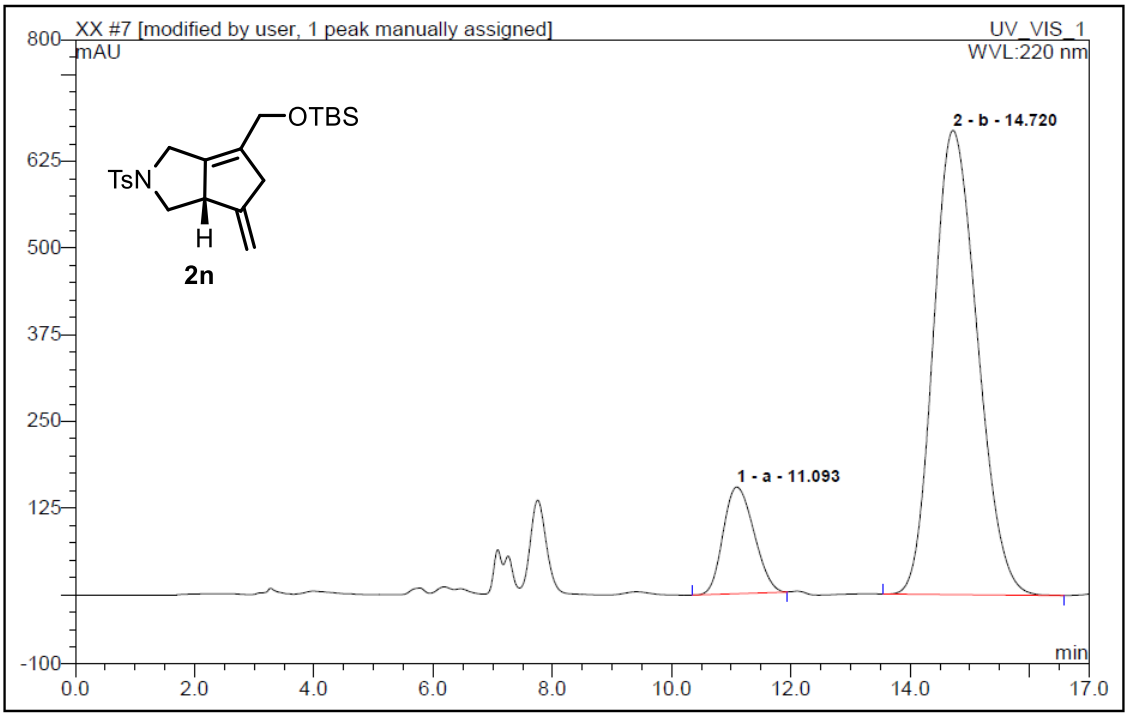
No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area(ident.) %	Amount mg/l	Type
2	21.30	a	342.007	240.925	49.91	n.a.	BMB^
2	31.07	b	241.372	241.794	50.09	n.a.	BMB^
Total:			583.379	482.719	100.00	0.000	



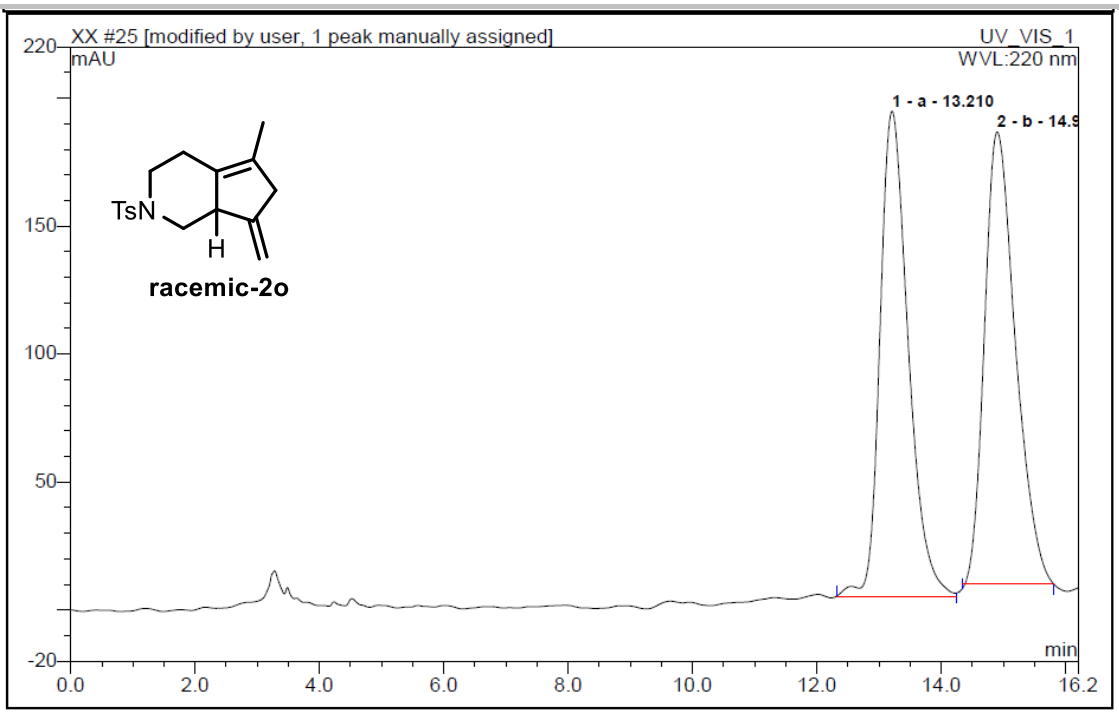
No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area(ident.) %	Amount mg/l	Type
2	21.32	a	36.482	25.611	6.71	n.a.	BMB^
2	30.86	b	351.288	356.354	93.29	n.a.	BMB^
Total:			387.770	381.966	100.00	0.000	



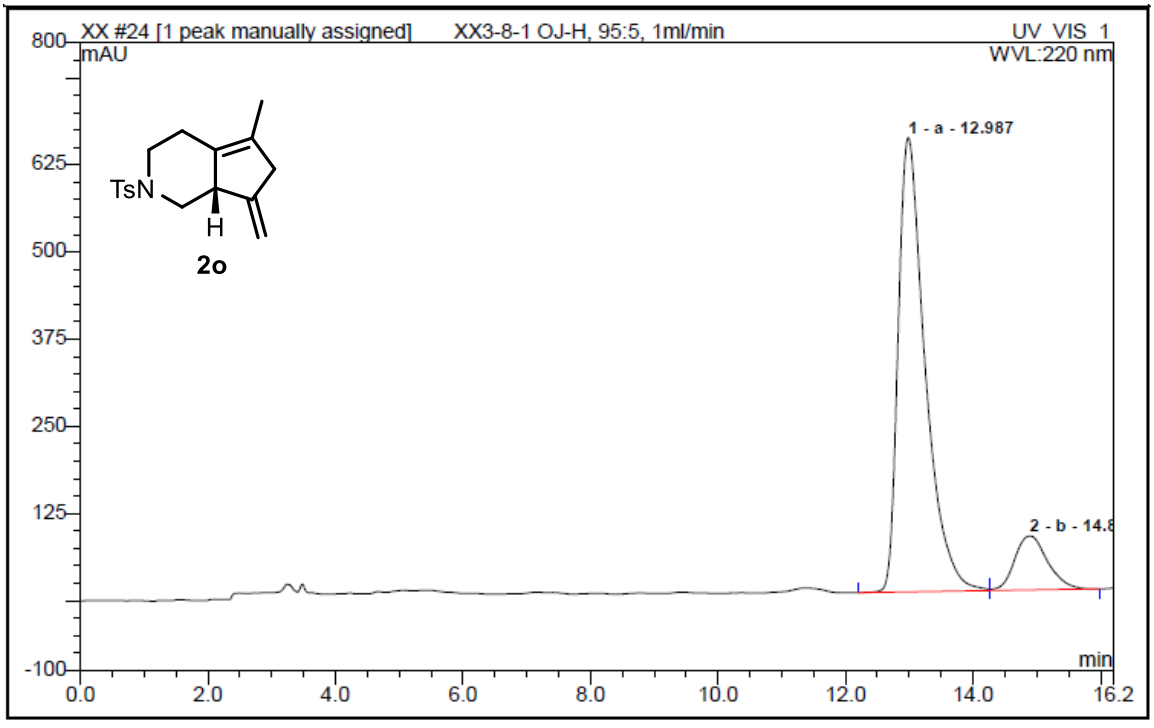
No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area(ident.) %	Amount mg/l	Type
2	10.78	a	137.790	79.202	50.04	n.a.	BMB^
2	14.34	b	98.629	79.073	49.96	n.a.	BMB
Total:			236.419	158.274	100.00	0.000	



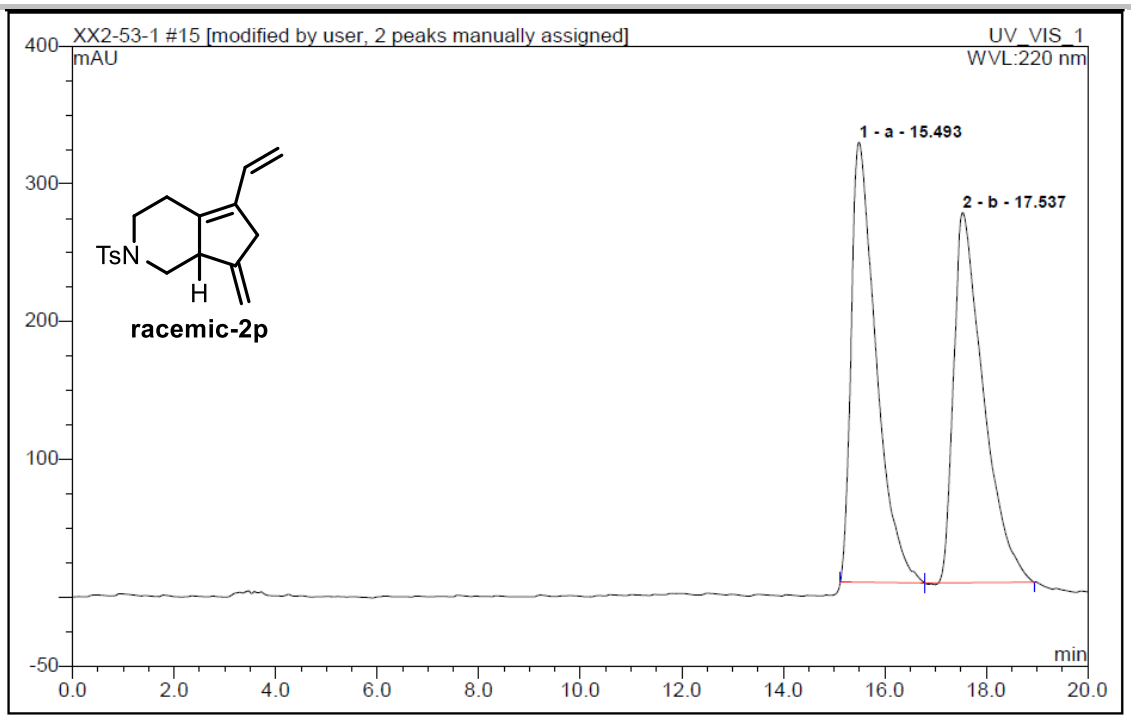
No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area(ident.) %	Amount mg/l	Type
2	11.09	a	153.759	92.064	13.85	n.a.	BMB^
2	14.72	b	669.498	572.767	86.15	n.a.	BMB
Total:			823.257	664.831	100.00	0.000	



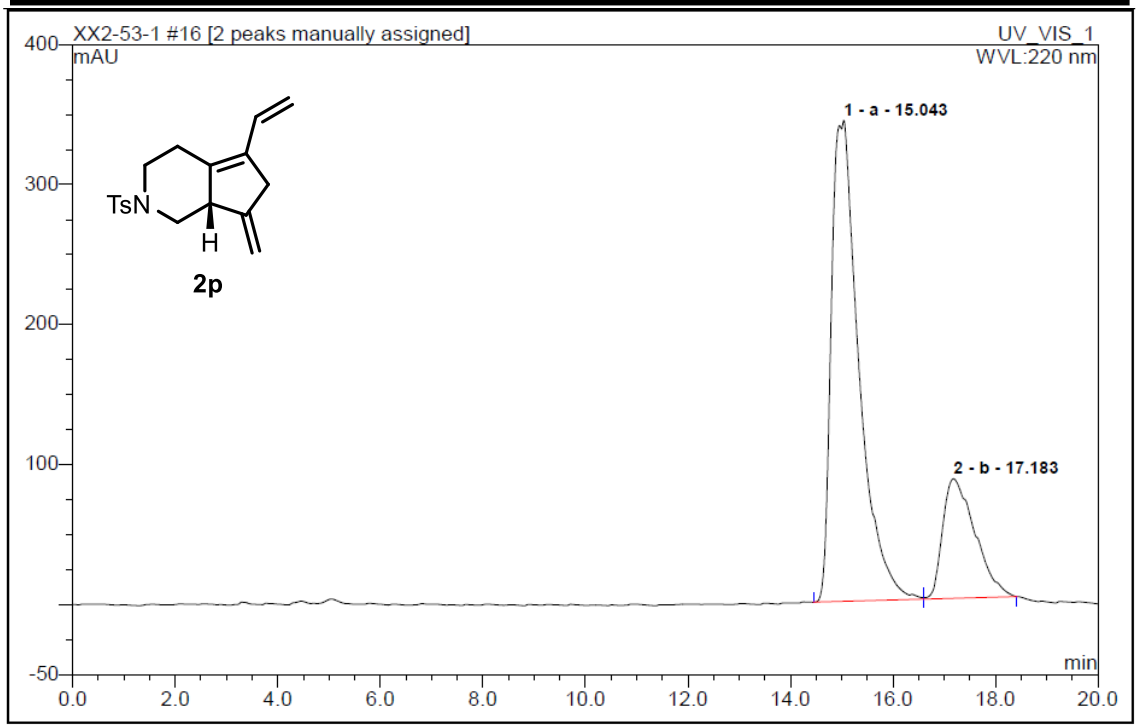
No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area(ident.) %	Amount mg/l	Type
2	13.21	a	189.564	99.918	49.46	n.a.	BM *^
2	14.90	b	176.761	102.111	50.54	n.a.	MB*
Total:			366.325	202.030	100.00	0.000	



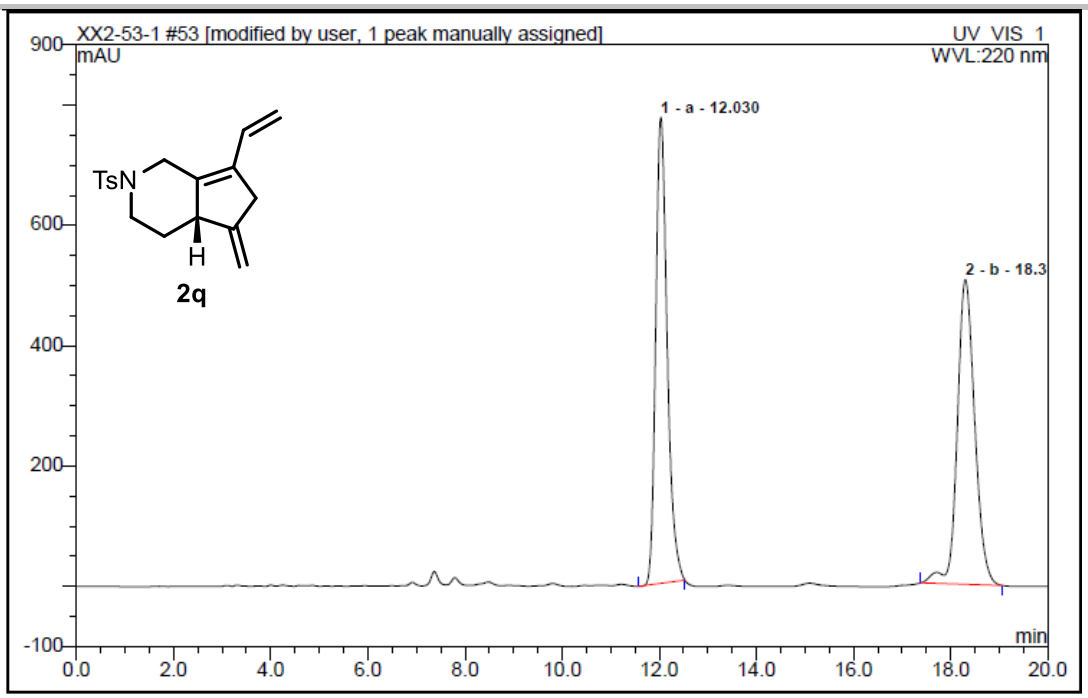
No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area(ident.) %	Amount mg/l	Type
2	12.99	a	651.439	319.282	87.31	n.a.	BM ^
2	14.89	b	77.470	46.389	12.69	n.a.	MB
Total:			728.909	365.672	100.00	0.000	



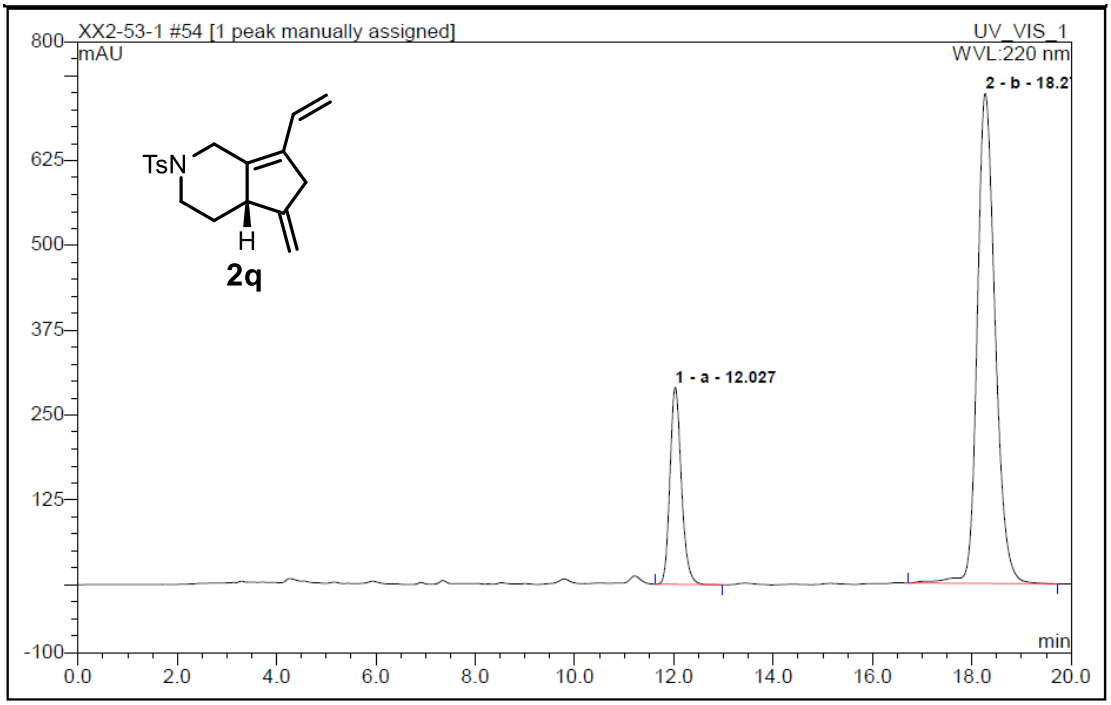
No.	Ret.Time min		Peak Name	Height mAU	Area mAU*min	Rel.Area(ident.) %	Amount mg/l	Type
2	15.49	a		319.400	182.292	49.96	n.a.	BMb*^
2	17.54	b		268.706	182.585	50.04	n.a.	bMB*^
Total:				588.107	364.877	100.00	0.000	



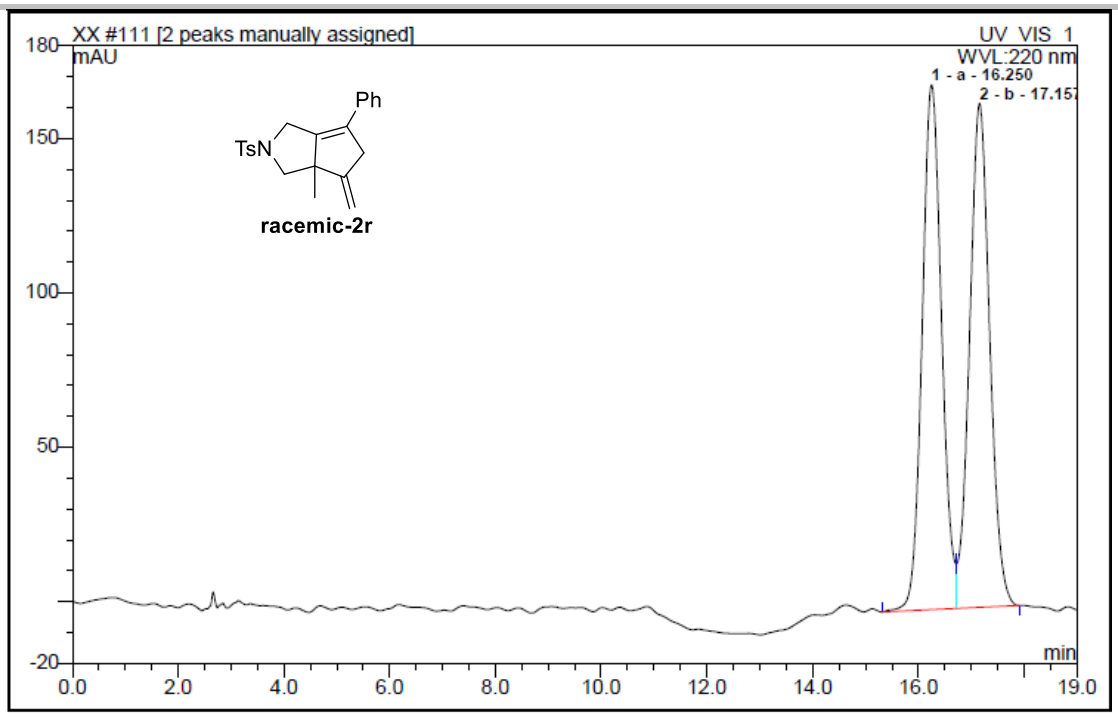
No.	Ret.Time min		Peak Name	Height mAU	Area mAU*min	Rel.Area(ident.) %	Amount mg/l	Type
2	15.04	a		343.683	214.418	77.45	n.a.	BM ^
2	17.18	b		85.360	62.445	22.55	n.a.	MB^
Total:				429.043	276.862	100.00	0.000	



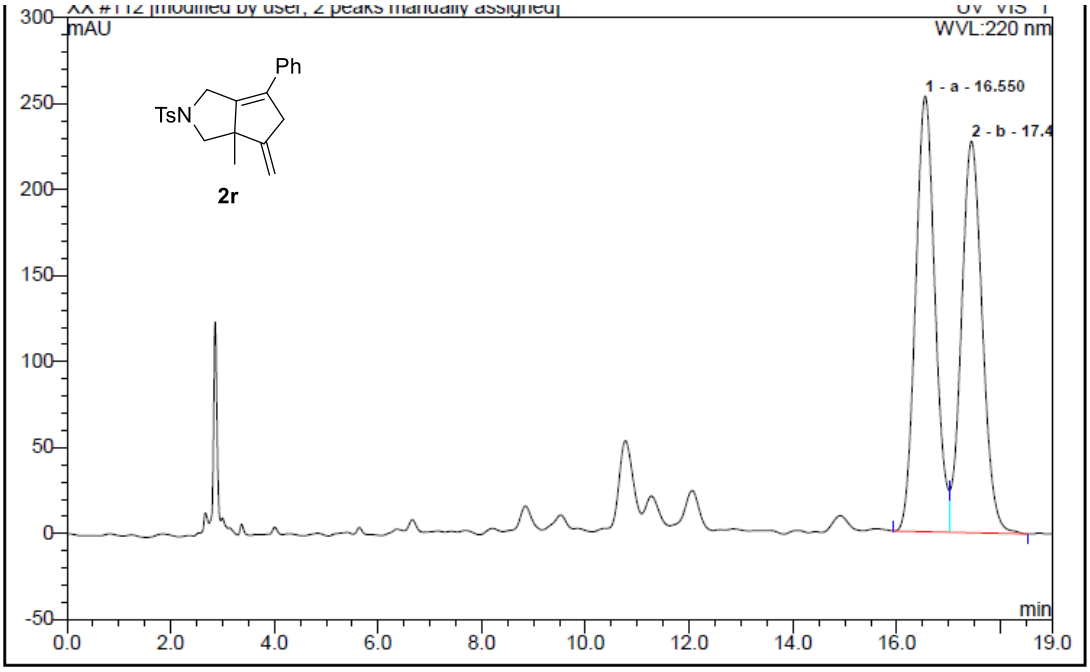
No.	Ret.Time min		Peak Name	Height mAU	Area mAU*min	Rel.Area(ident.) %	Amount mg/l	Type
2	12.03	a		774.499	211.510	50.03	n.a.	BMB*
2	18.30	b		506.201	211.239	49.97	n.a.	BMB*^
Total:				1280.701	422.749	100.00	0.000	



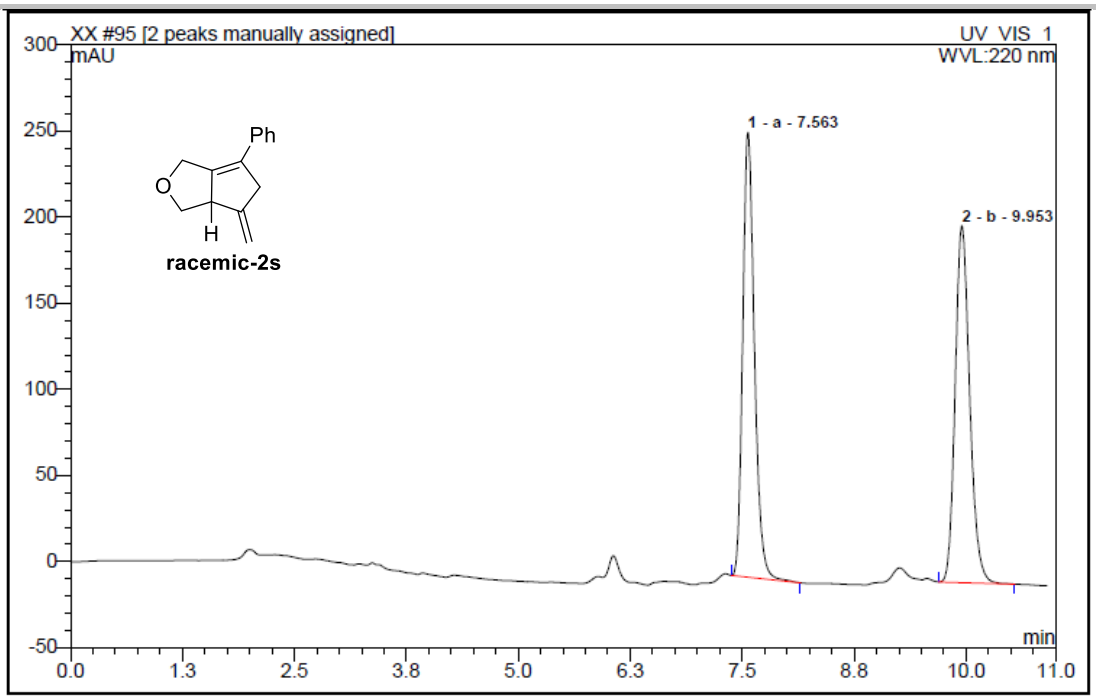
No.	Ret.Time min		Peak Name	Height mAU	Area mAU*min	Rel.Area(ident.) %	Amount mg/l	Type
2	12.03	a		290.205	77.532	20.35	n.a.	BMB
2	18.27	b		722.212	303.471	79.65	n.a.	BMB^
Total:				1012.417	381.002	100.00	0.000	



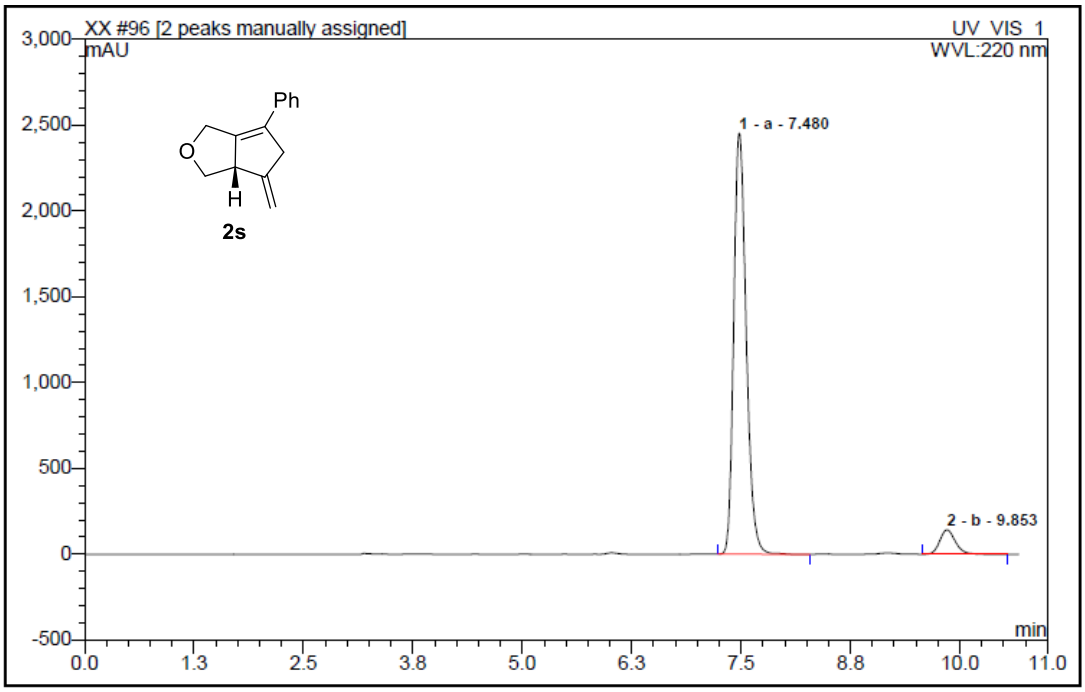
No.	Ret.Time min		Peak Name	Height mAU	Area mAU*min	Rel.Area(ident.) %	Amount mg/l	Type
2	16.25	a		169.881	72.349	50.06	n.a.	BM ^
2	17.16	b		163.233	72.188	49.94	n.a.	MB^
Total:				333.113	144.537	100.00	0.000	



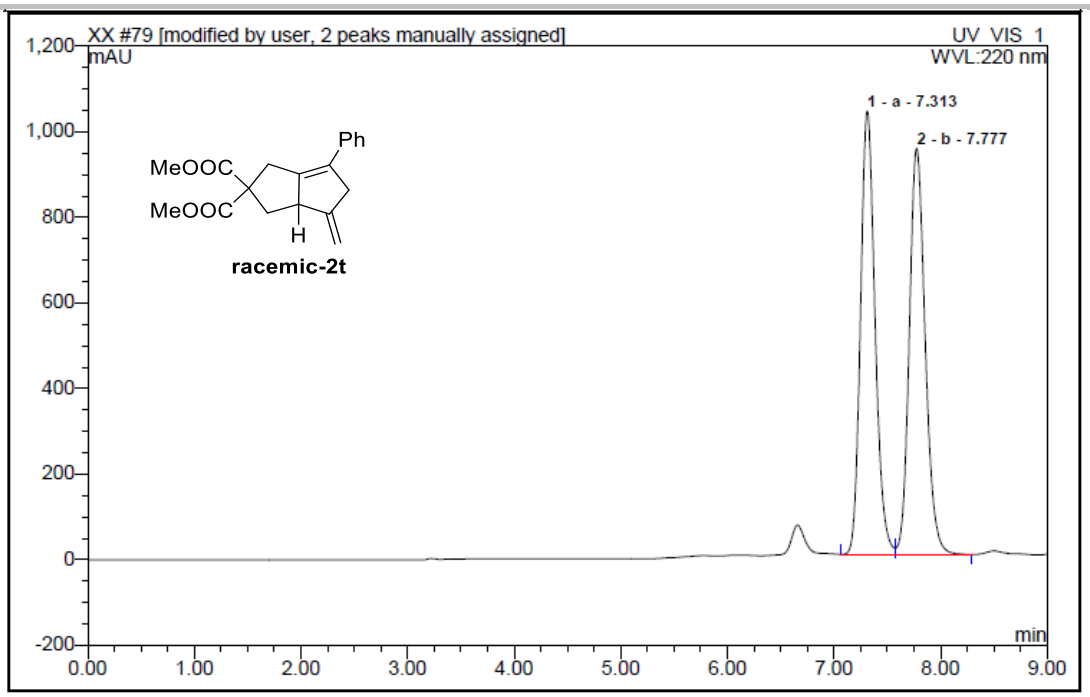
No.	Ret.Time min		Peak Name	Height mAU	Area mAU*min	Rel.Area(ident.) %	Amount mg/l	Type
2	16.55	a		253.300	109.982	50.85	n.a.	BM ^
2	17.44	b		227.634	106.309	49.15	n.a.	MB^
Total:				480.934	216.291	100.00	0.000	



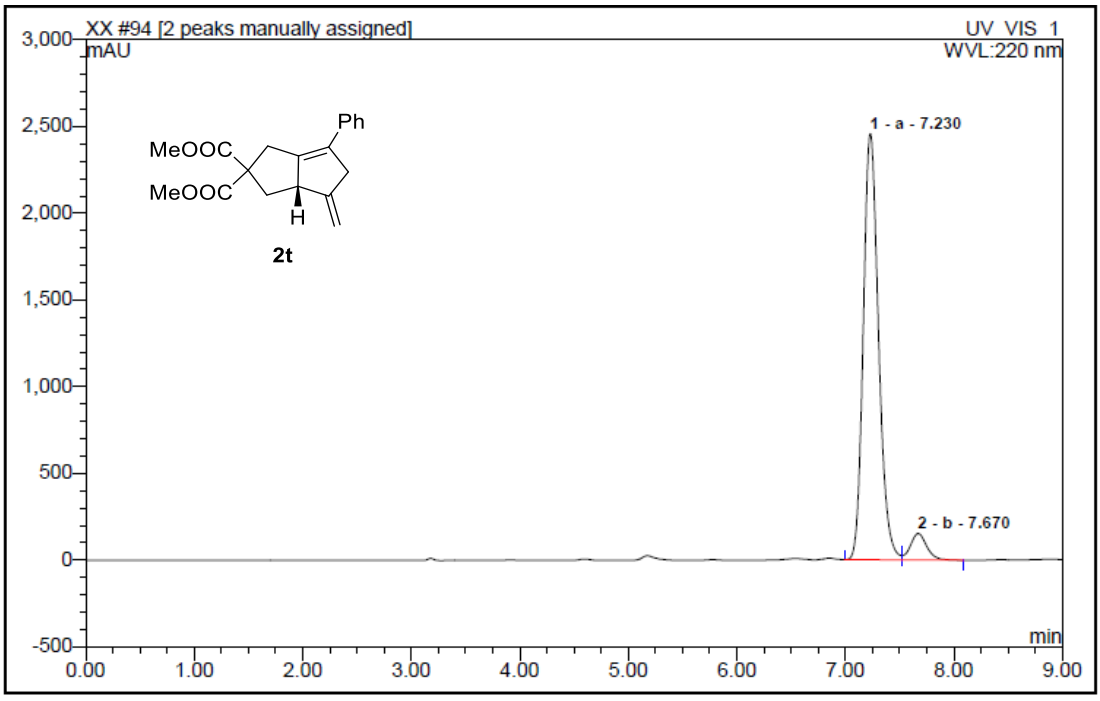
No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area(ident.) %	Amount mg/l	Type
2	7.56	a	258.326	39.003	50.04	n.a.	BMB^
2	9.95	b	207.185	38.935	49.96	n.a.	BMB^
Total:			465.512	77.938	100.00	0.000	



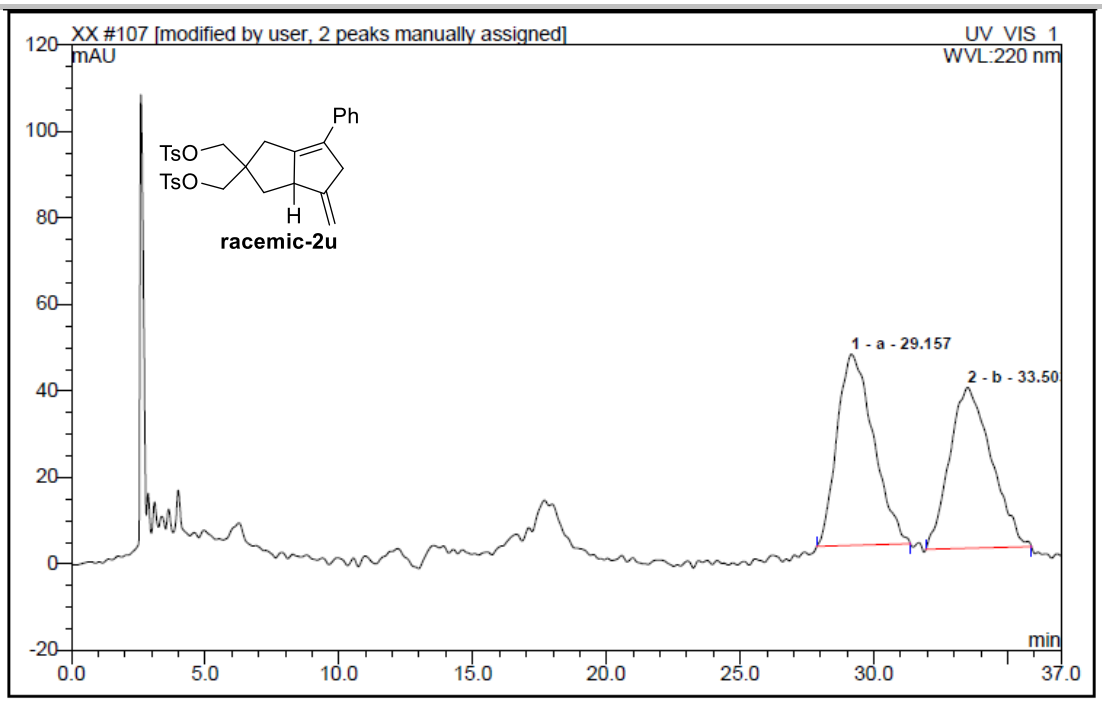
No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area(ident.) %	Amount mg/l	Type
2	7.48	a	2451.806	405.360	93.26	n.a.	BMB^
2	9.85	b	141.547	29.292	6.74	n.a.	BMB^
Total:			2593.352	434.652	100.00	0.000	



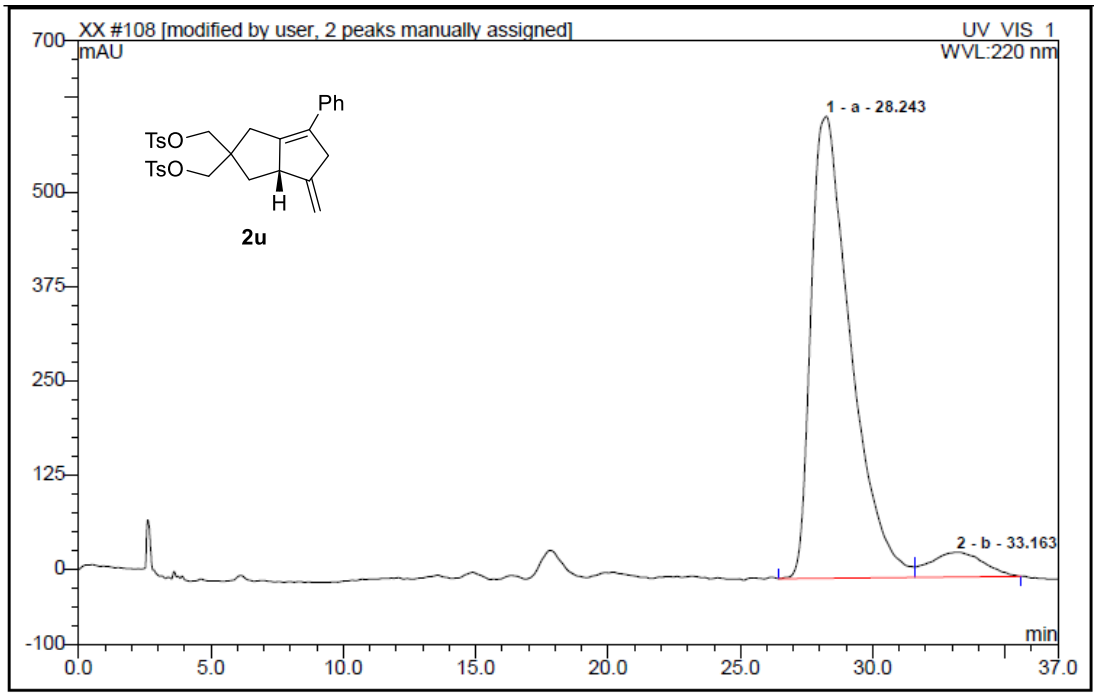
No.	Ret.Time min		Peak Name	Height mAU	Area mAU*min	Rel.Area(ident.) %	Amount mg/l	Type
2	7.31	a		1036.235	163.612	49.92	n.a.	BM *^
2	7.78	b		948.621	164.154	50.08	n.a.	MB^
Total:				1984.856	327.765	100.00	0.000	



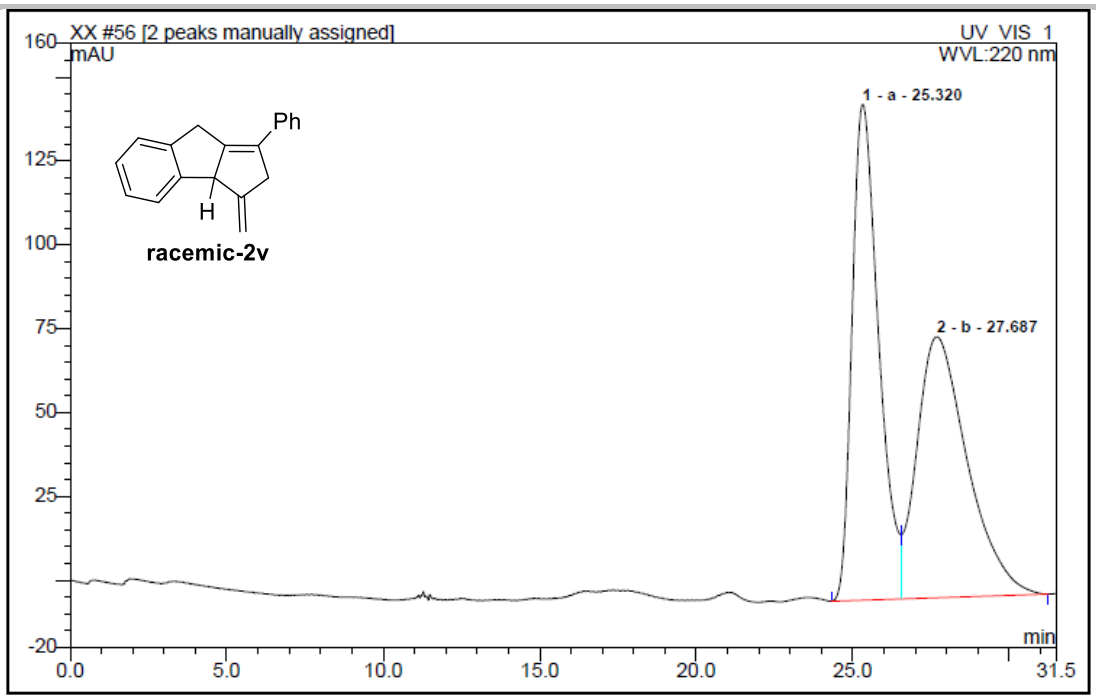
No.	Ret.Time min		Peak Name	Height mAU	Area mAU*min	Rel.Area(ident.) %	Amount mg/l	Type
2	7.23	a		2455.615	398.706	93.75	n.a.	BM ^
2	7.67	b		152.483	26.569	6.25	n.a.	MB^
Total:				2608.098	425.275	100.00	0.000	



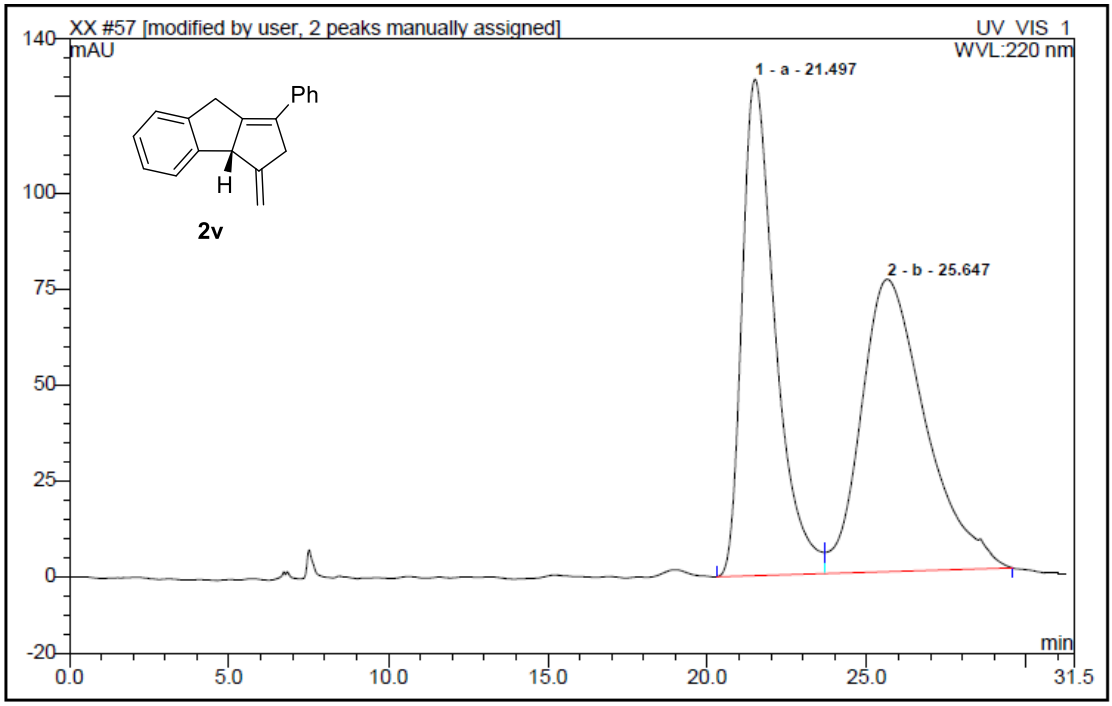
No.	Ret.Time min		Peak Name	Height mAU	Area mAU*min	Rel.Area(ident.) %	Amount mg/l	Type
2	29.16	a		44.177	69.914	50.84	n.a.	BMB*^
2	33.50	b		37.140	67.608	49.16	n.a.	BMB*^
Total:				81.317	137.522	100.00	0.000	



No.	Ret.Time min		Peak Name	Height mAU	Area mAU*min	Rel.Area(ident.) %	Amount mg/l	Type
2	28.24	a		611.953	1063.291	93.34	n.a.	BM ^
2	33.16	b		32.823	75.920	6.66	n.a.	MB^
Total:				644.776	1139.211	100.00	0.000	



No.	Ret.Time min		Peak Name	Height mAU	Area mAU*min	Rel.Area(ident.) %	Amount mg/l	Type
2	25.32	a		147.775	145.017	49.84	n.a.	BM ^
2	27.69	b		77.783	145.973	50.16	n.a.	MB^
Total:				225.558	290.990	100.00	0.000	



No.	Ret.Time min		Peak Name	Height mAU	Area mAU*min	Rel.Area(ident.) %	Amount mg/l	Type
2	21.50	a		129.213	155.633	46.59	n.a.	BM *^
2	25.65	b		76.151	178.388	53.41	n.a.	MB*^
Total:				205.365	334.021	100.00	0.000	

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