Angewandte Chemie
Eine Zeitschrift der Gesellschaft Deutscher Chemiker

Supporting Information

Rhodium(I)-Catalyzed Bridged [5+2] Cycloaddition of *cis*-Allene-vinylcyclopropanes to Synthesize the Bicyclo[4.3.1]decane Skeleton

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Supporting Information

Contents

1. General

Air and moisture sensitive reactions were carried out in oven-dried glassware sealed with rubber septa under a positive pressure of dry argon. Similarly 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. 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.

Tetrahydrofuran, 1,2-dimethoxyethane and toluene were distilled from sodium and benzophenone prior to use. Dioxane, 1,2-dichloroethane and chlorobenzene (SuperDry, with molecular sieves) were purchased from J&K and used directly. Synthetic reagents were purchased from Acros, Aldrich, and Alfa Aesar and used without further purification, unless otherwise indicated.

NMR spectra were measured on Bruker ARX 400 (^{1}H at 400 MHz, ^{13}C at 101 MHz) nuclear magnetic resonance spectrometers. ^{1}H-NMR spectra are reported relative to Me_4Si (0.00 ppm) or residual solvent signals (C_6D_6: 7.16 ppm). Data for ^{1}H-NMR spectra are reported as follows: chemical shift (ppm, s = singlet, brs = broad singlet, d = doublet, t = triplet, q = quartet, dd = doublet of doublets, dt = doublet of triplets, dm = doublet of multiplet, ddd = doublet of doublet of doublets, tdd = triplet of doublet of doublets, m = multiplet), coupling constant (Hz), and integration. Data for ^{13}C-NMR are reported in terms of chemical shift (ppm) relative to residual solvent peak ($CDCl_3$: 77.0 ppm, C_6D_6: 128.0 ppm). ^{13}C signals are analyzed as follows: (+) = CH3/CH, (−) = CH2, quaternary carbons and other carbons with no attached protons are not marked. The assignment resulted from DEPT-135°. Infrared spectra were recorded on Bruker Tensor 27 fourier transform infrared spectrometer (FT-IR) and were reported in wavenumbers (cm^{-1}). High-resolution mass spectra (HRMS) were recorded on Bruker Apex IV FTMS mass spectrometer (ESI) and ThermoFisher Q Exactive GC GC–MS mass spectrometer (EI).

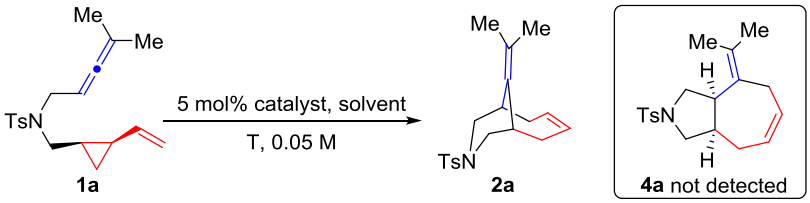
Abbreviations:

acac = acetylacetone
Bs = *p*-bromobenzenesulfonyl
Boc = *t*-butoxycarbonyl
COD = 1,5-cyclooctadiene
COE = cyclooctene
DCE = 1,2-dichloroethane
DCM = dichloromethane
DIAD = diisopropyl azodicarboxylate
DMSO = dimethyl sulphoxide
EA = ethyl acetate
MS = molecular sieve
Ms = methylsulfonyl
NBD = norbornadiene
Ns = *p*-nitrobenzenesulfonyl
PDC = pyridinium dichromate
PE = petroleum ether
TBS = *t*-butyldimethylsilyl
TBAF = tetrabutylammonium fluoride
THF = tetrahydrofuran
TLC = thin layer chromatography
Ts = *p*-toluenesulfonyl

2. Screening Reaction Conditions

We commenced our study with NTs-tethered *cis*-allene-VCP **1a** as the standard substrate. At first, we tried different rhodium catalysts (entries 1−6) and no reaction occurred when $[Rh(COD)Cl]_2$ or $[Rh(COE)_2Cl]_2$ was used. Other catalysts such as $[Rh(NBD)_2]BF_4$ and $Rh(CO)(PPh_3)_2Cl$ lead to decomposition of the substrates. Only when $[Rh(CO)_2Cl]_2$ was used, a new highly symmetrical bicyclo[4.3.1]decane cycloadduct could be isolated in 77% yield after 4 h (entry 3). Here, the inner double bond of the allene act as the 2π component and participate in the [5+2] cycloadditions, which is called here as the bridged [5+2] reaction, in an opposite manner compared to previously reported normal [5+2] cycloadditions. We then investigated how solvents affected the reaction outcome (entries 7−10), finding that DCE and DME both gave similar yields and aromatic solvent such as toluene could slow down the reaction and gave only modest yield after 8 h. Increasing the reaction temperature also had no benefit to the improvement of the reaction yield (entry 11). Finally we chose dioxane as solvent and the desired bicyclo[4.3.1]decane cycloadduct **2a** could be obtained in 80% yield when using 0.2 mmol scale starting material (entry 12).

Table S1: Selected optimization conditions with allene **1a**



1a **2a** **4a** not detected

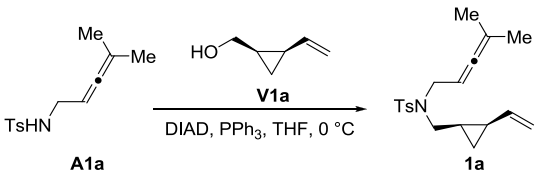
entry[a]	solvent	catalyst	T	time	yield[c]
1	dioxane	$[Rh(COD)Cl]_2$	80	4h	NR
2	dioxane	$[Rh(COE)_2Cl]_2$	80	4h	NR
3	dioxane	$[Rh(CO)_2Cl]_2$	80	4h	77%
4	dioxane	$[Rh(NBD)_2]BF_4$[b]	80	4h	decomposed
5	dioxane	$Rh(acac)(CO)_2$[b]	80	4h	NR
6	dioxane	$Rh(CO)(PPh_3)_2Cl$[b]	80	3h	slowly decomposed
7	DCE	$[Rh(CO)_2Cl]_2$	80	4h	74%
8	DME	$[Rh(CO)_2Cl]_2$	80	5h	74%
9	toluene	$[Rh(CO)_2Cl]_2$[b]	80	8h	57%
10	C_6H_5Cl	$[Rh(CO)_2Cl]_2$[b]	80	8h	46%
11	dioxane	$[Rh(CO)_2Cl]_2$	100	2h	75%
12	**dioxane**	**$[Rh(CO)_2Cl]_2$**	**80**	**4h**	**80%[d,e]**
13[f]	dioxane	$[Rh(CO)_2Cl]_2$	80	5h	NR

[a]0.1 mmol substrate was used. [b]10 mol% catalyst loading.[c]Isolated yields. [d]0.2 mmol substrate was used. [e]Average yield of two runs. [f]The reaction was performed under 1 atm CO in order to get some CO insertion products.

3. Experimental Procedures and Characterization Data

3.1 Synthesis of Substrates

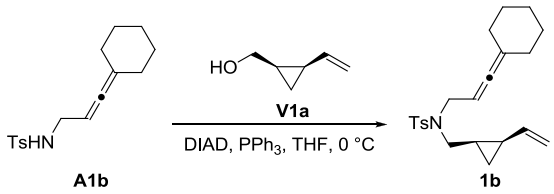
Substrate (1a)



To a stirred solution of **V1a**[1] (84 mg, 0.86 mmol), tosylamide **A1a**[2] (260 mg, 1.03 mmol), and PPh_3 (452 mg, 1.72 mmol) in anhydrous THF (5 mL) was added DIAD (348 mg, 1.72 mmol) at 0 ℃ under N_2. The mixture was then stirred overnight at room temperature. 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 product **1a** (152 mg, 53%).

1a: light yellow oil, TLC R_f = 0.72 (PE/EA, 5:1). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.70 (d, J = 8.2 Hz, 2H), 7.28 (d, J = 8.2 Hz, 2H), 5.53 (ddd, J = 17.0, 10.2, 8.5 Hz, 1H), 5.12 (ddd, J = 17.0, 1.7, 0.6 Hz, 1H), 5.00 (dd, J = 10.2, 1.7 Hz, 1H), 4.77–4.68 (m, 1H), 3.92 (dd, J = 14.2, 5.8 Hz, 1H), 3.87 (dd, J = 14.2, 5.8 Hz, 1H), 3.30 (dd, J = 14.5, 6.1 Hz, 1H), 3.14 (dd, J = 14.5, 8.0 Hz, 1H), 2.41 (s, 3H), 1.65 (s, 3H), 1.64 (s, 3H), 1.69–1.53 (m, 1H), 1.25–1.17 (m, 1H), 0.97–0.90 (m, 1H), 0.45–0.39 (m, 1H). ^{13}C NMR (101 MHz, $CDCl_3$): δ 203.0, 142.9, 137.9, 136.7 (+), 129.6 (+), 127.1 (+), 115.4 (–), 96.7, 84.7 (+), 46.7 (–), 46.1 (–), 21.5 (+), 20.4 (+), 20.3 (+), 19.7 (+), 17.0 (+), 11.7 (–). IR (KBr): υ 2982, 2916, 2863, 1447, 1342, 1158, 1094, 981 cm^{-1}. HRMS (ESI) calcd for $C_{19}H_{26}NO_2S$ ($[M+H]^+$): 332.1679. Found: 332.1680.

Substrate (1b)

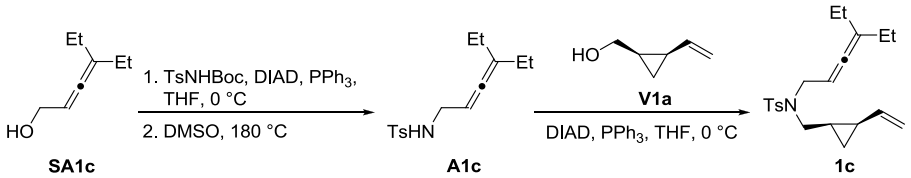


To a stirred solution of **V1a** (216 mg, 2.20 mmol), tosylamide **A1b**[3] (696 mg, 2.39 mmol), and PPh_3 (1.15 g, 4.38 mmol) in anhydrous THF (10 mL) was added DIAD (890 mg, 4.40 mmol) at 0 ℃ under N_2. The mixture was then stirred for 2 h at room temperature. The reaction mixture was concentrated and the crude product was purified by flash column chromatography on silica gel (eluted with PE/EA 20:1) to afford product **1b** (463 mg, 56%).

1b: light yellow oil, TLC R_f = 0.74 (PE/EA, 5:1). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.71 (d, J = 8.3 Hz, 2H), 7.28 (d, J = 8.3 Hz, 2H), 5.52 (ddd, J = 17.0, 10.2, 8.6 Hz, 1H), 5.12 (ddd, J = 17.0, 1.7, 0.6 Hz, 1H), 5.00 (dd, J = 10.2, 1.7 Hz, 1H), 4.75–4.68 (m, 1H), 3.97–3.86 (m, 2H), 3.32 (dd, J = 14.5, 6.0 Hz, 1H), 3.14 (dd, J = 14.5, 8.1 Hz, 1H), 2.41 (s, 3H), 2.10–2.00 (m, 4H), 1.61–1.46 (m, 7H), 1.24–1.15 (m, 1H), 0.97–0.90 (m, 1H), 0.45–0.39 (m, 1H). ^{13}C NMR (101 MHz, $CDCl_3$): δ 199.8, 142.9, 137.9, 136.8 (+), 129.6 (+), 127.1 (+), 115.4 (–), 103.8, 84.4 (+), 46.9 (–), 46.0 (–), 31.2 (–), 27.1 (–), 25.9 (–), 21.5 (+), 19.6 (+), 17.0 (+), 11.8 (–). IR (KBr): υ 2929, 2854, 1446,

1344, 1159, 1094, 968 cm^{-1}. HRMS (ESI) calcd for $C_{22}H_{30}NO_2S$ ($[M+H]^+$): 372.1992. Found: 372.2000.

Substrate (1c)



To a stirred solution of **SA1c**[4] (602 mg, 4.77 mmol), TsNHBoc[5] (1.55 g, 5.71 mmol), and PPh_3 (2.50 g, 9.53 mmol) in anhydrous THF (25 mL) was added DIAD (1.93 g, 9.54 mmol) at 0 ℃ under N_2. The mixture was then stirred for 6 h at room temperature. The reaction mixture was concentrated and the crude product was purified by flash column chromatography on silica gel (eluted with PE/EA 20:1) to afford intermediate, which was used directly in the following step.

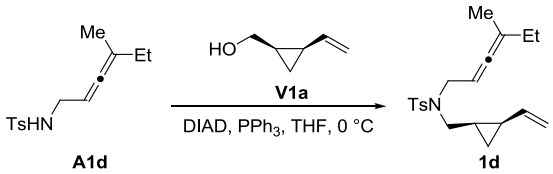
A stirred solution of the above intermediate in DMSO (50 mL) was immersed in a preheated oil bath at 180 ℃ for 20 min. The mixture was cooled to rt and diluted with ether. The solution was washed 5 times with water, and dried over $MgSO_4$. After removing the solvent, the crude product was purified by flash column chromatography on silica gel (eluted with PE/EA 10:1 then 5:1) to afford tosylamide **A1c** (1.15 g, 86%, 2 steps).

A1c: white solid, m.p. = 63–65 ℃, TLC R_f = 0.42 (PE/EA, 5:1). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.75 (d, J = 8.2 Hz, 2H), 7.31 (d, J = 8.2 Hz, 2H), 5.20–5.09 (m, 1H), 4.48–4.32 (m, 1H), 3.56–3.48 (m, 2H), 2.43 (s, 3H), 1.93 (qd, J = 7.3, 3.1 Hz, 4H), 0.92 (t, J = 7.3 Hz, 6H). ^{13}C NMR (101 MHz, $CDCl_3$): δ 199.5, 143.4, 136.9, 129.7 (+), 127.1 (+), 112.6, 89.6 (+), 42.2 (–), 25.4 (–), 21.5 (+), 12.2 (+). IR (KBr): υ 3280, 2966, 2932, 1327, 1161, 1094 cm^{-1}. HRMS (ESI) calcd for $C_{15}H_{22}NO_2S$ ($[M+H]^+$): 280.1366. Found: 280.1365.

To a stirred solution of **V1a** (80 mg, 0.82 mmol), tosylamide **A1c** (273 mg, 0.98 mmol), and PPh_3 (430 mg, 1.64 mmol) in anhydrous THF (4 mL) was added DIAD (332 mg, 1.64 mmol) at 0 ℃ under N_2. The mixture was then stirred overnight at room temperature. The reaction mixture was concentrated and the crude product was purified by flash column chromatography on silica gel (eluted with PE/EA 20:1) to afford product **1c** (238 mg, 81%).

1c: colorless oil, TLC R_f = 0.74 (PE/EA, 5:1). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.71 (d, J = 8.2 Hz, 2H), 7.28 (d, J = 8.2 Hz, 2H), 5.53 (ddd, J = 17.0, 10.2, 8.6 Hz, 1H), 5.12 (ddd, J = 17.0, 1.6, 0.6 Hz, 1H), 5.00 (dd, J = 10.2, 1.6 Hz, 1H), 4.97–4.90 (m, 1H), 3.94 (dd, J = 15.2, 6.9 Hz, 1H), 3.88 (dd, J = 15.2, 6.9 Hz, 1H), 3.32 (dd, J = 14.5, 6.0 Hz, 1H), 3.17 (dd, J = 14.5, 8.1 Hz, 1H), 2.42 (s, 3H), 1.98–1.89 (m, 4H), 1.60–1.54 (m, 1H), 1.26–1.17 (m, 1H), 0.96 (t, J = 7.4 Hz, 6H), 0.94–0.88 (m, 1H), 0.47–0.40 (m, 1H). ^{13}C NMR (101 MHz, $CDCl_3$): δ 201.4, 142.9, 137.8, 136.7 (+), 129.6 (+), 127.1 (+), 115.4 (–), 109.7, 88.6 (+), 47.1 (–), 46.3 (–), 25.5 (–), 25.4 (–), 21.5 (+), 19.8 (+), 17.0 (+), 12.31 (+), 12.28 (+), 11.8 (–). IR (KBr): υ 2967, 2932, 1455, 1345, 1157, 1092, 908 cm^{-1}. HRMS (ESI) calcd for $C_{21}H_{30}NO_2S$ ($[M+H]^+$): 360.1992. Found: 360.1998.

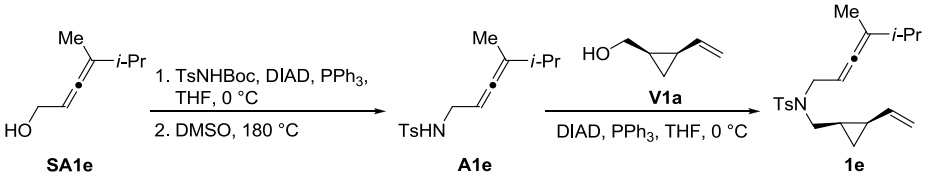
Substrate (1d)



To a stirred solution of **V1a** (198 mg, 2.02 mmol), tosylamide **A1d**[6] (589 mg, 2.22 mmol), and PPh_3 (1.05 g, 4.00 mmol) in anhydrous THF (10 mL) was added DIAD (809 mg, 4.00 mmol) at 0 ℃ under N_2. The mixture was then stirred for 2 h at room temperature. The reaction mixture was concentrated and the crude product was purified by flash column chromatography on silica gel (eluted with PE/EA 50:1 then 20:1) to afford product **1d** (532 mg, 76%).

1d: colorless oil, TLC R_f = 0.63 (PE/EA, 5:1). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.71 (d, J = 8.3 Hz, 2H), 7.28 (d, J = 8.3 Hz, 2H), 5.58–5.47 (m, 1H), 5.15–5.09 (m, 1H), 5.03–4.96 (m, 1H), 4.87–4.78 (m, 1H), 3.99–3.91 (m, 1H), 3.91–3.78 (m, 1H), 3.38–3.24 (m, 1H), 3.21–3.08 (m, 1H), 2.41 (s, 3H), 1.92 (qd, J = 7.4, 2.8 Hz, 2H), 1.65 (d, J = 2.8 Hz, 3H), 1.60–1.52 (m, 1H), 1.26–1.16 (m, 1H), 0.96 (t, J = 7.4 Hz, 3H), 0.94–0.88 (m, 1H), 0.46–0.39 (m, 1H). ^{13}C NMR (101 MHz, $CDCl_3$): δ 202.22 & 202.18, 142.9, 137.9 & 137.8, 136.73 & 136.69 (+), 129.6 (+), 127.13 & 127.12 (+), 115.4 & 115.3 (–), 102.91 & 102.90, 86.56 & 86.54 (+), 47.0 & 46.8 (–), 46.2 & 46.1 (–), 26.89 & 26.86 (–), 21.5 (+), 19.9 & 19.6 (+), 18.78 & 18.75 (+), 17.1 & 16.9 (+), 12.18 & 12.16 (+), 11.9 & 11.7 (–). IR (KBr): υ 2971, 1449, 1340, 1158, 1095, 902 cm^{-1}. HRMS (ESI) calcd for $C_{20}H_{28}NO_2S$ ([M+H]$^+$): 346.1835. Found: 346.1837.

Substrate (1e)



To a stirred solution of **SA1e**[7] (265 mg, 2.10 mmol), TsNHBoc (684 mg, 2.52 mmol), and PPh_3 (1.10 g, 4.19 mmol) in anhydrous THF (10 mL) was added DIAD (850 mg, 4.20 mmol) at 0 ℃ under N_2. The mixture was then stirred for 4 h at room temperature. The reaction mixture was concentrated and the crude product was purified by flash column chromatography on silica gel (eluted with PE/EA 20:1) to afford intermediate, which was used directly in the following step.

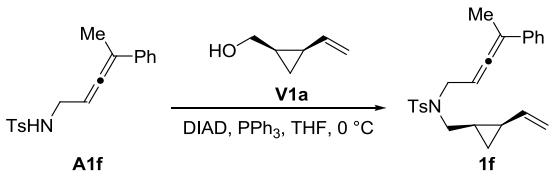
A stirred solution of the above intermediate in DMSO (20 mL) was immersed in a preheated oil bath at 180 ℃ for 20 min. The mixture was cooled to rt and diluted with ether. The solution was washed 5 times with water, and dried over $MgSO_4$. After removing the solvent, the crude product was purified by flash column chromatography on silica gel (eluted with PE/EA 10:1 then 5:1) to afford tosylamide **A1e** (386 mg, 66%, 2 steps).

A1e: light yellow oil, TLC R_f = 0.40 (PE/EA, 5:1). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.75 (d, J = 8.3 Hz, 2H), 7.31 (d, J = 8.3 Hz, 2H), 5.06–4.98 (m, 1H), 4.40 (brs, 1H), 3.50–3.47 (m, 2H), 2.43 (s, 3H), 2.14–2.02 (m, 1H), 1.64 (d, J = 2.8 Hz, 3H), 0.96 (d, J = 6.8 Hz, 6H). ^{13}C NMR (101 MHz, $CDCl_3$): δ 199.6, 143.4, 137.0, 129.7 (+), 127.1 (+), 110.0, 87.7 (+), 42.2 (–), 31.8 (+), 21.6 (+), 21.5 (+), 21.2 (+), 17.2 (+). IR (KBr): υ 3281, 2962, 2926, 2870, 1425, 1327, 1161, 1094 cm^{-1}. HRMS (ESI) calcd for $C_{15}H_{22}NO_2S$ ([M+H]$^+$): 280.1366. Found: 280.1366.

To a stirred solution of **V1a** (94 mg, 0.96 mmol), tosylamide **A1e** (340 mg, 1.22 mmol), and PPh_3 (582 mg, 2.22 mmol) in anhydrous THF (5 mL) was added DIAD (449 mg, 2.22 mmol) at 0 ℃ under N_2. The mixture was then stirred overnight at room temperature. The reaction mixture was concentrated and the crude product was purified by flash column chromatography on silica gel (eluted with PE/EA 20:1) to afford product **1e** (215 mg, 62%).

1e: colorless oil, TLC R_f = 0.73 (PE/EA, 5:1). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.71 (d, J = 8.1 Hz, 2H), 7.28 (d, J = 8.1 Hz, 2H), 5.59–5.47 (m, 1H), 5.17–5.08 (m, 1H), 5.03–4.97 (m, 1H), 4.87–4.78 (m, 1H), 4.00–3.97 (m, 1H), 3.90–3.76 (m, 1H), 3.41–3.23 (m, 1H), 3.23–3.07 (m, 1H), 2.42 (s, 3H), 2.13–2.03 (m, 1H), 1.64 (d, J = 2.7 Hz, 3H), 1.60–1.53 (m, 1H), 1.27–1.14 (m, 1H), 1.00–0.99 (d, J = 2.4 Hz, 3H), 0.97 (d, J = 2.4 Hz, 3H), 0.95–0.89 (m, 1H), 0.46–0.39 (m, 1H). ^{13}C NMR (101 MHz, $CDCl_3$): δ 201.6 & 201.5, 142.9, 137.9 & 137.8, 136.74 & 136.69 (+), 129.6 (+), 127.12 & 127.11 (+), 115.4 & 115.3 (–), 107.24 & 107.20, 86.9 & 86.8 (+), 47.1 & 46.9 (–), 46.23 & 46.18 (–), 31.89 & 31.86 (+), 21.5 (+), 21.41 & 21.40 (+),21.2 (+), 19.9 & 19.6 (+), 17.2 & 17.0 (+), 17.0 & 16.8 (+), 12.0 & 11.7 (–). IR (KBr): υ 2963, 2926, 1452, 1345, 1158, 912 cm^{-1}. HRMS (ESI) calcd for $C_{21}H_{30}NO_2S$ ($[M+H]^+$): 360.1992. Found: 360.1997.

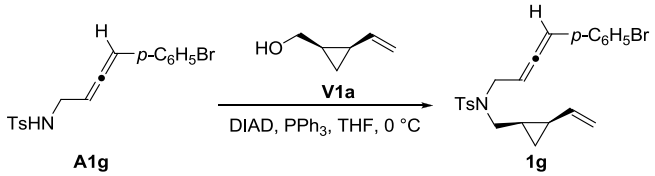
Substrate (1f)



To a stirred solution of **V1a** (190 mg, 1.94 mmol), tosylamide **A1f**[8] (704 mg, 2.25 mmol), and PPh_3 (1.05 g, 4.00 mmol) in anhydrous THF (10 mL) was added DIAD (808 mg, 4.00 mmol) at 0 ℃ under N_2. The mixture was then stirred for 3 h at room temperature. The reaction mixture was concentrated and the crude product was purified by flash column chromatography on silica gel (eluted with PE/EA 20:1) to afford product **1f** (447 mg, 58%).

1f: colorless oil, TLC R_f = 0.65 (PE/EA, 5:1). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.72 (d, J = 8.1 Hz, 2H), 7.34–7.26 (m, 6H), 7.24–7.17 (m, 1H), 5.51–5.32 (m, 1H), 5.30–5.21 (m, 1H), 5.12–5.02 (m, 1H), 4.98–4.89 (m, 1H), 4.17–3.89 (m, 2H), 3.36–3.26 (m, 1H), 3.25–3.10 (m, 1H), 2.41 (s, 3H), 2.10–2.00 (m, 3H), 1.57–1.47 (m, 1H), 1.21–1.09 (m, 1H), 0.92–0.83 (m, 1H), 0.41–0.30 (m, 1H). ^{13}C NMR (101 MHz, $CDCl_3$): δ 205.3 & 205.2, 143.1, 137.7, 136.58 & 136.56 (+), 136.4 & 136.3, 129.6 (+), 128.35 & 128.34 (+), 127.1 (+), 127.0 (+), 125.8 & 125.7 (+), 115.44 & 115.39 (–), 102.13 & 102.10, 89.0 & 88.9 (+), 46.5 & 46.4 (–), 46.2 & 46.1 (–), 21.5 (+), 19.63 & 19.60 (+), 17.02 & 16.96 (+), 16.94 & 16.93 (+), 11.72 & 11.66 (–). IR (KBr): υ 2922, 1447, 1339, 1157, 1093, 903 cm^{-1}. HRMS (ESI) calcd for $C_{24}H_{28}NO_2S$ ($[M+H]^+$): 394.1835. Found: 394.1839.

Substrate (1g)

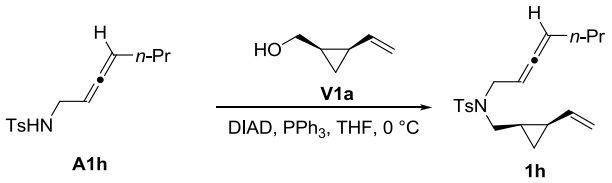


To a stirred solution of **V1a** (149 mg, 1.52 mmol), tosylamide **A1g**[9] (630 mg, 1.66 mmol),

and PPh_3 (798 mg, 3.04 mmol) in anhydrous THF (10 mL) was added DIAD (615 mg, 3.04 mmol) at 0 ℃ under N_2. The mixture was then stirred for 4 h at room temperature. The reaction mixture was concentrated and the crude product was purified by flash column chromatography on silica gel (eluted with PE/EA 20:1) to afford product **1g** (447 mg, 64%).

1g: yellow oil, TLC R_f = 0.50 (PE/EA, 5:1). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.74–7.69 (m, 2H), 7.44–7.37 (m, 2H), 7.31–7.26 (m, 2H), 7.11–7.03 (m, 2H), 6.13–6.01 (m, 1H), 5.52–5.35 (m, 2H), 5.15–5.04 (m, 1H), 5.01–4.91 (m, 1H), 4.13–3.95 (m, 2H), 3.30–3.12 (m, 2H), 2.42 (s, 3H), 1.60–1.50 (m, 1H), 1.21–1.11 (m, 1H), 0.95–0.85 (m, 1H), 0.44–0.30 (m, 1H). ^{13}C NMR (101 MHz, $CDCl_3$): δ 206.03 & 205.95, 143.2, 137.5, 136.42 & 136.39 (+), 132.6, 131.8 (+), 129.7 (+), 128.3 (+), 127.2 (+), 121.0, 115.63 & 115.61 (–), 95.32 & 95.27 (+), 91.7 & 91.6 (+), 46.7 & 46.6 (–), 45.7 & 45.6 (–), 21.5 (+), 19.71 & 19.68 (+), 17.1 & 16.9 (+), 11.53 & 11.50 (–). IR (KBr): υ 3299, 3071, 3001, 2924, 2866, 2255, 1951, 1635, 1597, 1489, 1341, 1157 cm^{-1}. HRMS (ESI) calcd for $C_{23}H_{25}BrNO_2S$ ($[M+H]^+$): 458.0784. Found: 458.0785.

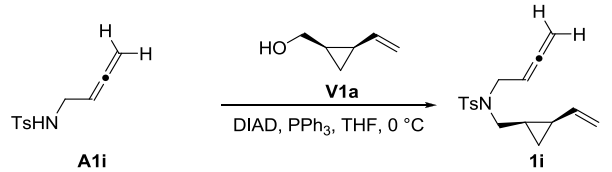
Substrate (1h)



To a stirred solution of **V1a** (199 mg, 2.03 mmol), tosylamide **A1h**[10] (584 mg, 2.20 mmol), and PPh_3 (1.05 g, 4.00 mmol) in anhydrous THF (10 mL) was added DIAD (814 mg, 4.02 mmol) at 0 ℃ under N_2. The mixture was then stirred for 4 h at room temperature. The reaction mixture was concentrated and the crude product was purified by flash column chromatography on silica gel (eluted with PE/EA 20:1) to afford product **1h** (506 mg, 72%).

1h: yellow oil, TLC R_f = 0.61 (PE/EA, 5:1). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.70 (d, J = 8.2 Hz, 2H), 7.28 (d, J = 8.2 Hz, 2H), 5.59–5.47 (m, 1H), 5.16–5.05 (m, 2H), 5.04–4.97 (m, 1H), 4.90–4.78 (m, 1H), 4.02–3.80 (m, 2H), 3.36–3.24 (m, 1H), 3.19–3.06 (m, 1H), 2.42 (s, 3H), 1.99–1.86 (m, 2H), 1.65–1.51 (m, 1H), 1.44–1.32 (m, 2H), 1.25–1.15 (m, 1H), 0.97–0.85 (m, 1H), 0.90 (t, J = 7.4 Hz, 3H) 0.47–0.38 (m, 1H). ^{13}C NMR (101 MHz, $CDCl_3$): δ 205.1 & 205.0, 143.0, 137.8, 136.7 & 136.6 (+), 129.6 (+), 127.1 (+), 115.41 & 115.40 (–), 92.34 & 92.33 (+), 86.7 & 86.6 (+), 46.6 & 46.5 (–), 46.3 & 46.2 (–), 30.7 & 30.6 (–), 22.4 & 22.3 (–), 21.5 (+), 19.8 & 19.7 (+), 17.2 & 17.0 (+), 13.58 & 13.57 (+), 11.8 & 11.6 (–). IR (KBr): υ 3074, 2960, 2870, 1962, 1635, 1451, 1345, 1158, 1093 cm^{-1}. HRMS (ESI) calcd for $C_{20}H_{28}NO_2S$ ($[M+H]^+$): 346.1835. Found: 346.1836.

Substrate (1i)

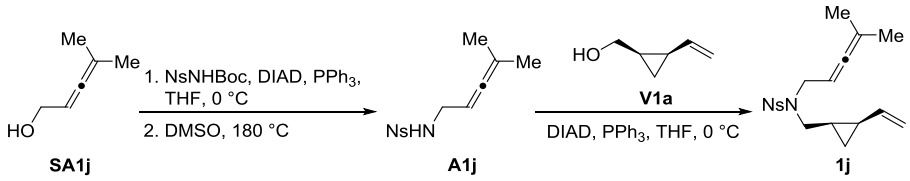


To a stirred solution of **V1a** (200 mg, 2.04 mmol), tosylamide **A1i**[11] (491 mg, 2.20 mmol), and PPh_3 (1.05 g, 4.00 mmol) in anhydrous THF (10 mL) was added DIAD (809 mg, 4.00 mmol)

at 0 ℃ under N_2. The mixture was then stirred for 2 h at room temperature. The reaction mixture was concentrated and the crude product was purified by flash column chromatography on silica gel (eluted with PE/EA 20:1) to afford product **1i** (339 mg, 55%).

1i: light yellow oil, TLC R_f = 0.61 (PE/EA, 5:1). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.70 (d, J = 8.3 Hz, 2H), 7.29 (d, J = 8.3 Hz, 2H), 5.54 (ddd, J = 17.0, 10.2, 8.5 Hz, 1H), 5.12 (ddd, J = 17.0, 1.6, 0.8 Hz, 1H), 5.01 (dd, J = 10.2, 1.6 Hz, 1H), 4.95–4.86 (m, 1H), 4.74–4.67 (m, 2H), 4.04–3.86 (m, 2H), 3.28 (dd, J = 14.5, 6.3 Hz, 1H), 3.16 (dd, J = 14.5, 7.8 Hz, 1H), 2.42 (s, 3H), 1.63–1.54 (m, 1H), 1.26–1.15 (m, 1H), 0.99–0.89 (m, 1H), 0.47–0.38 (m, 1H). ^{13}C NMR (101 MHz, $CDCl_3$): δ 209.2, 143.1, 137.6, 136.6 (+), 129.6 (+), 127.1 (+), 115.5 (–), 86.2 (+), 76.2 (–), 46.4 (–), 45.8 (–), 21.5 (+), 19.8 (+), 17.1 (+), 11.5 (–). IR (KBr): υ 3069, 3000, 2925, 2867, 1955, 1634, 1446, 1341, 1157, 1092 cm^{-1}. HRMS (ESI) calcd for $C_{17}H_{22}NO_2S$ ($[M+H]^+$): 304.1366. Found: 304.1362.

Substrate (1j)



To a stirred solution of **SA1j**[12] (488 mg, 4.97 mmol), NsNHBoc[13] (1.81 g, 5.99 mmol), and PPh_3 (2.62 g, 10 mmol) in anhydrous THF (25 mL) was added DIAD (2.02 g, 10 mmol) at 0 ℃ under N_2. The mixture was then stirred for 3 h at room temperature. The reaction mixture was concentrated and the crude product was purified by flash column chromatography on silica gel (eluted with PE/EA 20:1, then 10:1, then 5:1) to afford intermediate, which was used directly in the following step.

A stirred solution of the above intermediate in DMSO (42 mL) was immersed in a preheated oil bath at 180 ℃ for 20 min. The mixture was cooled to rt and diluted with ether. The solution was washed 5 times with water, and dried over $MgSO_4$. After removing the solvent, the crude product was purified by flash column chromatography on silica gel (eluted with PE/EA 10:1 then 5:1) to afford tosylamide **A1j** (939 mg, 80%, 2 steps).

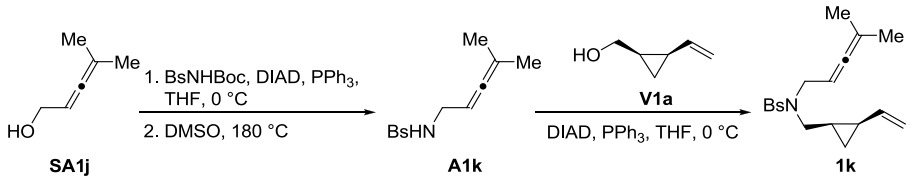
A1j: light yellow solid, m.p. = 72–74 ℃, TLC R_f = 0.52 (PE/EA, 3:1). ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.37 (d, J = 8.9 Hz, 2H), 8.06 (d, J = 8.9 Hz, 2H), 4.98–4.87 (m, 1H), 4.65 (t, J = 5.4 Hz, 1H), 3.65–3.54 (m, 2H), 1.65 (d, J = 2.9 Hz, 6H). ^{13}C NMR (101 MHz, $CDCl_3$): δ 201.1, 150.0, 146.1, 128.3 (+), 124.4 (+), 100.0, 85.3 (+), 77.0, 42.2 (–), 20.4 (+). IR (KBr): υ 3294, 3107, 2913, 1531, 1411, 1348, 1164, 1095, 854 cm^{-1}. HRMS (EI) calcd for $C_{12}H_{14}O_4N_2S$ ($[M]^+$): 282.0669. Found: 282.0668.

To a stirred solution of **V1a** (200 mg, 2.04 mmol), tosylamide **A1j** (621 mg, 2.20 mmol), and PPh_3 (1.05 g, 4.00 mmol) in anhydrous THF (10 mL) was added DIAD (809 mg, 4.00 mmol) at 0 ℃ under N_2. The mixture was then stirred overnight at room temperature. The reaction mixture was concentrated and the crude product was purified by flash column chromatography on silica gel (eluted with PE/EA 20:1) to afford product **1j** (502 mg, 68%).

1j: light yellow oil, TLC R_f = 0.47 (PE/EA, 5:1). ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.34 (d, J = 8.9 Hz, 2H), 8.01 (d, J = 8.9 Hz, 2H), 5.53 (ddd, J = 17.0, 10.2, 8.4 Hz, 1H), 5.14 (ddd, J = 17.0, 1.6, 0.7 Hz, 1H), 5.03 (dd, J = 10.2, 1.6 Hz, 1H), 4.77–4.67 (m, 1H), 4.02–3.89 (m, 2H), 3.34 (dd, J =

14.6, 6.3 Hz, 1H), 3.23 (dd, *J* = 14.6, 7.8 Hz, 1H), 1.65 (s, 3H), 1.64 (s, 3H), 1.62–1.56 (m, 1H), 1.22–1.12 (m, 1H), 0.99–0.92 (m, 1H), 0.48–0.40 (m, 1H). ^{13}C NMR (101 MHz, $CDCl_3$): δ 203.2, 149.8, 146.9, 136.2 (+), 128.2 (+), 124.3 (+), 115.8 (–), 97.4, 84.2 (+), 46.7 (–), 46.3 (–), 20.27 (+), 20.26 (+), 19.7 (+), 16.8 (+), 11.5 (–). IR (KBr): υ 3105, 3078, 2982, 2914, 2868, 1968, 1724, 1531, 1448, 1349, 1159, 1093 cm^{-1}. HRMS (ESI) calcd for $C_{18}H_{23}N_2O_4S$ ([M+H]$^+$): 363.1373. Found: 363.1373.

Substrate (1k)



To a stirred solution of **SA1j** (490 mg, 4.99 mmol), BsNHBoc[14] (2.02 g, 6.00 mmol), and PPh_3 (2.62 g, 10 mmol) in anhydrous THF (25 mL) was added DIAD (2.02 g, 10 mmol) at 0 ℃ under N_2. The mixture was then stirred overnight at room temperature. The reaction mixture was concentrated and the crude product was purified by flash column chromatography on silica gel (eluted with PE/EA 20:1) to afford intermediate, which was used directly in the following step.

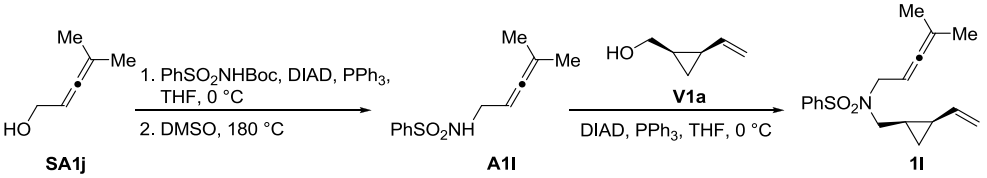
A stirred solution of the above intermediate in DMSO (50 mL) was immersed in a preheated oil bath at 180 ℃ for 20 min. The mixture was cooled to rt and diluted with ether. The solution was washed 5 times with water, and dried over $MgSO_4$. After removing the solvent, the crude product was purified by flash column chromatography on silica gel (eluted with PE/EA 10:1 then 5:1) to afford tosylamide **A1k** (1.29 g, 81%, 2 steps).

A1k: white solid, m.p. = 82–85 ℃, TLC R_f = 0.27 (PE/EA, 5:1). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.74 (d, *J* = 8.7 Hz, 2H), 7.66 (d, *J* = 8.7 Hz, 2H), 4.96–4.86 (m, 1H), 4.50 (t, *J* = 5.4 Hz, 1H), 3.57–3.49 (m, 2H), 1.64 (d, *J* = 2.9 Hz, 6H). ^{13}C NMR (101 MHz, $CDCl_3$): δ 201.0, 139.2, 132.4 (+), 128.7 (+), 127.6, 99.8, 85.5 (+), 42.1 (–), 20.4 (+). IR (KBr): υ 3263, 2979, 2909, 2854, 1575, 1468, 1404, 1337, 1165 cm^{-1}. HRMS (ESI) calcd for $C_{12}H_{15}BrNO_2S$ ([M+H]$^+$): 316.0001. Found: 315.9994.

To a stirred solution of **V1a** (196 mg, 2.00 mmol), tosylamide **A1k** (696 mg, 2.20 mmol), and PPh_3 (1.05 g, 4.00 mmol) in anhydrous THF (10 mL) was added DIAD (809 mg, 4.00 mmol) at 0 ℃ under N_2. The mixture was then stirred overnight at room temperature. The reaction mixture was concentrated and the crude product was purified by flash column chromatography on silica gel (eluted with PE/EA 50:1 then 20:1) to afford product **1k** (541 mg, 68%).

1k: colorless oil, TLC R_f = 0.73 (PE/EA, 5:1). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.71–7.66 (m, 2H), 7.65–7.60 (m, 2H), 5.53 (ddd, *J* = 17.0, 10.2, 8.5 Hz, 1H), 5.13 (ddd, *J* = 17.0, 1.7, 0.7 Hz, 1H), 5.02 (dd, *J* = 10.2, 1.7 Hz, 1H), 4.77–4.68 (m, 1H), 3.93 (dd, *J* = 14.5, 6.1 Hz, 1H), 3.88 (dd, *J* = 14.5, 6.0 Hz, 1H), 3.30 (dd, *J* = 14.5, 6.2 Hz, 1H), 3.16 (dd, *J* = 14.5, 7.9 Hz, 1H), 1.65 (s, 3H), 1.64 (s, 3H), 1.62–1.54 (m, 1H), 1.23–1.15 (m, 1H), 0.98–0.91 (m, 1H), 0.46–0.39 (m, 1H). ^{13}C NMR (101 MHz, $CDCl_3$): δ 203.1, 140.0, 136.5 (+), 132.2 (+), 128.6 (+), 127.1, 115.6 (–), 97.0, 84.4 (+), 46.7 (–), 46.2 (–), 20.32 (+), 20.31 (+), 19.7 (+), 16.9 (+), 11.6 (–). IR (KBr): υ 3080, 2984, 2922, 2863, 1457, 1344, 1161, 1082 cm^{-1}. HRMS (ESI) calcd for $C_{18}H_{23}BrNO_2S$ ([M+H]$^+$): 396.0627. Found: 396.0638.

Substrate (1l)



To a stirred solution of **SA1j** (490 mg, 4.99 mmol), $PhSO_2NHBoc$[15] (1.54 g, 5.98 mmol), and PPh_3 (2.62 g, 10 mmol) in anhydrous THF (25 mL) was added DIAD (2.02 g, 10 mmol) at 0 ℃ under N_2. The mixture was then stirred overnight at room temperature. The reaction mixture was concentrated and the crude product was purified by flash column chromatography on silica gel (eluted with PE/EA 20:1 then 10:1) to afford intermediate, which was used directly in the following step.

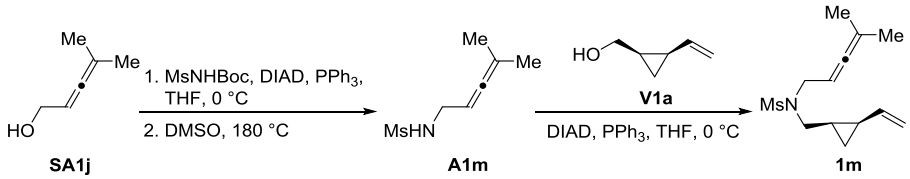
A stirred solution of the above intermediate in DMSO (50 mL) was immersed in a preheated oil bath at 180 ℃ for 20 min. The mixture was cooled to rt and diluted with ether. The solution was washed 5 times with water, and dried over $MgSO_4$. After removing the solvent, the crude product was purified by flash column chromatography on silica gel (eluted with PE/EA 5:1 then 3:1) to afford tosylamide **A1l** (909 mg, 77%, 2 steps).

A1l: white solid, m.p. = 82–85 ℃, TLC R_f = 0.27 (PE/EA, 5:1). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.92–7.82 (m, 2H), 7.62–7.47 (m, 3H), 4.99–4.84 (m, 1H), 4.53 (brs, 1H), 3.61–3.44 (m, 2H), 1.63 (d, J = 2.9 Hz, 6H). ^{13}C NMR (101 MHz, $CDCl_3$): δ 201.0, 140.0, 132.6 (+), 129.1 (+), 127.1 (+), 99.5, 85.6 (+), 42.1 (–), 20.4 (+). IR (KBr): υ 3267, 2987, 2913, 1450, 1411, 1324, 1159, 1093 cm^{-1}. HRMS (ESI) calcd for $C_{12}H_{16}NO_2S$ ($[M+H]^+$): 238.0896. Found: 238.0898.

To a stirred solution of **V1a** (186 mg, 1.90 mmol), tosylamide **A1l** (521 mg, 2.20 mmol), and PPh_3 (1.05 g, 4.00 mmol) in anhydrous THF (10 mL) was added DIAD (809 mg, 4.00 mmol) at 0 ℃ under N_2. The mixture was then stirred overnight at room temperature. The reaction mixture was concentrated and the crude product was purified by flash column chromatography on silica gel (eluted with PE/EA 50:1 then 20:1) to afford product **1l** (379 mg, 63%).

1l: yellow oil, TLC R_f = 0.70 (PE/EA, 5:1). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.86–7.80 (m, 2H), 7.58–7.45 (m, 3H), 5.53 (ddd, J = 17.0, 10.2, 8.5 Hz, 1H), 5.12 (ddd, J = 17.0, 1.7, 0.7 Hz, 1H), 5.00 (dd, J = 10.2, 1.7 Hz, 1H), 4.76–4.68 (m, 1H), 3.98–3.85 (m, 2H), 3.32 (dd, J = 14.5, 6.1 Hz, 1H), 3.17 (dd, J = 14.5, 8.0 Hz, 1H), 1.64 (s, 3H), 1.63 (s, 3H), 1.60–1.54 (m, 1H), 1.24–1.16 (m, 1H), 0.97–0.89 (m, 1H), 0.45–0.38 (m, 1H). ^{13}C NMR (101 MHz, $CDCl_3$): δ 203.1, 140.8, 136.6 (+), 132.2 (+), 129.0 (+), 127.0 (+), 115.4 (–), 96.8, 84.6 (+), 46.7 (–), 46.1 (–), 20.33 (+), 20.32 (+), 19.7 (+), 17.0 (+), 11.7 (–). IR (KBr): υ 3071, 2982, 2912, 2864, 1722, 1635, 1447, 1344, 1158, 1094, 979 cm^{-1}. HRMS (ESI) calcd for $C_{18}H_{24}NO_2S$ ($[M+H]^+$): 318.1522. Found: 318.1523.

Substrate (1m)



To a stirred solution of **SA1j** (352 mg, 3.59 mmol), MsNHBoc[16] (839 mg, 4.30 mmol), and PPh_3 (1.89 g, 7.20 mmol) in anhydrous THF (18 mL) was added DIAD (1.45 g, 7.17 mmol) at 0 ℃ under N_2. The mixture was then stirred overnight at room temperature. The reaction mixture was concentrated and the crude product was purified by flash column chromatography on silica gel (eluted with PE/EA 20:1 then 10:1) to afford intermediate, which was used directly in the following step.

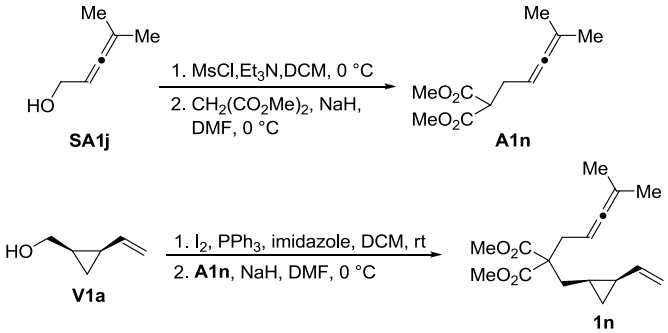
A stirred solution of the above intermediate in DMSO (35 mL) was immersed in a preheated oil bath at 180 ℃ for 20 min. The mixture was cooled to rt and diluted with ether. The solution was washed 5 times with water, and dried over $MgSO_4$. After removing the solvent, the crude product was purified by flash column chromatography on silica gel (eluted with PE/EA 2:1) to afford tosylamide **A1m** (365 mg, 58%, 2 steps).

A1m: colorless oil, TLC R_f = 0.18 (PE/EA, 3:1). ^{1}H NMR (400 MHz, $CDCl_3$): δ 5.12–5.03 (m, 1H), 4.39 (brs, 1H), 3.74–3.64 (m, 2H), 2.97 (s, 3H), 1.72 (d, J = 2.9 Hz, 6H). ^{13}C NMR (101 MHz, $CDCl_3$): δ 201.1, 99.7, 86.2 (+), 42.1 (–), 40.9 (+), 20.5 (+). IR (KBr): υ 3286, 2982, 2913, 1437, 1410, 1317, 1151 cm^{-1}. HRMS (ESI) calcd for $C_7H_{14}NO_2S$ ($[M+H]^+$): 176.0740. Found: 176.0741.

To a stirred solution of **V1a** (180 mg, 1.83 mmol), tosylamide **A1m** (360 mg, 2.05 mmol), and PPh_3 (970 mg, 3.70 mmol) in anhydrous THF (10 mL) was added DIAD (748 mg, 3.70 mmol) at 0 ℃ under N_2. The mixture was then stirred for 2.5 h at room temperature. The reaction mixture was concentrated and the crude product was purified by flash column chromatography on silica gel (eluted with PE/EA 20:1) to afford product **1m** (213 mg, 45%).

1m: light yellow oil, TLC R_f = 0.46 (PE/EA, 5:1). ^{1}H NMR (400 MHz, $CDCl_3$): δ 5.58 (ddd, J = 17.0, 10.2, 8.6 Hz, 1H), 5.16 (ddd, J = 17.0, 1.6, 8.6 Hz, 1H), 5.05 (dd, J = 10.2, 1.6 Hz, 1H), 5.00–4.92 (m, 1H), 3.95 (dd, J = 15.5, 6.6 Hz, 1H), 3.88 (dd, J = 15.5, 6.5 Hz, 1H), 3.31 (dd, J = 14.6, 6.6 Hz, 1H), 3.24 (dd, J = 14.6, 7.5 Hz, 1H), 2.88 (s, 3H), 1.71 (s, 3H), 1.70 (s, 3H), 1.67–1.60 (m, 1H), 1.32–1.24 (dd, J = 13.9, 6.4 Hz, 1H), 1.04–0.96 (m, 1H), 0.52–0.44 (m, 1H). ^{13}C NMR (101 MHz, $CDCl_3$): δ 203.1, 136.6 (+), 115.6 (–), 97.1, 84.6 (+), 46.1 (–), 45.9 (–), 39.9 (+), 20.40 (+), 19.7 (+), 17.1 (+), 11.5 (–). IR (KBr): υ 2982, 2932, 2861, 1332, 1147, 965 cm^{-1}. HRMS (ESI) calcd for $C_{13}H_{22}NO_2S$ ($[M+H]^+$): 256.1366. Found: 256.1370.

Substrate (1n)



To a stirred solution of **SA1j** (740 mg, 7.54 mmol) and Et_3N (1.01 g, 9.98 mmol) in anhydrous DCM (50 mL) was added MsCl (916 mg, 8.00 mmol) dropwise at 0 ℃ under N_2. The resulting mixture was stirred for 1 hour at 0 ℃, and then quenched by saturated $NaHCO_3$ solution.

The layers were separated, and the aqueous layers were extracted with ether. The combined organic layer was washed with brine, dried over $MgSO_4$ and concentrated. The crude product was used directly without further purification.

To a solution of dimethyl malonate (1.98 g, 15.0 mol) in DMF (50 mL) was added NaH (60% purity, 300 mg, 7.5 mmol) and stirred at 0 ℃ for 30 min. Then a solution of the above mesylate product in THF (20 mL) was added and the reaction mixture was allowed to slowly warm to rt and stirred overnight. Saturated aqueous NH_4Cl was added to quench the reaction, and the mixture was extracted with ether. The combined extract was washed with water and brine, dried over $MgSO_4$, and concentrated. After removing the solvent, the crude product was purified by flash column chromatography on silica gel (eluted with PE/EA 50:1 then 20:1) to afford **A1n** (842 mg, 53%, 2 steps).

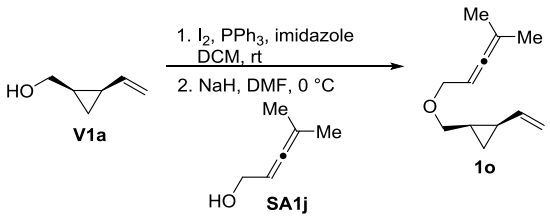
A1n: colorless oil, TLC R_f = 0.50 (PE/EA, 5:1). ^{1}H NMR (400 MHz, $CDCl_3$): δ 5.05–4.96 (m, 1H), 3.74 (s, 6H), 3.51 (t, J = 7.5 Hz, 1H), 2.56 (dd, J = 7.5, 5.8 Hz, 2H), 1.65 (d, J = 2.9 Hz, 6H). ^{13}C NMR (101 MHz, $CDCl_3$): δ 201.7, 169.5, 97.6, 85.5 (+), 52.5 (+), 51.1 (+), 28.2 (–), 20.5 (+). IR (KBr): υ 2982, 2954, 1755, 1738, 1437, 1338, 1275, 1226, 1153 cm^{-1}. HRMS (ESI) calcd for $C_{11}H_{17}O_4$ ($[M+H]^+$): 213.1121. Found: 213.1117.

To a stirred solution of **V1a** (450 mg, 4.59 mmol), PPh_3 (1.44 g, 5.49 mmol) and imidazole (383 mg, 5.62 mmol) in anhydrous DCM (15 mL) was added I_2 (1.71 g, 6.74 mmol) slowly and the resulting mixture was stirred for 1 hour in dark. Saturated aqueous $Na_2S_2O_3$ was added to quench the reaction. The layers were separated, and the aqueous layers were extracted with ether. The combined organic layer was dried over $MgSO_4$ and concentrated. The crude product was used directly without further purification.

To a solution of **A1n** (842 mg, 3.97 mol) in DMF (20 mL) was added NaH (60% purity, 192 mg, 4.80 mmol) and stirred at 0 ℃ for 30 min. Then a solution of the above iodide in DMF (5 mL) was added and the reaction mixture was allowed to slowly warm to rt and stirred overnight. Saturated aqueous NH_4Cl was added to quench the reaction, and the mixture was extracted with ether. The combined extract was washed with water and brine, dried over $MgSO_4$, and concentrated. After removing the solvent, the crude product was purified by flash column chromatography on silica gel (eluted with PE/EA 50:1) to afford **1n** (840 mg, 72%, 2 steps).

1n: colorless oil, TLC R_f = 0.56 (PE/EA, 5:1). ^{1}H NMR (400 MHz, $CDCl_3$): δ 5.54 (ddd, J = 17.0, 10.2, 8.8 Hz, 1H), 5.11 (ddd, J = 17.0, 1.8, 0.5 Hz, 1H), 4.99 (dd, J = 10.2, 1.8 Hz, 1H), 4.82–4.72 (m, 1H), 3.72 (s, 3H), 3.70 (s, 3H), 2.73–2.60 (m, 2H), 2.27–2.14 (m, 1H), 1.81–1.71 (m, 1H), 1.65 (s, 3H), 1.64 (s, 3H) 1.54–1.44 (m, 1H), 0.95–0.82 (m, 2H), 0.27–0.17 (m, 1H). ^{13}C NMR (101 MHz, $CDCl_3$): δ 203.7, 171.7, 171.6, 137.6 (+), 114.7 (–), 95.1, 82.8 (+), 57.9, 52.3 (+), 52.2 (+), 32.9 (–), 31.4 (–), 20.5 (+), 19.2 (+), 13.6 (+), 12.5 (–). IR (KBr): υ 2982, 2951, 1736, 1439, 1288, 1215 cm^{-1}. HRMS (ESI) calcd for $C_{17}H_{24}NaO_4$ ($[M+Na]^+$): 315.1567. Found: 315.1566.

Substrate (1o)

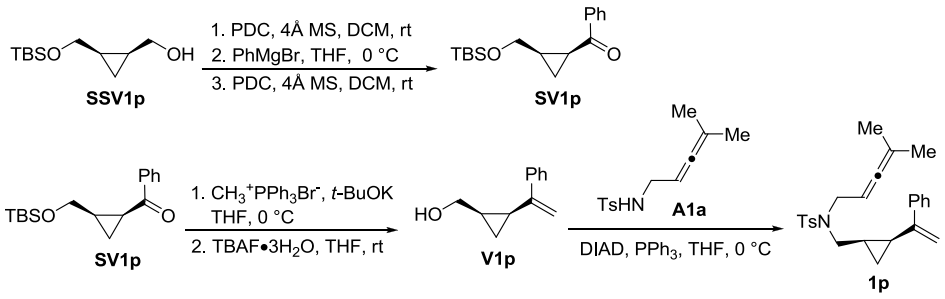


To a stirred solution of **V1a** (282 mg, 2.87 mmol), PPh_3 (906 mg, 3.45 mmol) and imidazole (245 mg, 3.60 mmol) in anhydrous DCM (10 mL) was added I_2 (1.09 g, 4.29 mmol) slowly and the resulting mixture was stirred for 1 hour in dark. Saturated aqueous $Na_2S_2O_3$ was added to quench the reaction. The layers were separated, and the aqueous layers were extracted with ether. The combined organic layer was dried over $MgSO_4$ and concentrated. The crude product was used directly without further purification.

To a solution of S**A1j** (245 mg, 2.50 mol) in DMF (10 mL) was added NaH (60% purity, 120 mg, 3.0 mmol) and stirred at 0 ℃ for 30 min. Then a solution of the above iodide in DMF (4 mL) was added and the reaction mixture was allowed to slowly warm to rt and stirred overnight. Saturated aqueous NH_4Cl was added to quench the reaction, and the mixture was extracted with ether. The combined extract was washed with water and brine, dried over $MgSO_4$, and concentrated. After removing the solvent, the crude product was purified by flash column chromatography on silica gel (eluted with PE/EA 50:1) to afford **1o** (295 mg, 66%, 2 steps).

1o: colorless oil, TLC R_f = 0.44 (PE/EA, 20:1). ^{1}H NMR (400 MHz, $CDCl_3$): δ 5.62 (ddd, J = 17.0, 10.2, 8.3 Hz, 1H), 5.14 (ddd, J = 17.0, 1.8, 0.7 Hz, 1H), 5.09–5.02 (m, 1H), 5.01 (dd, J = 10.2, 1.8 Hz, 1H), 3.99–3.90 (d, J = 6.8 Hz, 2H), 3.49 (dd, J = 10.3, 6.7 Hz, 1H), 3.37 (dd, J = 10.3, 7.7 Hz, 1H), 1.70 (s, 3H), 1.69 (s, 3H), 1.67–1.58 (m, 1H), 1.39–1.26 (m, 1H), 1.01–0.90 (m, 1H), 0.48–0.41 (m, 1H). ^{13}C NMR (101 MHz, $CDCl_3$): δ 202.8, 137.0 (+), 114.9 (–), 95.8, 86.4 (+), 69.3 (–), 69.2 (–), 20.42 (+), 20.41 (+), 19.4 (+), 18.0 (+), 10.6 (–). IR (KBr): υ 2982, 2857, 1635, 1449, 1091, 988, 899 cm^{-1}. HRMS (EI) calcd for $C_{12}H_{18}O$ ([M]$^+$): 178.1352. Found: 178.1349.

Substrate (1p)



The preparation of compound **SV1p** was based on the reported procedure from the Ph.D. thesis of Dr. Ye Siyu[17].

SSV1p[18] (1.64g 7.59 mmol) was dissolved in DCM (25 mL), then PDC (5.26 g, 13.98 mmol) and 4 Å MS (1.0 g) were added successively. The resulting mixture was stirred for 9 h at rt. After the accomplishment of the oxidation reaction, the mixture was filtered and the filtrate was concentrated. To a solution of the above crude product in THF (10 mL) at 0 ℃ was added PhMgBr (1 M, 14 mL, 14 mmol), and the resulting mixture was stirred for 1 h at 0 ℃. After that, saturated aqueous NH_4Cl was added to quench the reaction, and the mixture was extracted with ether. The combined extract was washed with water and brine, dried over Na_2SO_4, and concentrated. The crude product alcohol was dissolved in DCM (25 mL). Then PDC (5.50 g, 14.62 mmol) and 4 Å MS (1.0 g) were added successively. The resulting mixture was stirred for 2 h at rt. The mixture was filtered and the filtrate was concentrated. The crude product was purified by flash column chromatography (eluted with PE/EA 80:1) to afford **SV1p** (1.30 g, 59% for 3 steps).

SV1p: colorless oil, TLC R_f = 0.78 (PE/EA, 5:1). ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.05–7.98 (m, 2H), 7.57–7.49 (m, 1H), 7.48–7.39 (m, 2H), 3.89 (dd, J = 11.0, 5.2 Hz, 1H), 3.39 (dd, J = 11.0, 9.2 Hz, 1H), 2.81–2.73 (m, 1H), 1.97–1.83 (m, 1H), 1.49–1.38 (m, 1H), 1.15–1.06 (m, 1H), 0.71 (s, 9H), -0.09 (s, 3H), -0.22 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$): δ 198.1, 138.7, 132.4 (+), 128.3 (+), 128.2 (+), 60.8 (–), 27.3 (+), 25.7 (+), 22.8 (+), 18.1, 11.1 (–), -5.6 (+), -5.7 (+). IR (KBr): υ 2935, 2928, 2857, 1672, 1599, 1581 cm^{-1}. HRMS (ESI) calcd for $C_{17}H_{26}NaO_2Si$ ([M+Na]$^+$): 313.1594. Found: 313.1592.

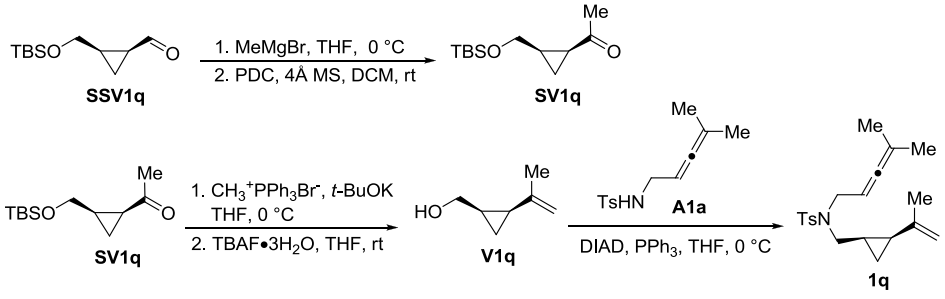
To a mixture of methyltriphenylphosphonium bromide (2.50 g, 7.0 mmol) and *t*-BuOK (713 mg, 6.35 mmol) in round bottle was added THF (20 mL) under an argon atmosphere at 0 ℃, and the resulting solution was stirred for 30 min at 0 ℃. Then a solution of ketone **SV1p** (923 mg, 3.18 mmol) in THF (10 mL) was added dropwise at 0 ℃, and the resulting mixture was stirred for 2 h at room temperature. After that, saturated aqueous NH_4Cl was added to quench the reaction, and the mixture was extracted with ether. The combined extract was washed with water and brine, dried over $MgSO_4$, and concentrated. The crude product was purified by flash column chromatography (eluted with PE/EA, 50:1) to afford intermediate alkene.

The intermediate alkene was dissolved in THF (30 mL) and TBAF $3H_2O$ (2.0 g, 6.34 mmol) was added. The resulting solution was stirred for 18 h at rt. After removing the solvent, the crude product was purified by flash column chromatography on silica gel (eluted with PE/EA 5:1 then 3:1) to afford alcohol **V1p** (526 mg, 95%, 2 steps). The intermediate alcohol was used directly in the next reaction.

To a stirred solution of **V1p** (526 mg, 3.02 mmol), tosylamide **A1a** (829 mg, 3.30 mmol), and PPh_3 (1.57 g, 5.98 mmol) in anhydrous THF (15 mL) was added DIAD (1.21 g, 5.98 mmol) at 0 ℃ under N_2. The mixture was then stirred for 2 h at room temperature. The reaction mixture was concentrated and the crude product was purified by flash column chromatography on silica gel (eluted with PE/EA 20:1) to afford product **1p** (754 mg, 61%).

1p: colorless oil, TLC R_f = 0.53 (PE/EA, 5:1). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.61 (d, J = 8.3 Hz, 2H), 7.56–7.51 (m, 2H), 7.37–7.27 (m, 3H), 7.22 (d, J = 8.3 Hz, 2H), 5.55–5.51 (m, 1H), 5.01–4.98 (m, 1H), 4.71–4.62 (m, 1H), 3.88 (dd, J = 15.1, 6.8 Hz, 1H), 3.79 (dd, J = 15.1, 7.0 Hz, 1H), 3.30 (dd, J = 14.5, 4.4 Hz, 1H), 2.77 (dd, J = 14.5, 9.9 Hz, 1H), 2.39 (s, 3H), 1.95–1.85 (m, 1H), 1.65–1.59 (m, 6H), 1.53–1.44 (m, 1H), 1.01–0.92 (m, 1H), 0.86–0.78 (m, 1H). ^{13}C NMR (101 MHz, $CDCl_3$): δ 203.0, 144.0, 142.8, 141.1, 137.7, 129.5 (+), 128.3 (+), 127.7 (+), 127.1 (+), 125.8 (+), 112.7 (–), 96.6, 84.6 (+), 47.4 (–), 45.9 (–), 21.4 (+), 21.1 (+), 20.4 (+), 20.2 (+), 17.0 (+), 9.3 (–). IR (KBr): υ 2984, 2919, 1966, 1609, 1447, 1338, 1158, 1099 cm^{-1}. HRMS (ESI) calcd for $C_{25}H_{30}NO_2S$ ([M+H]$^+$): 408.1992. Found: 408.1982.

Substrate (1q)



To a solution of **SSV1q**[18] (857 mg, 4.0 mmol) in THF (10 mL) at 0 ℃ was added MeMgBr (3 M, 1.5 mL, 4.5 mmol), and the resulting mixture was stirred for 15 min at 0 ℃. After that, saturated aqueous NH_4Cl was added to quench the reaction, and the mixture was extracted with ether. The combined extract was washed with water and brine, dried over Na_2SO_4. After concentrated, the crude product was purified by flash column chromatography on silica gel (eluted with PE/EA 5:1) and used directly.

The product alcohol was dissolved in DCM (20 mL), then PDC (1.50 g, 3.99 mmol) and 4 Å MS (1.0 g) were added successively. The resulting mixture was stirred for 1 h at rt. The mixture was filtered and the filtrate was concentrated. The crude product was purified by flash column chromatography (eluted with PE/EA 20:1) to afford **SV1q** (374 mg, 41% for 2 steps).

SV1q: colorless oil, TLC R_f = 0.67 (PE/EA, 5:1). ^{1}H NMR (400 MHz, $CDCl_3$): δ 3.84 (dd, J = 11.0, 5.2 Hz, 1H), 3.37 (dd, J = 11.0, 9.4 Hz, 1H), 2.29 (s, 3H), 2.16–2.08 (m, 1H), 1.73–1.61 (m, 1H), 1.20–1.12 (m, 1H), 0.98–0.90 (m, 1H), 0.86 (s, 9H), 0.02 (s, 3H), -0.01 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$): δ 206.2, 60.5 (–), 31.8 (+), 26.7 (+), 25.9 (+), 25.5 (+), 18.3, 11.7 (–), -5.40 (+), -5.44 (+). IR (KBr): υ 2956, 2931, 2858, 1702, 1378, 1255, 1166, 1080 cm^{-1}. HRMS (ESI) calcd for $C_{12}H_{25}O_2Si$ ($[M+H]^+$): 229.1618. Found: 229.1622.

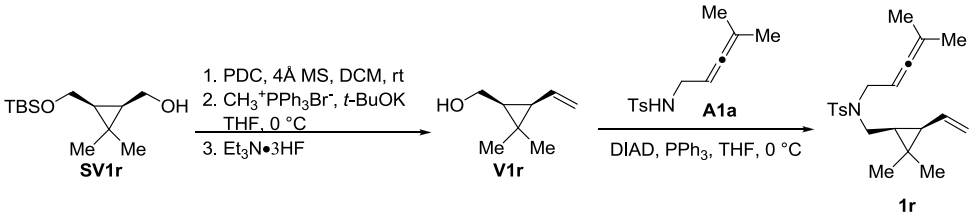
To a mixture of methyltriphenylphosphonium bromide (1.27 g, 3.56 mmol) and *t*-BuOK (361 mg, 3.22 mmol) in round bottle was added THF (16 mL) under an argon atmosphere at 0 ℃, and the resulting solution was stirred for 30 min at 0 ℃. Then a solution of ketone **SV1q** (370 mg, 1.62 mmol) in THF (4 mL) was added dropwise at 0 ℃, and the resulting mixture was stirred for 30 min at room temperature. After that, saturated aqueous NH_4Cl was added to quench the reaction, and the mixture was extracted with ether. The combined extract was washed with water and brine, dried over $MgSO_4$, and concentrated. The crude product was purified by flash column chromatography (eluted with PE/EA, 100:1) to afford intermediate alkene (345 mg, 94%).

The intermediate alkene (259 mg, 1.14 mmol) was dissolved in THF (4.5 mL) and TBAF $3H_2O$ (720 mg, 2.28 mmol) was added. The resulting solution was stirred overnight at rt. After removing the solvent, the crude product was purified by flash column chromatography on silica gel (eluted with PE/EA 5:1) to afford alcohol **V1q** (111 mg, 86%). The intermediate alcohol was used directly in the next reaction.

To a stirred solution of **V1q** (111 mg, 0.99 mmol), tosylamide **A1a** (274 mg, 1.09 mmol), and PPh_3 (524 mg, 2.00 mmol) in anhydrous THF (10 mL) was added DIAD (404 g, 2.00 mmol) at 0 ℃ under N_2. The mixture was then stirred for 2 h at room temperature. The reaction mixture was concentrated and the crude product was purified by flash column chromatography on silica gel (eluted with PE/EA 20:1) to afford product **1q** (196 mg, 57%).

1q: colorless oil, TLC R_f = 0.70 (PE/EA, 5:1). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.69 (d, J = 8.3 Hz, 2H), 7.27 (d, J = 8.3 Hz, 2H), 4.86–4.78 (m, 1H), 4.76–4.66 (m, 1H), 4.62–4.56 (m, 1H), 3.95–3.82 (m, 2H), 3.38 (dd, J = 14.3, 5.0 Hz, 1H), 2.82 (dd, J = 14.3, 9.3 Hz, 1H), 2.41 (s, 3H), 1.79 (s, 3H), 1.67–1.60 (m, 6H), 1.48–1.41 (m, 1H), 1.27–1.17 (m, 1H), 0.80–0.72 (m, 1H), 0.62–0.54 (m, 1H). ^{13}C NMR (101 MHz, $CDCl_3$): δ 203.0, 142.9, 142.1, 137.8, 129.5 (+), 127.1 (+), 111.3 (–), 96.7, 84.7 (+), 47.1 (–), 45.6 (–), 24.4 (+), 22.5 (+), 21.5 (+), 20.4 (+), 20.3 (+), 15.9 (+), 9.0 (–). IR (KBr): υ 3079, 2980, 2915, 1968, 1647, 1599, 1450, 1343, 1157, 1095 cm^{-1}. HRMS (ESI) calcd for $C_{20}H_{28}NO_2S$ ($[M+H]^+$): 346.1835. Found: 346.1829.

Substrate (1r)



Compound **SV1r**[19] (3.66 g, 15.0 mmol) was dissolved in DCM (75 mL), then PDC (8.45 g, 22.5 mmol) and 4 Å MS (3.0 g) were added successively. The resulting mixture was stirred for 4 h at rt. The mixture was filtered and the filtrate was concentrated. The crude product was purified by flash column chromatography (eluted with PE/EA 20:1) to afford aldehyde and used directly.

To a mixture of methyltriphenylphosphonium bromide (5.71 g, 16.0 mmol) and *t*-BuOK (1.68 g, 15.0 mmol) in round bottle was added THF (50 mL) under an argon atmosphere at 0 ℃, and the resulting solution was stirred for 20 min at 0 ℃. Then a solution of the above aldehyde in THF (20 mL) was added dropwise at 0 ℃, and the resulting mixture was stirred for 2 h at room temperature. After that, saturated aqueous NH_4Cl was added to quench the reaction, and the mixture was extracted with ether. The combined extract was washed with water and brine, dried over $MgSO_4$, and concentrated. The crude product was purified by flash column chromatography (eluted with PE/EA, 50:1) to afford intermediate alkene (1.70 g, 47% for 2 steps).

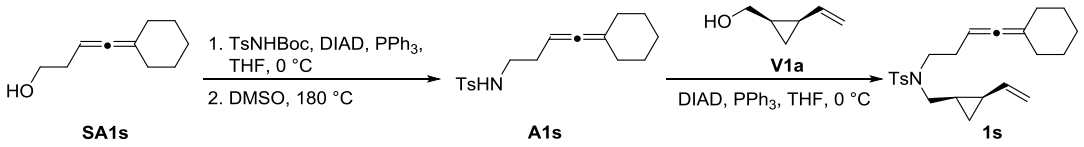
The intermediate alkene (1.70 g, 7.07 mmol) was dissolved in THF (14 mL) and Et_3N 3HF (1.40 g, 8.68 mmol) was added. The resulting solution was stirred overnight at rt. After removing the solvent, the crude product was purified by flash column chromatography on silica gel (eluted with PE/EA 3:1 then 2:1) to afford alcohol **V1r** (693 mg, 78%).

V1r: colorless oil, TLC R_f = 0.25 (PE/EA, 5:1). ^{1}H NMR (400 MHz, $CDCl_3$): δ 5.68–5.56 (m, 1H), 5.21 (dd, J = 16.9, 2.0 Hz, 1H), 5.06 (dd, J = 10.3, 2.0 Hz, 1H), 3.77 (dd, J = 11.6, 7.6 Hz, 1H), 3.69 (dd, J = 11.6, 8.1 Hz, 1H), 1.48–1.40 (m, 1H), 1.41 (brs, 1H), 1.20–1.14 (m, 1H), 1.13 (s, 3H), 1.12 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$): δ 134.4 (+), 116.1 (–), 60.2 (–), 32.2 (+), 31.4 (+), 28.7 (+), 22.0, 15.4 (+). IR (KBr): υ 3334, 2989, 2948, 2868, 1632, 1454, 1377, 1020, 897 cm^{-1}. HRMS (EI) calcd for $C_8H_{14}O$ ($[M+H]^+$): 126.1039. Found: 126.1039.

To a stirred solution of **V1r** (127 mg, 1.01 mmol), tosylamide **A1a** (301 mg, 1.20 mmol), and PPh_3 (525 mg, 2.00 mmol) in anhydrous THF (10 mL) was added DIAD (404 g, 2.00 mmol) at 0 ℃ under N_2. The mixture was then stirred for 6 h at room temperature. The reaction mixture was concentrated and the crude product was purified by flash column chromatography on silica gel (eluted with PE/EA 20:1) to afford product **1r** (276 mg, 76%).

1r: colorless oil, TLC R_f = 0.67 (PE/EA, 5:1). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.71 (d, J = 8.3 Hz, 2H), 7.28 (d, J = 8.3 Hz, 2H), 5.56–5.44 (m, 1H), 5.15 (dd, J = 16.9, 1.9 Hz, 1H), 5.02 (dd, J = 10.3, 2.0 Hz, 1H), 4.71–4.63 (m, 1H), 3.88 (dd, J = 15.5, 6.7 Hz, 1H), 3.81 (dd, J = 15.5, 6.8 Hz, 1H), 3.35 (dd, J = 14.4, 7.3 Hz, 1H), 3.24 (dd, J = 14.4, 6.7 Hz, 1H), 2.41 (s, 3H), 1.66–1.60 (m, 6H), 1.40–1.33 (m, 1H), 1.07 (s, 3H), 1.05 (s, 3H), 1.03–0.97 (m, 1H). ^{13}C NMR (101 MHz, $CDCl_3$): δ 202.9, 142.9, 137.8, 134.3 (+), 129.6 (+), 127.1 (+), 116.0 (–), 96.7, 84.7 (+), 46.3 (–), 43.0 (–), 31.2 (+), 28.4 (+), 28.1 (+), 21.5 (+), 21.4, 20.3 (+), 20.3 (+), 15.5 (+). IR (KBr): υ 2981, 2942, 2866, 1452, 1344, 1159, 1095 cm^{-1}. HRMS (ESI) calcd for $C_{21}H_{30}NO_2S$ ($[M+H]^+$): 360.1991. Found: 360.1998.

Substrate (1s)



To a stirred solution of **SA1s**[20] (609 mg, 4.00 mmol), TsNHBoc (1.19 g, 4.39 mmol), and PPh_3 (2.10 g, 8.01 mmol) in anhydrous THF (20 mL) was added DIAD (1.62 g, 8.01 mmol) at 0 ℃ under N_2. The mixture was then stirred overnight at room temperature. The reaction mixture was concentrated and the crude product was purified by flash column chromatography on silica gel (eluted with PE/EA 20:1 then 10:1) to afford intermediate.

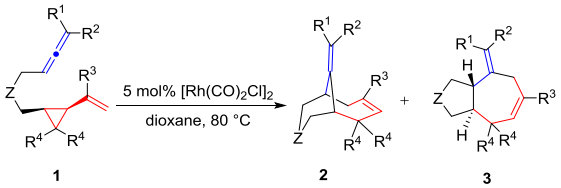
A stirred solution of the achieved intermediate in DMSO (40 mL) was immersed in a preheated oil bath at 180 ℃ for 20 min. The mixture was cooled to rt and diluted with ether. The solution was washed 5 times with water, and dried over $MgSO_4$. After removing the solvent, the crude product was purified by flash column chromatography on silica gel (eluted with PE/EA 5:1) to afford tosylamide **A1s** (1.10 g, 90%, 2 steps).

A1s: colorless oil, TLC R_f = 0.32 (PE/EA, 5:1). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.75 (d, J = 8.2 Hz, 2H), 7.31 (d, J = 8.2 Hz, 2H), 4.90–4.77 (m, 1H), 4.59 (t, J = 6.0 Hz, 1H), 3.08–2.97 (m, 2H), 2.43 (s, 3H), 2.15–2.00 (m, 6H), 1.64–1.45 (m, 6H). ^{13}C NMR (101 MHz, $CDCl_3$): δ 198.8, 143.3, 137.0, 129.6 (+), 127.1 (+), 103.8, 84.9 (+), 42.4 (–), 31.5 (–), 29.0 (–), 27.2 (–), 25.9 (–), 21.5 (+). IR (KBr): υ 3281, 2927, 2853, 1444, 1327, 1161, 1094 cm^{-1}. HRMS (ESI) calcd for $C_{17}H_{24}NO_2S$ ($[M+H]^+$): 306.1522. Found: 306.1525.

To a stirred solution of **V1a** (99 mg, 1.01 mmol), tosylamide **A1s** (366 mg, 1.20 mmol), and PPh_3 (524 mg, 2.00 mmol) in anhydrous THF (5 mL) was added DIAD (404 mg, 2.00 mmol) at 0 ℃ under N_2. The mixture was then stirred for 5 h at room temperature. The reaction mixture was concentrated and the crude product was purified by flash column chromatography on silica gel (eluted with PE/EA 20:1) to afford product **1s** (217 mg, 56%).

1s: colorless oil, TLC R_f = 0.56 (PE/EA, 5:1). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.69 (d, J = 8.3 Hz, 2H), 7.28 (d, J = 8.3 Hz, 2H), 5.54 (ddd, J = 17.0, 10.2, 8.3 Hz, 1H), 5.11 (ddd, J = 17.0, 1.6, 0.7 Hz, 1H), 5.02 (dd, J = 10.2, 1.4 Hz, 1H), 4.91–4.82 (m, 1H), 3.35–3.08 (m, 4H), 2.42 (s, 3H), 2.25–2.14 (m, 2H), 2.12–2.02 (m, 4H), 1.64–1.46 (m, 7H), 1.20–1.07 (m, 1H), 0.97–0.88 (m, 1H), 0.43–0.34 (m, 1H). ^{13}C NMR (101 MHz, $CDCl_3$): δ 198.9, 142.9, 137.5, 136.3 (+), 129.5 (+), 127.1 (+), 115.6 (–), 103.1, 85.1 (+), 47.4 (–), 47.2 (–), 31.6 (–), 28.7 (–), 27.4 (–), 26.1 (–), 21.5 (+), 20.0 (+), 17.4 (+), 11.2 (–). IR (KBr): υ 2927, 2853, 1447, 1341, 1157, 1093 cm^{-1}. HRMS (ESI) calcd for $C_{23}H_{32}NO_2S$ ($[M+H]^+$): 386.2148. Found: 386.2138.

3.2 Bridged [5+2] Cycloaddition

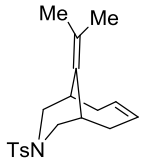


1 2 3

General procedure: A solution of $[Rh(CO)_2Cl]_2$ (3.9 mg, 0.01 mmol, 5 mol%) and substrate (0.20 mmol) in anhydrous dioxane (4 mL, 0.05 M) was continuously stirred at 80 ℃ under N_2 atmosphere. When TLC indicated the disappearance of the starting material, the reaction mixture was cooled to room temperature and concentrated. The crude mixture was submitted to flash column chromatography on silica gel to afford the corresponding product(s).

For substrate **1p** and **1q**, 10 mol% $[Rh(CO)_2Cl]_2$ was used.
For substrate **1p**, the reaction was conducted at 100 ℃.
For substrate **1n**, decomposition was observed when cationic Rh catalyst (10 mol% $[Rh(CO)_2Cl]_2$ + 20 mol% AgOTf) was used.

Product (2a)

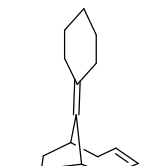


2a

Reaction time: 4 h. Eluted with PE/EA 20:1
Run 1: 66.4 mg **1a** was converted to 52.8 mg **2a**, yield 80%. Run 2: 66.4 mg **1a** was converted to 53.0 mg **2a**, yield 80%. So the average yield of two runs was 80%.

2a: white solid, m.p. = 174–177 ℃, TLC R_f = 0.60 (PE/EA, 5:1). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.59 (d, J = 8.2 Hz, 2H), 7.27 (d, J = 8.2 Hz, 2H), 5.66–5.56 (m, 2H), 3.64 (d, J = 11.1 Hz, 2H), 3.04–2.97 (m, 2H), 2.40 (s, 3H), 2.46–2.34 (m, 4H), 2.34–2.23 (m, 2H), 1.65 (s, 6H). ^{13}C NMR (101 MHz, $CDCl_3$): δ 143.0, 133.0, 131.0, 129.4 (+), 127.6 (+), 127.4 (+), 124.9, 52.5 (–), 35.0 (–), 34.2 (+), 21.4 (+), 19.6 (+). IR (KBr): υ 2924, 2837, 1458, 1339, 1165, 988 cm^{-1}. HRMS (ESI) calcd for $C_{19}H_{26}NO_2S$ ($[M+H]^+$): 332.1679. Found: 332.1678.

Product (2b)

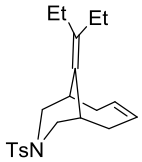


2b

Reaction time: 4 h. Eluted with PE/EA 20:1
Run 1: 74.9 mg **1b** was converted to 53.7 mg **2b**, yield 72%. Run 2: 74.3 mg **1b** was converted to 54.7 mg **2b**, yield 74%. So the average yield of two runs was 73%.

2b: colorless oil, TLC R_f = 0.73 (PE/EA, 5:1). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.59 (d, J = 8.2 Hz, 2H), 7.28 (d, J = 8.2 Hz, 2H), 5.67–5.55 (m, 2H), 3.65 (d, J = 11.1 Hz, 2H), 3.11–3.01 (m, 2H), 2.48–2.34 (m, 4H), 2.40 (s, 3H), 2.31–2.18 (m, 4H), 2.06–1.96 (m, 2H), 1.60–1.35 (m, 6H). ^{13}C NMR (101 MHz, $CDCl_3$): δ 143.0, 134.2, 133.0, 129.4 (+), 127.8, 127.7 (+), 127.3 (+), 52.6 (–), 36.1 (–), 33.6 (+), 30.0 (–), 28.7 (–), 27.0 (–), 21.4 (+). IR (KBr): υ 2924, 2848, 1453, 1342, 1164, 985 cm^{-1}. HRMS (ESI) calcd for $C_{22}H_{30}NO_2S$ ($[M+H]^+$): 372.1991. Found: 372.2003.

Product (2c)



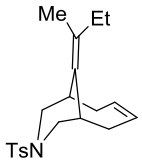
2c

Reaction time: 4 h. Eluted with PE/EA 20:1

Run 1: 72.2 mg **1c** was converted to 53.1 mg **2c**, yield 74%. Run 2: 71.9 mg **1c** was converted to 51.5 mg **2c**, yield 72%. So the average yield of two runs was 73%.

2c: white solid, m.p. = 115–117 ℃, TLC R_f = 0.65 (PE/EA, 5:1). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.59 (d, J = 8.2 Hz, 2H), 7.28 (d, J = 8.2 Hz, 2H), 5.69–5.57 (m, 2H), 3.68 (d, J = 11.1 Hz, 2H), 3.01–2.88 (m, 2H), 2.53–2.44 (m, 2H), 2.41 (s, 3H), 2.37 (dd, J = 11.1, 3.4 Hz, 2H), 2.34–2.24 (m, 2H), 2.00 (qd, J = 7.5, 2.4 Hz, 4H), 0.92 (t, J = 7.5 Hz, 6H). ^{13}C NMR (101 MHz, $CDCl_3$): δ 143.0, 137.5, 133.3, 131.2, 129.4 (+), 127.7 (+), 127.6 (+), 52.7 (–), 34.9 (–), 33.7 (+), 24.3 (–), 21.5 (+), 14.3 (+). IR (KBr): υ 2964, 2930, 2872, 1462, 1339, 1166, 946 cm^{-1}. HRMS (ESI) calcd for $C_{21}H_{30}NO_2S$ ($[M+H]^+$): 360.1992. Found: 360.1989.

Product (2d)



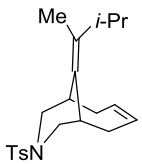
2d

Reaction time: 4 h. Eluted with PE/EA 20:1

Run 1: 69.3 mg **1d** was converted to 55.9 mg **2d**, yield 81%. Run 2: 69.7 mg **1d** was converted to 54.6 mg **2d**, yield 78%. So the average yield of two runs was 80%.

2d: white solid, m.p. = 127–130 ℃, TLC R_f = 0.60 (PE/EA, 5:1). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.59 (d, J = 8.2 Hz, 2H), 7.28 (d, J = 8.2 Hz, 2H), 5.67–5.57 (m, 2H), 3.70–3.60 (m, 2H), 3.04–2.91 (m, 2H), 2.40 (s, 3H), 2.50–2.23 (m, 6H), 2.12–1.90 (m, 2H), 1.64 (s, 3H), 0.92 (t, J = 7.5 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$): δ 143.0, 133.1, 131.0, 130.8, 129.4 (+, Ar), 127.6 (+, Ar & C=C), 127.3 (+, C=C), 52.7 (–), 52.4 (–), 35.4 (–), 34.6 (–), 34.1 (+), 33.9 (+), 26.7 (–), 21.4 (+), 17.1 (+), 13.5 (+). IR (KBr): υ 2967, 2926, 2874, 2831, 1597, 1460, 1336, 1166, 977 cm^{-1}. HRMS (ESI) calcd for $C_{20}H_{28}NO_2S$ ($[M+H]^+$): 346.1835. Found: 346.1834.

Product (2e)



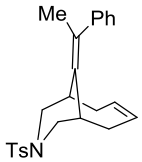
2e

Reaction time: 5 h. Eluted with PE/EA 20:1

Run 1: 72.3 mg **1e** was converted to 55.4 mg **2e**, yield 77%. Run 2: 72.6 mg **1e** was converted to 56.9 mg **2e**, yield 78%. So the average yield of two runs was 78%.

2e: colorless oil, TLC R_f = 0.68 (PE/EA, 5:1). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.59 (d, J = 8.2 Hz, 2H), 7.28 (d, J = 8.2 Hz, 2H), 5.66–5.57 (m, 2H), 3.70–3.60 (m, 2H), 3.15–3.05 (m, 1H), 3.00–2.92 (m, 1H), 2.91–2.80 (m, 1H), 2.41 (s, 3H), 2.50–2.19 (m, 6H), 1.53 (s, 3H), 0.94 (d, J = 6.8 Hz, 3H), 0.89 (d, J = 6.8 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$): δ 143.0, 134.4, 133.0, 129.9, 129.4 (+), 127.6 (+), 127.4 (+), 127.2 (+), 52.7 (–), 52.4 (–), 35.6 (–), 34.6 (–), 34.2 (+), 33.6 (+), 29.1 (+), 21.4 (+), 21.3 (+), 20.9 (+), 11.3 (+). IR (KBr): υ 2962, 2872, 1461, 1341, 1165, 1089, 981 cm^{-1}. HRMS (ESI) calcd for $C_{21}H_{30}NO_2S$ ([M+H]$^+$): 360.1992. Found: 360.1987.

Product (2f)



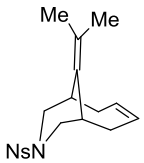
2f

Reaction time: 6 h. Eluted with PE/EA 20:1

Run 1: 79.0 mg **1f** was converted to 47.1 mg **2f**, yield 60%. Run 2: 79.1 mg **1f** was converted to 51.5 mg **2f**, yield 65%. So the average yield of two runs was 62%.

2f: light yellow oil, TLC R_f = 0.51 (PE/EA, 5:1). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.58 (d, J = 8.2 Hz, 2H), 7.31–7.25 (m, 4H), 7.24–7.18 (m, 1H), 7.06–6.98 (m, 2H), 5.74–5.63 (m, 2H), 3.79–3.71 (m, 1H), 3.58–3.43 (m, 1H), 3.15–3.07 (m, 1H), 2.66–2.43 (m, 4H), 2.41 (s, 3H), 2.36–2.27 (m, 2H), 2.20–2.11 (m, 1H), 1.91 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$): δ 144.1, 143.1, 134.3, 133.3, 131.9, 129.4 (+), 128.3 (+), 128.2 (+), 127.7 (+), 127.5 (+), 127.1 (+), 126.2 (+), 52.7 (–), 52.3 (–), 35.1 (+), 34.6 (–), 33.9 (+), 33.8 (–), 21.4 (+), 20.3 (+). IR (KBr): υ 3018, 2912, 2841, 1599, 1454, 1340, 1164, 981 cm^{-1}. HRMS (ESI) calcd for $C_{24}H_{28}NO_2S$ ([M+H]$^+$): 394.1835. Found: 394.1836.

Product (2j)



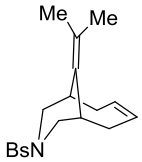
2j

Reaction time: 4 h. Eluted with PE/EA 10:1

Run 1: 73.3 mg **1j** was converted to 56.6 mg **2j**, yield 77%. Run 2: 72.6 mg **1j** was converted to 58.2 mg **2j**, yield 80%. So the average yield of two runs was 78%.

2j: light yellow solid, m.p. = 208–211 ℃, TLC R_f = 0.42 (PE/EA, 5:1). ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.34 (d, J = 8.8 Hz, 2H), 7.89 (d, J = 8.8 Hz, 2H), 5.65–5.57 (m, 2H), 3.71 (d, J = 11.3 Hz, 2H), 3.08–3.00 (m, 2H), 2.49 (dd, J = 11.3, 3.7 Hz, 2H), 2.46–2.36 (m, 2H), 2.36–2.26 (m, 2H), 1.67 (s, 6H). ^{13}C NMR (101 MHz, $CDCl_3$): δ 149.9, 142.6, 130.4, 128.6 (+), 127.3 (+), 125.6, 124.1 (+), 52.3 (–), 35.0 (–), 34.1 (+), 19.7 (+). IR (KBr): υ 2917, 2882, 1529, 1350, 1168 cm^{-1}. HRMS (ESI) calcd for $C_{18}H_{23}N_2O_4S$ ($[M+H]^+$): 363.1373. Found: 363.1373.

Product (2k)



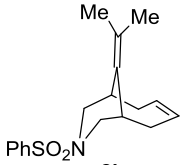
2k

Reaction time: 7 h. Eluted with PE/EA 20:1

Run 1: 79.0 mg **1k** was converted to 58.1 mg **2k**, yield 74%. Run 2: 79.0 mg **1k** was converted to 61.1 mg **2k**, yield 77%. So the average yield of two runs was 76%.

2k: white solid, m.p. = 169–172 ℃, TLC R_f = 0.70 (PE/EA, 5:1). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.63 (d, J = 8.7 Hz, 2H), 7.57 (d, J = 8.7 Hz, 2H), 5.66–5.57 (m, 2H), 3.64 (d, J = 11.2 Hz, 2H), 3.06–2.97 (m, 2H), 2.46–2.36 (m, 4H), 2.35–2.24 (m, 2H), 1.66 (s, 6H). ^{13}C NMR (101 MHz, $CDCl_3$): δ 135.3, 132.1 (+), 130.7, 129.1 (+), 127.4 (+), 127.3, 125.3, 52.4 (–), 35.0 (–), 34.2 (+), 19.6 (+). IR (KBr): υ 3089, 3000, 2905, 2831, 1571, 1462, 1338, 1168, 995 cm^{-1}. HRMS (ESI) calcd for $C_{18}H_{23}BrNO_2S$ ($[M+H]^+$): 396.0627. Found: 396.0623.

Product (2l)



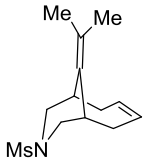
2l

Reaction time: 3 h. Eluted with PE/EA 20:1

Run 1: 64.0 mg **1l** was converted to 48.7 mg **2l**, yield 76%. Run 2: 63.5 mg **1l** was converted to 46.1 mg **2l**, yield 72%. So the average yield of two runs was 74%.

2l: white solid, m.p. = 142–145 ℃, TLC R_f = 0.50 (PE/EA, 5:1). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.74–7.67 (m, 2H), 7.57–7.52 (m, 1H), 7.52–7.45 (m, 2H), 5.67–5.56 (m, 2H), 3.67 (d, J = 11.2 Hz, 2H), 3.06–2.97 (m, 2H), 2.47–2.37 (m, 4H), 2.34–2.24 (m, 2H), 1.66 (s, 6H). ^{13}C NMR (101 MHz, $CDCl_3$): δ 136.2, 132.3 (+), 131.0, 128.8 (+), 127.6 (+), 127.4 (+), 125.0, 52.4 (–), 35.0 (–), 34.2 (+), 19.6 (+). IR (KBr): υ 3000, 2926, 2832, 1445, 1337, 1170, 1090 cm^{-1}. HRMS (ESI) calcd for $C_{18}H_{24}NO_2S$ ($[M+H]^+$): 318.1522. Found: 318.1528.

Product (2m)



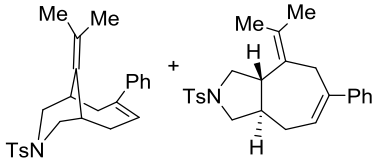
2m

Reaction time: 3 h. Eluted with PE/EA 10:1

Run 1: 51.5 mg **1m** was converted to 37.4 mg **2m**, yield 73%. Run 2: 51.4 mg **1m** was converted to 39.7 mg **2m**, yield 77%. So the average yield of two runs was 75%.

2m: white solid, m.p. = 129–132 ℃, TLC R_f = 0.21 (PE/EA, 5:1). ^{1}H NMR (400 MHz, $CDCl_3$): δ 5.64–5.54 (m, 2H), 3.66 (d, J = 11.5 Hz, 2H), 3.12–3.03 (m, 2H), 2.85 (dd, J = 11.5, 3.7 Hz, 2H), 2.71 (s, 3H), 2.44–2.27 (m, 4H), 1.73 (s, 6H). ^{13}C NMR (101 MHz, $CDCl_3$): δ 130.8, 127.3 (+), 125.4, 52.2 (–), 35.0 (–), 34.9 (+), 34.2 (+), 19.7 (+). IR (KBr): υ 2998, 2933, 2878, 2834, 1324, 1153, 991 cm^{-1}. HRMS (ESI) calcd for $C_{13}H_{22}NO_2S$ ([M+H]$^+$): 256.1366. Found: 256.1364.

Product (2p) and product (3p)



2p **3p**

Reaction time: 3 h. Eluted with PE/EA 20:1

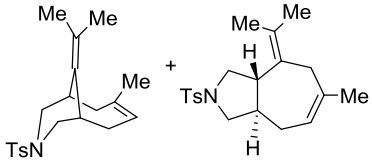
Run 1: 82.4 mg **1p** was converted to **2p** and **3p** (57.3 mg, 1:7), yield 70%. Run 2: 82.4 mg **1p** was converted to **2p** and **3p** (57.3 mg, 1:7), yield 70%. So the average yield of two runs was 70%.

Pure **3p** could be achieved by recrystallization from DCM/PE, and **2p** was enriched in the mother liquor.

2p: colorless oil, TLC R_f = 0.47 (PE/EA, 5:1). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.71 (d, J = 8.2 Hz, 2H), 7.31–7.22 (m, 5H), 7.14–7.08 (m, 2H), 5.67–5.59 (m, 1H), 3.55–3.43 (m, 3H), 3.32–3.23 (m, 1H), 3.18–3.09 (m, 1H), 3.08–3.01 (m, 1H), 2.67–2.58 (m, 1H), 2.52–2.43 (m, 1H), 2.40 (s, 3H), 2.20–2.10 (m, 2H), 1.62 (s, 3H), 1.55 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$): δ 143.3, 143.2, 141.6, 132.8, 129.6 (+), 128.3, 128.1 (+), 127.7 (+), 126.7 (+), 126.3, 125.7 (+), 124.9 (+), 53.0 (–), 50.3 (–), 43.1 (+), 39.9 (+), 32.2 (–), 27.8 (–), 21.5 (+), 21.2 (+), 20.2 (+). IR (KBr): υ 3026, 2923, 1597, 1343, 1164, 1097, 1034 cm^{-1}. HRMS (ESI) calcd for $C_{25}H_{30}NO_2S$ ([M+H]$^+$): 408.1992. Found: 408.1997.

3p: white solid, m.p. = 180–183 ℃, TLC R_f = 0.47 (PE/EA, 5:1). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.75 (d, J = 8.2 Hz, 2H), 7.34 (d, J = 8.2 Hz, 2H), 7.30–7.16 (m, 5H), 5.60–5.50 (m, 1H), 3.80–3.69 (m, 1H), 3.58–3.48 (m, 1H), 3.27–3.14 (m, 2H), 2.92–2.80 (m, 2H), 2.65–2.49 (m, 3H), 2.44 (s, 3H), 2.09–1.93 (m, 1H), 1.60 (s, 3H), 1.56 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$): δ 146.0, 143.3, 140.2, 134.5, 129.7 (+), 128.6, 128.4, 128.1 (+), 127.4 (+), 126.4 (+), 126.0 (+), 125.2 (+), 52.8 (–), 51.9 (–), 48.6 (+), 40.4 (+), 32.4 (–), 31.6 (–), 21.5 (+), 21.0 (+), 20.8 (+). IR (KBr): υ 2984, 2866, 1596, 1456, 1343, 1157, 1092, 1014 cm^{-1}. HRMS (ESI) calcd for $C_{25}H_{30}NO_2S$ ([M+H]$^+$): 408.1992. Found: 408.1981.

Product (2q) and product (3q)



Reaction time: 4 h. Eluted with PE/EA 20:1

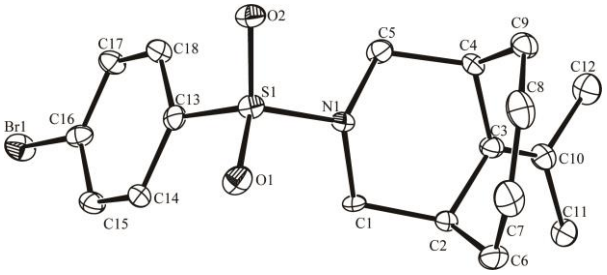
Run 1: 68.4 mg **1q** was converted to **2q** and **3q** (50.5 mg, 3:1), yield 74%. Run 2: 71.8 mg **1q** was converted to **2q** and **3q** (55.1 mg, 3:1), yield 77%. So the average yield of two runs was 76%.

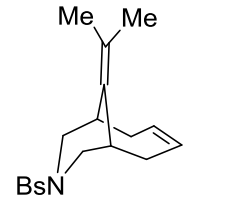
2q and **3q** was separated by preparative thin layer chromatography.

2q: colorless oil, TLC R_f = 0.61 (PE/EA, 5:1). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.59 (d, J = 8.2 Hz, 2H), 7.28 (d, J = 8.2 Hz, 2H), 5.42–5.34 (m, 1H), 3.68–3.60 (m, 2H), 3.01–2.90 (m, 2H), 2.40 (s, 3H), 2.45–2.34 (m, 4H), 2.28–2.16 (m, 2H), 1.74 (s, 3H), 1.63 (s, 3H), 1.62 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$): δ 143.0, 135.4, 133.4, 131.8, 129.4 (+), 127.5 (+), 124.1, 121.7 (+), 51.85 (–), 51.83 (–), 38.5 (–), 34.1 (+), 33.4 (+), 33.2 (–), 27.2 (+), 21.4 (+), 19.59 (+), 19.58 (+). IR (KBr): υ 2966, 2923, 2857, 1456, 1340, 1165, 1093 cm^{-1}. HRMS (ESI) calcd for $C_{20}H_{28}NO_2S$ ($[M+H]^+$): 346.1835. Found: 346.1828.

3q: colorless oil, TLC R_f = 0.52 (PE/EA, 5:1). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.73 (d, J = 8.2 Hz, 2H), 7.32 (d, J = 8.2 Hz, 2H), 5.17–5.09 (m, 1H), 3.74–3.63 (m, 1H), 3.53–3.43 (m, 1H), 2.88–2.69 (m, 3H), 2.67–2.56 (m, 1H), 2.53–2.38 (m, 2H), 2.44 (s, 3H), 2.35–2.25 (m, 1H), 1.87–1.75 (m, 1H), 1.72 (s, 3H), 1.67 (s, 3H), 1.58 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$): δ 143.3, 135.8, 134.5, 129.6 (+), 128.6, 127.5, 127.4 (+), 120.4 (+), 53.0 (–), 51.9 (–), 48.4 (+), 40.5 (+), 32.1 (–), 31.9 (–), 27.8 (+), 21.5 (+), 20.7 (+, 2C). IR (KBr): υ 2920, 2873, 1447, 1345, 1093, 1041 cm^{-1}. HRMS (ESI) calcd for $C_{20}H_{28}NO_2S$ ($[M+H]^+$): 346.1835. Found: 346.1834.

4. Crystallographic Data of Compound 2k





2k CCDC 1535695

Table S3.1 Crystal data and structure refinement for exp_7579-1.

Identification code	exp_7579-1
Empirical formula	$C_{18}H_{22}NO_2SBr$
Formula weight	396.33
Temperature/K	180.01(10)
Crystal system	monoclinic
Space group	$P2_1/n$
a/Å	17.4506(17)
b/Å	11.1673(9)
c/Å	18.3316(16)
α/°	90
β/°	100.091(10)
γ/°	90
Volume/Å^3	3517.1(6)
Z	8
ρ_{calc}g/cm^3	1.497
μ/mm^{-1}	2.465
F(000)	1632.0
Crystal size/mm^3	0.1 × 0.1 × 0.05
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	5.984 to 58.502
Index ranges	-23 ≤ h ≤ 16, -14 ≤ k ≤ 14, -25 ≤ l ≤ 23
Reflections collected	15641
Independent reflections	7947 [R_{int} = 0.0713, R_{sigma} = 0.1211]
Data/restraints/parameters	7947/0/419
Goodness-of-fit on F^2	1.027
Final R indexes [I>=2σ (I)]	R_1 = 0.0835, wR_2 = 0.1880
Final R indexes [all data]	R_1 = 0.1541, wR_2 = 0.2394
Largest diff. peak/hole / e Å^{-3}	3.82/-1.08

Table S3.2 Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic

Displacement Parameters ($Å^2 \times 10^3$) for exp_7579-1. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
Br1	2035.6(5)	7371.6(7)	11407.0(4)	40.3(2)
Br2	945.6(5)	3399.7(7)	-3298.8(4)	44.7(3)
C1	3788(4)	3092(5)	9685(3)	22.6(13)
C2	3864(4)	1749(5)	9575(3)	24.3(14)
C3	3142(4)	1194(5)	9097(3)	25.6(14)
C4	2820(4)	1909(5)	8420(3)	26.2(14)
C5	2756(4)	3236(5)	8593(4)	28.2(15)
C6	4613(4)	1434(6)	9269(4)	35.1(16)
C7	4675(4)	1793(6)	8510(4)	38.1(17)
C8	4142(5)	1936(6)	7909(4)	38.2(18)
C9	3277(4)	1724(6)	7781(4)	30.8(15)
C10	2852(4)	135(6)	9262(3)	29.4(15)
C11	3183(5)	-624(5)	9901(4)	36.4(17)
C12	2149(4)	-449(6)	8784(4)	41.1(18)
C13	3279(4)	5819(5)	9580(4)	26.7(14)
C14	3695(4)	5989(5)	10293(3)	26.2(14)
C15	3327(4)	6440(5)	10830(4)	28.6(15)
C16	2541(4)	6733(6)	10661(4)	28.6(15)
C17	2123(4)	6559(6)	9958(4)	30.8(15)
C18	2491(4)	6110(6)	9420(4)	29.3(15)
C19	1419(4)	3488(5)	450(4)	25.7(14)
C20	2013(4)	3477(5)	1166(3)	23.8(13)
C21	2440(4)	2290(5)	1293(3)	23.6(13)
C22	1920(4)	1202(6)	1135(4)	27.5(14)
C23	1348(4)	1315(5)	419(3)	26.3(14)
C24	1647(4)	3834(6)	1838(4)	37.9(17)
C25	1081(5)	3028(7)	2097(4)	39.0(17)
C26	1015(4)	1853(7)	2080(4)	38.4(18)
C27	1499(4)	909(6)	1796(4)	34.6(16)
C28	3198(4)	2220(6)	1558(4)	28.5(14)
C29	3728(4)	3295(7)	1758(4)	41.5(18)
C30	3636(4)	1046(6)	1751(4)	38.0(17)
C31	241(4)	2769(6)	-1013(4)	27.9(14)
C32	315(4)	3931(6)	-1262(4)	32.1(16)
C33	518(4)	4122(6)	-1943(4)	32.7(16)
C34	657(4)	3123(5)	-2364(4)	28.3(15)
C35	603(4)	1958(5)	-2126(4)	29.4(15)

C36	387(4)	1794(6)	-1428(4)	29.1(15)
N1	3521(3)	3685(4)	8967(3)	24.4(12)
N2	911(3)	2449(4)	412(3)	20.8(11)
O1	4552(2)	5237(4)	9132(3)	30.2(10)
O2	3352(3)	5485(4)	8190(2)	29.3(10)
O3	-287(3)	3633(4)	110(3)	30.2(10)
O4	-329(3)	1426(4)	-62(3)	30.8(11)
S1	3724.9(9)	5097.8(13)	8906.1(9)	24.8(4)
S2	59.4(9)	2544.6(12)	-100.7(9)	22.7(4)

Table S3.3 Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for exp_7579-1. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Br1	37.7(5)	55.0(5)	29.6(4)	-7.5(3)	9.9(3)	4.2(3)
Br2	55.5(6)	43.6(4)	38.8(5)	8.4(3)	19.1(4)	5.4(4)
C1	26(4)	24(3)	16(3)	4(2)	-4(3)	6(3)
C2	28(4)	22(3)	20(3)	1(3)	-3(3)	1(3)
C3	25(4)	31(3)	20(3)	-1(3)	3(3)	4(3)
C4	25(4)	26(3)	24(3)	-6(3)	-4(3)	0(3)
C5	22(4)	25(3)	36(4)	5(3)	0(3)	-3(3)
C6	26(4)	34(4)	41(4)	0(3)	-5(3)	2(3)
C7	28(4)	44(4)	46(5)	-11(3)	17(4)	-3(3)
C8	46(5)	35(4)	38(4)	-7(3)	20(4)	-9(3)
C9	42(4)	29(3)	21(3)	1(3)	2(3)	-2(3)
C10	34(4)	35(3)	21(3)	-1(3)	10(3)	-1(3)
C11	50(5)	18(3)	38(4)	10(3)	2(4)	-9(3)
C12	41(5)	34(4)	49(5)	2(3)	11(4)	-9(3)
C13	26(4)	17(3)	36(4)	5(3)	0(3)	-5(3)
C14	23(4)	24(3)	29(4)	-2(3)	-2(3)	-2(3)
C15	31(4)	33(3)	20(3)	1(3)	0(3)	-2(3)
C16	25(4)	32(3)	28(4)	9(3)	3(3)	0(3)
C17	22(4)	37(4)	32(4)	-3(3)	0(3)	-4(3)
C18	31(4)	31(3)	24(3)	-2(3)	0(3)	-1(3)
C19	27(4)	22(3)	27(3)	1(3)	1(3)	-4(3)
C20	21(3)	28(3)	20(3)	2(3)	-3(3)	-7(3)
C21	19(3)	30(3)	21(3)	1(3)	0(3)	-2(3)
C22	23(4)	31(3)	26(3)	3(3)	0(3)	7(3)
C23	33(4)	25(3)	20(3)	-2(3)	0(3)	0(3)

C24	34(4)	38(4)	41(4)	-3(3)	3(3)	1(3)
C25	39(5)	51(4)	24(4)	-2(3)	-3(3)	7(4)
C26	30(4)	68(5)	19(3)	11(3)	7(3)	1(4)
C27	27(4)	36(4)	40(4)	12(3)	3(3)	-1(3)
C28	20(3)	44(4)	20(3)	4(3)	-1(3)	2(3)
C29	27(4)	58(5)	36(4)	6(4)	-3(3)	-9(4)
C30	25(4)	58(4)	30(4)	10(3)	2(3)	12(3)
C31	16(3)	41(4)	24(3)	-8(3)	-4(3)	3(3)
C32	33(4)	27(3)	33(4)	-1(3)	-3(3)	4(3)
C33	33(4)	29(3)	35(4)	2(3)	0(3)	5(3)
C34	27(4)	27(3)	29(4)	-3(3)	1(3)	2(3)
C35	23(4)	23(3)	39(4)	-2(3)	-3(3)	2(3)
C36	26(4)	33(3)	25(3)	2(3)	-2(3)	2(3)
N1	27(3)	23(2)	20(3)	0(2)	-5(2)	1(2)
N2	19(3)	25(3)	17(3)	-2(2)	-1(2)	-4(2)
O1	17(2)	29(2)	45(3)	4(2)	6(2)	-1.5(18)
O2	29(3)	33(2)	24(2)	5.6(19)	-1(2)	2.3(19)
O3	20(2)	34(2)	36(3)	-5(2)	2(2)	3.8(19)
O4	27(3)	31(2)	33(3)	-1(2)	0(2)	-9.6(19)
S1	23.6(9)	26.5(8)	24.1(8)	2.3(6)	3.5(7)	1.0(6)
S2	16.6(8)	28.7(8)	22.0(8)	-2.1(6)	1.0(6)	-1.1(6)

Table S3.4 Bond Lengths for exp_7579-1.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Br1	C16	1.892(7)	C20	C21	1.519(8)
Br2	C34	1.894(7)	C20	C24	1.537(9)
C1	C2	1.523(8)	C21	C22	1.514(9)
C1	N1	1.474(7)	C21	C28	1.329(9)
C2	C3	1.533(9)	C22	C23	1.509(9)
C2	C6	1.549(9)	C22	C27	1.559(9)
C3	C4	1.499(9)	C23	N2	1.477(7)
C3	C10	1.342(9)	C24	C25	1.474(10)
C4	C5	1.524(9)	C25	C26	1.317(11)
C4	C9	1.541(9)	C26	C27	1.499(10)
C5	N1	1.477(8)	C28	C29	1.520(10)
C6	C7	1.471(10)	C28	C30	1.527(9)
C7	C8	1.321(11)	C31	C32	1.388(9)
C8	C9	1.506(10)	C31	C36	1.377(9)
C10	C11	1.479(9)	C31	S2	1.774(7)

C10	C12	1.525(10)	C32	C33	1.374(9)
C13	C14	1.392(9)	C33	C34	1.402(9)
C13	C18	1.392(9)	C34	C35	1.380(9)
C13	S1	1.767(7)	C35	C36	1.407(9)
C14	C15	1.362(9)	N1	S1	1.626(5)
C15	C16	1.391(9)	N2	S2	1.616(5)
C16	C17	1.379(9)	O1	S1	1.438(4)
C17	C18	1.364(9)	O2	S1	1.426(4)
C19	C20	1.523(9)	O3	S2	1.439(4)
C19	N2	1.455(7)	O4	S2	1.429(4)

Table S3.5 Bond Angles for exp_7579-1.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
N1	C1	C2	110.2(5)	C23	C22	C27	111.3(5)
C1	C2	C3	113.1(5)	N2	C23	C22	110.0(5)
C1	C2	C6	111.7(5)	C25	C24	C20	119.7(6)
C3	C2	C6	111.3(5)	C26	C25	C24	131.4(7)
C4	C3	C2	114.1(5)	C25	C26	C27	131.1(7)
C10	C3	C2	122.1(6)	C26	C27	C22	119.5(5)
C10	C3	C4	123.7(6)	C21	C28	C29	124.5(6)
C3	C4	C5	112.2(5)	C21	C28	C30	124.1(6)
C3	C4	C9	112.9(5)	C29	C28	C30	111.3(6)
C5	C4	C9	110.7(5)	C32	C31	S2	118.9(5)
N1	C5	C4	109.5(5)	C36	C31	C32	121.4(6)
C7	C6	C2	119.2(6)	C36	C31	S2	119.3(5)
C8	C7	C6	131.6(7)	C33	C32	C31	119.8(6)
C7	C8	C9	130.6(7)	C32	C33	C34	118.2(6)
C8	C9	C4	119.9(6)	C33	C34	Br2	117.8(5)
C3	C10	C11	125.0(6)	C35	C34	Br2	118.9(5)
C3	C10	C12	123.1(6)	C35	C34	C33	123.2(6)
C11	C10	C12	111.9(6)	C34	C35	C36	117.0(6)
C14	C13	C18	120.0(6)	C31	C36	C35	120.2(6)
C14	C13	S1	119.8(5)	C1	N1	C5	112.4(5)
C18	C13	S1	119.9(5)	C1	N1	S1	117.3(4)
C15	C14	C13	119.6(6)	C5	N1	S1	119.2(4)
C14	C15	C16	119.8(6)	C19	N2	C23	111.9(5)
C15	C16	Br1	119.6(5)	C19	N2	S2	117.8(4)
C17	C16	Br1	119.4(5)	C23	N2	S2	118.9(4)
C17	C16	C15	121.0(6)	N1	S1	C13	105.4(3)

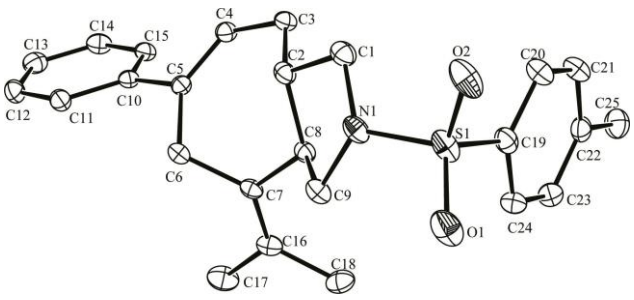
C18	C17	C16	119.2(6)	O1	S1	C13	107.0(3)
C17	C18	C13	120.4(6)	O1	S1	N1	107.8(3)
N2	C19	C20	110.6(5)	O2	S1	C13	108.7(3)
C19	C20	C24	111.9(5)	O2	S1	N1	106.7(3)
C21	C20	C19	112.4(5)	O2	S1	O1	120.3(3)
C21	C20	C24	111.4(5)	N2	S2	C31	105.0(3)
C22	C21	C20	114.1(5)	O3	S2	C31	106.6(3)
C28	C21	C20	122.5(6)	O3	S2	N2	106.6(3)
C28	C21	C22	123.2(6)	O4	S2	C31	109.6(3)
C21	C22	C27	111.6(5)	O4	S2	N2	108.0(3)
C23	C22	C21	112.5(5)	O4	S2	O3	120.0(3)

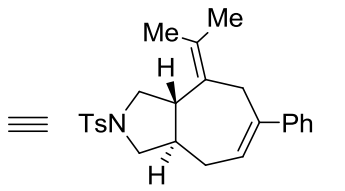
Table S3.6 Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for exp_7579-1.

Atom	*x*	*y*	*z*	U(eq)
H1A	3412	3246	10020	27
H1B	4298	3426	9917	27
H2	3917	1372	10076	29
H4	2279	1612	8242	31
H5A	2586	3687	8127	34
H5B	2364	3356	8916	34
H6A	5058	1795	9607	42
H6B	4680	555	9303	42
H7	5192	1949	8438	46
H8	4337	2219	7488	46
H9A	3185	890	7606	37
H9B	3040	2253	7369	37
H11A	3639	-226	10188	55
H11B	3338	-1398	9722	55
H11C	2791	-749	10216	55
H12A	1931	95	8382	62
H12B	1753	-622	9089	62
H12C	2309	-1197	8575	62
H14	4232	5792	10404	31
H15	3607	6553	11318	34
H17	1584	6749	9850	37
H18	2209	5995	8933	35
H19A	1104	4229	426	31
H19B	1693	3485	20	31

H20	2411	4100	1113	29
H22	2265	506	1078	33
H23A	1630	1298	-5	32
H23B	982	631	367	32
H24A	2077	3965	2260	45
H24B	1387	4616	1724	45
H25	696	3427	2314	47
H26	588	1553	2282	46
H27A	1157	210	1651	41
H27B	1901	651	2217	41
H29A	3433	4033	1624	62
H29B	4163	3254	1486	62
H29C	3929	3292	2291	62
H30A	3287	371	1594	57
H30B	3817	1005	2288	57
H30C	4084	1010	1496	57
H32	226	4591	-961	39
H33	563	4911	-2125	39
H35	709	1297	-2419	35
H36	340	1008	-1243	35

5. Crystallographic Data of Compound 3p





3p CCDC 1535693

Table S4.1 Crystal data and structure refinement for exp_7693.

Identification code	exp_7693
Empirical formula	$C_{25}H_{29}NO_2S$
Formula weight	407.55
Temperature/K	180.00(10)
Crystal system	triclinic
Space group	P-1
a/Å	8.7615(6)
b/Å	11.4755(7)
c/Å	11.7322(7)
α/°	72.319(5)
β/°	85.982(5)
γ/°	71.472(6)
Volume/Å^3	1065.16(13)
Z	2
ρ_{calc}g/cm^3	1.271
μ/mm^{-1}	0.173
F(000)	436.0
Crystal size/mm^3	0.1 × 0.1 × 0.05
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	6.098 to 52.044
Index ranges	-10 ≤ h ≤ 10, -14 ≤ k ≤ 9, -14 ≤ l ≤ 14
Reflections collected	6671
Independent reflections	4165 [R_{int} = 0.0248, R_{sigma} = 0.0454]
Data/restraints/parameters	4165/6/265
Goodness-of-fit on F^2	1.039
Final R indexes [I>=2σ (I)]	R_1 = 0.0475, wR_2 = 0.1145
Final R indexes [all data]	R_1 = 0.0651, wR_2 = 0.1292
Largest diff. peak/hole / e Å^{-3}	0.24/-0.46

Table S4.2 Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$) for exp_7693. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
S1	4346.9(6)	7892.4(6)	7780.6(4)	38.64(18)
O1	3046.5(18)	7671.8(19)	7298.4(14)	54.3(5)
O2	4037.5(19)	8708.0(16)	8532.4(13)	49.5(5)
N1	5318(2)	8514.7(17)	6643.3(14)	33.0(4)
C10	11512(2)	8529.1(18)	2989.4(16)	27.0(4)
C7	8082(2)	7329.1(18)	4348.4(16)	25.7(4)
C8	7435(2)	7557.2(18)	5525.3(16)	25.6(4)
C2	7854(2)	8605.2(19)	5854.0(16)	28.1(4)
C4	10650(2)	8355.8(18)	5027.7(16)	28.7(4)
C15	13142(2)	7863.2(19)	3243.8(17)	30.7(5)
C3	9627(2)	8301(2)	6109.7(16)	29.9(4)
C5	10284(2)	8403.7(18)	3924.5(16)	26.5(4)
C12	12223(3)	9509(2)	975.6(18)	37.8(5)
C11	11067(3)	9353.7(19)	1825.7(17)	32.4(5)
C6	8671(2)	8383(2)	3520.7(16)	29.1(4)
C21	7797(3)	5140(2)	10037.0(18)	37.7(5)
C14	14288(3)	8036(2)	2393.0(19)	37.1(5)
C16	8145(2)	6265(2)	4086.6(18)	30.9(5)
C22	8023(3)	4070(2)	9667.1(17)	34.2(5)
C13	13826(3)	8864(2)	1253.5(19)	38.6(5)
C20	6646(3)	6296(2)	9501.1(18)	36.8(5)
C19	5691(2)	6389(2)	8567.3(17)	32.6(5)
C9	5605(2)	7977(2)	5613.4(17)	31.1(5)
C1	6797(2)	8760(2)	6919.2(17)	33.3(5)
C18	7527(3)	5221(2)	4894(2)	41.2(5)
C23	7028(3)	4173(2)	8744.2(19)	41.0(5)
C25	9290(3)	2822(2)	10248(2)	45.9(6)
C17	8835(3)	5963(2)	2955(2)	46.9(6)
C24	5870(3)	5317(2)	8200.3(19)	39.4(5)

Table S4.3 Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for exp_7693. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
S1	25.5(3)	54.8(4)	27.2(3)	-12.3(2)	0.3(2)	-0.8(2)

O1	26.3(8)	91.2(14)	38.0(9)	-13.4(9)	-1.2(7)	-13.6(9)
O2	43.2(9)	59.3(11)	32.2(8)	-20.5(7)	1.9(7)	9.1(8)
N1	30.7(9)	40.2(10)	25.3(8)	-13.7(7)	0.5(7)	-3.2(8)
C10	34.4(11)	24.2(10)	26.2(9)	-10.7(8)	-0.9(8)	-10.8(9)
C7	21.3(9)	27.9(11)	26.5(9)	-9.9(8)	-5.3(7)	-2.7(8)
C8	28.5(10)	23.2(10)	23.1(9)	-6.7(8)	-3.5(8)	-4.6(8)
C2	34.7(11)	24.6(10)	23.6(9)	-8.4(8)	-1.8(8)	-5.7(9)
C4	32.1(10)	26.1(10)	29.1(10)	-8.7(8)	-2.3(8)	-9.8(9)
C15	35.5(11)	30.8(11)	29.1(10)	-11.4(8)	-3.0(9)	-11.5(9)
C3	38.4(11)	29.6(11)	25.6(9)	-11.2(8)	-2.2(8)	-12.3(9)
C5	32.7(10)	20.7(10)	26.6(9)	-7.1(8)	-2.1(8)	-8.2(8)
C12	53.2(14)	36.5(12)	24.7(10)	-8.7(9)	2.7(10)	-16.3(11)
C11	37.8(11)	29.8(11)	28.7(10)	-7.9(8)	-2.6(9)	-9.4(9)
C6	31.2(10)	33.4(11)	23.5(9)	-9.4(8)	-2.8(8)	-9.3(9)
C21	38.3(12)	45.9(14)	28.9(10)	-13.8(10)	-6.0(9)	-9(1)
C14	34.3(11)	40.7(13)	41.8(12)	-20.3(10)	1.4(10)	-11.3(10)
C16	24.7(10)	30.8(11)	37.6(11)	-16.2(9)	-4.5(8)	-2.4(9)
C22	37.0(12)	37.1(12)	28.2(10)	-7.3(9)	7.4(9)	-15(1)
C13	43.6(13)	45.3(14)	36.9(12)	-21.3(10)	11.7(10)	-21.1(11)
C20	39.2(12)	41.5(13)	29.1(10)	-15.1(9)	-2.3(9)	-6.6(10)
C19	25.7(10)	44.8(13)	25.8(10)	-8.7(9)	2.0(8)	-10.8(9)
C9	29(1)	37.1(12)	25.8(10)	-12.2(9)	-0.7(8)	-5.3(9)
C1	37.6(12)	32.6(12)	29.4(10)	-12.9(9)	-0.6(9)	-6.9(9)
C18	41.6(13)	30.9(12)	54.9(14)	-17.1(10)	-2.7(11)	-11.3(10)
C23	54.2(14)	39.1(13)	37.1(12)	-12.2(10)	1.5(11)	-23.6(12)
C25	50.4(14)	37.7(14)	42.4(13)	-6.6(10)	2.5(11)	-9.3(11)
C17	45.0(14)	51.2(15)	52.0(14)	-33.7(12)	3.5(11)	-8.3(12)
C24	42.2(13)	50.1(14)	33.1(11)	-10.8(10)	-5.4(10)	-24.1(11)

Table S4.4 Bond Lengths for exp_7693.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
S1	O1	1.4293(17)	C4	C3	1.499(3)
S1	O2	1.4262(16)	C4	C5	1.336(3)
S1	N1	1.6318(17)	C15	C14	1.382(3)
S1	C19	1.763(2)	C5	C6	1.531(3)
N1	C9	1.489(2)	C12	C11	1.385(3)
N1	C1	1.486(3)	C12	C13	1.372(3)
C10	C15	1.393(3)	C21	C22	1.376(3)
C10	C5	1.490(3)	C21	C20	1.380(3)

C10	C11	1.402(3)	C14	C13	1.384(3)
C7	C8	1.521(2)	C16	C18	1.509(3)
C7	C6	1.512(3)	C16	C17	1.511(3)
C7	C16	1.331(3)	C22	C23	1.391(3)
C8	C2	1.521(3)	C22	C25	1.500(3)
C8	C9	1.526(3)	C20	C19	1.383(3)
C2	C3	1.511(3)	C19	C24	1.384(3)
C2	C1	1.523(3)	C23	C24	1.376(3)

Table S4.5 Bond Angles for exp_7693.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
O1	S1	N1	106.68(9)	C10	C5	C6	116.48(16)
O1	S1	C19	108.31(11)	C4	C5	C10	118.15(18)
O2	S1	O1	120.43(10)	C4	C5	C6	125.34(17)
O2	S1	N1	106.41(10)	C13	C12	C11	120.8(2)
O2	S1	C19	107.73(10)	C12	C11	C10	120.6(2)
N1	S1	C19	106.50(9)	C7	C6	C5	113.76(15)
C9	N1	S1	118.73(14)	C22	C21	C20	121.7(2)
C1	N1	S1	116.86(13)	C15	C14	C13	120.1(2)
C1	N1	C9	109.53(15)	C7	C16	C18	123.45(18)
C15	C10	C5	121.48(17)	C7	C16	C17	124.2(2)
C15	C10	C11	117.61(18)	C18	C16	C17	112.37(19)
C11	C10	C5	120.88(18)	C21	C22	C23	118.0(2)
C6	C7	C8	115.05(16)	C21	C22	C25	121.2(2)
C16	C7	C8	121.89(18)	C23	C22	C25	120.8(2)
C16	C7	C6	123.05(17)	C12	C13	C14	119.47(19)
C7	C8	C9	115.77(15)	C21	C20	C19	119.5(2)
C2	C8	C7	115.84(15)	C20	C19	S1	120.09(17)
C2	C8	C9	101.77(15)	C20	C19	C24	119.8(2)
C8	C2	C1	102.64(15)	C24	C19	S1	119.99(16)
C3	C2	C8	114.11(16)	N1	C9	C8	103.50(15)
C3	C2	C1	113.99(16)	N1	C1	C2	103.75(15)
C5	C4	C3	129.34(19)	C24	C23	C22	121.2(2)
C14	C15	C10	121.35(19)	C23	C24	C19	119.8(2)
C4	C3	C2	114.59(16)				

Table S4.6 Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for exp_7693.

Atom	*x*	*y*	*z*	U(eq)
H8	7881	6733	6177	31
H2	7492	9421	5180	34
H4	11712	8356	5143	34
H15	13472	7278	4018	37
H3A	9761	8917	6500	36
H3B	10025	7428	6684	36
H12	11903	10068	190	45
H11	9963	9810	1619	39
H6A	7851	9225	3463	35
H6B	8781	8273	2711	35
H21	8451	5081	10678	45
H14	15395	7584	2591	45
H13	14613	8986	668	46
H20	6511	7022	9772	44
H9A	5083	8638	4869	37
H9B	5193	7235	5769	37
H1A	7330	8129	7674	40
H1B	6543	9640	6989	40
H18A	7231	5398	5660	62
H18B	8369	4387	5033	62
H18C	6579	5201	4514	62
H23	7150	3442	8485	49
H25A	10341	2855	9921	69
H25B	9033	2114	10088	69
H25C	9323	2682	11113	69
H17A	7961	6034	2436	70
H17B	9589	5086	3159	70
H17C	9404	6575	2536	70
H24	5195	5369	7575	47

6. DFT Calculations

6.1 Computational Details and Discussion

All DFT calculations were performed with the Gaussian 09 software package[21]. Geometry optimizations of all the minima and transition states involved were carried out at the B3LYP level of theory[22]. The LANL2DZ[23] basis set and pseudopotential were used for Rh and the 6-31G(d) basis set[24] for the other atoms. The key word "5D" was used to specify that five d-type orbitals were used for all elements in the calculations. Frequency calculations at the same level were performed to validate each structure as either a minimum or a transition state and to evaluate its zero-point energy and the thermal corrections at 298 K. Key transition-state structures were confirmed to connect corresponding reactants and products by intrinsic reaction coordinate (IRC) calculations[25].

To improve the calculation accuracy, single-point energies calculations and solvent effects were computed at the M06-2X level of theory[26] with the SDD[27] basis set and pseudopotential for Rh and the 6-311+G(d,p) basis set[24] for the other atoms. Solvation energies in dioxane (ε = 2.2099) were evaluated by IEFPCM calculations with radii and non-electrostatic terms for SMD solvation model[28].

The final free energies reported in the article (ΔG_{sol}) are the large basis set single-point energies in dioxane solvent with the gas-phase Gibbs free energy corrections (at 298 K).

DFT-calculated free energy surface of the two competing pathways when R = H is shown in Figure S1. **TS2a-H** is favored by 3.2 kcal, so the bicycle[4.3.1]decane cycloadduct **2-H** would be predominantly generated. This is because, transition state **TS2b-H** for allene's *trans* insertion into the C2-Rh bond suffers strong repulsion between internal hydrogen atoms in the allene moiety with those in the VCP moiety (the corresponding H…H distances are 2.10 A and 2.16 A, within the sum of van de Waals radius, see Figure S2).

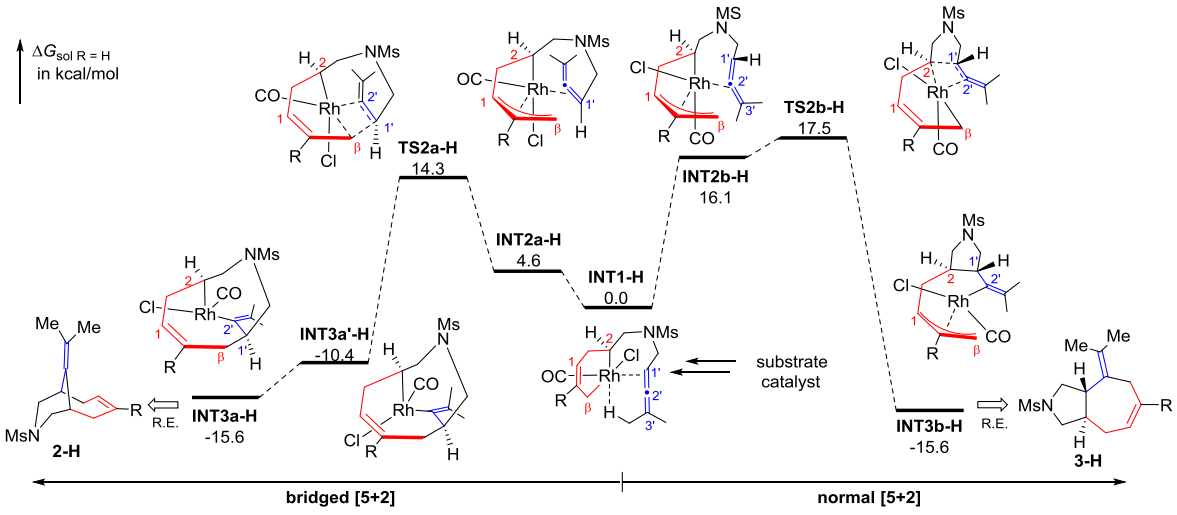


Figure S1. DFT-calculated free energy surfaces of the two competing pathways when R = H

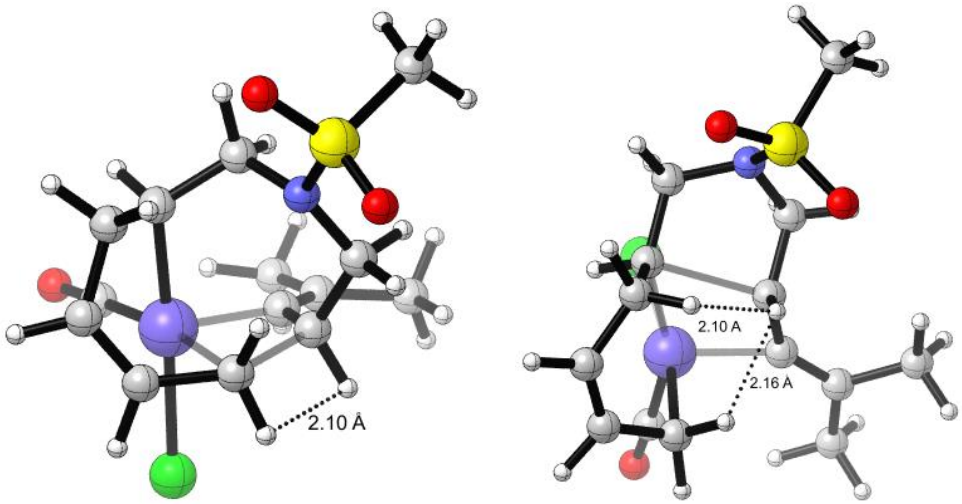


Figure S2. DFT-calculated structures[29] of transition states **TS2a-H** and **TS2b-H** (C gray; H white; O red; S yellow; N blue; Rh purple; Cl green).

The reaction for substrate with R = Ph was also calculated (Figure S3). We found that, the bridged [5+2] pathway via **TS2a-Ph** becomes a little more difficult with an activation Gibbs free energy 17.2 kcal/mol. This additional increase of energy comes from steric repulsion between Ph group and Cl atom (Figure S4). In the present case, the two [5+2] pathways have similar activation energies and consequently both cycloadducts should be obtained, agreeing with the experimental observation.

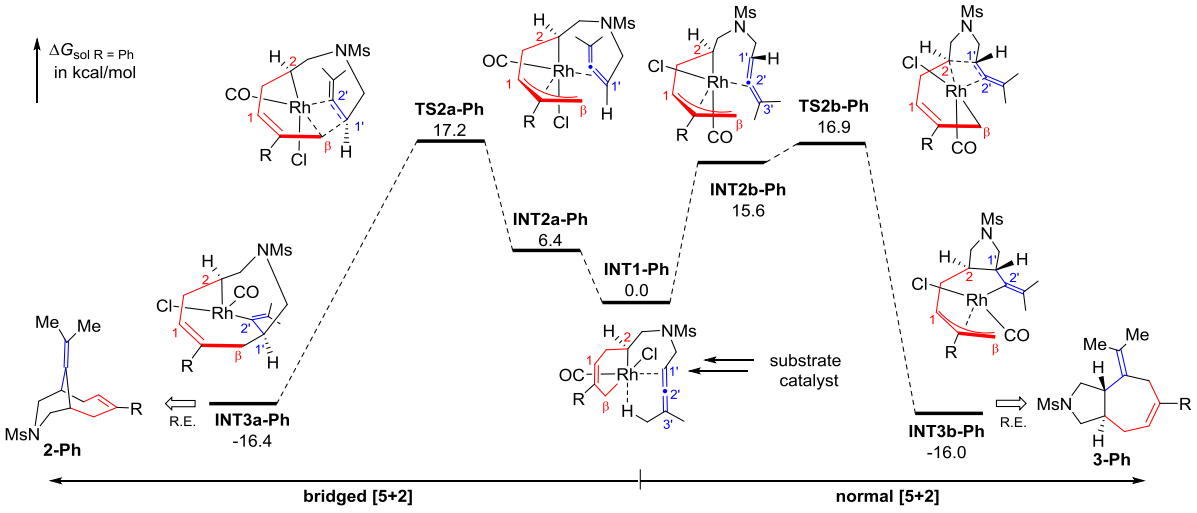


Figure S3. DFT-calculated free energy surfaces of the two competing pathways when R = Ph

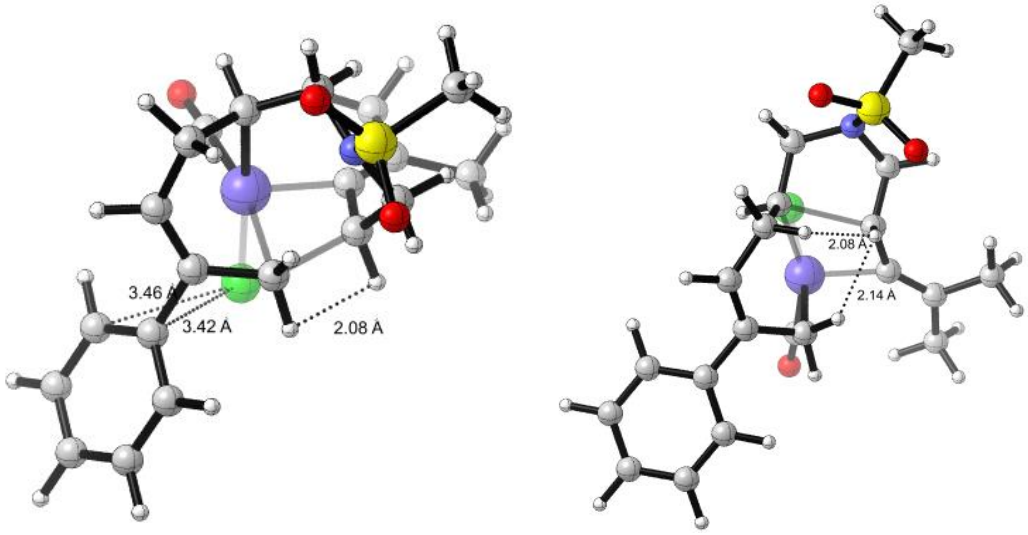


Figure S4. DFT-calculated structures of transition states **TS2a-Ph** and **TS2b-Ph** (C gray; H white; O red; S yellow; N blue; Rh purple; Cl green).

The inverse insertion of the inner double bond into Rh-C2 bond (**TS2d**), the *trans* insertion to Rh-Cβ bond (**TS2c**) and the *cis* insertion (**TS2e** and **TS2f**) were also considered. These pathways can be ruled out because of their high energy barriers compared to other favored transition states in the above mentioned Figures (Figure S5). For the transition states **TS2e-H** and **TS2e-Ph** corresponding to allene's *cis* insertion into the C2-Rh bond, there exists a strong repulsion between the two H atoms in the forming five membered rings. This could explain why previously reported *cis* bicyclo[5.3.0]decane product could not be observed (Figure S6).

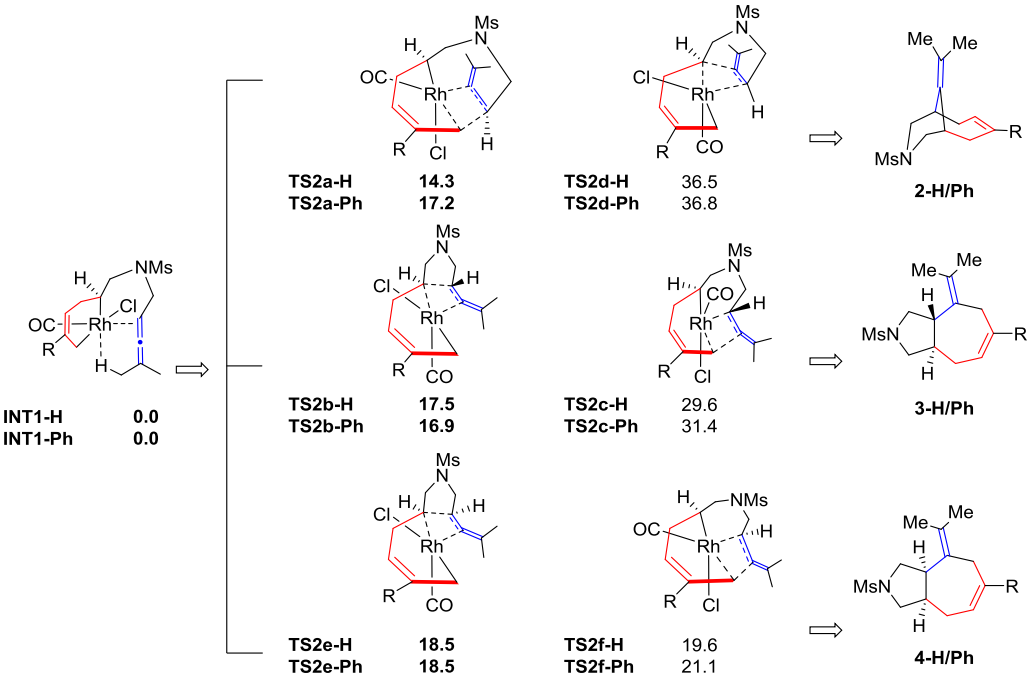


Figure S5. Other possible transition states (energies in kcal/mol).

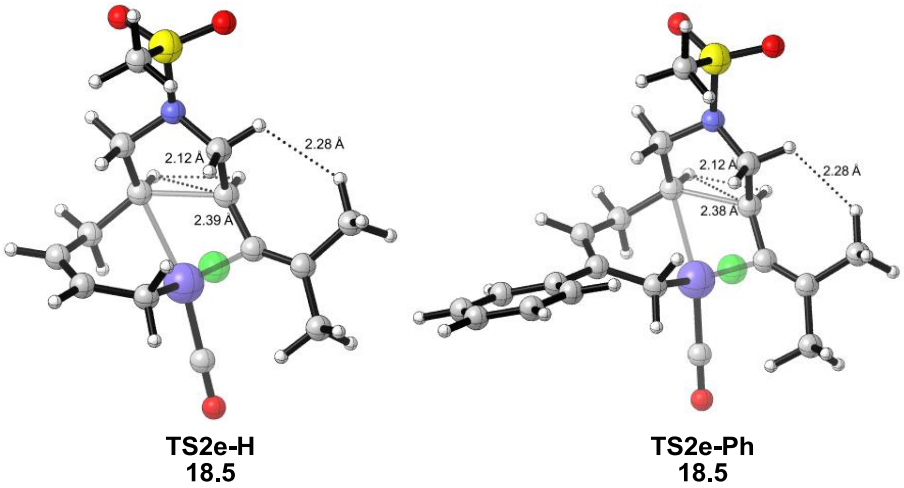


Figure S6. DFT-calculated structures of transition states **TS2e-H** and **TS2e-Ph** (C gray; H white; O red; S yellow; N blue; Rh purple; Cl green).

The situations for tether Z = CH_2 and CE_2 were also calculated (Figures S7-10). When Z = CH_2 (or CE_2), the bridged [5+2] pathway via **TS2a-CH$_2$** (or **TS2a-CE$_2$**) becomes difficult with an activation Gibbs free energy 20.9 kcal/mol (24.0 kcal/mol when Z = CE_2). The normal [5+2] pathway via **TS2b-CH$_2$** (or **TS2b-CE$_2$**) also becomes more difficult with an activation Gibbs free energy 21.3 kcal/mol (21.4 kcal/mol when Z = CE_2). These additional increases of activation energy come from steric repulsion between substituents of the C tether (H atom or CO_2Me group) and H atom in VCP moity (Figure S8). This can explain why no reaction occurred when C-tethered substrates **1n** was used. Further increase of the reaction temperature for this substrate resulted in the decomposition of substrates because of other side reactions. Figure S7 also gives the whole catalytic cycle of the bridged [5+2] reaction for the substrate with N tether, which includes ligand exchange, cyclopropane cleavage, allene insertion and reductive elimination. The overall activation free energy for the bridged [5+2] reaction is 28.5 kcal/mol. This agrees with the reaction conditions (heating at 80 ℃). We did not use DFT calculations to understand why substrate with O tether failed. Experimentally, the substrate decomposed and maybe other side reactions are easier than the key elementary steps in both normal and bridged [5+2] pathways.

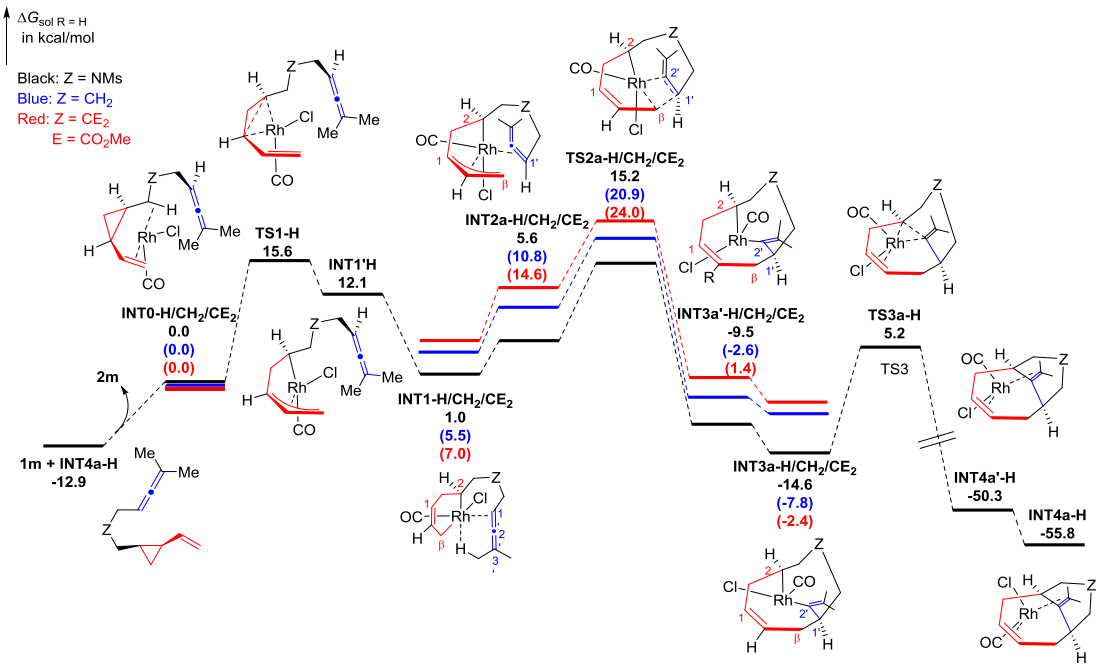


Figure S7. DFT-calculated free energy surfaces of bridged [5+2] pathway when Z = NMs, CH_2 and CE_2 (E = CO_2Me).

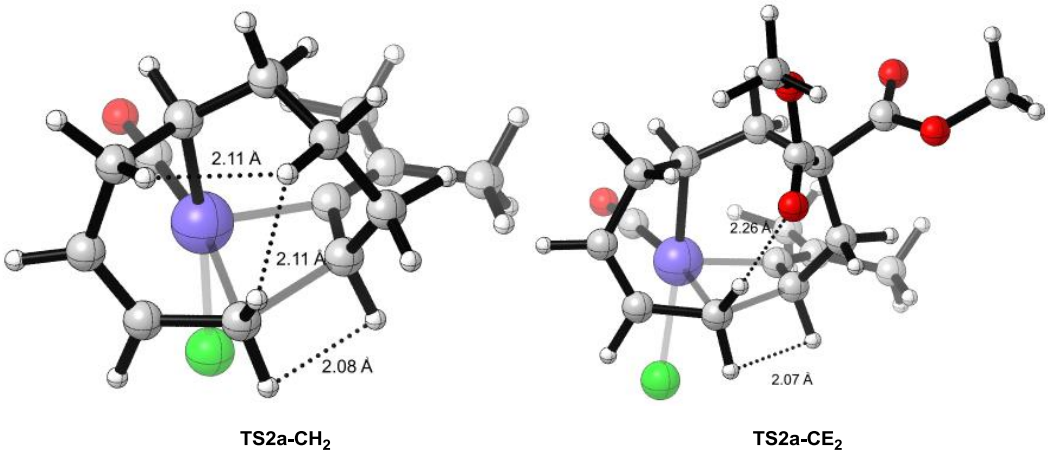


Figure S8. DFT-calculated structures of transition states **TS2a-CH_2** and **TS2a-CE_2** (C gray; H white; O red; Rh purple; Cl green).

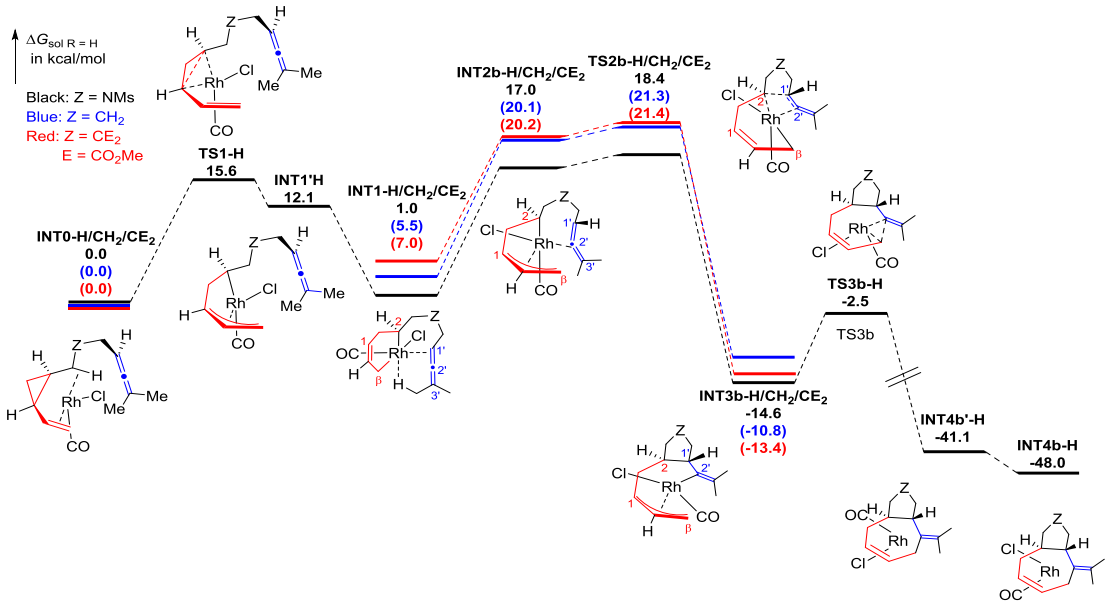


Figure S9. DFT-calculated free energy surfaces of normal [5+2] pathway when Z = NMs, CH_2 and CE_2 (E = CO_2Me).

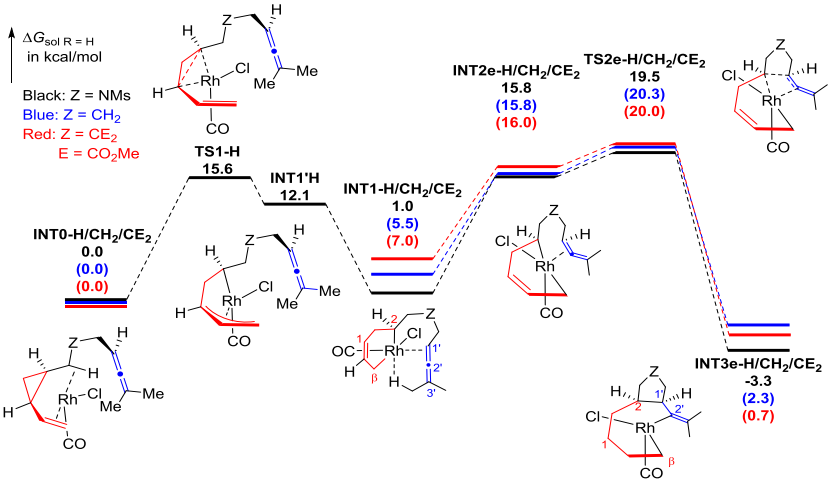


Figure S10. DFT-calculated free energy surfaces of *cis* insertion pathway when Z = NMs, CH_2 and CE_2 (E = CO_2Me).

We also checked how the computational methods affect the calculation results (Table S5). At the B3LYP level using a larger basis set (6-311+G(d,p) for all elements and SDD pseudopotential and basis set for Rh), **TS2a-H** is a little higher in energy than **TS2b-H** (about 1.0 kcal/mol in the gas phase and 2.0 kcal/mol in dioxane solution), which is not consistent with the experimental results. However, single point energy calculations using B3LYP-D3[30] with the above mentioned lager basis set in both gas phase and solution showed that **TS2a-H** is favored by 2.1 and 1.1 kcal/mol, respectively. This suggested that dispersion energy calculations are critical to understand the regiochemistry. M06-2X calculations to consider the dispersion effects also showed that **TS2a-H** is lower in energy than **TS2b-H** by about 3.3 kcal/mol in dioxane solution. Therefore, single-point energies and solvent effects were computed at the M06-2X level of theory with the SDD basis set and pseudopotential for Rh and the 6-311+G(d,p) basis set for the other atoms in the present investigation.

Table S5: Calculation results using different computational methods (*ΔG* in kcal/mol, others in Hartree/Particle)

	ΔG ***(TS2a-TS2b)***	***G*** ***TS2a-H***	***G*** ***TS2b-H***
B3LYP/6-31G(d)/LANL2DZ in the gas phase	0.1	-1794.038040	-1794.038144
B3LYP/6-311+G(d,p)/SDD//B3LYP/6-31G(d)/LANL2DZ in the gas phase	1.0	-1795.424854	-1795.426428
B3LYP/6-311+G(d,p)/SDD//B3LYP/6-31G(d)/LANL2DZ in dioxane	2.0	-1795.445763	-1795.448914
B3LYP-D3/6-311+G(d,p)/SDD//B3LYP/6-31G(d)/LANL2DZ In the gas phase	-2.1	-1795.540759	-1795.537462
B3LYP-D3/6-311+G(d,p)/SDD//B3LYP/6-31G(d)/LANL2DZ in dioxane	-1.1	-1795.561668	-1795.559948
M06-2X/6-311+G(d,p)/SDD//B3LYP/6-31G(d)/LANL2DZ in dioxane	-3.3	-1794.876671	-1794.871351
M06-2X/6-311+G(d,p)/SDD//M06-2X/6-31G(d)/LANL2DZ in dioxane	-2.9	-1794.877037	-1794.872453

6.2 Computed Energies of All Stationary Points

Table S6: Sum of electronic and thermal enthalpies (***H***, in Hartree), sum of electronic and thermal free energies (***G***, in Hartree), thermal correction to enthalpies (***TCH***, in Hartree), thermal correction to Gibbs free energy (***TCG***, in Hartree), and total energy in dioxane with non-electrostatic terms (E_{sol}, in Hartree).

	TCH	***TCG***	***H***	***G***	E_{sol}
1m	0.343444	0.271121	-1110.881533	-1110.953856	-1111.130086
2m	0.347493	0.282858	-1110.951084	-1111.015719	-1111.210132
INT0-H	0.360349	0.274595	-1793.978268	-1794.064022	-1795.175537
TS1-H	0.359015	0.275168	-1793.964724	-1794.048571	-1795.151258
INT1'-H	0.359828	0.273850	-1793.970840	-1794.056818	-1795.155549
INT1-H	0.359733	0.277549	-1793.978797	-1794.060982	-1795.176935
INT2a-H	0.360214	0.280853	-1793.979553	-1794.058914	-1795.172909
TS2a-H	0.360183	0.283565	-1793.961422	-1794.038040	-1795.160236
INT3a'-H	0.363030	0.286078	-1793.998405	-1794.075357	-1795.202112
INT3a-H	0.362954	0.285776	-1794.004751	-1794.081929	-1795.210002
TS3a-H	0.361456	0.286873	-1793.977499	-1794.052081	-1795.179543
INT4a'-H	0.364898	0.288092	-1794.055567	-1794.132374	-1795.269164
INT4a-H	0.365052	0.288434	-1794.066554	-1794.143171	-1795.278277
INT2b-H	0.359200	0.278079	-1793.962167	-1794.043289	-1795.151884
TS2b-H	0.358577	0.279937	-1793.960970	-1794.039610	-1795.151503
INT3b-H	0.362629	0.283476	-1794.009168	-1794.088320	-1795.207685
TS3b-H	0.361127	0.282988	-1793.988619	-1794.066757	-1795.187843
INT4b'-H	0.364297	0.286804	-1794.043631	-1794.121124	-1795.253194

INT4b-H	0.364587	0.286103	-1794.053810	-1794.132294	-1795.263531
TS2c-H	0.358876	0.281707	-1793.939050	-1794.016219	-1795.133868
TS2d-H	0.358834	0.281417	-1793.932688	-1794.010105	-1795.122702
INT2e-H	0.357807	0.278328	-1793.960159	-1794.039638	-1795.154077
TS2e-H	0.358206	0.279374	-1793.951649	-1794.030481	-1795.149284
INT3e-H	0.361165	0.361165	-1793.984926	-1793.984926	-1795.187737
TS2f-H	0.359534	0.281325	-1793.955558	-1794.033766	-1795.149533
INT1-Ph	0.445714	0.353759	-2024.946447	-2025.038402	-2026.199956
INT2a-Ph	0.445536	0.354338	-2024.939797	-2025.030995	-2026.190342
TS2a-Ph	0.445684	0.357631	-2024.918912	-2025.006966	-2026.176342
INT3a-Ph	0.448832	0.359724	-2024.968735	-2025.057844	-2026.231993
INT2b-Ph	0.445007	0.352496	-2024.929037	-2025.021549	-2026.173875
TS2b-Ph	0.444546	0.354198	-2024.927246	-2025.017594	-2026.173401
INT3b-Ph	0.448306	0.358572	-2024.974831	-2025.064565	-2026.230236
TS2c-Ph	0.444614	0.356192	-2024.899693	-2024.988115	-2026.152328
TS2d-Ph	0.444811	0.356220	-2024.898266	-2024.986857	-2026.143816
TS2e-Ph	0.444500	0.354972	-2024.917978	-2025.007506	-2026.171624
TS2f-Ph	0.445114	0.355855	-2024.915294	-2025.004552	-2026.168389
INT0-CH_2	0.328993	0.252962	-1190.102058	-1190.178089	-1191.267439
INT1-CH_2	0.328397	0.258677	-1190.100346	-1190.170067	-1191.264355
INT2a-CH_2	0.328785	0.260235	-1190.097671	-1190.166220	-1191.257568
TS2a-CH_2	0.329071	0.264112	-1190.079342	-1190.144300	-1191.245288
INT3a'-CH_2	0.331609	0.266026	-1190.114550	-1190.180134	-1191.284600
INT3a-CH_2	0.331499	0.265376	-1190.121263	-1190.187386	-1191.292226
INT0-CE_2	0.423859	0.325309	-1645.738486	-1645.837037	-1646.989816
INT1-CE_2	0.423324	0.332511	-1645.735960	-1645.826773	-1646.985886
INT2a-CE_2	0.423908	0.333895	-1645.730552	-1645.820565	-1646.975154
TS2a-CE_2	0.423919	0.337222	-1645.712250	-1645.798947	-1646.963526
INT3a'-CE_2	0.426490	0.338910	-1645.745453	-1645.833033	-1647.001187
INT3a-CE_2	0.426591	0.339458	-1645.750968	-1645.838102	-1647.007730
INT2b-CH_2	0.327633	0.258296	-1190.083893	-1190.153230	-1191.240695
TS2b-CH_2	0.327066	0.259525	-1190.082197	-1190.149738	-1191.240051
INT3b-CH_2	0.331047	0.263211	-1190.129107	-1190.196943	-1191.294912
INT2b-CE_2	0.422562	0.331427	-1645.721554	-1645.812689	-1646.963807
TS2b-CE_2	0.422112	0.332955	-1645.720643	-1645.809801	-1646.963305
INT3b-CE_2	0.426043	0.336799	-1645.772064	-1645.861308	-1647.022683
INT2e-CH_2	0.326521	0.258400	-1190.087345	-1190.155467	-1191.247646
TS2e-CH_2	0.327164	0.260398	-1190.077816	-1190.144581	-1191.242518
INT3e-CH_2	0.329777	0.262058	-1190.103805	-1190.171525	-1191.272859
INT2e-CE_2	0.421361	0.330541	-1645.724083	-1645.814904	-1646.969628
TS2e-CE_2	0.421981	0.332562	-1645.716211	-1645.716211	-1646.965194
INT3e-CE_2	0.424797	0.335189	-1645.745462	-1645.835070	-1646.998536

6.3 Coordinates of All Stationary Points

1m

C	-4.52489000	-1.18026800	-0.33790300
C	-5.83357500	-1.07085700	-0.09261900
C	-3.48962500	-1.35919600	0.70654600
C	-2.13419000	-0.65655600	0.64957200
C	-2.21978400	-2.14152600	0.41689100
H	-3.89585900	-1.47303100	1.70991600
H	-2.08931800	-2.50403700	-0.60110900
H	-1.84952600	-2.82313900	1.17818300
H	-2.12494200	-0.07087900	-1.43261400
C	-1.79271200	0.32180600	-0.46289000
H	-2.31436500	1.26916300	-0.31071000
H	1.30128300	0.10844900	-1.74344600
C	0.57834600	-0.38260700	-1.08973000
H	-0.02368200	-1.06085900	-1.70768500
C	1.30585300	-1.17477400	-0.01638400
H	0.67619600	-1.68430500	0.71490200
H	-6.55542100	-0.95071000	-0.89502400
H	-6.23017400	-1.09916200	0.92010400
H	-4.17978700	-1.15217700	-1.37142400
H	-1.75237800	-0.34948600	1.62251000
N	-0.36071700	0.62777100	-0.57575300
S	0.22597400	2.13437000	-0.14286700
O	1.44184400	2.37083200	-0.92569900
O	-0.89849200	3.07466400	-0.17420800
C	2.61147800	-1.27834800	0.05350400
C	3.91832100	-1.38622500	0.09790200
C	0.73814000	1.98657200	1.58444700
H	1.17553500	2.94474100	1.87584200
H	-0.13914300	1.77128400	2.19805000
H	1.47599400	1.18607500	1.66127100
C	4.64772700	-2.49595600	-0.63236000
H	5.22839600	-3.10581200	0.07310500
H	3.95723900	-3.15226400	-1.16835800
H	5.36028600	-2.07737000	-1.35573000
C	4.77864600	-0.41300500	0.87723000
H	5.50437900	0.07440300	0.21282400
H	4.18120200	0.36546500	1.35847000
H	5.35428800	-0.93899400	1.65108500

2m

C	-0.55840400	2.45357800	0.66785600
C	-1.03560400	1.41655200	1.65614400

C	-0.55841500	2.45324700	-0.66898400
C	-1.02332800	-0.08521000	-1.27394800
C	-1.03563700	1.41573500	-1.65675200
H	-0.19498000	3.36294400	-1.14734400
H	-0.44727300	1.52714300	-2.57865600
H	-2.06933400	1.67049900	-1.94088500
C	-1.02332100	-0.08457300	1.27406200
H	-1.49364100	-0.60258600	2.11514000
H	-2.06929000	1.67147000	1.94018000
H	-0.44721400	1.52840300	2.57797800
H	-0.19496100	3.36351300	1.14575900
H	-1.49369600	-0.60359900	-2.11477400
N	1.09566800	-0.26806000	0.00008500
C	-1.80436400	-0.38385200	0.00012400
C	-3.08128000	-0.82686900	0.00018200
C	-3.89674700	-1.09865000	-1.24751500
H	-4.24376000	-2.14171200	-1.25844900
H	-4.80193400	-0.47554100	-1.25199500
H	-3.37047600	-0.91401000	-2.18511200
C	-3.89703400	-1.09781200	1.24789300
H	-4.80316300	-0.47607100	1.25077500
H	-4.24249200	-2.14137900	1.26040700
H	-3.37162100	-0.91074800	2.18548100
C	0.40306100	-0.67444100	1.22194400
H	0.32828800	-1.77606900	1.27336800
H	0.98137900	-0.32600500	2.07980500
C	0.40305100	-0.67505000	-1.22156300
H	0.98135300	-0.32703100	-2.07960500
H	0.32827900	-1.77670300	-1.27244400
S	2.76977100	-0.20875200	0.00005200
O	3.17565500	0.37634600	1.27941200
O	3.17562700	0.37591400	-1.27951400
C	3.34505700	-1.92774900	0.00032800
H	4.43718700	-1.90174500	0.00030100
H	2.98445000	-2.43076700	0.90052400
H	2.98441800	-2.43106600	-0.89968900

INT0-H

Rh	2.11552800	0.54724500	-0.20053300
C	1.56321300	1.64366800	1.65120400
C	1.25263600	2.40809400	0.51742000
C	0.61265300	0.84739300	2.49325600
C	-0.31115600	-0.26805000	1.99436000
C	-0.89553300	1.04155900	2.42870400

H	1.01772700	0.65088300	3.48205200
H	-1.27553500	1.71096400	1.66113100
H	-1.44141500	1.08778700	3.36730300
H	-0.14283700	0.17962300	-0.12476800
C	-0.25156800	-0.70356700	0.54076300
H	0.62124200	-1.35503300	0.41626000
H	-2.99248900	-0.30499200	0.90411500
C	-2.70257200	-0.72860700	-0.06473700
H	-3.44624300	-1.48592000	-0.32588500
C	-2.67500900	0.35282400	-1.12648500
H	-2.29644200	0.04438300	-2.10349400
H	1.88912600	3.24137000	0.23494800
H	0.23720500	2.46990800	0.13208300
H	2.49011400	1.88085900	2.16862100
H	-0.41509000	-1.11061300	2.67304900
N	-1.40939200	-1.42859300	0.02788200
S	-1.38237500	-3.11715700	0.21473600
O	-0.55929000	-3.44235000	1.38616600
O	-2.76876100	-3.58202600	0.11402800
C	3.75970800	1.27860800	-0.41808700
O	4.80179900	1.74999100	-0.55246100
Cl	2.64505800	-1.28130900	-1.60168900
C	-0.48504500	-3.66485300	-1.24830200
H	-0.35513400	-4.74586600	-1.15499300
H	-1.08370500	-3.42400000	-2.12830700
H	0.48614600	-3.16492400	-1.29136300
C	-3.12906400	1.57206900	-0.95506600
C	-3.64042900	2.77200400	-0.80634600
C	-5.11232600	3.03428600	-1.05988000
H	-5.23783300	3.78627100	-1.85045600
H	-5.64090500	2.12615100	-1.35987700
H	-5.59372900	3.43439100	-0.15736700
C	-2.81293800	3.96979600	-0.38907200
H	-3.20143700	4.40526300	0.54140000
H	-1.76132200	3.71237600	-0.23658100
H	-2.86383600	4.75575100	-1.15437400

TS1-H

C	-1.14960900	-0.89763500	2.12377300
C	-0.34706200	0.46400900	0.87972000
Rh	-2.20336100	-0.59369800	0.04325900
C	-3.73942300	-1.32157600	-0.85866700
O	-4.67514200	-1.74849000	-1.36613900
Cl	-2.87422800	1.58223800	-0.73707500

C	-1.21982900	-2.53018100	0.26735500
H	-0.18589800	-2.37455800	-0.02824800
H	-1.70122900	-3.38504000	-0.19708300
C	-1.71872800	-2.05760400	1.50159300
H	-2.60203700	-2.49819400	1.95482600
H	-1.77268500	-0.39046900	2.85645100
C	0.24278200	-0.39025000	1.97648200
H	0.94870100	-1.14702300	1.62879300
H	0.63778600	0.14049400	2.84441800
H	-0.74848200	1.40012300	1.25115700
C	0.41745400	0.61305600	-0.44371100
H	-0.22693700	1.08918900	-1.18233100
H	0.71961100	-0.35481500	-0.85339700
C	3.32201500	-0.31393200	-0.98418000
H	3.44978200	0.07808300	-1.99492700
C	2.91095400	0.70239000	0.05828000
H	3.68213500	1.47404100	0.13250700
H	2.82012400	0.22590900	1.04149700
N	1.66883300	1.39842200	-0.34551300
S	1.56082300	3.03294200	0.13357600
O	2.90849300	3.58915100	-0.03320900
O	0.88489500	3.18023600	1.43231600
C	0.48076200	3.72727400	-1.12921900
H	0.44013700	4.79794300	-0.91469700
H	0.92393300	3.55077500	-2.11035700
H	-0.52072500	3.29689400	-1.05289700
C	3.56468200	-1.57849800	-0.73377500
C	3.85004900	-2.83501500	-0.48306700
C	2.82051900	-3.93906600	-0.61095200
H	3.15759600	-4.69603500	-1.33167000
H	2.67950000	-4.45418400	0.34899600
H	1.85218700	-3.55804300	-0.94710300
C	5.24250200	-3.26087900	-0.06154000
H	5.21495400	-3.76039900	0.91631800
H	5.65697700	-3.98265300	-0.77815500
H	5.92429700	-2.40944500	0.00461100

INT1’-H

C	-1.12008400	-1.68448900	1.73907400
C	-0.32163900	0.25141500	0.58911200
Rh	-2.23975500	-0.47888800	0.12795200
C	-4.21506600	-1.01561100	-0.13721200
O	-5.33557900	-1.17370800	-0.29242400
Cl	-2.69287800	1.48168600	-1.13303800

C	-1.34977200	-2.25607700	-0.62119100
H	-0.33238300	-2.01762400	-0.91559100
H	-1.93015700	-2.76410000	-1.38646400
C	-1.67215400	-2.50736100	0.75414400
H	-2.51033800	-3.15186100	1.00718500
H	-1.55620000	-1.72086800	2.73482300
C	0.15183400	-0.87716000	1.51115600
H	0.92007700	-1.51007000	1.04958000
H	0.55438900	-0.51338700	2.46270800
H	-0.60381500	1.13376200	1.16928100
C	0.56322300	0.65856200	-0.58590400
H	-0.03532800	1.23537000	-1.29242500
H	0.92899200	-0.21896900	-1.13029900
C	3.51883000	-0.22955000	-0.79902800
H	3.79896300	0.23841000	-1.74474900
C	2.96093400	0.71071100	0.24747300
H	3.71356500	1.46570100	0.49003900
H	2.72882400	0.16163800	1.16847900
N	1.78839500	1.44164100	-0.28051400
S	1.58995700	3.01950700	0.31870600
O	2.93969300	3.58576300	0.43556100
O	0.69575600	3.06507600	1.48732600
C	0.74003700	3.83764300	-1.04410700
H	0.66477600	4.88707500	-0.74937400
H	1.34113900	3.73610600	-1.94866000
H	-0.25963000	3.41799300	-1.17356100
C	3.70532700	-1.51578000	-0.62396800
C	3.92618700	-2.79728500	-0.44287900
C	2.90539700	-3.85281900	-0.81686500
H	3.32312700	-4.54638400	-1.55917000
H	2.62797500	-4.45469900	0.05938100
H	1.99697900	-3.41191500	-1.23699900
C	5.23116100	-3.30304900	0.13932900
H	5.04864200	-3.87954400	1.05646500
H	5.73246700	-3.97768600	-0.56790700
H	5.91352200	-2.48320000	0.37686100

INT1-H

C	0.38412200	-1.61946500	0.23912900
C	0.14004600	1.23927700	-0.93074700
Rh	-1.35178600	-0.37180800	0.21544100
C	-1.91401700	-1.14844300	-1.67196700
H	-1.40654300	-0.49248700	-2.38943800
H	-2.99185000	-0.95678600	-1.74281800

C	-1.58441500	-2.58070800	-1.91729100
H	-2.37524100	-3.23140900	-2.29202700
C	-0.36561200	-3.08881400	-1.68875600
H	-0.15534700	-4.13528400	-1.89699500
C	0.73800900	-2.23595300	-1.11690600
H	1.04177200	-1.44832000	-1.81848700
H	1.64341900	-2.84133700	-0.95958300
H	0.09615200	-2.41702900	0.93014800
N	2.10612100	0.21639300	0.09573600
H	0.35798600	0.69140700	-1.84704400
C	-1.03121800	1.86452600	-0.81068800
C	-2.08953000	2.64144800	-0.80974000
C	-3.42005200	2.27126600	-0.19821500
H	-3.44041200	1.25283300	0.20013500
H	-3.64917200	2.94700200	0.63442600
H	-4.21885200	2.37041000	-0.94428100
C	-1.99875700	4.01725400	-1.44310000
H	-2.74242300	4.11588800	-2.24423000
H	-2.21970100	4.78853100	-0.69420500
H	-1.00899200	4.21443100	-1.86231900
C	-2.27159200	-1.75431200	1.07091900
Cl	-1.18535500	0.84277400	2.40420700
O	-2.83937200	-2.58998300	1.61271200
S	3.76643000	0.25835700	-0.13683100
O	4.20891800	-1.13097200	-0.27722000
O	4.02296200	1.25642100	-1.17778300
C	4.47542200	0.89167900	1.40230200
H	4.09413200	1.89874700	1.58502100
H	4.20883000	0.22106200	2.22202300
H	5.56027000	0.91730100	1.27525000
C	1.33646200	1.45737800	-0.02252900
H	1.00228400	1.81777000	0.95682000
H	1.98006200	2.20752700	-0.49267000
C	1.52636200	-0.85480000	0.91407000
H	2.31832900	-1.59172800	1.09451800
H	1.18951200	-0.45849800	1.87798800

INT2a-H

O	-3.72517500	-0.44119500	1.71799400
C	-2.74383000	-0.41613300	1.12781700
Rh	-1.17837700	-0.55860000	-0.02279100
C	-0.64045300	-2.67960000	-0.60039400
C	0.18935300	-1.80776400	-1.34545500
C	-0.60352500	-2.66464100	0.79936300

C	0.23822500	-0.53533500	1.56135100
C	0.54098600	-2.03886000	1.59063500
H	-1.35833200	-3.23726000	1.33347100
H	1.50373400	-2.26279500	1.11785800
H	0.57752900	-2.44446200	2.60836500
Cl	-2.90151900	-0.70794000	-1.89110700
H	1.09203100	1.44459600	1.58930700
C	1.41511600	0.41482500	1.38490700
H	2.19548400	0.15699500	2.11075100
H	1.90764900	0.95383100	-1.94534100
C	1.41053900	1.20288300	-1.00699700
H	1.60152800	2.26682600	-0.78473600
C	-0.10281300	1.04018300	-1.19739900
H	-0.43332300	0.80663400	-2.20749300
H	-0.02073200	-1.69930500	-2.40411700
H	1.19728700	-1.58174400	-1.02387600
H	-1.48404000	-3.15392900	-1.09345300
H	-0.30462700	-0.23706400	2.46185400
N	2.01126400	0.35798400	0.03895600
C	-1.00487400	1.60837600	-0.32600800
C	-1.53383500	2.71534500	0.17800300
C	-2.48827400	2.81696300	1.33996100
H	-2.21491400	3.66637300	1.97885200
H	-3.51246100	3.00032000	0.98803000
H	-2.49723100	1.92021000	1.95939800
C	-1.20835500	4.04341100	-0.48664100
H	-2.13034500	4.51948200	-0.84668700
H	-0.75070800	4.73779000	0.23124400
H	-0.53495800	3.92643300	-1.33952900
S	3.64012000	-0.02182500	-0.11150000
O	3.93713300	-1.01089300	0.92911600
O	3.87571400	-0.31089800	-1.52798200
C	4.56903700	1.47705300	0.29517100
H	4.30141400	2.26771900	-0.40922700
H	4.34158500	1.77274600	1.32167900
H	5.63028800	1.23553900	0.20044900

TS2a-H

O	-3.37012800	-0.57604200	2.32255700
C	-2.60026600	-0.54149000	1.46852300
Rh	-1.38064600	-0.54453100	0.06693100
C	-0.59630900	-2.23481700	-1.23130000
C	0.09089600	-1.01988700	-1.75510000
C	-0.32798200	-2.83684800	-0.02968100

C	0.26795700	-0.90010600	1.39404100
C	0.69769900	-2.31833600	0.96396900
H	-0.88289000	-3.74096700	0.21231800
H	1.69575900	-2.31328600	0.50897600
H	0.75340000	-2.99193100	1.82572600
Cl	-3.24324300	-0.41229400	-1.60778200
H	0.99335000	1.11769800	1.72164500
C	1.38338900	0.14533500	1.39544600
H	2.14691100	-0.17085000	2.11565200
H	2.05136500	1.07031700	-1.83212700
C	1.47100000	1.19313500	-0.91561800
H	1.54255300	2.24551200	-0.59918200
C	-0.01025300	0.91108100	-1.21246700
H	-0.29196400	1.19440400	-2.22573200
H	-0.22112200	-0.82892300	-2.77633300
H	1.16758800	-1.05658900	-1.62616800
H	-1.39388800	-2.63371900	-1.85026000
H	-0.14271900	-0.92347400	2.40637700
N	2.05501000	0.30401200	0.09089500
C	-0.96949400	1.38683200	-0.21974900
C	-1.39229400	2.59418800	0.15503200
C	-2.44011000	2.85214800	1.20786100
H	-2.08126600	3.58952000	1.93924100
H	-3.34544800	3.27273600	0.74970000
H	-2.72777700	1.94925400	1.74603900
C	-0.86975800	3.85330800	-0.51476600
H	-1.70837000	4.43241900	-0.92431300
H	-0.35999900	4.50682900	0.20711700
H	-0.17847400	3.64843000	-1.33679900
S	3.69750300	-0.02868800	-0.03233300
O	3.98031500	-1.12728000	0.89481500
O	3.99936600	-0.14014400	-1.46228700
C	4.56337200	1.43252300	0.58998100
H	4.30526200	2.29381300	-0.03011200
H	4.27881200	1.59911700	1.63111800
H	5.63451400	1.22885800	0.52088100

INT3a'-H

O	-2.17054400	0.32204500	2.99649700
C	-1.96489400	-0.02132000	1.92022100
Rh	-1.50038000	-0.67983200	0.22837000
C	-0.54422200	-1.07553300	-1.99351300
C	0.46441500	0.03647400	-2.18070900
C	-0.38953300	-2.16622800	-1.18663700

C	0.38466200	-1.32954500	0.95830800
C	0.73651500	-2.31841600	-0.17666800
H	-1.14608700	-2.94790300	-1.24961200
H	1.70896500	-2.08778800	-0.62114800
H	0.77969800	-3.34913800	0.18940100
Cl	-3.74274900	-1.12953200	-0.68882300
H	1.12953000	0.38059200	2.07286900
C	1.50922200	-0.38196700	1.37793800
H	2.25967000	-0.97466000	1.91363400
H	2.35285700	1.90537100	-0.99579200
C	1.59707500	1.47323000	-0.33676800
H	1.36098700	2.20784600	0.44763700
C	0.31731700	1.23812800	-1.19007700
H	0.25927600	2.13813000	-1.81087600
H	0.35062600	0.41188400	-3.20253200
H	1.47913700	-0.36594200	-2.10329000
H	-1.42604700	-1.05376000	-2.62964800
H	0.07411100	-1.86968600	1.86179600
N	2.18935700	0.27811100	0.25998800
C	-0.97205500	1.21180500	-0.39034800
C	-1.78658600	2.26961700	-0.22418600
C	-3.14009100	2.27584800	0.45859500
H	-3.06390100	2.64644000	1.49067900
H	-3.80656600	2.96856300	-0.07000900
H	-3.62495900	1.29893700	0.45626500
C	-1.43982700	3.66086300	-0.74579900
H	-2.09711900	3.92878200	-1.58425700
H	-1.62714300	4.39823700	0.04564400
H	-0.40563500	3.78842800	-1.06892000
S	3.82794700	-0.00777300	0.02661600
O	4.08196200	-1.39257100	0.43348100
O	4.15797500	0.46392900	-1.32127600
C	4.69966800	1.06210900	1.19688300
H	4.45765400	2.10411000	0.97665500
H	4.40104000	0.79743500	2.21350300
H	5.76994000	0.88855900	1.06253000

INT3a-H

O	2.19415000	-0.17999000	-2.88475400
C	1.98565800	-0.24715600	-1.75898900
Rh	1.54870400	-0.44146100	0.05805200
C	0.49762200	-0.04420700	2.29401600
C	-0.61705800	0.95472500	2.04124900
C	0.51440200	-1.36541900	1.94782400

C	-0.18870800	-1.52631000	-0.38763500
C	-0.51301600	-2.01758300	1.02923400
H	1.30468100	-1.99951600	2.33804800
H	-1.53662900	-1.75997800	1.31745400
H	-0.40089100	-3.10368000	1.08027800
Cl	2.83416200	-2.58017300	0.08166900
C	-0.43956100	1.77598500	0.72595400
H	-0.54516200	2.83760200	0.97766700
H	-0.63194700	1.64435900	2.89183000
H	-1.58297500	0.44184700	2.03423000
H	1.30588000	0.30088100	2.93790600
H	0.22533700	-2.32243900	-1.00818200
N	-2.07102800	0.15861600	-0.41275200
S	-3.70268800	-0.14244100	-0.14360200
O	-3.85176400	-1.59576600	-0.02564900
O	-4.13459100	0.76034500	0.92639800
C	-4.56445300	0.36340800	-1.65196900
H	-4.19836000	-0.23369900	-2.48993100
H	-5.62973400	0.17798600	-1.49568300
H	-4.38974600	1.42765300	-1.82371900
C	0.95093300	1.54269100	0.17473800
C	1.86212400	2.51848900	-0.01873100
C	3.30035100	2.27353100	-0.44140400
H	3.49187900	2.66564200	-1.45065200
H	3.98595700	2.80393600	0.23339600
H	3.59802500	1.22033000	-0.42571100
C	1.60587800	4.00300200	0.18839100
H	2.20305500	4.38857600	1.02665900
H	1.92705700	4.56113800	-0.70201900
H	0.56183300	4.26092100	0.37420400
C	-1.29435100	-0.82568500	-1.16522000
H	-0.88697400	-0.35752500	-2.07182600
H	-1.98034400	-1.61952800	-1.48750100
C	-1.58684200	1.53593100	-0.29875800
H	-2.43734800	2.14445300	0.01451600
H	-1.25608600	1.89333300	-1.28493500

TS3a-H

O	3.90045900	1.52268500	-1.48111900
C	3.08751700	0.90920300	-0.95443600
Rh	1.89149700	-0.31673900	-0.07310200
C	0.73698800	-1.87461600	1.14795100
C	-0.41550700	-1.18003900	1.84619000
C	0.75922600	-2.21846300	-0.18914600

C	-0.12824000	-0.12584100	-1.20604800
C	-0.23806200	-1.67546800	-1.18612600
H	1.49694400	-2.94199000	-0.52513300
H	-1.26119200	-1.98742300	-0.94269500
H	-0.00975400	-2.06006700	-2.18567300
Cl	3.92669000	-1.48366800	0.40329400
C	-0.54462600	0.35531300	1.63038100
H	-0.33426100	0.84217000	2.58917500
H	-0.32642100	-1.37416300	2.91923500
H	-1.34971900	-1.65786600	1.52660000
H	1.48638100	-2.34100700	1.78214000
H	0.37362200	0.24150100	-2.10065200
N	-2.35037500	0.14975700	-0.03944000
S	-3.88586700	-0.47931900	-0.28618000
O	-3.83251700	-1.25583900	-1.52798600
O	-4.30497300	-1.08606600	0.97913700
C	-4.96837200	0.93760000	-0.58874500
H	-4.62228900	1.46561900	-1.47996700
H	-5.97673300	0.54937900	-0.75040600
H	-4.95396400	1.59175500	0.28580300
C	0.39197500	0.96750500	0.58471600
C	0.51840600	2.31617200	0.45287200
C	1.07967000	3.03818500	-0.75044400
H	1.19474900	2.39710000	-1.62590100
H	0.40388600	3.85870000	-1.03095100
H	2.05178500	3.50377400	-0.53698300
C	0.06911600	3.29782400	1.52237100
H	0.87397100	4.02111200	1.71075500
H	-0.79910800	3.88663300	1.19018300
H	-0.18397200	2.83620900	2.47847000
C	-1.52717800	0.52680900	-1.19083400
H	-1.44930000	1.61753500	-1.27079200
H	-2.03590000	0.15026600	-2.08598100
C	-2.00588200	0.71660600	1.26747400
H	-2.69118400	0.29758000	2.00721300
H	-2.12610600	1.80863000	1.25680600

INT4a'-H

O	4.50275500	1.67406300	-0.00077300
C	3.59429600	0.96965100	-0.00047400
Rh	2.14012500	-0.24463900	0.00003100
C	0.61961500	-1.90122500	0.68668800
C	-0.50186900	-1.27047200	1.48416600
C	0.61963200	-1.90124800	-0.68663800

C	-0.60317800	0.26769000	-1.27655300
C	-0.50166800	-1.27027600	-1.48417900
H	1.33572800	-2.53103400	-1.20657000
H	-1.44964800	-1.74578800	-1.19668300
H	-0.36136400	-1.47576000	-2.54952700
Cl	3.83125000	-1.92172400	0.00001200
C	-0.60333200	0.26752400	1.27678700
H	-0.14432400	0.74746900	2.14146000
H	-0.36176900	-1.47618300	2.54949500
H	-1.44976800	-1.74593900	1.19635700
H	1.33571500	-2.53100400	1.20662700
H	-0.14404800	0.74773700	-2.14110100
N	-2.70874500	0.29160200	-0.00000300
S	-4.26397600	-0.32219600	-0.00009600
O	-4.44378300	-1.01100600	-1.27993700
O	-4.44401800	-1.01079300	1.27982900
C	-5.37371100	1.10602100	-0.00033100
H	-5.19541300	1.69786700	-0.90088100
H	-6.39706600	0.72325100	-0.00042600
H	-5.19563200	1.69799300	0.90018000
C	0.10237200	0.74553000	0.00019600
C	0.95225200	1.85438300	0.00030000
C	1.27262900	2.64528900	-1.26082200
H	1.31606100	2.03829400	-2.16556500
H	0.51050600	3.42549100	-1.40685000
H	2.23446800	3.15660800	-1.16220000
C	1.27301800	2.64473500	1.26166500
H	2.23502600	3.15575700	1.16306600
H	0.51120400	3.42517200	1.40807500
H	1.31639800	2.03739300	2.16617600
C	-2.07512900	0.74459100	-1.23844200
H	-2.10713400	1.84467800	-1.30445400
H	-2.62565800	0.32851700	-2.08454700
C	-2.07524200	0.74452100	1.23851700
H	-2.62589800	0.32844600	2.08453600
H	-2.10718200	1.84460600	1.30456500

INT4a-H

Rh	2.14309500	-0.38219500	0.00007100
C	0.62201900	-1.79342700	0.70326800
C	-0.48683900	-1.14844000	1.50923800
C	0.62210100	-1.79331500	-0.70355000
C	-0.64399900	0.37862800	-1.27696500
C	-0.48667000	-1.14820400	-1.50954100

H	1.14949100	-2.59958900	-1.20960200
H	-1.42857300	-1.66214200	-1.26728300
H	-0.30907800	-1.32177200	-2.57578600
C	-0.64410400	0.37844000	1.27692100
H	-0.21122100	0.88958800	2.13680200
H	-0.30938400	-1.32220500	2.57547400
H	-1.42872300	-1.66231200	1.26676800
H	1.14934900	-2.59978500	1.20925000
H	-0.21107300	0.88993000	-2.13673100
N	-2.74752000	0.30643600	-0.00009600
S	-4.27106900	-0.38002500	-0.00018900
O	-4.41851700	-1.07713000	-1.27997700
O	-4.41859200	-1.07731200	1.27949100
C	-5.44772500	0.99345400	-0.00012400
H	-5.29704800	1.59309000	-0.90048900
H	-6.45186100	0.56281800	-0.00018100
H	-5.29709700	1.59296500	0.90033100
C	0.04036000	0.87823200	0.00004400
C	0.91347600	1.94512900	0.00016200
C	1.35505000	2.67951800	-1.25011700
H	1.22873300	2.11971800	-2.17716700
H	0.77958500	3.61342700	-1.33324600
H	2.41192400	2.94462000	-1.16702000
C	1.35496100	2.67929700	1.25059400
H	2.41187800	2.94429500	1.16767700
H	0.77958700	3.61325800	1.33375700
H	1.22844300	2.11939100	2.17755400
C	-2.13492000	0.79242000	-1.23605500
H	-2.21177600	1.89032000	-1.29466500
H	-2.66749500	0.35855300	-2.08467400
C	-2.13501000	0.79226900	1.23596600
H	-2.66765300	0.35830600	2.08449300
H	-2.21185500	1.89016400	1.29470100
Cl	4.06402500	1.09518200	0.00029400
C	3.45236200	-1.68982300	0.00003800
O	4.25205000	-2.51576600	0.00002000

INT2b-H

C	0.60342300	-1.53949100	0.32285100
C	0.26395700	0.94934400	-0.38942100
Rh	-1.31810200	-0.50915600	0.11725000
C	-1.43037100	-0.95760500	-1.95227000
H	-0.63160300	-0.40252300	-2.45012100
H	-2.39132300	-0.64092600	-2.35888200

C	-1.22347400	-2.41861500	-1.98924800
H	-2.04448100	-3.04926700	-2.32976400
C	-0.06828700	-2.99798700	-1.60427200
H	0.04748900	-4.07696600	-1.68226500
C	1.05553300	-2.21135100	-0.97400400
H	1.46566400	-1.47696000	-1.68224200
H	1.90114900	-2.87125800	-0.73589500
H	-0.00742900	-2.25061000	0.90044900
N	2.26931200	0.29308100	0.91227400
H	0.74200700	0.65779500	-1.32233500
C	-1.04358900	1.45603900	-0.44164800
C	-1.74864600	2.55476900	-0.68743700
C	-3.24594600	2.70263400	-0.64421000
H	-3.76553000	1.76137000	-0.47220200
H	-3.53829900	3.39925600	0.15298500
H	-3.61317800	3.12740200	-1.58780800
C	-1.00438900	3.82844500	-1.05428500
H	-1.33966300	4.19778300	-2.03282200
H	-1.21569800	4.62108100	-0.32396600
H	0.07784900	3.68212600	-1.10060300
C	1.66918100	-1.00455800	1.26787400
H	2.47833000	-1.73616500	1.35459500
H	1.21477400	-0.86856200	2.25241700
C	1.24311900	1.32089700	0.69942900
H	0.72377500	1.47824200	1.64869400
H	1.73199900	2.25992900	0.41306500
C	-3.31615300	-0.46405600	0.35023400
O	-4.42943000	-0.55142700	0.58776300
Cl	-1.40370500	-0.41390000	2.64338500
S	3.59967600	0.30392700	-0.13756000
O	4.14616200	-1.05717500	-0.17033900
O	3.25830000	1.00195100	-1.38767700
C	4.76161800	1.35196000	0.75662800
H	5.00306000	0.87172400	1.70573000
H	5.65275500	1.44883700	0.13189700
H	4.30979600	2.33229800	0.92100000

TS2b-H

C	0.60219000	-1.44788200	0.28641300
C	0.32776600	0.77215800	-0.36806500
Rh	-1.49819600	-0.48106100	0.17568900
C	-1.62217600	-1.02174300	-1.87545800
H	-0.85435900	-0.44080500	-2.39397000
H	-2.59557600	-0.76489500	-2.29441000

C	-1.34498000	-2.47459200	-1.89280700
H	-2.15353600	-3.14439500	-2.18508200
C	-0.15652500	-3.00753100	-1.55089000
H	-0.01223200	-4.08393500	-1.61343900
C	0.98517900	-2.18548000	-0.99976800
H	1.37601100	-1.49542700	-1.76137900
H	1.83664000	-2.83581400	-0.75930200
H	-0.07952900	-2.08095000	0.87198100
N	2.36093000	0.25644700	0.92552900
H	0.78175700	0.46156600	-1.30650500
C	-0.97186800	1.36043000	-0.44749700
C	-1.52448300	2.53077800	-0.75589100
C	-2.99609700	2.85075000	-0.73103000
H	-3.61496200	1.99844400	-0.45457600
H	-3.19701200	3.65827100	-0.01415400
H	-3.32595500	3.21050600	-1.71496300
C	-0.64037300	3.68991500	-1.18385500
H	-0.95486200	4.06301400	-2.16776900
H	-0.73502400	4.52836900	-0.48063200
H	0.41563400	3.41590900	-1.25250700
C	1.70383000	-1.01964500	1.24840900
H	2.46438000	-1.80312000	1.30272300
H	1.25666500	-0.89044100	2.23751400
C	1.32237600	1.25788900	0.66177500
H	0.81648100	1.47972300	1.60555300
H	1.78427900	2.17642300	0.28558100
C	-3.40835800	-0.32295300	0.32845200
O	-4.54476600	-0.27561100	0.46447600
Cl	-1.38263400	-0.25274100	2.67117800
S	3.68247100	0.21876400	-0.14674800
O	4.15321600	-1.16917200	-0.22083800
O	3.35840300	0.96569900	-1.37246300
C	4.90682200	1.17698500	0.76244400
H	5.11986000	0.66515000	1.70181400
H	5.80135900	1.23118600	0.13741700
H	4.51290200	2.17839400	0.94654000

INT3b-H

C	0.72292300	-1.26560500	-0.65927400
C	0.65815000	0.25856700	-0.40877200
Rh	-2.16371300	-0.36730200	0.16896500
C	-2.86717500	-0.06623800	-1.86706500
H	-2.11648000	0.51537500	-2.39374300
H	-3.88288300	0.30497900	-1.97695900

C	-2.70103500	-1.48149400	-1.70955400
H	-3.59674800	-2.05452700	-1.46510200
C	-1.49304000	-2.11750600	-1.46626200
H	-1.56948400	-3.11868700	-1.04602100
C	-0.09286300	-1.72395500	-1.88235500
H	-0.10791400	-0.93916700	-2.64796800
H	0.37082000	-2.60779900	-2.34098100
H	0.33836300	-1.78184700	0.22611800
N	2.73787400	-0.55653000	0.36319100
H	1.16714000	0.70960500	-1.27392800
C	-0.67754700	0.97249300	-0.31735600
C	-0.82979900	2.28131900	-0.58880100
C	-2.13217000	3.04791400	-0.65973400
H	-3.00569200	2.40449100	-0.76946100
H	-2.27374000	3.66999200	0.23480600
H	-2.11005900	3.73542000	-1.51492000
C	0.36179200	3.18807800	-0.87343300
H	0.28808000	3.59611300	-1.89107400
H	0.33911800	4.04873800	-0.19141500
H	1.33795800	2.71454300	-0.76933200
C	2.24137100	-1.49273000	-0.69278000
H	2.66836900	-1.25471000	-1.67309900
H	2.51609000	-2.52174800	-0.44400200
C	1.63728000	0.36506200	0.77220200
H	1.17386500	0.00148800	1.69564600
H	2.02013300	1.37380400	0.92839600
C	-2.92865100	0.93354700	1.29464700
O	-3.43241200	1.64520300	2.04012000
Cl	-1.51089300	-1.64419600	2.14404900
S	4.25283800	0.14412700	0.07633700
O	4.95944000	-0.73702500	-0.85886200
O	4.11425700	1.57994600	-0.21968100
C	5.03278500	0.00423000	1.69347500
H	5.11369400	-1.05289700	1.94974800
H	6.02165600	0.46243400	1.61555400
H	4.42702200	0.53692700	2.42948500

TS3b-H

C	0.68066200	-1.26890300	-0.44666200
C	0.74653400	0.27811500	-0.55605000
Rh	-2.11423300	-0.25818700	0.14704200
C	-2.69946700	0.99839200	1.42896200
O	-3.11416200	1.72999700	2.21145400
Cl	-3.13754700	-1.95153300	1.48329200

C	-1.77934100	0.40208500	-2.07660700
H	-0.84791700	0.45206000	-2.63481900
H	-2.45863100	1.20768700	-2.33260100
C	-2.34647700	-0.92806300	-1.93024100
H	-3.42129600	-1.06831800	-2.01249500
C	-1.54890000	-1.97455100	-1.50883800
H	-2.05161700	-2.89959000	-1.24218100
C	-0.03075500	-2.02278300	-1.58134900
H	0.31723900	-1.63915900	-2.55167500
H	0.26761200	-3.07669600	-1.54238900
H	0.16772100	-1.51615300	0.49247800
C	2.16152800	-1.64986700	-0.28304600
H	2.66614100	-1.73413500	-1.25130300
H	2.28343200	-2.60008500	0.24685100
N	2.71908300	-0.52522900	0.51406700
C	1.71274400	0.56109700	0.61505200
H	1.17736000	0.48012900	1.56958900
H	2.20688800	1.52826200	0.56976000
H	1.28807300	0.51770300	-1.48835600
S	4.32998000	-0.08957700	0.21831600
O	4.90605500	-1.10015600	-0.67494000
O	4.39909500	1.33921800	-0.12140000
C	5.08628200	-0.29013000	1.84061600
H	4.98551200	-1.33240700	2.14735700
H	6.13994900	-0.01753000	1.74323700
H	4.58598600	0.37356300	2.54848600
C	-0.56818500	1.05432700	-0.52980900
C	-0.61834900	2.41340100	-0.56483900
C	-1.89238100	3.22149300	-0.62165200
H	-2.79560800	2.60942800	-0.61617800
H	-1.94945600	3.90605400	0.23630100
H	-1.90502600	3.85540100	-1.51990700
C	0.62301900	3.28718000	-0.58951300
H	0.43847600	4.17384600	-1.20832400
H	0.87564500	3.65839700	0.41382000
H	1.50566800	2.78261200	-0.98909500

INT4b'-H

C	-0.78639900	-1.24844600	-0.17172900
C	-0.89123000	0.03898800	0.69019000
Rh	2.16226400	-0.00870200	-0.17757500
C	2.23171700	1.15530000	-1.63632900
O	2.26418000	1.82979800	-2.56923000
Cl	3.83806800	-1.29087800	-1.26998900

C	0.92046400	-0.40760900	2.38436200
H	0.06504100	-0.93624600	2.82323100
H	1.39789100	0.14189800	3.19571600
C	1.87841700	-1.36912100	1.71788000
H	2.91934200	-1.41714000	2.03208500
C	1.42429900	-2.21766200	0.74715600
H	2.14041200	-2.88288600	0.27476700
C	-0.04808300	-2.44939900	0.43794000
H	-0.55556100	-2.75754600	1.36570800
H	-0.12809100	-3.29346000	-0.25565900
H	-0.24003400	-0.96804500	-1.08075900
C	-2.25658600	-1.51258500	-0.54188000
H	-2.76736900	-2.11318700	0.21706000
H	-2.35278700	-2.02336000	-1.50637600
N	-2.84861300	-0.14732500	-0.60813700
C	-1.83822500	0.86195100	-0.20024700
H	-1.34008800	1.22430900	-1.10507700
H	-2.32033200	1.69670300	0.30755400
H	-1.49270300	-0.21316600	1.57904700
S	-4.44808500	0.04861700	-0.08574500
O	-4.93026600	-1.23880400	0.42702300
O	-4.52661700	1.26373900	0.73455800
C	-5.32493700	0.37782300	-1.62416500
H	-5.19503800	-0.47501500	-2.29276000
H	-6.38052300	0.50882900	-1.37384700
H	-4.92227400	1.28836400	-2.07131600
C	0.44586300	0.52554700	1.24751300
C	1.14178800	1.72005100	1.03095900
C	2.24529700	2.19699200	1.96740000
H	2.82883700	1.39756800	2.42498700
H	2.94484400	2.83694000	1.42181200
H	1.80871600	2.80712900	2.77374600
C	0.58379700	2.88156500	0.22335700
H	1.39274100	3.49079000	-0.19007900
H	-0.06332400	2.58772100	-0.59904300
H	0.00541400	3.53146600	0.89554400

INT4b-H

C	0.79352300	-1.10904500	0.13350700
C	0.98595200	0.17210700	-0.72189700
Rh	-2.25509100	-0.23987100	0.17570900
C	-0.91425400	-0.06895000	-2.38112700
H	-0.10260500	-0.57573200	-2.92268400
H	-1.42310000	0.55874100	-3.11412100

C	-1.87338300	-1.08279500	-1.79363200
H	-2.81744700	-1.25390900	-2.30618400
C	-1.42486000	-2.02044400	-0.85333600
H	-2.08036800	-2.86915300	-0.66845200
C	0.03552300	-2.27831900	-0.50392800
H	0.56172000	-2.60397100	-1.41629700
H	0.07387100	-3.12673800	0.18922800
H	0.23981600	-0.80927200	1.03481800
C	2.23534800	-1.46341700	0.54165000
H	2.71448700	-2.11478700	-0.19593200
H	2.27287200	-1.96362600	1.51598900
N	2.92320500	-0.14818900	0.59651100
C	1.99536200	0.92654100	0.16359600
H	1.52145000	1.34999500	1.05352600
H	2.54912900	1.70614900	-0.35930200
H	1.55089300	-0.12474700	-1.62033800
S	4.54205400	-0.07631800	0.11082500
O	4.94378600	-1.40686500	-0.36004700
O	4.72689700	1.10989700	-0.73437800
C	5.40427500	0.22847200	1.66272500
H	5.20214900	-0.59829500	2.34603000
H	6.47176300	0.28354900	1.43574300
H	5.05321300	1.17359800	2.08077000
C	-0.31814100	0.77896800	-1.23936700
C	-0.89640400	1.97371000	-0.89854900
C	-2.15723000	2.50242400	-1.55783400
H	-2.74285800	1.75845400	-2.09783500
H	-2.80606800	2.94090800	-0.79266500
H	-1.88678100	3.30916500	-2.25529400
C	-0.31412000	2.98394100	0.06812500
H	-0.70435900	3.97850700	-0.17053600
H	-0.63188800	2.75894600	1.09328000
H	0.77307000	3.04082300	0.02886800
C	-3.68293600	-1.24157600	0.73363100
O	-4.58726500	-1.87044100	1.07105000
Cl	-2.66614200	1.28021000	1.96184300

TS2c-H

Rh	-1.02326000	-0.52952600	0.31523100
C	-2.67720000	-1.65979200	-1.13542300
C	-2.52573900	-0.21852900	-1.46523500
C	-1.78036400	-2.65028800	-1.38679900
C	0.40995700	-1.79060800	-0.67494700
C	-0.36553900	-2.40092700	-1.85124900

H	-2.06027400	-3.66850200	-1.12540000
H	-0.36067200	-1.71042400	-2.70748200
H	0.11043500	-3.32789300	-2.19911500
H	2.56222800	-1.90545000	-0.80245700
C	1.77997000	-1.17739500	-1.03203300
H	1.83330500	-0.96731700	-2.11318700
H	1.76989400	1.87111300	-1.30466900
C	1.28501000	1.24817700	-0.53161100
H	1.20423500	1.83855100	0.38174700
C	-0.05673600	0.79666900	-1.05046200
H	0.02888500	0.32086400	-2.02728900
H	-3.45167100	0.32339100	-1.31111600
H	-2.09848900	-0.04409400	-2.45223400
H	-3.59439100	-1.92531900	-0.61679800
H	0.53484200	-2.54922900	0.09987800
N	2.09021600	0.03430100	-0.25298700
S	3.66490000	0.27205100	0.28834200
O	3.62209900	1.44579100	1.16006200
O	4.16160000	-1.02493300	0.74915500
C	4.64426200	0.72332200	-1.16753000
H	4.24505300	1.63957100	-1.60824400
H	5.66643400	0.89379300	-0.82147900
H	4.62640300	-0.09909300	-1.88623700
C	-1.33624600	1.34394600	-0.78820500
C	-1.96229100	2.50446100	-0.57240700
C	-3.36384400	2.62731000	-0.03424400
H	-3.41754300	3.46267800	0.67491200
H	-4.07611400	2.85609300	-0.84117900
H	-3.68372100	1.72283300	0.48767900
C	-1.26482300	3.80634900	-0.91109100
H	-1.87011500	4.39324100	-1.61598500
H	-1.14465200	4.42129200	-0.00928700
H	-0.27846200	3.65312400	-1.35756700
Cl	-2.88163100	-0.44225100	1.93718700
C	0.09813300	-0.52075000	1.84042600
O	0.70525500	-0.45046500	2.81081400

TS2d-H

Rh	-1.55907200	0.00010200	-0.32924300
C	-2.03827800	-2.70912100	0.23767500
C	-1.53983500	-2.00308200	-0.96830300
C	-1.68189100	-2.48600500	1.51684200
C	0.14871100	-0.60037500	1.17348200
C	-0.82411500	-1.38977300	2.09134300

H	-2.13312300	-3.12617700	2.27495700
H	-0.19851200	-1.82292700	2.89374800
H	-1.48941900	-0.67284800	2.58856600
H	-2.18951500	-2.15953100	-1.83168300
H	-0.52517200	-2.26626100	-1.25708000
H	-2.80011300	-3.47040200	0.06145900
H	0.63273200	0.11745500	1.82721900
C	0.23607300	0.41932600	-1.44667100
H	-0.03512400	1.01218700	-2.32065700
C	1.34094000	-0.59967600	-1.71636200
H	0.97491000	-1.49429500	-2.23462500
H	2.07244700	-0.12997500	-2.37927200
N	2.05076600	-1.02533000	-0.50363700
S	3.45275900	-0.18100700	-0.06187000
O	3.71552400	0.83987400	-1.08328300
O	3.37841200	0.17140700	1.36175500
C	4.72755800	-1.44711800	-0.22625800
H	4.76235500	-1.77511500	-1.26643200
H	5.67688700	-0.99148500	0.06530900
H	4.48895700	-2.28112300	0.43647300
C	1.21358700	-1.54439000	0.58900900
H	0.75455200	-2.46673400	0.22368700
H	1.87481500	-1.83974300	1.41112000
C	0.26070100	1.06793900	-0.18456600
C	0.60217200	2.21296600	0.41452600
C	1.41173400	3.22383000	-0.37102500
H	1.63723500	2.88748600	-1.38456700
H	0.87212400	4.17852800	-0.41810500
H	2.36690500	3.40847000	0.13719600
C	0.28134700	2.57582500	1.83862800
H	-0.63408300	2.09269600	2.18821400
H	1.11954100	2.29825900	2.49478900
H	0.15147000	3.66004800	1.92911400
C	-2.92472600	0.36912500	-1.62391700
O	-3.69771200	0.65998500	-2.41922300
Cl	-3.01616300	1.11784500	1.35714500

INT2e-H

C	0.48386900	-1.53138000	0.50624700
C	0.09645900	1.12143400	0.60444500
Rh	-1.35444600	-0.49307900	0.10896700
H	-1.93030700	-0.33559300	-2.50421800
C	-1.01730800	-0.62658000	-1.97262100
H	-0.24677300	0.09460500	-2.27808100

C	-0.60317800	-2.02165600	-2.35630100
C	-0.27867700	-2.97459600	-1.47668300
H	0.04261900	-3.96102600	-1.80170500
C	-0.34054500	-2.69674800	0.00802700
H	-0.16949800	-3.57738600	0.64304700
H	-1.43681000	-2.51052200	0.28365900
H	0.56503100	-1.49910900	1.59242800
H	0.13250400	1.03471000	1.69002200
N	2.29510100	0.08633600	0.27353100
C	-3.35470000	-0.37395500	-0.03127800
O	-4.49458200	-0.35196900	0.01924000
Cl	-1.87096300	-0.58478900	2.58112500
C	-1.07129300	1.57906200	-0.00534300
C	-1.70683900	2.63880000	-0.48927800
C	-1.13850000	4.02253400	-0.22884800
H	-1.87226600	4.63965700	0.30652900
H	-0.22449100	3.99091300	0.36982300
H	-0.91863300	4.53579900	-1.17484000
C	-2.99353600	2.61829900	-1.27366500
H	-3.82178700	3.02478500	-0.67748300
H	-2.90187200	3.25477400	-2.16321000
H	-3.26819400	1.61656600	-1.60674800
S	3.96322000	0.33572400	0.27338300
O	4.18472800	1.65759500	0.86045400
O	4.56872100	-0.87368000	0.83024200
C	4.46268200	0.43150600	-1.46465900
H	4.21881400	-0.50834500	-1.96480000
H	3.95584000	1.27322900	-1.94194500
H	5.54331300	0.59113600	-1.47792200
C	1.43444600	1.21438500	-0.08576700
H	1.92399800	2.12512100	0.27667300
H	1.29917800	1.30210400	-1.17456500
C	1.79674900	-1.21972800	-0.16938200
H	2.53124400	-1.96843900	0.15007100
H	1.70570400	-1.27148400	-1.26234600
H	-0.53712600	-2.24131400	-3.42472600

TS2e-H

C	0.47296200	-1.27118900	0.75173900
C	0.22700300	0.84587500	0.60358300
Rh	-1.65116100	-0.44432300	0.06202900
H	-1.99361200	-0.59180600	-2.62875200
C	-1.15214600	-0.78163700	-1.95459400
H	-0.37247000	-0.05814400	-2.23312700

C	-0.65654900	-2.18871300	-2.11141100
C	-0.24589100	-2.97614900	-1.11022900
H	0.12802700	-3.97468900	-1.32618300
C	-0.28688100	-2.56446400	0.34731600
H	0.16237300	-3.34507800	0.98170800
H	-1.33119400	-2.55991300	0.72925200
H	0.47139000	-1.18719100	1.83595500
H	0.24848200	0.91561500	1.69018900
N	2.47431100	0.04598100	0.39845100
C	-3.46868700	-0.24836500	-0.36855400
O	-4.58603800	-0.13546500	-0.60235000
Cl	-2.20906500	-0.36359900	2.49516400
C	-0.95082600	1.41628100	-0.01906200
C	-1.35848200	2.62125900	-0.41140900
C	-0.54047900	3.86065800	-0.09664800
H	-1.15659900	4.58155400	0.45678600
H	0.34341400	3.64963000	0.50994400
H	-0.21634000	4.36177200	-1.01884400
C	-2.65362700	2.89872200	-1.13278100
H	-3.36957000	3.40043400	-0.46768100
H	-2.47664200	3.57620200	-1.97840600
H	-3.12330600	1.99415800	-1.52003200
S	4.13235300	0.24615400	0.17904800
O	4.42615700	1.63018900	0.54878800
O	4.77363600	-0.89295400	0.83356400
C	4.43691100	0.08850600	-1.59861400
H	4.13852300	-0.90671500	-1.93517200
H	3.88811800	0.86673900	-2.13357200
H	5.51083300	0.22372500	-1.74647300
C	1.56319600	1.08292100	-0.06831700
H	1.95075600	2.05811200	0.23880700
H	1.44136700	1.08188500	-1.16393000
C	1.87531400	-1.26203600	0.16419800
H	2.47852600	-2.02172300	0.67165300
H	1.82893300	-1.51057900	-0.90675200
H	-0.61343900	-2.58279600	-3.12972100

INT3e-H

C	0.63967100	-1.23697300	0.64849000
C	0.50337000	0.31556300	0.73320500
Rh	-2.13650800	-0.45985500	-0.13399100
H	-2.57870900	-0.52888100	-2.63187300
C	-1.77702600	0.03882000	-2.13422300
H	-1.92295900	1.09544200	-2.36916200

C	-0.42068400	-0.41172700	-2.59405300
C	0.39468600	-1.26995200	-1.96974100
H	1.34963100	-1.52622800	-2.42256800
C	0.08965600	-1.90630400	-0.63933900
H	0.43082300	-2.95054600	-0.62968400
H	-1.01594800	-2.06692400	-0.54551900
H	0.12615700	-1.70974200	1.49186800
H	0.63176900	0.54768600	1.79988500
N	2.71598600	-0.30853300	0.00500300
C	-3.65293600	0.55254300	0.04495700
O	-4.65111700	1.10250300	0.18149900
Cl	-2.93468300	-2.00585900	1.56411100
C	-0.78868200	1.00520400	0.28634400
C	-0.97381200	2.33505700	0.34497300
C	0.01164800	3.24953400	1.06236700
H	-0.54582200	3.99926600	1.63786400
H	0.67074000	2.72789200	1.75910100
H	0.63819200	3.80232200	0.34891600
C	-2.13478100	3.11661300	-0.22775400
H	-2.83756600	3.42471900	0.55903600
H	-1.76144800	4.03965800	-0.68955200
H	-2.69224500	2.57546500	-0.99259400
S	4.35542900	0.03670100	0.25925600
O	4.51344400	1.30009800	0.99339500
O	4.96517100	-1.19835000	0.75959000
C	4.93428000	0.32060100	-1.42310900
H	4.80426100	-0.59689500	-1.99856900
H	4.36783100	1.14362600	-1.86416800
H	5.99161900	0.58777600	-1.35598000
C	1.76585700	0.83084400	-0.01725000
H	2.19922400	1.70302400	0.47582700
H	1.52184100	1.09047800	-1.05092800
C	2.15439800	-1.42395800	0.80442100
H	2.43847100	-1.35620900	1.86229100
H	2.51197900	-2.38308400	0.42294300
H	-0.08799500	0.01754100	-3.54215700

TS2f-H

C	0.47320600	0.50812400	1.76603800
Rh	1.27491400	-0.65267400	-0.12173700
C	0.12163900	0.77348600	-1.23420900
H	0.69002900	0.96210300	-2.14701200
C	-1.34304600	0.45969600	-1.50792600
H	-1.42321700	-0.11266900	-2.44524100

H	-1.86678900	1.41160100	-1.64451600
N	-2.00156700	-0.27138100	-0.42552000
C	-1.72722600	-1.71686000	-0.42071100
H	-2.48730000	-2.20307800	0.20100100
H	-1.83910800	-2.09628600	-1.44859400
C	-0.34063200	-2.06823900	0.10662400
H	0.01166800	-2.95159700	-0.43041600
C	-0.25627900	-2.36345800	1.61193300
H	-1.04358400	-1.83199600	2.16181500
H	-0.38847300	-3.43157400	1.82181400
C	1.10689100	-1.88431200	2.06359800
H	1.86116800	-2.60567700	2.36771400
C	1.39165700	-0.54258200	2.18306800
H	2.38374000	-0.24222600	2.50725100
H	0.70884000	1.47038800	2.19220300
H	-0.58972800	0.29103300	1.75916400
S	-3.47760600	0.27491200	0.15952400
O	-3.71289100	-0.44550900	1.41367600
O	-3.43934700	1.73812600	0.11065000
C	-4.74175200	-0.26922500	-1.01619800
H	-5.70788100	0.06862900	-0.63412500
H	-4.54363500	0.18589600	-1.98921600
H	-4.72661900	-1.35918700	-1.08397000
C	0.51949800	1.56326100	-0.13427300
C	0.91743400	2.81563800	0.09018400
C	0.53447000	3.87553700	-0.92564300
H	-0.09366600	3.48559500	-1.72970600
H	-0.00885100	4.69520500	-0.43692800
H	1.44221300	4.30682900	-1.36864900
C	1.73031300	3.31675900	1.25796500
H	2.26216800	4.22928100	0.96920500
H	1.09354000	3.58389200	2.11424900
H	2.47655300	2.58323700	1.57174900
C	1.92758400	-1.66720600	-1.54998700
O	2.33916000	-2.25012800	-2.45159000
Cl	3.57015100	0.42873000	-0.16047300

INT1-Ph

C	0.47084400	-1.09278900	1.06837400
C	1.72414300	0.76773200	-1.05722600
Rh	-0.10217800	0.91258300	0.60369500
C	-1.45320300	0.19543800	-0.85513300
H	-0.83397800	0.05442400	-1.74820100
H	-2.12443900	1.04383300	-1.02705900

C	-2.19836000	-1.05542600	-0.49930800
C	-1.49962400	-2.14655200	-0.12355500
H	-2.01087400	-3.08310900	0.08387600
C	-0.00213200	-2.10844000	0.02246600
H	0.48579300	-1.91828700	-0.94338100
H	0.37089600	-3.09165300	0.34155800
H	-0.05634200	-1.28689300	2.00771000
N	2.93881200	-0.89667200	0.34608200
H	1.37113400	-0.02328500	-1.71674300
C	1.22213400	1.99655300	-1.18233200
C	0.87649400	3.23175800	-1.46334300
C	-0.22520200	3.98940000	-0.76041900
H	-0.76220800	3.38208900	-0.02602000
H	0.19532100	4.84754400	-0.22260500
H	-0.94937100	4.36994500	-1.49207100
C	1.62416700	3.98313400	-2.54878100
H	0.92783400	4.31280900	-3.33043500
H	2.09269000	4.88176200	-2.12725900
H	2.40191000	3.37155400	-3.01291200
C	-1.40918400	0.77515900	1.93449600
Cl	1.28991400	2.26531000	2.19572100
O	-2.19184700	0.70495700	2.76865400
S	3.49323900	-2.19300800	-0.57211700
O	3.00694200	-3.42213500	0.06319500
O	3.24456400	-1.92673100	-1.99619300
C	5.27907200	-2.12119400	-0.32277000
H	5.65564100	-1.15053600	-0.65145300
H	5.48763000	-2.28087100	0.73607800
H	5.71948200	-2.91719700	-0.92787400
C	2.97958800	0.43472500	-0.26347200
H	3.12636300	1.17174600	0.53032700
H	3.83648000	0.48383600	-0.94458300
C	1.96513400	-1.11869100	1.42118400
H	2.17382400	-2.10857500	1.84412900
H	2.16336400	-0.37071300	2.19310700
C	-3.68433700	-1.06990000	-0.56473600
C	-4.37357300	-0.38468600	-1.58162500
C	-4.44481400	-1.77706100	0.38434600
C	-5.76565600	-0.42061600	-1.65764700
H	-3.81186900	0.16030900	-2.33538200
C	-5.83646300	-1.81256700	0.31021100
H	-3.93505200	-2.28365700	1.19890400
C	-6.50424000	-1.13507200	-0.71232500
H	-6.27407600	0.10776800	-2.46010400

H	-6.40096200	-2.36055100	1.06024700
H	-7.58921900	-1.15813600	-0.76776200

INT2a-Ph

O	-1.73301900	2.98924100	1.85987200
C	-1.14239300	2.18869000	1.29105400
Rh	-0.38699500	0.73229300	0.23715500
C	-1.58684200	-1.26397000	0.36206500
C	-0.55756400	-1.34677800	-0.62273500
C	-1.17920500	-0.91824300	1.66568100
C	1.01461100	0.10430700	1.70104500
C	0.24139300	-1.12014100	2.18933400
H	-1.95922800	-0.71062600	2.39379500
H	0.66866600	-2.04863200	1.79399900
H	0.23180000	-1.21008100	3.28224100
Cl	-2.05844500	1.53480400	-1.50700700
H	2.94458000	0.85101200	1.08781500
C	2.44124400	-0.11692100	1.21613700
H	2.99191700	-0.68427200	1.97579000
H	2.35061100	-0.82442400	-2.11734500
C	2.39438300	-0.10156300	-1.30183200
H	3.29101500	0.52637200	-1.44382200
C	1.17116600	0.81851000	-1.39643400
H	0.53926900	0.68474200	-2.27202200
H	-0.86026800	-1.37230000	-1.66443700
H	0.39428300	-1.80497700	-0.38957000
H	1.03635900	0.88157300	2.46948200
N	2.51370300	-0.86775700	-0.04946000
C	1.11802300	2.01869700	-0.72693500
C	1.59318500	3.24648900	-0.57217500
C	1.24892600	4.21814300	0.52781900
H	2.14510100	4.76931900	0.83920500
H	0.52143500	4.96255000	0.17703300
H	0.83456000	3.72647000	1.40851200
C	2.54531800	3.79161400	-1.62464000
H	2.11356700	4.68550000	-2.09488200
H	3.49748300	4.09813200	-1.17042400
H	2.75118800	3.06328400	-2.41317900
S	3.39661100	-2.29495300	-0.09819100
O	3.20680100	-2.95058200	1.19923800
O	3.04328500	-2.96673400	-1.35101300
C	5.14161300	-1.82731600	-0.21042200
H	5.30154600	-1.25246300	-1.12535800
H	5.41346300	-1.24352500	0.67174600

H	5.72319700	-2.75152100	-0.24308600
C	-3.02655400	-1.37673800	0.00563600
C	-3.40912800	-2.36008900	-0.91876100
C	-4.02472200	-0.60150400	0.61657400
C	-4.75496900	-2.56912100	-1.22127800
H	-2.64973200	-2.97963400	-1.38748600
C	-5.36696300	-0.80812300	0.31245400
H	-3.74937300	0.19618200	1.29940000
C	-5.73777300	-1.79443400	-0.60590200
H	-5.03227000	-3.33895500	-1.93607100
H	-6.12523600	-0.18708300	0.78111700
H	-6.78634900	-1.95240300	-0.84290200

TS2a-Ph

O	-1.24067000	3.11000400	2.43306100
C	-0.95510000	2.28781600	1.68081000
Rh	-0.55057400	0.93345000	0.47738900
C	-1.36295500	-1.26632100	0.26229500
C	-0.34352300	-1.06271700	-0.83085800
C	-1.00156300	-1.31622300	1.58892100
C	1.00441300	0.16879000	1.72831300
C	0.41553900	-1.19679000	2.12134900
H	-1.78988500	-1.55070500	2.30047000
H	1.02525100	-2.02292600	1.73270600
H	0.39883300	-1.31592000	3.21024600
Cl	-2.44928900	1.72301900	-0.95246000
H	2.75699000	1.13469900	0.88784800
C	2.41431800	0.12251100	1.13708800
H	3.09019500	-0.28507000	1.89768800
H	2.20665000	-1.03754200	-2.07776600
C	2.17975500	-0.20541300	-1.37134300
H	2.90984400	0.55033300	-1.70055800
C	0.79436400	0.45829600	-1.41711100
H	0.35891000	0.43603600	-2.41536700
H	-0.82459700	-1.16043100	-1.79718600
H	0.50748500	-1.72487800	-0.70663000
H	1.05796700	0.82150400	2.60338900
N	2.53525500	-0.74015700	-0.05510300
C	0.70247100	1.78647400	-0.81091200
C	1.18192300	2.98556800	-1.13963900
C	0.92735600	4.25444600	-0.36632500
H	1.87024300	4.78200900	-0.16591400
H	0.29736300	4.93749900	-0.95191400
H	0.42758100	4.07372000	0.58496300

C	2.00614400	3.18727700	-2.39944300
H	1.54235200	3.96101600	-3.02587400
H	3.01933500	3.54119100	-2.16191300
H	2.09508200	2.28259900	-3.00728000
S	3.58488800	-2.05100100	-0.01285400
O	3.56201600	-2.57319800	1.35568100
O	3.24708300	-2.90037300	-1.15864000
C	5.24209400	-1.38573400	-0.30180000
H	5.27214900	-0.90936300	-1.28426500
H	5.48156900	-0.67070900	0.48831700
H	5.93935300	-2.22628900	-0.27158200
C	-2.77191800	-1.57756300	-0.12758300
C	-3.02118200	-2.49242800	-1.16217200
C	-3.86431200	-1.04632600	0.57537100
C	-4.32582000	-2.86950000	-1.48297400
H	-2.19208600	-2.93811700	-1.70576200
C	-5.16623100	-1.42387900	0.25586600
H	-3.69125600	-0.30203900	1.34575200
C	-5.40282900	-2.33670500	-0.77473300
H	-4.49678100	-3.58421400	-2.28343500
H	-5.99926700	-0.98792300	0.80034000
H	-6.41964200	-2.62485800	-1.02711400

INT3a-Ph

O	-0.08989500	3.65824100	1.57377900
C	0.24047100	2.73514100	0.97738000
Rh	0.66188400	1.25050200	-0.08407200
C	0.85416000	-1.18777500	-0.92884300
C	-0.21675300	-1.89557700	-0.10440100
C	0.52097600	-0.25528200	-1.88404300
C	-1.19614100	1.28989900	-1.03509700
C	-0.88792800	0.27589100	-2.14127100
H	1.29180900	0.09796800	-2.56014000
H	-1.63076700	-0.52663700	-2.16583000
H	-0.89385300	0.77801300	-3.11244700
Cl	1.60671500	2.78653300	-1.81667700
H	-2.43804100	1.71648000	0.69024700
C	-2.45193400	1.07205600	-0.19938300
H	-3.28982500	1.39990700	-0.82727100
H	-2.59216500	-1.78206300	1.64059300
C	-2.06489000	-0.85838700	1.39507100
H	-2.18572700	-0.15996300	2.23617100
C	-0.55257600	-1.20404700	1.25707000
H	-0.39516600	-1.94545400	2.04843200

H	0.11190300	-2.91529900	0.10127900
H	-1.12621600	-1.98739700	-0.70231600
H	-1.20182600	2.31362500	-1.41370600
N	-2.71087300	-0.31034300	0.20123600
C	0.38006800	-0.03811300	1.50934200
C	1.17044200	0.06370500	2.59835400
C	2.20393700	1.15536300	2.81323400
H	1.92540200	1.80816800	3.65300900
H	3.17169300	0.70627700	3.07466600
H	2.37740100	1.78614000	1.93669600
C	1.18568800	-0.91978500	3.75893900
H	2.13620000	-1.47072800	3.78760700
H	1.11618700	-0.37139000	4.70854000
H	0.37539200	-1.65077100	3.74752600
S	-4.08128200	-1.07713100	-0.39659400
O	-4.32209500	-0.53405700	-1.73646200
O	-3.90093400	-2.51429100	-0.17548100
C	-5.45471500	-0.54119500	0.65216000
H	-5.26017000	-0.85008800	1.68143300
H	-5.55517200	0.54402400	0.58171600
H	-6.35904200	-1.02705900	0.27828700
C	2.28127300	-1.61909100	-0.80092100
C	2.62553400	-2.93565400	-0.44622400
C	3.33181600	-0.71508800	-1.06576600
C	3.95957500	-3.33556200	-0.36558700
H	1.85476500	-3.67443700	-0.25544600
C	4.66342900	-1.11415000	-0.97479900
H	3.11112500	0.31577800	-1.33207000
C	4.98575700	-2.42713000	-0.62492600
H	4.19345900	-4.36294600	-0.09981200
H	5.45003500	-0.39206900	-1.17556500
H	6.02452900	-2.73768500	-0.55440800

INT2b-Ph

C	0.70931900	-1.14740600	0.95759100
C	1.51309200	0.73273800	-0.66811900
Rh	-0.33704500	0.72076600	0.53684400
C	-1.30034700	-0.12375800	-1.15185400
H	-0.52797100	-0.36400700	-1.88558900
H	-1.98897100	0.60432500	-1.57827400
C	-1.96683100	-1.33110500	-0.59908700
C	-1.20475700	-2.35307800	-0.13411800
H	-1.68666200	-3.26874000	0.20072900
C	0.29480700	-2.26563700	0.00235200

H	0.77527800	-2.14981900	-0.98031200
H	0.69413900	-3.21096900	0.39509200
H	0.04413600	-1.16026700	1.83516400
N	3.17165400	-0.62276600	0.57879400
H	1.43887100	-0.02513000	-1.44497300
C	0.72718600	1.88835300	-0.78856500
C	0.66739700	3.08158600	-1.36902500
C	-0.42414900	4.10789700	-1.22541600
H	-1.27295200	3.75228600	-0.64335400
H	-0.03631000	5.01188700	-0.73691900
H	-0.79180300	4.41342700	-2.21389500
C	1.80592000	3.50128200	-2.28487200
H	1.42332400	3.73001700	-3.28864000
H	2.28379800	4.41572300	-1.90842500
H	2.57164700	2.72736800	-2.38260100
C	2.13510300	-1.13948100	1.48886700
H	2.41934100	-2.15567600	1.77899600
H	2.16489900	-0.50204800	2.37627400
C	2.83001800	0.71192700	0.07197000
H	2.80612600	1.39824100	0.92294800
H	3.61484400	1.04360400	-0.61818900
C	-1.85071500	2.00244200	0.91069800
O	-2.71684400	2.65628400	1.26345400
Cl	0.43521700	1.53375500	2.79899500
S	3.89831300	-1.69939200	-0.50975600
O	3.58083200	-3.06074300	-0.06414900
O	3.62385700	-1.28279600	-1.89427000
C	5.64989900	-1.40643600	-0.20240200
H	5.86925400	-1.66928400	0.83324500
H	6.20839100	-2.04396900	-0.89191500
H	5.87733800	-0.35575500	-0.39315900
C	-3.45401100	-1.40383900	-0.55815000
C	-4.23241800	-0.91686700	-1.62302800
C	-4.12015200	-1.97088700	0.54299600
C	-5.62387000	-1.00723600	-1.59434100
H	-3.74332900	-0.48742800	-2.49302500
C	-5.51127300	-2.05983600	0.57332400
H	-3.53863400	-2.32328200	1.39040500
C	-6.26955900	-1.57884900	-0.49616100
H	-6.20422000	-0.63367800	-2.43393100
H	-6.00356800	-2.49498400	1.43900500
H	-7.35392800	-1.64333500	-0.47128400

TS2b-Ph

C	0.75461600	-1.09563300	0.83105900
C	1.50638900	0.59948100	-0.54972900
Rh	-0.47463300	0.84425900	0.55582600
C	-1.41147300	-0.03372300	-1.13421100
H	-0.62311600	-0.21184100	-1.87021000
H	-2.14323600	0.65114200	-1.55991800
C	-2.00888900	-1.29573600	-0.61778600
C	-1.20549500	-2.30924400	-0.21315500
H	-1.65318100	-3.24902900	0.10133300
C	0.29809900	-2.20306300	-0.12246700
H	0.74776100	-2.08691100	-1.11938100
H	0.71400900	-3.14719900	0.25359800
H	0.04409500	-1.02851100	1.66747600
N	3.24276800	-0.66109900	0.65667800
H	1.45413900	-0.13949300	-1.34593900
C	0.74061400	1.79332800	-0.73572400
C	0.82006800	2.93814500	-1.40890200
C	-0.19447100	4.05138600	-1.38533400
H	-1.05417800	3.83389400	-0.75327500
H	0.26715400	4.97759400	-1.01741300
H	-0.55793000	4.25975600	-2.40070500
C	2.01936300	3.20343700	-2.30312000
H	1.68678800	3.43417200	-3.32406800
H	2.58193000	4.07697400	-1.94677800
H	2.70348600	2.35268500	-2.35934900
C	2.13541700	-1.18475100	1.47152400
H	2.35055000	-2.22438900	1.73227800
H	2.12088500	-0.58472700	2.38528500
C	2.84930900	0.65555300	0.14309900
H	2.81501000	1.35283300	0.98490800
H	3.59417400	1.00898900	-0.57706800
C	-1.90249300	2.10985300	0.78800300
O	-2.75970500	2.84307600	0.98550800
Cl	0.44354200	1.59800700	2.76205100
S	3.97977300	-1.72620400	-0.45004700
O	3.61897300	-3.09276400	-0.05527000
O	3.75247500	-1.26127200	-1.82768200
C	5.72368700	-1.47541600	-0.07689600
H	5.90259600	-1.76629800	0.95900100
H	6.29263800	-2.10774500	-0.76263800
H	5.97509400	-0.42477500	-0.23444800
C	-3.49155700	-1.42472500	-0.53821000
C	-4.31646500	-0.94927500	-1.57268100
C	-4.10580000	-2.03411900	0.57010800

C	-5.70226100	-1.09192900	-1.50834400
H	-3.86792000	-0.48701500	-2.44768800
C	-5.49163700	-2.17479500	0.63670700
H	-3.48827900	-2.37862700	1.39492900
C	-6.29622000	-1.70498000	-0.40325600
H	-6.31875500	-0.72609200	-2.32527700
H	-5.94350400	-2.64165300	1.50792400
H	-7.37644800	-1.80962500	-0.35017900

INT3b-Ph

C	1.23729200	-1.22476000	-0.47271200
C	1.61532500	0.26998600	-0.43107200
Rh	-1.21730700	0.52657400	0.41395000
C	-2.01135800	0.74269800	-1.60411900
H	-1.17229700	0.96154600	-2.25737700
H	-2.85903600	1.41201200	-1.71522900
C	-2.27398500	-0.61344600	-1.20344400
C	-1.21064000	-1.47734000	-0.91837500
H	-1.47210400	-2.36744800	-0.35074500
C	0.17185700	-1.54885900	-1.53352800
H	0.26968500	-0.87879500	-2.39569600
H	0.30457200	-2.57204800	-1.91179000
H	0.84215200	-1.50908300	0.50765400
N	3.46028500	-1.01654300	0.29161300
H	2.12673800	0.46047600	-1.38698200
C	0.52809500	1.32473000	-0.34288400
C	0.69732100	2.58316600	-0.78859100
C	-0.35729200	3.66239100	-0.89796500
H	-1.37587500	3.27503800	-0.86620500
H	-0.24725200	4.40737000	-0.09778100
H	-0.23230900	4.20428500	-1.84426500
C	2.05291100	3.08850700	-1.26899800
H	1.99707800	3.36291400	-2.33176700
H	2.31681600	4.00528300	-0.72476800
H	2.87674800	2.38588800	-1.14482400
C	2.62162600	-1.87364400	-0.60383100
H	2.98719300	-1.85659200	-1.63673000
H	2.63624100	-2.91013200	-0.25536500
C	2.71336700	0.22914800	0.64386500
H	2.27648300	0.12975000	1.64316200
H	3.37829000	1.09319700	0.61935000
C	-1.49495000	2.12851300	1.38900100
O	-1.71478500	3.03164700	2.06078500
Cl	-0.65320200	-0.61079500	2.50985200

S	5.08191300	-0.84124900	-0.15427300
O	5.41738200	-1.99203100	-0.99919300
O	5.34771900	0.52749100	-0.62733800
C	5.92070000	-1.03071000	1.42827500
H	5.71007100	-2.02811200	1.81634100
H	6.99012000	-0.90268800	1.24437300
H	5.56189700	-0.26269100	2.11669700
C	-3.65570400	-0.95953400	-0.73984400
C	-4.75054600	-0.59009500	-1.53933500
C	-3.89760600	-1.65676600	0.45783500
C	-6.05102400	-0.92149600	-1.16237500
H	-4.57829600	-0.06224500	-2.47323400
C	-5.20182400	-1.97197000	0.83898700
H	-3.07227600	-1.91915800	1.11403000
C	-6.28107400	-1.61126400	0.02999900
H	-6.88429200	-0.64010600	-1.80033000
H	-5.37202300	-2.49549700	1.77546100
H	-7.29514300	-1.86208500	0.32847800

TS2c-Ph

Rh	-0.15550700	-0.07477000	0.40111300
C	-2.21582800	-0.66956600	-1.09794400
C	-1.60680200	0.69765500	-1.29814200
C	-1.58504100	-1.82333600	-1.45172200
C	0.79367400	-1.63382500	-0.71214900
C	-0.14474700	-1.92044400	-1.88907200
H	-2.15033000	-2.74933400	-1.37911400
H	0.04872500	-1.20808200	-2.70638700
H	0.05956000	-2.91667700	-2.30639600
H	2.82328700	-2.36292800	-0.88928700
C	2.27750700	-1.43949800	-1.09753400
H	2.36427700	-1.24261700	-2.17928300
H	3.09789300	1.49758800	-1.35174300
C	2.49724600	1.02016100	-0.55678300
H	2.62884500	1.59205800	0.36229500
C	1.05932500	0.96078700	-1.00526400
H	0.96559900	0.50862900	-1.99191000
H	-2.32854000	1.47131700	-1.06670500
H	-1.20344400	0.80973700	-2.30548700
H	0.70435100	-2.44196600	0.01766800
N	2.94458000	-0.37542300	-0.32469000
S	4.54442800	-0.59587600	0.14515400
O	4.87101900	0.53180000	1.01784000
O	4.67658700	-1.98557100	0.58419600

C	5.54794000	-0.42018800	-1.35292300
H	5.40420200	0.57709100	-1.77431200
H	6.59062200	-0.54909900	-1.05316100
H	5.26757000	-1.19483600	-2.07014400
C	-0.02044800	1.81690000	-0.66408100
C	-0.28934900	3.09757200	-0.38645700
C	-1.57786500	3.58699000	0.22106200
H	-1.37114800	4.40909900	0.91710900
H	-2.24862300	3.99253700	-0.55137900
H	-2.09668500	2.79997200	0.77319800
C	0.73338600	4.16373900	-0.72209000
H	0.28985300	4.92676500	-1.37705500
H	1.05990600	4.68116300	0.18980400
H	1.61699500	3.75965300	-1.22381600
Cl	-1.76302200	0.49290100	2.16600300
C	0.99660700	-0.47383300	1.85435000
O	1.64810100	-0.63054800	2.78436200
C	-3.62433600	-0.73421000	-0.60510200
C	-4.60737300	0.11073900	-1.14573000
C	-4.01139000	-1.67661100	0.36063600
C	-5.93834200	0.01010200	-0.74153900
H	-4.33733200	0.83611100	-1.90905000
C	-5.34109000	-1.77614600	0.76666500
H	-3.25609700	-2.30737500	0.81839700
C	-6.30993800	-0.93418500	0.21694000
H	-6.68508300	0.66716600	-1.17951500
H	-5.61721000	-2.50211900	1.52654500
H	-7.34536500	-1.00878700	0.53803300

TS2d-Ph

Rh	0.34361000	1.06997900	0.37163100
C	2.26621800	-0.82758700	-0.42607600
C	1.43057400	-0.67657000	0.80248200
C	1.76926300	-0.72033900	-1.68208700
C	-0.80862300	-0.21202200	-1.21979700
C	0.42197500	-0.25352200	-2.16669600
H	2.46159800	-0.91960600	-2.49947600
H	0.12455100	-0.89553900	-3.01709700
H	0.55816800	0.74973200	-2.59074300
H	2.03696600	-0.55666900	1.70076500
H	0.72513900	-1.48542200	0.96926500
H	-1.61343500	0.19211500	-1.82463800
C	-1.34884300	0.32893100	1.48013800
H	-1.41761800	0.88494400	2.41551400

C	-1.71015500	-1.14845700	1.61761600
H	-0.89682700	-1.74667000	2.04556500
H	-2.55353200	-1.22293300	2.30919900
N	-2.12336800	-1.76832900	0.35145800
S	-3.77551600	-1.76836800	-0.03390200
O	-4.50892900	-1.21128400	1.10881700
O	-3.96420700	-1.23417100	-1.38899700
C	-4.14676900	-3.53235000	-0.10828300
H	-3.96122500	-3.97030600	0.87367200
H	-5.20027200	-3.62974400	-0.38115700
H	-3.51570500	-3.99833300	-0.86752300
C	-1.18479300	-1.63634000	-0.77363400
H	-0.29020100	-2.20683700	-0.51095800
H	-1.62154500	-2.14451500	-1.64034200
C	-1.76609700	0.97664900	0.28747500
C	-2.69906000	1.80209000	-0.19757700
C	-3.89736800	2.12599500	0.67033100
H	-3.87138800	1.61483400	1.63435600
H	-3.95522000	3.20946800	0.83705100
H	-4.81867200	1.82101900	0.15751100
C	-2.68547300	2.41723200	-1.56982600
H	-1.67047300	2.54595300	-1.95273100
H	-3.26681900	1.79325700	-2.26461500
H	-3.16780700	3.40078800	-1.54400000
C	1.34044800	1.98857400	1.72960300
O	1.86173400	2.56940900	2.56920300
Cl	0.88829600	2.96507300	-1.15791400
C	3.72202800	-1.09573500	-0.23311500
C	4.16305700	-2.00290800	0.74651900
C	4.68923700	-0.44661500	-1.02040200
C	5.52130900	-2.26770900	0.91955900
H	3.43457700	-2.52263800	1.36371600
C	6.04768300	-0.70980000	-0.84618300
H	4.36990800	0.28973200	-1.75225700
C	6.46940600	-1.62308400	0.12237300
H	5.83882200	-2.98116300	1.67555000
H	6.77830000	-0.18979200	-1.46009400
H	7.52816400	-1.82501000	0.26013600

TS2e-Ph

C	0.89307100	-0.14202200	1.54621100
C	1.83459700	0.72948400	-0.14458900
Rh	-0.21700900	1.67034400	0.49361900
H	-2.16452900	0.80931200	-1.18507000

C	-1.43166300	0.30750100	-0.54739700
H	-0.76467800	-0.24553000	-1.22310800
C	-2.11773300	-0.63330300	0.41636200
C	-1.64180200	-0.84054400	1.66029800
H	-2.10876300	-1.58974000	2.29470200
C	-0.48326700	-0.08245000	2.26944300
H	-0.26570100	-0.46990800	3.27726500
H	-0.77356300	0.96494900	2.51353700
H	1.64705800	0.30133900	2.19252600
H	2.59286000	1.16622800	0.50377500
N	2.42406800	-1.54535600	0.31163700
C	-1.35739500	3.09973600	0.06856600
O	-2.04473500	3.98819100	-0.16399600
Cl	1.12024200	3.15978100	1.98481900
C	1.12733000	1.68594300	-0.97462600
C	1.32910400	2.30410200	-2.13607600
C	2.64671100	2.16126600	-2.87619700
H	3.08626400	3.15297500	-3.04628700
H	3.38276300	1.56438700	-2.33246100
H	2.49436200	1.70749600	-3.86488700
C	0.34090000	3.22972600	-2.80065100
H	0.67965500	4.27245900	-2.73280400
H	0.25867500	2.99052400	-3.86893600
H	-0.65622000	3.16654400	-2.36419000
S	3.26201700	-2.97658600	0.02077300
O	4.42559900	-2.60864300	-0.78501400
O	3.38447400	-3.64928000	1.31292900
C	2.18648100	-3.99728200	-1.01789600
H	1.25365900	-4.20224000	-0.48800500
H	1.99834200	-3.48419600	-1.96361800
H	2.72158500	-4.93160800	-1.20262100
C	2.23024700	-0.59181600	-0.77261900
H	3.17540500	-0.46668000	-1.30754200
H	1.45964900	-0.91563700	-1.49123500
C	1.23071000	-1.56952400	1.14732600
H	1.44163600	-2.15308900	2.04906300
H	0.37132500	-2.02410600	0.63090000
C	-3.32177800	-1.36593500	-0.06960300
C	-3.43914800	-1.74602300	-1.41845200
C	-4.38032100	-1.68722900	0.79990700
C	-4.55765700	-2.44327900	-1.87466100
H	-2.64200200	-1.50419400	-2.11533400
C	-5.49936800	-2.38184500	0.34431800
H	-4.33523300	-1.36336600	1.83566500

C	-5.59237600	-2.76639700	-0.99529300
H	-4.62051300	-2.73318400	-2.92029600
H	-6.30685800	-2.61127600	1.03458800
H	-6.46719500	-3.30313600	-1.35182300

TS2f-Ph

C	0.38600800	-1.12191300	-0.43017500
Rh	0.27439400	1.17702800	0.12385400
C	-1.18670400	0.54785800	1.55427600
H	-1.05391800	1.20669600	2.41480300
C	-2.63977800	0.44493300	1.11320600
H	-3.13231400	1.41915000	1.25824700
H	-3.13410700	-0.28626900	1.76119700
N	-2.80440000	0.01185000	-0.27338600
C	-2.60022400	1.07778600	-1.26612900
H	-3.03813300	0.74517500	-2.21387800
H	-3.15302300	1.97100300	-0.93477400
C	-1.13301000	1.43296500	-1.48159900
H	-1.07875800	2.50028200	-1.70919500
C	-0.42357000	0.67350900	-2.60668700
H	-0.89649900	-0.30206900	-2.78198400
H	-0.47749300	1.22162900	-3.55530800
C	1.02204700	0.47191100	-2.20257400
H	1.80264500	0.94475100	-2.79306200
C	1.40461700	-0.45166400	-1.24665600
H	0.75651100	-2.00126400	0.07289600
H	-0.59413700	-1.27223200	-0.87043800
S	-3.85200000	-1.24780800	-0.63199100
O	-3.53704000	-1.66734000	-2.00045600
O	-3.78973700	-2.18582500	0.49105300
C	-5.52297600	-0.55180800	-0.65973100
H	-6.20877600	-1.36420900	-0.91122400
H	-5.76090400	-0.15325200	0.32900900
H	-5.57573500	0.23058300	-1.41993000
C	-0.32232200	-0.56900000	1.55059000
C	0.19097000	-1.41793900	2.44023000
C	-0.54410900	-1.59675300	3.75530800
H	-1.48220900	-1.03886500	3.79675600
H	-0.77120700	-2.65749200	3.92581600
H	0.09703800	-1.26467600	4.58288900
C	1.45082900	-2.23230000	2.29815300
H	1.87786500	-2.41780500	3.28954500
H	1.24759600	-3.21901500	1.85581000
H	2.20508000	-1.71607400	1.70177900

C	0.19975700	3.02062800	0.42533300
O	0.14127200	4.14550100	0.65635800
Cl	2.25615800	1.37295600	1.70107500
C	2.84536300	-0.81413100	-1.09518700
C	3.21050400	-2.17014200	-1.08519300
C	3.85831900	0.15652500	-1.05526700
C	4.55323600	-2.54733000	-1.04267300
H	2.44234600	-2.93739300	-1.14051800
C	5.19890900	-0.22207800	-1.01145900
H	3.59093100	1.20647300	-1.01073500
C	5.55186400	-1.57343300	-1.00602000
H	4.81621200	-3.60174400	-1.04438200
H	5.96905100	0.54272100	-0.96364600
H	6.59796300	-1.86506400	-0.96792200

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Rh	-2.03059400	-0.15475100	-0.19087200
C	-0.99533600	-1.46015700	1.24699400
C	-0.62210100	-1.81438900	-0.05752600
C	-0.25097600	-0.58474700	2.20021300
C	0.43921600	0.73084600	1.83355300
C	1.26957700	-0.46400200	2.19798100
H	-0.71180500	-0.57083900	3.18422900
H	1.80168700	-0.96826300	1.39568600
H	1.77933400	-0.49107300	3.15772500
H	0.70419800	0.57033100	-0.31943600
C	0.40572000	1.31361300	0.42825200
H	-0.62375300	1.65346500	0.19450000
H	3.08019600	1.73170900	1.22839900
C	2.81980500	2.23991700	0.29377400
H	3.35877700	3.19856600	0.29387100
C	3.29845200	1.42125900	-0.88858800
H	3.09730700	1.85294000	-1.87344200
H	-1.03592300	-2.71227000	-0.50679400
H	0.31664300	-1.48735500	-0.49762300
H	-1.74195600	-2.08427800	1.73387200
H	0.33733700	1.49115600	2.60737800
C	-3.43873800	-1.23726100	-0.52104800
O	-4.33359600	-1.93392000	-0.72757300
Cl	-3.20021400	1.75835900	-0.90936900
C	3.93713300	0.27759400	-0.82304900
C	4.61210900	-0.84760500	-0.77073200
C	6.12616600	-0.85951300	-0.68928300
H	6.55488800	-1.39740900	-1.54590600

H	6.53873700	0.15242800	-0.67596000
H	6.46199100	-1.38282100	0.21655800
C	3.93615600	-2.20331100	-0.80075600
H	4.17120200	-2.77856400	0.10537200
H	2.84900300	-2.11684800	-0.88304700
H	4.29589600	-2.79443600	-1.65392300
C	1.30958300	2.54908300	0.24897200
H	1.06759000	3.28587500	1.02612300
H	1.06718600	3.02276300	-0.71103100

INT1-CH_2

C	1.86870800	0.83047600	0.22084800
C	-0.97713600	1.44749700	-0.86372300
Rh	0.16380300	-0.47273300	0.20788100
C	0.71104900	-1.19077400	-1.70824000
H	0.23661300	-0.48836800	-2.40433800
H	0.19914800	-2.15619900	-1.80256000
C	2.17309100	-1.30649500	-1.96844400
H	2.55638900	-2.25543500	-2.34535100
C	3.02125400	-0.29369900	-1.74426500
H	4.08301800	-0.39822000	-1.95511600
C	2.52492200	1.00348500	-1.15716400
H	1.83695800	1.50711000	-1.85042700
H	3.36781500	1.69917000	-1.01987800
H	2.56612800	0.28262000	0.86008700
H	-0.38341900	1.51577000	-1.77705500
C	-1.88146000	0.46943200	-0.78347300
C	-2.91712000	-0.33832100	-0.81256700
C	-2.93652000	-1.73129900	-0.22847700
H	-1.99320300	-2.00696100	0.25061000
H	-3.71816100	-1.80337700	0.53763000
H	-3.16413600	-2.46865200	-1.00948400
C	-4.20570900	0.13198800	-1.46170500
H	-4.49235100	-0.54637700	-2.27592500
H	-5.02085500	0.12215000	-0.72661800
H	-4.11803100	1.14301600	-1.86747800
C	1.23842500	-1.76926300	1.01671600
Cl	-0.91397300	-0.05420400	2.42766700
O	1.88412900	-2.56732500	1.52829300
C	-0.87635300	2.63332000	0.07459400
H	-1.31708500	2.37304800	1.04097000
H	-1.48012700	3.44519900	-0.35930900
C	1.49860800	2.12466600	0.94858500
H	2.46017000	2.63490100	1.13429800

H	1.08825800	1.86979900	1.93036800
C	0.56789000	3.12430100	0.24692400
H	0.54903700	4.04494300	0.84307600
H	0.97929100	3.40704600	-0.73246900

INT2a-CH_2

O	-0.11219900	-2.63186600	1.98371800
C	0.04357100	-1.73098400	1.29296300
Rh	0.50104500	-0.36306600	-0.01318600
C	2.66944700	-0.31959200	-0.61569800
C	1.95077800	0.56132600	-1.46721200
C	2.68267500	-0.10157300	0.76552500
C	0.75317800	1.20236000	1.40921400
C	2.28871700	1.23264400	1.39495100
H	3.10720200	-0.87480600	1.40153500
H	2.67993500	2.06132800	0.79206400
H	2.72128600	1.33593200	2.39768800
Cl	0.30961000	-2.28503300	-1.69152600
H	-1.04965400	2.36298500	1.46826500
C	-0.00335900	2.50688800	1.17060400
H	0.40796400	3.26125200	1.86328700
H	-0.54610000	2.73383600	-2.29317400
C	-0.85247200	2.39116600	-1.29769000
H	-1.88444700	2.74232200	-1.15449400
C	-0.92246300	0.86448100	-1.32211800
H	-0.73294600	0.37225000	-2.27409600
H	1.78704400	0.24537700	-2.49176100
H	1.98428500	1.62895200	-1.29783900
H	2.96533400	-1.29387900	-0.99356600
H	0.41890400	0.77799700	2.35855900
C	-1.61091600	0.16245400	-0.36066000
C	-2.78518300	-0.10735100	0.19452500
C	-3.03633500	-0.87312700	1.46882000
H	-3.85510600	-0.40661700	2.03103700
H	-3.34525300	-1.90514400	1.25414500
H	-2.16282700	-0.90786900	2.12054500
C	-4.04553800	0.34751600	-0.52405400
H	-4.67371600	-0.51959000	-0.76992800
H	-4.64671100	1.00476000	0.11915400
H	-3.82390800	0.87638400	-1.45446400
C	0.03116200	3.10318500	-0.24407400
H	1.06726200	3.16191800	-0.59532400
H	-0.31091900	4.14471800	-0.19263700

TS2a-CH_2

O	-0.26779600	-2.51722000	2.29663100
C	-0.04924300	-1.76832700	1.45050600
Rh	0.36317500	-0.60872800	0.06109200
C	2.20323500	-0.38202000	-1.24911000
C	1.25498400	0.66044400	-1.74865800
C	2.87217500	-0.33084400	-0.05580900
C	1.23411700	0.81956000	1.40888700
C	2.70898300	0.80059400	0.94594200
H	3.55470200	-1.14554800	0.17642600
H	3.00871000	1.74855600	0.47901600
H	3.38709300	0.64991500	1.79325600
Cl	-0.35007500	-2.31596300	-1.64627900
H	-0.45553600	2.06956100	1.88103800
C	0.56706200	2.19510300	1.50568500
H	1.10927600	2.76132800	2.28251200
H	-0.10359300	3.20411300	-1.80824200
C	-0.41241400	2.68127200	-0.89289300
H	-1.41502000	3.05448200	-0.65033900
C	-0.58510800	1.19265600	-1.20779800
H	-0.94614400	1.00010600	-2.21722400
H	0.97963100	0.43671000	-2.77402900
H	1.65185100	1.66451800	-1.63673900
H	2.32168600	-1.25726900	-1.87993400
H	1.17644400	0.35684300	2.39598900
C	-1.32793900	0.40953500	-0.21849100
C	-2.60845000	0.38357300	0.15091800
C	-3.19102800	-0.53642900	1.19374600
H	-3.77740100	0.03358800	1.92786300
H	-3.87767500	-1.25608500	0.72753400
H	-2.43085900	-1.10243700	1.73134000
C	-3.63770900	1.28086700	-0.51498400
H	-4.46054700	0.67096300	-0.91176900
H	-4.08409800	1.97991400	0.20643700
H	-3.22901800	1.86313700	-1.34494700
C	0.55168000	3.07893700	0.24680900
H	1.57191900	3.15932500	-0.14843600
H	0.28727300	4.10063300	0.54631000

INT3a'-CH_2

O	-1.51201200	0.06432200	2.88655900
C	-1.16225900	-0.21767300	1.82964800
Rh	-0.45508900	-0.75664200	0.18169100
C	0.76038200	-0.94311300	-1.93613300

C	1.59270200	0.31781700	-2.00738000
C	1.01263800	-2.01329500	-1.12742300
C	1.43212200	-1.11817100	1.09659700
C	2.05179300	-1.99768300	-0.01718600
H	0.40409400	-2.90650300	-1.26461700
H	3.00566000	-1.60215200	-0.38174500
H	2.24184200	-3.01684300	0.33627000
Cl	-2.49853300	-1.54171900	-0.96767200
H	1.71281000	0.58737800	2.38356800
C	2.31434500	-0.02108200	1.69542300
H	3.06764400	-0.52485900	2.32544900
H	3.00605300	2.50777900	-0.65881100
C	2.27954500	1.93522700	-0.06411100
H	1.82591500	2.65266800	0.63208900
C	1.15790600	1.46945900	-1.03519100
H	0.98133800	2.33615400	-1.68056800
H	1.53179800	0.68900000	-3.03575700
H	2.64517300	0.06871400	-1.83552900
H	-0.05094500	-1.04274400	-2.65330600
H	1.09836800	-1.76156800	1.92049800
C	-0.17916100	1.20823500	-0.36050000
C	-1.16320600	2.11864000	-0.25209100
C	-2.55779600	1.89281500	0.29734600
H	-2.63986300	2.24365500	1.33595100
H	-3.27409300	2.48471200	-0.28626300
H	-2.87802600	0.85176100	0.23764100
C	-0.98863300	3.56312000	-0.71125900
H	-1.58839000	3.75485400	-1.61178100
H	-1.37074600	4.23614100	0.06745900
H	0.04164900	3.85767600	-0.91603100
C	3.08093600	0.90024600	0.73761100
H	3.69457100	0.29635600	0.05719800
H	3.80742900	1.46413400	1.33805000

INT3a-CH_2

O	0.57420100	-1.93770400	2.47951900
C	0.56627200	-1.41740100	1.45757800
Rh	0.61068000	-0.46937700	-0.16366700
C	-0.06871400	1.01992800	-2.04124000
C	-1.29720600	1.75705000	-1.53881300
C	1.22305400	1.23238700	-1.65401500
C	1.25710400	1.28737700	0.79319800
C	1.60739000	2.10226400	-0.46349300
H	2.02742300	0.75420500	-2.20396200

H	1.08222500	3.06321300	-0.49287300
H	2.68259600	2.30012100	-0.49273600
Cl	2.99811200	-1.16097500	-0.46723700
H	0.11151700	1.15720400	2.60799800
C	0.36829000	1.91506900	1.85656700
H	1.02360300	2.63217500	2.38304100
H	-2.92540000	2.60929500	0.82835600
C	-2.11099700	1.88216300	0.95489100
H	-2.43687800	1.20298300	1.75435900
C	-2.03538100	1.04664600	-0.35560900
H	-3.08271100	0.94062500	-0.65945900
H	-1.98671000	1.84424000	-2.38582700
H	-1.02070700	2.78115700	-1.26717500
H	-0.22549000	0.35714900	-2.89128900
H	2.16318400	0.89940100	1.25880300
C	-1.45745600	-0.34463400	-0.18440000
C	-2.18476200	-1.47830300	-0.26374400
C	-1.59860000	-2.87933300	-0.22543400
H	-1.88069700	-3.40588600	0.69781900
H	-1.99713800	-3.47598600	-1.05734400
H	-0.50791900	-2.91052600	-0.31256600
C	-3.69568300	-1.53239300	-0.42857200
H	-3.96812900	-1.97140200	-1.39890000
H	-4.12701500	-2.18986000	0.33930400
H	-4.19538000	-0.56587100	-0.34428900
C	-0.89376500	2.68253900	1.44060800
H	-0.63050100	3.44978000	0.70176700
H	-1.22524600	3.24798500	2.32174500

INT0-CE_2

Rh	-2.69597500	-0.73947100	-0.23282100
C	-1.60498700	-2.51161800	0.40205500
C	-1.50230500	-2.39917100	-0.99331200
C	-0.65695700	-2.00054400	1.43098900
C	0.31386000	-0.82033600	1.27949700
C	0.85212500	-2.21759800	1.35296400
H	-1.06979100	-2.08346500	2.43332000
H	1.23010500	-2.64808500	0.42985100
H	1.36279200	-2.55480500	2.25094600
H	0.78338100	-0.57853800	-0.83020000
C	0.43972200	0.02227300	0.01484100
H	-0.52708500	0.46205400	-0.28402800
H	2.85842100	0.21585900	1.45208300
C	2.87258700	0.76124400	0.50590700

H	3.46316200	1.66899200	0.67831500
C	3.53429100	-0.06924000	-0.57531000
H	3.50519700	0.33517700	-1.59006700
H	-2.07617400	-3.07296900	-1.62247300
H	-0.64138000	-1.95193300	-1.48091500
H	-2.30453300	-3.24888000	0.79222300
H	0.39553800	-0.24470100	2.19943000
C	-4.26382900	-1.51658900	-0.66532200
O	-5.26341000	-2.02119900	-0.94169100
Cl	-3.62567900	1.38000500	0.14080900
C	4.18349400	-1.19019400	-0.37141100
C	4.87668800	-2.28810800	-0.17936000
C	6.35175000	-2.23864500	0.16845200
H	6.94432200	-2.77367700	-0.58617000
H	6.71911100	-1.21119700	0.23103500
H	6.53977700	-2.73258500	1.13160000
C	4.26578100	-3.66889200	-0.30009100
H	4.35127200	-4.21748600	0.64787000
H	3.21035800	-3.62639800	-0.58133600
H	4.79794100	-4.25927800	-1.05830400
C	1.42470200	1.21491300	0.16452800
C	0.90957300	2.13923700	1.28218400
C	1.43818300	1.99154600	-1.16100800
O	0.98334600	1.59202400	-2.21009500
O	1.41931200	2.26330800	2.37489900
O	2.07610700	3.16988500	-1.01970000
O	-0.22940000	2.73683200	0.90087300
C	-0.88773400	3.56512300	1.87778500
H	-0.30721300	4.47651900	2.04595200
H	-1.86312200	3.79095200	1.45008500
H	-0.99554300	3.02495300	2.82081100
C	2.14880100	3.98405500	-2.20396700
H	1.14399400	4.22888000	-2.55709800
H	2.68334600	4.88552900	-1.90442700
H	2.68943800	3.45964400	-2.99609900

INT1-CE$_2$

C	0.02357600	1.53617900	0.65291900
C	0.09070200	-0.89883700	-1.18156400
Rh	1.67993300	0.21617600	0.30875300
C	2.31036600	1.43636100	-1.30069300
H	1.72442300	1.08050600	-2.15635000
H	3.35866800	1.16009900	-1.46618900
C	2.14115000	2.90180500	-1.09921200

H	3.00936500	3.54721600	-1.23645500
C	0.96578500	3.43637300	-0.74039800
H	0.85591000	4.50979300	-0.60540700
C	-0.22286200	2.54547000	-0.48126500
H	-0.52415000	2.03123200	-1.40310800
H	-1.08834600	3.15440000	-0.17796900
H	0.37835200	2.09862900	1.52047000
H	-0.09982400	-0.11506400	-1.91041800
C	1.23932400	-1.57689700	-1.26001500
C	2.24115100	-2.39149100	-1.50280700
C	3.59247500	-2.31422600	-0.83217100
H	3.67751000	-1.47597400	-0.13534000
H	3.77613100	-3.22971900	-0.25668400
H	4.38600700	-2.22525400	-1.58549200
C	2.05707200	-3.51143900	-2.51023600
H	2.79924900	-3.42664800	-3.31458100
H	2.21308400	-4.48256500	-2.02264000
H	1.05949600	-3.50458700	-2.95659700
C	2.67848700	1.24842900	1.51725200
Cl	1.45337100	-1.52237700	2.09657400
O	3.29390700	1.85758100	2.26841500
C	-1.10067900	-1.35776200	-0.36575300
H	-0.74944100	-1.97607200	0.46442800
H	-1.73035900	-1.97334200	-1.01811500
C	-1.18128500	0.73328700	1.14867700
H	-1.89498100	1.47028800	1.54416400
H	-0.86907500	0.12760600	2.00201800
C	-1.96698400	-0.20147700	0.19571300
C	-2.65129100	0.55472200	-0.95574500
C	-3.10552700	-0.84008500	1.02583800
O	-2.49122700	0.34209100	-2.13905600
O	-3.25474000	-0.73619800	2.21998000
O	-3.92211200	-1.56239800	0.22818400
O	-3.48506100	1.50244300	-0.48043200
C	-4.20939200	2.24965100	-1.47407800
H	-3.51772100	2.80169600	-2.11581400
H	-4.81087100	1.57776200	-2.09124100
H	-4.84612000	2.93549500	-0.91519400
C	-5.01548200	-2.21869900	0.89445100
H	-5.56277300	-2.74127500	0.10975900
H	-4.63914000	-2.92432100	1.63930500
H	-5.65536300	-1.48376400	1.38958200

INT2a-CE$_2$

O	-3.95024800	0.37540000	1.93216700
C	-3.04919300	0.14359300	1.26364200
Rh	-1.68803900	-0.41906900	-0.02161000
C	-1.78660600	-2.59942300	-0.60389200
C	-0.87139700	-1.93412900	-1.46376900
C	-1.54123100	-2.62801000	0.77079100
C	-0.16619900	-0.76865500	1.41268600
C	-0.17112000	-2.30362600	1.36369200
H	-2.32251900	-3.00180800	1.42857000
H	0.61257200	-2.71270700	0.71825600
H	-0.04947800	-2.76210500	2.35317200
Cl	-3.56827100	-0.08240300	-1.71351000
H	0.88161400	1.07572500	1.55363600
C	1.12024600	0.04080600	1.30259500
H	1.81756200	-0.29812100	2.08171900
H	1.32891700	-0.29000800	-2.06450500
C	1.16662100	0.50196300	-1.33094800
H	1.65422500	1.39064800	-1.75568000
C	-0.31683100	0.84054700	-1.29715000
H	-0.80645400	0.75686800	-2.26753900
H	-1.19612500	-1.74381000	-2.48160400
H	0.19711400	-2.03620100	-1.31855000
H	-2.78163900	-2.84060400	-0.96634400
H	-0.62277300	-0.46718700	2.35851700
C	-0.93440800	1.62325600	-0.34890600
C	-1.07712800	2.82702300	0.18886700
C	-1.88031800	3.19097000	1.41031800
H	-1.30155200	3.86698700	2.05281700
H	-2.79697900	3.72652400	1.12825500
H	-2.16429700	2.32357000	2.00557800
C	-0.38361100	4.00379500	-0.47864900
H	-1.11742800	4.77715000	-0.74281300
H	0.33952000	4.46520000	0.20750100
H	0.14235100	3.71070400	-1.39088200
C	1.93965100	0.09923800	-0.02071600
C	2.65621700	-1.24938600	-0.23722900
C	3.04572300	1.15880000	0.19074200
O	2.46190800	-2.03249900	-1.14415300
O	3.05578300	2.01342400	1.04614900
O	3.53537500	-1.48379500	0.75540600
O	4.00037100	1.04072300	-0.75719300
C	5.07248200	1.99701800	-0.68276700
H	5.74029400	1.75041200	-1.50828400
H	4.68660100	3.01408600	-0.78953700

H	5.59265900	1.91090600	0.27467700
C	4.27399500	-2.71489100	0.66283000
H	3.59600800	-3.57171200	0.69579700
H	4.84531000	-2.74607500	-0.26813100
H	4.93997000	-2.71884000	1.52568800

TS2a-CE$_2$

O	-3.55535700	0.07048600	2.51935500
C	-2.87179500	-0.09723500	1.60884600
Rh	-1.81148700	-0.43388400	0.12268000
C	-1.44585600	-2.31012700	-1.10024600
C	-0.61815600	-1.26044400	-1.77150000
C	-1.15105600	-2.87807200	0.10934900
C	-0.12790000	-0.98565300	1.32561400
C	0.06037400	-2.46854600	0.92895100
H	-1.81190300	-3.65567100	0.48607000
H	0.95962700	-2.64033200	0.32849100
H	0.15448300	-3.10553500	1.81574000
Cl	-3.78209100	-0.09325100	-1.39916600
H	0.75604700	0.93872800	1.64700100
C	1.08458600	-0.05107700	1.32195400
H	1.78338100	-0.39935700	2.09477700
H	1.69702500	0.28138200	-2.10532800
C	1.22791500	0.73565400	-1.22862400
H	1.44513900	1.80809800	-1.28734200
C	-0.29381800	0.64983600	-1.36548200
H	-0.60834400	0.91786300	-2.37379000
H	-1.00987000	-1.07901700	-2.76717100
H	0.44008700	-1.50628400	-1.77712300
H	-2.35770600	-2.60095000	-1.61216100
H	-0.50568500	-0.96129900	2.34959000
C	-1.08687800	1.35761800	-0.35830700
C	-1.26772900	2.64520900	-0.06547600
C	-2.16052800	3.16454000	1.03293200
H	-1.61491100	3.87601300	1.66812800
H	-3.01504000	3.70738400	0.60648200
H	-2.55251400	2.37177800	1.66937600
C	-0.59056900	3.74087200	-0.87082100
H	-1.33753500	4.47593600	-1.19855300
H	0.14420400	4.28637700	-0.26202200
H	-0.08385200	3.36829100	-1.76538600
C	1.94809100	0.16538000	0.04356700
C	2.72283100	-1.11612900	-0.32461900
C	3.02824300	1.21236300	0.41175500

O	2.65167300	-1.72359400	-1.37365500
O	3.00966500	1.94347500	1.37364100
O	3.51881100	-1.49810800	0.69130900
O	3.99294100	1.24215400	-0.53309700
C	5.03809300	2.20932800	-0.32549700
H	5.71371300	2.09378500	-1.17306900
H	4.62307900	3.22005900	-0.29757200
H	5.55896800	2.01073700	0.61460900
C	4.32381700	-2.66706000	0.45415900
H	3.68859200	-3.53897600	0.27767200
H	4.97052500	-2.51294900	-0.41294700
H	4.91510900	-2.80006100	1.36001500

INT3a'-CE$_2$

O	-2.20861800	1.31214900	2.80349400
C	-2.13871800	0.66509100	1.85831900
Rh	-1.91139400	-0.50175500	0.40534100
C	-1.26694300	-1.67025300	-1.63950200
C	-0.17861000	-0.81398300	-2.24911200
C	-1.10960000	-2.46865600	-0.54362300
C	-0.01712000	-1.11343500	1.14154000
C	0.13751800	-2.41792700	0.32339700
H	-1.92283900	-3.14063700	-0.27247800
H	1.02704700	-2.43185900	-0.30963200
H	0.19166200	-3.29616700	0.97607100
Cl	-4.29159500	-0.95370900	-0.07223600
H	0.81751800	0.76968900	1.75333600
C	1.17130200	-0.16487400	1.30984200
H	1.84441800	-0.60455900	2.05792600
H	2.08531500	0.97249500	-1.90275800
C	1.37554700	0.98840900	-1.07000600
H	1.28571200	2.03489400	-0.75433200
C	-0.02457700	0.62458600	-1.64373200
H	-0.08318500	1.29212100	-2.51022100
H	-0.41316700	-0.70825200	-3.31329800
H	0.78191500	-1.33229100	-2.19856000
H	-2.21193500	-1.73633200	-2.17368400
H	-0.33002500	-1.37637100	2.15968000
C	-1.20099200	1.02550500	-0.76837400
C	-1.85799700	2.19495200	-0.87483700
C	-3.12826200	2.59057800	-0.14704700
H	-2.91023000	3.20603400	0.73714900
H	-3.74482100	3.21037100	-0.80996700
H	-3.73546300	1.73328200	0.14828600

C	-1.39479800	3.31180300	-1.80469700
H	-2.09026500	3.42219800	-2.64824100
H	-1.41203700	4.26429300	-1.25895400
H	-0.38790200	3.18776600	-2.20641600
C	2.06441400	0.22505600	0.10421400
C	2.89185200	-0.96476200	-0.41765800
C	3.10844000	1.23500400	0.65283600
O	2.97902700	-1.32912200	-1.57160100
O	2.99183400	1.88860700	1.66344000
O	3.55738100	-1.56266600	0.59217800
O	4.16021700	1.33908800	-0.18569600
C	5.17152600	2.28827200	0.19822200
H	5.93165500	2.23400800	-0.58114100
H	4.74801900	3.29421800	0.25534900
H	5.59352300	2.02219100	1.17061800
C	4.42269700	-2.64700500	0.21306300
H	3.84668400	-3.45365000	-0.24798100
H	5.17967500	-2.29916300	-0.49420100
H	4.88574500	-2.98686600	1.13952700

INT3a-CE$_2$

O	-2.16449700	0.94028100	2.84962300
C	-2.10802800	0.47862300	1.80230300
Rh	-1.93708000	-0.36335500	0.12575200
C	-1.26620000	-0.89865300	-2.20093900
C	-0.08871000	0.01126500	-2.50524100
C	-1.24114100	-1.99851300	-1.39225600
C	-0.17557700	-1.34736400	0.70108600
C	-0.05646000	-2.31314300	-0.48920300
H	-2.08815600	-2.67678100	-1.37656200
H	0.87805500	-2.19725900	-1.04319900
H	-0.11969000	-3.34804800	-0.13978700
Cl	-3.32983600	-2.23882000	1.03176000
H	0.64655100	0.24833900	1.87530200
C	1.00336800	-0.51048600	1.17469800
H	1.62148600	-1.18589600	1.78348100
H	2.18436300	1.58052700	-1.41593600
C	1.38419600	1.32762300	-0.71409200
H	1.24462500	2.20398000	-0.06865400
C	0.06318100	1.22732300	-1.53507500
H	0.15158300	2.11114000	-2.17716600
H	-0.24490600	0.40059600	-3.51725900
H	0.83641600	-0.56772500	-2.54395800
H	-2.16307700	-0.74605700	-2.80008700

H	-0.57250400	-1.87813300	1.56702900
C	-1.21612300	1.37532100	-0.73156900
C	-1.97870200	2.48863700	-0.74271100
C	-3.33856400	2.60489100	-0.07589500
H	-3.30243700	3.27589300	0.79450800
H	-4.06296200	3.04299200	-0.77605000
H	-3.75798700	1.64817000	0.25037900
C	-1.61222000	3.78755200	-1.44465900
H	-2.28825300	3.98115500	-2.28967900
H	-1.73794800	4.62934700	-0.74962300
H	-0.58731600	3.82750100	-1.81786700
C	1.96932200	0.19649900	0.19101800
C	2.79921600	-0.80665400	-0.63271000
C	3.00040000	0.93960500	1.08597500
O	2.97822500	-0.77800500	-1.83164100
O	2.81977400	1.26992500	2.23526700
O	3.35236500	-1.74005500	0.17011700
O	4.12042200	1.22811000	0.39378800
C	5.12455800	1.96654200	1.11412500
H	5.94391200	2.10590400	0.40897900
H	4.72678700	2.93073400	1.44038900
H	5.45714200	1.40201300	1.98877800
C	4.21615600	-2.68921700	-0.47951500
H	3.66368100	-3.25819200	-1.23180300
H	5.05027600	-2.17396800	-0.96231000
H	4.57383400	-3.34647600	0.31306400

INT2b-CH_2

C	2.08766800	0.17882000	0.16393600
C	-0.02473900	1.48266600	-0.67152800
Rh	0.02858700	-0.56474300	0.18439800
C	0.21618500	-1.29936100	-1.79950900
H	0.27603400	-0.42767500	-2.45764900
H	-0.66754900	-1.87855900	-2.07041800
C	1.46209100	-2.09737900	-1.81183500
H	1.38812900	-3.16617200	-2.01311900
C	2.67249000	-1.55954900	-1.57228700
H	3.56423300	-2.18062300	-1.62236200
C	2.83486000	-0.12304600	-1.13793900
H	2.51739500	0.56252100	-1.93902600
H	3.89909500	0.10170500	-0.97358300
H	2.19373400	-0.68344800	0.84528000
H	0.48408300	1.44730400	-1.63624600
C	-1.26602100	0.82611900	-0.58828000

C	-2.56391500	0.98357600	-0.82476700
C	-3.65421300	-0.02866900	-0.59282700
H	-3.27287500	-1.01663700	-0.33748800
H	-4.31638300	0.29781300	0.22057800
H	-4.27804400	-0.12725300	-1.49097800
C	-3.04892400	2.31128200	-1.38272700
H	-3.55048700	2.16232100	-2.34878300
H	-3.78614100	2.76492400	-0.70665300
H	-2.23457700	3.02598200	-1.52659100
C	2.46309000	1.44675200	0.90452000
H	3.56289200	1.50339400	0.94024600
H	2.10576000	1.35562800	1.93393700
C	0.38391700	2.63905500	0.20053900
H	-0.07042500	2.54084000	1.19089400
H	-0.02067600	3.55355500	-0.26333400
C	-1.30498500	-1.97190700	0.71590800
O	-1.96909000	-2.80808500	1.12130700
Cl	-0.04991400	-0.09793800	2.66671700
C	1.90791200	2.74286400	0.30080100
H	2.19283800	3.59739500	0.92516100
H	2.33530700	2.92271300	-0.69644800

TS2b-CH_2

C	2.06968200	0.05214900	0.11336300
C	0.31861100	1.41216000	-0.61637300
Rh	-0.14625200	-0.67157200	0.24565600
C	0.02202800	-1.44220700	-1.73073800
H	0.13124200	-0.57331400	-2.38723400
H	-0.88115700	-1.97987600	-2.02199700
C	1.22831800	-2.30170900	-1.72890300
H	1.08971000	-3.37261800	-1.87784200
C	2.47513400	-1.83563700	-1.53242800
H	3.31901200	-2.52131700	-1.56423400
C	2.76334800	-0.39489500	-1.18004500
H	2.50694300	0.26827900	-2.02017400
H	3.84434600	-0.26018600	-1.03337600
H	1.99384000	-0.81058000	0.79181000
H	0.80031400	1.33428900	-1.59133500
C	-1.03313900	0.93783100	-0.56272200
C	-2.25334500	1.36804000	-0.87506800
C	-3.53767000	0.60423900	-0.68215100
H	-3.38320300	-0.40265000	-0.29750000
H	-4.19424000	1.13510900	0.02058600
H	-4.08470100	0.52800100	-1.63171400

C	-2.43752700	2.74728900	-1.48379400
H	-2.95215000	2.67175200	-2.45146900
H	-3.06680100	3.37369200	-0.83719400
H	-1.49127300	3.26960900	-1.64520800
C	2.66720300	1.20816500	0.89333100
H	3.75948700	1.07764200	0.90983900
H	2.30858400	1.13477600	1.92434800
C	0.77168500	2.58876100	0.20976600
H	0.29352600	2.55191200	1.19325700
H	0.42479400	3.50125200	-0.29833100
C	-1.62288300	-1.82296500	0.63640000
O	-2.47590400	-2.53860000	0.91042300
Cl	-0.10487200	-0.04455400	2.66776300
C	2.29380500	2.58356700	0.33569300
H	2.64414800	3.38335800	0.99706600
H	2.75746000	2.74911400	-0.64719000

INT3b-CH_2

C	2.12511100	-0.54400300	-0.41220000
C	1.57190200	0.84663200	-0.01524600
Rh	-0.97573800	-0.63388500	-0.01331800
C	-1.46701300	-0.26345500	-2.09406200
H	-0.87096600	0.57595100	-2.43937100
H	-2.52569200	-0.18963100	-2.33027100
C	-0.89628500	-1.58024000	-2.05520200
H	-1.59508200	-2.41723500	-2.02166500
C	0.40802100	-1.86572600	-1.68631500
H	0.59261600	-2.89610000	-1.38740000
C	1.65442300	-1.02012300	-1.80199500
H	1.49668200	-0.16406900	-2.46931800
H	2.42874800	-1.64618400	-2.26607900
H	1.78597300	-1.27440600	0.33116700
H	2.04039300	1.53975000	-0.73253400
C	0.08199400	1.13337900	-0.12696000
C	-0.43341000	2.36195100	-0.31212400
C	-1.88486700	2.71806900	-0.54838400
H	-2.49769300	1.86357200	-0.83621600
H	-2.33061000	3.17326800	0.34714300
H	-1.95800300	3.46912500	-1.34614300
C	0.44281900	3.60808200	-0.30016200
H	0.40207800	4.11190800	-1.27624000
H	0.05793300	4.32506000	0.43767300
H	1.48808500	3.41835200	-0.05725300
C	3.63124800	-0.33908000	-0.17984800

H	4.07060100	0.23258400	-1.00890100
H	4.17274400	-1.28919400	-0.11804500
C	2.25985900	1.06120800	1.35258100
H	1.71550900	0.50208900	2.12116000
H	2.27231400	2.11265400	1.65637800
C	-2.21947800	0.22866500	1.09952200
O	-2.99763100	0.66845100	1.81956900
Cl	-0.29753300	-2.01722000	1.88047000
C	3.69052100	0.47511800	1.14603800
H	3.96784700	-0.16735700	1.98759900
H	4.44477300	1.26695100	1.08924600

INT2b-CE$_2$

C	0.11481900	1.44399700	-0.75348900
C	-0.14125900	-0.47571700	0.95532600
Rh	-1.72400600	0.32189100	-0.37657900
C	-2.26275500	1.63798100	1.20128800
H	-1.54368100	1.47383500	2.00879900
H	-3.26189300	1.39924100	1.56768900
C	-2.15965500	2.99352300	0.61959600
H	-3.06835300	3.58911800	0.53205700
C	-0.99541200	3.50786100	0.18031200
H	-0.96168200	4.52037900	-0.21597300
C	0.26959000	2.68612700	0.13200700
H	0.58921300	2.40872900	1.14723000
H	1.09308300	3.28899600	-0.27836400
H	-0.47183300	1.72391900	-1.64530500
H	0.11143700	0.28203800	1.69193500
C	-1.40150200	-1.09102000	1.07574400
C	-2.05092400	-2.04657600	1.73104200
C	-3.50177800	-2.42058300	1.58334600
H	-4.05213900	-1.75282000	0.92192800
H	-3.59569600	-3.44021700	1.18593300
H	-3.99779700	-2.41446800	2.56317800
C	-1.28937900	-2.87918000	2.74937300
H	-1.75191600	-2.78666900	3.74150900
H	-1.32352100	-3.94307800	2.47862300
H	-0.24140100	-2.58071900	2.83423800
C	1.37371500	0.74915400	-1.23886600
H	2.08640100	1.50855000	-1.58666000
H	1.11188800	0.13296600	-2.10114900
C	1.04630800	-1.16765400	0.33975300
H	0.71576900	-1.83970200	-0.45712200
H	1.51927900	-1.76866400	1.12704200

C	-3.62704000	-0.12326100	-0.82009700
O	-4.68428800	-0.32562800	-1.20221200
Cl	-1.30207100	-0.96660100	-2.50395700
C	2.08598500	-0.17740000	-0.22791800
C	2.76600500	0.61218700	0.90122200
C	3.18858300	-0.96467200	-0.96042000
O	3.74150300	1.40207200	0.40961600
O	3.86374200	-1.74554700	-0.08790100
O	2.47984100	0.56203100	2.07931200
O	3.42110000	-0.92238100	-2.14479100
C	4.46380700	2.18149600	1.37930500
H	4.93962100	1.52818900	2.11487200
H	5.21251700	2.73209000	0.80980400
H	3.78906700	2.86927900	1.89561000
C	4.91046700	-2.54931600	-0.66142100
H	5.66076800	-1.91365700	-1.13855100
H	5.34494900	-3.10046000	0.17277700
H	4.49877400	-3.23580300	-1.40556900

TS2b-CE$_2$

C	0.12080600	1.37765700	-0.71480300
C	-0.09375600	-0.32292800	0.88059100
Rh	-1.87403900	0.25387900	-0.42976300
C	-2.42181500	1.65766300	1.07329200
H	-1.73356400	1.49382700	1.90790300
H	-3.43856000	1.47826800	1.42459800
C	-2.25099000	2.99148800	0.45401800
H	-3.14290900	3.59738400	0.29404000
C	-1.06055900	3.48121700	0.06188200
H	-1.00178500	4.47898300	-0.36743900
C	0.21191700	2.66843500	0.11103300
H	0.50130900	2.45758400	1.15070500
H	1.04122600	3.26008600	-0.30260100
H	-0.51471100	1.57093700	-1.59239200
H	0.14843300	0.45325400	1.60017800
C	-1.35008200	-0.97998100	1.07058400
C	-1.88089600	-1.92346600	1.84361600
C	-3.30492000	-2.41226500	1.79390800
H	-3.91382700	-1.88174000	1.06337200
H	-3.33217800	-3.48089500	1.54117500
H	-3.78074100	-2.30690500	2.77841700
C	-1.02266400	-2.60607600	2.89494000
H	-1.47696500	-2.49149400	3.88855700
H	-0.95560500	-3.68467200	2.69827800

H	-0.00798300	-2.20286600	2.94091200
C	1.40219600	0.75317800	-1.23895400
H	2.06514400	1.54858500	-1.60184900
H	1.14941500	0.12331800	-2.09473900
C	1.09686900	-1.08739000	0.36166000
H	0.77408800	-1.80173300	-0.40103300
H	1.52729000	-1.64435500	1.20224200
C	-3.70670700	-0.23459500	-0.74234000
O	-4.79227500	-0.50602400	-0.98934300
Cl	-1.29337500	-1.11363100	-2.44249300
C	2.15490700	-0.14058800	-0.23277500
C	2.84144600	0.68003000	0.86896700
C	3.24058700	-0.94873700	-0.96121400
O	3.83800400	1.42751900	0.35609600
O	3.91189500	-1.72386000	-0.08162700
O	2.53697900	0.68704300	2.04350000
O	3.46234700	-0.92574600	-2.14827000
C	4.56449600	2.23489800	1.30025700
H	5.02001700	1.60469000	2.06806300
H	5.32934500	2.74678000	0.71642700
H	3.89689100	2.95591600	1.77903100
C	4.94466400	-2.55030600	-0.64902400
H	5.70157800	-1.93168500	-1.13789500
H	5.37512400	-3.09608400	0.19072600
H	4.51950000	-3.24086600	-1.38165400

INT3b-CE$_2$

C	0.39611700	-0.19901700	-1.42008200
C	0.20708900	0.78190300	-0.23927000
Rh	-2.44294700	-0.48817500	-0.09265200
C	-3.44539400	0.87165100	-1.45863100
H	-2.84523000	1.77353700	-1.53473900
H	-4.50147000	1.04948300	-1.27141600
C	-3.10444800	-0.28610100	-2.23435500
H	-3.88896000	-1.03184800	-2.37148700
C	-1.81184900	-0.71440200	-2.49348500
H	-1.71706700	-1.75596900	-2.79539000
C	-0.53436100	0.08488400	-2.61557100
H	-0.74027900	1.15917300	-2.69588300
H	-0.04934400	-0.21879100	-3.55323500
H	0.19388200	-1.21545200	-1.06532400
H	0.56885500	1.74798900	-0.62085500
C	-1.17816100	1.08599700	0.30461700
C	-1.49743000	2.24230200	0.91267100

C	-2.87040600	2.67781400	1.37519500
H	-3.67972600	2.09878600	0.92939600
H	-2.95977200	2.60742900	2.46819200
H	-3.02942800	3.73344000	1.11899400
C	-0.44603800	3.30142800	1.22410800
H	-0.67205100	4.22846300	0.67818100
H	-0.48682400	3.55315100	2.29264100
H	0.57968200	3.01216800	0.99478000
C	1.91428100	-0.10285900	-1.64285000
H	2.16583100	0.80146800	-2.21103800
H	2.32606900	-0.96565100	-2.16996300
C	1.27144900	0.25532300	0.74154900
H	0.91653200	-0.67384400	1.19873300
H	1.52243300	0.96023300	1.53458700
C	-3.17229500	-0.29288900	1.62943900
O	-3.63604500	-0.27389300	2.67899200
Cl	-1.42342600	-2.58676300	0.62371200
C	2.50122000	-0.02095600	-0.18761600
C	3.49398600	1.13958300	-0.11118300
C	3.19458400	-1.32904000	0.20350500
O	4.68301500	0.79648300	-0.64461600
O	3.66043000	-1.24692100	1.46700400
O	3.24662600	2.24924600	0.31239300
O	3.29310100	-2.31754500	-0.48751100
C	5.67903200	1.83329700	-0.66846300
H	5.90305100	2.17009000	0.34698400
H	6.55859500	1.38130500	-1.12714500
H	5.33058500	2.68511100	-1.25836900
C	4.28974700	-2.43720100	1.97193900
H	5.15514000	-2.70147800	1.35844400
H	4.59805400	-2.19471000	2.98919700
H	3.58253400	-3.27051900	1.97175600

INT2e-CH_2

C	2.02153900	0.37841900	0.56393800
C	-0.45586000	1.53082400	0.72627800
Rh	0.12980300	-0.54286700	0.09086500
H	-0.30738200	-0.70048000	-2.54912000
C	0.44835900	-0.16806100	-1.96110000
H	0.29995900	0.90011400	-2.16779600
C	1.83464100	-0.58528200	-2.37092100
C	2.79778400	-0.92203700	-1.50775300
H	3.79685800	-1.18473300	-1.84693700
C	2.52086700	-0.92444500	-0.02270100

H	3.34125400	-1.32164900	0.59173000
H	1.75219100	-1.74691900	0.18890300
H	2.02481200	0.35926300	1.65510700
H	-0.39150200	1.40420300	1.80798400
C	-1.06275700	-2.13273000	-0.18103300
O	-1.70484300	-3.07709100	-0.20235200
Cl	-0.09012200	-1.18755900	2.53758200
C	-1.44978900	0.82984200	0.04474300
C	-2.67473000	0.90258900	-0.46239300
C	-3.54244600	2.10223800	-0.12540000
H	-4.46576300	1.77768200	0.37345900
H	-3.03290000	2.80869800	0.53503800
H	-3.84329400	2.63464900	-1.03814800
C	-3.33418700	-0.12623600	-1.34514000
H	-4.13620400	-0.65063700	-0.80742200
H	-3.80161100	0.36377900	-2.20938600
H	-2.63218400	-0.87023700	-1.72457800
C	0.21155500	2.76052600	0.16258800
H	-0.33811100	3.62336700	0.57084400
H	0.08750700	2.79746500	-0.92532400
C	2.49384700	1.69514200	0.00306100
H	3.54928000	1.82070200	0.29633000
H	2.47719600	1.68932500	-1.09122800
H	2.05951800	-0.57125800	-3.44028400
C	1.69174300	2.88379300	0.54116500
H	2.09957000	3.82136000	0.14513600
H	1.78711100	2.93206800	1.63468700

TS2e-CH_2

C	1.93226200	0.20901100	0.68770000
C	0.28634100	1.54191200	0.49514400
Rh	-0.19571200	-0.73318100	0.07843900
H	-0.39661700	-1.21905700	-2.58701000
C	0.34357600	-0.71597200	-1.95571600
H	0.35968700	0.33326700	-2.28252200
C	1.69508400	-1.34574300	-2.12013100
C	2.56092400	-1.57471900	-1.12656800
H	3.53572300	-2.00513100	-1.34612200
C	2.25519100	-1.26916100	0.32416400
H	3.11971800	-1.51303700	0.96135400
H	1.49753100	-1.98073300	0.72559900
H	1.87159800	0.28292800	1.77235000
H	0.25927700	1.64925500	1.58030000
C	-1.63945600	-1.87077400	-0.26858100

O	-2.52438800	-2.57898900	-0.45399900
Cl	-0.59715700	-0.93466200	2.54447800
C	-0.97577400	1.08847600	-0.06380100
C	-2.12678100	1.64216900	-0.44079300
C	-2.41250200	3.11027000	-0.18183100
H	-3.34436400	3.21168800	0.39062700
H	-1.62177100	3.60665400	0.38515700
H	-2.55792200	3.65648800	-1.12406800
C	-3.26916200	0.89678200	-1.08618500
H	-4.09455700	0.75382500	-0.37511600
H	-3.67052200	1.47674900	-1.92764000
H	-2.97328800	-0.08199200	-1.46484400
C	1.05366500	2.63177000	-0.22992200
H	0.56739100	3.59173700	-0.01431400
H	0.99190200	2.47756800	-1.31345400
C	2.94659000	1.16577300	0.07548900
H	3.91622000	0.98122400	0.56021900
H	3.07426800	0.93237700	-0.98732600
H	1.99039000	-1.61290500	-3.13791200
C	2.50517400	2.61514700	0.23793300
H	3.13342900	3.30062800	-0.34095400
H	2.56492800	2.92312000	1.29037700

INT3e-CH_2

C	1.84570500	-1.02724600	0.67092800
C	1.53508100	0.51126300	0.72630400
Rh	-1.02130200	-0.54157000	-0.12862000
H	-1.47344700	-0.70335400	-2.63278000
C	-0.70404900	-0.08489400	-2.14478700
H	-0.90368500	0.95722700	-2.40517600
C	0.67292000	-0.47250000	-2.59868800
C	1.55138900	-1.23011700	-1.93260100
H	2.51420700	-1.45029200	-2.39067800
C	1.30841800	-1.80404300	-0.56134100
H	1.72735000	-2.81824400	-0.49930000
H	0.22104100	-2.05120700	-0.44266000
H	1.40179800	-1.51514800	1.54394400
H	1.58981000	0.76082900	1.79794000
C	-2.63139000	0.32418500	-0.00289200
O	-3.68293300	0.77335200	0.10353400
Cl	-1.68491300	-2.04840000	1.67010500
C	0.18688600	1.05547900	0.24205100
C	-0.15358600	2.35571000	0.27205600
C	0.69130600	3.38881500	1.00743100

H	0.02723300	4.06059500	1.56676200
H	1.39226400	2.95157700	1.72070300
H	1.25928400	4.01795700	0.30816000
C	-1.38012000	2.99222800	-0.34323800
H	-2.13597300	3.23187400	0.41800900
H	-1.10017400	3.94416500	-0.81311100
H	-1.85006900	2.37950400	-1.11261400
C	2.77917300	1.14310600	0.04922700
H	2.87046700	2.21533000	0.23386500
H	2.71827900	0.99811800	-1.03390000
C	3.40593800	-1.10870900	0.73722400
H	3.73519100	-1.60902100	1.65346100
H	3.78647700	-1.70928000	-0.09709000
H	0.96458700	-0.08421600	-3.57763100
C	3.94047900	0.33932800	0.64872700
H	4.85888200	0.41417700	0.05649100
H	4.17316800	0.72042900	1.65105600

INT2e-CE$_2$

C	0.21392100	-1.35565700	0.81504500
C	-0.13716500	1.17635600	-0.00587400
Rh	-1.65141000	-0.44462600	0.23410000
H	-2.44655800	-1.18181800	-2.21614200
C	-1.49883800	-1.31557500	-1.68309400
H	-0.73984600	-0.78859500	-2.27640700
C	-1.15138300	-2.77591900	-1.57713600
C	-0.76317800	-3.37167200	-0.44521900
H	-0.49109000	-4.42415100	-0.42378300
C	-0.67423100	-2.58295200	0.84015200
H	-0.43983100	-3.18742900	1.72787300
H	-1.73313800	-2.26688900	1.13427400
H	0.38613800	-0.95751200	1.81322000
H	-0.01898200	1.48254800	1.03433500
C	-3.65358900	-0.33366700	0.22412200
O	-4.78621300	-0.26796400	0.35408500
Cl	-1.93393400	0.37999000	2.61621100
C	-1.36476500	1.43294500	-0.62226100
C	-2.03715300	2.28815300	-1.38284700
C	-1.43595300	3.65204200	-1.67211000
H	-2.10506200	4.44669700	-1.31503600
H	-0.46395700	3.78758100	-1.19066900
H	-1.31105500	3.80088200	-2.75330900
C	-3.39655000	2.05389100	-1.99031300
H	-4.15861100	2.67495100	-1.49962000

H	-3.38959200	2.33995100	-3.05021200
H	-3.71163300	1.01127200	-1.92919200
C	1.12283200	0.98999000	-0.81036400
H	1.60122200	1.97423100	-0.89252400
H	0.89422900	0.67000700	-1.82847200
C	1.46655800	-1.38469700	-0.02605900
H	2.18575800	-2.04635200	0.47497000
H	1.26768000	-1.80476700	-1.01542700
H	-1.19206900	-3.36111400	-2.49912100
C	2.13422600	-0.00060700	-0.19856300
C	3.31256600	-0.15880700	-1.17759700
C	2.69277000	0.49221900	1.14866800
O	3.28683600	0.14482900	-2.34923400
O	2.76234200	-0.16584500	2.16162800
O	4.37343800	-0.72763100	-0.57354800
O	3.11590500	1.76944500	1.05532100
C	5.51902800	-0.95908500	-1.41384800
H	5.88502000	-0.01540500	-1.82606600
H	6.26743800	-1.41385500	-0.76508700
H	5.25898600	-1.63152500	-2.23526100
C	3.67951300	2.32237700	2.25994900
H	3.96034500	3.34470700	2.00671900
H	2.94020300	2.31127000	3.06445300
H	4.55459300	1.74495800	2.56848100

TS2e-CE$_2$

C	0.19802900	-1.02586900	0.95820800
C	-0.01882600	0.88389500	0.02660800
Rh	-1.98138600	-0.38915500	0.22561100
H	-2.63286800	-1.52668000	-2.15331100
C	-1.72481000	-1.50200800	-1.54196800
H	-0.96342700	-0.99086700	-2.14744600
C	-1.28154900	-2.89170000	-1.19164700
C	-0.78396400	-3.25942700	-0.00533500
H	-0.45305700	-4.28402300	0.15066800
C	-0.65539400	-2.30996400	1.16756800
H	-0.17119300	-2.80896000	2.02155300
H	-1.65492000	-2.08190100	1.60359700
H	0.32470500	-0.54089300	1.92211800
H	0.10716600	1.36372800	0.99782800
C	-3.82993900	-0.26479300	-0.06233900
O	-4.96580200	-0.18467400	-0.20923700
Cl	-2.24211800	0.67672200	2.47903300
C	-1.25667500	1.24799600	-0.63874300

C	-1.69161800	2.23128700	-1.42390000
C	-0.82883200	3.44788300	-1.70545300
H	-1.37136800	4.36138100	-1.42717400
H	0.11308200	3.44168600	-1.15218200
H	-0.59925800	3.52758500	-2.77686100
C	-3.05932700	2.28329200	-2.05831100
H	-3.68880600	3.03907700	-1.56871700
H	-2.97473900	2.57443900	-3.11364800
H	-3.58014200	1.32640300	-2.01521500
C	1.22937500	0.78127800	-0.82503300
H	1.61667300	1.78994100	-1.00382600
H	1.00225200	0.34860200	-1.80234800
C	1.51980500	-1.35697000	0.28403900
H	2.11877100	-1.94858100	0.98595400
H	1.33944900	-1.96989500	-0.60442600
H	-1.35545700	-3.64453200	-1.98022300
C	2.28479300	-0.09147800	-0.13211200
C	3.40772800	-0.45554900	-1.11183700
C	2.89068900	0.60873600	1.09330100
O	3.34351200	-0.34523900	-2.31545600
O	2.83793600	0.20147300	2.23207600
O	4.46712000	-0.96908700	-0.45741300
O	3.48856400	1.76243300	0.73483100
C	5.57120000	-1.38078500	-1.28462400
H	5.95924900	-0.53017100	-1.85050100
H	6.32419900	-1.76225800	-0.59521200
H	5.25422700	-2.16047200	-1.98175900
C	4.10125500	2.50281200	1.80756400
H	4.52396200	3.39306200	1.34194800
H	3.35409600	2.77506600	2.55707300
H	4.88349200	1.90488500	2.28172500

INT3e-CE$_2$

C	0.28673900	-0.85740600	1.05281600
C	0.17716900	0.56334200	0.41684300
Rh	-2.51692000	-0.44090900	0.10660000
H	-3.10446700	-1.59036800	-2.07908900
C	-2.25290400	-0.91270500	-1.91309000
H	-2.36504300	-0.06291000	-2.59023200
C	-0.94242400	-1.59956700	-2.16083000
C	-0.10936800	-2.10244600	-1.24259900
H	0.81629600	-2.56896500	-1.57193900
C	-0.34388500	-2.02651300	0.24326900
H	-0.01626800	-2.95797900	0.72593600

H	-1.44419500	-2.08998300	0.45139300
H	-0.21713300	-0.86884600	2.02496200
H	0.35535400	1.25438000	1.25470000
C	-4.01864400	0.57798200	-0.14277400
O	-5.00873100	1.15160700	-0.23918200
Cl	-3.33177100	-1.10471800	2.30524900
C	-1.13178500	1.01232200	-0.24239900
C	-1.31691300	2.23512100	-0.76987400
C	-0.30940400	3.35932300	-0.56497200
H	-0.84773100	4.28744900	-0.33290600
H	0.39233900	3.17564300	0.25095400
H	0.26891400	3.55120400	-1.47953900
C	-2.50156200	2.70220000	-1.58618400
H	-3.17566500	3.33525400	-0.99194100
H	-2.14927800	3.32121300	-2.42151400
H	-3.08574300	1.88669100	-2.01308600
C	1.40752100	0.62705000	-0.52310700
H	1.68686200	1.64637300	-0.79367300
H	1.21400800	0.08525600	-1.44933300
C	1.81163600	-1.03054900	1.26726400
H	2.08986800	-0.71418800	2.27516800
H	2.12324200	-2.07417100	1.15847300
H	-0.65234000	-1.67397000	-3.21148100
C	2.54421400	-0.09632100	0.24948600
C	3.43972400	-0.91341000	-0.68575000
C	3.39620800	0.94611600	0.98840100
O	3.20354800	-1.18286800	-1.84325800
O	3.34842300	1.19175200	2.17340500
O	4.52605200	-1.36277200	-0.02344500
O	4.17916600	1.61912300	0.11980900
C	5.43163100	-2.17454000	-0.79048100
H	5.81228300	-1.61440600	-1.64835400
H	6.24161000	-2.43196000	-0.10781800
H	4.92800100	-3.07654200	-1.14807600
C	5.00188300	2.64933600	0.69431500
H	5.55853300	3.07661500	-0.13997600
H	4.38226800	3.41086800	1.17495900
H	5.68311600	2.22372700	1.43555200

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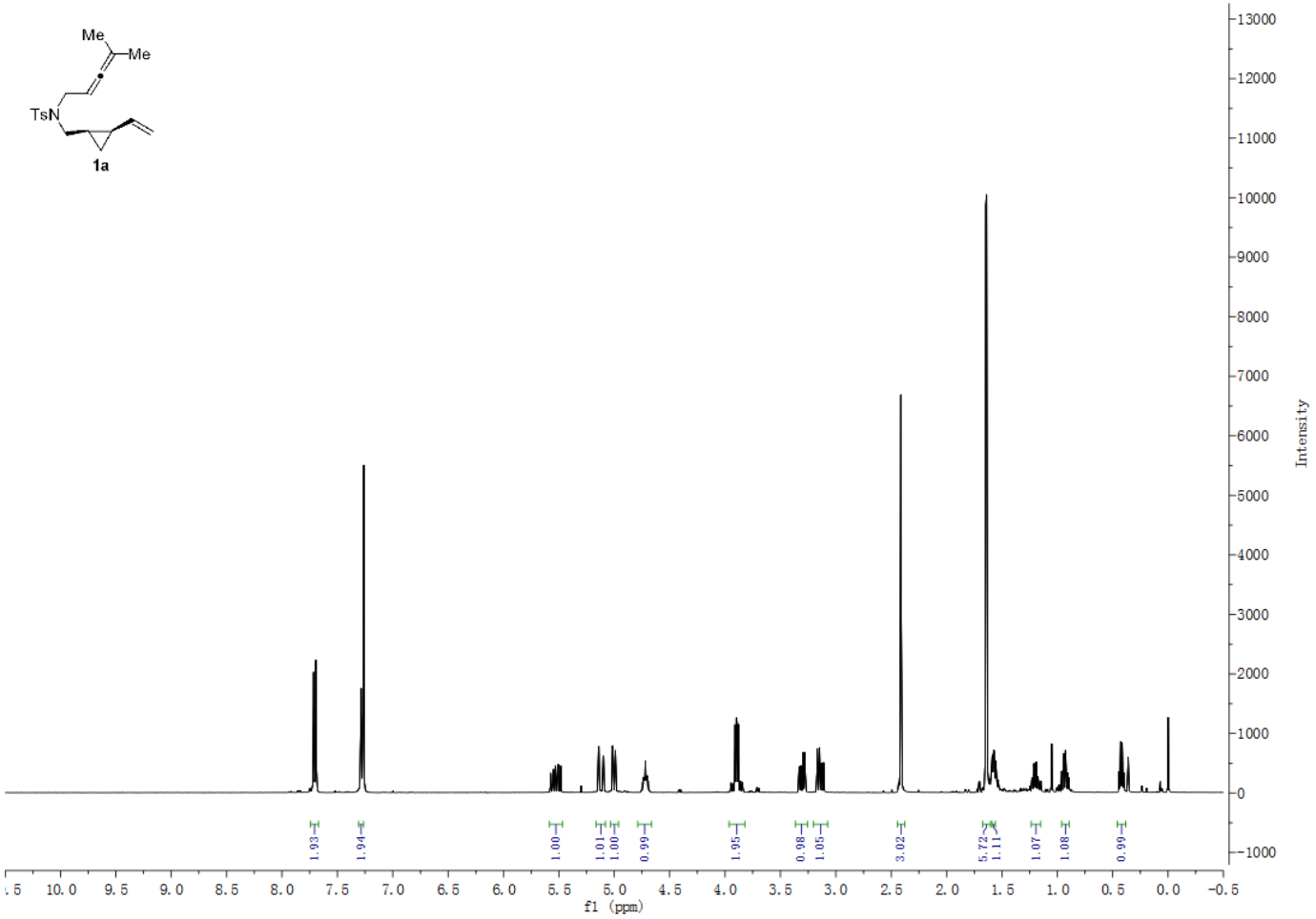
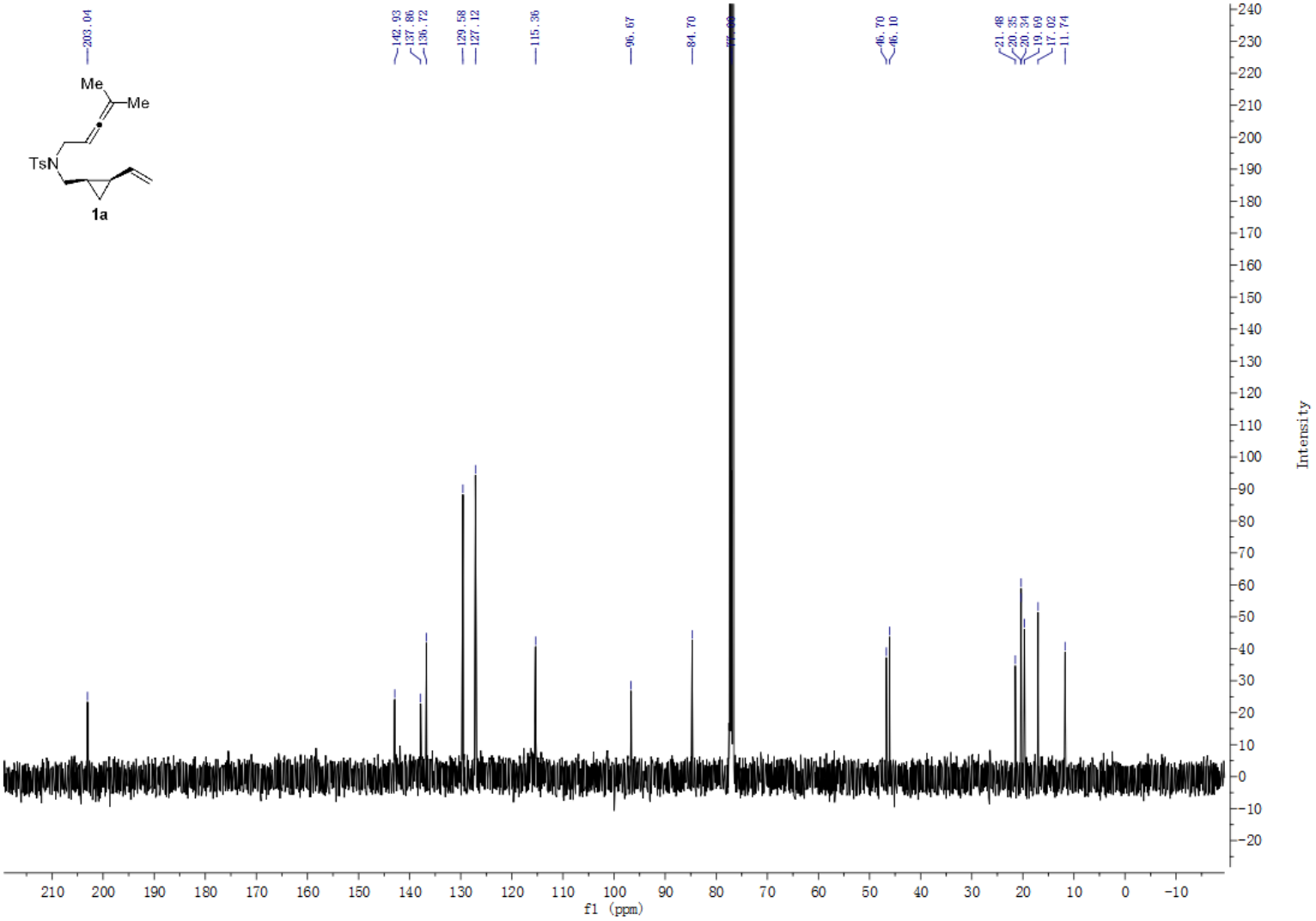
8. NMR Spectra of New Compounds

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136.72
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96.67
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77.48
46.70
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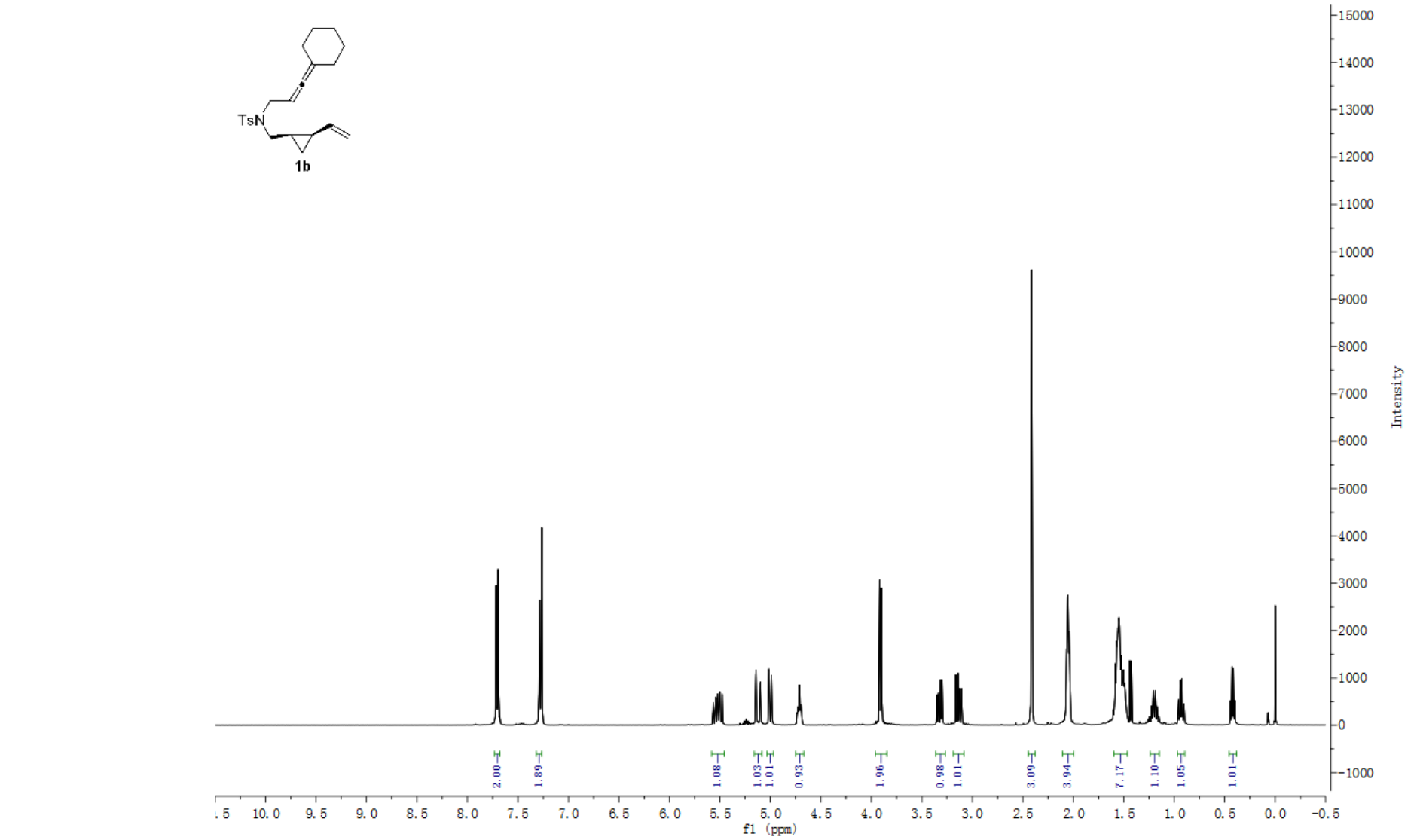
21.48
20.35
20.34
19.69
17.02
11.74
Me
Me
TsN
1a
f1 (ppm)
Intensity


TsN
1b
Intensity
f1 (ppm)
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1.01
0.93
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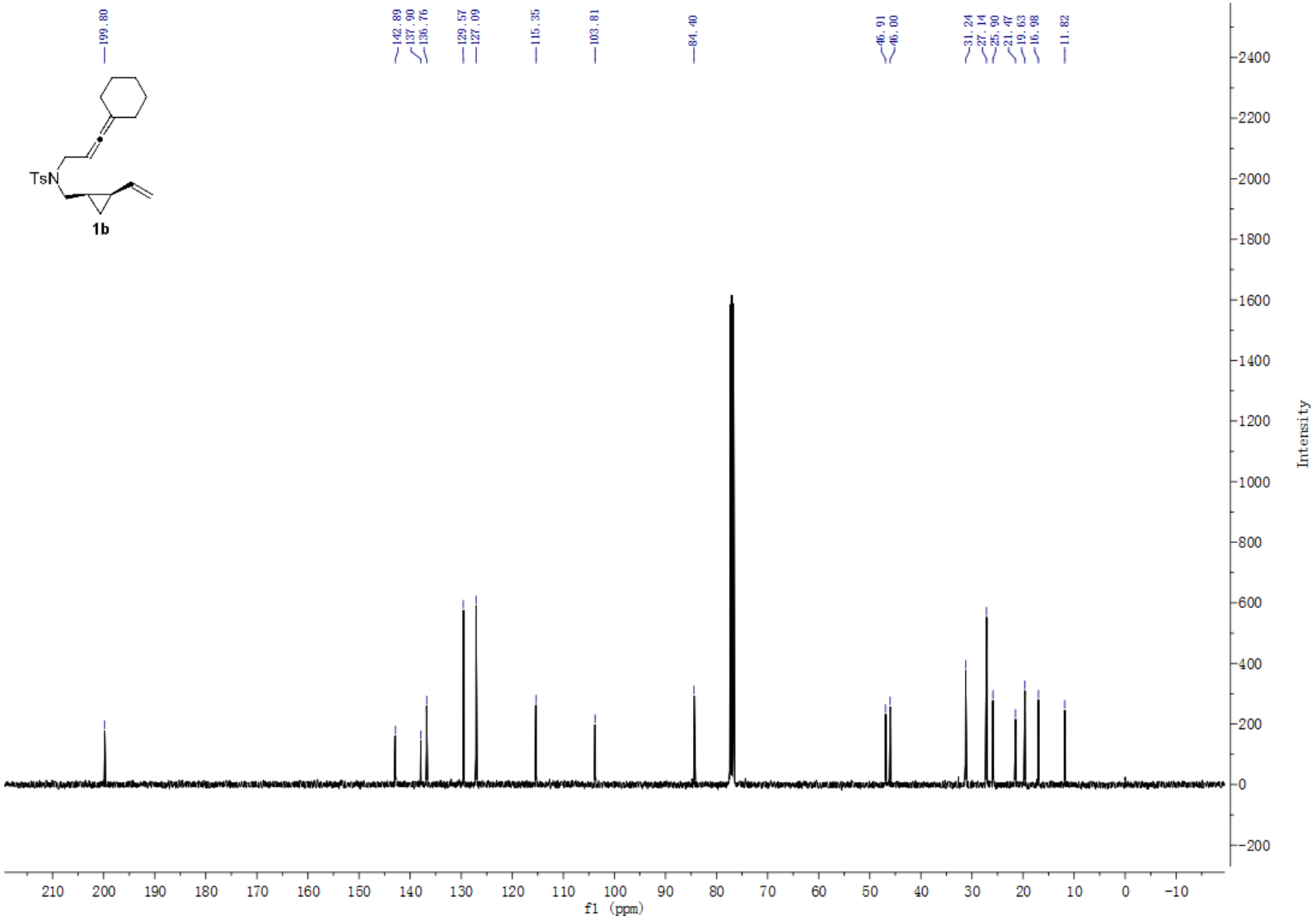
1.01
3.09
3.94
7.17
1.10
1.05
1.01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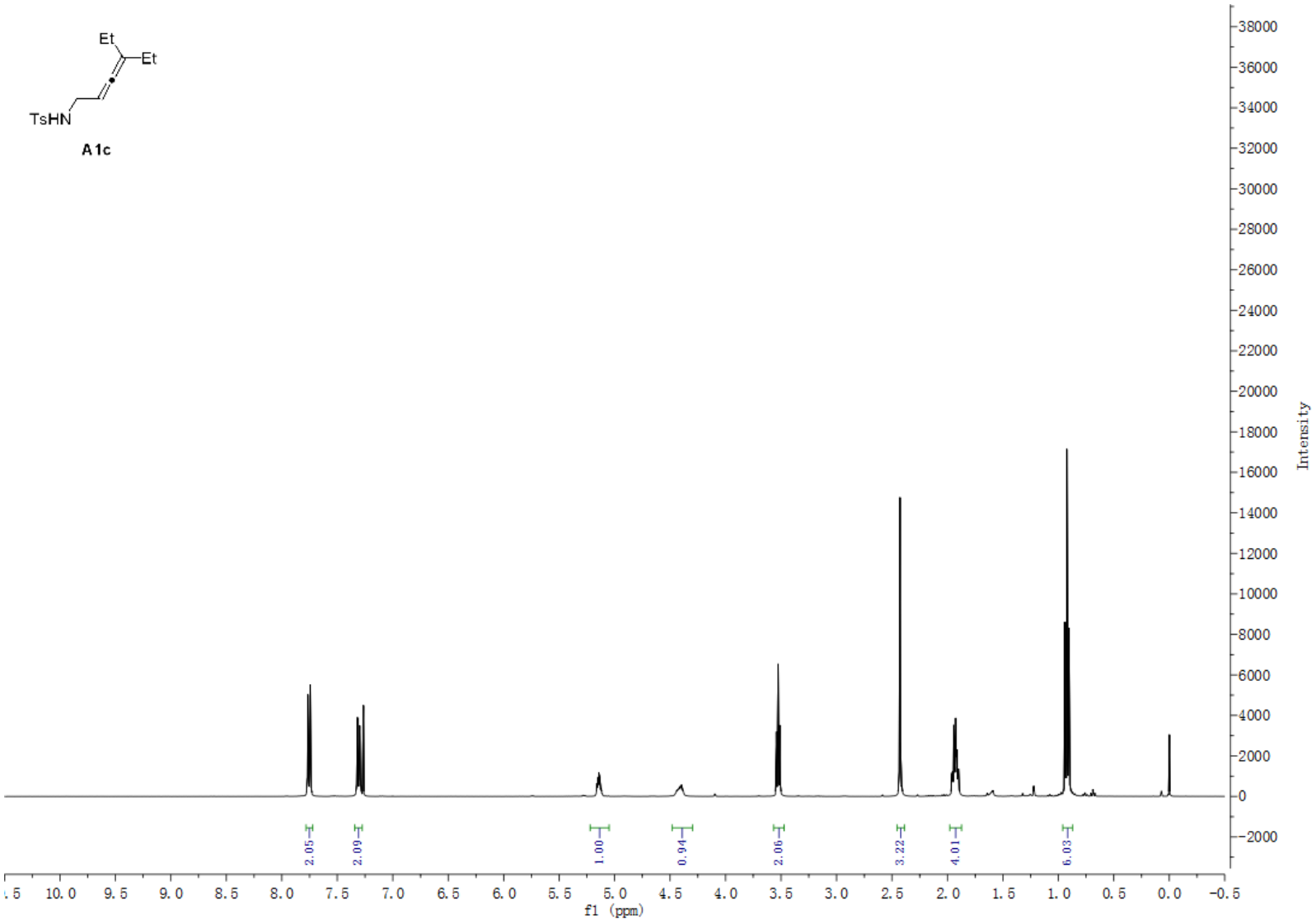
1b
Intensity
f1 (ppm)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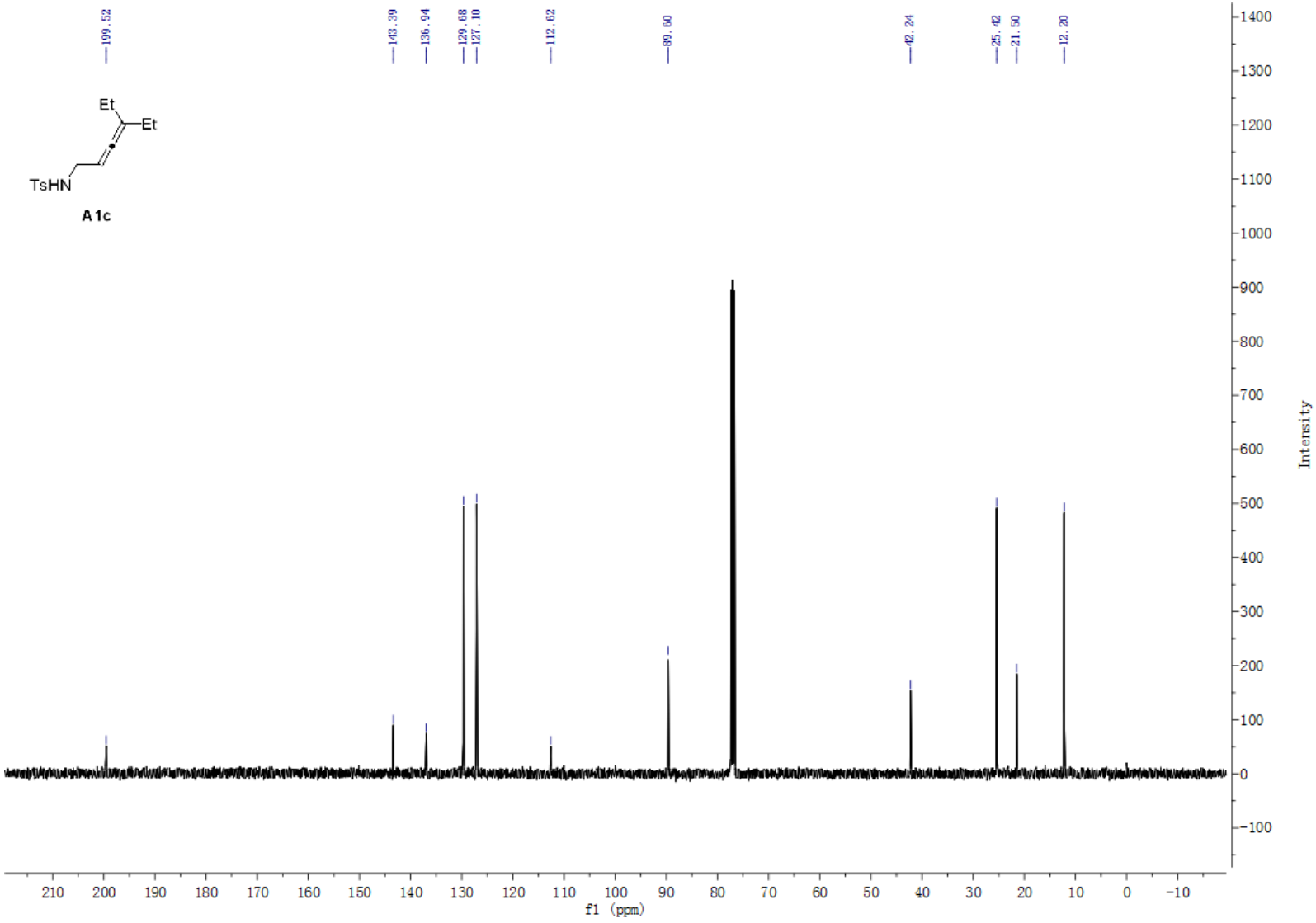
4.01
6.03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Et
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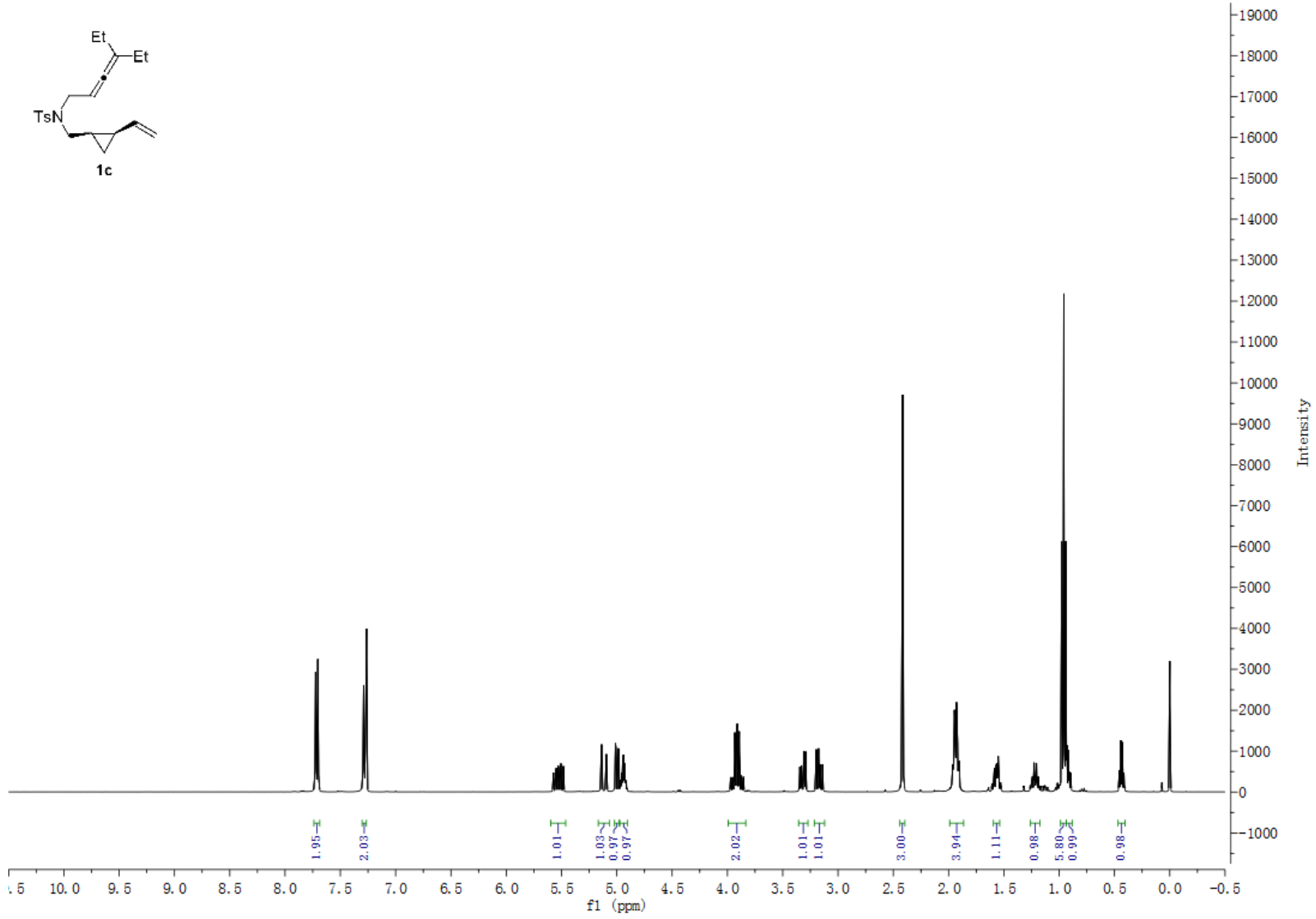
A1c
Intensity
f1 (ppm)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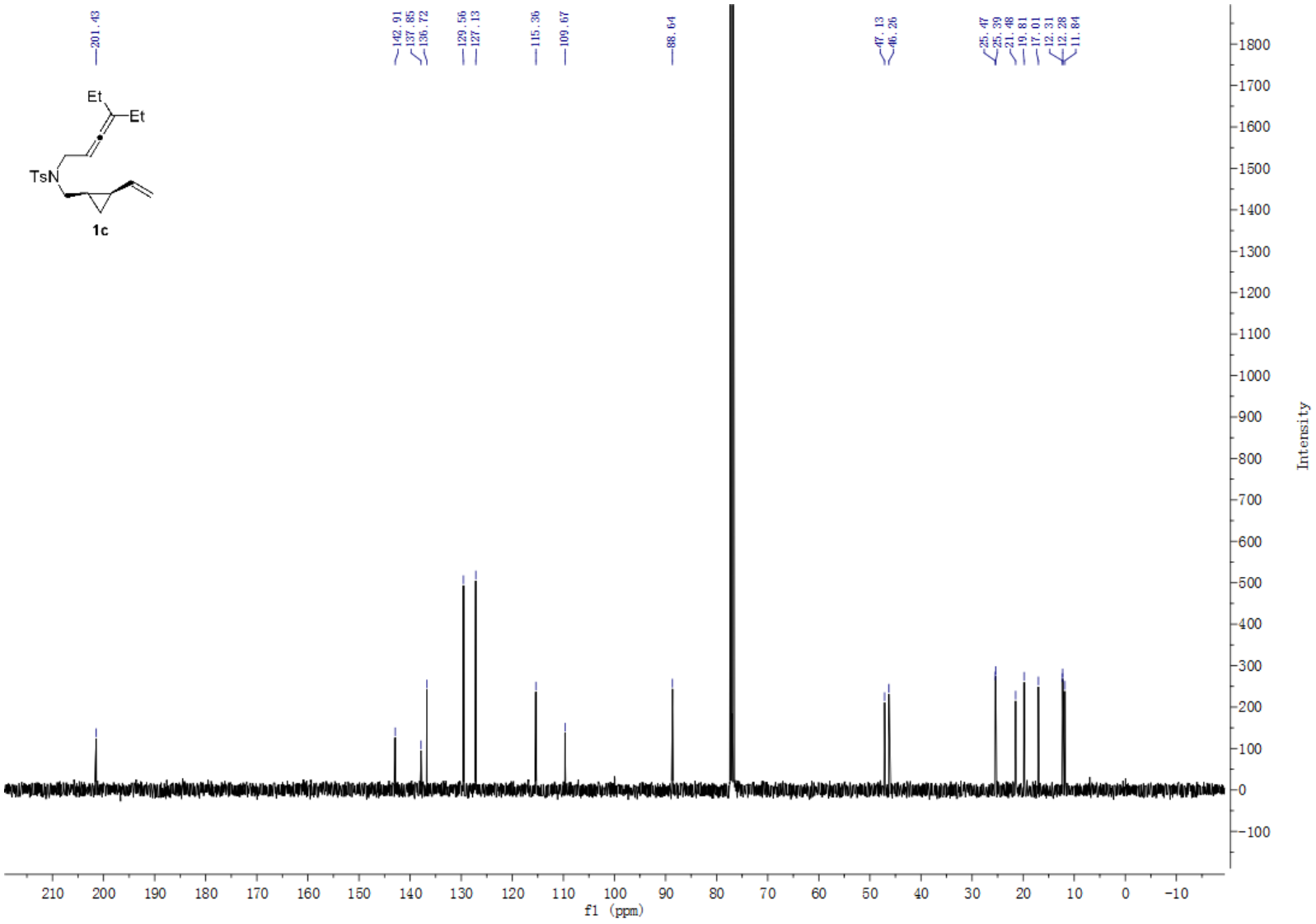
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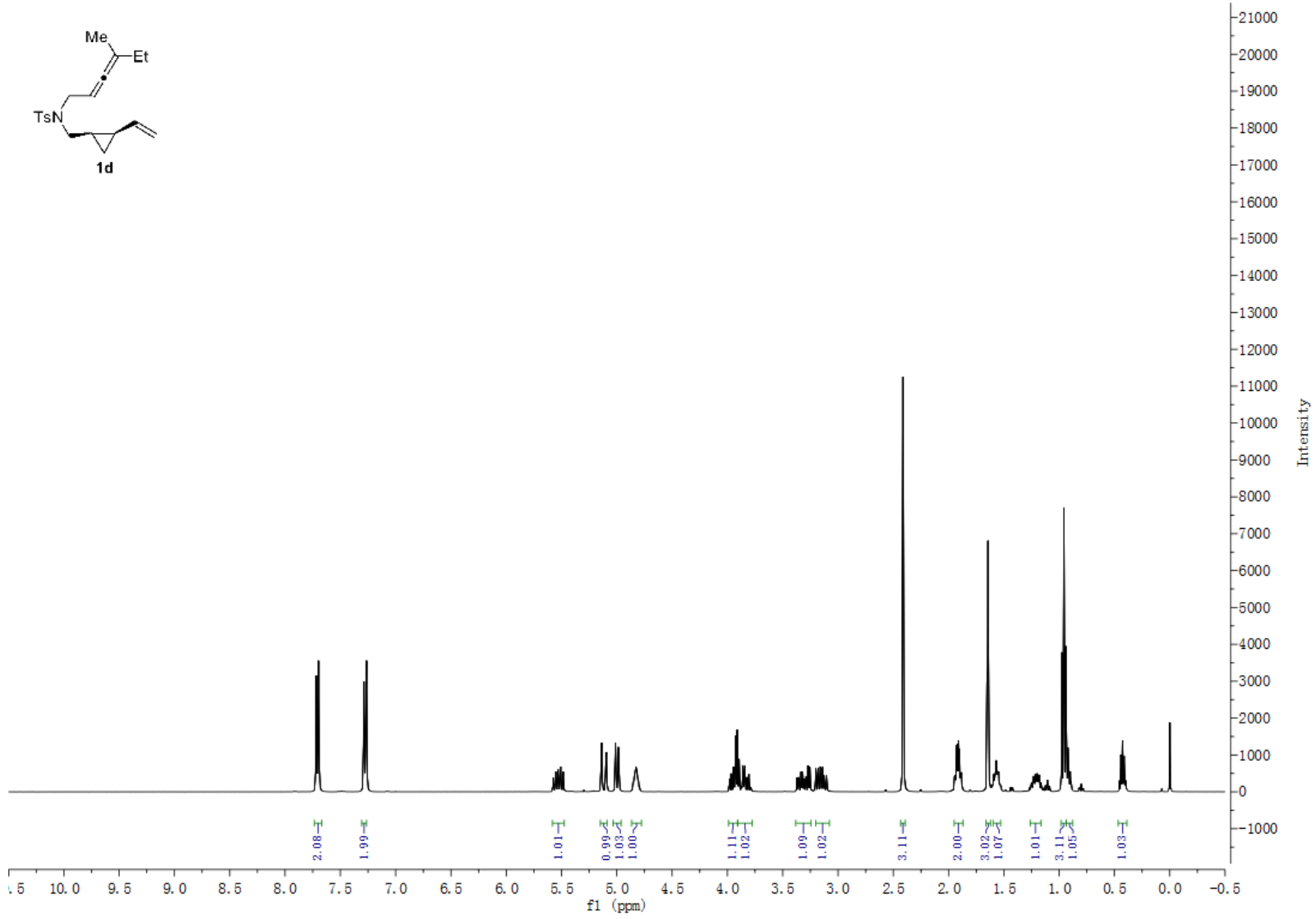
Intensity
f1 (ppm)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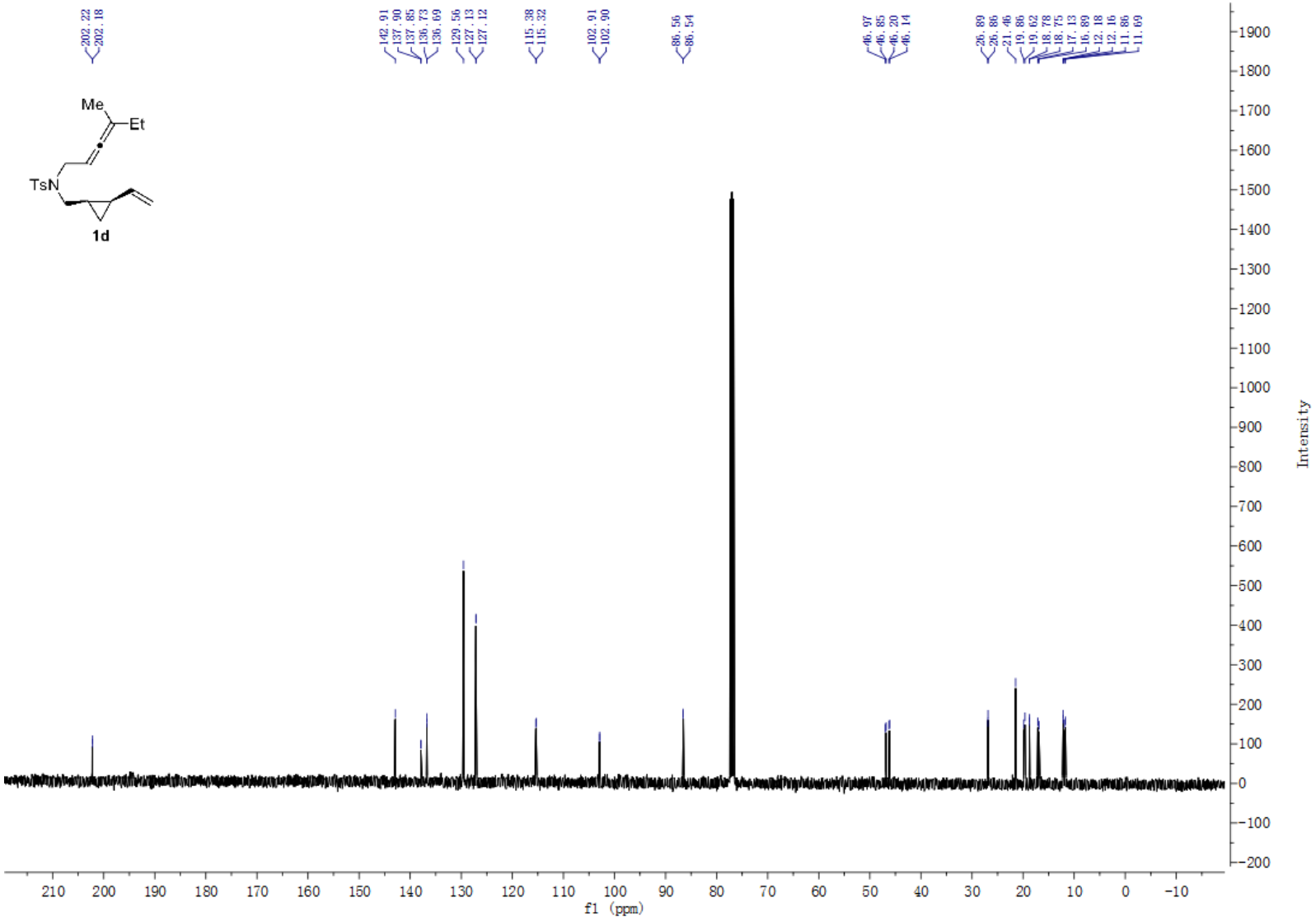
1.03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102.90
86.56
86.54
46.97
46.85
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46.14
26.89
26.86
21.46
19.86
19.62
18.78
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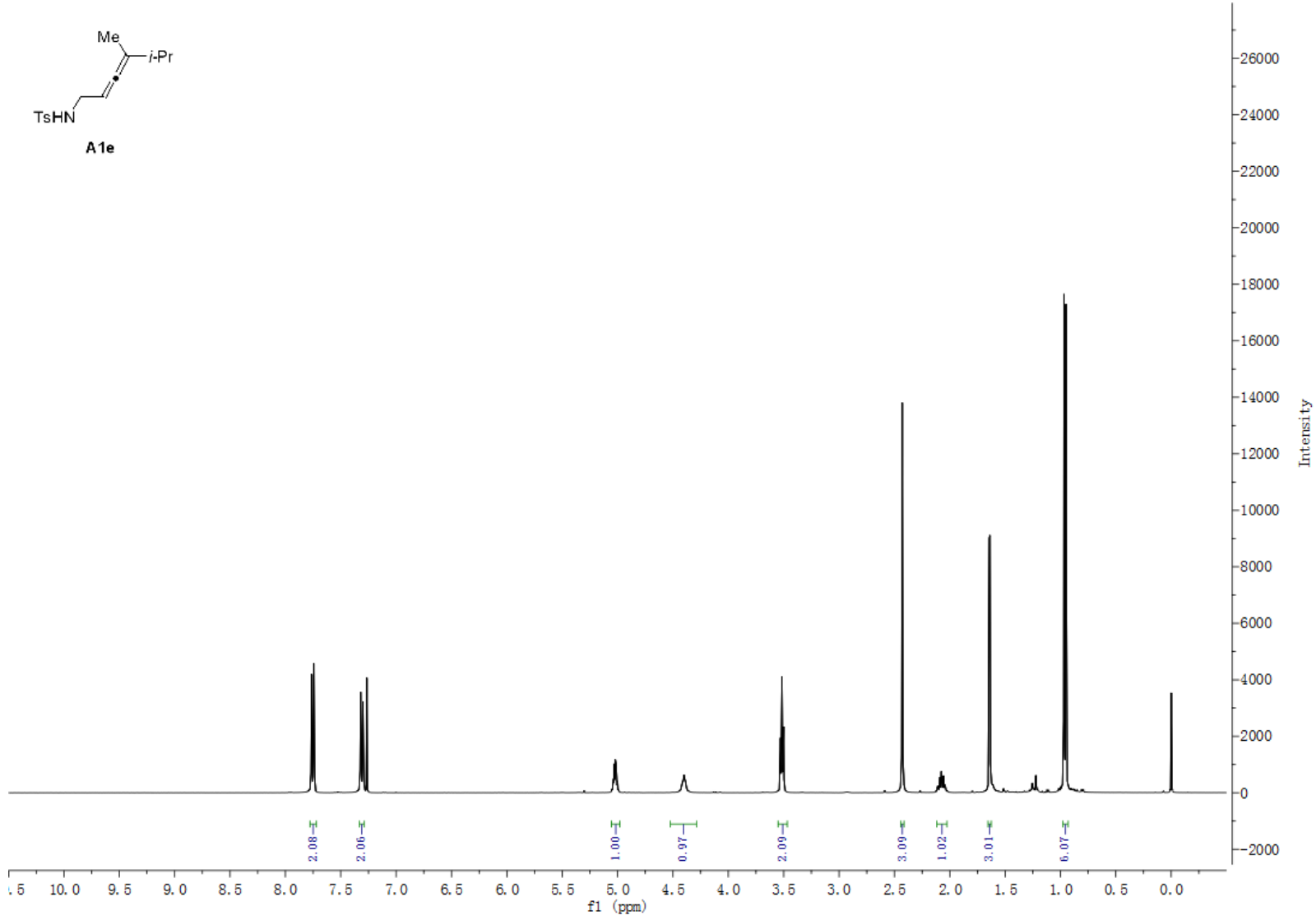
Et
TsN
1d
Intensity
f1 (ppm)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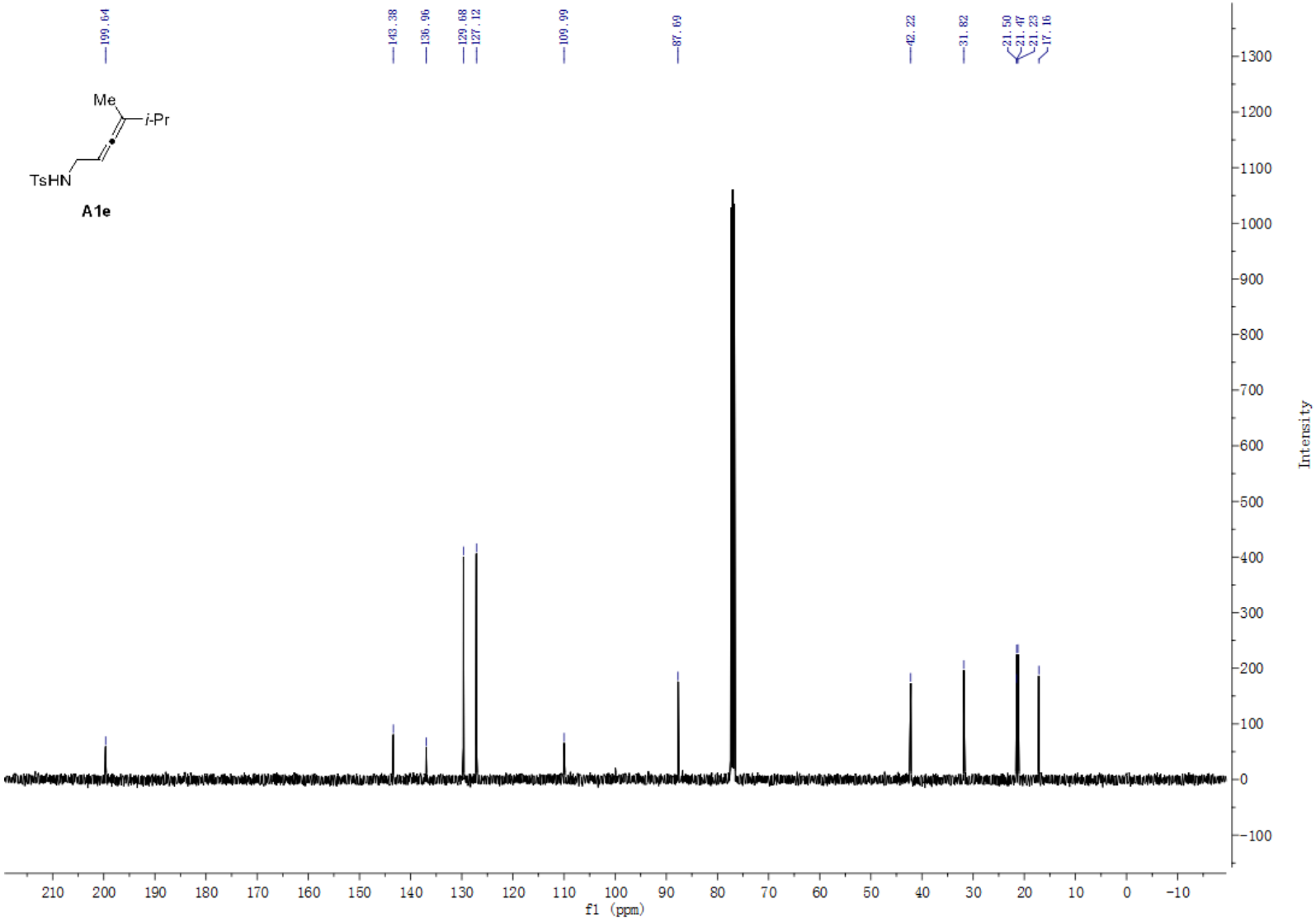
6.07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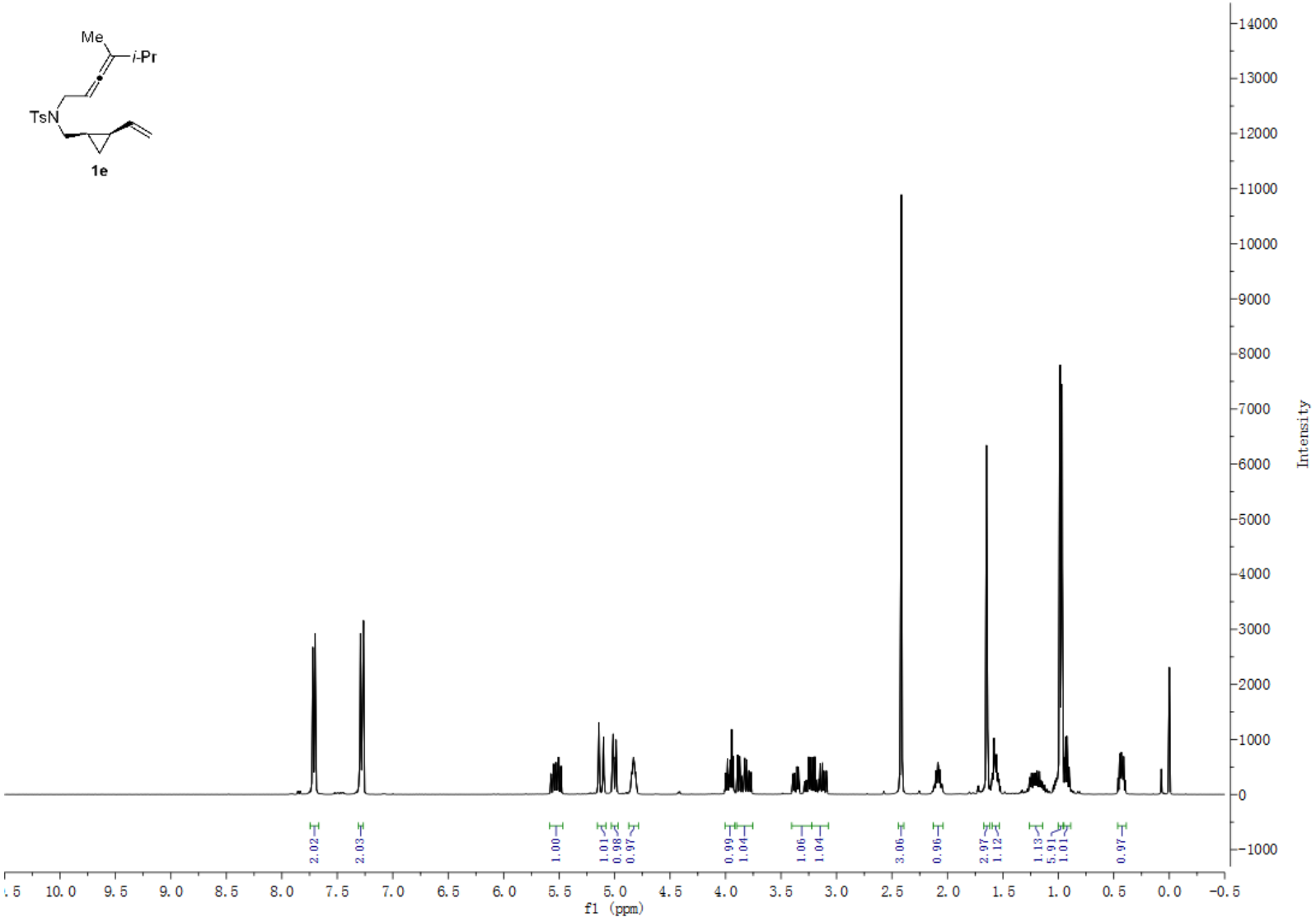
TsHN
A1e
Intensity
f1 (ppm)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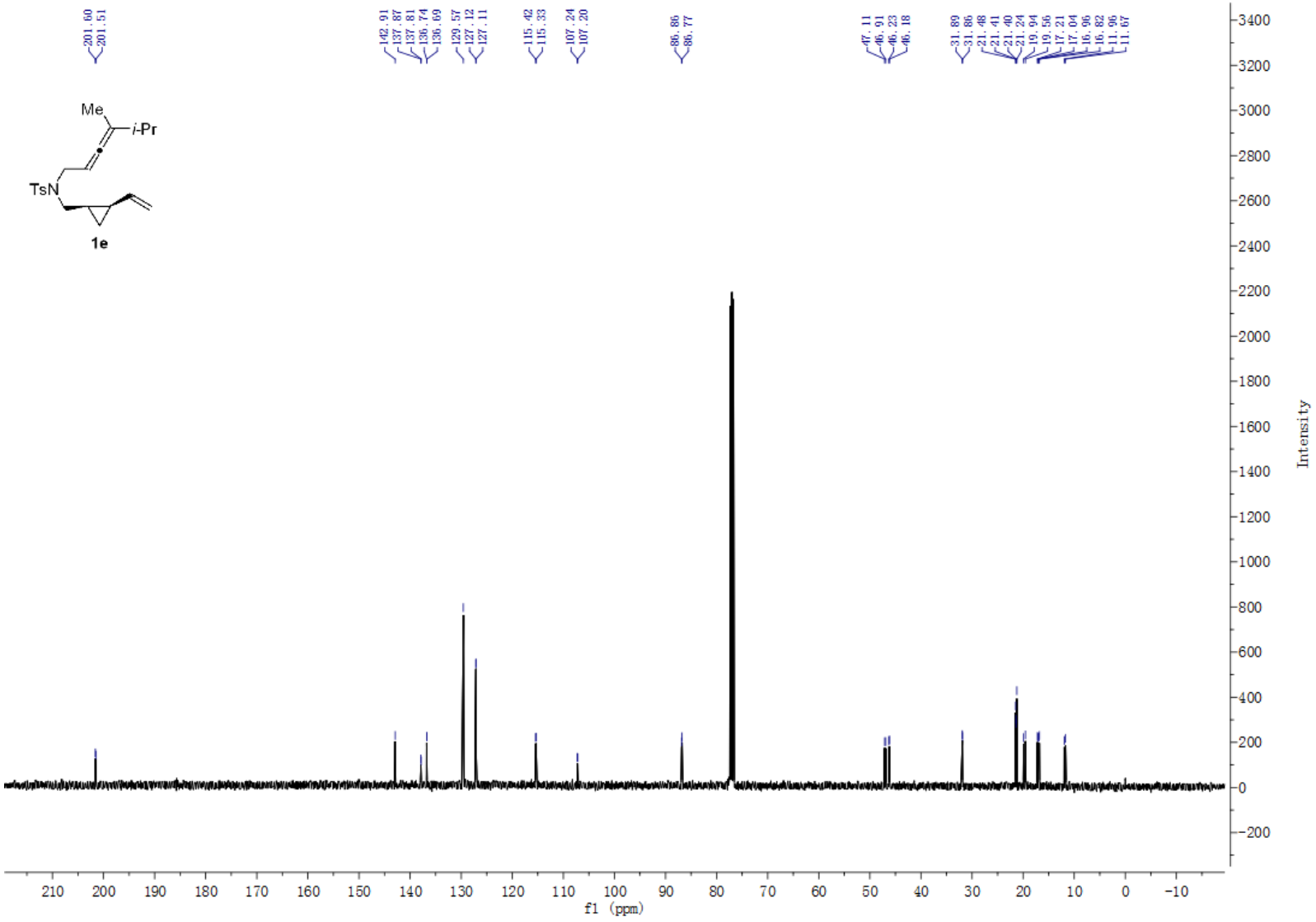
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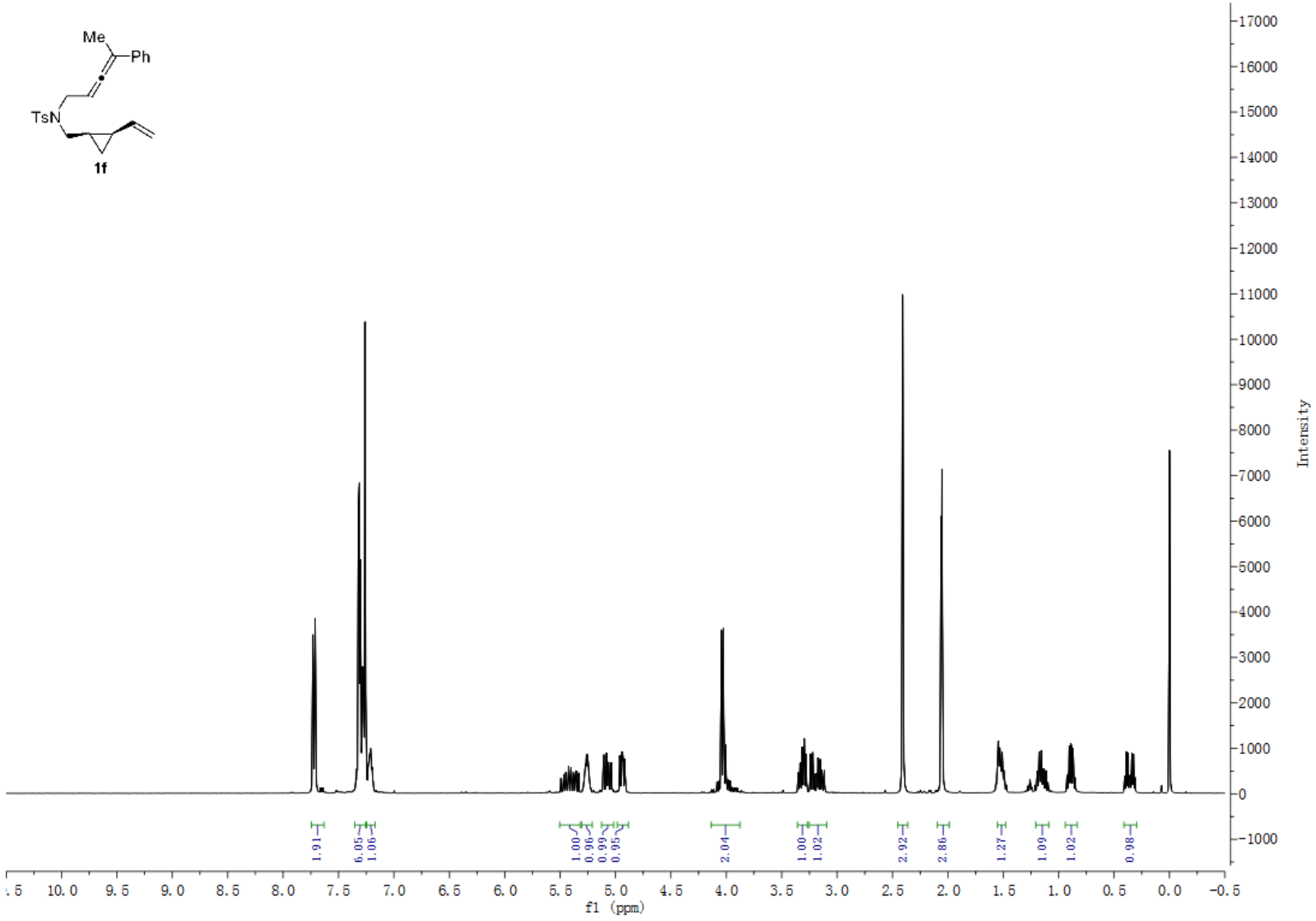
f1 (ppm)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1.27
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1.02
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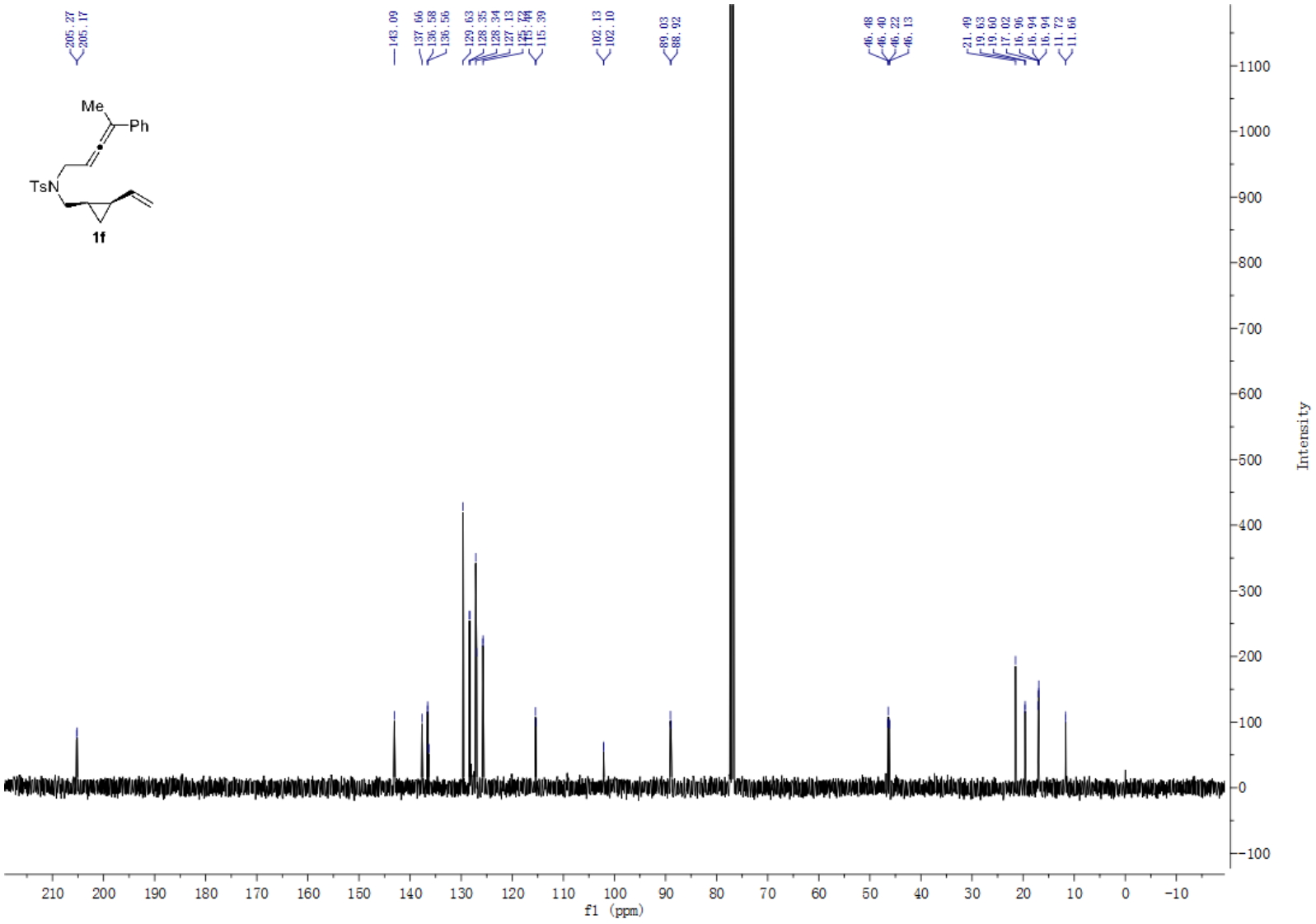
f1 (ppm)
Intensity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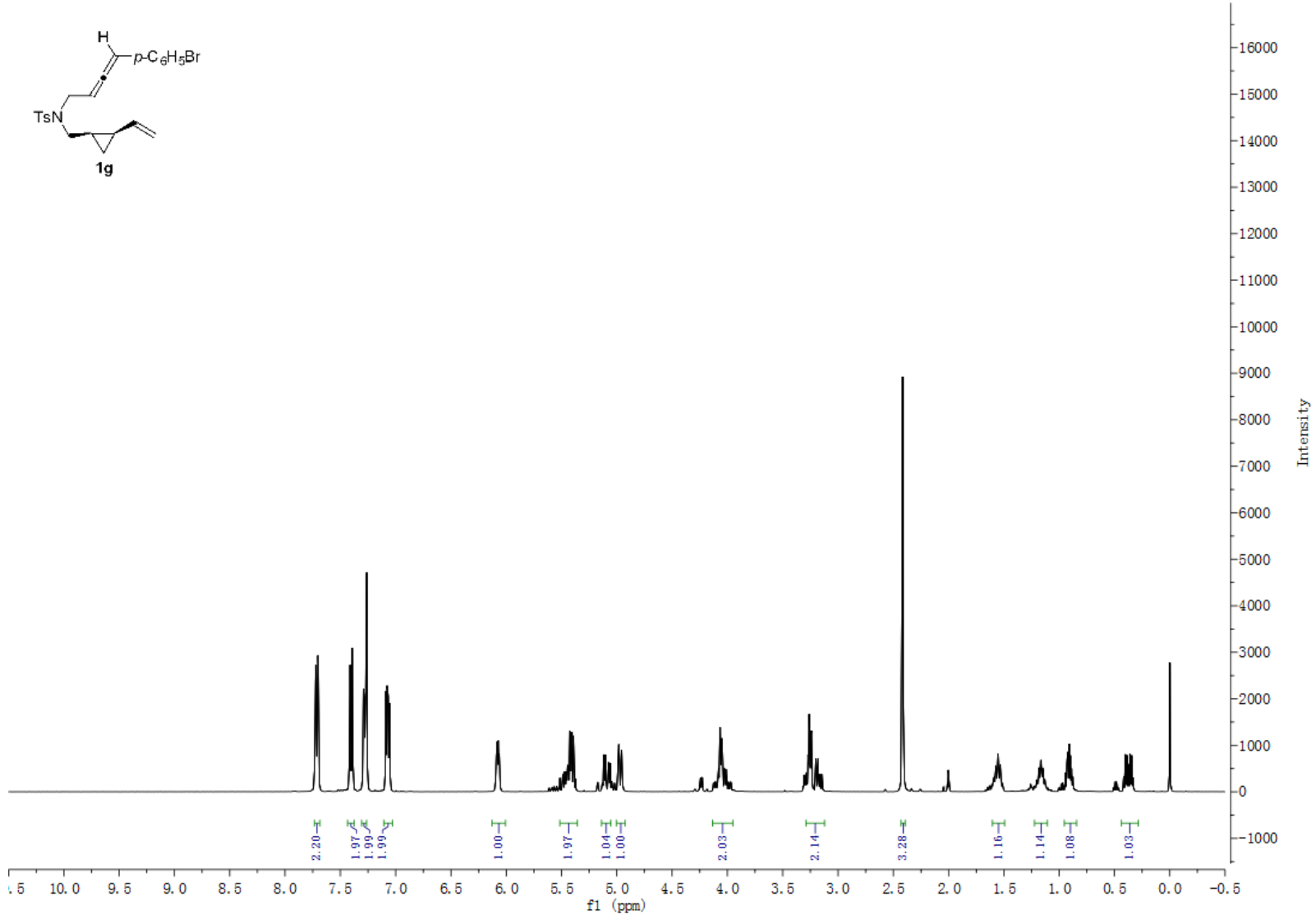
f1 (ppm)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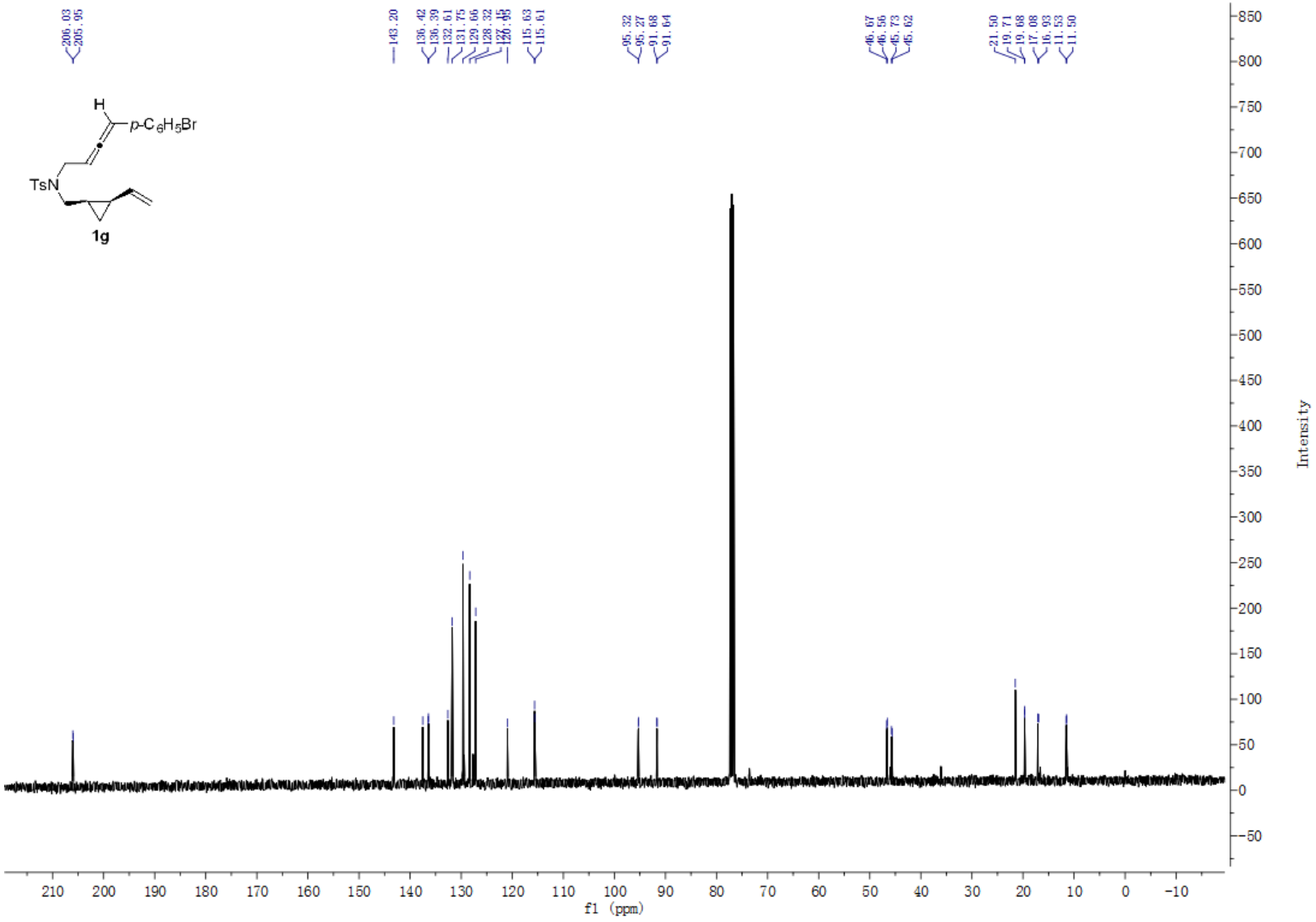
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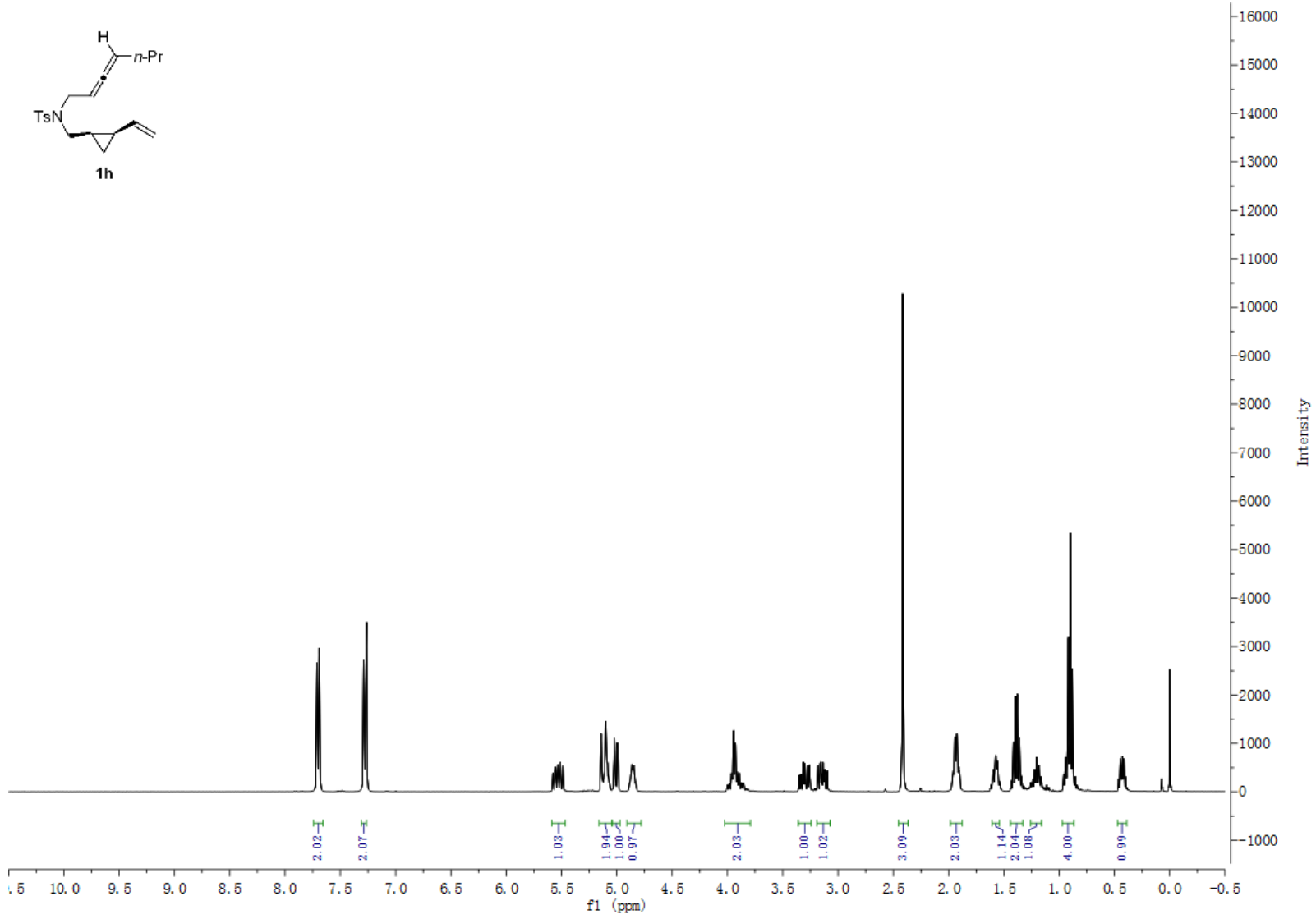
f1 (ppm)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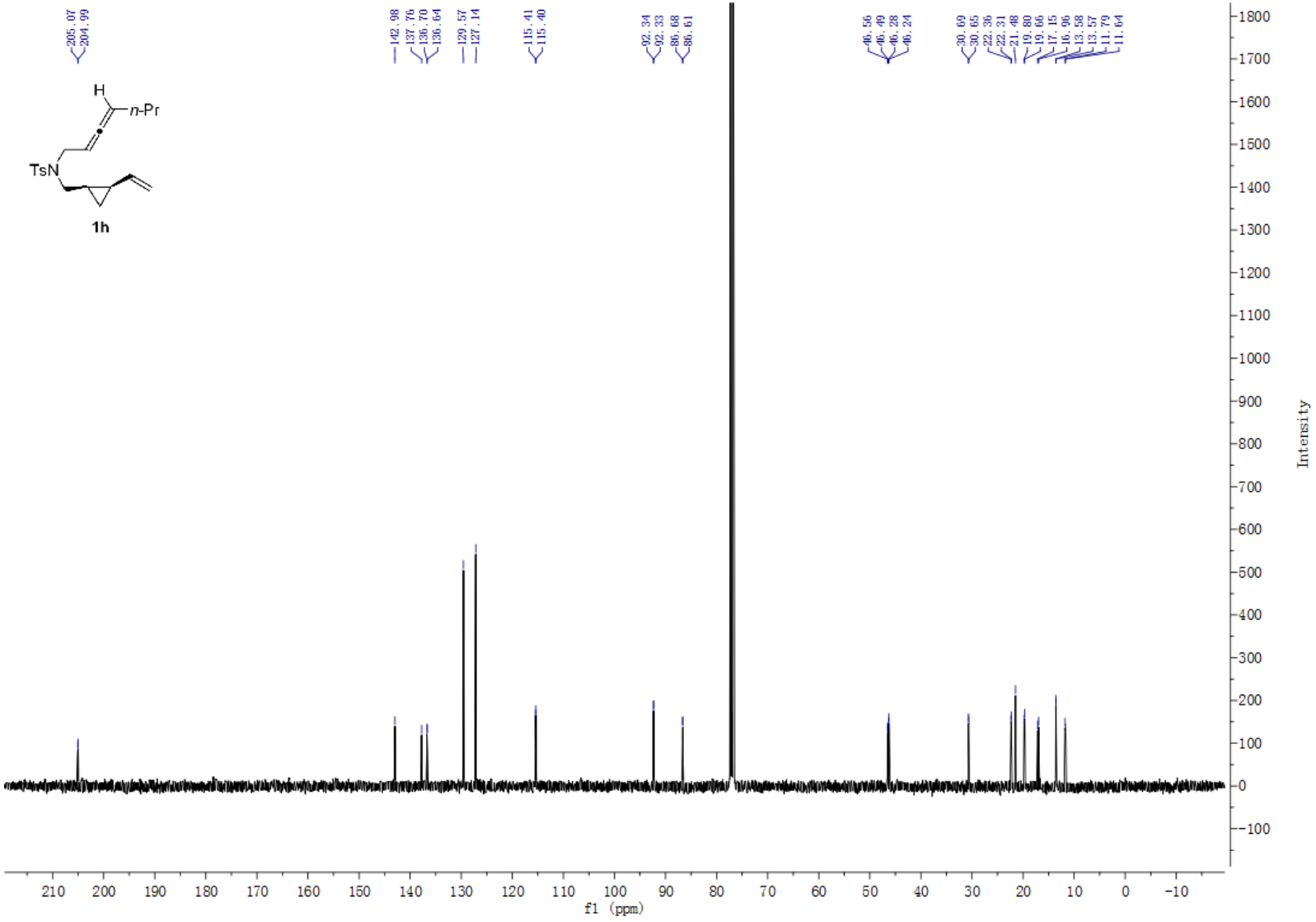
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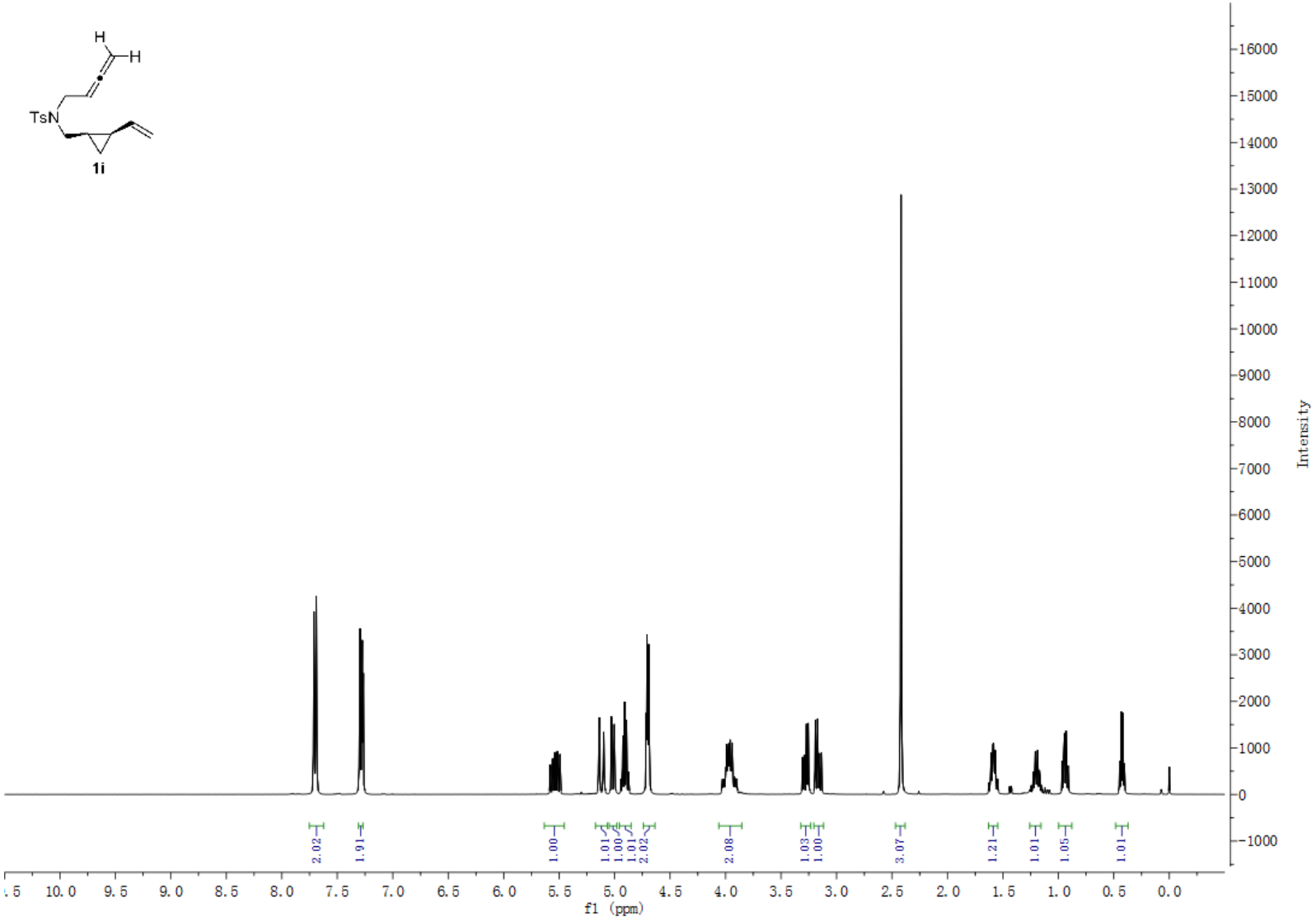
Intensity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6000
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4000
3000
2000
1000
0
-1000
Intensity
2.02
1.91
1.00
1.01
1.00
1.01
2.02
2.08
1.03
1.00
3.07
1.21
1.01
1.05
1.01
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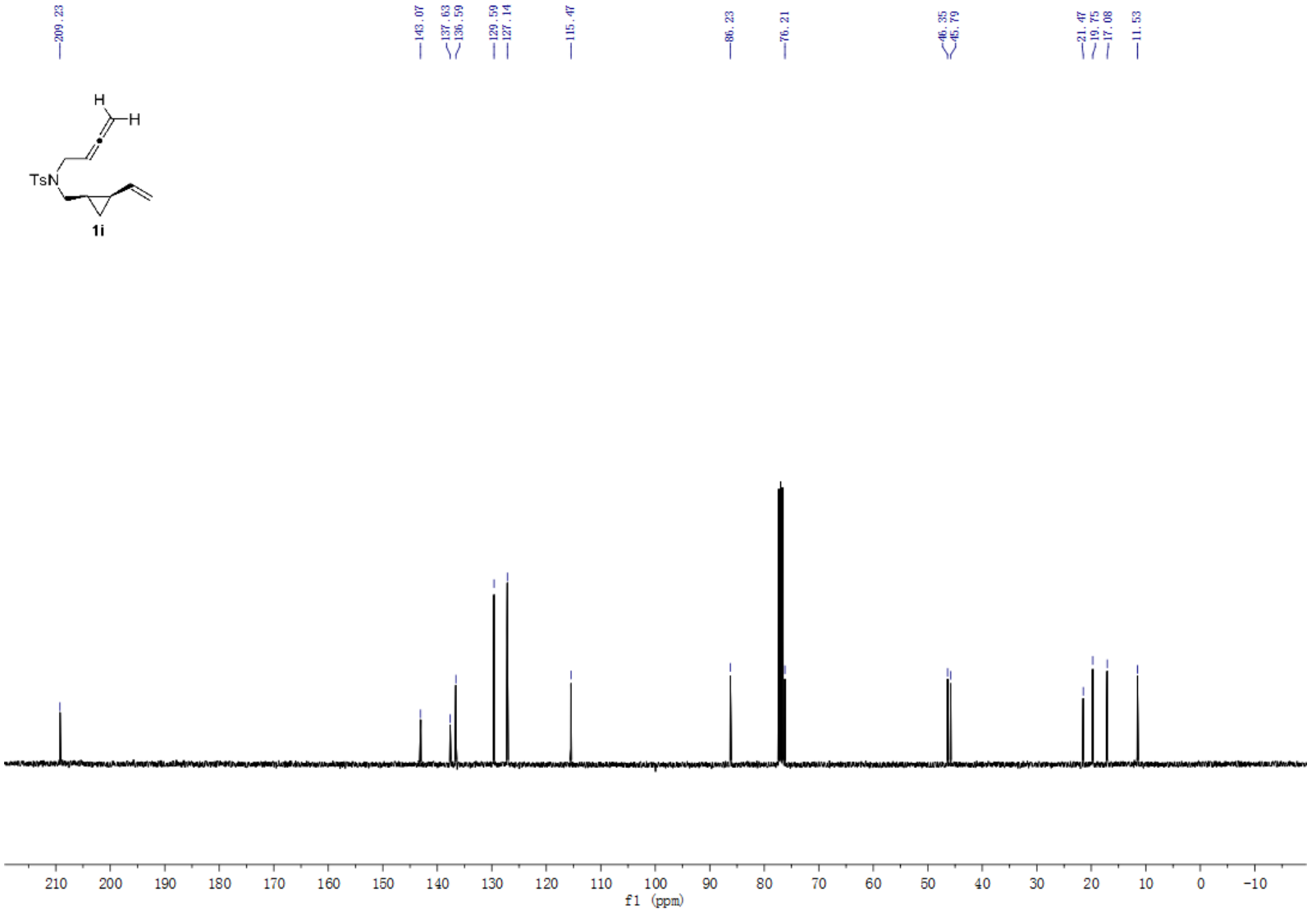
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1i
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190
180
170
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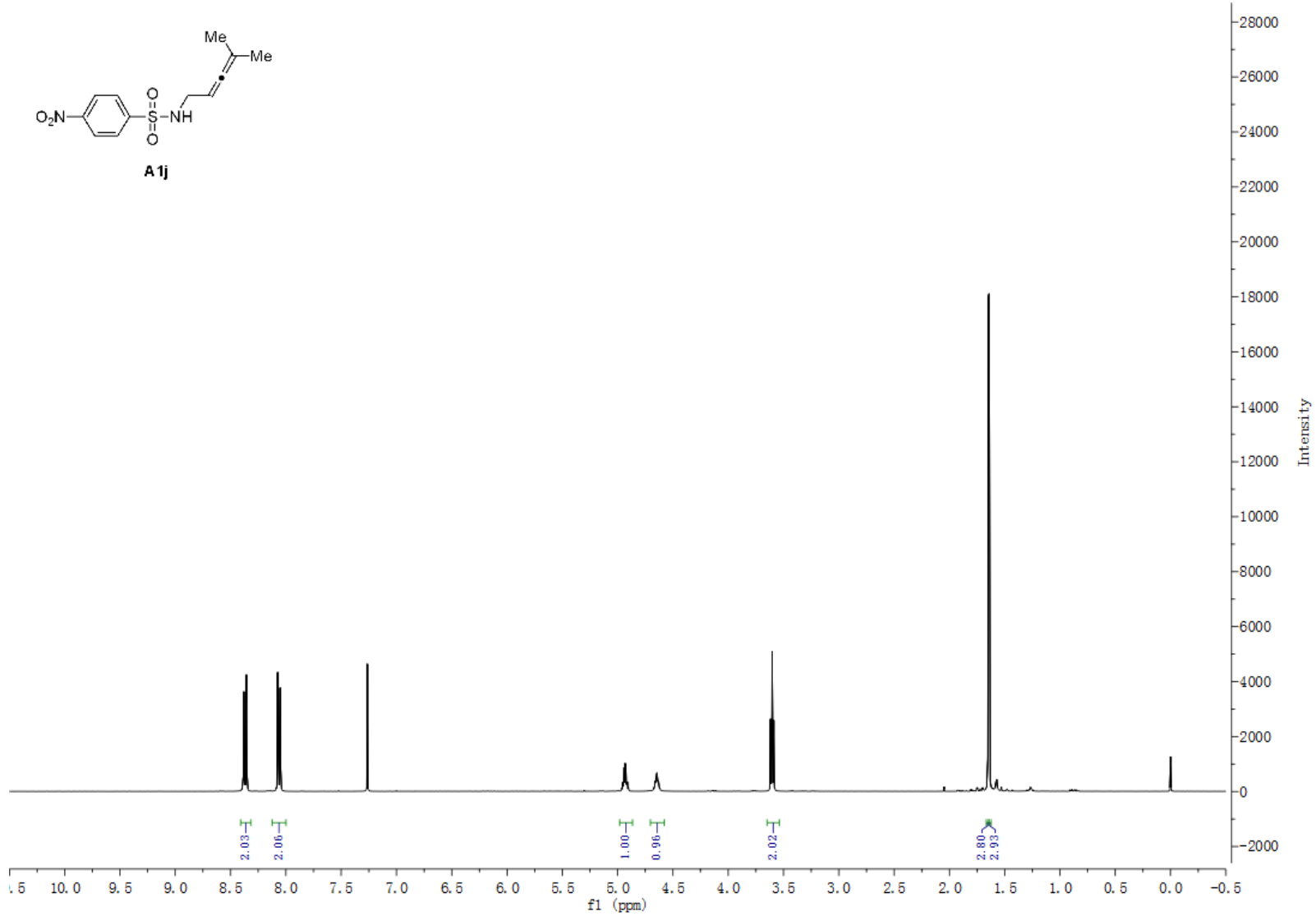
f1 (ppm)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12000
10000
8000
6000
4000
2000
0
-2000
Intensity
2.03
2.06
1.00
0.96
2.02
2.80
2.93
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
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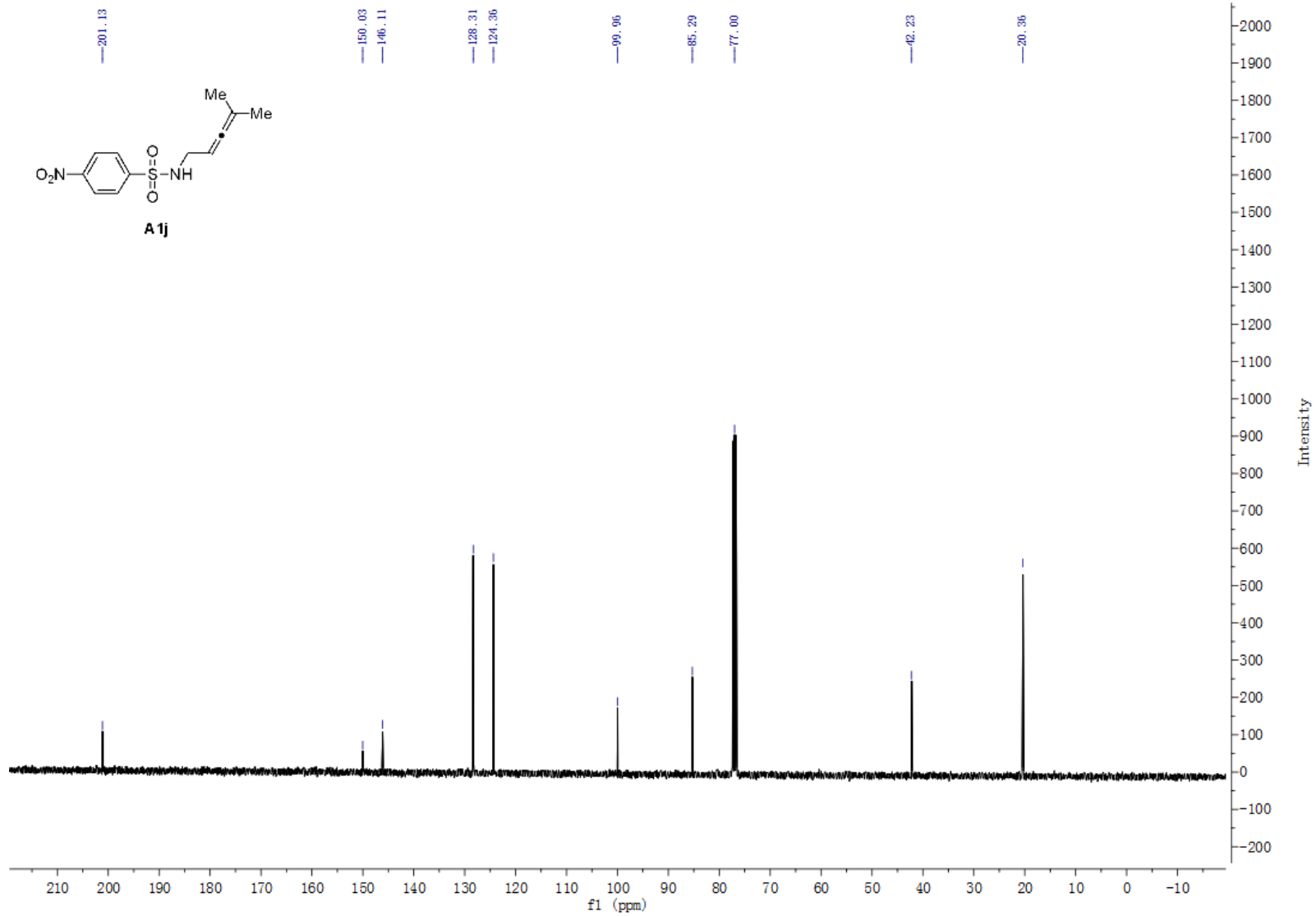
f1 (ppm)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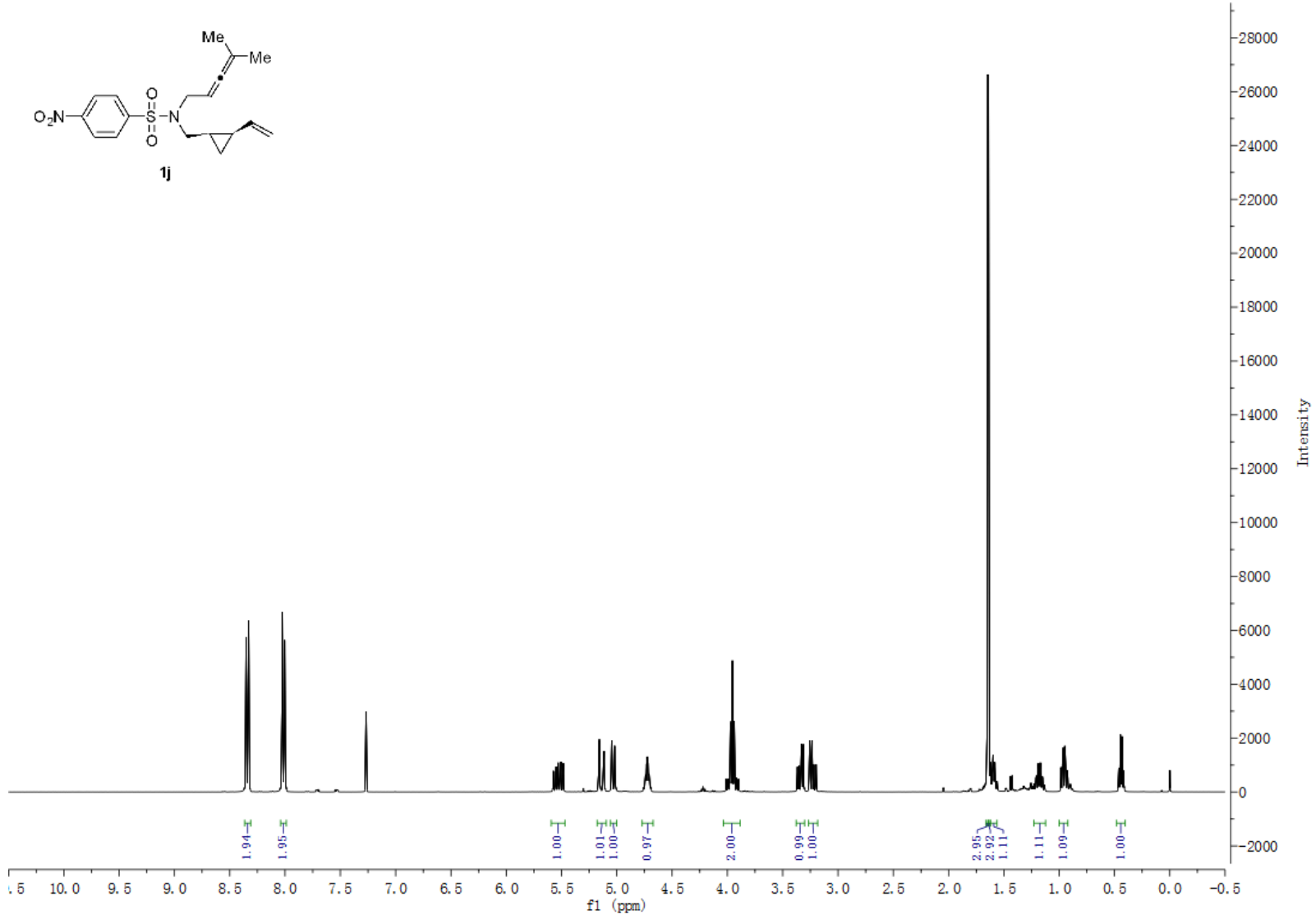
NH
O
O
A1j
Intensity
f1 (ppm)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S
O
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22000
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12000
10000
8000
6000
4000
2000
0
-2000
Intensity
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0.97
2.00
0.99
1.00
2.95
2.92
1.11
1.11
1.09
1.00
10.0
9.5
9.0
8.5
8.0
7.5
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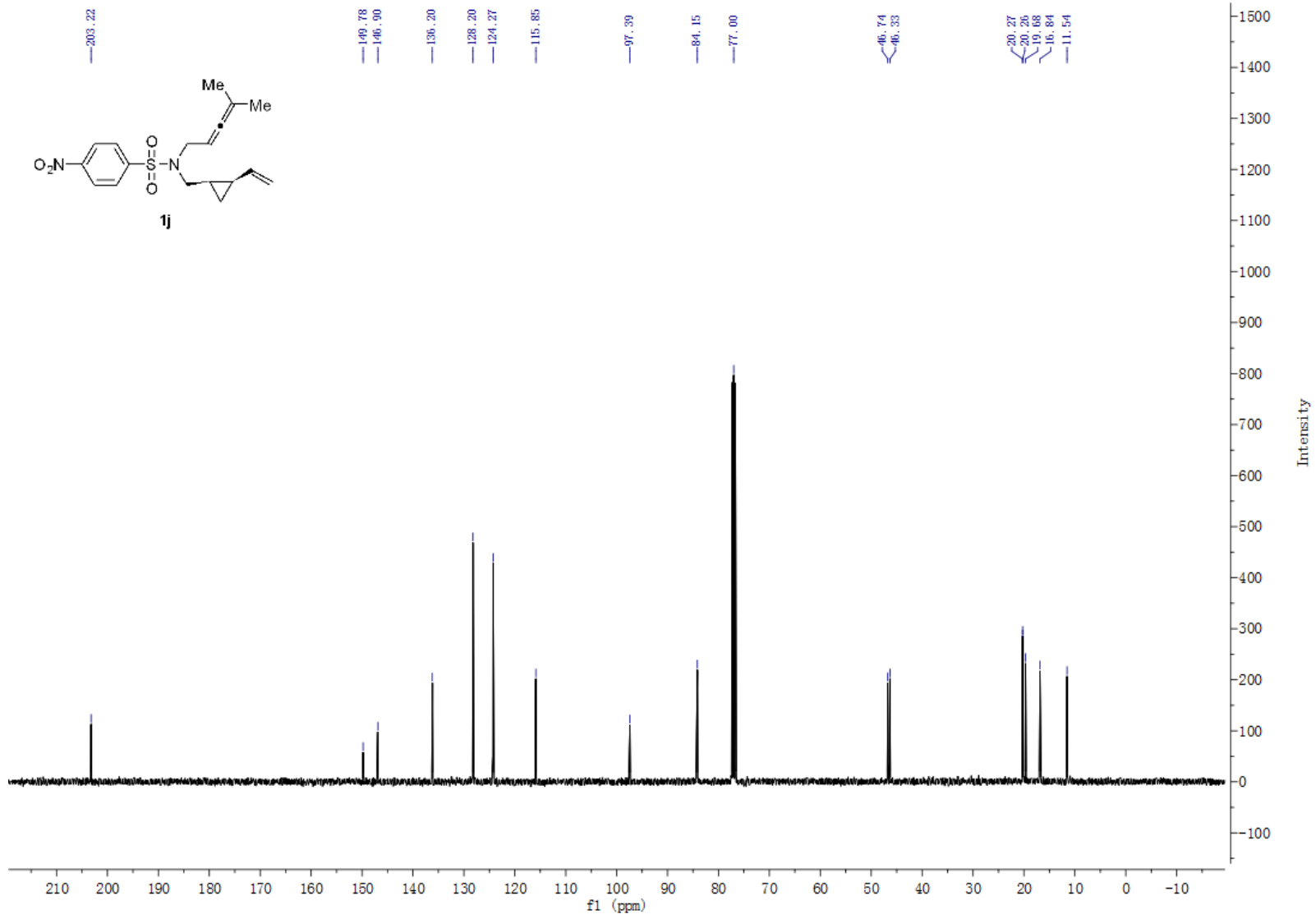
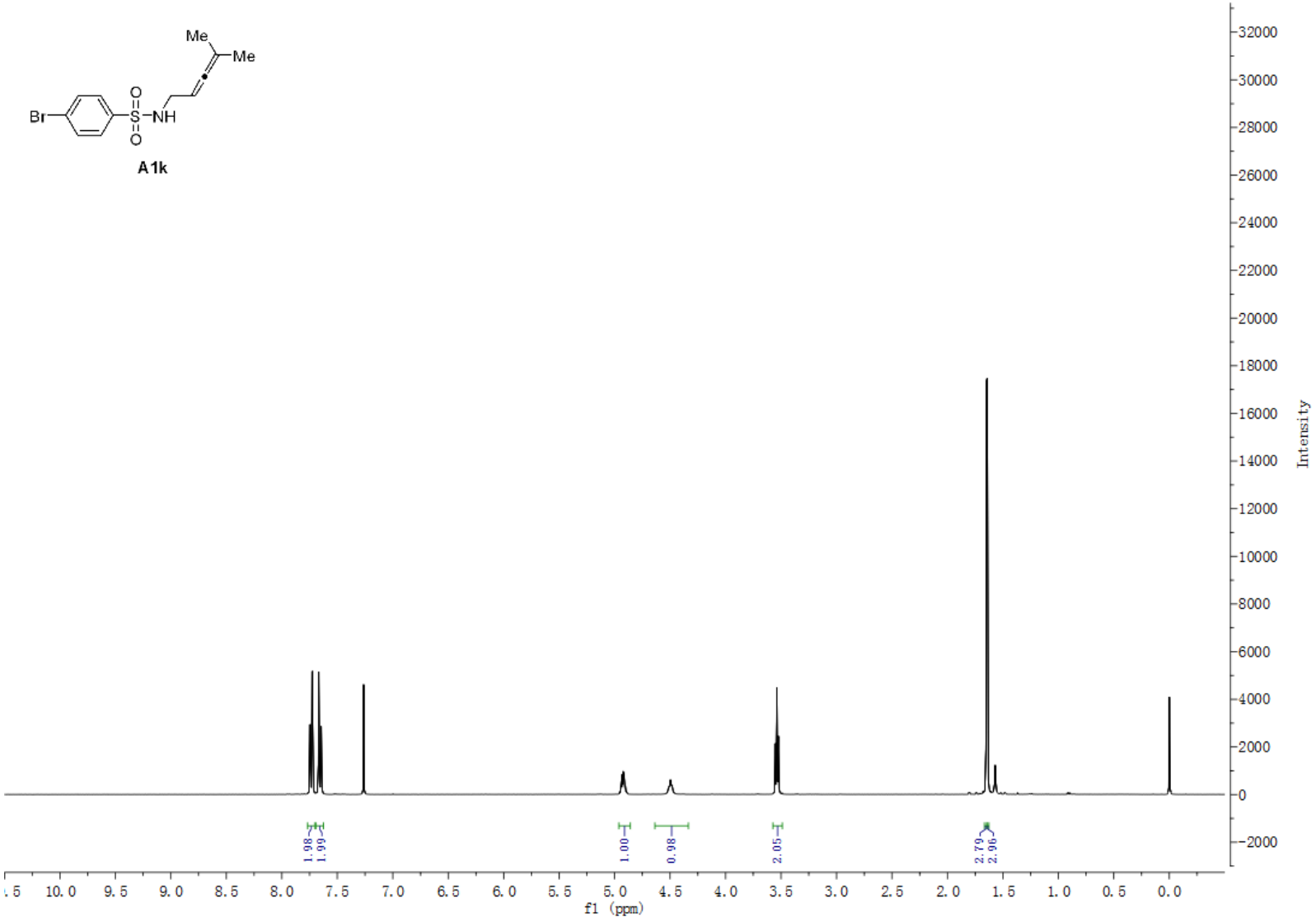
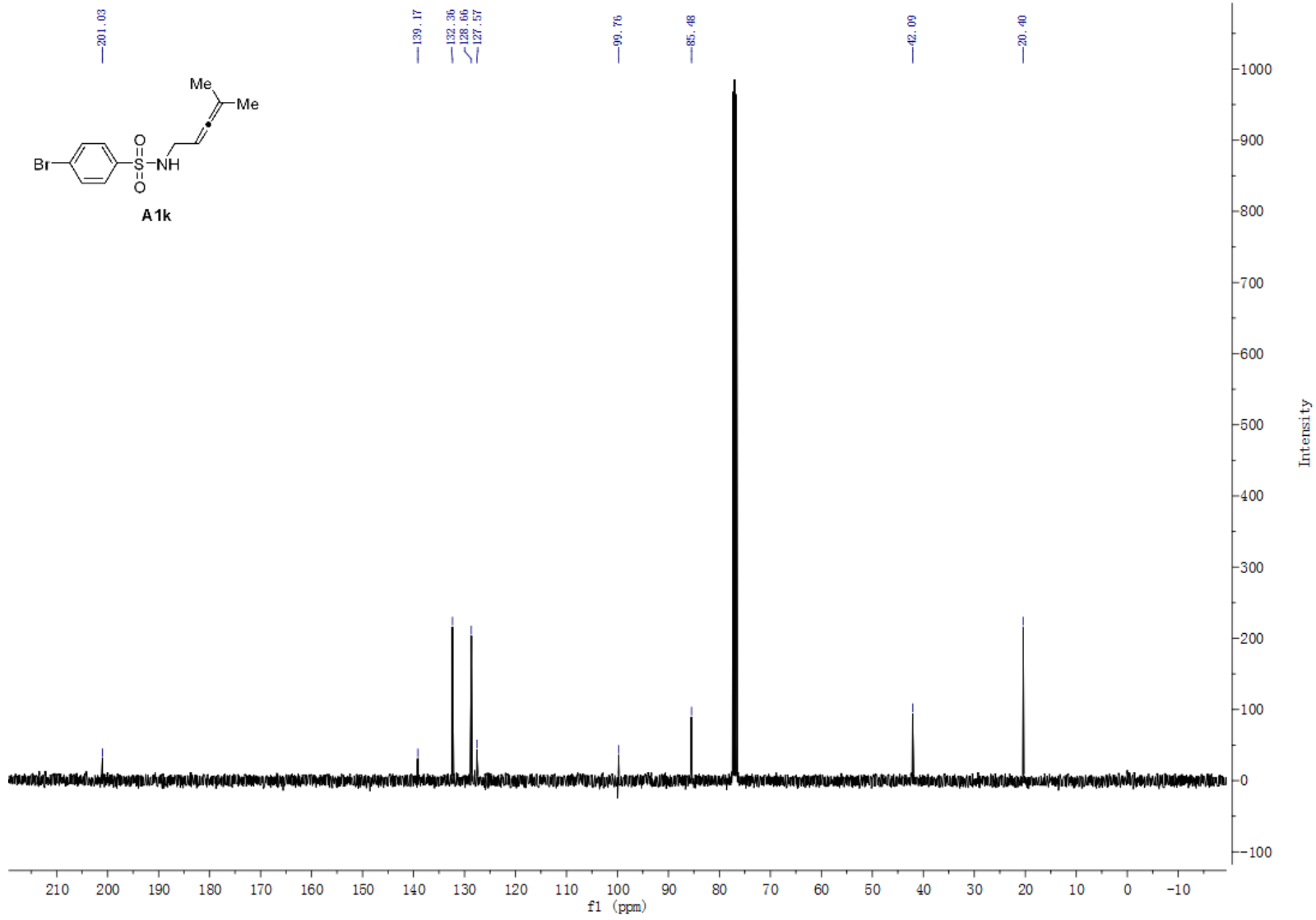
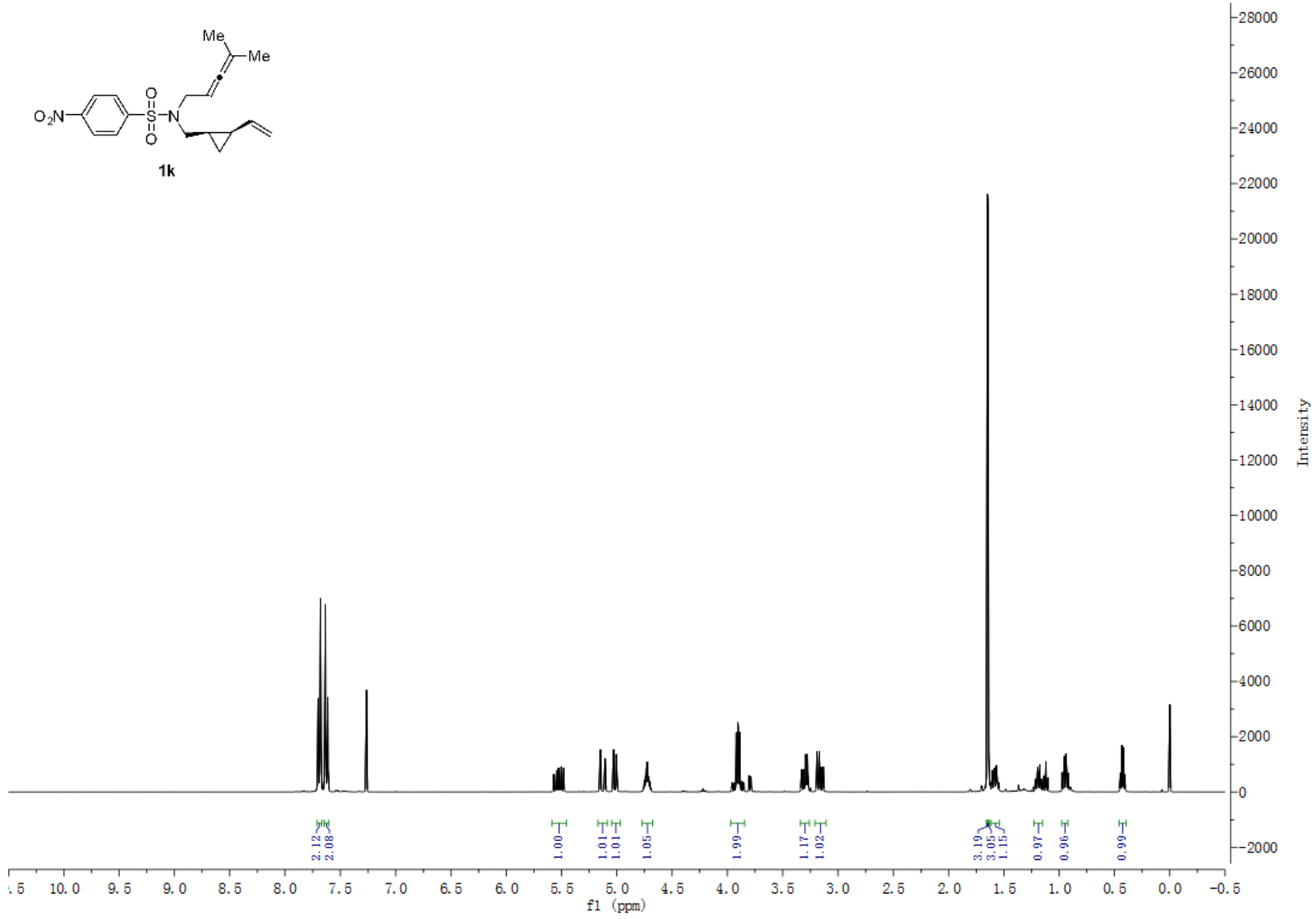
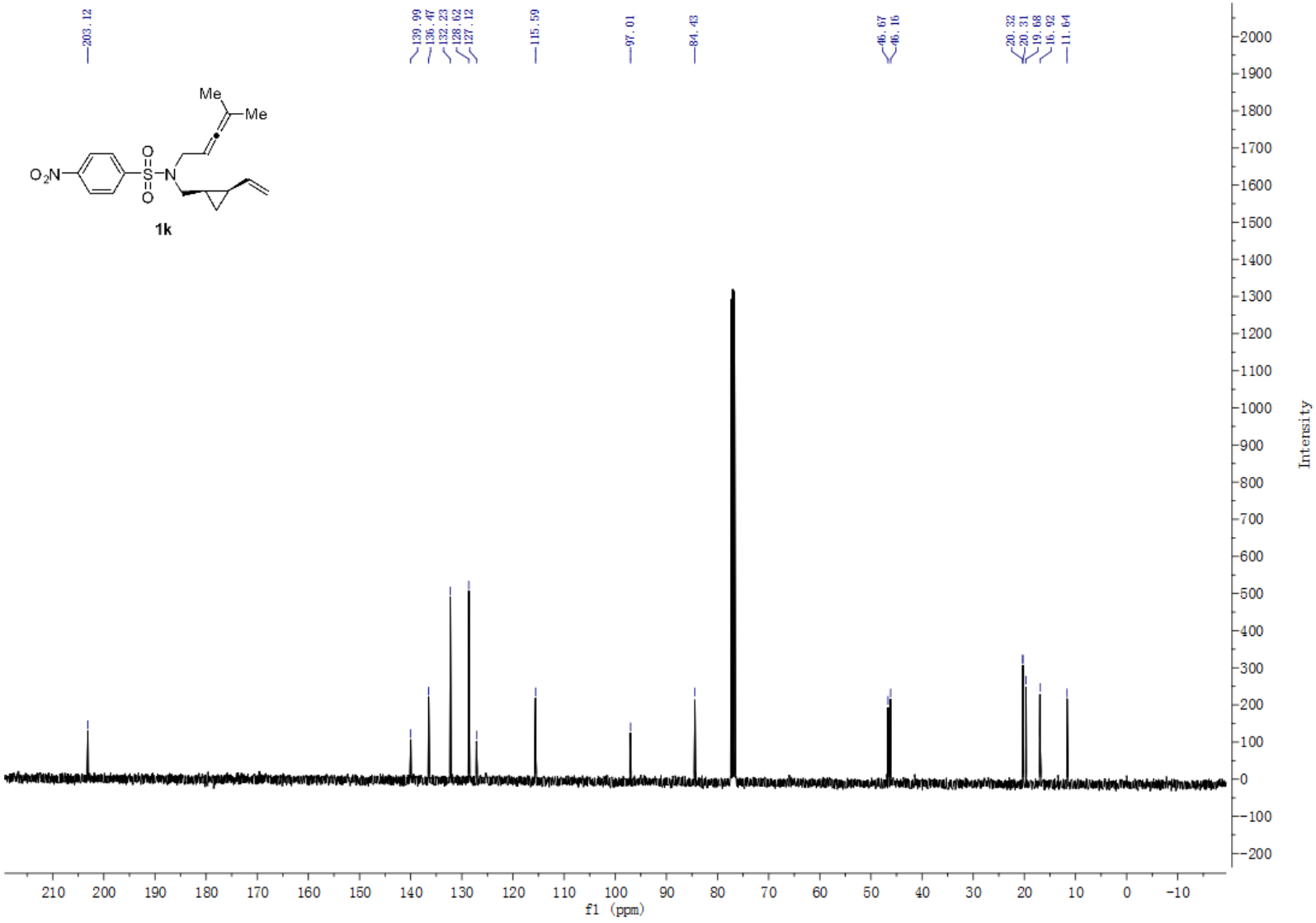
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

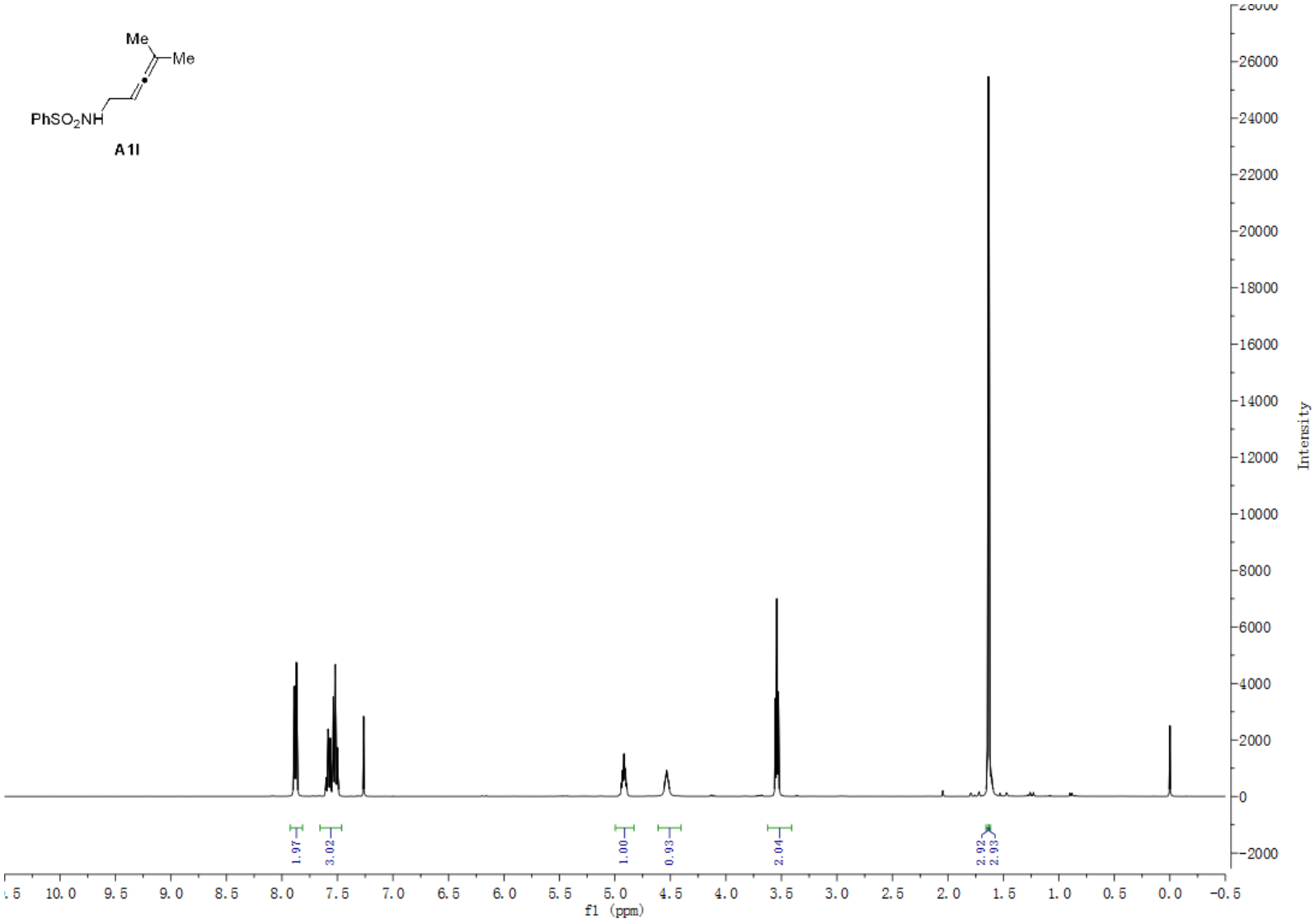

203.22
149.78
146.90
136.20
128.20
124.27
115.85
97.39
84.15
77.00
46.74
46.33
20.27
20.26
19.68
16.84
11.54
Me
Me
O2N
S
N
O
O
1j
Intensity
f1 (ppm)

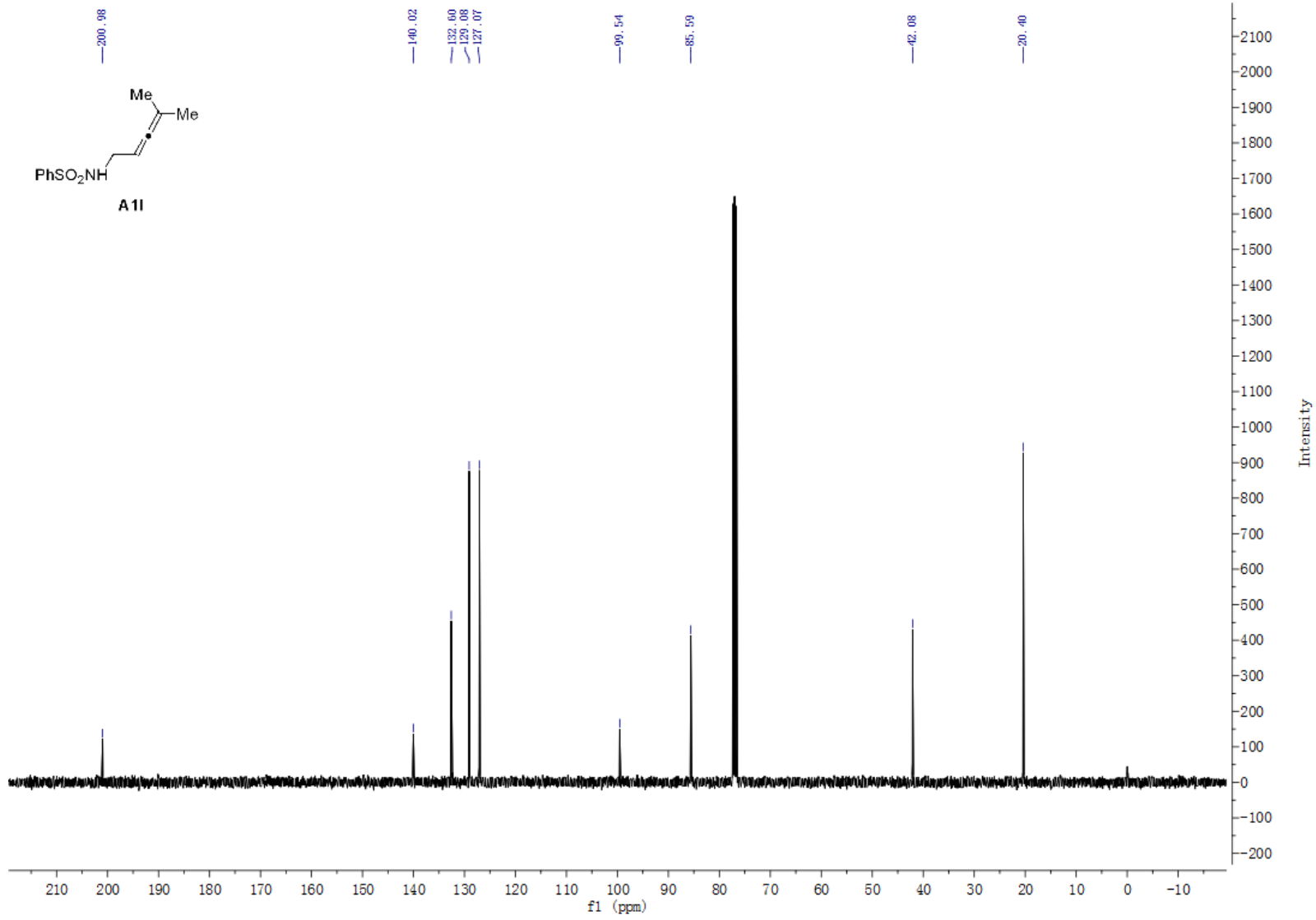

Me
Me
Br
O
S
NH
O
A1k
32000
30000
28000
26000
24000
22000
20000
18000
16000
14000
12000
10000
8000
6000
4000
2000
0
-2000
Intensity
1.98
1.99
1.00
0.98
2.05
2.79
2.96
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

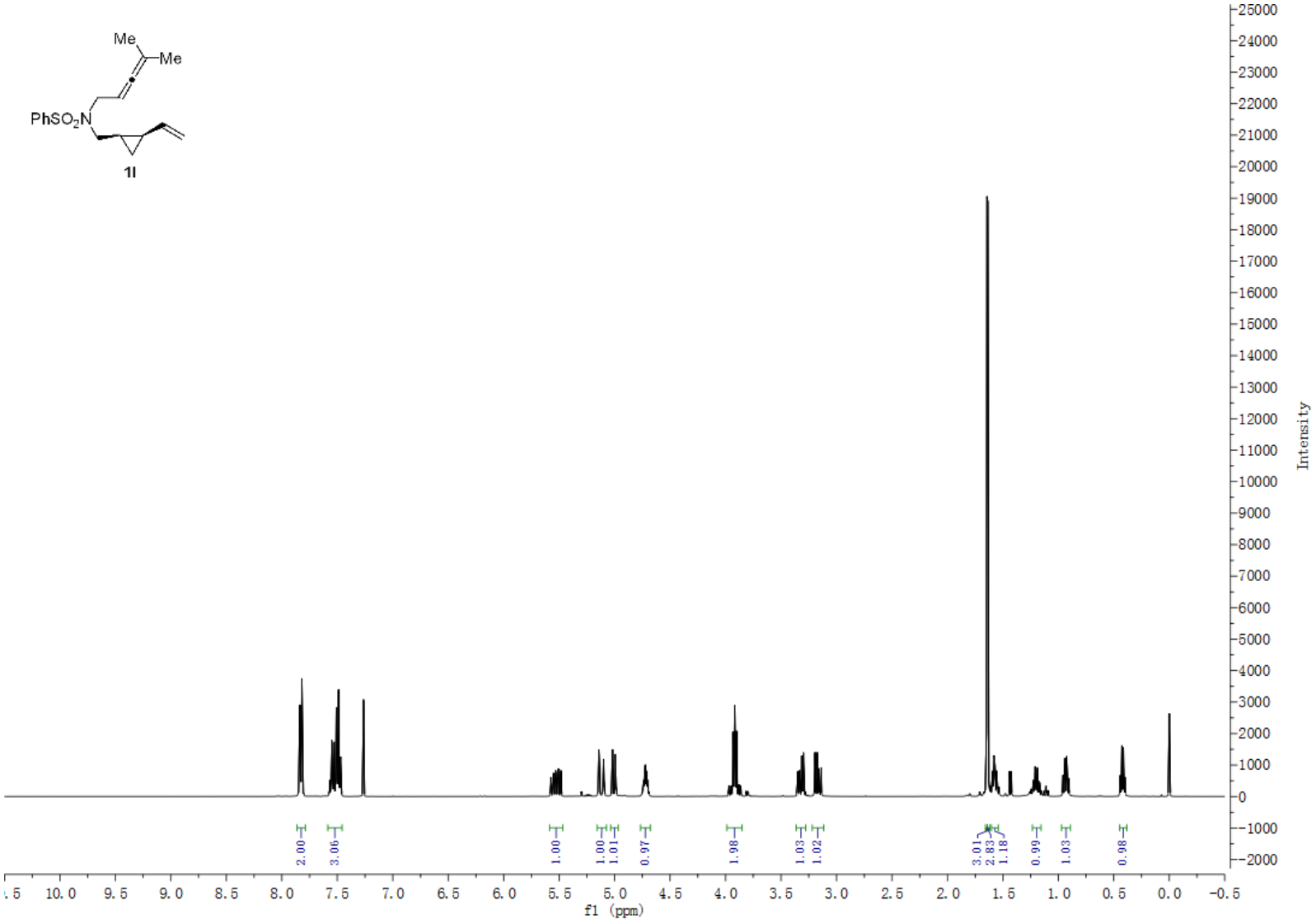

201.03
139.17
132.36
128.66
127.57
99.76
85.48
42.09
20.40
Me
Me
Br
O
S
NH
O
A1k
Intensity
1000
900
800
700
600
500
400
300
200
100
0
-100
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

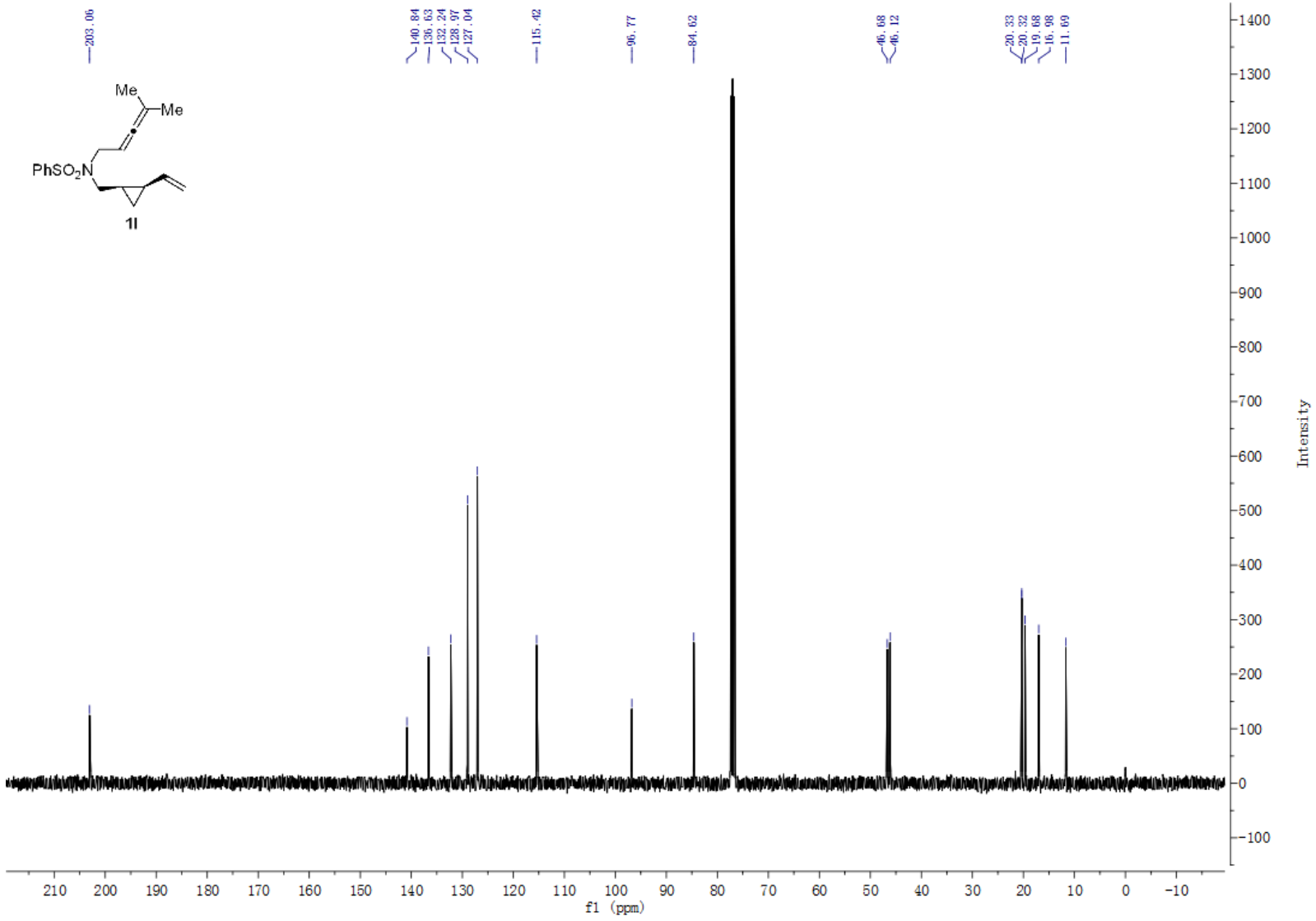

Me
Me
O2N
O
S
O
N
1k
28000
26000
24000
22000
20000
18000
16000
14000
12000
10000
8000
6000
4000
2000
0
-2000
Intensity
2.12
2.08
1.00
1.01
1.01
1.05
1.99
1.17
1.02
3.19
3.05
1.15
0.97
0.96
0.99
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

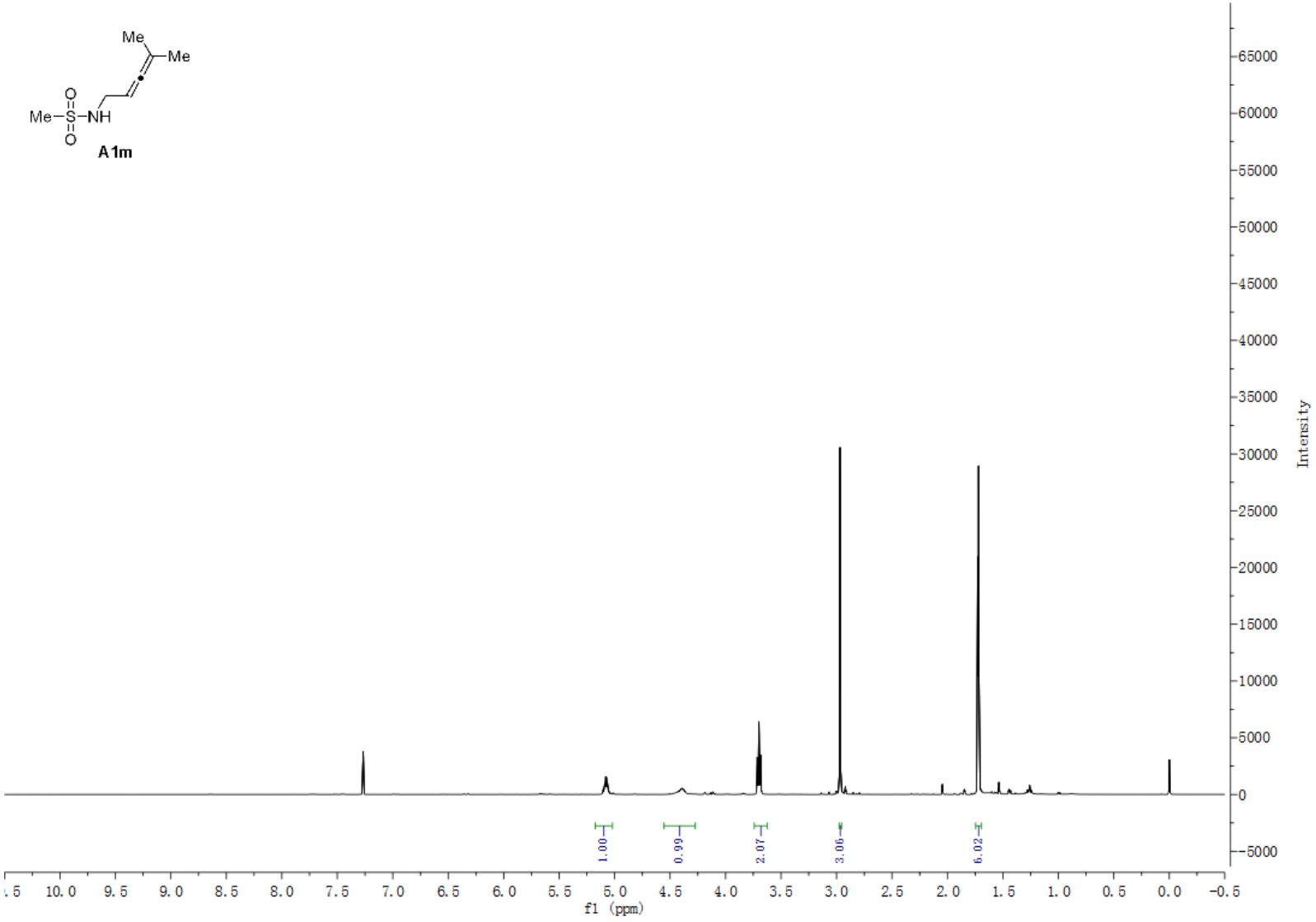

203.12
139.99
136.47
132.23
128.62
127.12
115.59
97.01
84.43
46.67
46.16
20.32
20.31
19.68
16.92
11.64
Me
Me
O2N
S
N
O
O
1k
Intensity
f1 (ppm)

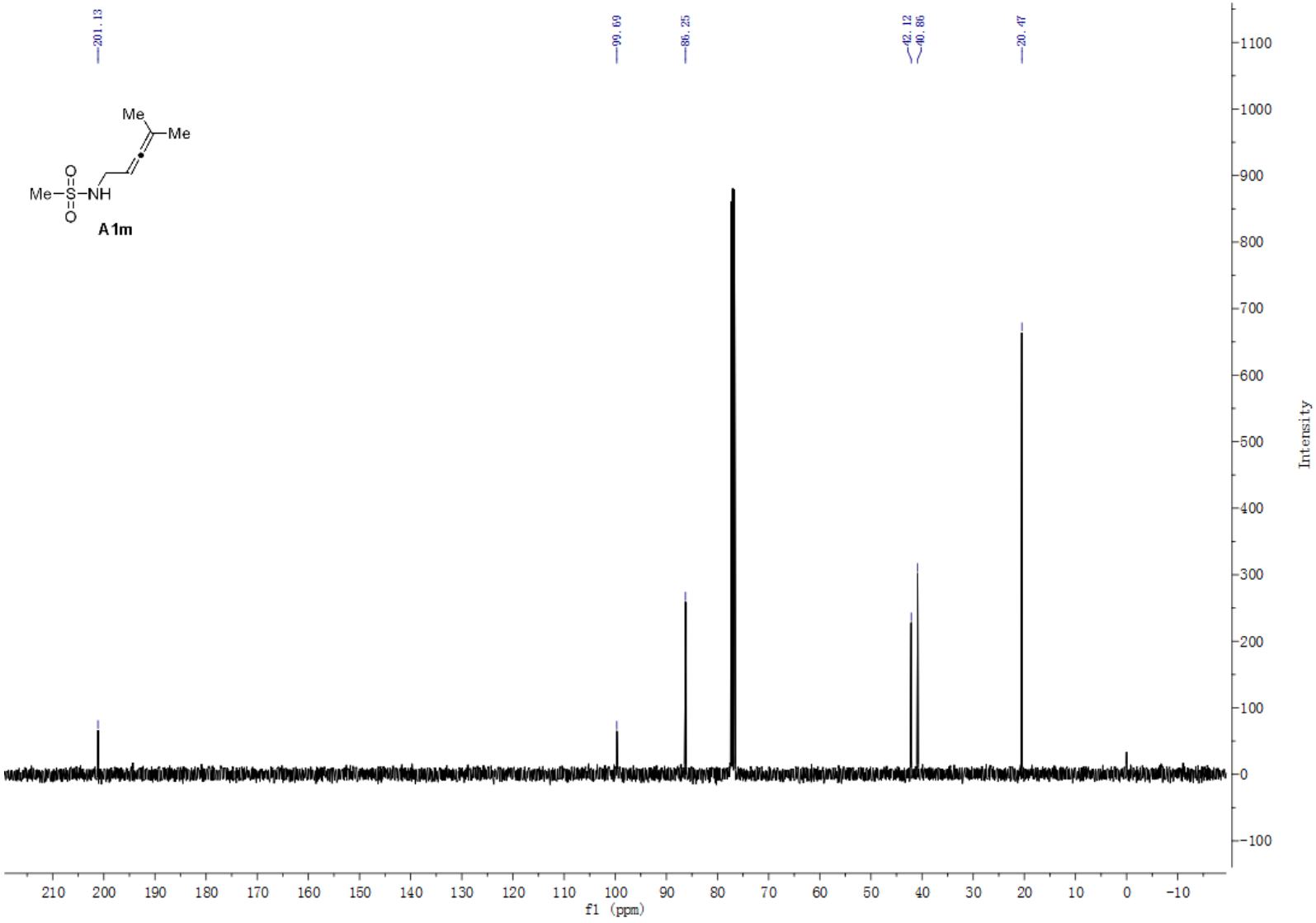

Me
Me
PhSO2NH
A1l
Intensity
f1 (ppm)
1.97
3.02
1.00
0.93
2.04
2.92
2.93

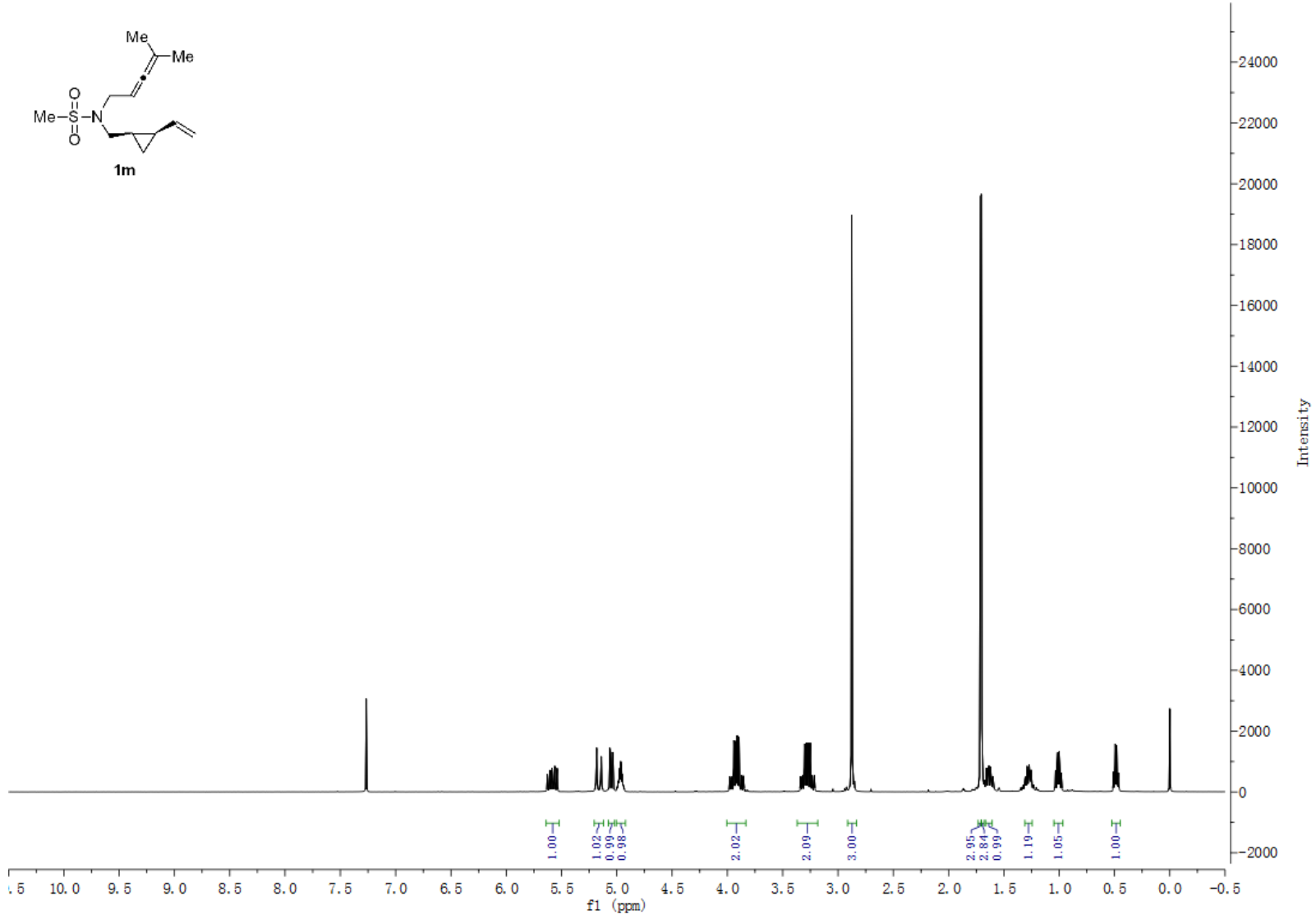

200.98
140.02
132.60
129.08
127.07
99.54
85.59
42.08
20.40
Me
Me
PhSO2NH
A1l
Intensity
f1 (ppm)

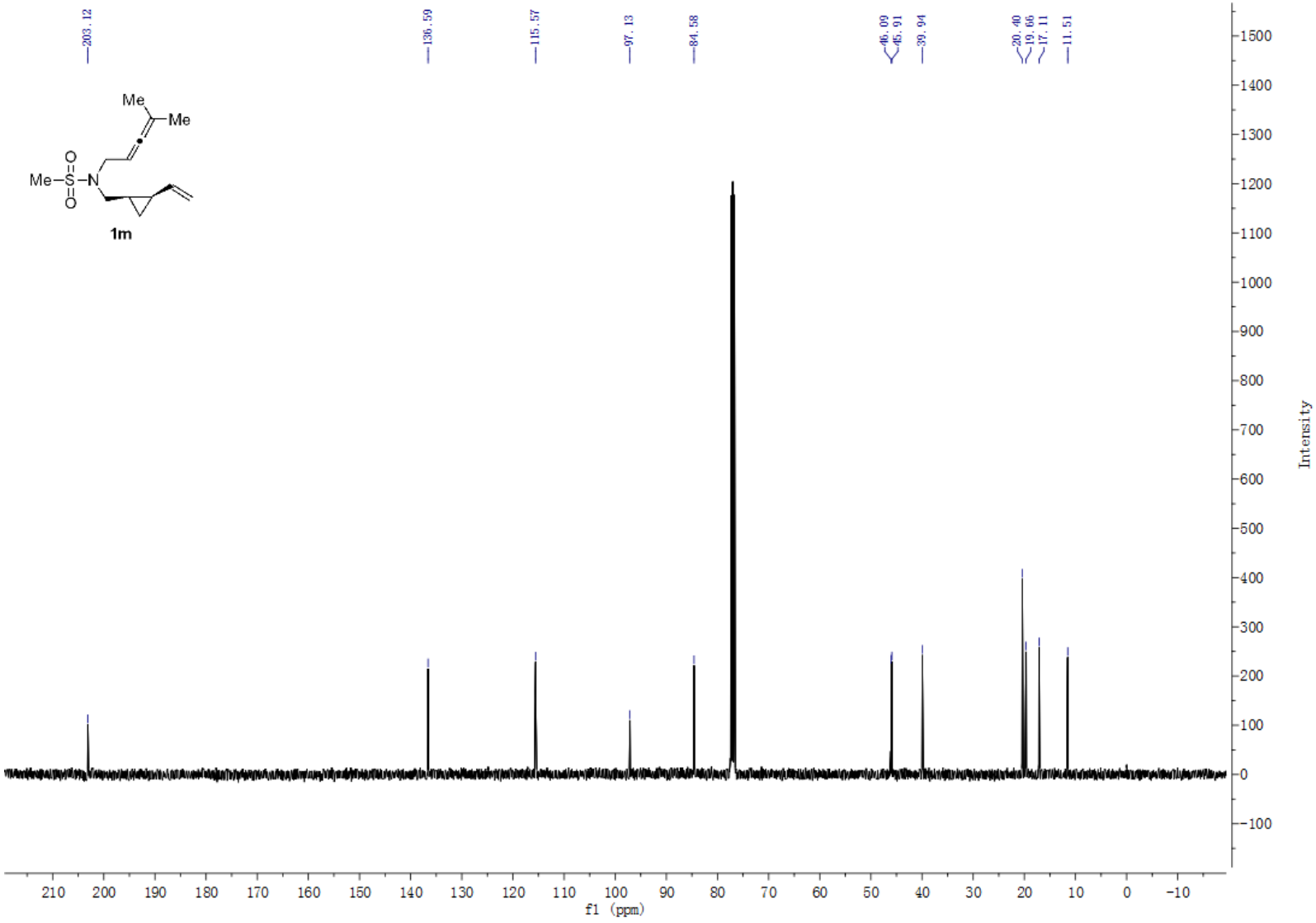

Me
Me
PhSO2N
1l
Intensity
f1 (ppm)
2.00
3.06
1.00
1.00
1.01
0.97
1.98
1.03
1.02
3.01
2.83
1.18
0.99
1.03
0.98

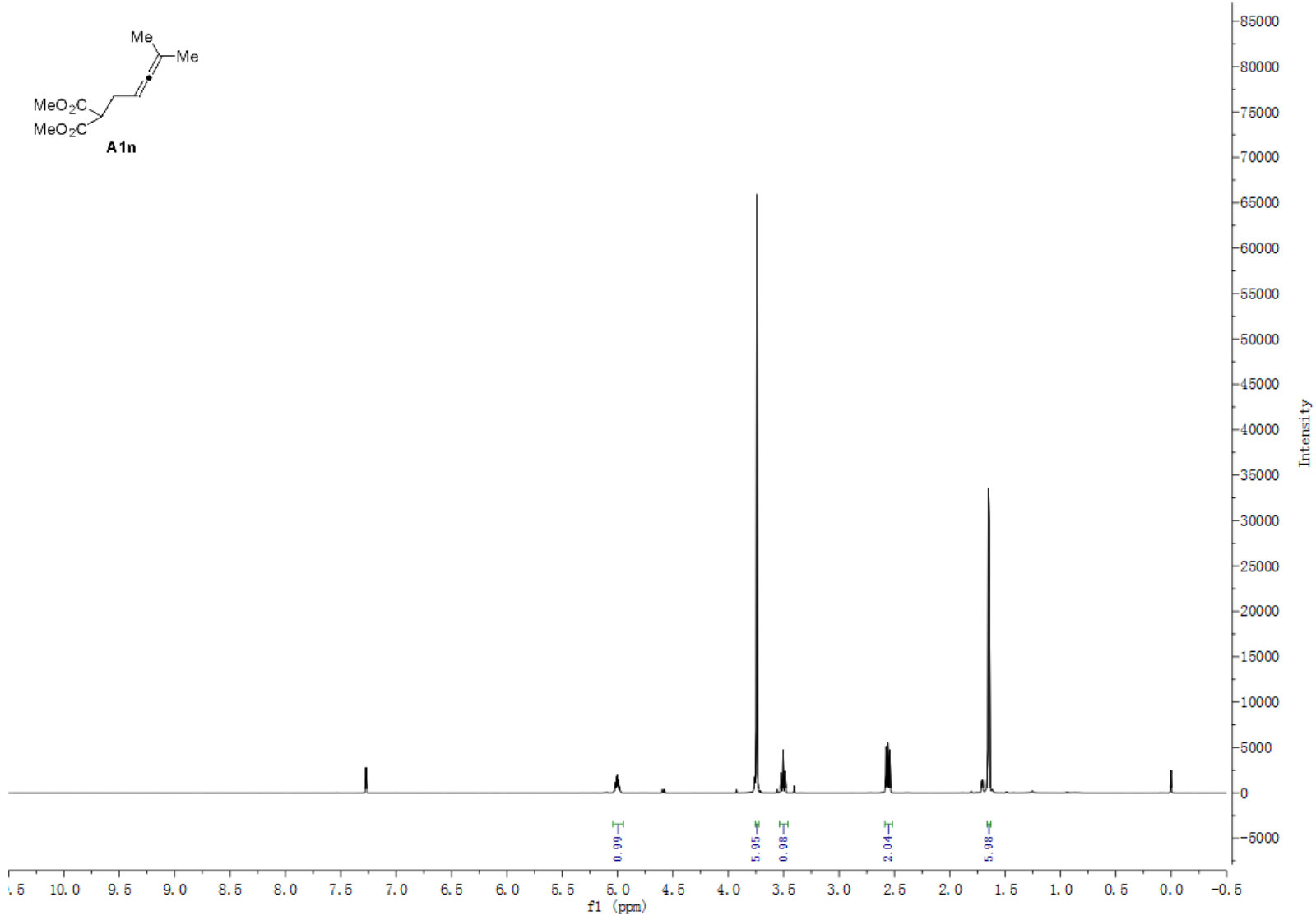

203.06
140.84
136.63
132.24
128.97
127.04
115.42
96.77
84.62
46.68
46.12
20.33
20.32
19.68
16.98
11.69
Me
Me
PhSO2N
1l
Intensity
f1 (ppm)

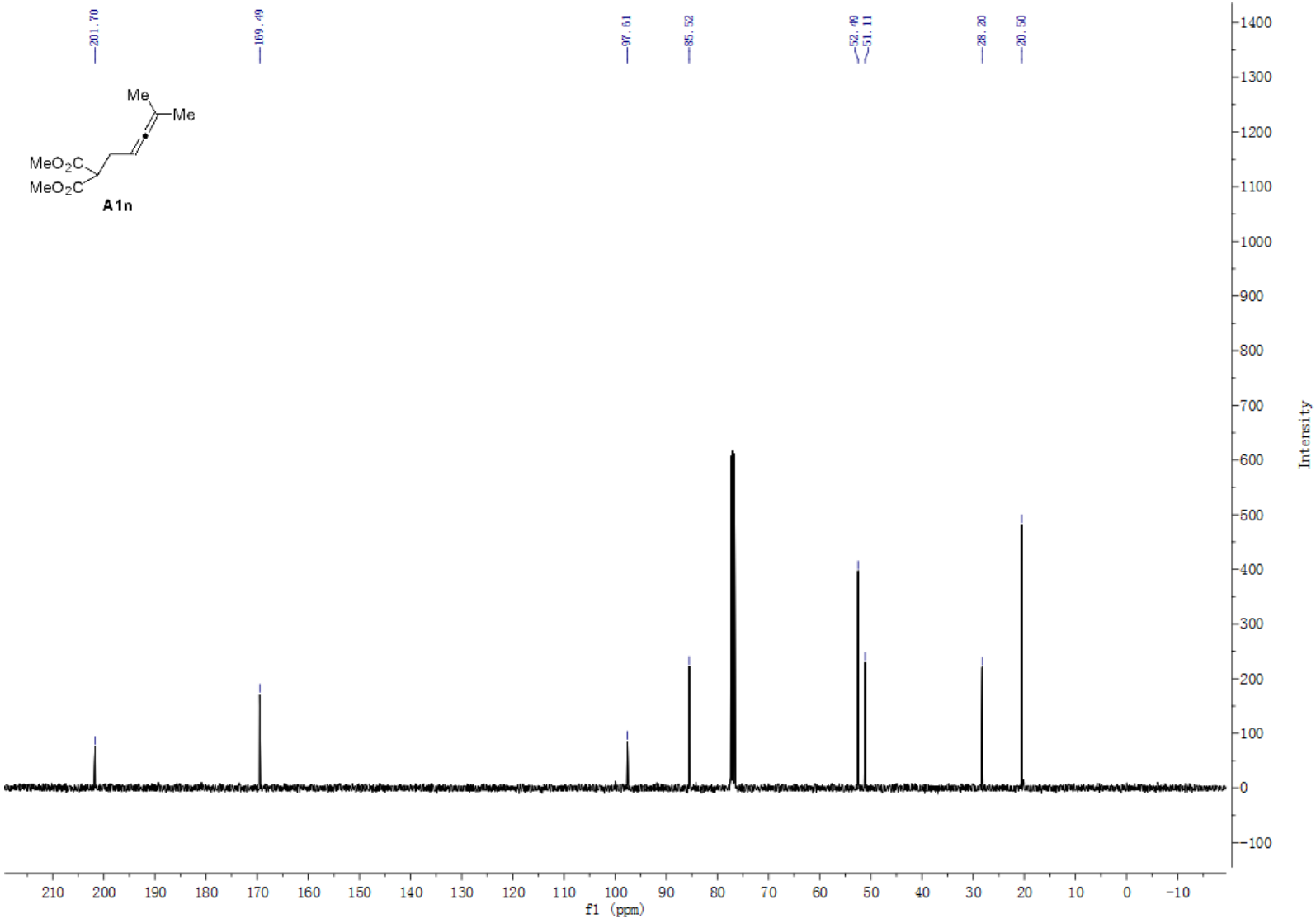

Me
Me
Me
S
NH
O
O
A1m
65000
60000
55000
50000
45000
40000
35000
30000
25000
20000
15000
10000
5000
0
-5000
Intensity
1.00
0.99
2.07
3.06
6.02
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

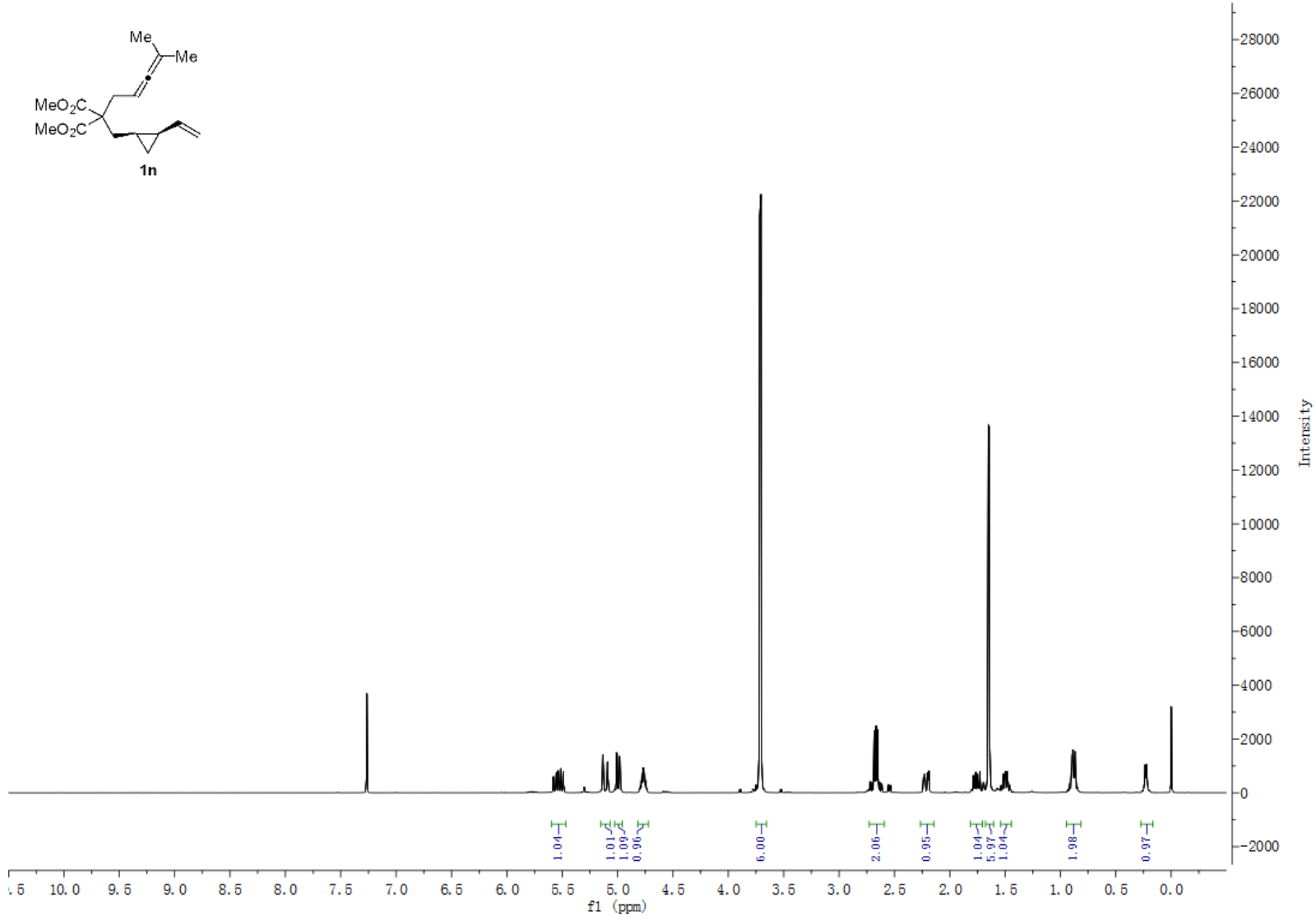

201.13
99.69
86.25
42.12
40.86
20.47
Me
Me
Me
S
O
O
NH
A1m
1100
1000
900
800
700
600
500
400
300
200
100
0
-100
Intensity
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

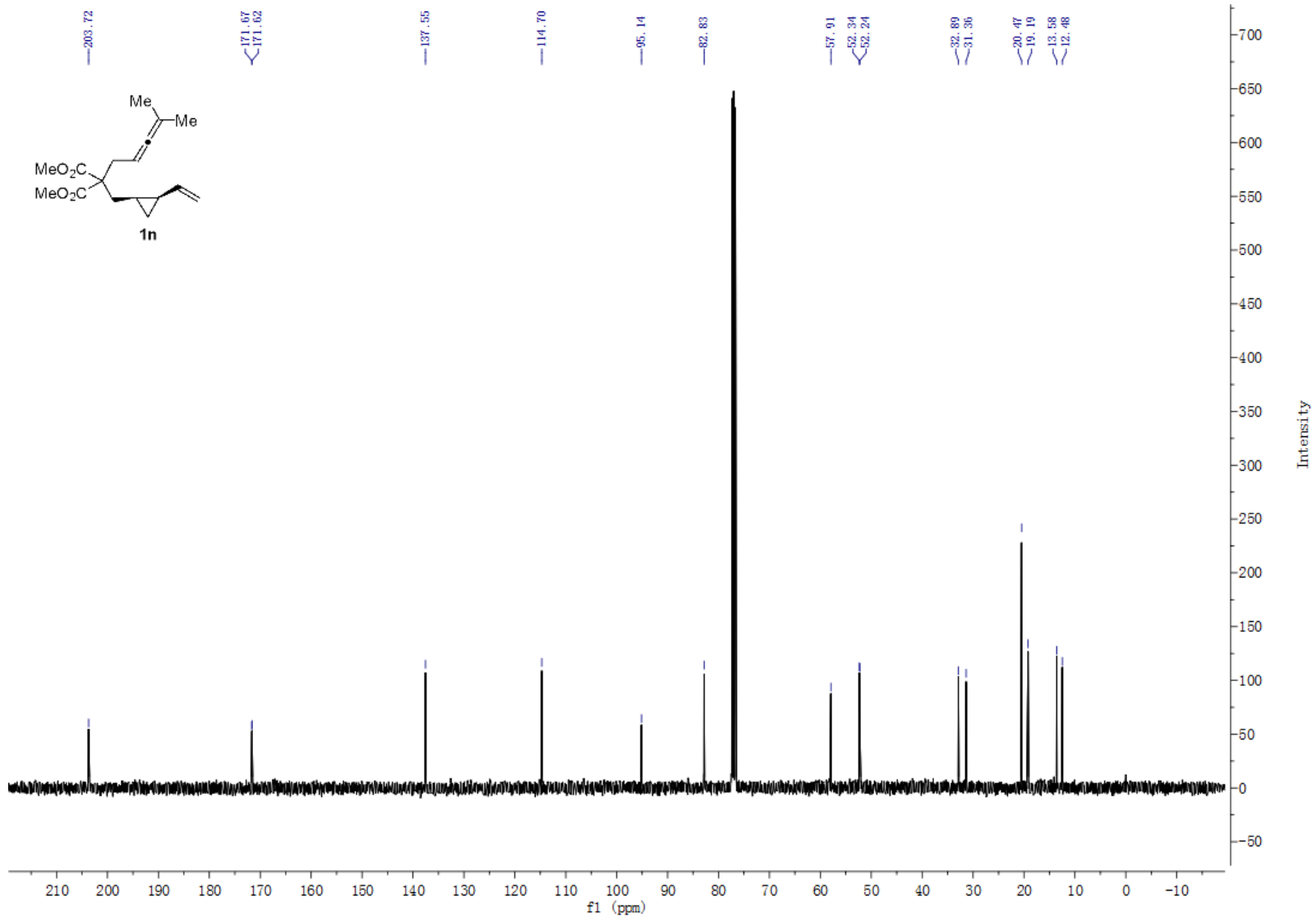

Me
Me
Me
S
N
O
O
1m
24000
22000
20000
18000
16000
14000
12000
10000
8000
6000
4000
2000
0
-2000
Intensity
1.00
1.02
0.99
0.98
2.02
2.09
3.00
2.95
2.84
0.99
1.19
1.05
1.00
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

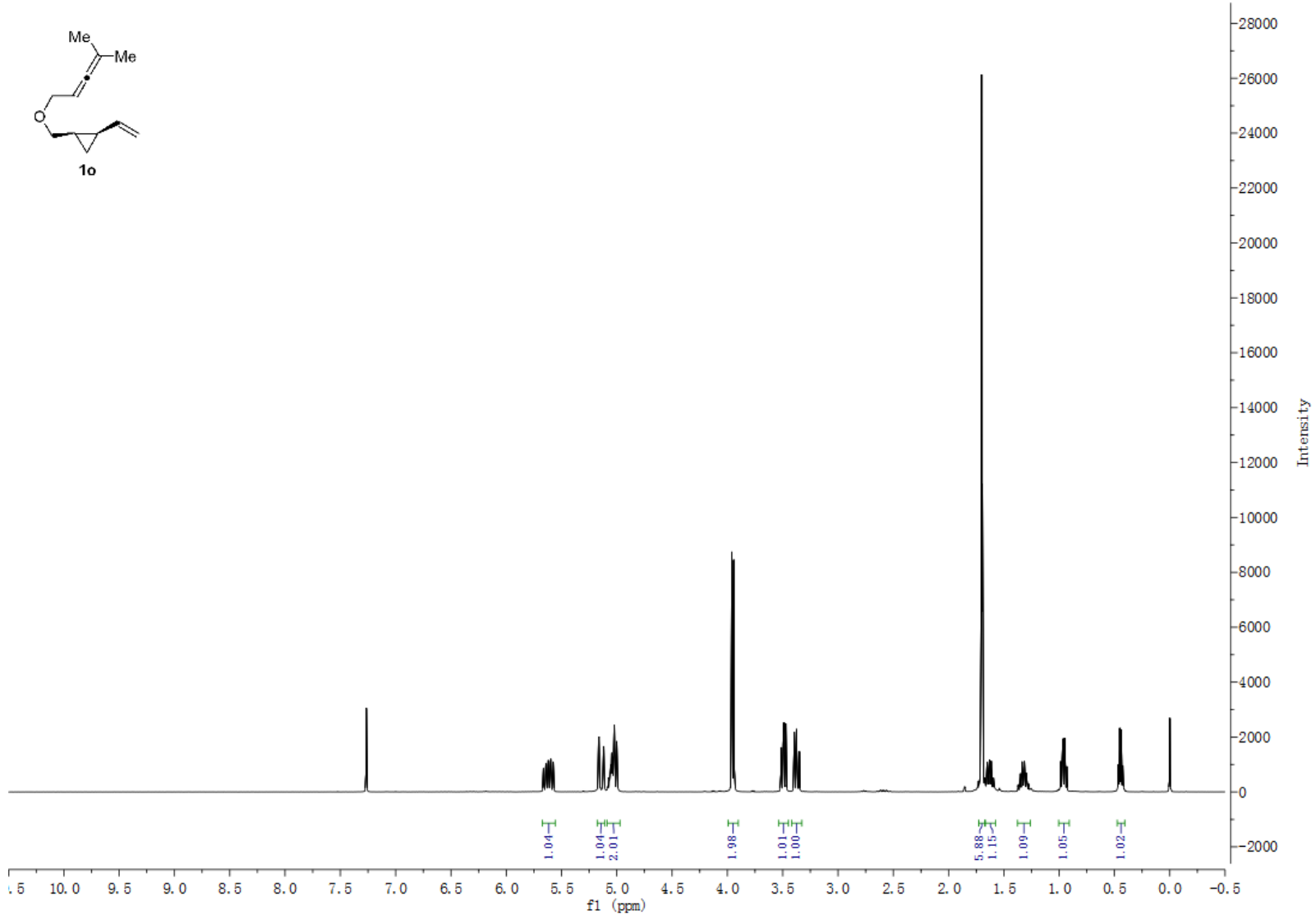

203.12
136.59
115.57
97.13
84.58
46.09
45.91
39.94
20.40
19.66
17.11
11.51
Me
Me
Me
O
S
O
N
1m
Intensity
f1 (ppm)

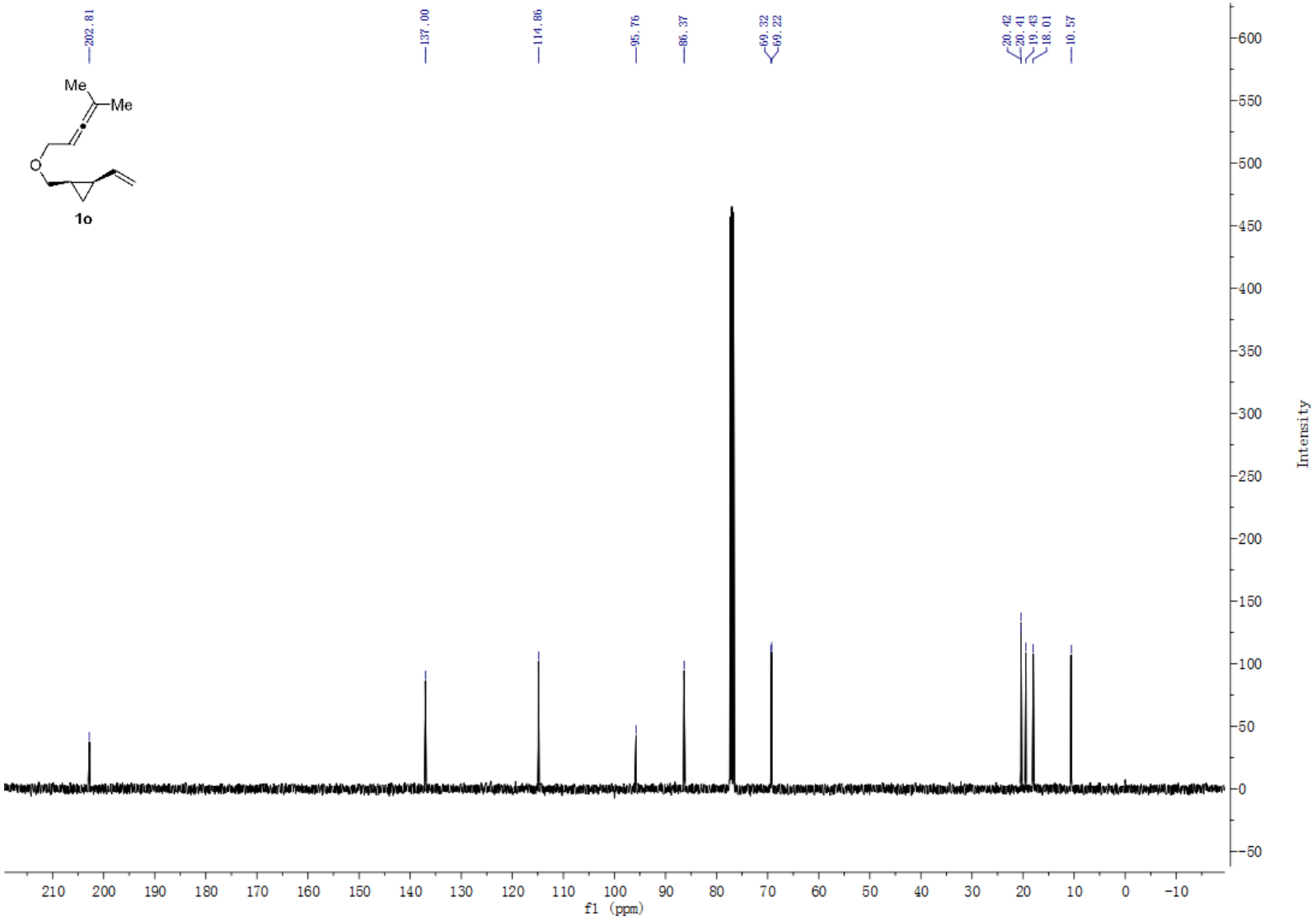

Me
Me
MeO2C
MeO2C
A1n
Intensity
f1 (ppm)
0.99
5.95
0.98
2.04
5.98

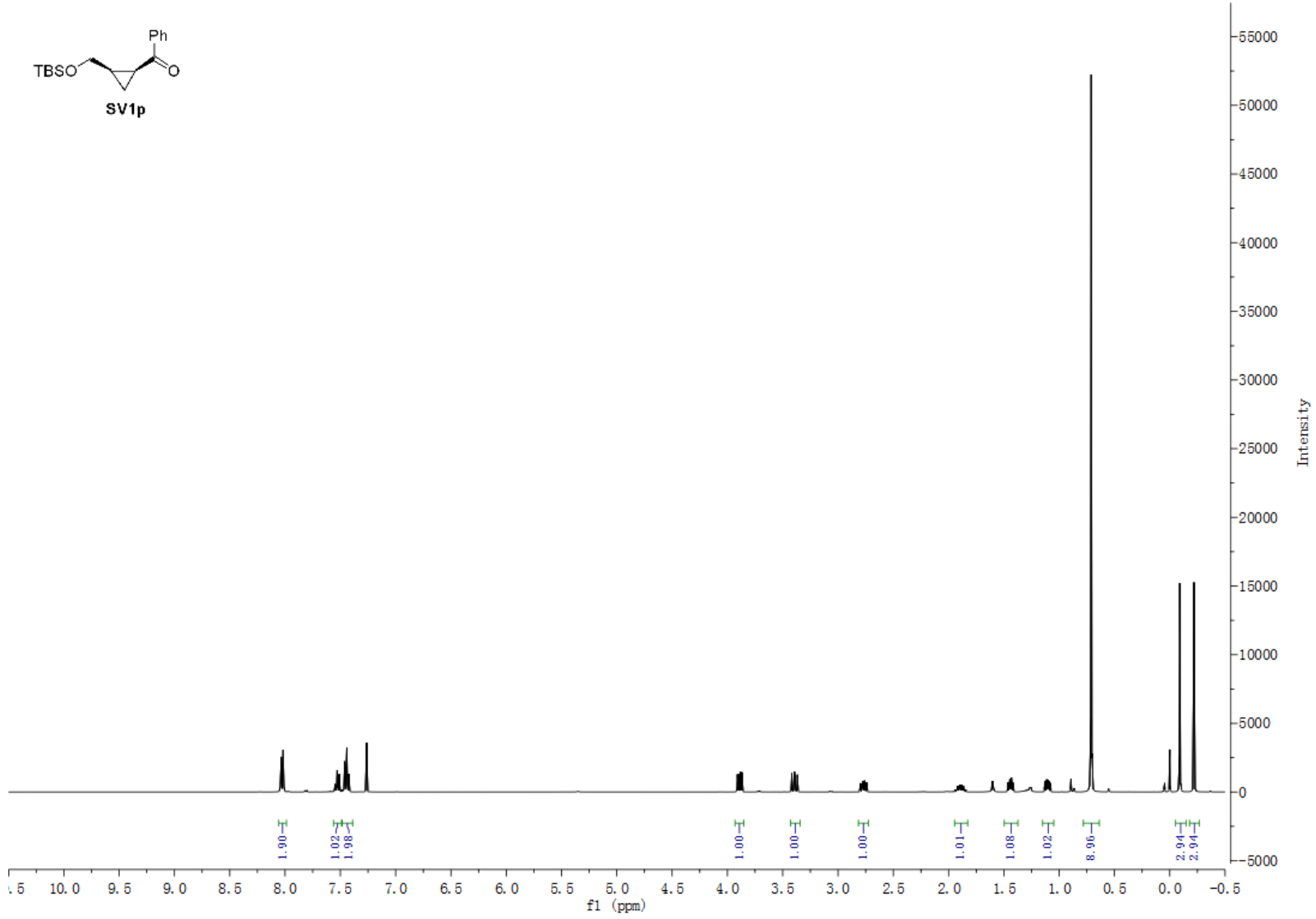

201.70
169.49
97.61
85.52
52.49
51.11
28.20
20.50
Me
Me
MeO2C
MeO2C
A1n
Intensity
f1 (ppm)

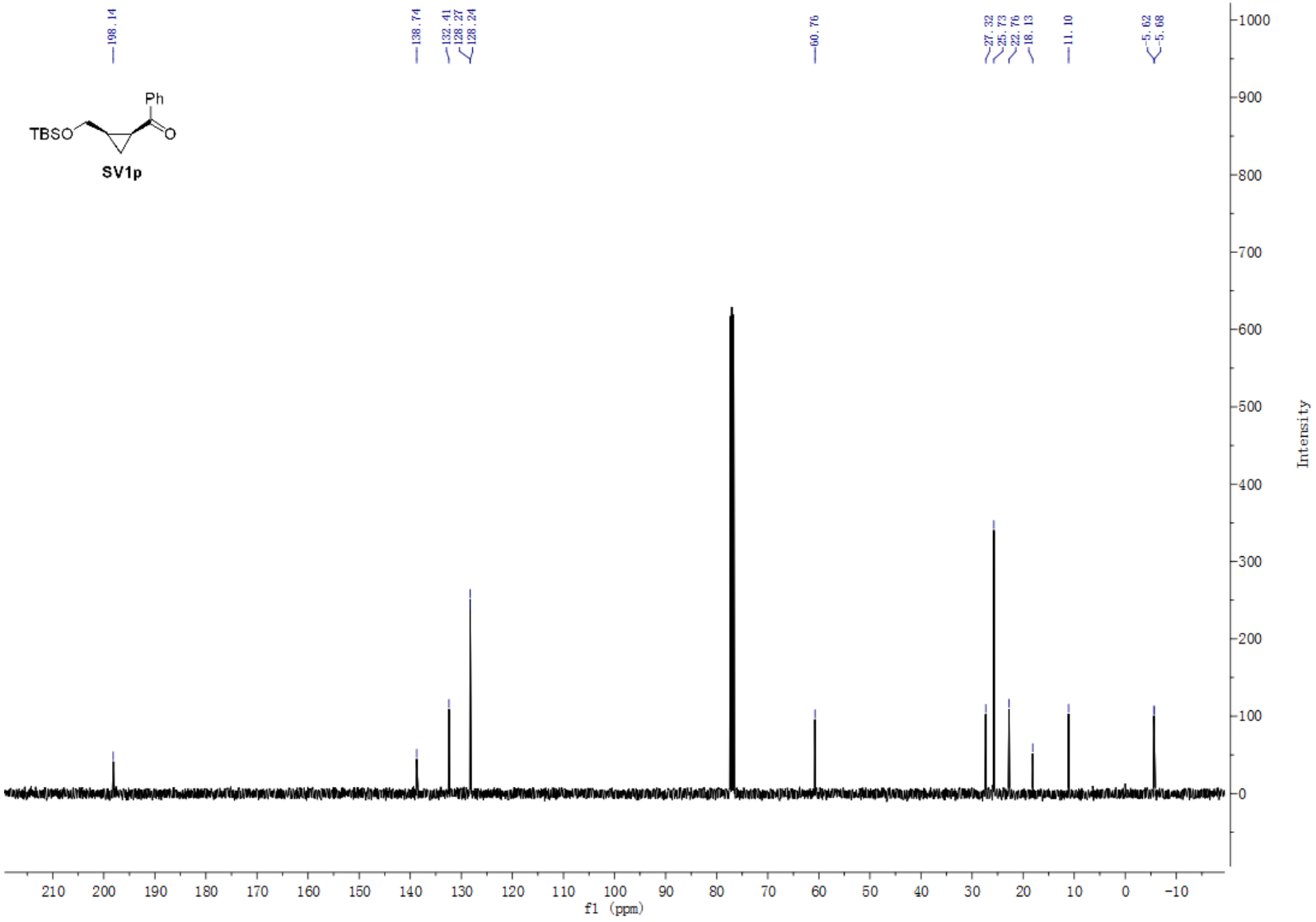

Me
Me
MeO2C
MeO2C
1n
Intensity
f1 (ppm)
1.04
1.01
1.09
0.96
6.00
2.06
0.95
1.04
5.97
1.04
1.98
0.97

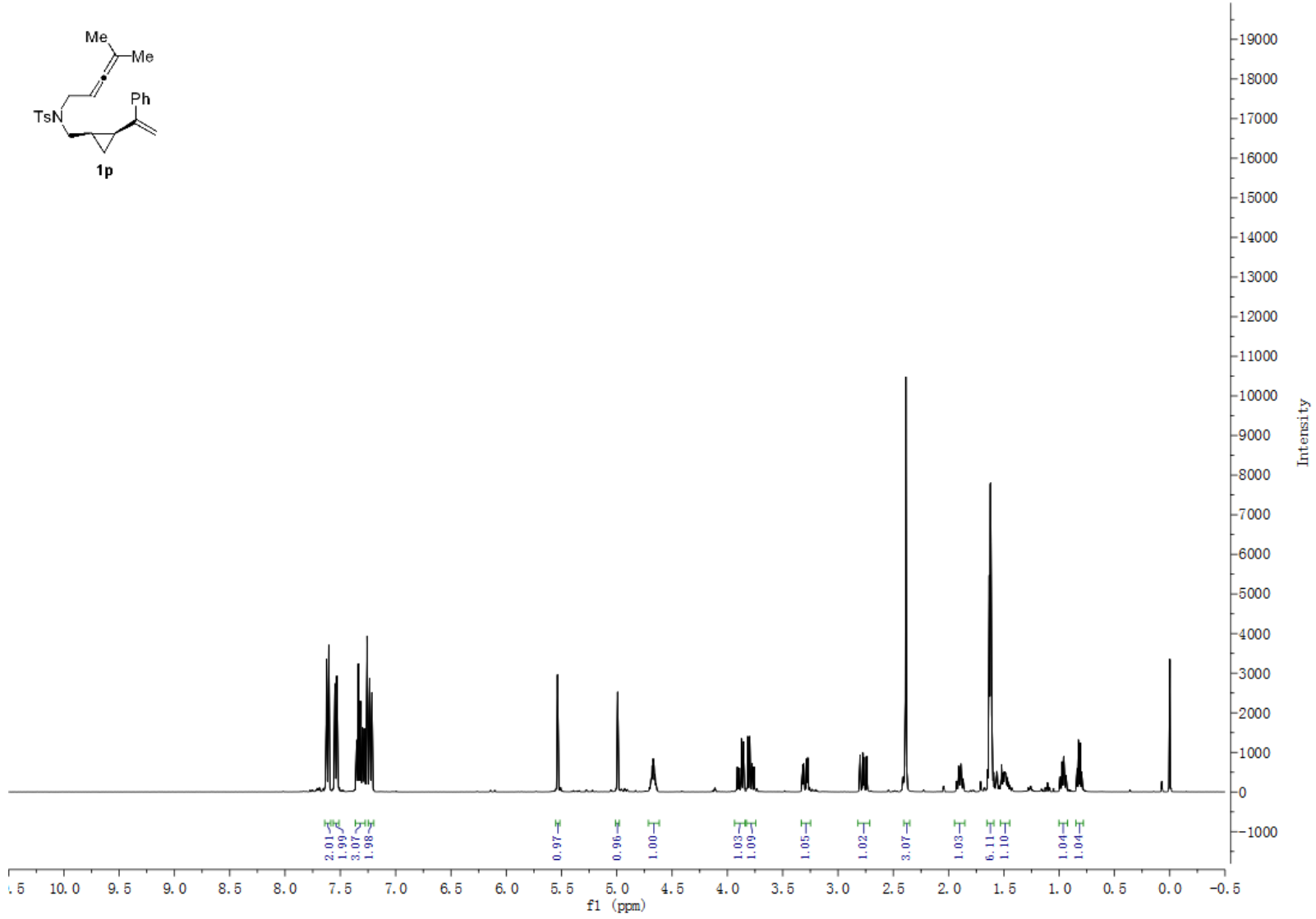

203.72
171.67
171.62
137.55
114.70
95.14
82.83
57.91
52.34
52.24
32.89
31.36
20.47
19.19
13.58
12.48
Me
Me
MeO2C
MeO2C
1n
Intensity
f1 (ppm)

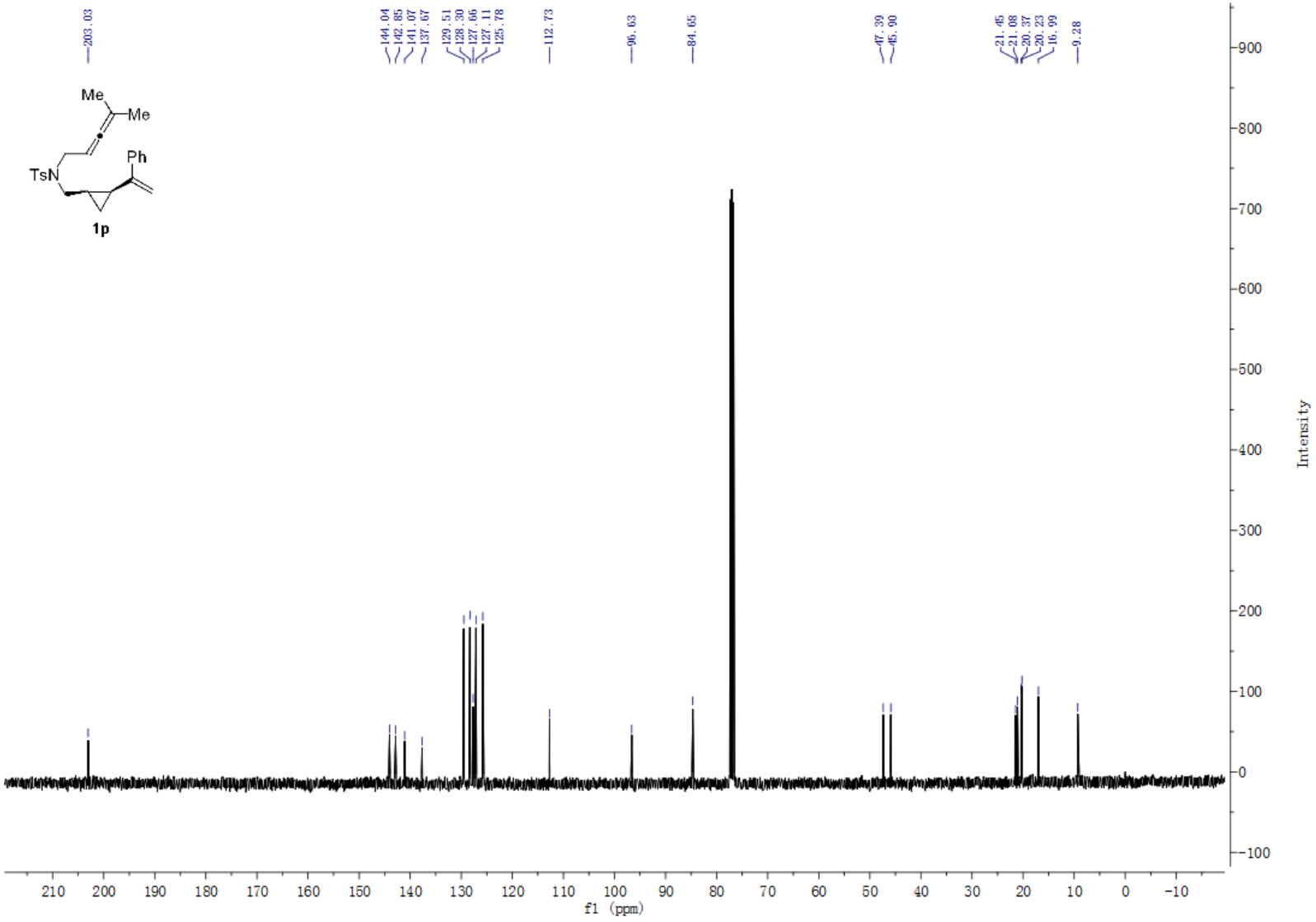

Me
Me
O
1o
28000
26000
24000
22000
20000
18000
16000
14000
12000
10000
8000
6000
4000
2000
0
-2000
Intensity
1.04
1.04
2.01
1.98
1.01
1.00
5.88
1.15
1.09
1.05
1.02
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

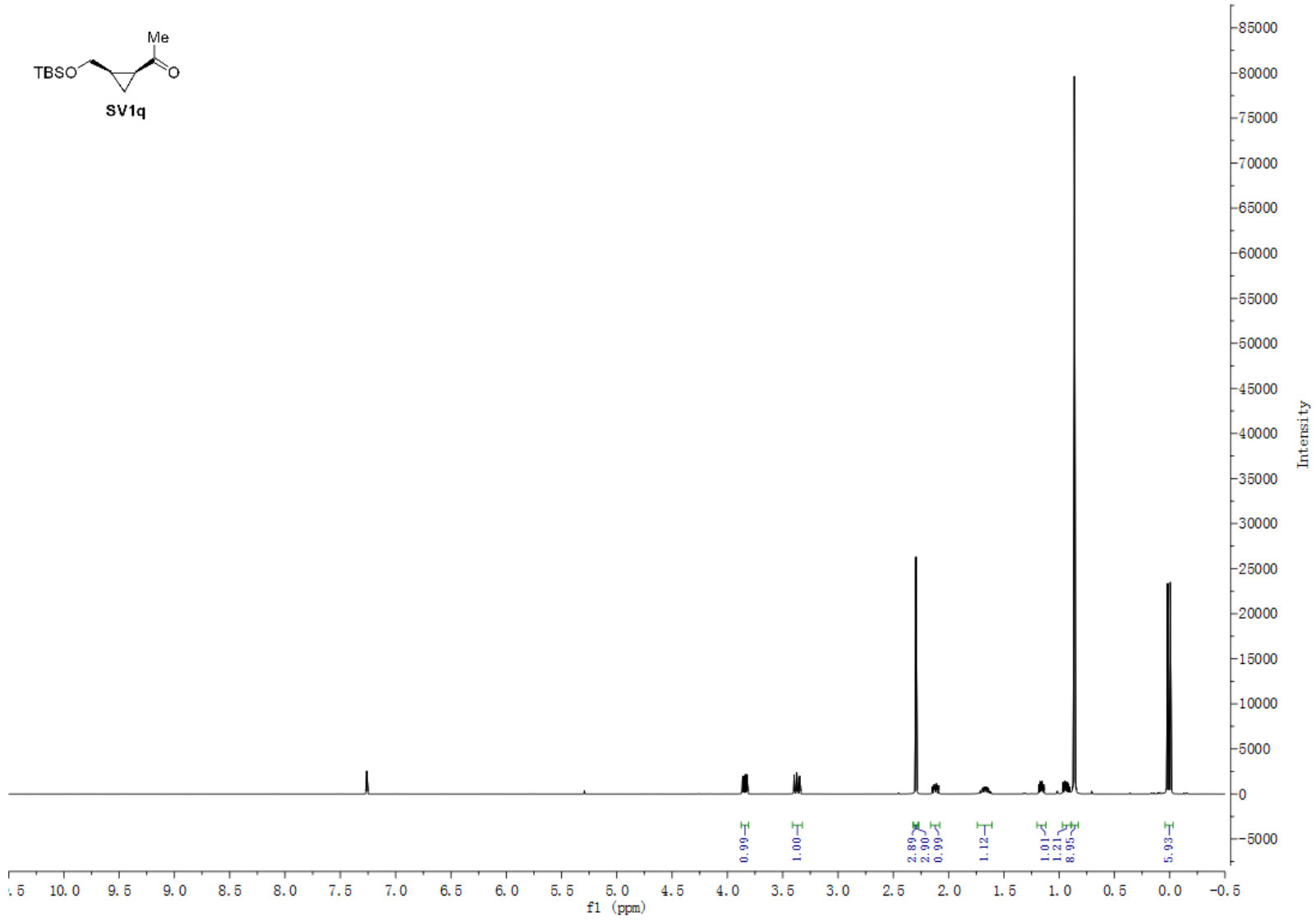

202.81
137.00
114.86
95.76
86.37
69.32
69.22
20.42
20.41
19.43
18.01
10.57
Me
Me
O
1o
Intensity
f1 (ppm)

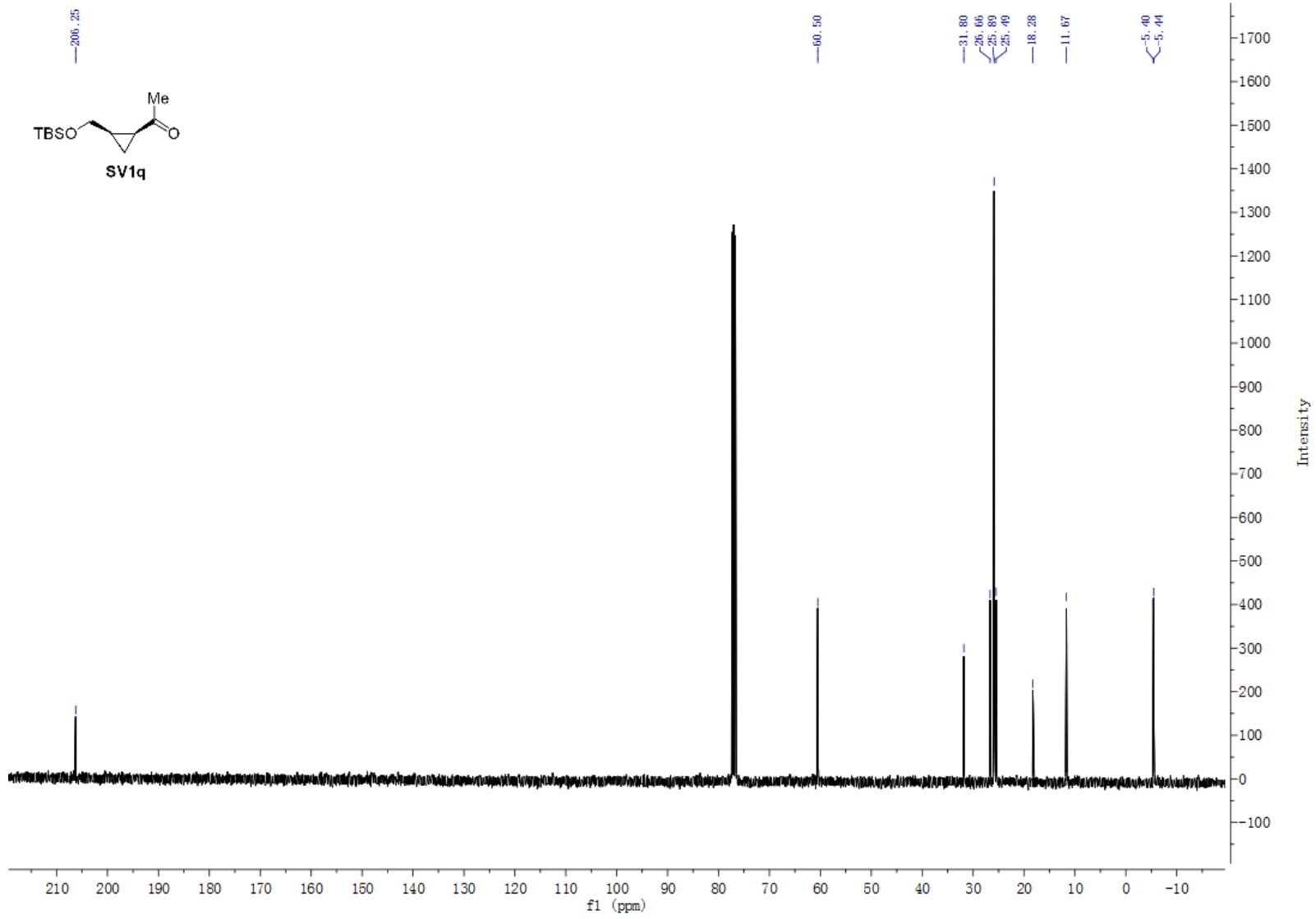

Ph
TBSO
O
SV1p
55000
50000
45000
40000
35000
30000
25000
20000
15000
10000
5000
0
-5000
Intensity
1.90
1.02
1.98
1.00
1.00
1.00
1.01
1.08
1.02
8.96
2.94
2.94
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

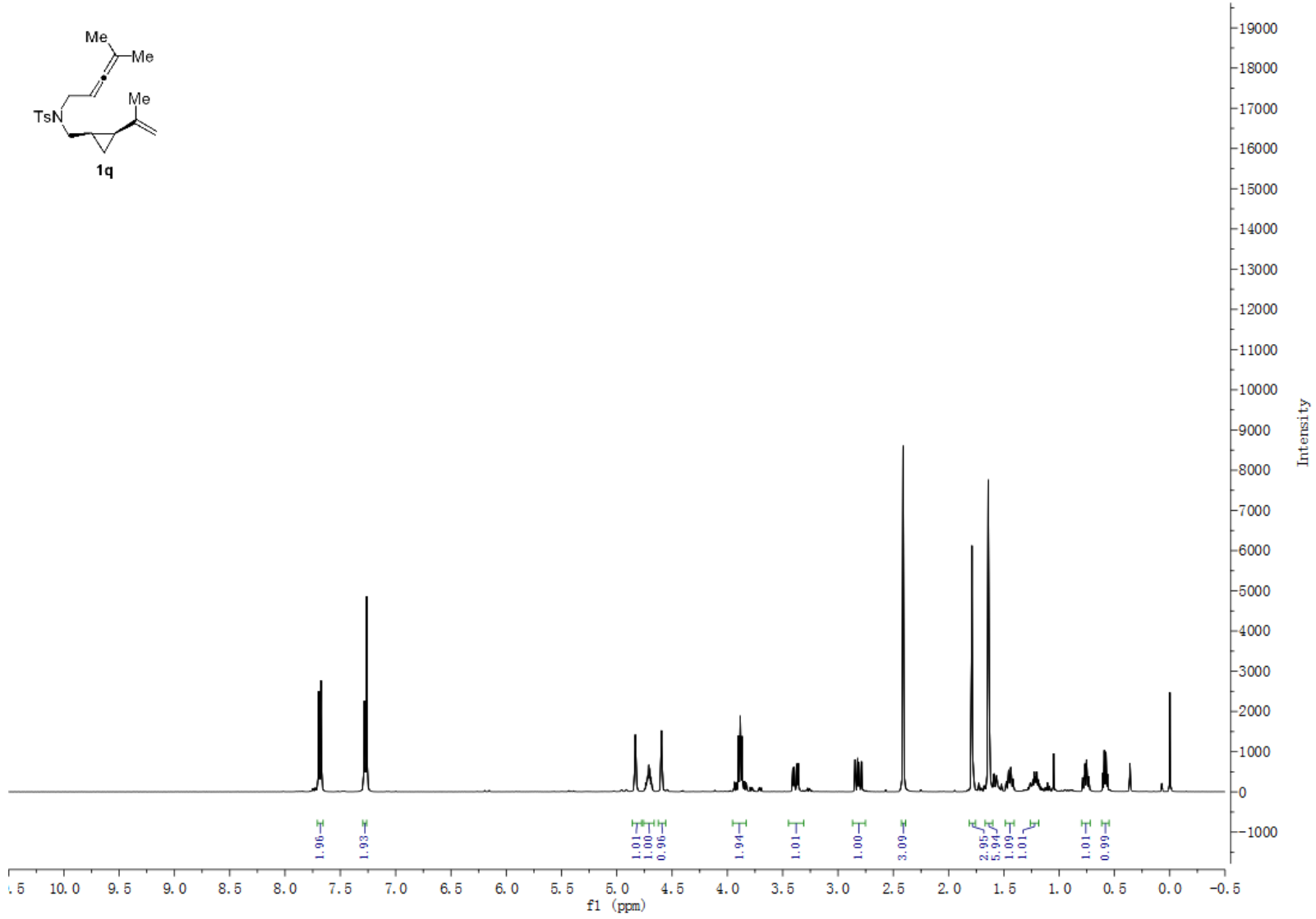

198.14
138.74
132.41
128.27
128.24
60.76
27.32
25.73
22.76
18.13
11.10
-5.62
-5.68
Ph
TBSO
O
SV1p
Intensity
f1 (ppm)

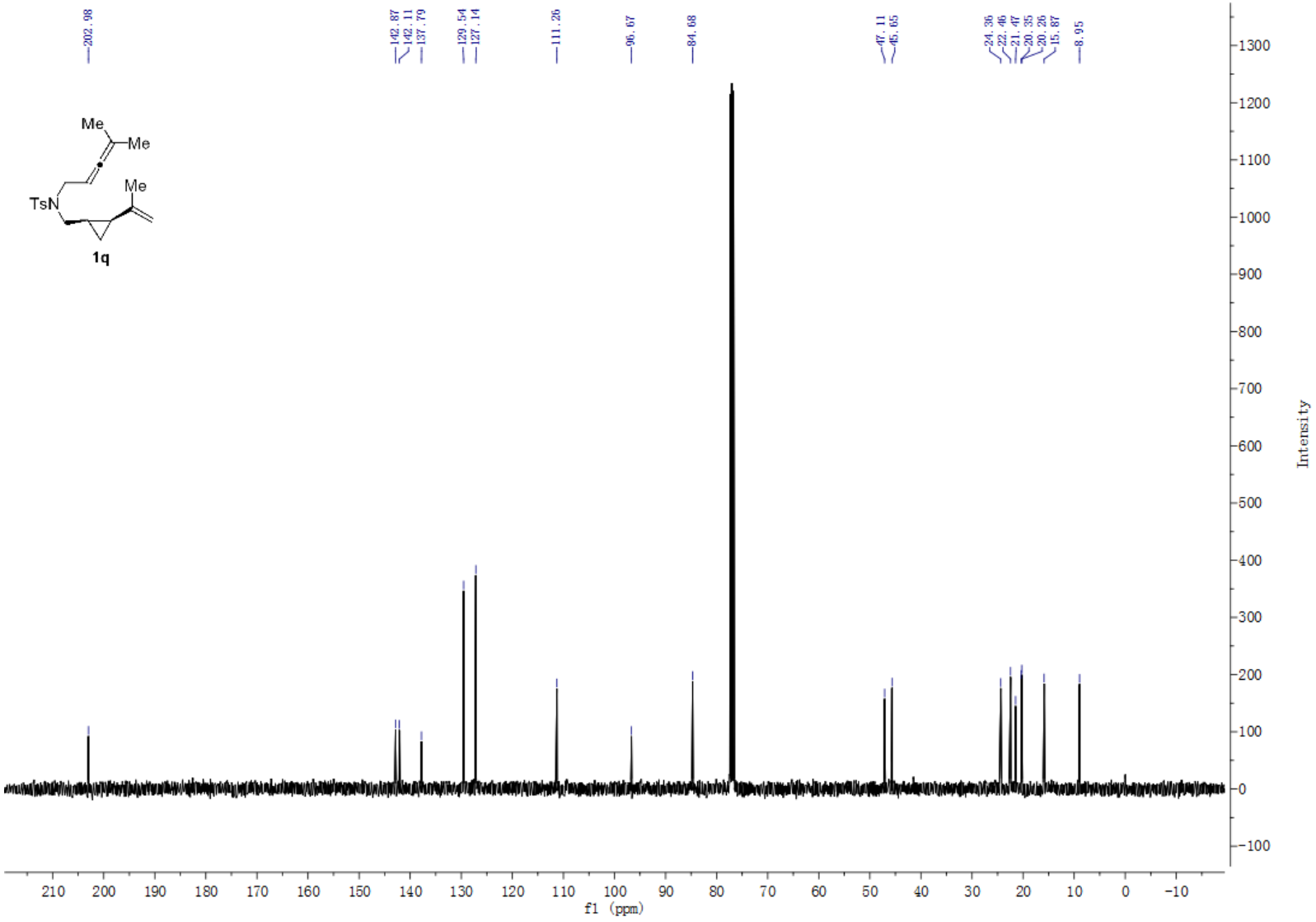

Me
Me
Ph
TsN
1p
Intensity
f1 (ppm)

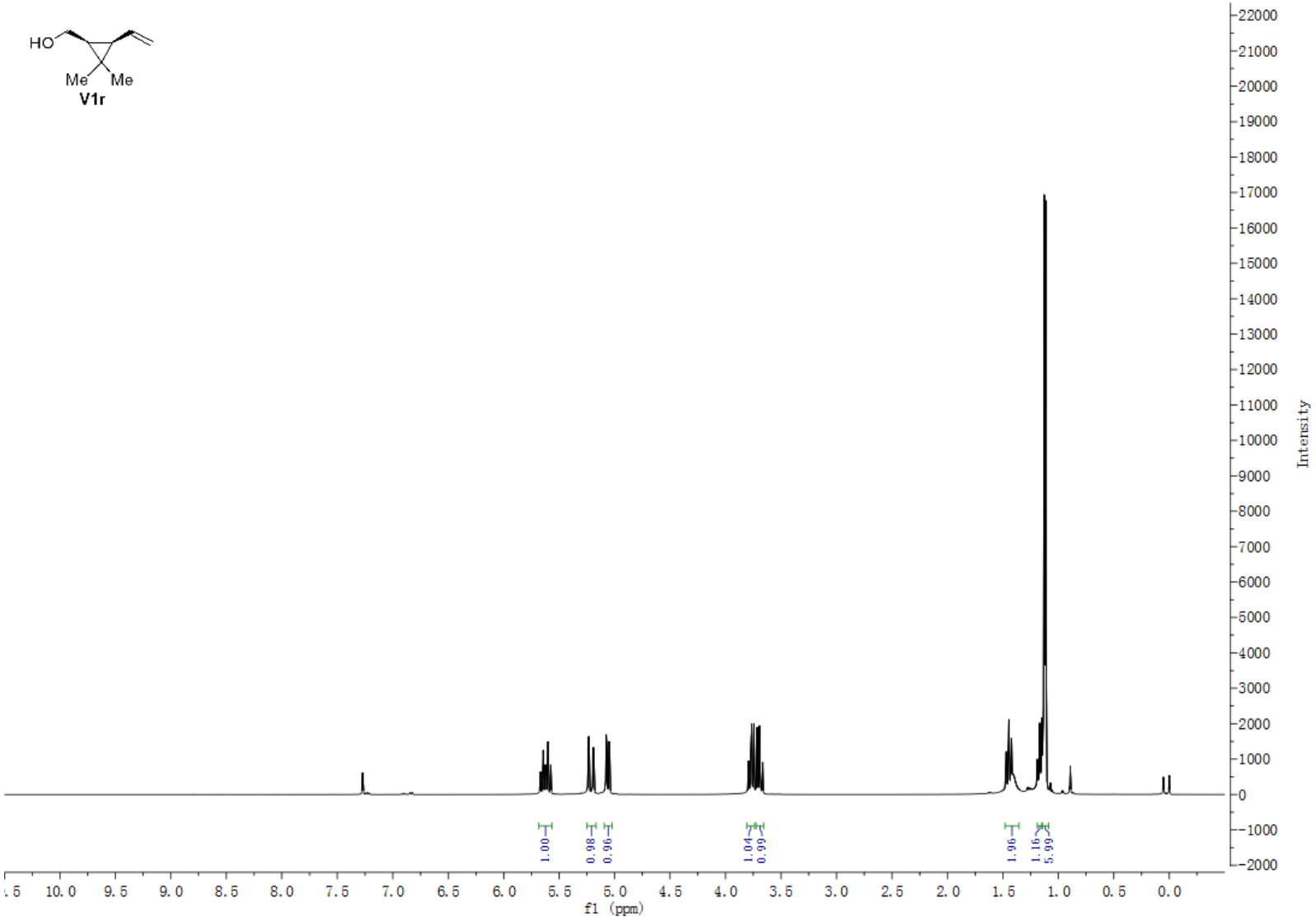

203.03
144.04
142.85
141.07
137.67
129.51
128.39
127.66
127.11
125.78
112.73
96.63
84.65
47.39
45.90
21.45
21.08
20.37
20.23
16.99
9.28
Me
Me
Ph
TsN
1p
Intensity
f1 (ppm)

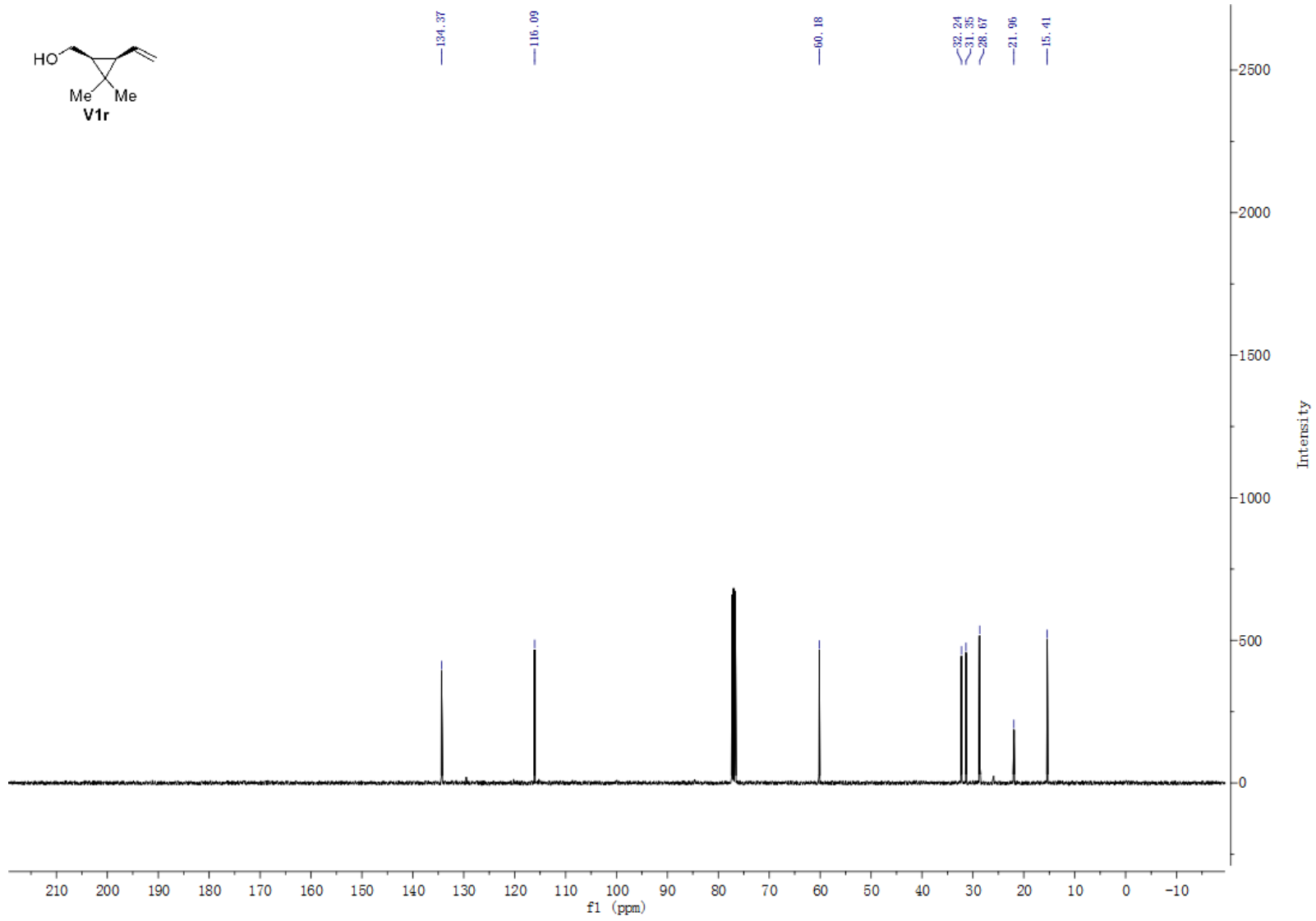

Me
TBSO
O
SV1q
Intensity
f1 (ppm)
0.99
1.00
2.89
2.90
0.99
1.12
1.01
1.21
8.95
5.93

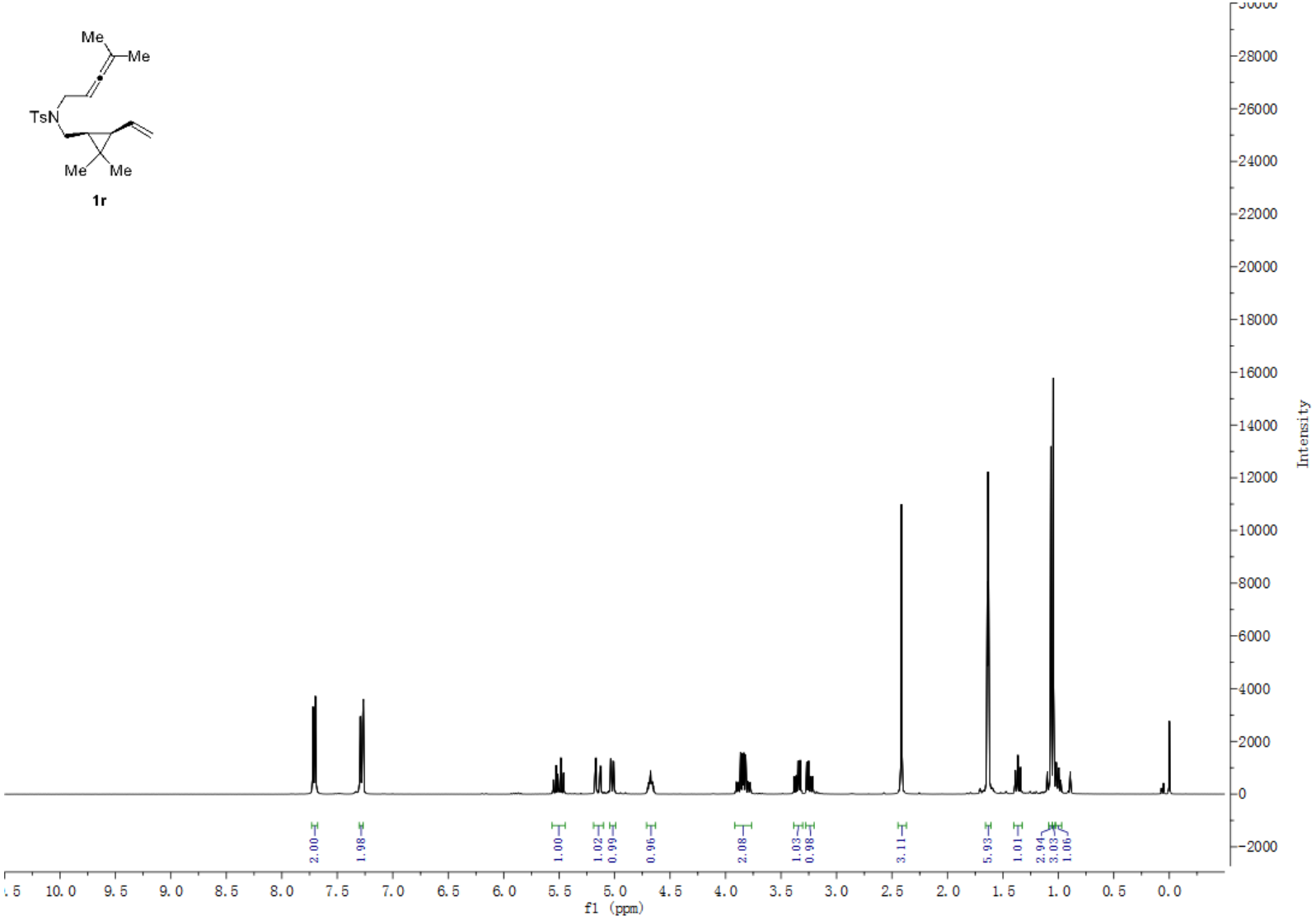

206.25
60.50
31.80
26.66
25.89
25.49
18.28
11.67
5.40
5.44
Me
TBSO
O
SV1q
Intensity
f1 (ppm)

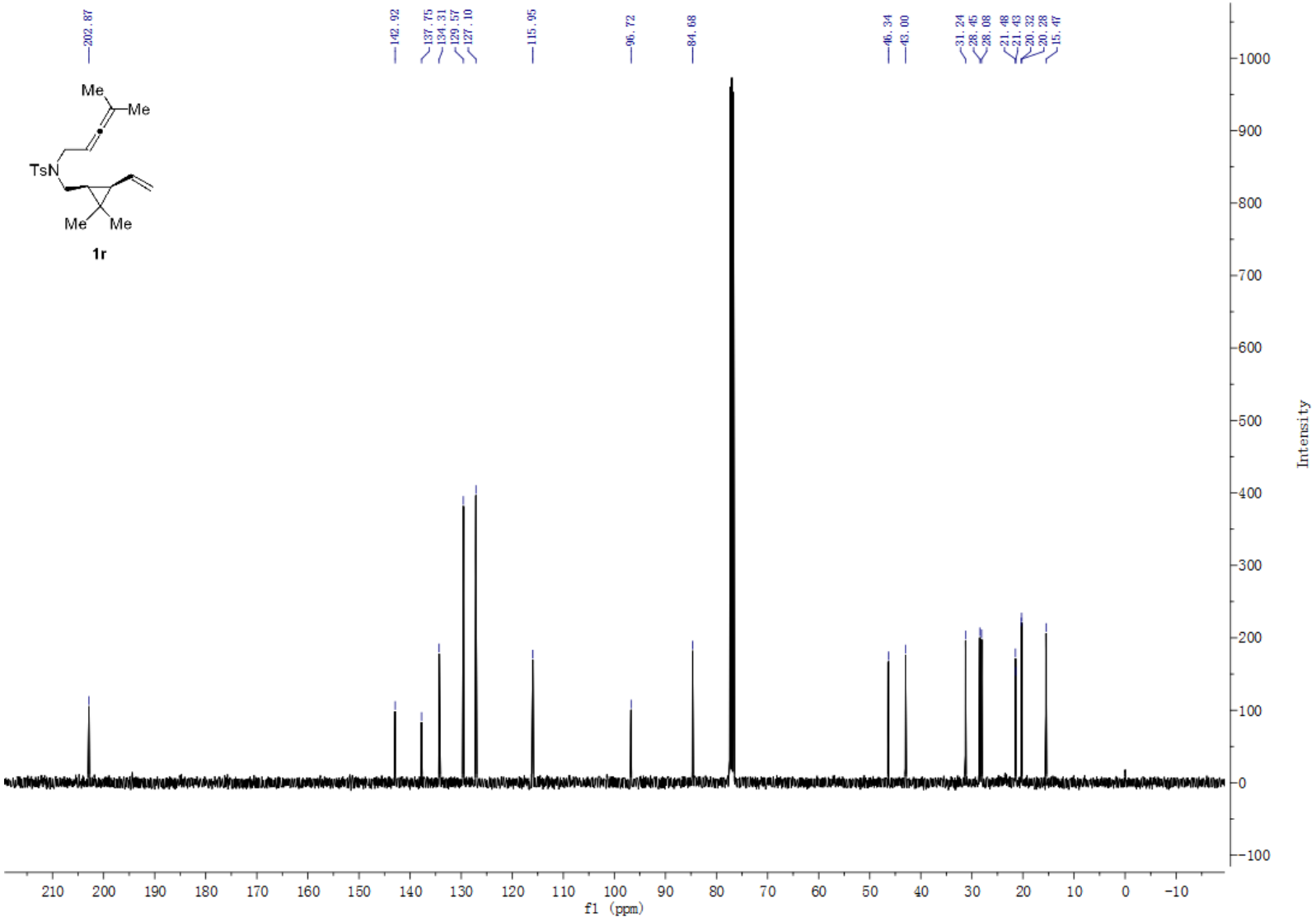

Me
Me
Me
TsN
1q
Intensity
f1 (ppm)

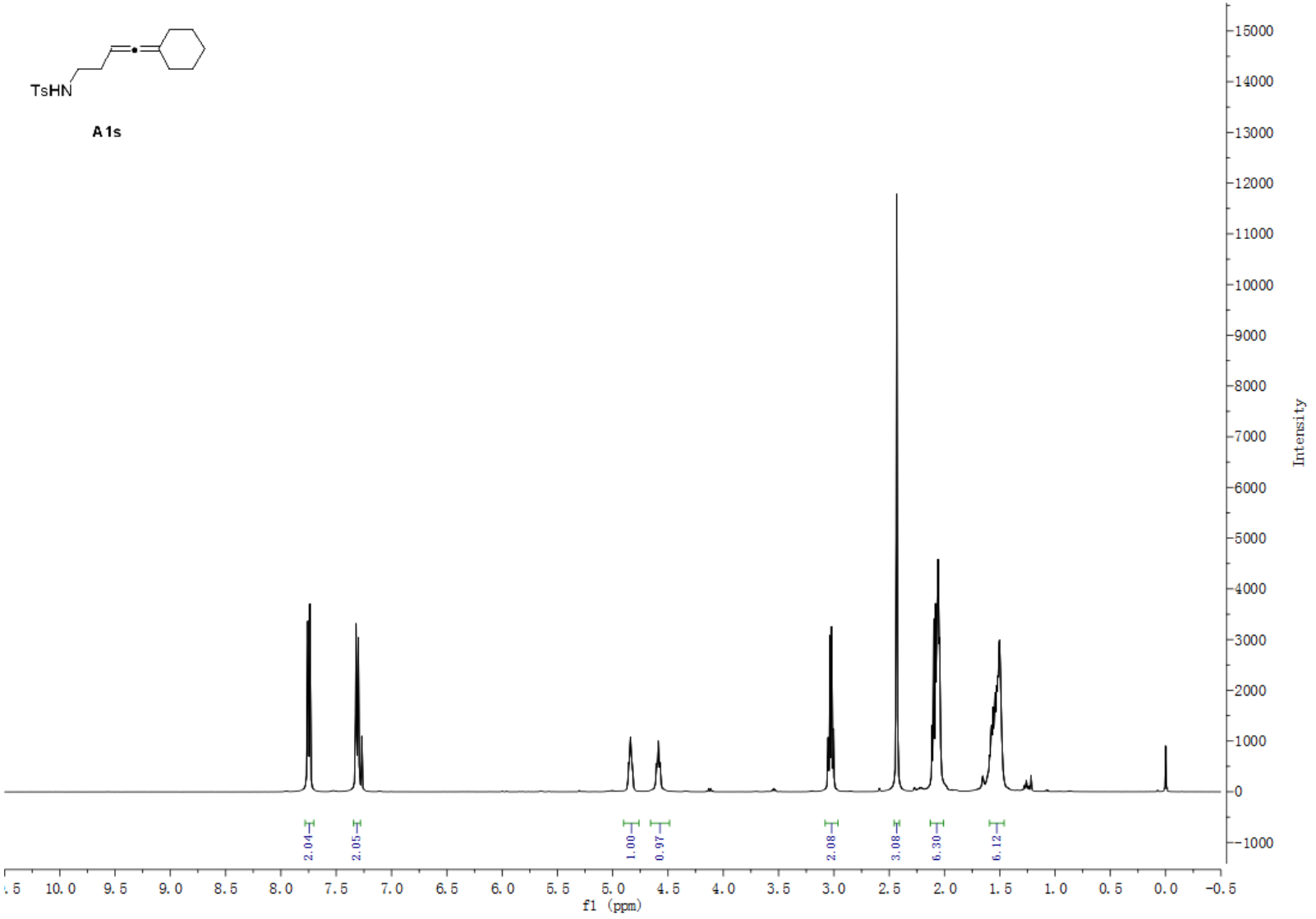

202.98
142.87
142.11
137.79
129.54
127.14
111.26
96.67
84.68
47.11
45.65
24.36
22.46
21.47
20.35
20.26
15.87
8.95
Me
Me
Me
TsN
1q
Intensity
f1 (ppm)

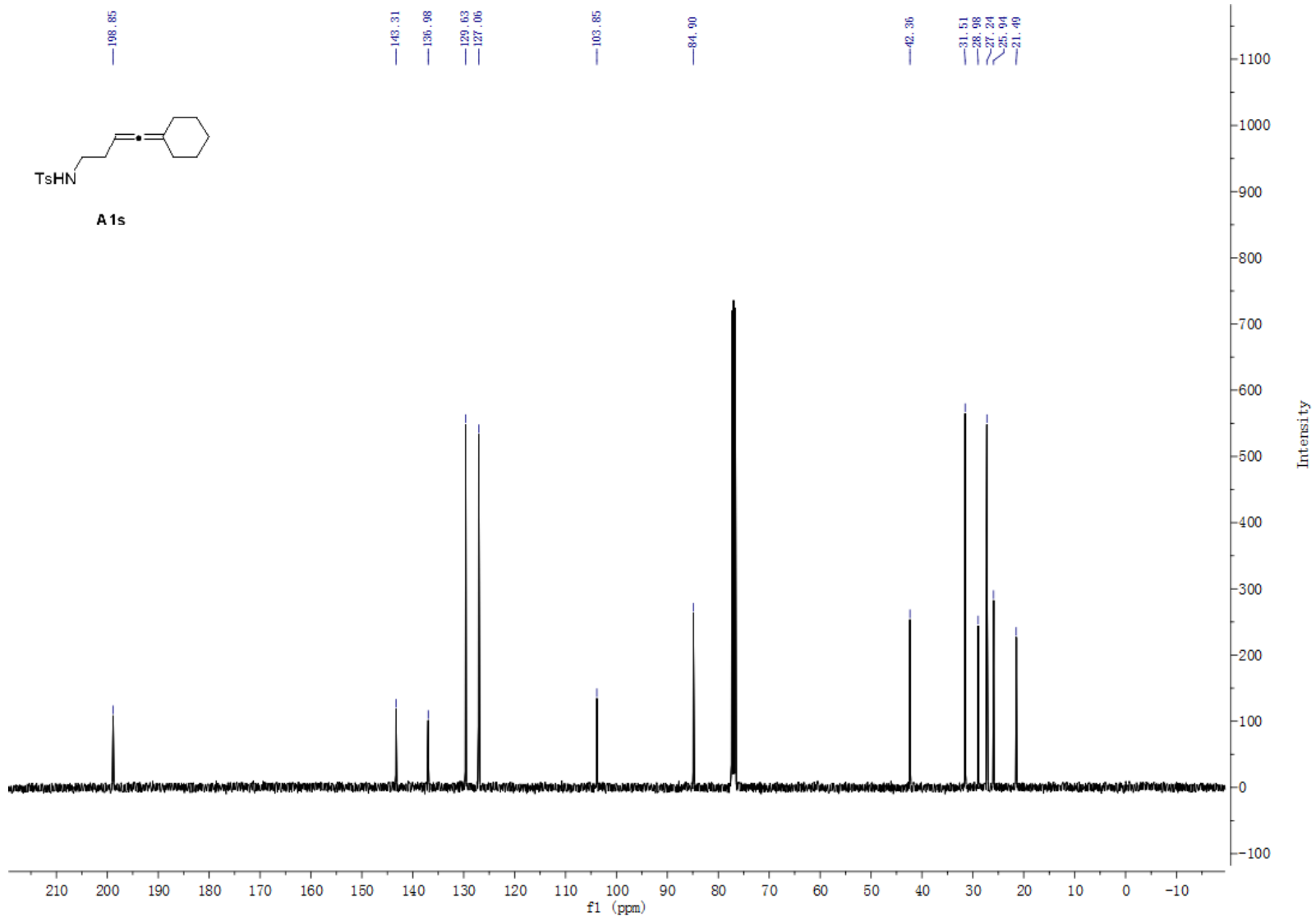

HO
Me
Me
V1r
1.00
0.98
0.96
1.04
0.99
1.96
1.16
5.99
f1 (ppm)
Intensity

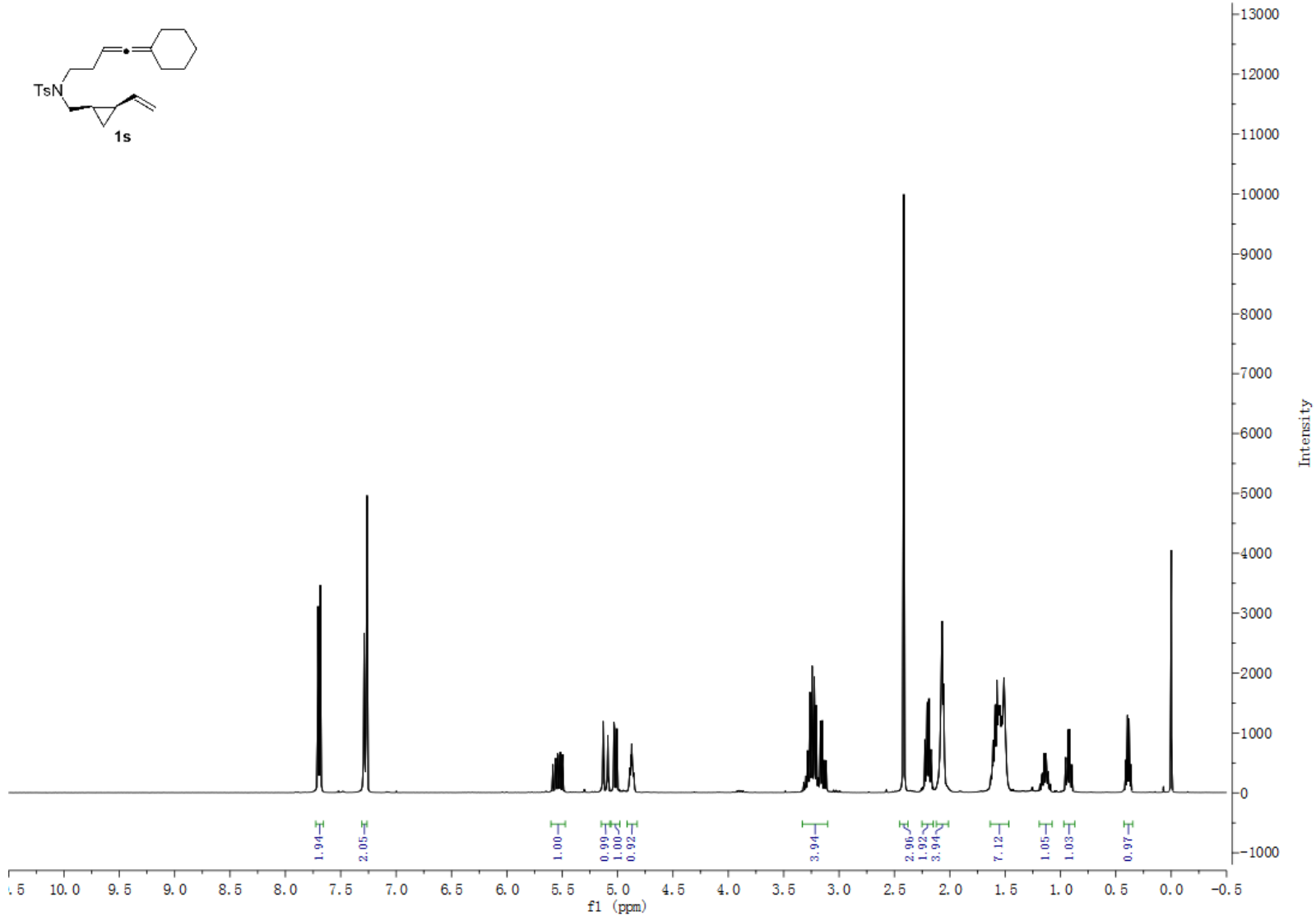

HO
Me
Me
V1r
134.37
116.09
60.18
32.24
31.35
28.67
21.96
15.41
2500
2000
1500
1000
500
0
Intensity
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

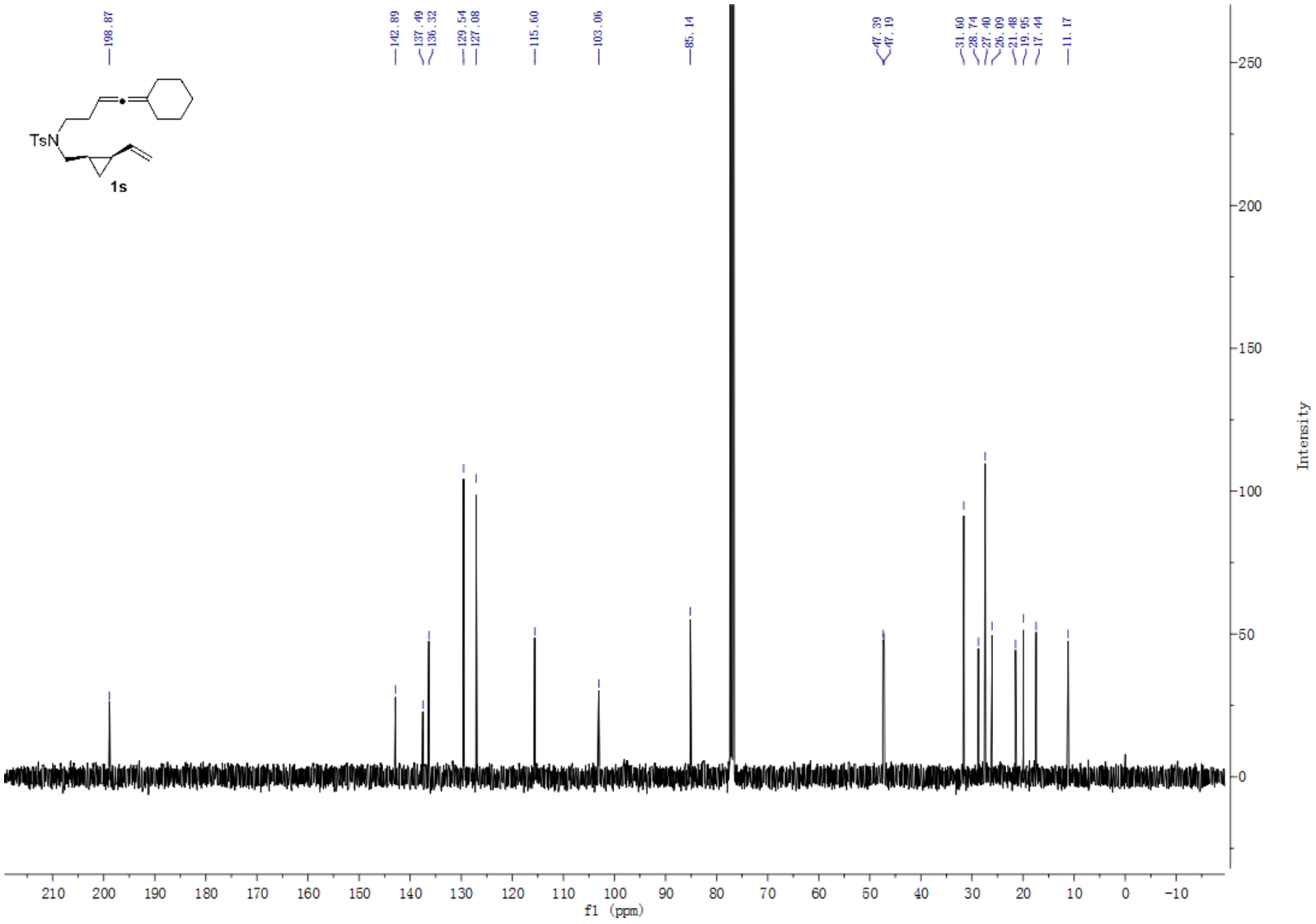

Me
Me
TsN
Me
Me
1r
Intensity
f1 (ppm)

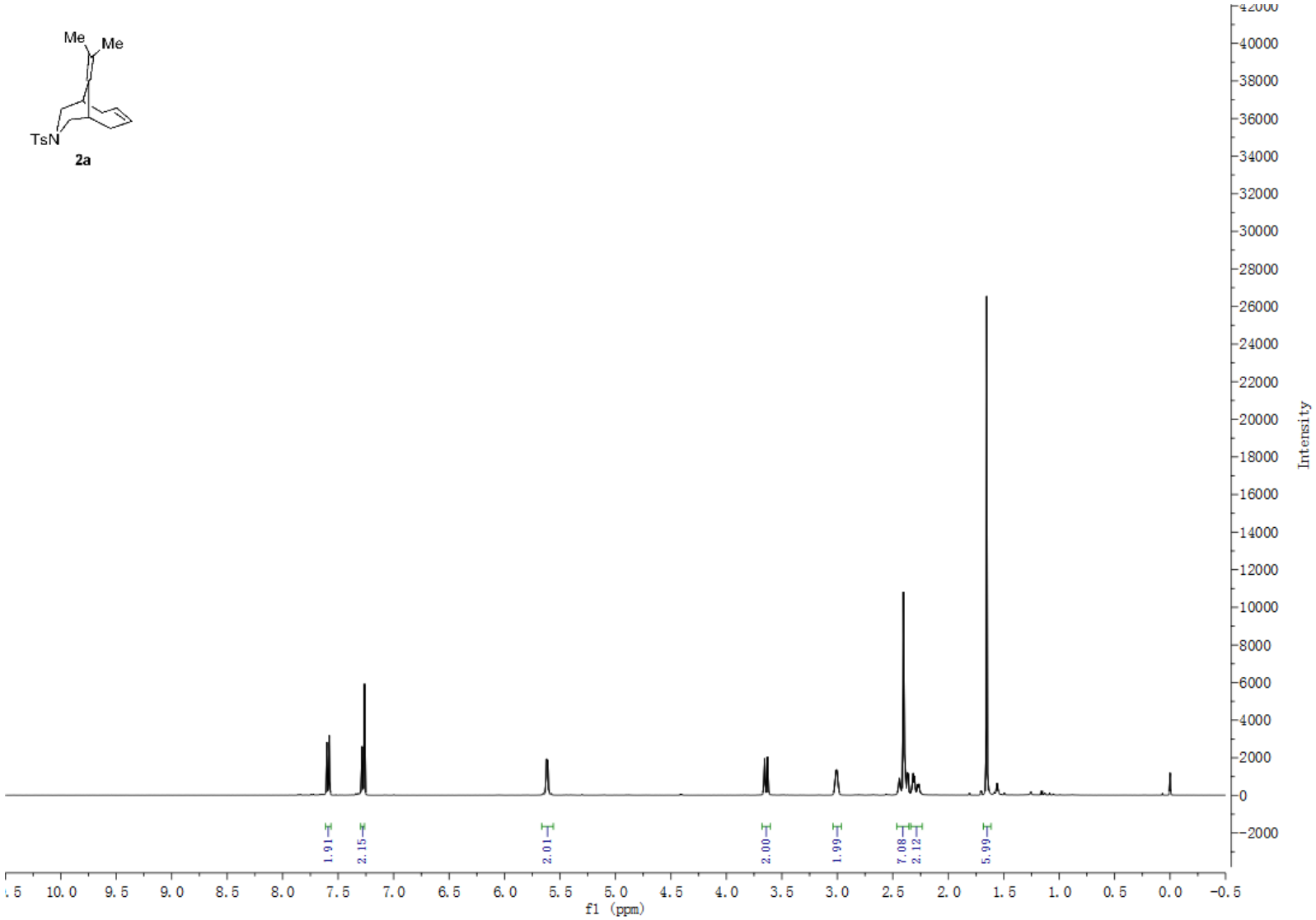

202.87
142.92
137.75
134.31
129.57
127.10
115.95
96.72
84.68
46.34
43.00
31.24
28.45
28.08
21.48
21.43
20.32
20.28
15.47
Me
Me
TsN
Me
Me
1r
Intensity
f1 (ppm)

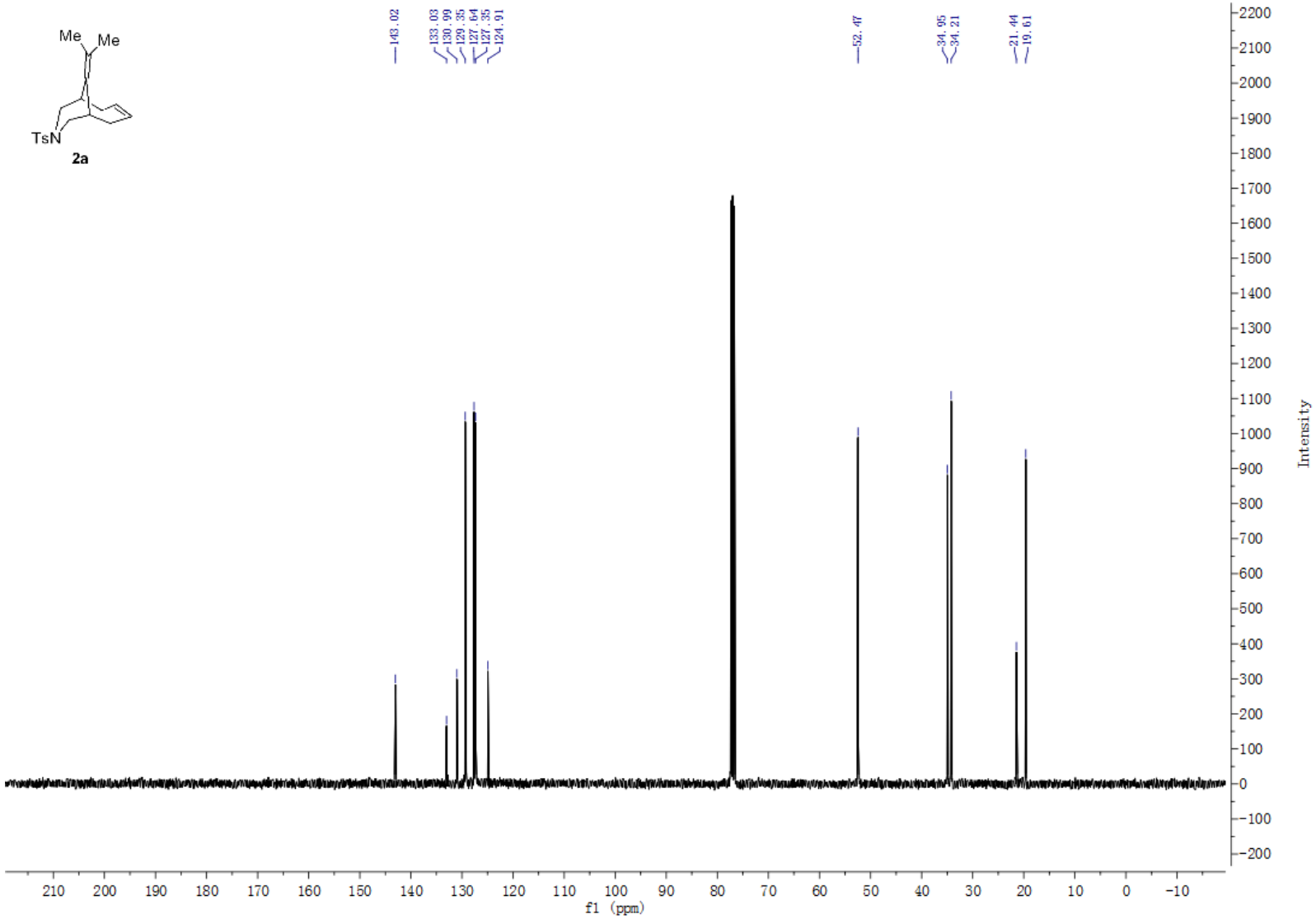

TsHN
A1s
2.04
2.05
1.00
0.97
2.08
3.08
6.30
6.12
f1 (ppm)
Intensity

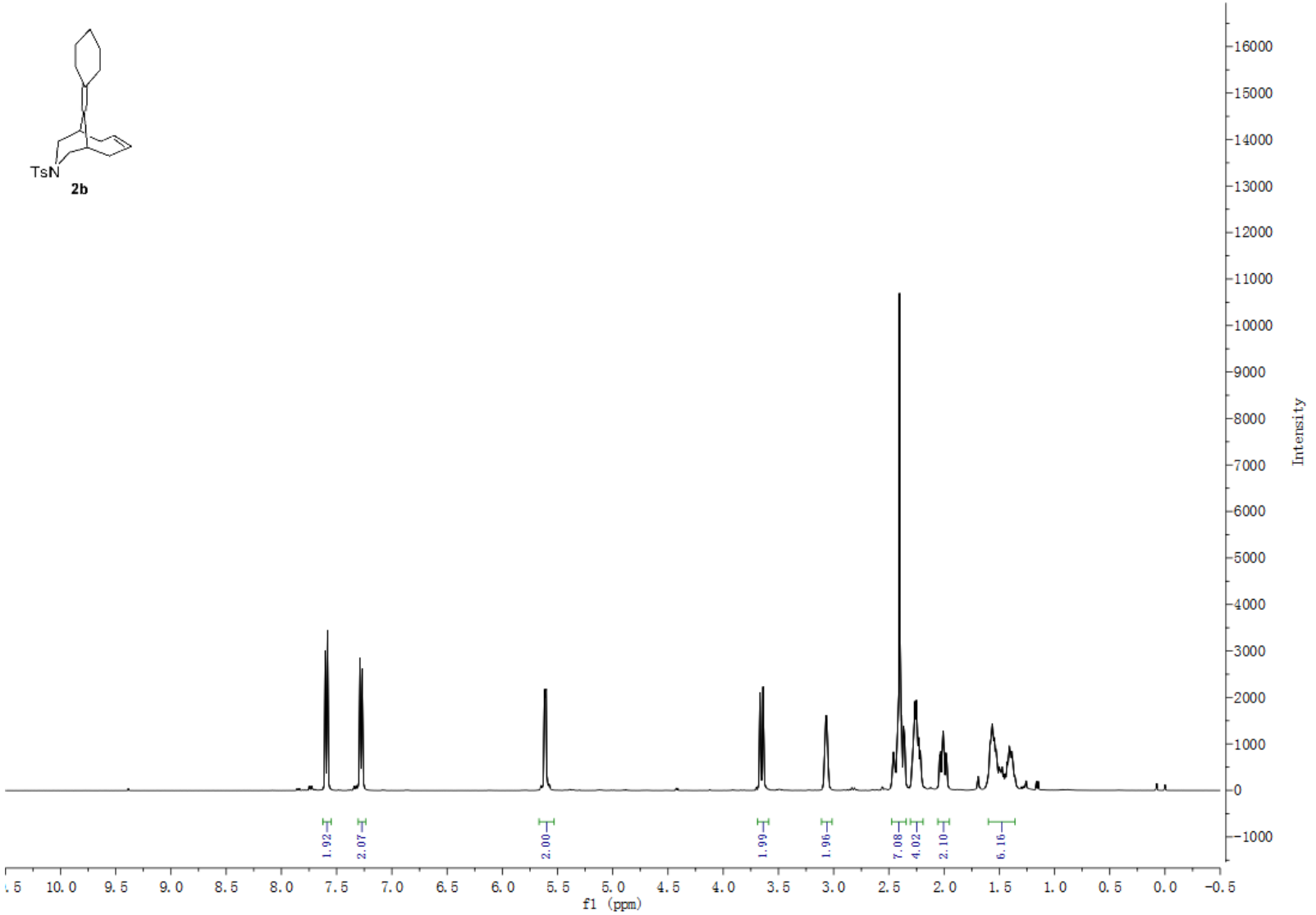

198.85
143.31
136.98
129.63
127.06
103.85
84.90
42.36
31.51
28.98
27.24
25.94
21.49
TsHN
A1s
Intensity
f1 (ppm)

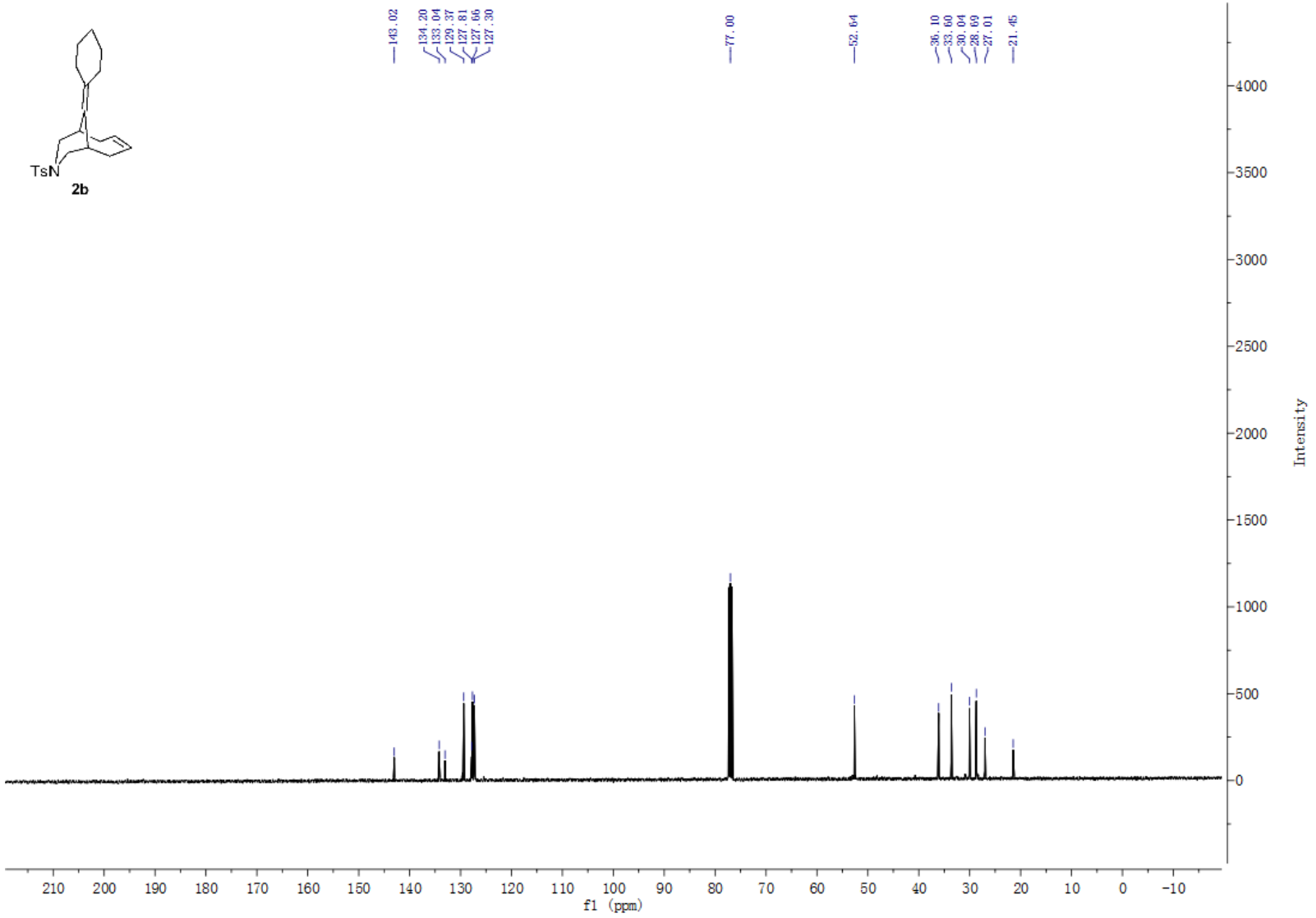

TsN
1s
1.94
2.05
1.00
0.99
1.00
0.92
3.94
2.96
1.92
3.94
7.12
1.05
1.03
0.97
f1 (ppm)
Intensity

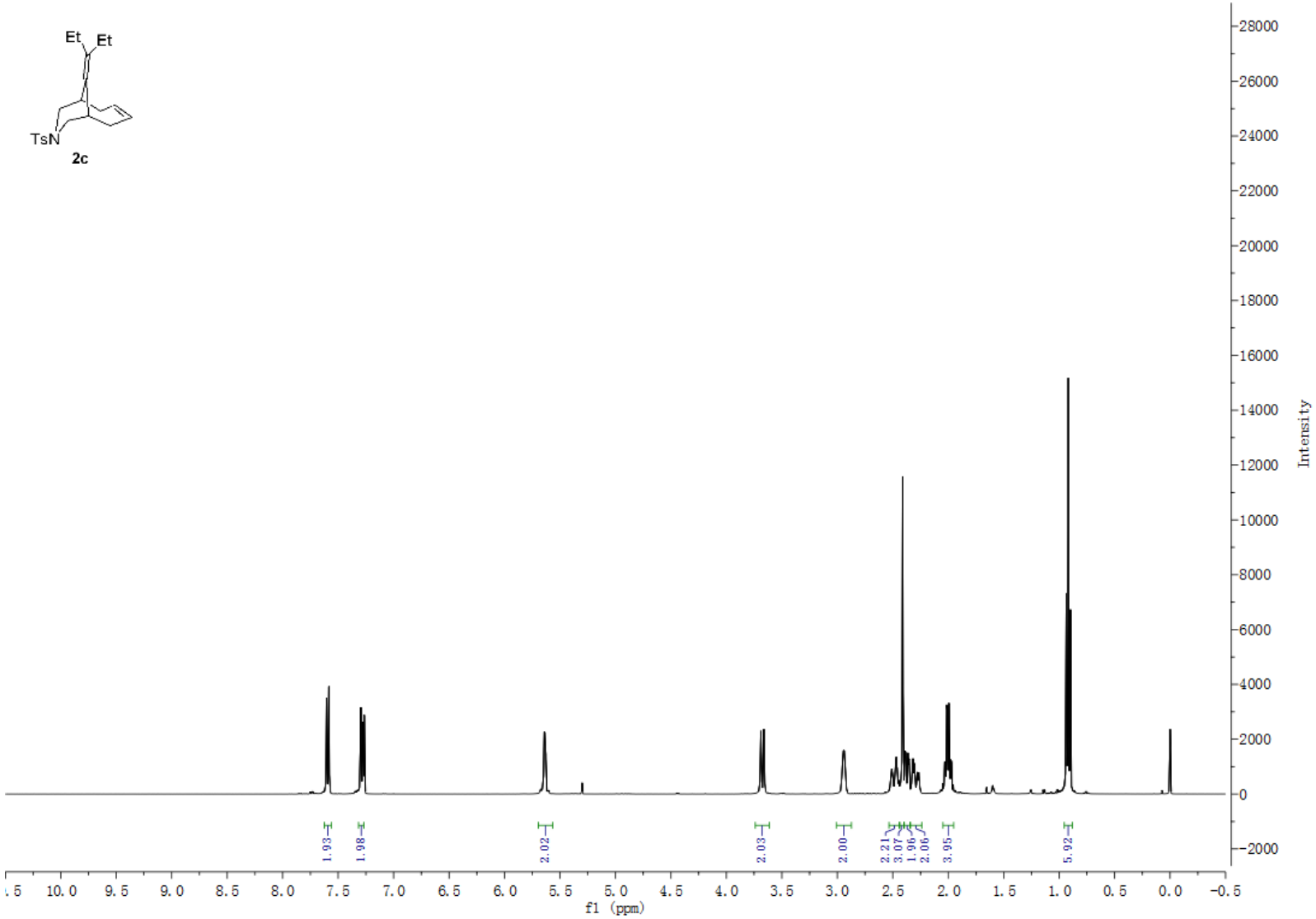

198.87
142.89
137.49
136.32
129.54
127.08
115.60
103.06
85.14
47.39
47.19
31.60
28.74
27.40
26.09
21.48
19.95
17.44
11.17
TsN
1s
Intensity
f1 (ppm)

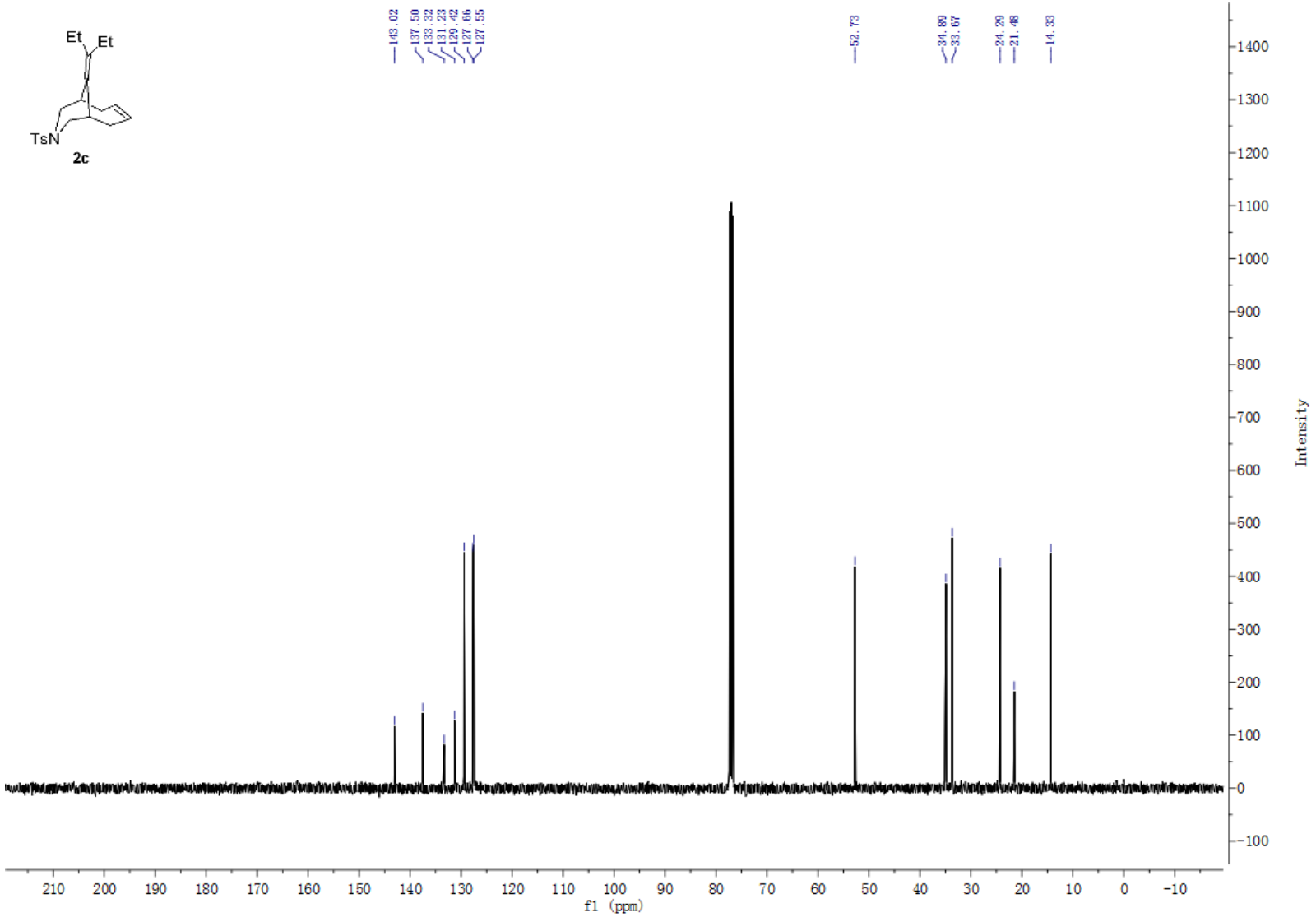

Me
Me
TsN
2a
Intensity
f1 (ppm)
1.91
2.15
2.01
2.00
1.99
7.08
2.12
5.99

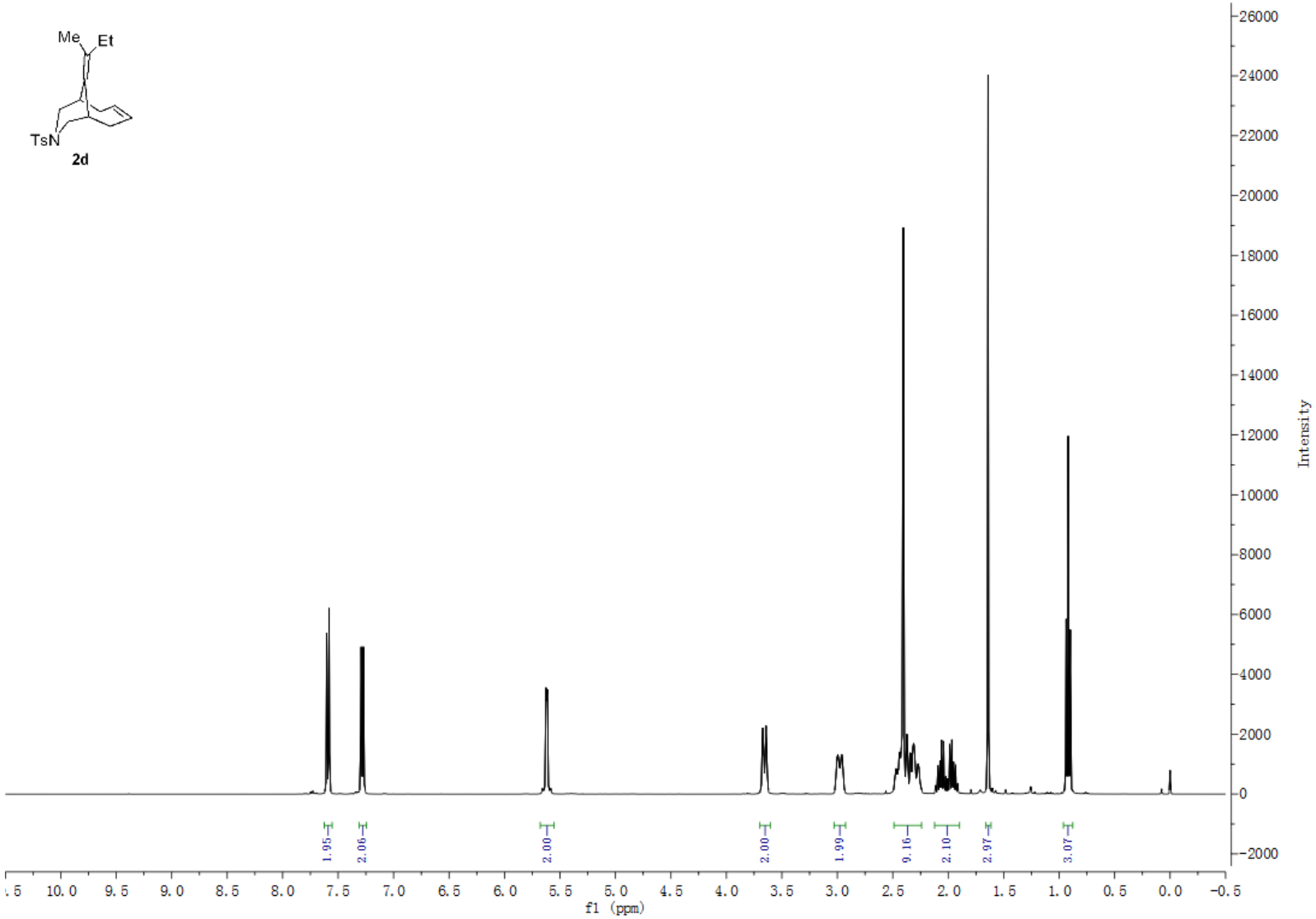

Me
Me
TsN
2a
143.02
133.03
130.99
129.35
127.64
127.35
124.91
52.47
34.95
34.21
21.44
19.61
Intensity
f1 (ppm)

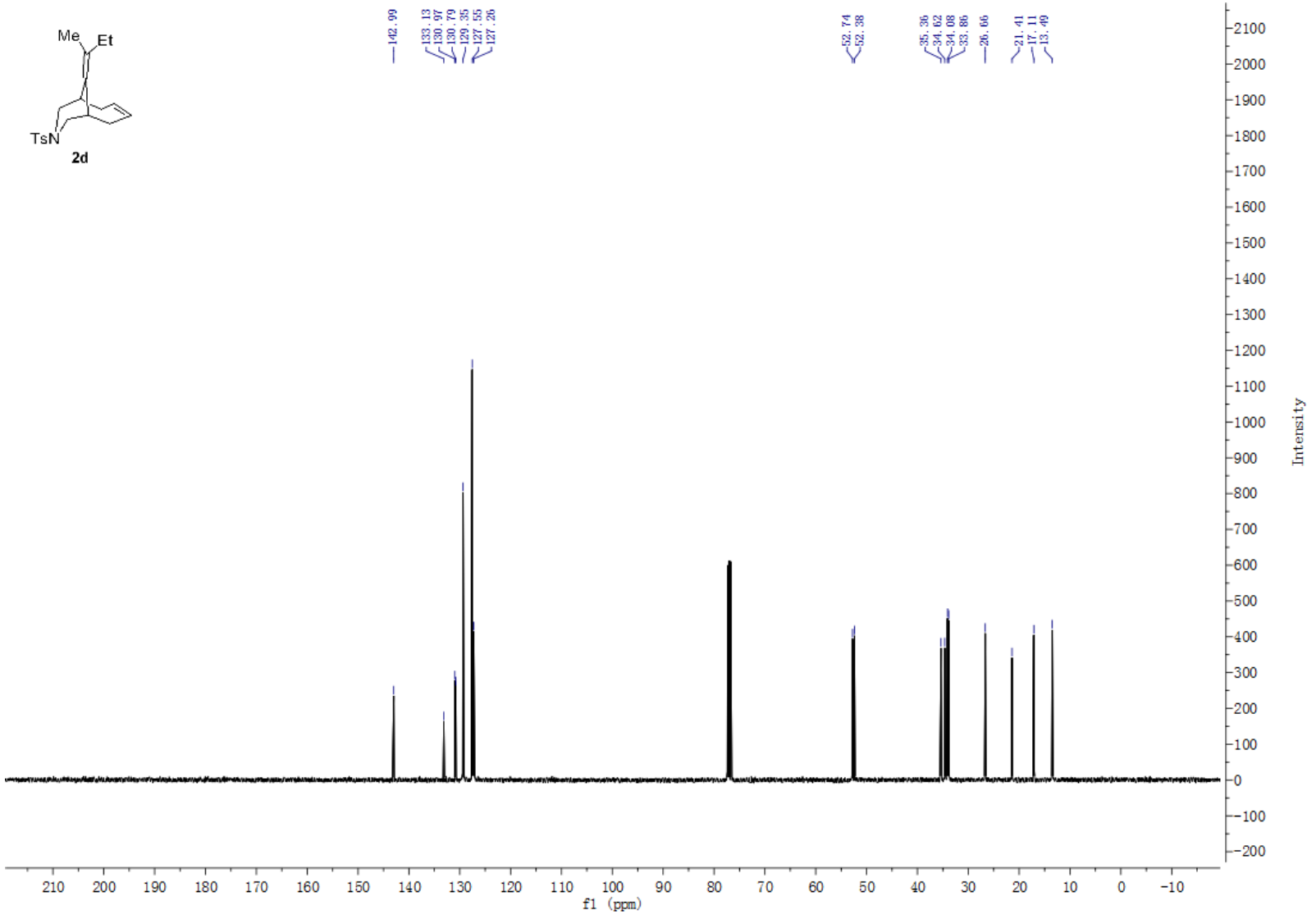

TsN
2b
16000
15000
14000
13000
12000
11000
10000
9000
8000
7000
6000
5000
4000
3000
2000
1000
0
-1000
Intensity
1.92
2.07
2.00
1.99
1.96
7.08
4.02
2.10
6.16
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

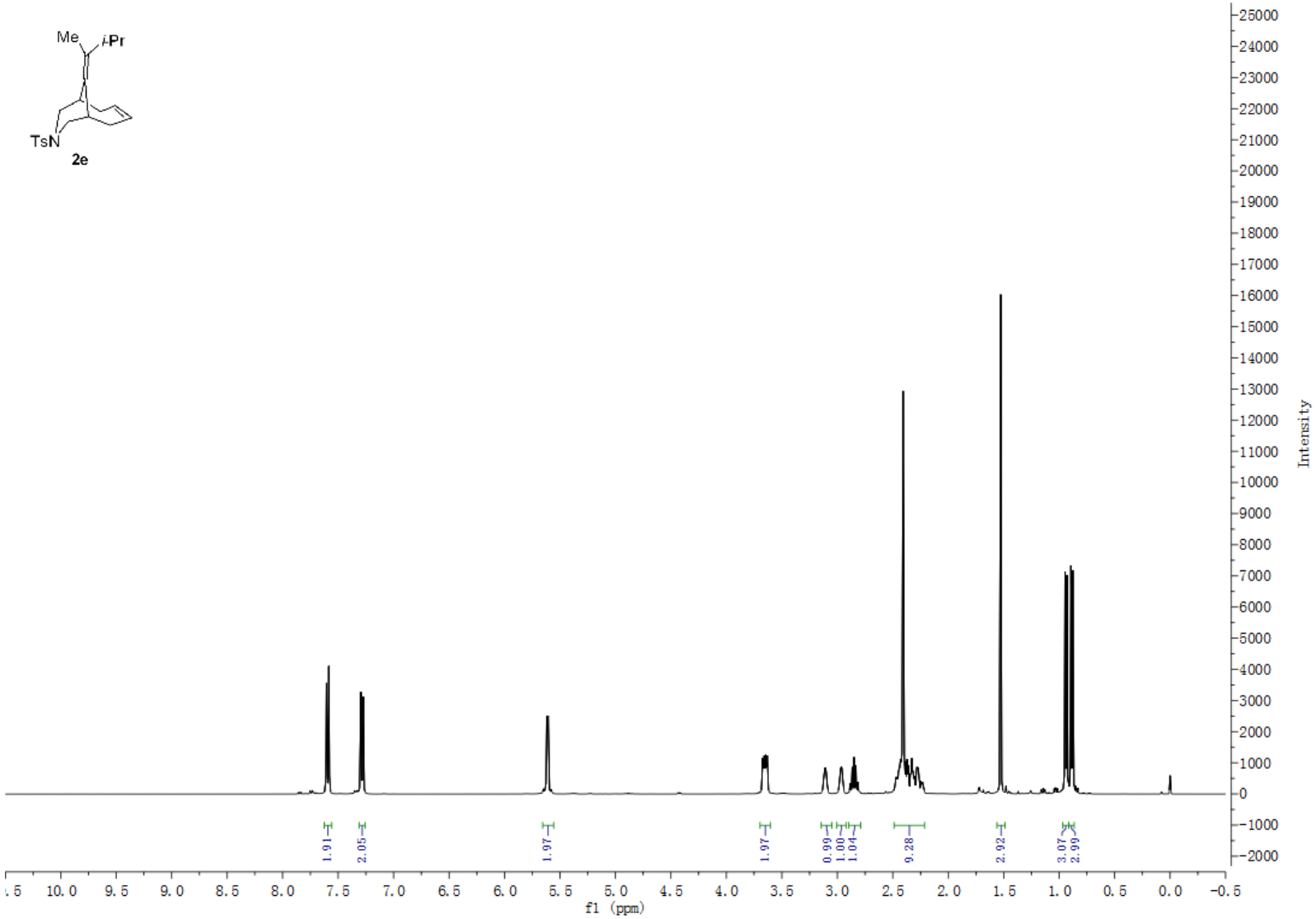

TsN
2b
143.02
134.20
133.04
129.37
127.81
127.66
127.30
77.00
52.64
36.10
33.60
30.04
28.69
27.01
21.45
Intensity
f1 (ppm)

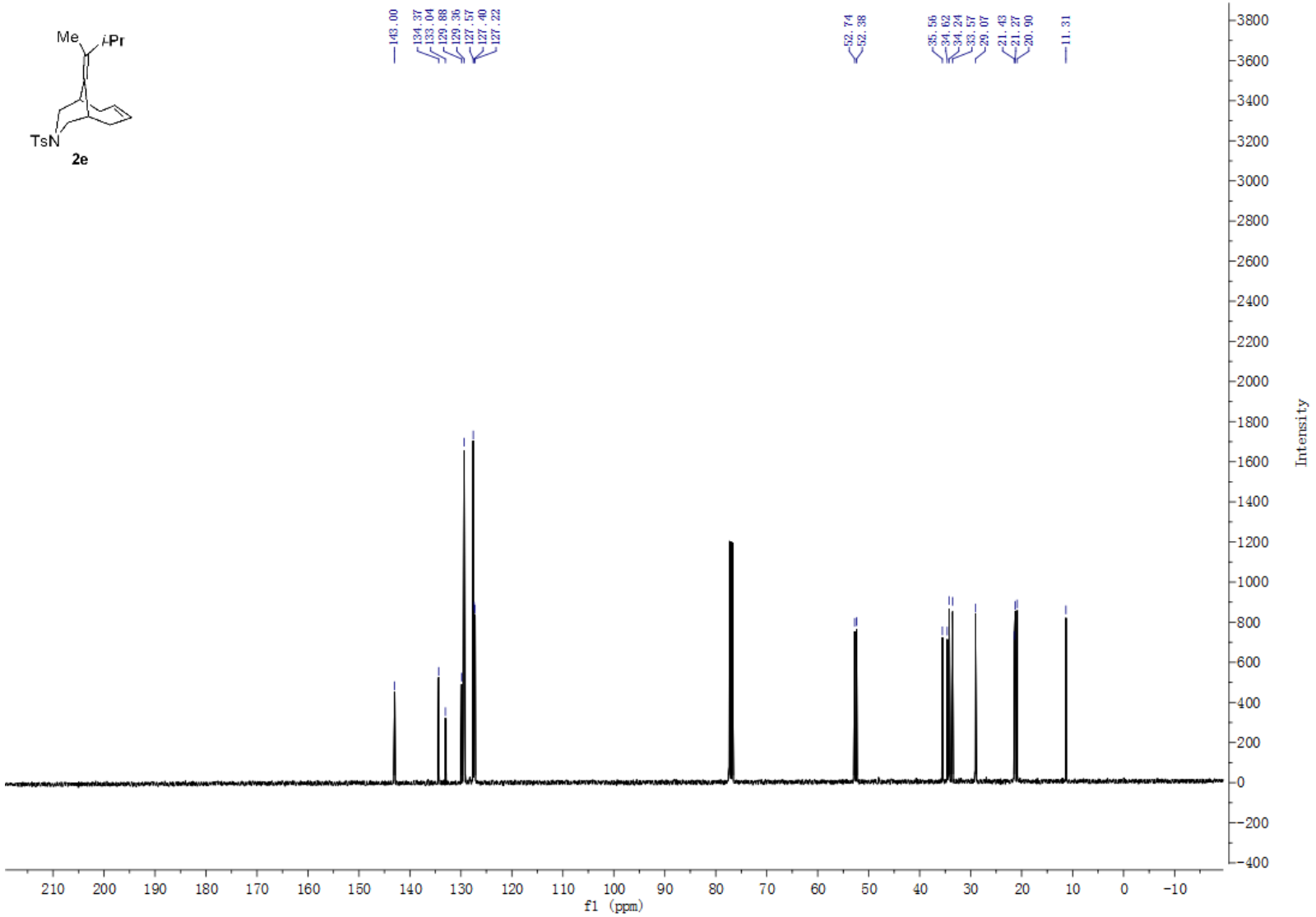

Et
Et
TsN
2c
28000
26000
24000
22000
20000
18000
16000
14000
12000
10000
8000
6000
4000
2000
0
-2000
Intensity
1.93
1.98
2.02
2.03
2.00
2.21
3.07
1.96
2.06
3.95
5.92
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

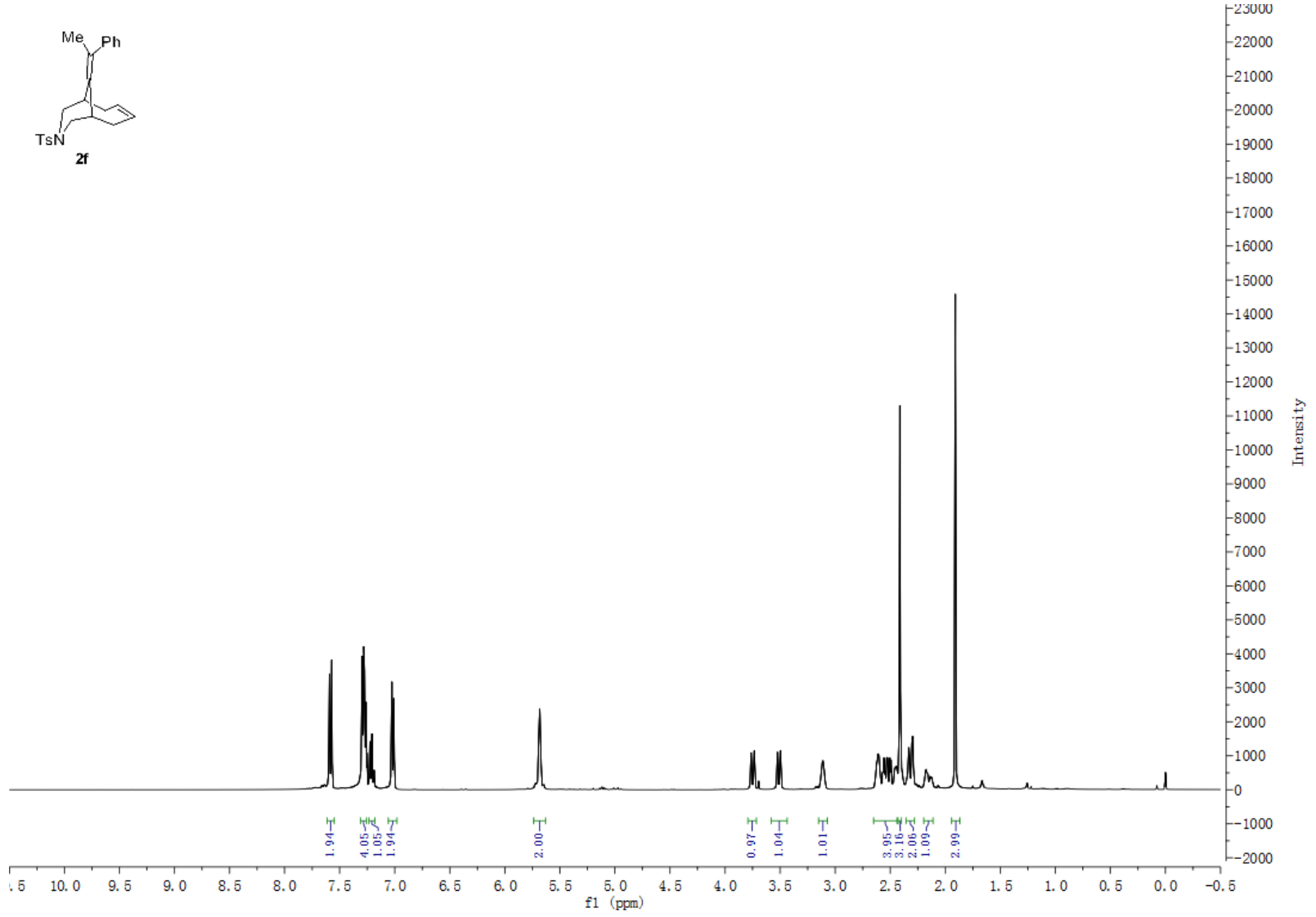

Et
Et
TsN
2c
143.02
137.59
133.32
131.23
129.42
127.66
127.55
52.73
34.89
33.67
24.29
21.48
14.33
Intensity
f1 (ppm)

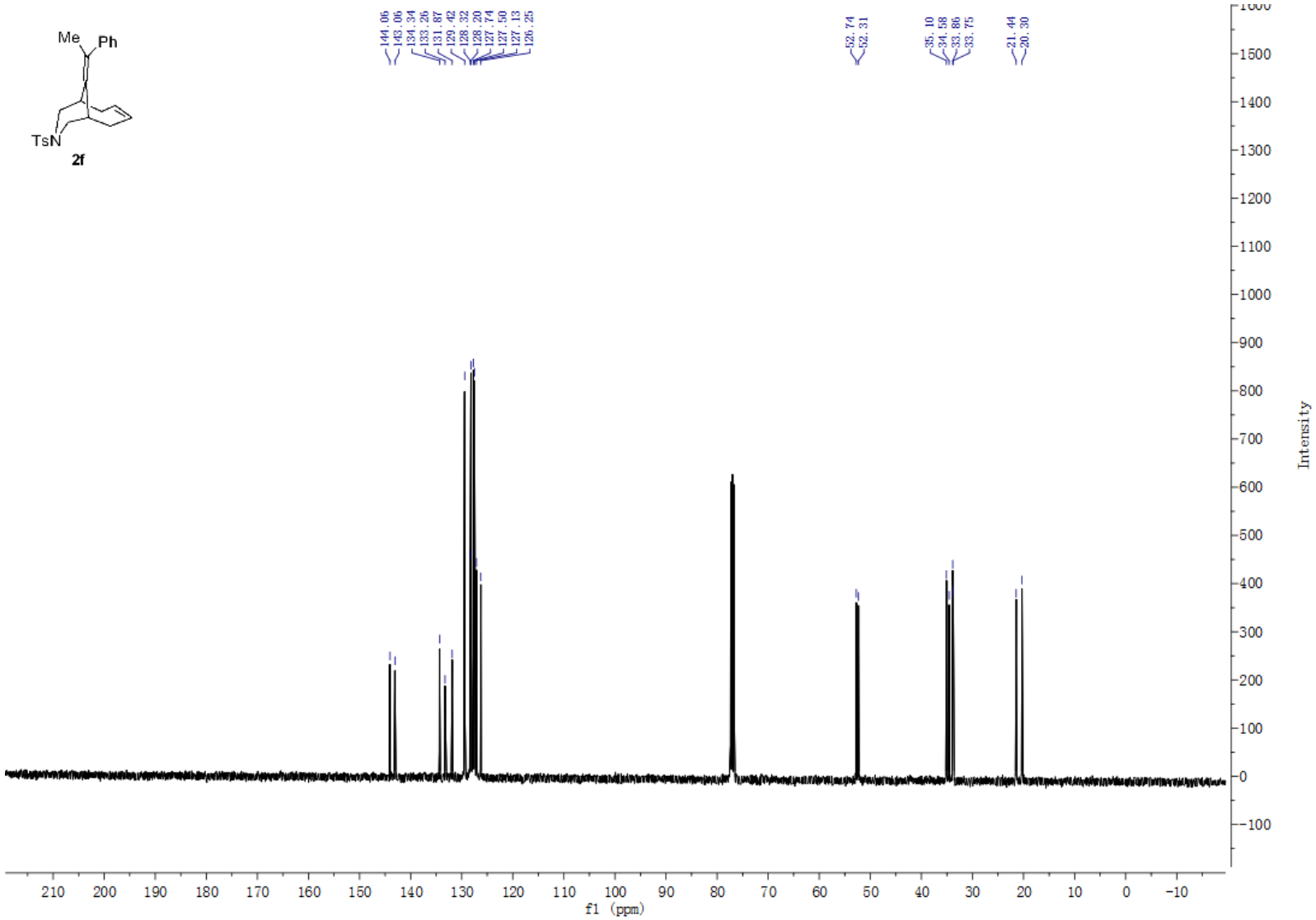

Me
Et
TsN
2d
1.95
2.06
2.00
2.00
1.99
9.16
2.10
2.97
3.07
f1 (ppm)
Intensity

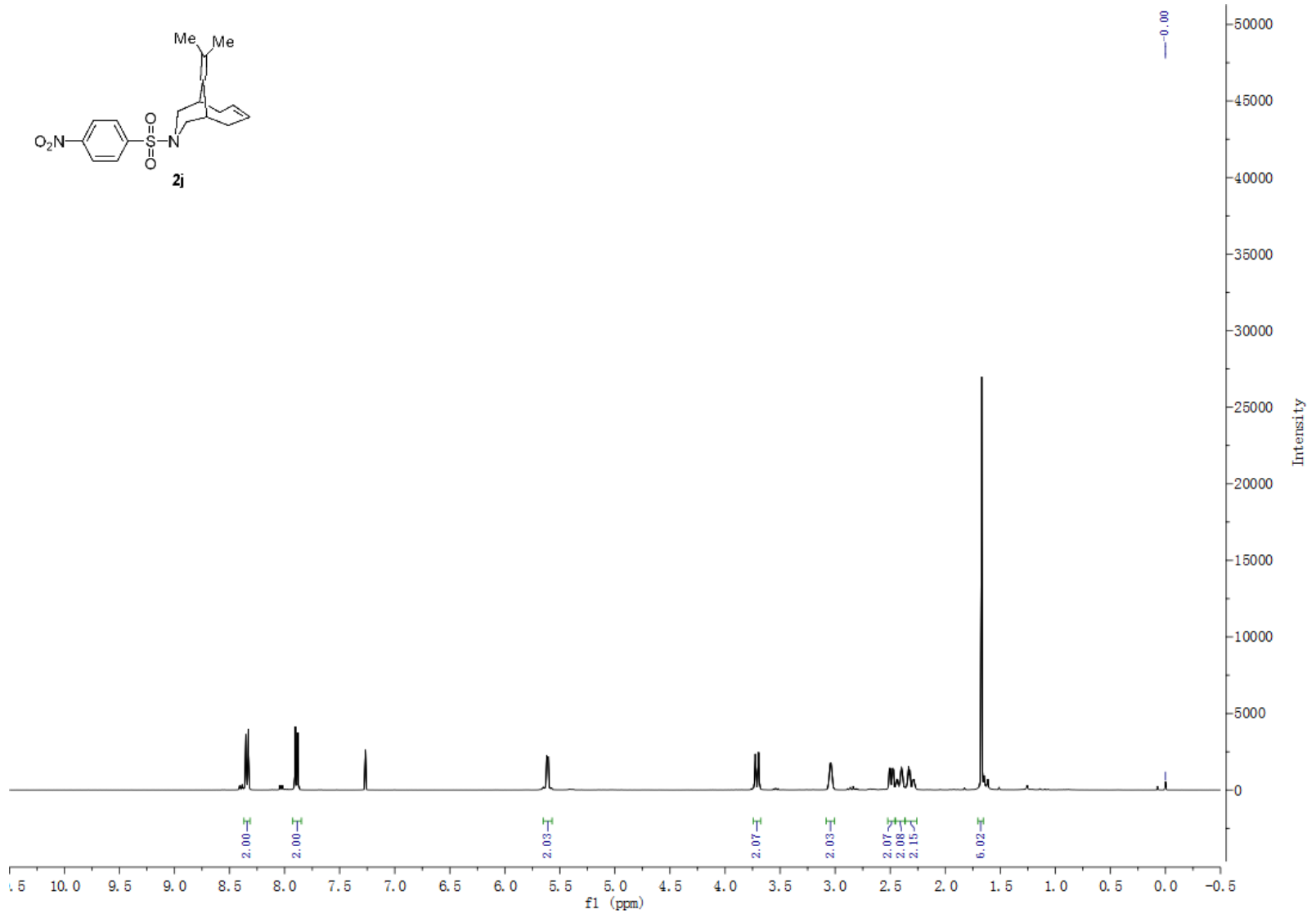

Me
Et
TsN
2d
142.99
133.13
130.97
130.79
129.35
127.55
127.26
52.74
52.38
35.36
34.62
34.08
33.86
26.66
21.41
17.11
13.49
Intensity
f1 (ppm)

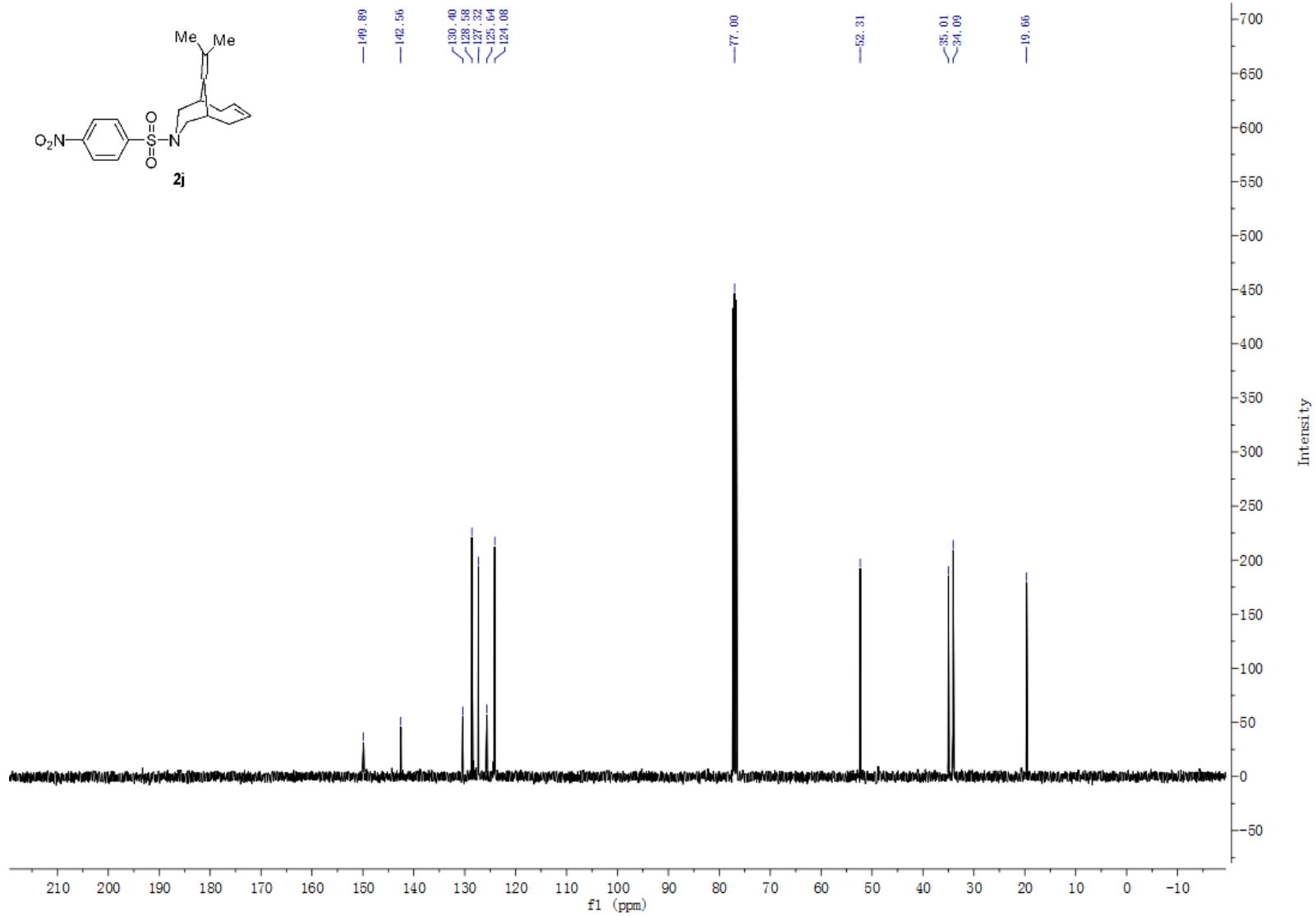

Me
iPr
TsN
2e
Intensity
f1 (ppm)
1.91
2.05
1.97
1.97
0.99
1.00
1.04
9.28
2.92
3.07
2.99

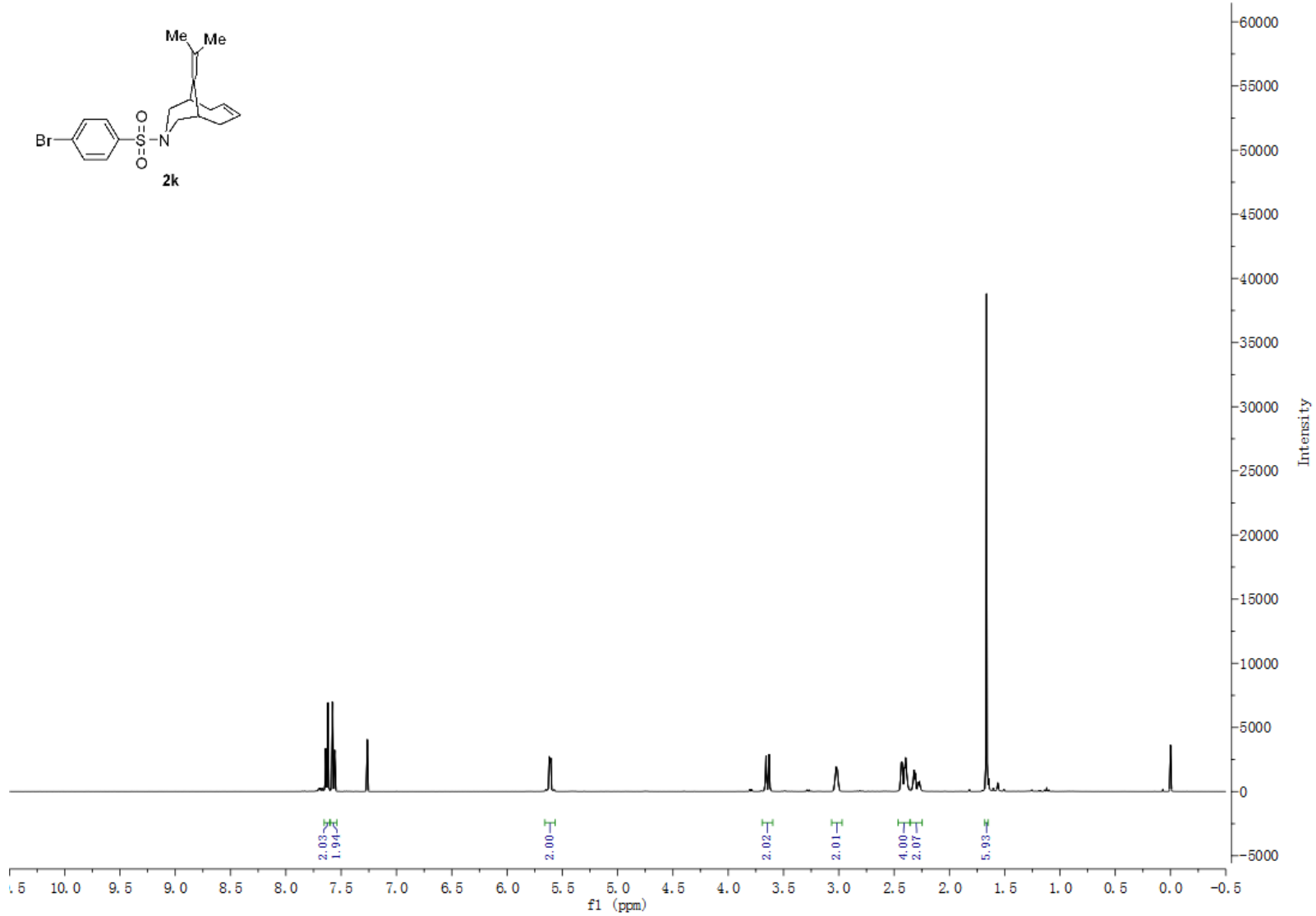

Me
iPr
TsN
2e
143.00
134.37
133.04
129.88
129.36
127.57
127.40
127.22
52.74
52.38
35.56
34.62
34.24
33.57
29.07
21.43
21.27
20.90
11.31
Intensity
f1 (ppm)

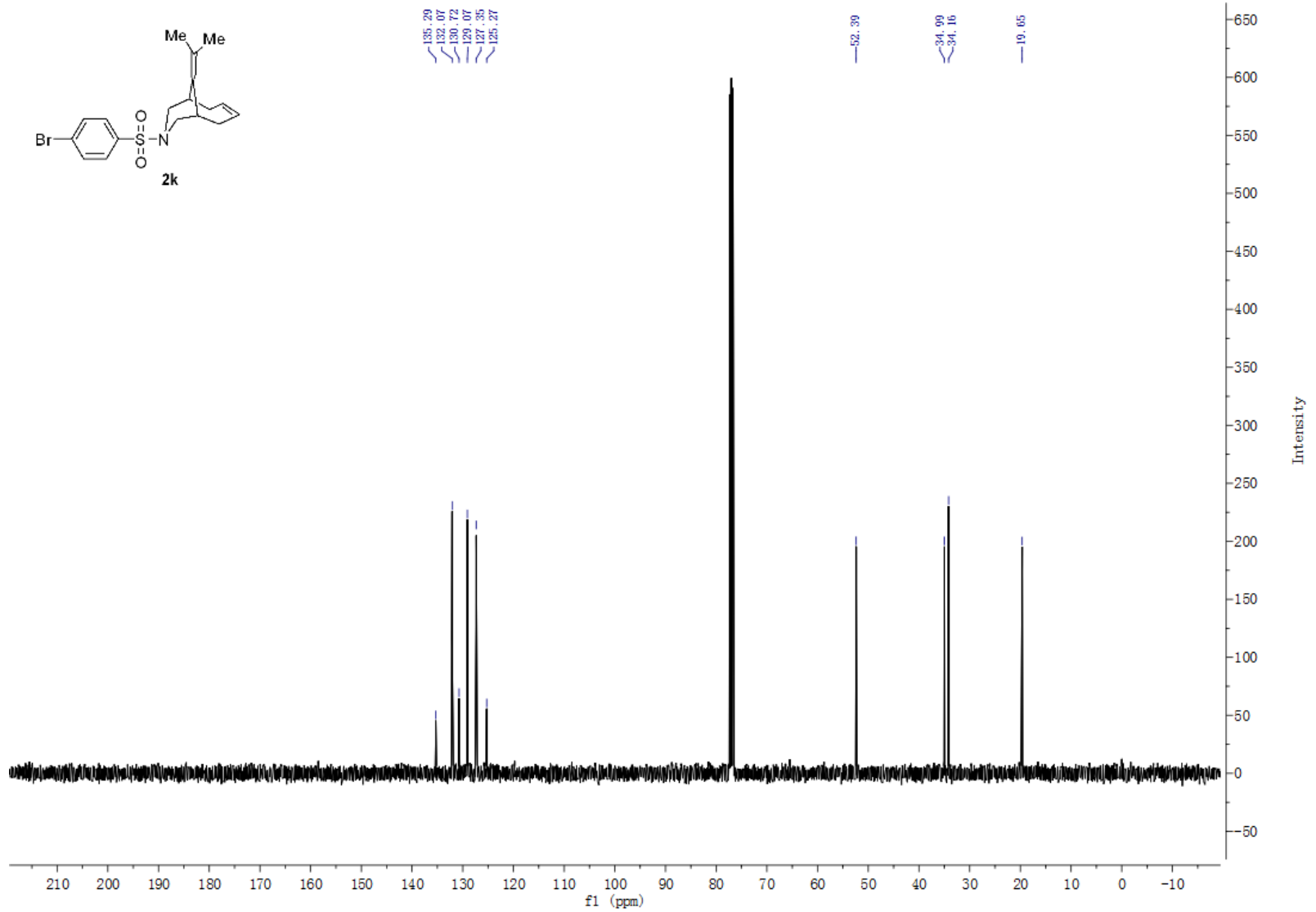

Me
Ph
TsN
2f
1.94
4.05
1.05
1.94
2.00
0.97
1.04
1.01
3.95
3.16
2.06
1.09
2.99
f1 (ppm)
Intensity

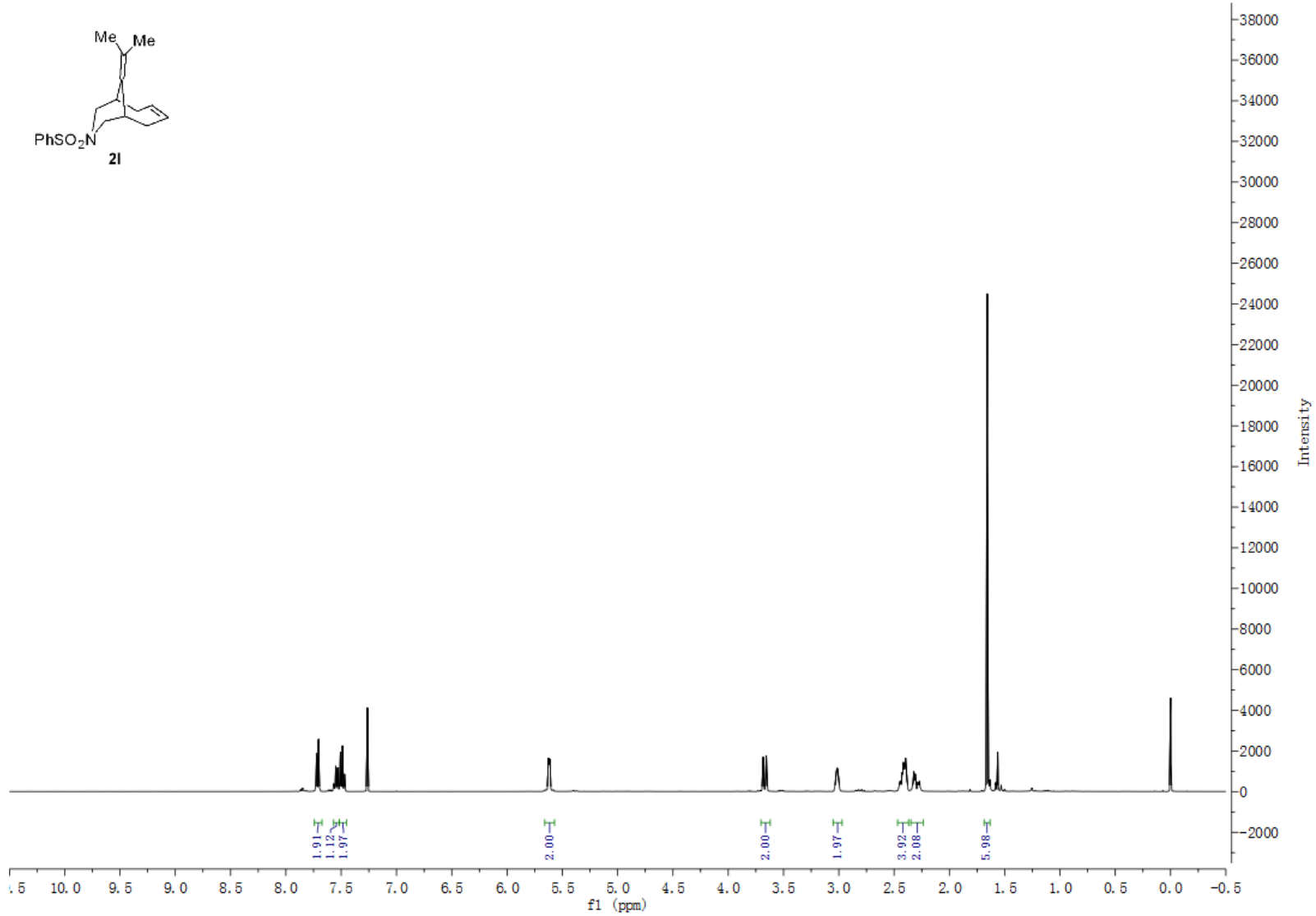

Me
Ph
TsN
2f
144.06
143.06
134.34
133.26
131.87
129.42
128.32
128.20
127.74
127.50
127.13
126.25
52.74
52.31
35.10
34.58
33.86
33.75
21.44
20.30
Intensity
f1 (ppm)

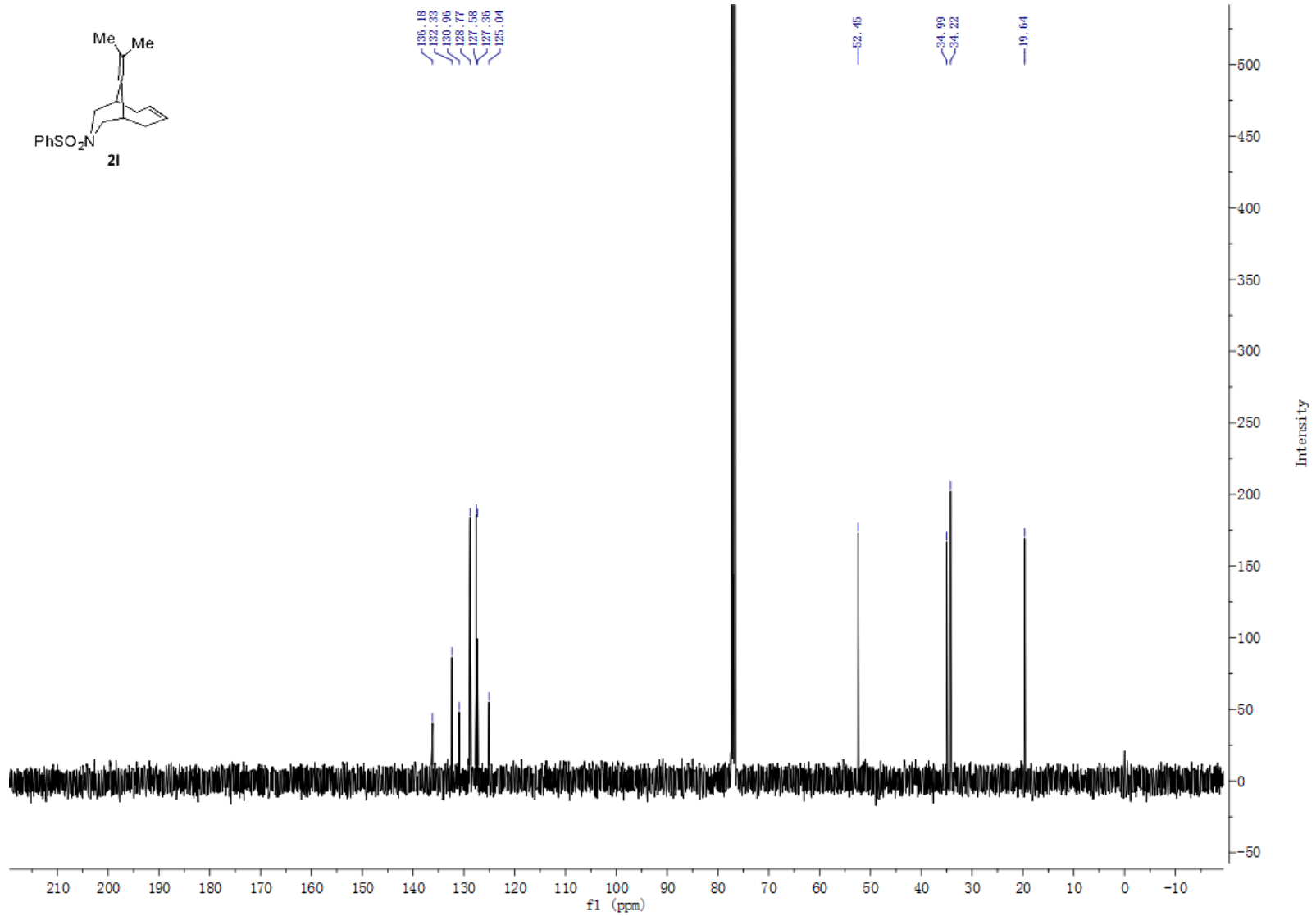

Me
Me
O2N
S
N
O
O
2j
-0.00
50000
45000
40000
35000
30000
25000
20000
15000
10000
5000
0
Intensity
2.00
2.00
2.03
2.07
2.03
2.07
2.08
2.15
6.02
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

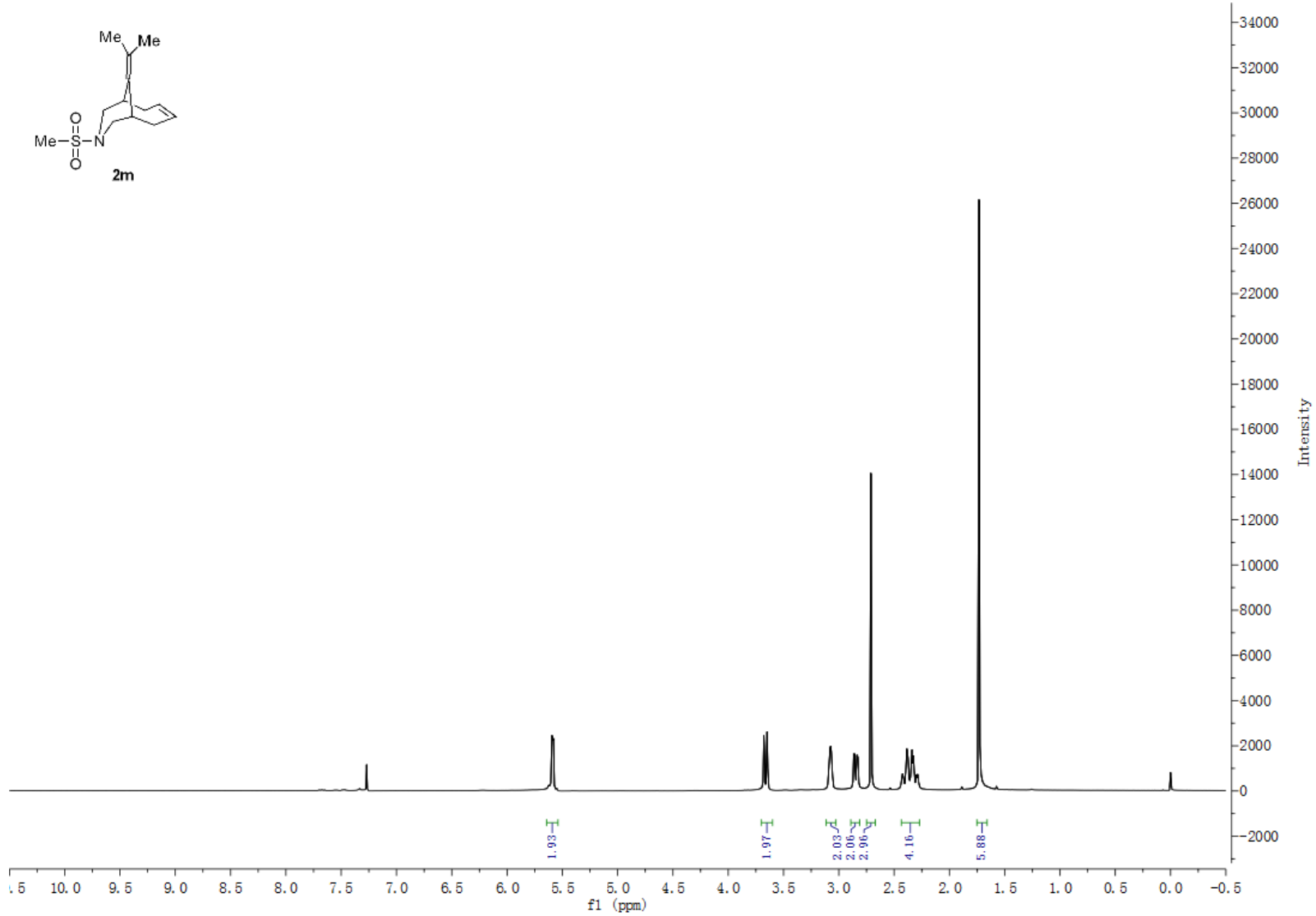

Me
Me
O2N
S
O
O
N
2j
149.89
142.56
130.40
128.58
127.32
125.64
124.08
77.00
52.31
35.01
34.09
19.66
Intensity
f1 (ppm)

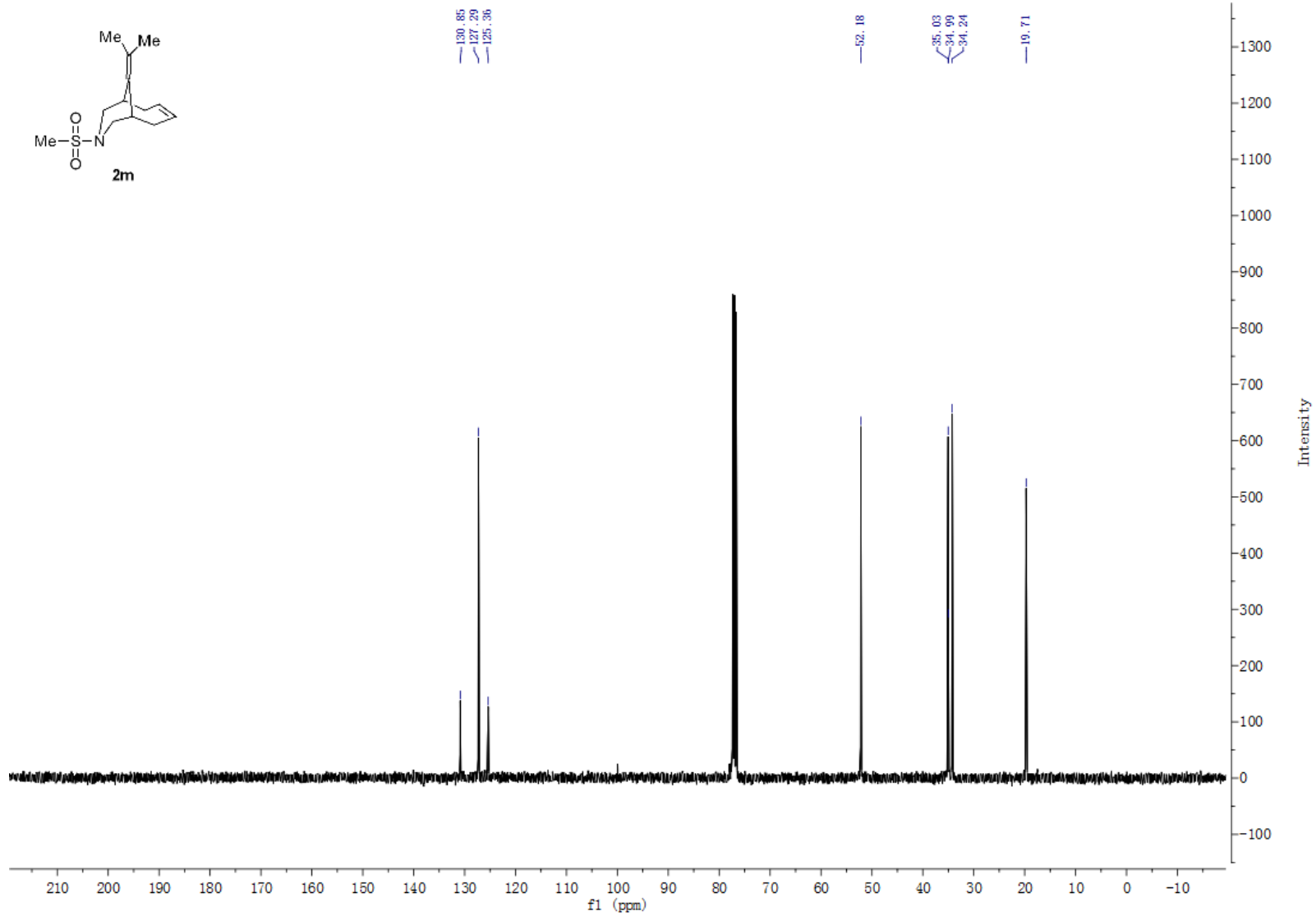

Me
Me
Br
S
O
O
N
2k
60000
55000
50000
45000
40000
35000
30000
25000
20000
15000
10000
5000
0
-5000
Intensity
2.03
1.94
2.00
2.02
2.01
4.00
2.07
5.93
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

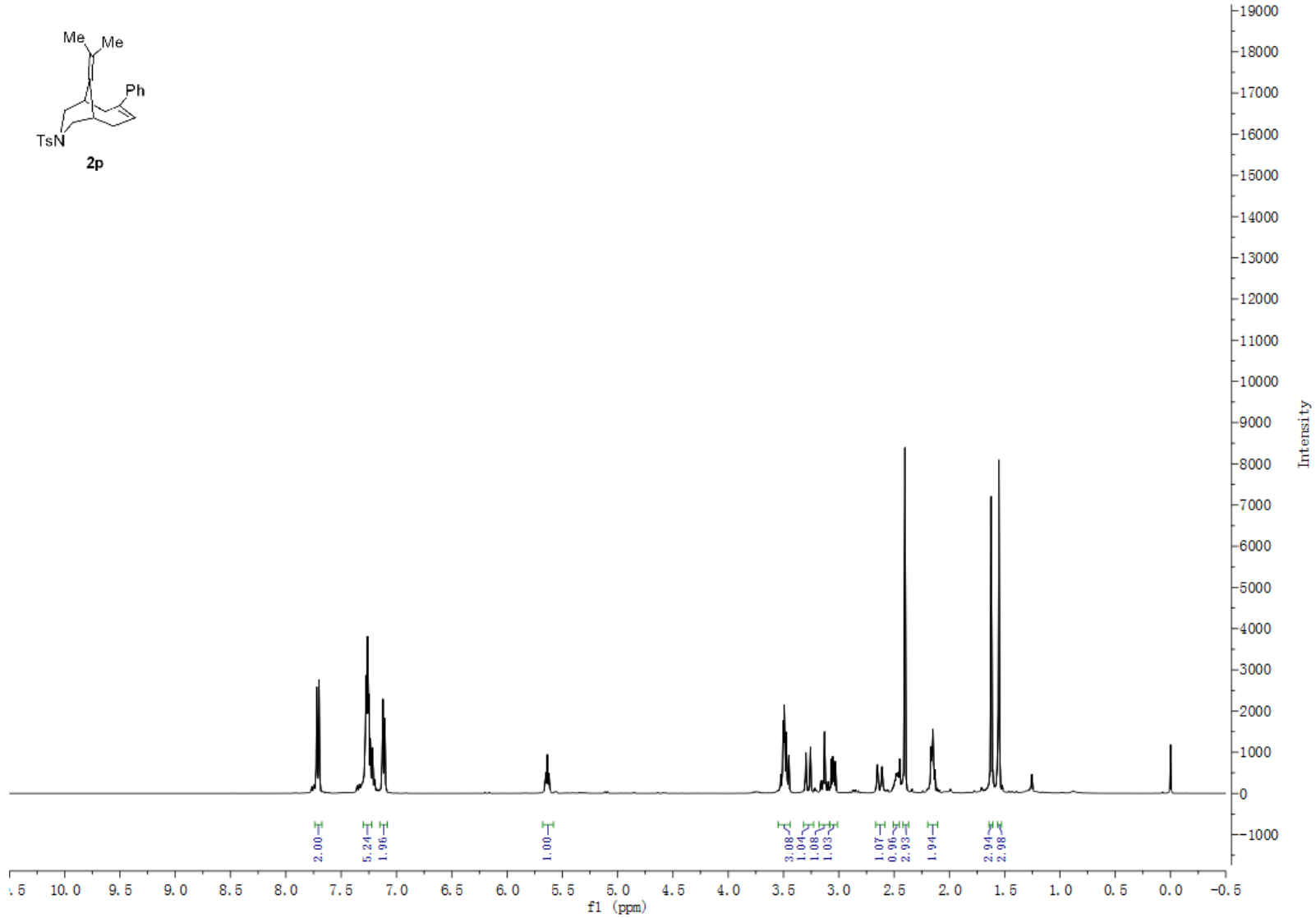

Me
Me
Br
S
O
O
N
2k
135.29
132.07
130.72
129.07
127.35
125.27
52.39
34.99
34.16
19.65
Intensity
f1 (ppm)

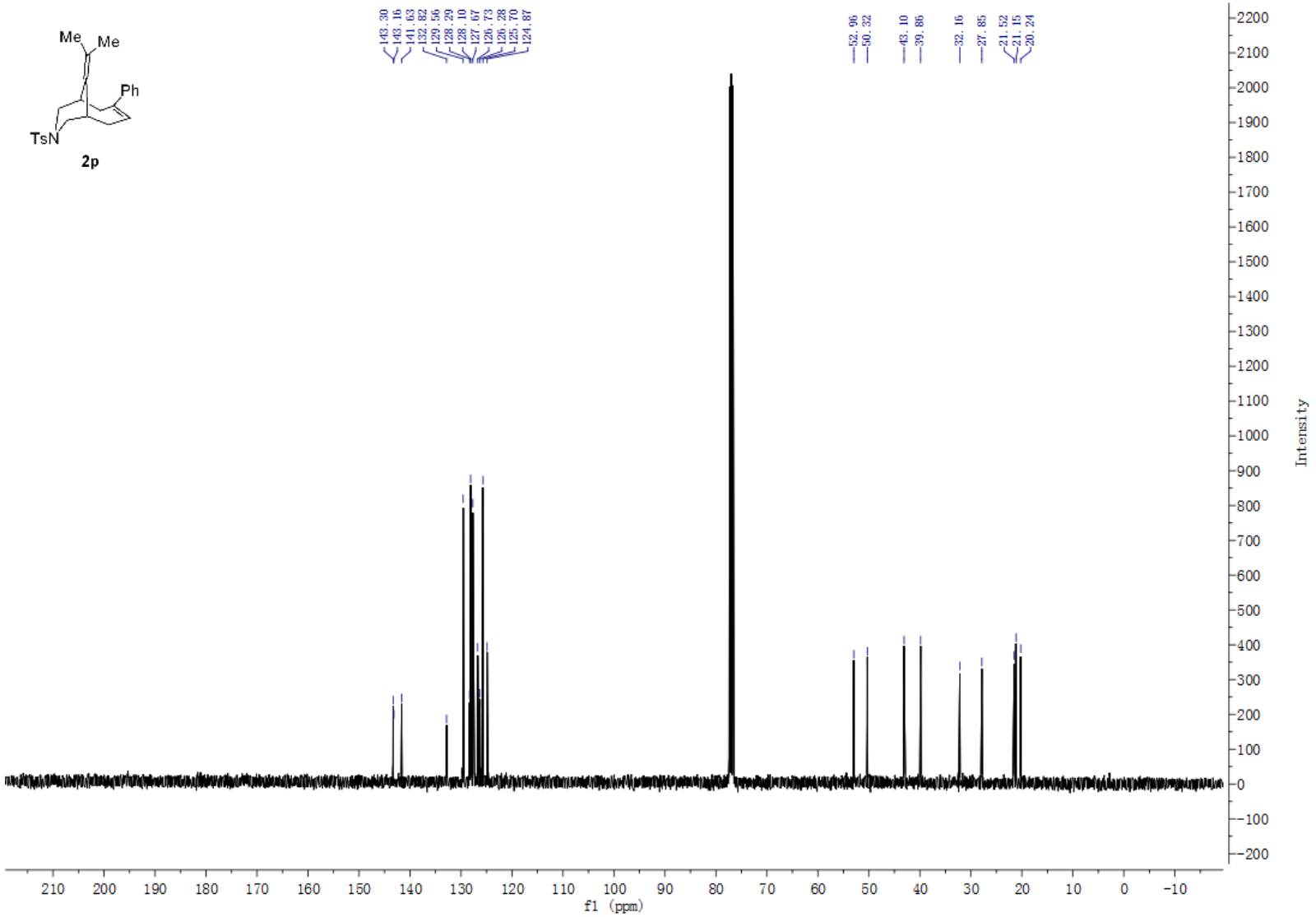

Me
Me
PhSO2N
2l
38000
36000
34000
32000
30000
28000
26000
24000
22000
20000
18000
16000
14000
12000
10000
8000
6000
4000
2000
0
-2000
Intensity
1.91
1.12
1.97
2.00
2.00
1.97
3.92
2.08
5.98
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

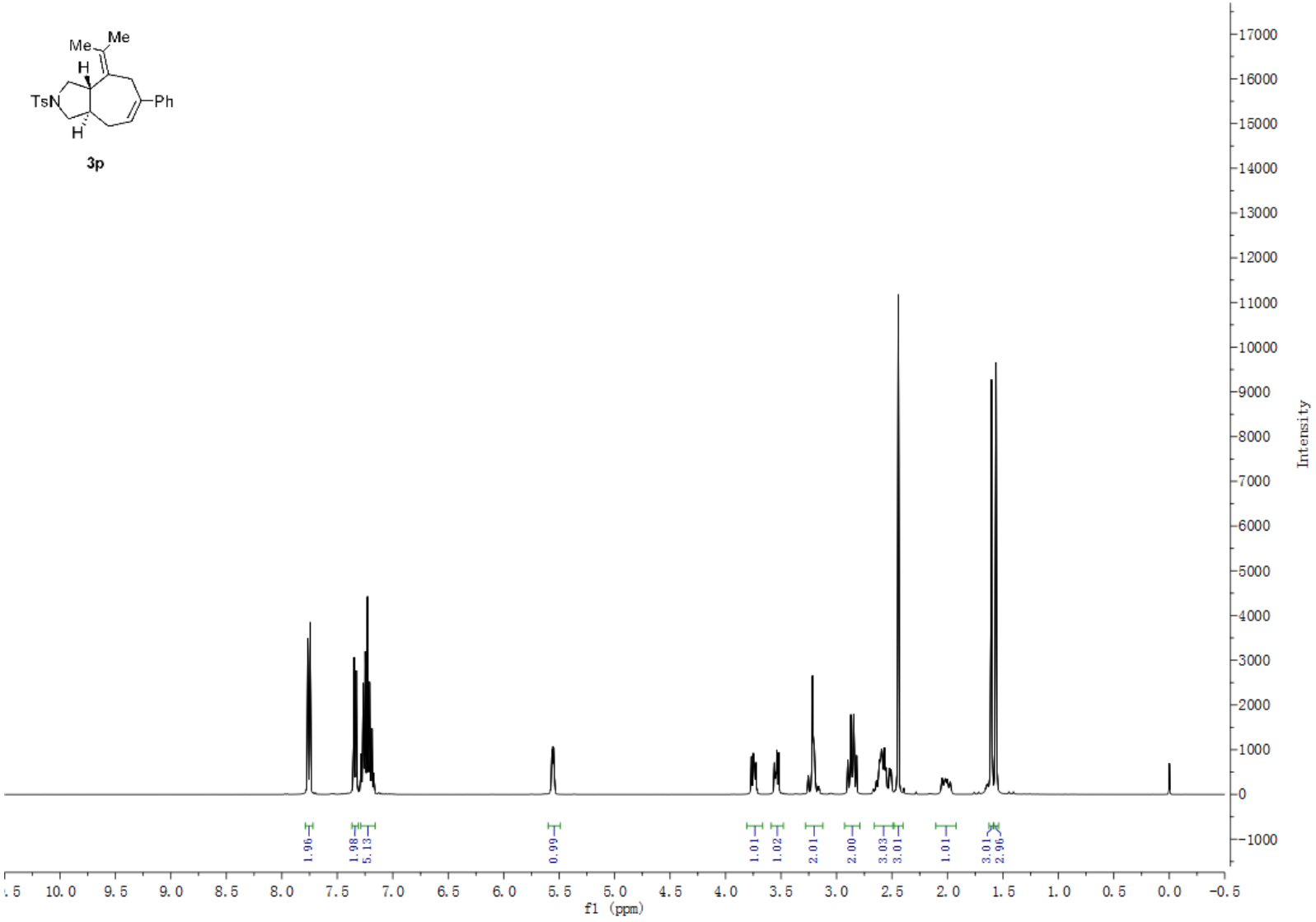

Me
Me
PhSO2N
2l
136.18
132.33
130.96
128.77
127.58
127.36
125.04
52.45
34.99
34.22
19.64
Intensity
f1 (ppm)

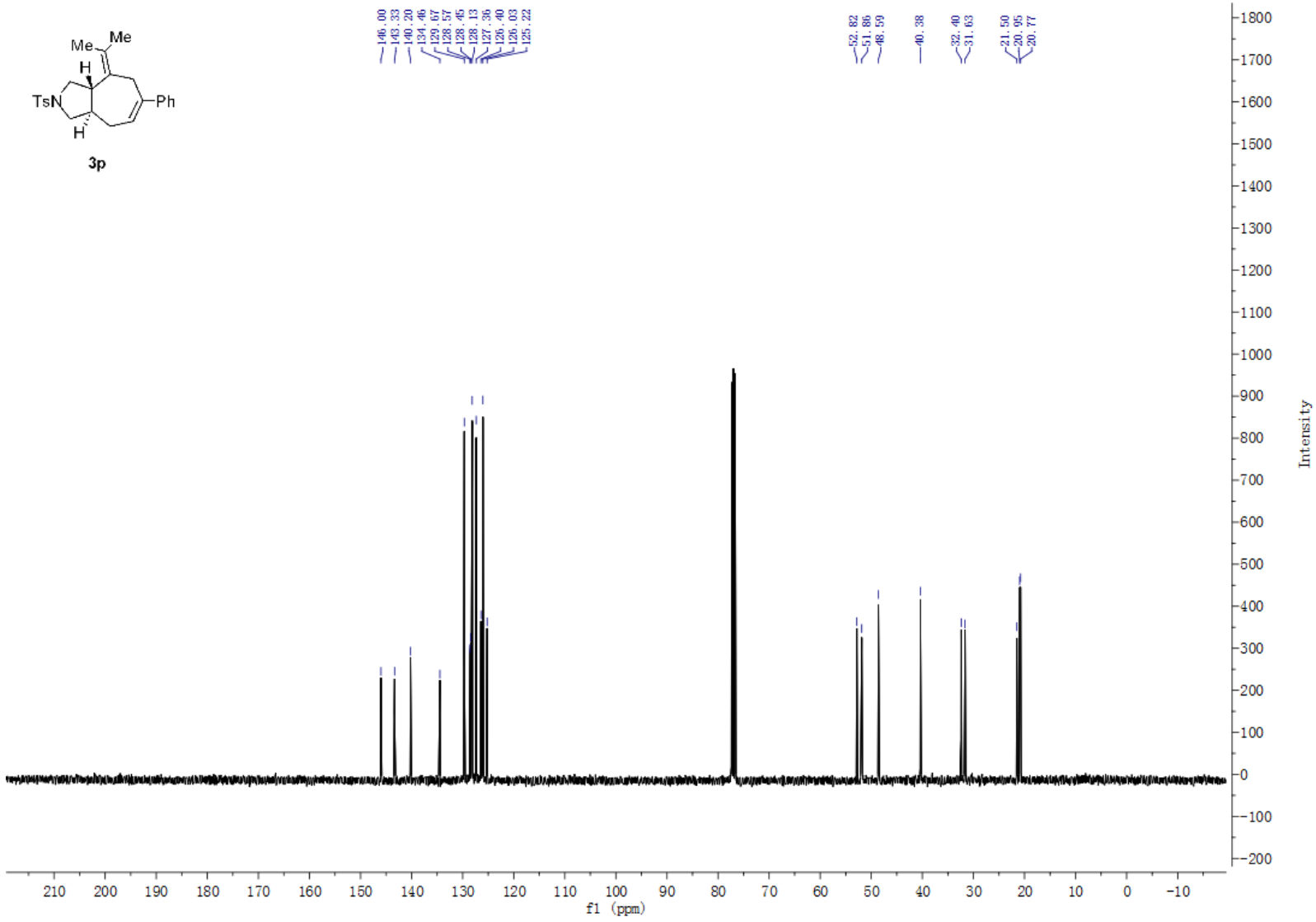

Me
Me
Me
S
N
O
O
2m
1.93
1.97
2.03
2.06
2.96
4.16
5.88
f1 (ppm)
Intensity

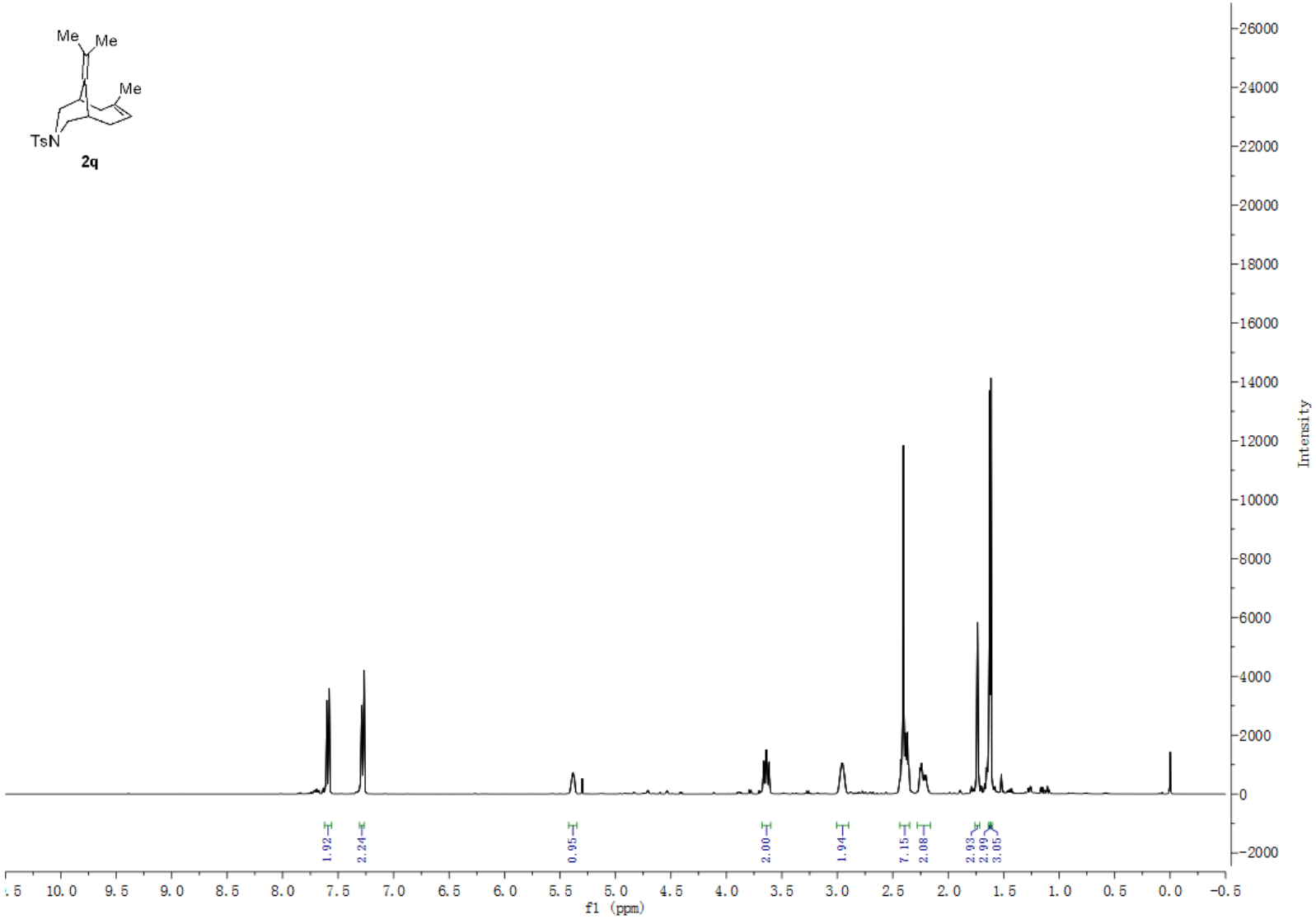

Me
Me
Me
S
N
O
O
2m
130.85
127.29
125.36
52.18
35.03
34.99
34.24
19.71
Intensity
f1 (ppm)

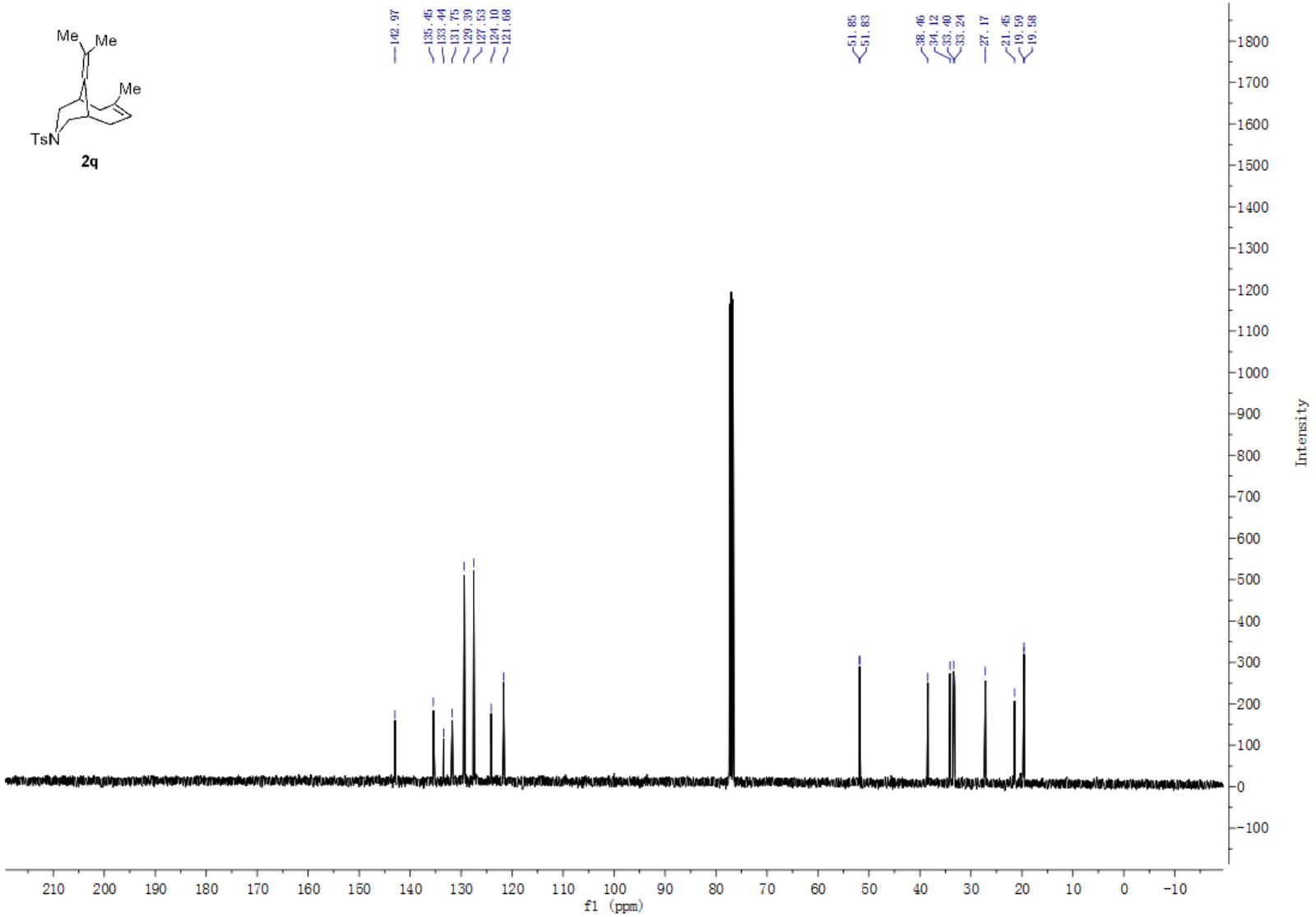

Me
Me
Ph
TsN
2p
Intensity
f1 (ppm)
2.00
5.24
1.96
1.00
3.08
1.04
1.08
1.03
1.07
0.96
2.93
1.94
2.94
2.98


Me
Me
Ph
TsN
2p
143.30
143.16
141.63
132.82
129.56
128.29
128.10
127.67
126.73
126.28
125.70
124.87
52.96
50.32
43.10
39.86
32.16
27.85
21.52
21.15
20.24
Intensity
f1 (ppm)


Me
Me
H
TsN
Ph
H
3p
Intensity
f1 (ppm)
1.96
1.98
5.13
0.99
1.01
1.02
2.01
2.00
3.03
3.01
1.01
3.01
2.96

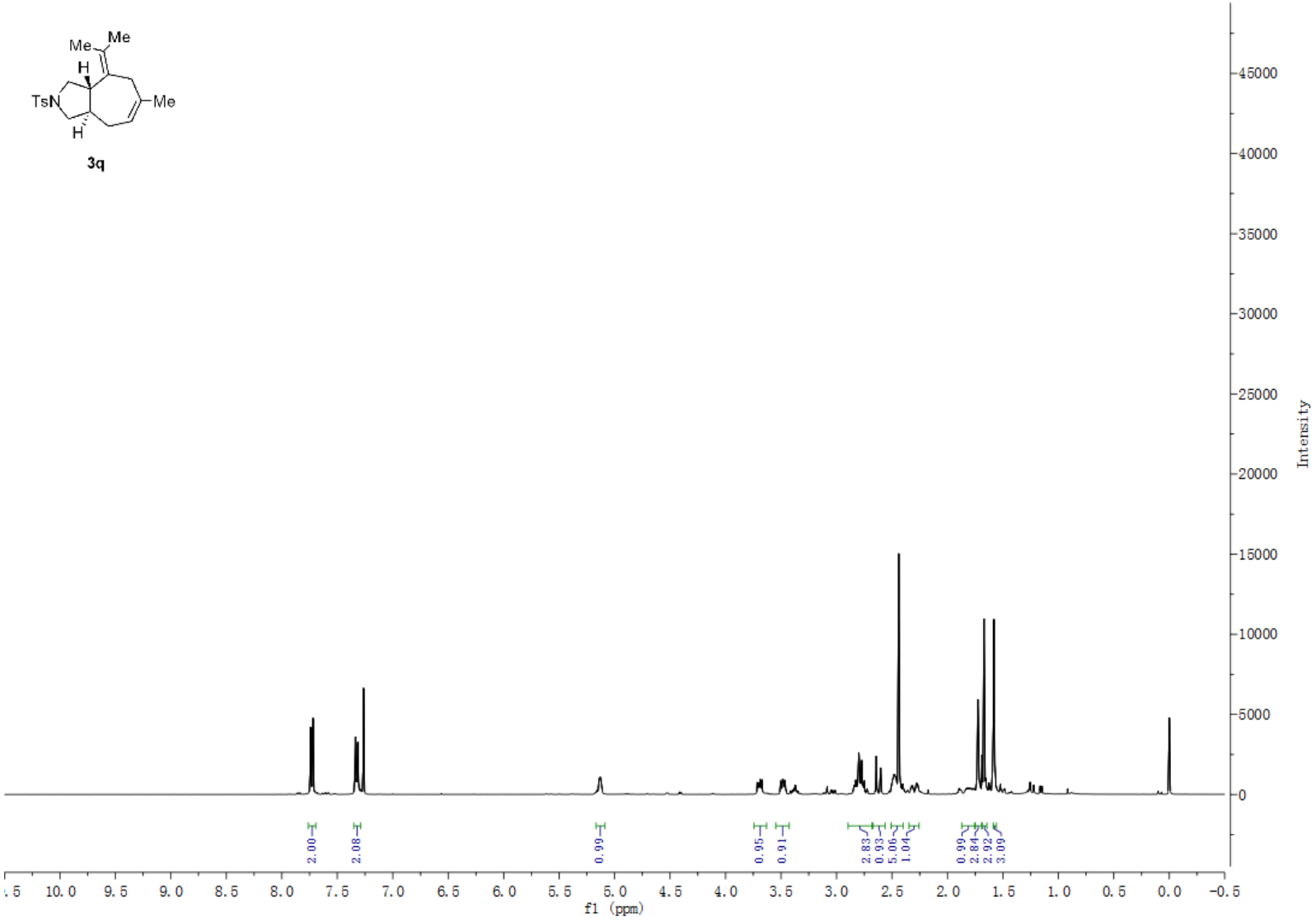

Me
Me
H
TsN
Ph
H
3p
146.00
143.33
140.20
134.46
129.67
128.57
128.45
128.13
127.36
126.40
126.03
125.22
52.82
51.86
48.59
40.38
32.40
31.63
21.50
20.95
20.77
Intensity
f1 (ppm)

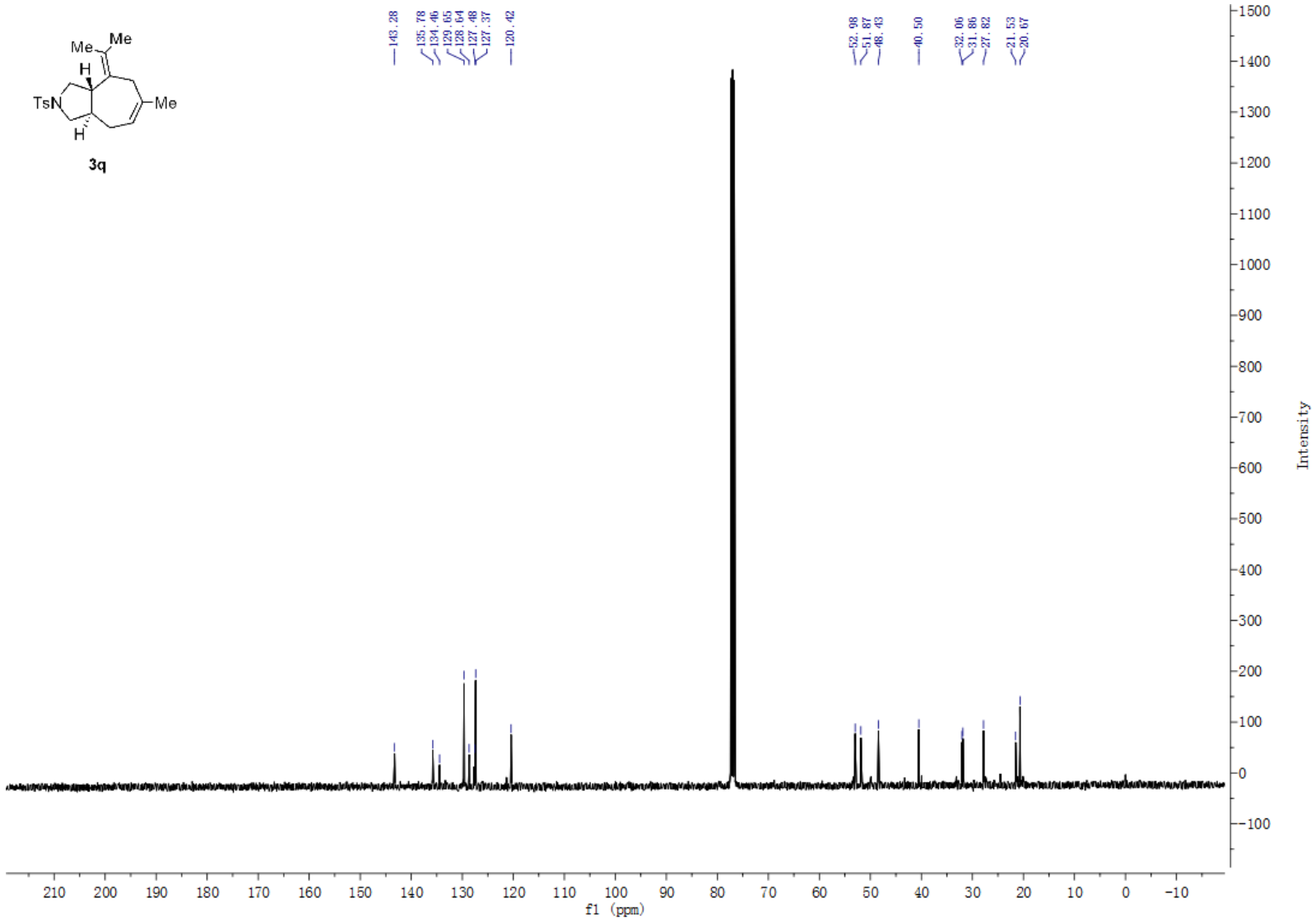

Me
Me
Me
TsN
2q
Intensity
f1 (ppm)
1.92
2.24
0.95
2.00
1.94
7.15
2.08
2.93
2.99
3.05


Me
Me
Me
TsN
2q
142.97
135.45
133.44
131.75
129.39
127.53
124.10
121.68
51.85
51.83
38.46
34.12
33.40
33.24
27.17
21.45
19.59
19.58
Intensity
f1 (ppm)

Me
Me
H
TsN
Me
H

3q


45000
40000
35000
30000
25000
20000
15000
10000
5000
0
Intensity
2.00
2.08
0.99
0.95
0.91
2.83
0.93
5.06
1.04
0.99
2.84
2.92
3.09
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)


Me
Me
H
TsN
Me
H
3q
143.28
135.78
134.46
129.65
128.64
127.48
127.37
120.42
52.98
51.87
48.43
40.50
32.06
31.86
27.82
21.53
20.67
Intensity
f1 (ppm)