Electronic Supplementary Material (ESI) for Chemical Science.

Diastereoselective ring opening of fully-substituted cyclopropanes *via* intramolecular Friedel–Crafts alkylation

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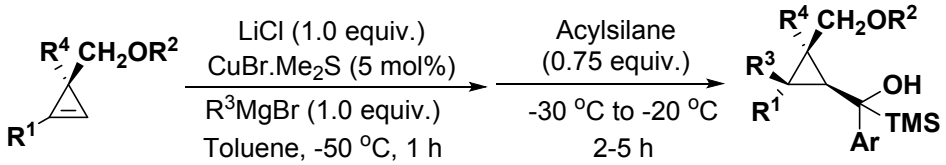
General information

All glassware was flame-dried under vacuum, and cooled under argon prior to use. Unless otherwise stated, all reactions were carried out under positive pressure of argon. Ether and THF were dried from Pure-Solv® Purification System (Innovative Technology©). The newly opened commercial grade dichloromethane was used directly. Toluene was distilled from sodium and benzophenone. Copper iodide, copper cyanide, copper bromide dimethyl sulfide, rhodium acetate dimer, methyllithium (1.6 M in diethyl ether), butyllithium (1.6 M in hexane), tert-butyllithium (1.7 M in pentane) were purchased from Aldrich. Methylmagnesium bromide (3.0 M in diethyl ether) was purchased from Acros. Ethylmagnesium bromide (2.0 M in diethyl ether), was prepared according to literatures and freshly titrated before using with butanol/1,10-phenanthroline. Anhydrous $FeCl_3$ (97% purity), purchased from Sigma Aldrich and used directly. Thin Layer Chromatography (TLC) was performed using Merck© silica gel 60 F254 plates. Column chromatography was performed using Bio-Labsilica gel 60A (0.040-0.063mm). ^{1}H-NMR and ^{13}C-NMR spectra were recorded on a Bruker©spectrometers AVIII400 or Bruker Avance 300 NMR using $CDCl_3$ (unless otherwise specified) as solvent. The GC chromatograms were recorded using Varian© 3800 apparatus with Varian© CP-Sil 8CB® column. HPLC chromatograms were recorded using Agilent© 1100 Series line with CHIRALPAK® AD-H or CHIRALCEL® OD. Acylsilanes and cyclopropenes were synthesized according to known procedures[1].

[1] (a) Y. Lou, T. P. Remarchuk, E. J. Corey, *J. Am. Chem. Soc.* 2005, ***127***, 14223. (b) D. Didier, P.-O. Delaye, M. Simaan, B. Island, G. Eppe, H. Eijsberg, A. Kleiner, P. Knochel, and I. Marek, *Chem. Eur. J.* 2014, ***20***, 1038.

General Procedure for Starting Materials[2]



All the starting materials were prepared according to the previously developed protocols in our group[3] with minor changes like increasing scale of the reaction from 1 mmol to 3 or 5 mmol.

Characterization of newly synthesized compounds:

((1R*,2R*,3S*)-2-butyl-3-(methoxymethyl)-2-methylcyclopropyl)-1-phenylethan-1-ol (3c)

R_f = 0.6 (ether/hexane = 1:10), colorless oil, 54% yield, 1:1 dr determined by ^{1}H-NMR. **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.52 (d, *J* = 7.8 Hz, 2H), 7.34 (t, *J* = 7.7 Hz, 2H), 7.22 (t, *J* = 7.3 Hz, 1H), 3.81 (dd, *J* = 11.0, 8.2 Hz, 1H), 3.64 (dd, *J* = 11.0, 8.6 Hz, 1H), 3.56 (s, 1H), 3.20 (s, 3H), 1.60 (s, 3H), 1.38 (s, 3H), 1.34 – 1.22 (m, 6H), 1.13 (d, *J* = 9.6 Hz, 1H), 1.04 – 0.98 (m, 1H), 0.90 (t, *J* = 7.1 Hz, 3H). **^{13}C NMR (400 MHz, $CDCl_3$)** δ 150.99, 128.04, 126.33, 124.57, 73.76, 69.43, 57.59, 44.35, 38.68, 30.49, 28.90, 26.32, 24.78, 23.00, 14.20, 12.95. **HRMS** (APCI) calcd. for $C_{18}H_{31}O2$ [M+3H]: 279.2319 found: 279.2351.

((1R*,2R*,3S*)-2-butyl-3-(methoxymethyl)-2-methylcyclopropyl)diphenylmethanol (3d)

R_f = 0.7 (ether/hexane = 1:10), colorless oil, 34% yield, 98:02 dr determined by ^{1}H-NMR. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.38 (dd, *J* = 15.0, 7.8 Hz, 4H), 7.27 – 7.05 (m, 6H), 3.97 (s, 1H), 3.80 (dd, *J* = 10.3, 8.4 Hz, 1H), 3.63 (t, *J* = 9.9 Hz, 1H), 3.21 (s, 3H), 1.59 (d, *J* = 9.3 Hz, 1H), 1.39 (d, *J* = 9.3 Hz, 1H), 1.23 – 0.93 (m, 6H), 0.86 (s, 3H), 0.75 (t, *J* = 6.6 Hz, 3H). **^{13}C NMR (400 MHz, $CDCl_3$)** δ 150.70, 147.79, 128.03, 127.61, 126.61, 126.31, 126.28, 70.08, 57.91, 43.78, 38.49, 28.45, 26.08, 24.34, 22.85, 14.16, 12.60, 0.92. **HRMS** (APCI) calcd. for $C_{23}H_{29}O$ [M-H2O+H]$^+$: 321.2213found: 321.2221.

((1R*,2R*,3S*)-2-butyl-3-(methoxymethyl)-2-methylcyclopropyl)(dimethyl(phenyl)silyl)(phenyl)methanol (3l)

R_f = 0.8 (ether/hexane = 1:10), colorless oil, 59% yield, 98:02 dr determined by ^{1}H-NMR. **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.28 – 7.15 (m, 5H), 7.09 (dd, *J* = 12.7, 5.0 Hz, 2H), 7.04 – 6.96 (m, 3H), 3.59 (dd, *J* = 10.3, 7.4 Hz, 1H), 3.46 (s, 1H), 3.33 (t, *J* = 10.2 Hz, 1H), 3.14 (s, 3H), 1.56 – 1.46 (m, 1H),

[2] (a) F. G. Zhang, G. Eppe, I. Marek, *Angew. Chem., Int. Ed*., 2016, ***55***, 714. (b) F.-G. Zhang, I. Marek, *J. Am. Chem. Soc.,* 2017, ***139***, 8364.

1.33 (d, *J* = 9.4 Hz, 1H), 1.19 – 1.01 (m, 5H), 0.75 (dd, *J* = 9.5, 4.5 Hz, 4H), 0.45 (s, 3H), 0.23 (s, 3H), 0.16 (s, 3H). **^{13}C NMR (400 MHz, $CDCl_3$)** δ 146.92, 136.25, 135.07, 129.20, 127.39, 126.99, 125.24, 124.56, 71.32, 70.51, 57.93, 43.58, 34.61, 28.69, 26.74, 24.48, 22.90, 14.29, 13.76, -5.64, -5.78. **HRMS** (APCI) calcd. for $C_{25}H_{36}OSi$ [M+H]: 380.2535. found: 380.2531.

((1R*,2R*,3S*)-2-butyl-3-(hydroxymethyl)-2-methylcyclopropyl)(4 fluorophenyl)(trimethylsilyl)methanol (3n)

R_f = 0.5 (ether/hexane = 3:7), colorless oil, 42% yield, 98:02 dr determined by ^{1}H-NMR. **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.30 – 7.22 (m, 2H), 7.05 – 6.93 (m, 2H), 4.19 (ddd, *J* = 11.1, 7.3, 3.7 Hz, 1H), 3.75 (td, *J* = 11.0, 5.9 Hz, 1H), 3.30 (s, 1H), 1.88 (dd, *J* = 5.6, 4.1 Hz, 1H), 1.70 (ddd, *J* = 13.4, 10.6, 4.3 Hz, 1H), 1.34 – 1.18 (m, 6H), 0.89 (ddd, *J* = 11.6, 9.1, 6.8 Hz, 3H), 0.60 (s, 3H), 0.04 – -0.03 (m, 9H). **^{13}C NMR (101 MHz, $CDCl_3$)** δ 160.55 (d, *J* = 285 Hz), 143.12 (d, *J* = 2.9 Hz), 126.17 (d, *J* = 7.6 Hz), 113.98 (d, *J* = 21.0 Hz), 71.25 (s), 60.74 (s), 43.63 (s), 34.35 (s), 29.26 (s), 28.72 (s), 24.57 (s), 22.86 (s), 14.19 (s), 13.61 (s), -4.10 (s). **HRMS** (APCI) calcd. for $C_{26}H_{37}FOSi$ [M+H]: 412.2598. found: 412.2601.

((1S*,2S*,3S*)-2-butyl-3-(methoxymethyl)-2-methyl-3-phenylcyclopropyl)(4-fluorophenyl)(trimethylsilyl)methanol (3r)

R_f = 0.7 (ether/hexane = 1:9), white solid, 72% yield, 98:02 dr determined by ^{1}H-NMR. **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.30 – 7.18 (m, 6H), 7.13 (dd, *J* = 9.7, 4.3 Hz, 1H), 6.88 (t, *J* = 8.9 Hz, 2H), 4.04 (s, 1H), 3.96 (d, *J* = 10.1 Hz, 1H), 3.84 (d, *J* = 10.1 Hz, 1H), 3.13 (s, 3H), 1.86 (s, 1H), 1.05 – 0.81 (m, 6H), 0.69 (s, 3H), 0.57 (t, *J* = 7.2 Hz, 3H), -0.00 (s, 9H). **^{13}C NMR (101 MHz, $CDCl_3$)** δ 159.94 (d, *J* = 183.2 Hz), 144.87, 143.05, 129.81 (d, *J* = 51.0 Hz), 127.91 (d, *J* = 25.3 Hz), 126.26, 126.16 (d, *J* = 5.1 Hz), 113.88 (d, *J* = 20.9 Hz), 70.62, 58.45, 40.77, 39.10, 36.90, 30.69, 28.04, 23.09, 14.79, 13.84, -3.44. **HRMS** (APCI) calcd. for $C_{26}H_{36}FO_2Si$ [M+H]: 427.2463, found: 427.2476.

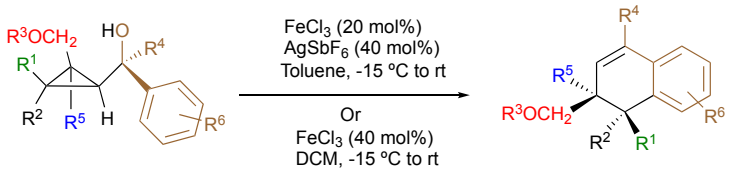
((1S*,2S*,3S*)-2-butyl-3-(hydroxymethyl)-2-methyl-3-phenylcyclopropyl)(m-tolyl)(trimethylsilyl)methanol (3s)

R_f = 0.5 (ether/hexane = 2:8), white solid, 42% yield, 98:02 dr determined by ^{1}H-NMR**. ^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.28 (d, *J* = 7.1 Hz, 2H), 7.22 (t, *J* = 7.6 Hz, 2H), 7.11 (dd, *J* = 8.7, 5.7 Hz, 1H), 7.07 – 7.03 (m, 2H), 6.83 (d, *J* = 5.2 Hz, 1H), 4.12 (d, *J* = 5.8 Hz, 1H), 3.66 (s, 1H), 2.23 (s, 3H), 1.90 (t, *J* = 5.9 Hz, 1H), 1.82 (s, 1H), 0.97-0.78 (m, 6H), 0.66 (s, 3H), 0.56 (t, *J* = 7.2 Hz, 3H), -0.00 (s, 9H). **^{13}C NMR (101 MHz, $CDCl_3$)** δ 146.73, 143.45, 135.99, 129.55, 127.98, 126.69, 126.12, 125.43, 124.89, 121.73, 70.70, 65.91, 42.40, 39.05, 36.33, 30.55, 27.84, 22.79, 21.38, 14.22, 13.54, -3.60. **HRMS** (APCI) calcd. for $C_{26}H_{37}O_2Si$ [M-H]: 409.2641, found: 409.2657.

((1S*,2S*,3S*)-2-butyl-3-(methoxymethyl)-3-(4-methoxyphenyl)-2-methylcyclopropyl)(4-fluorophenyl)(trimethylsilyl)methanol (3t)

R_f = 0.7 (ether/hexane = 2:8), crystalline solid, 65% yield, 98:02 dr determined by ^{1}H-NMR. **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.20 (t, *J* = 8.6 Hz, 4H), 6.89 (t, *J* = 8.5 Hz, 2H), 6.78 (d, *J* = 8.4 Hz, 2H), 4.03 (s, 1H), 3.93 (d, *J* = 10.0 Hz, 1H), 3.80 (d, *J* = 10.1 Hz, 1H), 3.73 (s, 3H), 3.15 (s, 3H), 1.81 (s, 1H), 1.15 – 0.79 (m, 6H), 0.68 (s, 3H), 0.60 (t, *J* = 7.1 Hz, 3H), -0.00 (s, 9H). **^{13}C NMR (101 MHz, $CDCl_3$)** δ 160.57(d, *J* = 245 Hz), 157.80, 143.08 (d, *J* = 3 Hz), 136.90, 130.42, 126.22(d, *J* = 6 Hz), 113.86(d, *J* = 21 Hz), 113.44, 70.64, 58.45, 55.25, 39.98, 39.08, 37.04, 30.64, 30.36, 29.00, 28.15, 23.14, 14.79, 13.91, -3.44. **HRMS** (APCI) calcd. for $C_{27}H_{38}FO_3Si$ [M-H]: 457.2569, found: 457.2567.

General procedure for diastereoselective intramolecular Friedel–Crafts alkylation



***Procedure* A:** A 15 mL dry Schlenk tube containing anhydrous $FeCl_3$ (20 mol%), $AgSbF_6$ (40 mol%) in 0.1 M Toluene and a septum was cooled down to –15 °C (bath temperature) using ice and rock salt. The cyclopropane derivative (0.3 mmol) was added at -15 °C and stirred for 0.5 to 3 h. After completion of the reaction (monitored by TLC), the reaction mixture was passed through a small silica pad and washed with diethyl ether (20 ml X 2) to remove all metal salts. Purification over silica gel column chromatography (hexane/diethyl ether or CH_2Cl_2/hexane) afforded the desired compound.

***Procedure* B:** A 15 mL dry Schlenk tube containing anhydrous $FeCl_3$ (40 mol%) in 0.1 M DCM and a septum was cooled down to –15 °C (bath temperature) using ice and rock salt. The cyclopropane derivative (0.3 mmol) was added at -15 °C and stirred for 0.5 to 3 h. After completion of the reaction (monitored by TLC), the reaction mixture was passed through a small silica pad and washed with diethyl ether (20 ml x 2) to remove all metal salts. Purification over silica gel column chromatography (hexane/diethyl ether or hexane/CH_2Cl_2) afforded the desired compound.

Optimization Studies:

S. No	Catalyst (mol%)	Additive (mol%)	Solvent	Temp/Time	NMR yields **4** (CP)	**6** (EP)
1	$FeCl_3$(20)	-	Toluene	rt/12h	58%	10%
2	**$FeCl_3$(20)**	**$AgSbF_6$(40)**	**Toluene**	**-15/3h**	**76%**	**8%**
Temperature Controls						
3	$FeCl_3$(20)	-	Toluene	0 to rt/3h	58%	10%
4	$FeCl_3$(20)	-	Toluene	-15 to rt/3h	66%	12%
5	$FeCl_3$(40)	-	Toluene	-15 to 0/3h	74%	6%
6	$FeCl_3$(40)	-	Toluene	-30 to 0/2.5h	72%	8%
7	**$FeCl_3$(40)**	**-**	**Toluene**	**-40 to 0/3h**	**76%**	**8%**
8	$FeCl_3$(50)	-	Toluene	-40 to 0/30min	69%	8%
9	$FeCl_3$(100)	-	Toluene	0/30min	58%	6%
10	$FeCl_3$(20)	-	Toluene	-40 to 0/3h	62%	13%
11	$FeCl_3$(40)	-	Toluene	rt/30min	58%	11%
Catalyst Screening						
	-	$AgSbF_6$(20)	Toluene	-20 to rt/12h	48% +SM	nd
	-	$AgSbF_6$(40)	Toluene	-20 to rt/12h	57% +SM	nd
	$AgNO_3$(20)	-	Toluene	0 to rt/12h	nr	nr
	$FeCl_2$(40)	-	Toluene	0 to rt/12h	nr	nr
	$Fe(acac)_3$(40)	-	Toluene	0 to rt/12h	nr	nr
	$Fe(ClO_4)_3$(40)	-	Toluene	0 to rt/12h	nr	nr
	$Cu(Otf)_2$(20)	-	Toluene	rt/12h	22% +SM	nd
	$ZrCl_4$(20)	-	Toluene	rt/12h	Multiple	nd
	$BF_3.OEt_2$ (20)		Toluene	rt/4h	48%	00
	$Bi(Otf)_3$(20)	-	DCM	-15 to rt/30min	40%	18%
	TsOH(100)	-	DCM	rt/30min	32%	10%
Solvent Screening						
	$FeCl_3$(40)	**-**	**DCM**	**-15 to rt/3h**	**81%**	**7%**
	$FeCl_3$(40)	-	TFE	-15 to rt/12h	35%	12%

*All the reactions were carried out with 0.3 mmol of **1a**

Characterization data of new Compounds

((3*R,4*S**)-4-butyl-3-(methoxymethyl)-4-methyl-3,4-dihydronaphthalen-1-yl)trimethylsilane (4a)**

Obtained as a colourless oil in 76% yield with method A and 74% yield with method B. R_f 0.7 (5:95 ether/hexane), *dr* 98:02. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.21 (t, *J* = 4.5 Hz, 1H), 7.15 (t, *J* = 4.4 Hz, 1H), 7.14 – 7.09 (m, 2H), 6.31 (d, *J* = 5.1 Hz, 1H), 3.45 (dd, *J* = 9.0, 5.2 Hz, 1H), 3.23 (s, 3H), 3.14 (t, *J* = 8.4 Hz, 1H), 2.51 – 2.42 (m, 1H), 1.58 – 1.47 (m, 3H), 1.22 – 1.17 (m, 2H), 1.15 (s, 3H), 1.01 (dt, *J* = 11.9, 7.3 Hz, 1H), 0.78 (t, *J* = 7.1 Hz, 3H), 0.21 (s, 9H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 142.83, 141.09, 137.01, 135.69, 127.13, 126.82, 125.83, 125.14, 72.84, 59.03, 43.03, 38.91, 38.88, 26.88, 23.45, 22.29, 14.14, -0.02. **^{29}Si NMR** (80 MHz, $CDCl_3$) δ -5.31. **HRMS** (APCI) calcd. for $C_{20}H_{33}OSi$ [M+H]: 317.2295 found: 317.2265.

(1S*, 2R*)-1-butyl-2-(methoxymethyl)-1,4-dimethyl-1,2-dihydronaphthalene (4c)

Obtained as a colourless oil in 32% yield with method B. R_f 0.8 (1:9 ether/hexane), *dr* 98:02. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.19 – 7.14 (m, 1H), 7.13 – 7.07 (m, 3H), 5.76 (dd, *J* = 5.4, 1.0 Hz, 1H), 3.39 (dd, *J* = 8.9, 5.3 Hz, 1H), 3.20 (s, 3H), 3.11 (t, *J* = 8.8 Hz, 1H), 2.48 – 2.37 (m, 1H), 1.99 (s, 3H), 1.49 (t, *J* = 5.6 Hz, 2H), 1.20 – 1.05 (m, 6H), 0.98 – 0.88 (m, 1H), 0.75 (t, *J* = 7.2 Hz, 3H).**^{13}C NMR** (101 MHz, $CDCl_3$) δ 143.04, 134.52, 131.02, 127.09, 126.94, 125.92, 124.90, 123.32, 73.33, 58.87, 42.46, 39.71, 39.25, 26.95, 23.35, 22.11, 19.47, 14.12. **HRMS** (APCl) calcd. for $C_{17}H_{23}$ [M+H]: 227.1794 found: 227.1801.

(1S* ,2R*)-1-butyl-2-(methoxymethyl)-1-methyl-4-phenyl-1,2-dihydronaphthalene (4d)

The title compound was obtained along with inseparable eliminated product. Obtained as a colourless oil in 56% yield with method B. R_f 0.6 (5:95 ether/hexane), *dr* 98:02. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.31 – 7.25 (m, 4H), 7.17 – 7.10 (m, 3H), 7.02 (td, *J* = 7.3, 1.7 Hz, 1H), 6.95 (d, *J* = 7.4 Hz, 1H), 5.97 (d, *J* = 5.5 Hz, 1H), 3.49 (dd, *J* = 8.9, 5.2 Hz, 1H), 3.24 (s, 3H), 3.22 – 3.16 (m, 1H), 2.61 (dt, *J* = 8.9, 5.4 Hz, 1H), 1.63 (dd, *J* = 10.7, 4.8 Hz, 2H), 1.23 (s, 3H), 1.21 – 1.11 (m, 4H), 0.77 (t, *J* = 7.1 Hz, 3H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 143.42, 140.93, 138.66, 133.85, 129.97, 129.39, 128.84, 128.20, 128.08, 127.44, 127.12, 126.21, 125.75, 125.00, 72.84, 58.99, 42.72, 39.37, 39.25, 26.96, 23.39, 22.19, 14.11. **HRMS** (ESI) calcd. for $C_{23}H_{28}NaO$ [M+Na]: 343.2038 found: 343.2031.

((3*R,4*R**)-4-butyl-3-(methoxymethyl)-4-methyl-3,4-dihydronaphthalen-1-yl)trimethylsilane (4e)**

Obtained as a colourless oil in 68% yield with method A. R_f 0.6 (5:95 ether/hexane), *dr* 98:02. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.25 – 7.21 (m, 2H), 7.12 (dd, *J* = 5.7, 3.4 Hz, 2H), 6.25 (d, *J* = 3.4 Hz, 1H), 3.61

(dd, *J* = 8.9, 4.4 Hz, 1H), 3.35 – 3.29 (m, 4H), 2.47 (dt, *J* = 9.6, 3.9 Hz, 1H), 1.70 – 1.60 (m, 1H), 1.29 (s, 3H), 1.10 (dt, *J* = 14.2, 7.9 Hz, 4H), 0.89 – 0.81 (m, 1H), 0.74 (t, *J* = 7.1 Hz, 3H), 0.21 (s, 9H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 142.83, 141.45, 137.33, 135.99, 126.96, 126.48, 125.90, 125.30, 72.79, 59.11, 44.69, 38.48, 34.40, 26.93, 24.31, 23.63, 14.16, -0.08. **^{29}Si NMR** (80 MHz, $CDCl_3$) δ -5.48. **HRMS** (ESI) calcd. for $C_{20}H_{32}NaOSi$ [M+Na]: 339.2120 found: 339.2163.

((3*R,4*S**)-4-ethyl-3-(methoxymethyl)-4-methyl-3,4-dihydronaphthalen-1-yl)trimethylsilane (4f)**

Obtained as a colourless oil in 68% yield with method A, R_f 0.7 (5:95 ether/hexane), *dr* 98:02. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.19 (dd, *J* = 6.0, 3.1 Hz, 1H), 7.13 (dt, *J* = 4.7, 2.9 Hz, 1H), 7.11 – 7.05 (m, 2H), 6.28 (d, *J* = 5.2 Hz, 1H), 3.42 (dd, *J* = 9.0, 5.2 Hz, 1H), 3.20 (s, 3H), 3.11 (t, *J* = 8.8 Hz, 1H), 2.45 (dt, *J* = 8.6, 5.2 Hz, 1H), 1.56 (dt, *J* = 7.3, 4.6 Hz, 2H), 1.12 (s, 3H), 0.68 (t, *J* = 7.5 Hz, 3H), 0.18 (s, 9H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 142.52, 141.04, 136.99, 135.67, 127.16, 126.80, 125.84, 125.30, 72.91, 59.01, 42.67, 39.07, 31.59, 21.73, 9.19, -0.02. **^{29}Si NMR** (80 MHz, $CDCl_3$) δ -5.33. **HRMS** (ESI) calcd. for $C_{18}H_{28}NaOSi$ [M+Na]: 311.1802 found: 311.1843.

((3*R,4*S**)-3-(methoxymethyl)-4-methyl-4-phenethyl-3,4-dihydronaphthalen-1-yl)trimethylsilane (4g)**

Obtained as a colourless oil in 69% yield with method A, R_f 0.6 (5:95 ether/hexane), *dr* 98:02. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.27 – 7.22 (m, 2H), 7.20 – 7.13 (m, 4H), 7.09 (d, *J* = 7.3 Hz, 1H), 7.02 (d, *J* = 7.1 Hz, 2H), 6.31 (d, *J* = 5.2 Hz, 1H), 3.49 (dd, *J* = 9.1, 5.4 Hz, 1H), 3.24 (s, 3H), 3.18 (d, *J* = 5.5 Hz, 1H), 2.57 – 2.47 (m, 2H), 2.30 (td, *J* = 12.8, 4.9 Hz, 1H), 1.86 (dtd, *J* = 18.7, 13.8, 4.9 Hz, 2H), 1.25 (s, 3H), 0.22 (s, 9H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 143.15, 142.01, 140.86, 137.30, 135.69, 128.45, 128.35, 127.29, 126.98, 126.10, 125.72, 125.31, 72.80, 59.04, 43.44, 41.43, 39.27, 31.38, 22.17, -0.03. **^{29}Si NMR** (80 MHz, $CDCl_3$) δ -5.19. **HRMS** (ESI) calcd. for $C_{24}H_{32}NaOSi$ [M+Na]: 387.2115 found: 387.2114.

((3*R,4*S**)-4-(2-(benzyloxy)ethyl)-3-(methoxymethyl)-4-methyl-3,4-dihydronaphthalen-1-yl)trimethylsilane (4h)**

Obtained as a colourless oil in 61% yield with method A and 62% with method B. R_f 0.6 (5:95 ether/hexane), *dr* 98:02. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.33 (dd, *J* = 7.7, 6.5 Hz, 2H), 7.30 – 7.26 (m, 4H), 7.25 – 7.22 (m, 1H), 7.21 – 7.14 (m, 2H), 6.36 (d, *J* = 5.2 Hz, 1H), 4.45 – 4.35 (m, 2H), 3.50 (ddd, *J* = 19.9, 8.8, 5.8 Hz, 2H), 3.36 (td, J = 8.8, 6.1 Hz, 1H), 3.26 (s, 3H), 3.20 (t, *J* = 8.7 Hz, 1H), 2.53 – 2.45 (m, 1H), 2.09 – 1.92 (m, 2H), 1.29 (s, 3H), 0.27 (s, 9H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 141.76, 140.92, 138.65, 137.10, 135.58, 128.43, 127.65, 127.56, 127.22, 126.99, 126.13, 125.09, 72.92, 72.60, 67.61, 58.97, 43.78, 38.45, 38.15, 22.62, -0.05. **^{29}Si NMR** (80 MHz, $CDCl_3$) δ -5.22. **HRMS** (ESI) calcd. for $C_{25}H_{34}NaO_2Si$ [M+Na]: 417.2220 found: 417.2220.

((3*R,4*S**)-4-butyl-3-(methoxymethyl)-4,6-dimethyl-3,4-dihydronaphthalen-1-yl)trimethylsilane (4i)**

Obtained as a colourless oil in 74% yield with method A and 78% with method B. R_f 0.7 (5:95 ether/hexane), *dr* 98:02. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.12 (d, *J* = 7.7 Hz, 1H), 6.97 (s, 1H), 6.92 (d, *J* = 8.7 Hz, 1H), 6.26 (d, J = 5.2 Hz, 1H), 3.45 (dd, *J* = 9.0, 5.2 Hz, 1H), 3.23 (s, 3H), 3.13 (t, *J* = 8.8 Hz, 1H), 2.48 – 2.42 (m, 1H), 2.29 (s, 3H), 1.57 – 1.44 (m, 2H), 1.22 – 1.12 (m, 6H), 1.08 – 0.99 (m, 1H), 0.79 (t, *J* = 7.1 Hz, 3H), 0.20 (s, 9H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 142.90, 140.07, 136.77, 136.33, 132.98, 127.04, 126.35, 126.02, 72.96, 59.00, 43.10, 39.12, 38.88, 26.90, 23.44, 22.28, 21.70, 14.14, -0.03. **^{29}Si NMR** (80 MHz, $CDCl_3$) δ -5.44. **HRMS** (APCl) calcd. for $C_{21}H_{35}OSi$ [M+H]: 331.2452 found: 331.2462.

((1*S,2*R**)-1-butyl-2-(methoxymethyl)-1-methyl-1,2-dihydrophenanthren-4-yl)trimethylsilane (4j)**

Obtained as a colourless oil in 68% yield with method A. R_f 0.7 (5:95 ether/hexane), *dr* 98:02. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.27 (dd, *J* = 6.7, 3.0 Hz, 1H), 7.74 – 7.67 (m, 1H), 7.57 (d, *J* = 8.4 Hz, 1H), 7.36 (d, *J* = 8.4 Hz, 1H), 7.33 – 7.25 (m, 2H), 6.47 (d, *J* = 5.8 Hz, 1H), 3.46 (dd, *J* = 8.8, 4.3 Hz, 1H), 3.17 (s, 3H), 3.09 (dd, *J* = 18.0, 8.9 Hz, 1H), 2.48 (ddd, *J* = 9.7, 5.7, 4.4 Hz, 1H), 1.89 – 1.69 (m, 2H), 1.62 (s, 3H), 1.51 (s, 3H), 1.16 (dt, *J* = 14.1, 5.8 Hz, 4H), 0.74 (t, *J* = 7.0 Hz, 3H), 0.18 (s, 9H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 141.36, 138.31, 138.14, 135.15, 133.83, 132.22, 129.01, 126.60, 126.26, 126.07, 124.54, 124.15, 74.11, 58.99, 45.92, 41.03, 38.89, 27.45, 25.32, 23.35, 13.97, 1.02, -0.00, -1.53. **^{29}Si NMR** (80 MHz, $CDCl_3$) δ -5.06. **HRMS** (APCl) calcd. for $C_{24}H_{35}OSi$ [M+H]: 367.2452 found: 367.2470.

((3*R,4*S**)-3-((benzyloxy)methyl)-4-butyl-4-methyl-3,4-dihydronaphthalen-1-yl)trimethylsilane (4k)**

Obtained as a colourless oil in 76% yield with method A. R_f 0.7 (5:95 ether/hexane), *dr* 97:03. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.29 – 7.24 (m, 2H), 7.24 – 7.19 (m, 4H), 7.16 – 7.12 (m, 1H), 7.10 (dd, *J* = 5.7, 3.5 Hz, 2H), 6.37 (d, *J* = 5.1 Hz, 1H), 4.43 (d, *J* = 12.2 Hz, 1H), 4.36 (d, *J* = 12.2 Hz, 1H), 3.57 (dd, *J* = 8.9, 5.2 Hz, 1H), 3.27 (t, *J* = 8.8 Hz, 1H), 2.54 (dt, *J* = 8.8, 5.1 Hz, 1H), 1.55 – 1.49 (m, 2H), 1.22 – 1.11 (m, 6H), 1.05 – 0.96 (m, 1H), 0.77 (t, *J* = 7.1 Hz, 3H), 0.22 (s, 9H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 142.88, 141.29, 138.80, 136.96, 135.65, 128.43, 127.52, 127.47, 127.14, 126.83, 125.80, 125.13, 73.17, 70.48, 43.21, 39.01, 38.92, 26.90, 23.44, 22.35, 14.14, -0.02. **^{29}Si NMR** (80 MHz, $CDCl_3$) δ -5.29. **HRMS** (APCl) calcd. for $C_{26}H_{37}OSi$ [M+H]: 393.2614found: 393.2608.

((3S*,4R*)-4-butyl-3-(methoxymethyl)-4-methyl-3,4-dihydronaphthalen-1-yl)dimethyl(phenyl)silane (4l)

Obtained as a colourless oil in 68% yield with method A. R_f 0.5 (1:9 ether/hexanes), *dr* 98:02. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.48 – 7.43 (m, 2H), 7.26 – 7.20 (m, 4H), 7.11 – 7.06 (m, 1H), 7.05 – 6.94 (m, 2H), 6.88 (td, *J* = 7.6, 1.2 Hz, 1H), 6.43 (d, *J* = 5.3 Hz, 1H), 3.45 (dd, *J* = 9.0, 5.2 Hz, 1H), 3.19 (s, 3H), 3.17 – 3.10 (m, 1H), 2.50 (dt, *J* = 8.6, 5.2 Hz, 1H), 1.57 – 1.50 (m, 2H), 1.20 – 1.10 (m, 6H), 0.97 (dd, *J* = 9.7, 5.4 Hz, 1H), 0.78 – 0.73 (m, 4H), 0.39 (d, *J* = 2.6 Hz, 6H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 145.27, 144.25, 141.05, 136.84, 136.46, 135.71, 130.61, 129.57, 129.41, 128.51, 127.44, 126.72, 74.52, 60.67, 45.23, 40.67, 40.52, 28.55, 25.10, 23.85, 15.80, 0.46, 0.00, **^{29}Si NMR** (80 MHz, $CDCl_3$) δ -8.79, **HRMS** (APCl) calcd. for $C_{25}H_{35}OSi$ [M+H]: 379.2452found: 379.2461.

((1*S,2*R**)-1-butyl-1-methyl-4-(trimethylsilyl)-1,2-dihydronaphthalen-2-yl)methanol (4m)**

Obtained as a colourless viscous oil in 49% yield with method A and 32% with method B. R_f 0.4 (15:85 ether/hexanes), *dr* 97:03. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.21 (dd, *J* = 6.2, 2.5 Hz, 1H), 7.16 – 7.07 (m, 3H), 6.31 (d, *J* = 5.6 Hz, 1H), 3.67 (dd, *J* = 10.6, 4.5 Hz, 1H), 3.54 – 3.45 (m, 1H), 2.34 (dt, *J* = 7.8, 5.1 Hz, 1H), 1.53 – 1.42 (m, 2H), 1.23 (s, 4H), 1.13 (ddd, *J* = 13.8, 9.1, 4.1 Hz, 3H), 1.00 – 0.91 (m, 1H), 0.76 (t, *J* = 7.2 Hz, 3H), 0.22 (s, 9H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 143.13, 139.60, 139.06, 135.29, 127.18, 127.17, 125.88, 125.20, 62.79, 45.93, 39.87, 38.56, 26.87, 23.37, 21.67, 14.12, -0.00. **^{29}Si NMR** (80 MHz, $CDCl_3$) δ -5.16. **HRMS** (APCl) calcd. for $C_{19}H_{29}Si$ [M+H]: 285.2039 found: 285.2052.

((1R*,2S*)-1-butyl-7-fluoro-1-methyl-4-(trimethylsilyl)-1,2-dihydronaphthalen-2-yl)methanol (4n)

Isolated as a colourless thick liquid in 42% yield with method A. R_f 0.3 (20% ether/hexanes), *dr* 98:02. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.17 (dd, *J* = 8.5, 6.0 Hz, 1H), 6.86 (dd, *J* = 10.6, 2.7 Hz, 1H), 6.78 (td, *J* = 8.3, 2.7 Hz, 1H), 6.28 (d, *J* = 5.7 Hz, 1H), 3.66 (dd, *J* = 10.7, 4.6 Hz, 1H), 3.49 (dd, *J* = 10.7, 7.8 Hz, 1H), 2.33 (dt, *J* = 7.7, 5.1 Hz, 1H), 1.51 – 1.37 (m, 2H), 1.22 (s, 3H), 1.18 – 1.10 (m, 3H), 1.01 – 0.90 (m, 1H), 0.77 (t, *J* = 7.2 Hz, 3H), 0.22 (s, 9H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 162.16 (d, *J* = 245.4 Hz), 146.31 (d, *J* = 6.5 Hz), 138.75 (d, *J* = 2.0 Hz), 138.23, 131.59 (d, *J* = 3.2 Hz), 128.44 (d, *J* = 8.0 Hz), 112.77 (d, *J* = 22.1 Hz), 112.25 (d, *J* = 20.9 Hz), 62.70, 45.71, 39.82, 38.97 (d, *J* = 1.3 Hz), 26.86, 23.41, 21.61, 14.17, -0.00. **HRMS** (APCl) calcd. for C19H30FOSi [M+H]: 321.1972found: 321.1982.

((1*S,2*R**)-1-butyl-1-methyl-4-(methyldiphenylsilyl)-1,2-dihydronaphthalen-2-yl)methanol (4o)**

Obtained as a colourless oil in 52% yield with method A. R_f 0.5 (15:85 ether/hexane), *dr* 97:03. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.48 (d, *J* = 7.3 Hz, 2H), 7.42 (d, *J* = 6.4 Hz, 2H), 7.34 – 7.23 (m, 6H), 7.12 (d, *J* = 7.5 Hz, 1H), 7.07 – 6.98 (m, 2H), 6.85 (t, *J* = 7.4 Hz, 1H), 6.24 (d, *J* = 5.8 Hz, 1H), 3.64 (dd, *J* = 10.5, 4.0 Hz, 1H), 3.57 – 3.45 (m, 1H), 2.32 (dd, *J* = 12.4, 5.4 Hz, 1H), 1.59 (dd, *J* = 16.2, 8.9 Hz, 1H), 1.49 (d, *J* = 13.0 Hz, 1H), 1.26 (s, 3H), 1.19 (s, 1H), 1.16 – 1.12 (m, 2H), 1.05 (s, 1H), 0.98 – 0.90 (m, 1H), 0.77 (t, *J* = 7.1 Hz, 3H), 0.69 (s, 3H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 145.07, 142.88, 136.77, 136.52, 135.45, 135.31, 135.22, 134.87, 129.47, 129.40, 128.33, 128.10, 128.03, 127.33, 125.92,

125.18, 62.86, 46.77, 40.03, 38.59, 26.92, 23.44, 21.66, 14.18, -2.38. **^{29}Si NMR** (80 MHz, $CDCl_3$) δ -10.98. **HRMS** (APCl) calcd. for $C_{29}H_{35}OSi$ [M+H]: 427.2457 found: 427.2451.

((3*R,4*R**)-4-butyl-3-(methoxymethyl)-3,4-dimethyl-3,4-dihydronaphthalen-1-yl)trimethylsilane (4p)**

Obtained as a colourless oil in 42% yield with method A. R_f 0.5 (5:95 ether/hexane), *dr* 99:01. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.22 – 7.19 (m, 1H), 7.18 – 7.15 (m, 1H), 7.15 – 7.10 (m, 2H), 5.89 (s, 1H), 3.17 (d, *J* = 8.9 Hz, 1H), 3.12 (s, 3H), 3.08 (d, *J* = 8.9 Hz, 1H), 1.83 – 1.72 (m, 1H), 1.24 (s, 3H), 1.20 (s, 3H), 1.12 (dd, *J* = 12.5, 3.5 Hz, 1H), 1.08 – 1.00 (m, 2H), 0.97 (t, *J* = 6.5 Hz, 1H), 0.70 (t, *J* = 7.0 Hz, 3H), 0.54 – 0.40 (m, 1H), 0.24 (s, 9H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 147.80, 141.86, 135.86, 135.64, 126.65, 126.47, 126.20, 125.65, 77.11, 59.47, 42.96, 42.22, 34.05, 27.30, 23.49, 18.33, 17.91, 14.10, -0.04. **^{29}Si NMR** (80 MHz, $CDCl_3$) δ -5.56. **HRMS** (ESI) calcd. for $C_{21}H_{34}NaOSi$ [M+Na]: 353.2271 found: 353.2206.

((3*S,4*R**)-4-butyl-3-(methoxymethyl)-4-methyl-3-phenyl-3,4-dihydronaphthalen-1-yl)trimethylsilane (4q)**

Obtained as a colourless oil in 60% yield with method A and 62% with method B. R_f 0.5 (5:95 ether/hexane), *dr* 98:02. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.28 (d, *J* = 7.4 Hz, 2H), 7.20 (t, *J* = 7.7 Hz, 2H), 7.14 – 7.07 (m, 2H), 7.06 – 6.97 (m, 3H), 6.43 (s, 1H), 3.99 (d, *J* = 9.2 Hz, 1H), 3.19 (d, *J* = 9.2 Hz, 1H), 2.94 (s, 3H), 1.76 – 1.63 (m, 1H), 0.99 (s, 3H), 0.72 (ddt, *J* = 14.6, 10.5, 7.4 Hz, 3H), 0.44 (t, *J* = 7.1 Hz, 4H), 0.25 – 0.18 (m, 1H), 0.17 – 0.08 (s, 9H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 147.61, 141.50, 140.58, 136.45, 135.01, 130.04, 127.39, 126.83, 126.60, 126.44, 126.39, 125.83, 74.57, 59.61, 52.97, 42.40, 34.16, 30.37, 26.29, 23.17, 17.39, 13.95. **^{29}Si NMR** (80 MHz, $CDCl_3$) δ -4.85. **HRMS** (APCl) calcd. for $C_{25}H_{33}Si$ [M+H]: 361.2346 found: 361.2360.

((3R*,4S*)-3-argio-4-butyl-6-fluoro-3-(methoxymethyl)-4-methyl-3,4-dihydronaphthalen-1-yl)trimethylsilane (4r)

Isolated as a colourless thick liquid in 63% yield with method A. R_f 0.5 (10% ether/hexanes), *dr* 98:02. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.41 – 7.36 (m, 2H), 7.31 (t, J = 7.6 Hz, 2H), 7.25 – 7.17 (m, 2H), 6.87 – 6.79 (m, 2H), 6.50 (s, 1H), 4.09 (d, J = 9.2 Hz, 1H), 3.28 (d, J = 9.2 Hz, 1H), 3.06 (s, 3H), 1.80 (td, J = 12.3, 4.2 Hz, 1H), 1.09 (s, 3H), 0.81 (d, J = 2.1 Hz, 5H), 0.57 (t, J = 7.1 Hz, 3H), 0.39 – 0.29 (m, 1H), 0.26(s, 9H). **^{13}C NMR** (101 MHz, $CDCl_3$) 162.99, 160.56, 146.84, 146.82, 143.89, 143.83, 141.27, 135.68, 131.38, 131.35, 130.07, 128.03, 127.95, 127.56, 126.61, 114.43, 114.11, 112.29, 112.08, 74.49, 59.69, 52.73, 42.79, 42.78, 34.09, 26.32, 23.21, 17.46, 14.01, 0.01. **^{29}Si NMR** (80 MHz, $CDCl_3$): -4.76 ppm. **HRMS** (TOF MS ES+) calcd. for C26H35OF NaSi [M+Na]: 433.2337 found: 433.2339.

((1S*,2R*)-2-argio-1-butyl-1,7-dimethyl-4-(trimethylsilyl)-1,2-dihydronaphthalen-2-yl)methanol (4s)

Isolated as an inseparable mixture of colourless thick liquid in 35% yield with method A. R_f 0.5 (25% ether/hexanes), single isomer. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.59 (dd, *J* = 7.3, 4.5 Hz, 4H), 7.52 (t, *J* = 7.6 Hz, 4H), 7.41 (t, *J* = 7.2 Hz, 2H), 7.29 (d, *J* = 6.7 Hz, 1H), 7.22 (s, 1H), 7.16 (d, *J* = 7.7 Hz, 2H), 7.08 (t, *J* = 8.4 Hz, 2H), 6.68 (s, 1H), 6.62 (s, 1H), 4.42 (ddd, *J* = 16.4, 11.2, 5.3 Hz, 2H), 3.88 (ddd, *J* = 31.2, 11.2, 6.6 Hz, 2H), 2.61 (s, 3H), 2.45 (s, 3H), 2.08 (td, *J* = 12.6, 3.8 Hz, 1H), 1.92 (td, *J* = 12.4, 4.3 Hz, 1H), 1.46 (s, 3H), 1.27 (s, 3H), 1.13 – 0.95 (m, 10H), 0.78 (t, *J* = 7.2 Hz, 3H), 0.73 (t, *J* = 7.1 Hz, 3H), 0.45 (s, 9H), 0.42 (s, 9H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 145.85, 145.57, 141.31, 140.96, 139.90, 138.54, 138.52, 137.21, 136.77, 136.65, 134.90, 134.47, 132.84, 130.49, 129.89, 127.74, 127.70, 127.57, 127.23, 126.49, 126.46, 126.35, 125.57, 64.24, 63.28, 55.47, 53.89, 45.50, 41.97, 36.93, 34.72, 26.28, 26.00, 25.75, 23.24, 22.99, 21.02, 20.78, 17.07, 13.82, 13.76, 0.10, 0.09. **^{29}Si NMR** (80 MHz, $CDCl_3$) δ -4.65 and -4.79. **HRMS** (APCl) calcd. for C26H35Si $[M-H2O+H]^+$: 375.2503; found: 375.2490.

((3R,4S)-4-butyl-6-fluoro-3-(methoxymethyl)-3-(4-methoxyphenyl)-4-methyl-3,4-dihydronaphthalen-1-yl)trimethylsilane (4t)

Isolated as a colourless thick liquid in 48% yield with method A. R_f 0.4 (10% ether/hexanes), *dr* 98:02. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.38 – 7.32 (m, 2H), 7.27 – 7.21 (m, 1H), 6.96 – 6.84 (m, 4H), 6.52 (s, 1H), 4.10 (d, *J* = 9.2 Hz, 1H), 3.83 (s, 3H), 3.31 (d, *J* = 9.2 Hz, 1H), 3.12 (s, 3H), 1.83 (td, *J* = 12.3, 4.3 Hz, 1H), 1.13 (s, 3H), 1.01 – 0.82 (m, 4H), 0.64 (t, *J* = 7.1 Hz, 3H), 0.45 – 0.34 (m, 1H), 0.31 (s, 9H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 161.75 (d, *J* = 245.0 Hz), 158.19, 147.08, 144.02 (d, *J* = 6.6 Hz), 135.62, 133.12, 131.38 (d, *J* = 3.2 Hz), 130.99, 127.95 (d, *J* = 8.0 Hz), 114.21 (d, *J* = 22.4 Hz), 113.04, 112.13 (d, *J* = 20.8 Hz), 74.63, 59.72, 55.32, 52.06, 42.91, 34.06, 26.32, 23.24, 17.45, 14.03, -0.00. **^{29}Si NMR** (80 MHz, $CDCl_3$) δ -4.83. **HRMS** (ESI) calcd. for $C_{27}H_{38}FO_2Si$ [M+Na]: 441.2620. found: 441.2606.

1-((1*S*,2*R*)-2-(methoxymethyl)-1-methyl-4-(trimethylsilyl)-1,2-dihydronaphthalen-1-yl)hexan-1-one (4w)

Obtained as a colourless oil in 70% yield with method A. R_f 0.7 (5:95 ether/hexane), *dr* 98:02. $[\alpha]_D^{20}$: +154.0 (c = 1.0, $CHCl_3$), HPLC (DAICEL Chiralpak IC, heptane / IPA = 99.5:0.5, 0.8 mL / min, 254 nm) t_R (major) = 4.29 min, t_R (minor) = 4.56 min. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.21 (dd, *J* = 6.2, 2.7 Hz, 1H), 7.15 (dd, *J* = 5.6, 3.8 Hz, 1H), 7.11 (dd, *J* = 5.9, 2.2 Hz, 2H), 6.31 (d, *J* = 5.1 Hz, 1H), 3.45 (dd, *J* = 9.0, 5.2 Hz, 1H), 3.23 (s, 3H), 3.18 – 3.12 (m, 1H), 2.52 – 2.43 (m, 1H), 1.52 (t, *J* = 4.4 Hz, 1H), 1.15 (s, 8H), 1.06 – 0.97 (m, 1H), 0.79 (t, *J* = 6.8 Hz, 3H), 0.21 (s, 9H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 142.86, 141.10, 137.02, 135.68, 127.13, 126.83, 125.82, 125.12, 72.85, 59.02, 43.02, 39.19, 38.96, 31.79, 30.04, 24.55, 22.74, 22.28, 14.21, -0.02. **^{29}Si NMR** (80 MHz, $CDCl_3$) δ -5.32. **HRMS** (ESI) calcd. for $C_{22}H_{36}NaOSi$ [M+Na]: 367.2433 found: 367.2473.

(S*)-(4-(4-(4-methoxyphenoxy)butyl)-3,3,4-trimethyl-3,4-dihydronaphthalen-1-yl)trimethylsilane (4x+5x)

Obtained as a colourless oil in 54% yield with method B. R_f 0.5 (5:95 ether/hexane), *dr* 98:02 for the two products.**^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.28 – 7.02 (m, 4H), 6.77 – 6.65 (m, 4H), 5.87 [s, 1H, (*66:33 from the both isomers*)], 3.78 – 3.58 [m, 5H, -OCH_2 (2H) and -OMe (3H))], 1.49 (m, 2H), 1.38 – 1.30 (m, 2H), 1.22 – 1.12 (m, 6H), 1.03 – 0.97 [m, 5H, -CH_3(3H), -CH_2(2H)], 0.20 – 0.14 (s, 9H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 153.75, 153.70, 153.35, 153.30, 150.86, 145.45, 141.85, 135.40, 135.07, 134.33 – 134.27, 127.05, 126.75, 126.66, 126.39, 126.17, 125.62, 125.51, 124.51, 115.60, 115.56, 114.68, 114.64, 114.60, 68.66, 55.84, 42.83, 40.51, 40.36, 38.73, 34.35, 30.42, 30.16, 29.82, 22.95, 22.28, 21.68, 17.53, -0.00, -0.07. **^{29}Si NMR** (80 MHz, $CDCl_3$) δ -5.56, -5.75. **HRMS** (TOF-ES) calcd. for $C_{27}H_{38}O_2SiNa$ [M+Na]: 445.2526 found: 445.2539.

((1*Z*,4*E*)-3-(methoxymethyl)-4-methyl-1-phenylocta-1,4-dien-1-yl)trimethylsilane (6a)

Obtained as a colourless oi, in 10-18% yield. R_f 0.8 (5:95 ether/hexane).**^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.21 (t, *J* = 3.8 Hz, 2H), 7.11 (t, *J* = 7.4 Hz, 1H), 6.87 (d, *J* = 6.9 Hz, 2H), 5.84 (d, *J* = 9.4 Hz, 1H), 4.96 (t, *J* = 7.1 Hz, 1H), 3.32 (d, *J* = 7.4 Hz, 1H), 3.28 – 3.23 (m, 1H), 3.16 (s, 3H), 2.96 (dd, *J* = 16.5, 7.2 Hz, 1H), 1.90 (q, *J* = 7.3 Hz, 2H), 1.76 (d, *J* = 10.7 Hz, 1H), 1.53 (s, 1H), 1.50 (s, 3H), 1.39 (s, 1H), 1.29 (dd, *J* = 14.7, 7.4 Hz, 2H), 0.83 (t, *J* = 7.4 Hz, 3H), -0.00 (s, 9H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 146.44, 142.43, 140.26, 134.90, 128.03, 128.00, 126.36, 125.46, 74.81, 58.75, 48.24, 30.06, 23.02, 14.34, 13.94, -1.44. **^{29}Si NMR** (80 MHz, $CDCl_3$) δ -4.66. **HRMS** (APCl) calcd. for $C_{20}H_{31}OSiH_2O$ [M-H2O+H]+: 333.2244; found: 333.2249.

((1*E*,4*E*)-3-(methoxymethyl)-4-methylocta-1,4-dien-1-yl)benzene (6b)

Obtained as a colourless oil in 70% yield. R_f 0.9 (5:95 ether/hexane).**^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.28 (d, *J* = 7.5 Hz, 2H), 7.21 (t, *J* = 7.6 Hz, 2H), 7.11 (t, *J* = 7.3 Hz, 1H), 6.34 (d, *J* = 16.0 Hz, 1H), 6.10 (dd, *J* = 16.0, 7.5 Hz, 1H), 5.23 (t, *J* = 7.2 Hz, 1H), 3.45 (dd, *J* = 11.6, 7.2 Hz, 2H), 3.29 (s, 3H), 3.06 (q, *J* = 7.2 Hz, 1H), 1.95 (dd, *J* = 14.8, 7.4 Hz, 2H), 1.56 (s, 3H), 1.31 (dd, *J* = 14.7, 7.3 Hz, 2H), 0.83 (t, *J* = 6.2 Hz, 3H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 137.74, 134.45, 130.68, 130.46, 128.56, 127.17, 127.10, 126.29, 74.72, 58.95, 51.70, 30.11, 22.98, 14.37, 13.95. **HRMS** (TOF-ES) calcd. for $C_{17}H_{24}NaO$ [M+Na]: 267.1725 found: 267.1725.

((3R,4S)-4-butyl-3-(methoxymethyl)-4-methyl-1,2,3,4-tetrahydronaphthalen-1-yl)trimethylsilane (7)

Obtained as a colourless oil in 82% yield with method A. R_f 0.7 (5:95 ether/hexane), *dr* 72:28. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.31 (ddd, *J* = 14.5, 7.4, 1.8 Hz, 1.8H), 7.24 – 7.19 (m, 1H), 7.15 – 7.02 (m, 3.6H), 3.70 (dd, *J* = 9.2, 3.3 Hz, 1H), 3.60 (dd, *J* = 9.3, 3.5 Hz, 0.4H), 3.44 (s, 3H), 3.41 (s, 1.2H), 3.32 – 3.27 (m, 1H), 3.18 (t, *J* = 9.1 Hz, 0.4H), 2.55 – 2.46 (m, 1.4H), 2.20 – 2.11 (m, 1.4H), 2.02 – 1.94 (m, 1.4H), 1.91 (dd, *J* = 11.9, 3.8 Hz, 1H), 1.81 (ddd, *J* = 14.5, 9.9, 5.0 Hz, 2H), 1.31 (ddd, *J* = 19.3, 9.3, 4.8 Hz, 3H), 1.18 (s, 1.2H), 1.14 (s, 3H), 0.89 (dd, *J* = 13.9, 6.7 Hz, 4.6H), 0.13 (s, 9H), 0.12 (s, 3.6H). **^{13}C**

NMR (101 MHz, $CDCl_3$) δ 145.34, 144.78, 141.05, 140.69, 129.67,129.65,129.26, 129.18, 128.04, 127.58, 126.23, 126.04, 125.72, 75.59, 75.29, 60.38, 60.35,60.32, 41.56, 40.65, 40.58, 40.32, 40.12, 39.40, 30.40, 29.38, 28.50, 28.23, 27.97, 27.15, 25.99, 25.13, 24.80, 24.72, 15.38, 0.44, -0.00. **HRMS** (APCl) calcd. for $C_{20}H_{35}OSi$ [M+H]: 319.2452 found: 319.2442.

(1*S,2*R**)-1-butyl-2-(methoxymethyl)-1-methyl-1,2-dihydronaphthalene (8)**

Obtained as a colourless oil in 50% yield. R_f 0.6 (5:95 ether/hexane), *dr* 94:06. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.09 (d, *J* = 7.9 Hz, 2H), 7.07 – 6.99 (m, 1H), 6.94 (d, *J* = 6.7 Hz, 1H), 6.37 (d, *J* = 9.6 Hz, 1H), 5.94 (dd, *J* = 9.6, 5.4 Hz, 1H), 3.42 (dd, *J* = 8.9, 5.2 Hz, 1H), 3.20 (s, 3H), 3.14 (t, *J* = 8.8 Hz, 1H), 2.46 (dd, *J* = 14.2, 5.3 Hz, 1H), 1.56 – 1.49 (m, 2H), 1.19 (s, 3H), 1.16 – 1.08 (m, 3H), 0.93 (dt, *J* = 12.1, 7.3 Hz, 1H), 0.75 (t, *J* = 7.2 Hz, 3H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 142.56, 132.97, 130.33, 127.41, 127.19, 126.72, 126.20, 125.09, 73.25, 59.00, 42.91, 39.73, 39.14, 26.99, 23.43, 21.80, 14.21. **HRMS** (TOF-ES) calcd. for $C_{17}H_{24}ONa$ [M+Na]+: 267.1750; found: 267.1749.

DFT Calculations

Computational details

The calculations were performed using Gaussian 09 Rev. D.01.[3] Geometry optimization, and frequency calculations of intermediates, transition structures and products were carried out at M062X[4]/6-311+G(d,p) level of theory with the Polarizable Continuum Model (IEFPCM) method[5] in dichloromethane. Frequency calculations 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. All transition-state structures were confirmed to connect corresponding reactants and products by intrinsic reaction coordinate (IRC) calculations.[6]

Three models, **3_H**, **3_Me** and **3_Ph** were considered for the theoretical investigations to represent the molecules **3a**, **3p** and **3q** used experimentally (Figure SI1).

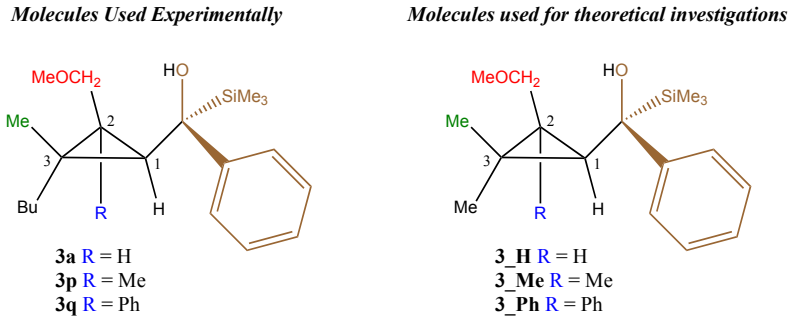
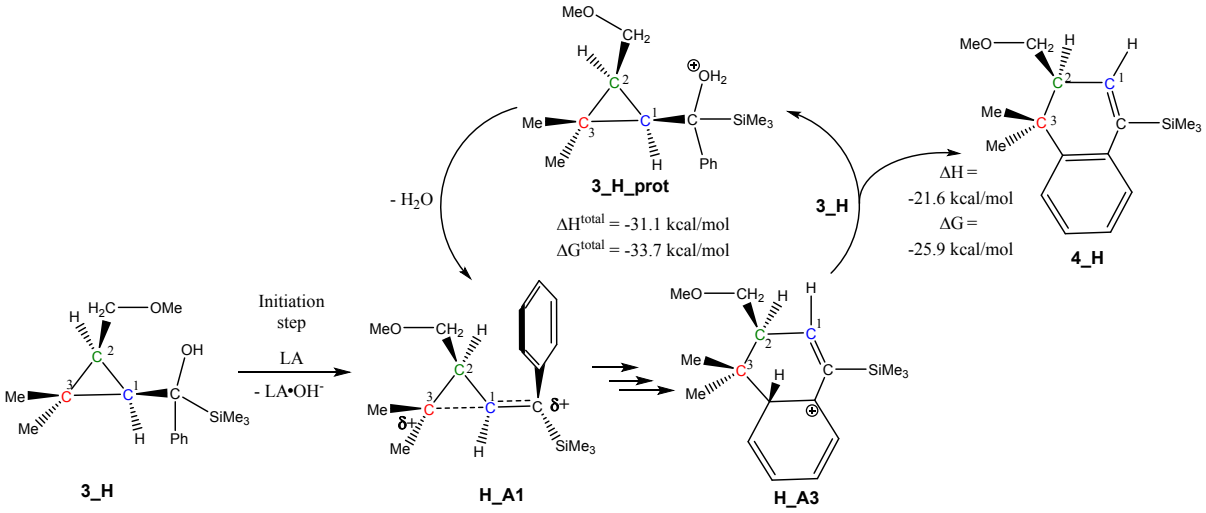


Figure SI1

Results and Discussion

1.1 Thermodynamics of the ring opening reaction of 3_H.

The proposed mechanism starts from the initiation step in which **3_H** reacts with the Lewis acid to produce the carbocation **H_A1** (Scheme SI1). Transformation of **H_A1** into **H_A3** will be discussed in details later. Deprotonation of to the ring-expanded **H_A3** produces the final product **4_H** while regenerating the protonated species **3_H_prot**. Dehydration of **3_H_prot** produces **H_A1** closing the catalytic cycle. The overall process of the cycle is essentially exothermic with enthalpy and Gibbs free energy of -31.1 and -33.7 kcal/mol respectively.



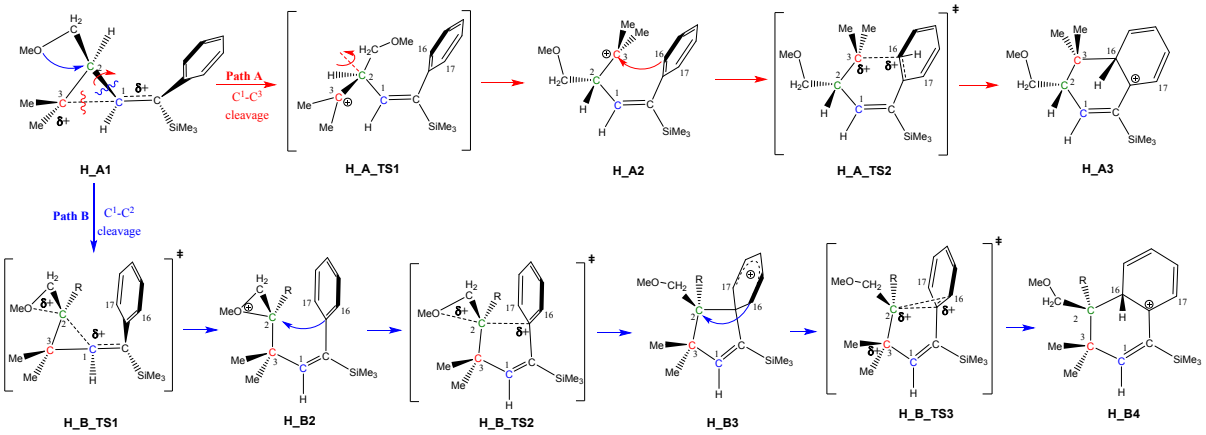
Scheme SI1

Initiation and deprotonation steps of **3_Me** and **3_Ph** followed a similar process to that of **3_H** and will not be discussed further. We will mainly focus our investigation to the ring-expansion **R_A1** to **R_A3** (R = H, Me, Ph) to rationalize the regio- and stereoselectivity of the reaction.

1.2 Investigation of the mechanisms of the ring expansion reactions of H_A1, Me_A1 and Ph_A1

2 R = H

Mechanisms for the ring expansion reactions via either C^1-C^3 or C^1-C^2 bonds cleavage were calculated and described in Path A and B respectively and presented in Scheme SI2 and Figure SI2.



Scheme SI2

Paths A and B are differing in the selectivity of the C-C bond cleavage. When C^1-C^3 are cleaved, it produces the tertiary cation **H_A2** and proceeds directly with very low-energy barriers (Figure SI2, Path A). In Path B, the cleavage of C^2-C^3 bond leads to a less stable secondary carbocation, which is concertedly stabilized by the MeO group producing the cyclic oxonium cation **H_B2**.

The Gibbs free energy of the highest transition state of Path A is -1.1 kcal/mol, while that of Path B is 13.5 kcal/mol rationalizing the complete regioselectivity of the ring-expansion.

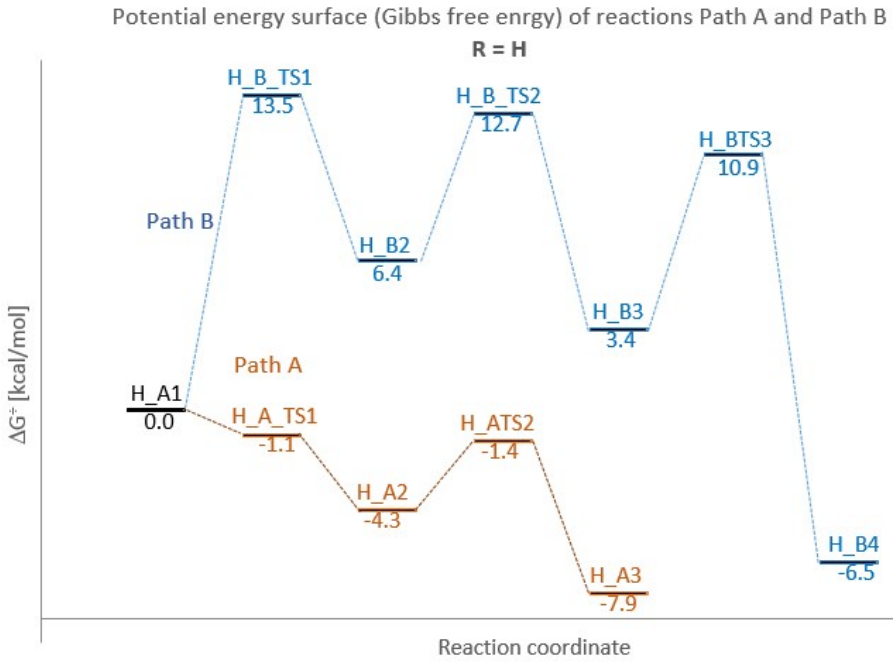
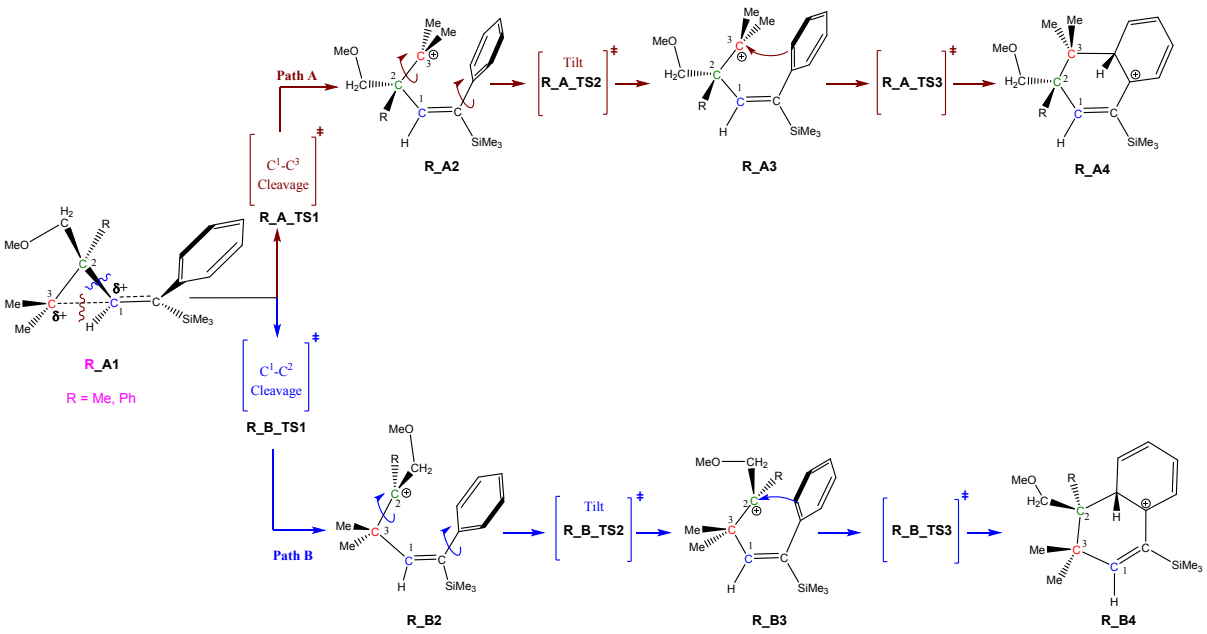


Figure SI2

3 R = Me, Ph

When the substituent R of the three-membered ring is either a methyl or a phenyl group (**Me_A1** and **Ph_A1** respectively), they both react very similarly and the general mechanism is presented in Scheme SI3. Path A for **Me_A1** and **Ph_A1** differed from the one described previously for **H_A1** by an additional step where the two methyl groups at the cationic carbon center and the phenyl ring slightly rotate (**R_A_TS2**) before ring closing. This C^1-C^2 bond cleavage of **Me_A1** and **Ph_A1** proceeded without MeO group participation (Scheme SI3).



Scheme SI3

4 Potential Energy Surface (PES) for R = Me

Both paths A and B are going through low PESs with the highest energies of 3.5 kcal/mol (**Me_A_TS2**, path A) and 5.0 kcal/mol (**Me_B_TS1**, path B) (Figure SI3). Supporting the selectivity of the C-C bond cleavage.

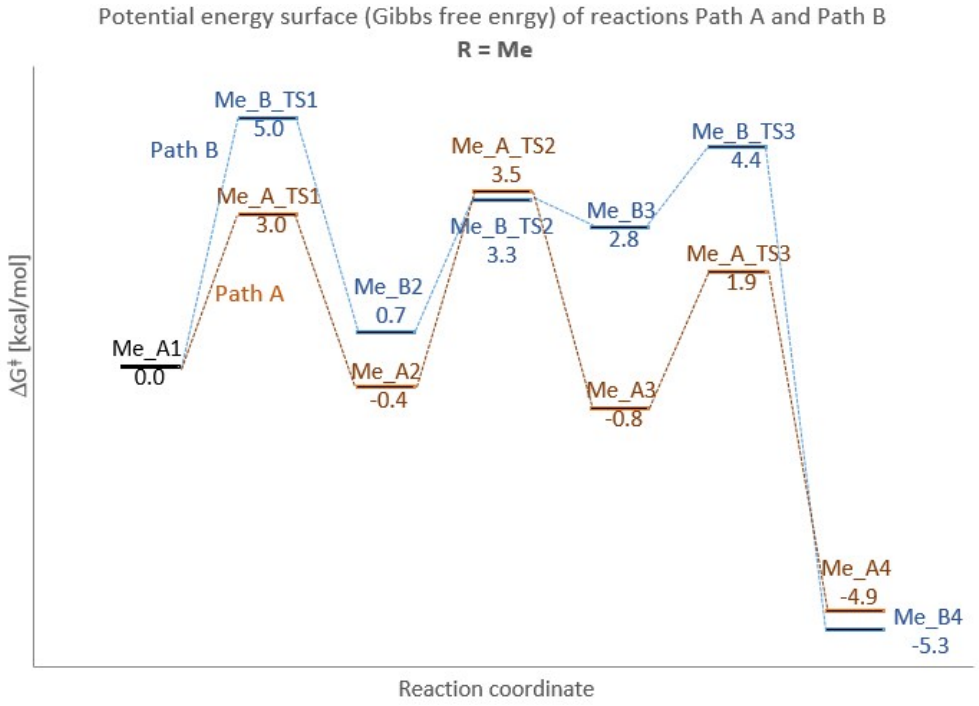
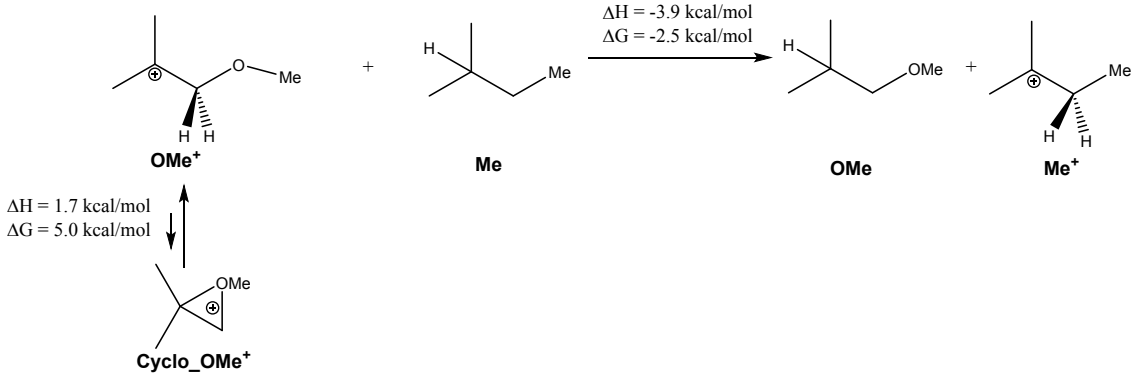


Figure SI3

Evaluation of destabilizing inductive effect of MeO

We noted that the tertiary carbocation **Me_B2** bearing a β-MeO substituent is higher in energy than the tertiary carbocation **Me_A2** (Figure SI3). To evaluate a potential negative inductive effect of the β-MeO substituent on the stability of the tertiary carbocation, the isodesmic reaction was calculated on a simple model (Scheme SI4). Indeed, the inductive effect of a β-OMe group on the carbocation (**OMe⁺**) is destabilizing relative to β-Me substituent on (**Me⁺**) by 2.5 kcal/mol.



Scheme SI4

5 R = Ph

When R is a phenyl group, the barriers of rate determining steps (RDSs) of paths A and B are 3.2 kcal/mol and 7.8 kcal/mol respectively (Figure SI4). The difference of 4.6 kcal/mol explains well the complete regioselectivity. Interestingly, RDS of Path B is not anymore, the first step, namely the cleavage of C^2-C^1 bond (**Ph_B_TS1**), but rather the last one (**Ph_B_TS3**). We also noted that the

product **Ph_B4** is by 8.5 kcal/mol higher in energy than **Ph_A4**. Scheme SI5 nicely demonstrates that this difference is due to the repulsive steric interactions between the phenyl ring and the two methyl groups in **Ph_B4** as compared to **Ph_A4**.

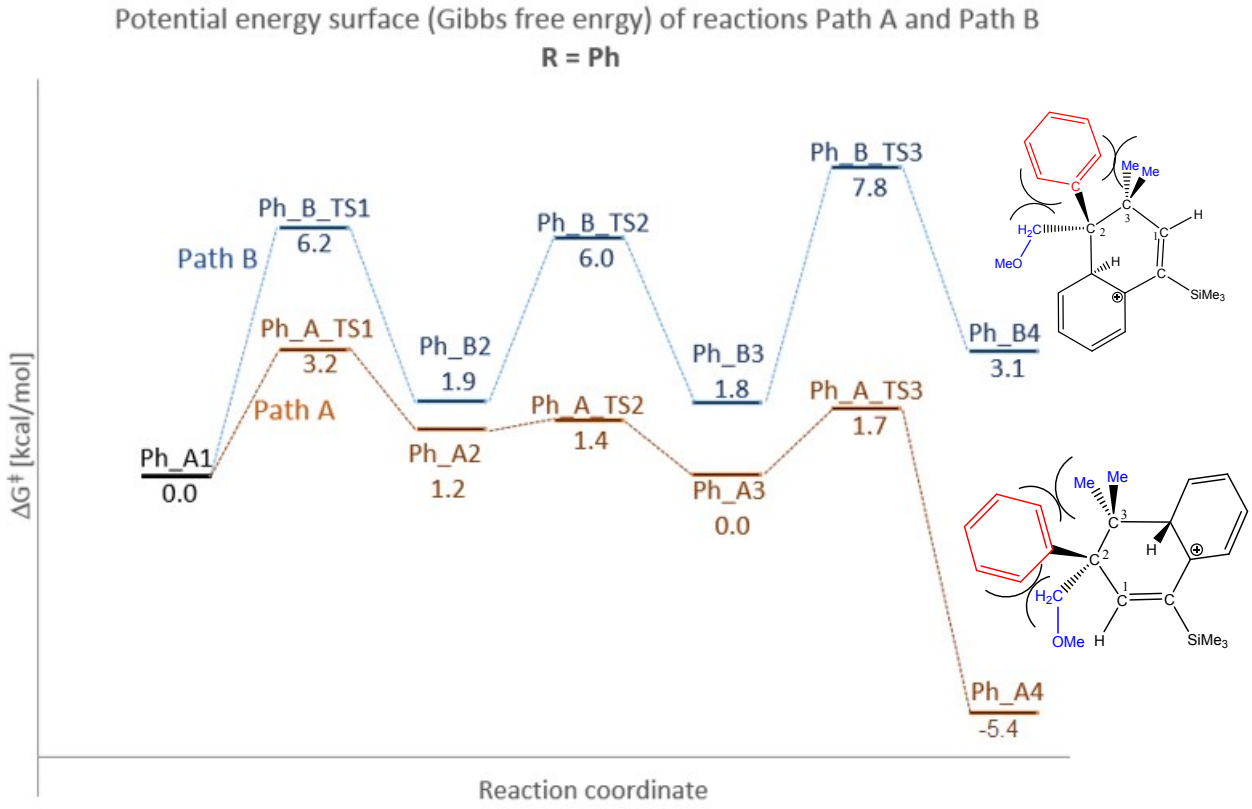
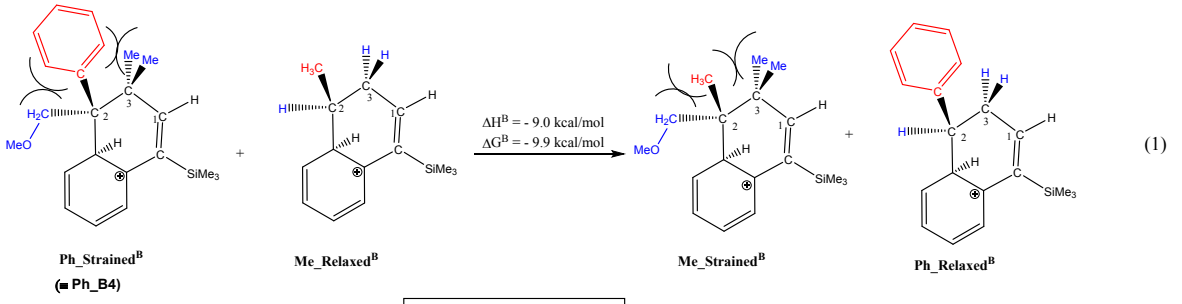


Figure SI4

Steric effects of Ph substituents

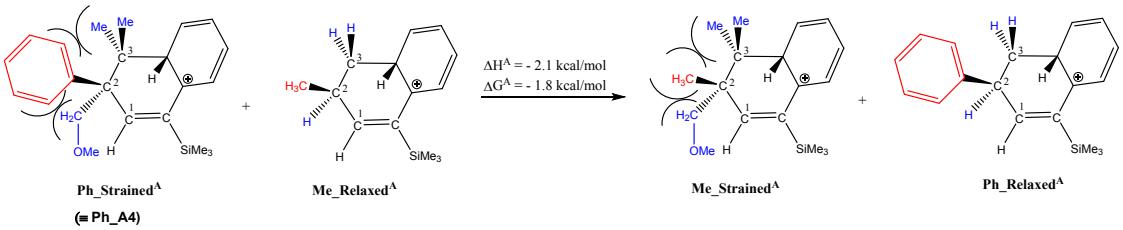
To evaluate the steric effects of the Ph substituent, two isodesmic reactions were calculated (Scheme SI5, eq. 1-2). In reaction 1, the relatively sterically bulky environment of Ph in **Ph_Strained**^{B} is changed to the less bulky environment in **Ph_Relaxed**^{B}, while the Me environment is changed from hydrogenated in **Me_Relaxed**^{B} to the more crowded one in **Me_Strained**^{B}. The negative Gibbs free energy (-9.9 kcal/mol) of this reaction indicates a higher repulsive strain (in **Ph_B4**) of Ph relative to the methyl at the same position. The analogous reaction for the **Ph_A4** product (Scheme SI5, eq.2) revealed significantly lower relative repulsive strain in **Ph_A4**, -1.8 kcal/mol. The strain in **Ph_A4** is lower than that in **Ph_B4** by 8.1 kcal/mol and is consistent with the energy difference of 8.5 kcal/mol between **Ph_A4** and **Ph_B4** (Figure SI4).



(1)

$\Delta\Delta H = \Delta H^{A} - \Delta H^{B} = 6.9$ kcal/mol

$\Delta\Delta G = \Delta G^{A} - \Delta G^{B} = 7.1$ kcal/mol



(2)

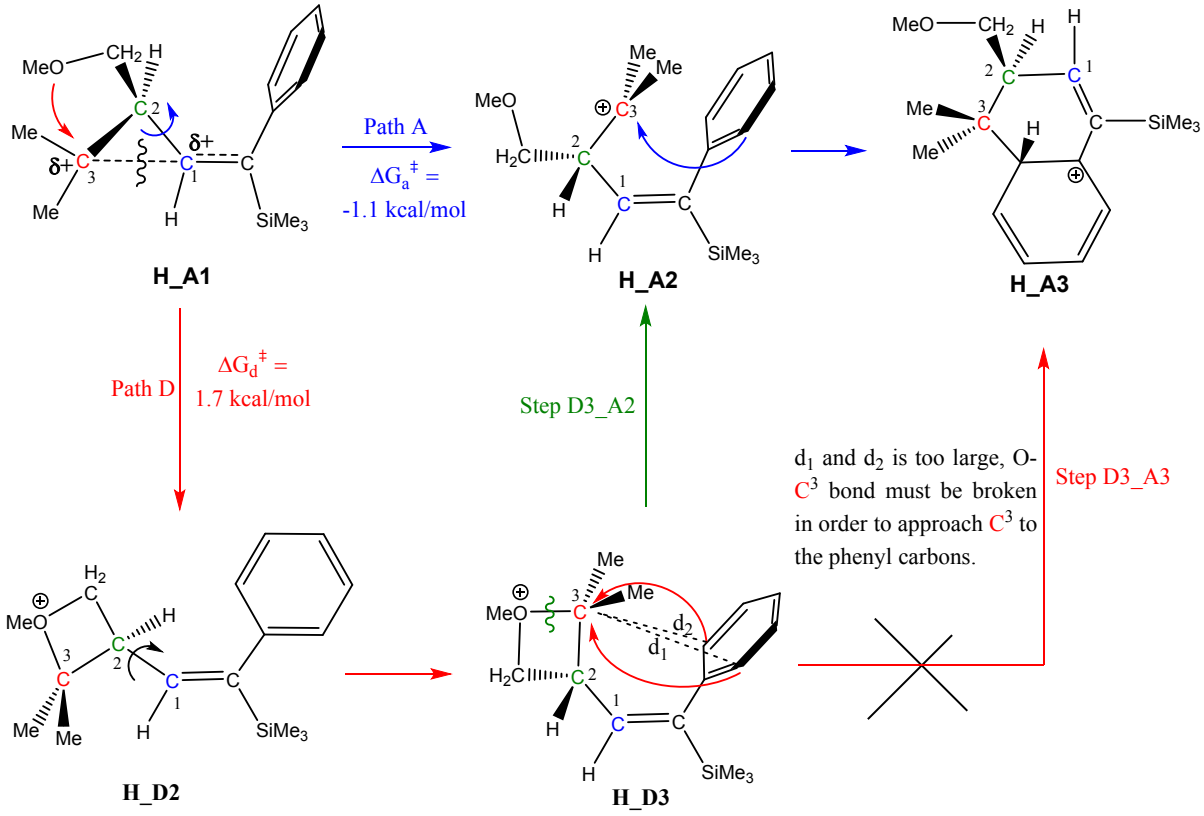
Scheme SI5

5.1 Understanding the stereospecificity

Neighboring participation of the methoxy group.

Our first hypothesis for the origin of the stereospecificity of the reaction was a potential intramolecular stabilization of the carbocation by the methoxy group. Participation of this MeO group during the C^1-C^3 bond cleavage was therefore theoretically investigated and presented in Scheme SI6.

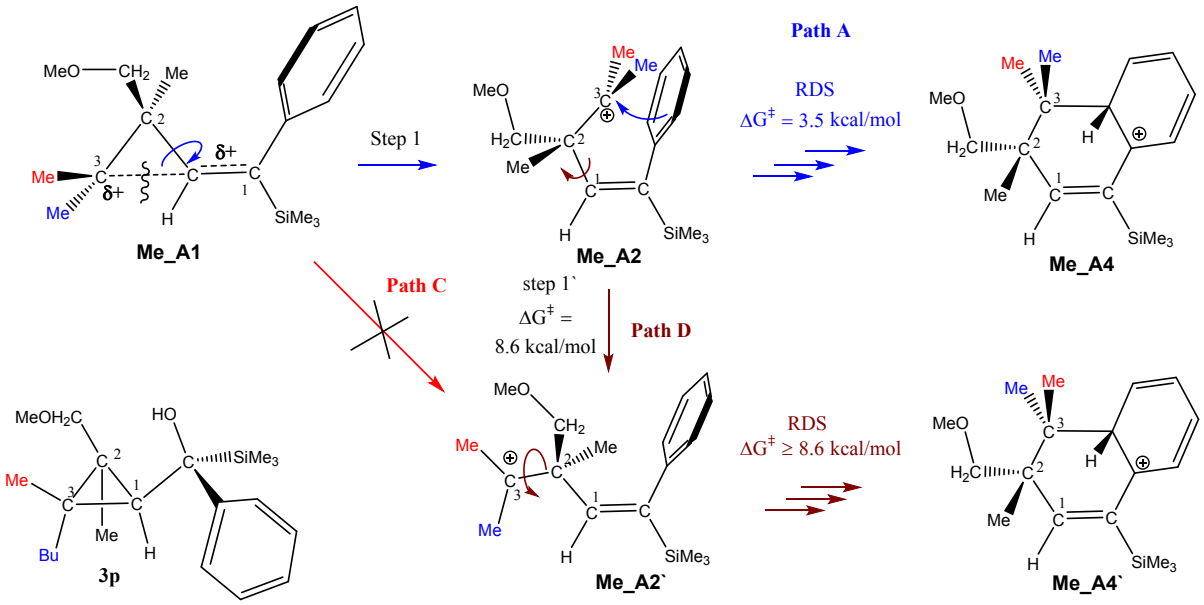
Coordination of the carbocation by the oxygen of the methoxy group produces the 4-membered oxonium ring **H_D2** (Path D). This step requires a barrier of 1.7 kcal/mol, which is higher than the barrier for the direct Path A of -1.1 kcal/mol. Moreover, the study of the geometry of chelated **H_D3** and the search of transition states for the step **D3** into **A3** led us to the conclusion that the direct (concerted) transformation **H_D3** -> **H_A3** (Step D3_A3) is impossible. C^3 is too remote from the phenyl in this constrained **H_D3** structure and cannot directly undergo a Friedel-Craft reaction. All our efforts resulted in the formation of the **H_A2** (via Step D3_A2) which ultimately produces **H_A3** – the product of the direct path A.



Scheme SI6

Stereospecificity of the ring expansion

To understand the complete stereospecificity for the ring expansion reaction of **3p**, we studied the mechanism on our model **Me_A1** as representative molecule of **3p**. In order to epimerize the stereocenter in C^3, a rotation around the C^3-C^2 bond has to occur. We could not locate potential pathways of low energy for this C^3-C^2 rotation in **Me_A2** as the system is geometrically blocked by the proximity of the aromatic ring (d[C^3-C^{ipso}] = 2.86A). The rotation along the C^2-C^3 bond becomes possible only when the rotamer **Me_A2`** is formed but with a relatively high barrier (8.6 kcal/mol) (Scheme SI7, Path D, Step 1`). The RDS for Path A is 3.5 kcal/mol, which by 5.1 kcal/mol lower in energy than that of Step 1`.



Scheme SI7

5.2 Geometries and energies of the calculated structures

5.2.1 Geometries for the Scheme SI1 and SI2 (R = H)

Name - **3_H**
Zero-point correction= 0.416620 (Hartree/Particle)
Thermal correction to Energy= 0.440528
Thermal correction to Enthalpy= 0.441473
Thermal correction to Gibbs Free Energy= 0.365348
Sum of electronic and zero-point Energies= -1104.036149
Sum of electronic and thermal Energies= -1104.012240
Sum of electronic and thermal Enthalpies= -1104.011296
Sum of electronic and thermal Free Energies= -1104.087420

Charge = 0 Multiplicity = 1

6	-0.425343	1.353478	-0.447740
6	0.835493	2.168414	-0.222198
6	-0.257092	2.151442	0.825907
1	-1.090936	1.860225	-1.142583
1	0.886812	3.075637	-0.818871
6	-0.596281	-0.145945	-0.681822
6	2.200345	1.605424	0.054574
1	2.792086	2.351710	0.606778
1	2.167522	0.694716	0.661480
8	2.842385	1.326167	-1.177162
6	4.157717	0.858021	-0.980853
1	4.161985	-0.059787	-0.379817
1	4.584284	0.647738	-1.961261
1	4.772695	1.613208	-0.475278
6	0.412557	-1.082656	-0.030448
6	0.225737	-1.588534	1.259106
6	1.545230	-1.497018	-0.739798
6	1.154823	-2.446093	1.839767
1	-0.647642	-1.299194	1.830812
6	2.472914	-2.360666	-0.165128
1	1.714630	-1.115193	-1.738226
6	2.287296	-2.834482	1.129924
1	0.987867	-2.817042	2.844497
1	3.347171	-2.660107	-0.732720
1	3.009889	-3.507281	1.576798
14	-2.455276	-0.594361	-0.327099
6	0.017877	1.536238	2.185311
1	0.705618	0.695902	2.155444
1	0.448135	2.300257	2.839984
1	-0.910903	1.192507	2.649517
6	-1.114193	3.398894	0.934610
1	-2.093508	3.163006	1.363710
1	-0.634462	4.137788	1.583753
1	-1.273705	3.856574	-0.044247
8	-0.472606	-0.255093	-2.123346
1	-0.539321	-1.186003	-2.364177

6 -2.671333 -2.428164 -0.682651
1 -2.406889 -2.671097 -1.716053
1 -2.053076 -3.040649 -0.021666
1 -3.715939 -2.716360 -0.536679
6 -3.485163 0.419515 -1.527343
1 -4.520361 0.066799 -1.515707
1 -3.491475 1.476215 -1.246031
1 -3.102559 0.337329 -2.546130
6 -3.084341 -0.176079 1.396559
1 -4.167225 -0.336966 1.399981
1 -2.661567 -0.777566 2.202432
1 -2.910949 0.879364 1.621042

Name - **3_H_Prot**
Zero-point correction= 0.424967 (Hartree/Particle)
Thermal correction to Energy= 0.451394
Thermal correction to Enthalpy= 0.452338
Thermal correction to Gibbs Free Energy= 0.370076
Sum of electronic and zero-point Energies= -1104.436894
Sum of electronic and thermal Energies= -1104.410467
Sum of electronic and thermal Enthalpies= -1104.409523
Sum of electronic and thermal Free Energies= -1104.491785

Charge = 1 Multiplicity = 1
6 -0.023022 -1.472190 -0.164089
6 1.515745 -1.855311 -0.299462
6 0.906955 -1.916509 -1.596580
1 -0.600828 -2.333271 0.144296
1 1.619103 -2.809700 0.211651
6 -0.631430 -0.253433 -0.102346
6 2.589456 -0.875145 0.086153
1 3.554078 -1.319017 -0.192977
1 2.495704 0.087091 -0.422899
8 2.526348 -0.699076 1.484727
6 3.556373 0.153145 1.965760
1 3.497939 1.134957 1.483681
1 3.409240 0.262255 3.038495
1 4.538451 -0.287739 1.772569
6 -0.064488 1.073572 -0.420786
6 -0.455653 1.745491 -1.584468
6 0.731853 1.732691 0.521859
6 0.003474 3.034092 -1.831558
1 -1.097099 1.251688 -2.305327
6 1.170307 3.028895 0.274184
1 0.982617 1.232487 1.449198
6 0.818162 3.678483 -0.905134
1 -0.285674 3.537081 -2.746321
1 1.785017 3.532844 1.010690
1 1.165746 4.686452 -1.095519

14 -2.464248 -0.183967 0.528260
6 1.155561 -0.889430 -2.658976
1 1.476851 0.076864 -2.283088
1 1.960792 -1.295145 -3.281126
1 0.277447 -0.765516 -3.293330
6 0.345251 -3.219246 -2.093688
1 -0.574898 -3.056597 -2.656034
1 1.085607 -3.645415 -2.778185
1 0.171042 -3.933833 -1.290739
8 -0.027226 -0.817712 2.762043
1 0.887942 -0.857251 2.443060
1 0.036364 -0.708889 3.715261
6 -2.541335 1.234692 1.738905
1 -1.837002 1.073400 2.556738
1 -2.298412 2.179130 1.245629
1 -3.550518 1.313186 2.151588
6 -2.902359 -1.833398 1.284505
1 -3.893906 -1.764371 1.739951
1 -2.938499 -2.630773 0.537935
1 -2.183110 -2.098937 2.061712
6 -3.503810 0.161068 -0.995910
1 -4.558803 0.058034 -0.726119
1 -3.352519 1.174777 -1.371305
1 -3.292430 -0.548748 -1.799510

Name - **4_H**
Zero-point correction= 0.389977 (Hartree/Particle)
Thermal correction to Energy= 0.411989
Thermal correction to Enthalpy= 0.412934
Thermal correction to Gibbs Free Energy= 0.339100
Sum of electronic and zero-point Energies= -1027.669346
Sum of electronic and thermal Energies= -1027.647334
Sum of electronic and thermal Enthalpies= -1027.646390
Sum of electronic and thermal Free Energies= -1027.720223

Charge = 0 Multiplicity = 1
6 0.223834 -1.120989 -0.399505
6 1.557472 -0.432618 -0.574650
6 1.620809 0.906621 0.210840
1 0.240153 -2.208260 -0.441946
1 1.686409 -0.196854 -1.642175
6 -0.936431 -0.480594 -0.199141
6 2.610680 -1.478398 -0.200821
1 2.485574 -1.776329 0.850976
1 2.428175 -2.374213 -0.812433
8 3.929097 -1.031225 -0.418109
6 4.878384 -2.019479 -0.080065
1 4.736995 -2.923375 -0.684834
1 5.866965 -1.606441 -0.275669

1 4.802582 -2.289064 0.980256
6 -0.909088 1.000686 -0.172240
6 0.315051 1.683416 -0.012825
6 -2.089892 1.738418 -0.314955
6 0.297825 3.078718 0.010381
6 -2.087424 3.127544 -0.298728
1 -3.030637 1.218880 -0.453161
6 -0.884565 3.800688 -0.131324
1 1.221237 3.628285 0.137631
1 -3.015425 3.674366 -0.416727
1 -0.859232 4.884004 -0.114021
14 -2.510788 -1.501126 0.061190
6 1.757898 0.646169 1.721948
1 0.960122 -0.005974 2.088193
1 2.722915 0.182577 1.945138
1 1.703198 1.592872 2.264166
6 2.827205 1.732806 -0.261102
1 2.968569 2.615253 0.365747
1 3.732254 1.133201 -0.204295
1 2.691712 2.063287 -1.294676
6 -3.674549 -1.378112 -1.414198
1 -4.490388 -2.097062 -1.293928
1 -4.119189 -0.389012 -1.539061
1 -3.142045 -1.627384 -2.335891
6 -3.376616 -0.941670 1.633984
1 -3.731497 0.089284 1.573080
1 -4.238738 -1.584160 1.834603
1 -2.696854 -1.013378 2.487429
6 -2.026918 -3.307368 0.249076
1 -1.594670 -3.711353 -0.670023
1 -1.310422 -3.455532 1.060773
1 -2.921555 -3.893073 0.479009

Name - **H_A1**
Zero-point correction= 0.400322 (Hartree/Particle)
Thermal correction to Energy= 0.423506
Thermal correction to Enthalpy= 0.424451
Thermal correction to Gibbs Free Energy= 0.348624
Sum of electronic and zero-point Energies= -1028.019127
Sum of electronic and thermal Energies= -1027.995943
Sum of electronic and thermal Enthalpies= -1027.994999
Sum of electronic and thermal Free Energies= -1028.070825

Charge = 1 Multiplicity = 1
6 -0.065408 -1.305646 -0.616558
6 -1.608754 -1.426189 -0.576241
6 -1.166925 -1.760488 0.769825
1 0.390546 -2.232678 -0.939771
1 -1.880278 -2.296056 -1.171390

6	0.783509	-0.288738	-0.270665
6	-2.577126	-0.286494	-0.805238
1	-2.340910	0.602096	-0.215177
1	-2.572386	-0.005005	-1.865886
8	-3.833479	-0.802206	-0.430778
6	-4.873338	0.140078	-0.623842
1	-4.946433	0.427431	-1.678295
1	-5.801478	-0.335211	-0.312733
1	-4.701961	1.037157	-0.018621
6	0.383531	1.095009	0.026763
6	0.756574	1.725784	1.221654
6	-0.264620	1.838092	-0.968963
6	0.432755	3.058924	1.434644
1	1.262542	1.161528	1.995807
6	-0.550202	3.182229	-0.764003
1	-0.513652	1.364559	-1.911998
6	-0.213956	3.791065	0.441315
1	0.696506	3.531180	2.372980
1	-1.038118	3.751070	-1.546124
1	-0.446774	4.836305	0.604478
14	2.689875	-0.613838	-0.370132
6	-1.351518	-0.824236	1.916640
1	-1.447540	0.219579	1.633875
1	-2.297209	-1.130193	2.380654
1	-0.562546	-0.942296	2.659908
6	-0.848336	-3.176538	1.131262
1	0.024603	-3.234288	1.783021
1	-1.709794	-3.546908	1.699453
1	-0.713481	-3.815962	0.260871
6	3.443887	-0.309068	1.318234
1	4.460349	-0.713022	1.308147
1	3.510367	0.754304	1.553097
1	2.892279	-0.814756	2.114415
6	3.316188	0.612185	-1.635278
1	4.395375	0.494609	-1.763272
1	2.838987	0.459270	-2.606025
1	3.119996	1.637194	-1.310552
6	2.953846	-2.387701	-0.897112
1	2.532835	-3.093853	-0.176160
1	2.528460	-2.594868	-1.881911
1	4.028657	-2.579406	-0.955335

Name - **H_A2**

Zero-point correction= 0.398014 (Hartree/Particle)
Thermal correction to Energy= 0.421386
Thermal correction to Enthalpy= 0.422330
Thermal correction to Gibbs Free Energy= 0.345899
Sum of electronic and zero-point Energies= -1028.025445
Sum of electronic and thermal Energies= -1028.002073

Sum of electronic and thermal Enthalpies= -1028.001129
Sum of electronic and thermal Free Energies= -1028.077560

Charge = 1 Multiplicity = 1

6	0.077637	-1.396251	0.627816
6	-1.425945	-1.141029	0.770369
6	-1.766106	0.229949	1.223833
1	0.373006	-2.411662	0.875096
1	-1.753327	-1.765515	1.618368
6	0.962919	-0.509920	0.168132
6	-2.180032	-1.619105	-0.463011
1	-1.959774	-0.973773	-1.325133
1	-1.848596	-2.633992	-0.714088
8	-3.551242	-1.599984	-0.152694
6	-4.359613	-1.961036	-1.258986
1	-4.109427	-2.967661	-1.610029
1	-5.394561	-1.941138	-0.923827
1	-4.228313	-1.249986	-2.082306
6	0.544049	0.870468	-0.187359
6	0.723218	1.926152	0.717730
6	0.012501	1.147533	-1.455856
6	0.322432	3.215774	0.386583
1	1.175390	1.727563	1.683928
6	-0.390866	2.435173	-1.783335
1	-0.078599	0.345202	-2.180407
6	-0.247095	3.470095	-0.859018
1	0.454847	4.020525	1.099694
1	-0.815622	2.634517	-2.759896
1	-0.562598	4.474003	-1.116492
14	2.791441	-0.965223	-0.106157
6	-2.636207	1.140536	0.482493
1	-2.877334	0.817953	-0.524206
1	-3.563034	1.224723	1.070899
1	-2.197920	2.146709	0.491297
6	-1.395061	0.592717	2.600686
1	-1.352655	1.668200	2.760114
1	-2.232460	0.203439	3.205250
1	-0.493467	0.085628	2.942486
6	3.146595	-0.682347	-1.924939
1	2.964898	0.360384	-2.198650
1	4.191530	-0.912491	-2.149509
1	2.515694	-1.316444	-2.553083
6	3.831735	0.185449	0.947159
1	4.893014	-0.037312	0.808403
1	3.668923	1.229182	0.666240
1	3.598091	0.073568	2.008806
6	3.049307	-2.755358	0.374735
1	2.433157	-3.424478	-0.231033
1	4.095468	-3.029354	0.215167
1	2.816627	-2.927604	1.428479

Name - **H_A3**
Zero-point correction= 0.401553 (Hartree/Particle)
Thermal correction to Energy= 0.423835
Thermal correction to Enthalpy= 0.424779
Thermal correction to Gibbs Free Energy= 0.351548
Sum of electronic and zero-point Energies= -1028.033371
Sum of electronic and thermal Energies= -1028.011089
Sum of electronic and thermal Enthalpies= -1028.010144
Sum of electronic and thermal Free Energies= -1028.083376

Charge = 1 Multiplicity = 1

6	0.076850	-1.196662	-0.528708
6	1.494149	-0.713436	-0.643212
6	1.699828	0.759697	-0.206795
1	-0.048905	-2.267434	-0.678769
1	1.754786	-0.778429	-1.713144
6	-1.008605	-0.446710	-0.231766
6	2.363991	-1.734575	0.099568
1	2.083279	-1.764436	1.162187
1	2.168988	-2.730298	-0.321874
8	3.727156	-1.418202	-0.031174
6	4.550039	-2.344714	0.651680
1	4.417084	-3.354724	0.248226
1	5.582265	-2.030881	0.507747
1	4.318272	-2.354647	1.722769
6	-0.796563	0.977871	-0.091469
6	0.407226	1.561181	-0.724373
6	-1.657045	1.795334	0.636407
6	0.563964	3.021238	-0.604308
1	0.379570	1.324489	-1.800372
6	-1.397186	3.150498	0.753278
1	-2.520159	1.376360	1.136614
6	-0.296853	3.780512	0.114251
1	1.395155	3.483947	-1.123211
1	-2.068609	3.759550	1.349462
1	-0.167745	4.850982	0.201287
14	-2.724382	-1.277095	-0.039099
6	1.817353	0.887364	1.314399
1	1.011700	0.365103	1.836735
1	2.769107	0.460058	1.637715
1	1.802508	1.937147	1.616480
6	2.938236	1.353982	-0.884544
1	3.173975	2.338549	-0.477234
1	3.788050	0.699039	-0.702785
1	2.797215	1.443778	-1.965302
6	-3.971221	-0.293526	-1.034361
1	-4.951614	-0.773058	-0.967420
1	-4.079179	0.733339	-0.678420
1	-3.683460	-0.260421	-2.088279

6 -3.205271 -1.361275 1.772706
1 -3.392484 -0.384468 2.222848
1 -4.123177 -1.948353 1.869598
1 -2.424733 -1.860134 2.352475
6 -2.573958 -3.014106 -0.721104
1 -2.202064 -3.019387 -1.748503
1 -1.920444 -3.640322 -0.108823
1 -3.564892 -3.476445 -0.723115

Name - **H_A_TS1**
Zero-point correction= 0.397347 (Hartree/Particle)
Thermal correction to Energy= 0.420665
Thermal correction to Enthalpy= 0.421609
Thermal correction to Gibbs Free Energy= 0.344528
Sum of electronic and zero-point Energies= -1028.019738
Sum of electronic and thermal Energies= -1027.996419
Sum of electronic and thermal Enthalpies= -1027.995475
Sum of electronic and thermal Free Energies= -1028.072557
1 imaginary frequency.
Charge = 1 Multiplicity = 1
6 0.057799 -1.489920 -0.298811
6 -1.496730 -1.535975 -0.262264
6 -1.704658 -1.396872 1.179818
1 0.486553 -2.479499 -0.422498
1 -1.762614 -2.557398 -0.550353
6 0.875634 -0.436155 -0.182458
6 -2.240353 -0.560107 -1.156131
1 -1.988692 0.481582 -0.934927
1 -1.969729 -0.759083 -2.200618
8 -3.611717 -0.792396 -0.931306
6 -4.433519 0.087773 -1.678118
1 -4.263091 -0.040568 -2.752104
1 -5.467411 -0.157827 -1.443823
1 -4.233876 1.129738 -1.404273
6 0.470139 0.971861 0.074022
6 0.492800 1.477589 1.377352
6 0.158985 1.831822 -0.983807
6 0.154973 2.804389 1.623587
1 0.765009 0.824868 2.200991
6 -0.178662 3.157932 -0.735169
1 0.170822 1.453211 -2.000686
6 -0.187900 3.645873 0.569215
1 0.163157 3.180392 2.639743
1 -0.431123 3.810710 -1.562258
1 -0.449393 4.679434 0.761571
14 2.764933 -0.693204 -0.386704
6 -2.280151 -0.186943 1.761177
1 -2.092562 0.714101 1.180105
1 -3.363896 -0.389006 1.657836

1 -2.050571 -0.058917 2.816610
6 -1.403099 -2.531073 2.063343
1 -0.813945 -2.206095 2.924441
1 -2.373330 -2.852891 2.472087
1 -0.936907 -3.368930 1.551613
6 3.308807 0.408779 -1.799984
1 3.107396 1.459775 -1.578918
1 4.383489 0.297354 -1.966925
1 2.792398 0.146981 -2.726771
6 3.576983 -0.165363 1.217040
1 4.659409 -0.301900 1.142271
1 3.384225 0.888610 1.430682
1 3.218737 -0.761248 2.060213
6 3.106905 -2.497031 -0.756325
1 2.609679 -2.823131 -1.673227
1 4.182449 -2.637418 -0.893822
1 2.790766 -3.148312 0.062409

Name - **H_A_TS2**

Zero-point correction= 0.399452 (Hartree/Particle)
Thermal correction to Energy= 0.421554
Thermal correction to Enthalpy= 0.422498
Thermal correction to Gibbs Free Energy= 0.349579
Sum of electronic and zero-point Energies= -1028.023119
Sum of electronic and thermal Energies= -1028.001018
Sum of electronic and thermal Enthalpies= -1028.000074
Sum of electronic and thermal Free Energies= -1028.072992
1 imaginary frequency.
Charge = 1 Multiplicity = 1
6 0.069038 -1.274479 -0.406855
6 1.495441 -0.802539 -0.620864
6 1.840281 0.594133 -0.195500
1 -0.046553 -2.349545 -0.523011
1 1.738543 -0.906854 -1.684476
6 -0.992887 -0.505998 -0.143409
6 2.430218 -1.759459 0.158806
1 2.161275 -1.760575 1.223359
1 2.274389 -2.769372 -0.240252
8 3.760295 -1.349314 -0.019794
6 4.679844 -2.208264 0.634388
1 4.610505 -3.224381 0.233095
1 5.676444 -1.811972 0.451218
1 4.487301 -2.231157 1.712015
6 -0.810586 0.953485 -0.050050
6 -0.115672 1.624930 -1.074518
6 -1.243448 1.684136 1.064430
6 0.127728 3.007726 -0.984023
1 0.087838 1.102537 -2.002961
6 -0.965307 3.036838 1.160152

1 -1.756454 1.175860 1.871965
6 -0.273574 3.705459 0.135747
1 0.632413 3.516771 -1.796758
1 -1.281077 3.587827 2.038410
1 -0.076159 4.766612 0.221238
14 -2.744806 -1.254410 -0.046163
6 1.823609 0.940686 1.240580
1 1.151479 0.320394 1.829809
1 2.857864 0.782900 1.581787
1 1.608610 2.002203 1.389454
6 2.776690 1.349682 -1.057595
1 2.898352 2.384096 -0.742835
1 3.729407 0.816329 -0.907212
1 2.535411 1.277158 -2.117146
6 -2.611216 -3.097070 -0.350348
1 -2.010877 -3.591952 0.417192
1 -3.612131 -3.536392 -0.323404
1 -2.176757 -3.316905 -1.328492
6 -3.517576 -0.931919 1.633852
1 -3.787438 0.117794 1.767114
1 -4.436846 -1.519091 1.716209
1 -2.855069 -1.230168 2.449930
6 -3.745877 -0.408633 -1.386016
1 -3.311376 -0.586984 -2.372753
1 -4.772953 -0.782524 -1.392711
1 -3.781449 0.671375 -1.218817

Name - **H_B2**

Zero-point correction= 0.400977 (Hartree/Particle)
Thermal correction to Energy= 0.423536
Thermal correction to Enthalpy= 0.424480
Thermal correction to Gibbs Free Energy= 0.350855
Sum of electronic and zero-point Energies= -1028.009102
Sum of electronic and thermal Energies= -1027.986544
Sum of electronic and thermal Enthalpies= -1027.985600
Sum of electronic and thermal Free Energies= -1028.059224

Charge = 1 Multiplicity = 1
6 0.257067 -1.527628 0.107895
6 -1.970393 -0.494048 -0.294504
6 -1.248513 -1.677588 0.305091
1 0.757073 -2.495639 0.090402
1 -1.758569 -0.286596 -1.339898
6 1.003188 -0.421842 -0.001025
6 -2.648311 0.569235 0.443340
1 -2.669521 0.556950 1.524192
1 -2.837607 1.516060 -0.050478
8 -3.468603 -0.545609 -0.090320
6 -4.347889 -0.294603 -1.232851

1 -3.880673 0.432401 -1.894907
1 -4.479564 -1.256154 -1.720434
1 -5.277866 0.080806 -0.815695
6 0.442820 0.958777 0.058921
6 0.153386 1.553322 1.292327
6 0.231809 1.698163 -1.110541
6 -0.376845 2.839817 1.352295
1 0.347338 1.000787 2.206064
6 -0.302101 2.981950 -1.050557
1 0.474619 1.254120 -2.070889
6 -0.613029 3.554742 0.180736
1 -0.600818 3.284232 2.315144
1 -0.471795 3.536639 -1.965940
1 -1.025238 4.555473 0.228013
14 2.892176 -0.531251 -0.175106
6 -1.552116 -1.848539 1.800283
1 -1.197333 -0.995314 2.381327
1 -2.623753 -1.985166 1.970426
1 -1.038375 -2.738675 2.166737
6 -1.724901 -2.920030 -0.469413
1 -1.183802 -3.799347 -0.116575
1 -2.791291 -3.091321 -0.306555
1 -1.540579 -2.811930 -1.541012
6 3.642114 0.309358 1.325418
1 4.733126 0.314554 1.255406
1 3.303572 1.346151 1.401174
1 3.362327 -0.209357 2.245833
6 3.411386 -2.330267 -0.264683
1 3.138272 -2.876230 0.641701
1 2.960738 -2.836367 -1.122085
1 4.497601 -2.390004 -0.374662
6 3.397602 0.380854 -1.736123
1 2.920022 -0.049672 -2.619980
1 3.127999 1.438560 -1.681172
1 4.480815 0.317392 -1.871752

Name - **H_B3**
Zero-point correction= 0.399911 (Hartree/Particle)
Thermal correction to Energy= 0.422640
Thermal correction to Enthalpy= 0.423584
Thermal correction to Gibbs Free Energy= 0.349294
Sum of electronic and zero-point Energies= -1028.013290
Sum of electronic and thermal Energies= -1027.990560
Sum of electronic and thermal Enthalpies= -1027.989616
Sum of electronic and thermal Free Energies= -1028.063906

Charge = 1 Multiplicity = 1
6 0.174026 -1.823882 0.103421
6 -1.476173 -0.152742 -0.220810

6	-1.311354	-1.629061	0.235410
1	0.610608	-2.818310	0.160005
1	-1.617280	-0.167321	-1.304125
6	0.903209	-0.716504	-0.048938
6	-2.611580	0.648428	0.411969
1	-2.518317	0.655631	1.499940
1	-2.581240	1.689483	0.059911
8	-3.864098	0.070902	0.129873
6	-4.329697	0.299307	-1.188997
1	-3.747583	-0.257754	-1.930602
1	-5.361175	-0.046708	-1.224581
1	-4.298008	1.366992	-1.432206
6	-0.019267	0.542528	-0.011490
6	0.046564	1.196499	1.301911
6	0.170837	1.444883	-1.149791
6	0.173917	2.549699	1.442058
1	-0.011289	0.560264	2.178954
6	0.297456	2.798772	-1.005886
1	0.176689	0.993304	-2.137808
6	0.288373	3.344848	0.288182
1	0.202593	3.009704	2.420744
1	0.407225	3.445441	-1.866011
1	0.385381	4.419576	0.402457
14	2.785977	-0.600862	-0.170040
6	-1.761481	-1.887483	1.680913
1	-1.247924	-1.247266	2.400754
1	-2.838176	-1.729403	1.774175
1	-1.543584	-2.923833	1.948620
6	-2.090087	-2.560297	-0.704329
1	-1.918872	-3.602716	-0.425394
1	-3.160942	-2.357522	-0.631675
1	-1.773149	-2.426853	-1.741568
6	3.382722	0.553535	1.183983
1	4.475932	0.556735	1.211424
1	3.056309	1.582336	1.007931
1	3.022069	0.241047	2.167423
6	3.459422	-2.332488	0.048443
1	3.088796	-3.003121	-0.730691
1	4.550542	-2.317385	-0.013153
1	3.181867	-2.746881	1.020684
6	3.251338	0.097821	-1.847659
1	2.821580	-0.495913	-2.658076
1	2.918763	1.132776	-1.963656
1	4.338929	0.089387	-1.962238

Name - **H_B4**

Zero-point correction= 0.402038 (Hartree/Particle)

Thermal correction to Energy= 0.424374

Thermal correction to Enthalpy= 0.425319

Thermal correction to Gibbs Free Energy= 0.351537
Sum of electronic and zero-point Energies= -1028.029297
Sum of electronic and thermal Energies= -1028.006961
Sum of electronic and thermal Enthalpies= -1028.006017
Sum of electronic and thermal Free Energies= -1028.079798

Charge = 1 Multiplicity = 1

6	0.359045	-1.381139	0.070435
6	-1.668822	0.081940	-0.266428
6	-1.141741	-1.353159	-0.002973
1	0.769204	-2.388092	0.132237
1	-1.559370	0.295071	-1.335442
6	1.211463	-0.329129	0.029783
6	-3.134028	0.294865	0.118387
1	-3.245278	0.273955	1.213977
1	-3.471595	1.276117	-0.236409
8	-3.930803	-0.702190	-0.467389
6	-5.295569	-0.554753	-0.122353
1	-5.681004	0.413687	-0.460073
1	-5.842849	-1.354416	-0.617799
1	-5.432515	-0.636465	0.962010
6	0.623557	0.988755	0.024717
6	-0.776768	1.131408	0.502046
6	1.321267	2.114435	-0.411545
6	-1.324878	2.506455	0.495883
1	-0.792529	0.811256	1.559266
6	0.712210	3.354548	-0.422135
1	2.333638	2.018743	-0.779923
6	-0.613273	3.564972	0.047490
1	-2.315338	2.658071	0.908088
1	1.271792	4.206459	-0.794227
1	-1.025111	4.564993	0.057023
14	3.101891	-0.638987	0.016495
6	-1.662356	-1.921743	1.334945
1	-1.426788	-1.272854	2.182668
1	-2.743876	-2.056693	1.280317
1	-1.206688	-2.895680	1.524213
6	-1.532904	-2.304452	-1.150185
1	-1.109190	-3.295975	-0.971374
1	-2.615222	-2.390005	-1.217700
1	-1.147351	-1.933991	-2.103270
6	3.896183	0.449164	1.320485
1	4.960693	0.210188	1.393354
1	3.811863	1.514871	1.097248
1	3.444391	0.269439	2.299410
6	3.804979	-0.293387	-1.688338
1	3.775882	0.761838	-1.967522
1	4.851366	-0.611138	-1.712702
1	3.263889	-0.861566	-2.448892
6	3.362232	-2.443041	0.443774
1	2.975282	-3.109934	-0.330384

1 4.435598 -2.631270 0.533401
1 2.897481 -2.707719 1.396746

Name - **H_B_TS1**
Zero-point correction= 0.398321 (Hartree/Particle)
Thermal correction to Energy= 0.421514
Thermal correction to Enthalpy= 0.422458
Thermal correction to Gibbs Free Energy= 0.345744
Sum of electronic and zero-point Energies= -1027.995345
Sum of electronic and thermal Energies= -1027.972152
Sum of electronic and thermal Enthalpies= -1027.971208
Sum of electronic and thermal Free Energies= -1028.047922
1 imaginary frequency.
Charge = 1 Multiplicity = 1
6 -0.223624 -1.315987 0.476102
6 -2.093247 -0.756691 -0.292754
6 -1.631653 -0.963343 1.067809
1 -0.105117 -2.389727 0.356020
1 -2.225983 -1.633426 -0.922164
6 0.796605 -0.510545 0.132115
6 -2.513202 0.526297 -0.882426
1 -2.250159 1.434780 -0.352445
1 -2.425760 0.622250 -1.961872
8 -3.806873 0.055978 -0.466439
6 -4.673895 -0.370992 -1.531805
1 -4.172850 -1.099547 -2.172037
1 -5.539106 -0.823671 -1.055722
1 -4.965112 0.503282 -2.114862
6 0.782401 0.975006 0.143118
6 1.249038 1.680294 1.257862
6 0.399404 1.681665 -0.999276
6 1.269743 3.069479 1.247157
1 1.572518 1.135324 2.138320
6 0.424098 3.073981 -1.007601
1 0.095866 1.137640 -1.888325
6 0.850537 3.770388 0.117983
1 1.614359 3.606825 2.122703
1 0.116803 3.611289 -1.897052
1 0.869036 4.853324 0.112813
14 2.467679 -1.280259 -0.414577
6 -1.698420 0.229375 2.011939
1 -1.326839 1.153832 1.577299
1 -2.736798 0.376567 2.317492
1 -1.104473 0.011673 2.900877
6 -2.215670 -2.220591 1.716043
1 -1.630348 -2.476978 2.600525
1 -3.245740 -2.026247 2.019186
1 -2.206445 -3.071123 1.032284
6 3.762864 -0.691480 0.803138

1 4.734416 -1.119070 0.541002
1 3.857070 0.396786 0.785853
1 3.519625 -1.001847 1.822296
6 2.325127 -3.146358 -0.409057
1 2.104459 -3.534380 0.588241
1 1.555443 -3.499407 -1.099814
1 3.278298 -3.576076 -0.729221
6 2.824302 -0.631820 -2.135605
1 2.041896 -0.924917 -2.839986
1 2.903430 0.457983 -2.139817
1 3.772549 -1.041394 -2.494452

Name - **H_B_TS2**
Zero-point correction= 0.398313 (Hartree/Particle)
Thermal correction to Energy= 0.421230
Thermal correction to Enthalpy= 0.422174
Thermal correction to Gibbs Free Energy= 0.346885
Sum of electronic and zero-point Energies= -1027.997734
Sum of electronic and thermal Energies= -1027.974817
Sum of electronic and thermal Enthalpies= -1027.973873
Sum of electronic and thermal Free Energies= -1028.049162
1 imaginary frequency.
Charge = 1 Multiplicity = 1
6 0.458932 -1.588038 0.030171
6 -1.712536 -0.496380 -0.257306
6 -1.050255 -1.721199 0.251245
1 0.978682 -2.543226 -0.013095
1 -1.679989 -0.341417 -1.332512
6 1.114182 -0.428775 -0.039345
6 -2.732503 0.284780 0.459934
1 -2.688674 0.244890 1.544227
1 -2.888438 1.297919 0.090920
8 -3.701440 -0.651750 -0.026637
6 -4.522492 -0.165555 -1.097974
1 -3.911357 0.207699 -1.923145
1 -5.117736 -1.011274 -1.432151
1 -5.165751 0.630699 -0.719748
6 0.359450 0.850003 0.046349
6 0.057767 1.418081 1.299755
6 0.032696 1.572495 -1.116688
6 -0.590287 2.643158 1.380673
1 0.348286 0.890102 2.201946
6 -0.614045 2.799765 -1.030264
1 0.295098 1.158471 -2.085078
6 -0.926137 3.335263 0.217006
1 -0.825033 3.065054 2.350420
1 -0.865979 3.341376 -1.933757
1 -1.424171 4.295031 0.284956
14 3.007944 -0.325092 -0.173398

6 -1.336328 -2.000195 1.731034
1 -0.997698 -1.180065 2.366516
1 -2.404316 -2.166604 1.892095
1 -0.801071 -2.901891 2.032242
6 -1.558802 -2.894731 -0.627356
1 -1.035240 -3.800618 -0.316921
1 -2.630347 -3.036037 -0.487341
1 -1.350531 -2.716488 -1.683777
6 3.615103 0.540545 1.374708
1 4.703214 0.643944 1.352520
1 3.185083 1.542257 1.459248
1 3.345214 -0.024737 2.270405
6 3.698579 -2.060067 -0.306749
1 3.314485 -2.574936 -1.190877
1 4.787557 -2.016012 -0.392370
1 3.457220 -2.658692 0.575082
6 3.425686 0.694114 -1.691635
1 3.022843 0.240609 -2.600632
1 3.024427 1.707430 -1.605843
1 4.510477 0.772222 -1.804015

Name - **H_B_TS3**
Zero-point correction= 0.399571 (Hartree/Particle)
Thermal correction to Energy= 0.421975
Thermal correction to Enthalpy= 0.422919
Thermal correction to Gibbs Free Energy= 0.349206
Sum of electronic and zero-point Energies= -1028.001583
Sum of electronic and thermal Energies= -1027.979179
Sum of electronic and thermal Enthalpies= -1027.978235
Sum of electronic and thermal Free Energies= -1028.051948
1 imaginary frequency.
Charge = 1 Multiplicity = 1
6 0.521174 -1.654828 0.036093
6 -1.431439 -0.239895 -0.326039
6 -0.989427 -1.655012 0.027247
1 1.024231 -2.614244 0.127658
1 -1.336448 -0.042370 -1.391094
6 1.178398 -0.498364 -0.064181
6 -2.776123 0.275707 0.165011
1 -2.891913 0.166569 1.250142
1 -2.902049 1.330047 -0.102937
8 -3.710440 -0.521735 -0.519622
6 -5.046631 -0.158217 -0.204910
1 -5.235191 0.887427 -0.468628
1 -5.697988 -0.804542 -0.789189
1 -5.244581 -0.305103 0.861868
6 0.323465 0.718439 -0.081088
6 -0.380811 1.081424 1.096501
6 0.441373 1.705376 -1.119605

6 -0.952151 2.362142 1.240736
1 -0.373103 0.393153 1.933490
6 -0.127284 2.936479 -0.970402
1 0.986491 1.444579 -2.019479
6 -0.819446 3.272916 0.223720
1 -1.469209 2.615812 2.157004
1 -0.036963 3.675221 -1.756996
1 -1.238279 4.266487 0.329536
14 3.069826 -0.330625 0.011167
6 -1.552712 -2.165389 1.360320
1 -1.280193 -1.530726 2.205349
1 -2.641464 -2.238409 1.308585
1 -1.157134 -3.163860 1.555643
6 -1.474554 -2.582183 -1.113019
1 -1.123668 -3.596258 -0.908976
1 -2.562756 -2.585290 -1.165541
1 -1.068611 -2.263109 -2.074998
6 3.446503 0.744699 1.500288
1 4.525120 0.884951 1.609426
1 2.991874 1.734002 1.390491
1 3.066792 0.293775 2.420398
6 3.703344 0.493031 -1.549956
1 3.413313 1.545453 -1.598889
1 4.796188 0.453034 -1.560672
1 3.339378 -0.011256 -2.448387
6 3.774317 -2.054371 0.189450
1 3.516440 -2.679732 -0.668996
1 4.864498 -2.000279 0.248197
1 3.413209 -2.544446 1.096646

Name - **H_D2**
Zero-point correction= 0.305037 (Hartree/Particle)
Thermal correction to Energy= 0.323261
Thermal correction to Enthalpy= 0.324205
Thermal correction to Gibbs Free Energy= 0.257896
Sum of electronic and zero-point Energies= -910.121173
Sum of electronic and thermal Energies= -910.102949
Sum of electronic and thermal Enthalpies= -910.102005
Sum of electronic and thermal Free Energies= -910.168315

Charge = 1 Multiplicity = 1
6 -0.175262 -0.089718 0.512710
6 -1.592969 0.412139 0.571239
6 -2.544682 -0.018519 -0.611968
1 -0.046084 -1.160216 0.743153
1 -1.627569 1.508903 0.661469
6 0.937449 0.638695 0.202354
6 -2.516216 -0.239523 1.624825
1 -2.252430 -1.279666 1.884862

1 -2.818440 0.345906 2.502993
8 -3.690651 -0.260131 0.616355
6 -4.701051 -1.361322 0.635611
1 -5.248433 -1.255551 1.583541
1 -5.363071 -1.173860 -0.220135
1 -4.200115 -2.339539 0.561661
6 2.261113 -0.045547 0.110229
6 2.379595 -1.290473 -0.564844
6 3.427937 0.529016 0.680863
6 3.619970 -1.947707 -0.651378
1 1.499095 -1.723611 -1.052593
6 4.665083 -0.136150 0.602054
1 3.364326 1.481874 1.215959
6 4.766599 -1.374046 -0.064836
1 3.695569 -2.899337 -1.186626
1 5.550893 0.313415 1.060768
1 5.732513 -1.882879 -0.134527
14 0.944277 2.524622 -0.248543
6 -2.251350 -1.349675 -1.263513
1 -1.981764 -2.133629 -0.537180
1 -3.090384 -1.692576 -1.891250
1 -1.373963 -1.207082 -1.922163
6 -3.078780 1.065991 -1.507235
1 -3.878930 0.699749 -2.172325
1 -3.442174 1.927266 -0.925368
1 -2.244593 1.417186 -2.146134
1 1.572271 2.662200 -1.611009
1 1.739646 3.299420 0.769397
1 -0.465652 3.069398 -0.292411

Name - **H_D3**

Zero-point correction= 0.429677 (Hartree/Particle)
Thermal correction to Energy= 0.453425
Thermal correction to Enthalpy= 0.454369
Thermal correction to Gibbs Free Energy= 0.378311
Sum of electronic and zero-point Energies= -1067.246522
Sum of electronic and thermal Energies= -1067.222774
Sum of electronic and thermal Enthalpies= -1067.221830
Sum of electronic and thermal Free Energies= -1067.297888

Charge = 1 Multiplicity = 1
6 0.150589 -1.244698 -0.446678
6 1.536355 -0.727355 -0.777296
6 2.267680 0.149516 0.295585
1 0.062692 -2.329442 -0.512253
6 -0.946677 -0.538816 -0.145286
6 2.657258 -1.764226 -0.602744
8 3.546094 -0.719916 -0.059620
6 4.591884 -1.062507 0.878473

1 5.325290 -1.644106 0.322725
1 5.027058 -0.124843 1.217850
1 4.175110 -1.634219 1.707351
6 -0.969802 0.950843 -0.069916
6 -1.021044 1.728752 -1.232272
6 -1.029732 1.601274 1.168166
6 -1.045152 3.118056 -1.157956
1 -1.064839 1.237401 -2.198147
6 -1.045381 2.990219 1.244048
1 -1.075811 1.012027 2.078579
6 -1.036788 3.753481 0.079897
1 -1.082239 3.704194 -2.068684
1 -1.082081 3.476189 2.211933
1 -1.055138 4.834897 0.137495
14 -2.625744 -1.407816 0.131658
6 1.914918 -0.134973 1.732290
1 1.704465 -1.188508 1.922073
1 2.701799 0.219026 2.401884
1 1.012195 0.428979 1.962456
6 2.564446 1.592180 0.013676
1 3.232530 2.007080 0.771547
1 2.996295 1.738046 -0.974643
1 1.615961 2.139053 0.064150
6 -3.260048 -0.960107 1.838168
1 -3.450961 0.111913 1.927663
1 -4.204618 -1.477401 2.027176
1 -2.560607 -1.254705 2.624874
6 -3.784089 -0.759287 -1.188843
1 -3.424005 -1.003049 -2.191437
1 -4.778671 -1.198589 -1.075297
1 -3.890569 0.326424 -1.119152
6 -2.382033 -3.260069 -0.020403
1 -2.029957 -3.548619 -1.013947
1 -1.680938 -3.646608 0.723942
1 -3.337711 -3.765247 0.142917
6 1.627031 -0.138514 -2.191008
1 1.175288 -0.836024 -2.898777
1 1.096340 0.808658 -2.254490
1 2.666853 0.024606 -2.487544
1 3.102958 -2.198642 -1.496061
1 2.478462 -2.512351 0.172160

5.2.2 Geometries for the Figure SI3 (R = Me)

Name - **Me_A1**
Zero-point correction= 0.426798 (Hartree/Particle)

Thermal correction to Energy= 0.452007
Thermal correction to Enthalpy= 0.452952
Thermal correction to Gibbs Free Energy= 0.371317
Sum of electronic and zero-point Energies= -1067.297743
Sum of electronic and thermal Energies= -1067.272533
Sum of electronic and thermal Enthalpies= -1067.271589
Sum of electronic and thermal Free Energies= -1067.353224

Charge = 1 Multiplicity = 1

6	-0.129092	-1.246921	-0.415826
6	-1.695394	-1.199848	-0.415228
6	-1.319447	-1.445920	0.972436
1	0.212222	-2.250249	-0.642032
6	0.837217	-0.309524	-0.192131
6	-2.422327	0.105099	-0.708120
1	-1.957649	0.976218	-0.245572
1	-2.441636	0.269906	-1.793842
8	-3.726657	-0.069156	-0.203772
6	-4.532047	1.076231	-0.414602
1	-4.636687	1.286393	-1.484509
1	-5.511700	0.865836	0.010118
1	-4.099566	1.951925	0.082419
6	0.637509	1.139282	-0.000331
6	1.012654	1.774775	1.188920
6	0.192948	1.909430	-1.082401
6	0.885753	3.153254	1.310984
1	1.369972	1.186708	2.026262
6	0.102881	3.290864	-0.964462
1	-0.065370	1.421399	-2.016046
6	0.436985	3.913774	0.234768
1	1.149282	3.634502	2.244902
1	-0.231331	3.879550	-1.810188
1	0.356076	4.989992	0.328087
14	2.689287	-0.863200	-0.303455
6	-1.415581	-0.381790	2.016105
1	-2.403832	-0.525691	2.470367
1	-0.665550	-0.520989	2.794600
1	-1.375217	0.633541	1.636251
6	-1.142350	-2.827272	1.520540
1	-0.370879	-2.841885	2.290633
1	-2.095410	-3.081671	2.001200
1	-0.932513	-3.584709	0.771784
6	-2.273083	-2.340829	-1.244663
1	-3.320103	-2.480033	-0.974725
1	-2.218014	-2.071975	-2.300490
1	-1.745274	-3.281964	-1.106633
6	3.395598	0.119287	-1.728111
1	3.320204	1.191823	-1.532234
1	4.451229	-0.129126	-1.864605
1	2.870401	-0.099727	-2.660648
6	3.528772	-0.429437	1.313340

1 4.519073 -0.894008 1.316388
1 3.664117 0.647324 1.428201
1 2.979061 -0.810335 2.177321
6 2.738451 -2.708049 -0.604055
1 2.247671 -3.262397 0.200772
1 2.275667 -2.985290 -1.554021
1 3.782326 -3.031453 -0.638190

Name - **Me_A2**
Zero-point correction= 0.426563 (Hartree/Particle)
Thermal correction to Energy= 0.451083
Thermal correction to Enthalpy= 0.452027
Thermal correction to Gibbs Free Energy= 0.374206
Sum of electronic and zero-point Energies= -1067.301519
Sum of electronic and thermal Energies= -1067.276999
Sum of electronic and thermal Enthalpies= -1067.276055
Sum of electronic and thermal Free Energies= -1067.353875

Charge = 1 Multiplicity = 1
6 0.136191 -1.362158 0.377149
6 -1.376527 -1.127367 0.508775
6 -1.678502 0.108551 1.284255
1 0.425099 -2.402456 0.510940
6 1.042726 -0.439278 0.043936
6 -1.990523 -1.157960 -0.896714
1 -1.666839 -0.286570 -1.479587
1 -1.621237 -2.056824 -1.408219
8 -3.392659 -1.193177 -0.791884
6 -4.023729 -1.184358 -2.060023
1 -3.719815 -2.054969 -2.650751
1 -5.097389 -1.221513 -1.887124
1 -3.774025 -0.271170 -2.611663
6 0.651972 0.983609 -0.139126
6 0.675831 1.867792 0.946445
6 0.269972 1.467604 -1.397634
6 0.248891 3.185739 0.797519
1 1.038515 1.517845 1.907054
6 -0.162093 2.779265 -1.543101
1 0.300111 0.804164 -2.255646
6 -0.189597 3.637288 -0.441558
1 0.260080 3.854225 1.650244
1 -0.478217 3.137012 -2.515747
1 -0.532415 4.658090 -0.558749
14 2.873869 -0.884346 -0.224462
6 -2.560362 1.150647 0.765173
1 -3.548244 0.668948 0.674077
1 -2.619287 2.021106 1.412446
1 -2.296271 1.425501 -0.261339
6 -1.287796 0.169868 2.700614

1	-1.165994	1.194846	3.044028
1	-2.166469	-0.234623	3.234393
1	-0.431277	-0.453818	2.949103
6	-1.979693	-2.303857	1.340098
1	-3.037242	-2.143403	1.545962
1	-1.881614	-3.203360	0.730312
1	-1.435239	-2.448396	2.271850
6	3.297977	-0.436495	-1.994833
1	3.139280	0.628791	-2.180769
1	4.348499	-0.660294	-2.198837
1	2.686828	-1.003533	-2.701474
6	3.878984	0.150396	0.972667
1	4.945931	-0.046970	0.839071
1	3.710506	1.217259	0.804346
1	3.618677	-0.079370	2.009131
6	3.110663	-2.714534	0.092379
1	2.842612	-2.982512	1.117519
1	2.514893	-3.323348	-0.592153
1	4.161353	-2.976906	-0.056997

Name - **Me_A3**

Zero-point correction= 0.426355 (Hartree/Particle)
Thermal correction to Energy= 0.450806
Thermal correction to Enthalpy= 0.451750
Thermal correction to Gibbs Free Energy= 0.373682
Sum of electronic and zero-point Energies= -1067.301899
Sum of electronic and thermal Energies= -1067.277448
Sum of electronic and thermal Enthalpies= -1067.276504
Sum of electronic and thermal Free Energies= -1067.354572

Charge = 1 Multiplicity = 1

6	-0.148406	-1.178585	0.246425
6	-1.550532	-0.622085	0.494726
6	-1.799122	0.759671	-0.000946
1	-0.141838	-2.265878	0.298121
6	1.002471	-0.520045	0.070805
6	-2.515945	-1.481981	-0.395899
1	-2.169840	-1.491661	-1.436090
1	-2.476835	-2.504649	0.000037
8	-3.809505	-0.950091	-0.299600
6	-4.769771	-1.736663	-0.988202
1	-4.804709	-2.748828	-0.573046
1	-5.735248	-1.254126	-0.852935
1	-4.531668	-1.789440	-2.055340
6	1.047451	0.961029	0.036712
6	0.551940	1.713528	1.108986
6	1.539908	1.636114	-1.087979
6	0.498721	3.107415	1.037634
1	0.244288	1.206620	2.017190

6 1.481762 3.020272 -1.158877
1 1.921495 1.067447 -1.928128
6 0.948763 3.761352 -0.100129
1 0.109753 3.673345 1.876062
1 1.844245 3.528284 -2.044715
1 0.903865 4.841771 -0.162356
14 2.646637 -1.484563 -0.018281
6 -1.570944 1.103339 -1.410141
1 -2.577627 1.119927 -1.859134
1 -1.189649 2.125402 -1.492292
1 -0.938394 0.400044 -1.944890
6 -2.602754 1.691183 0.792655
1 -2.614898 2.697806 0.381662
1 -3.616135 1.254049 0.706220
1 -2.357630 1.681906 1.852923
6 -1.929987 -0.847411 1.965779
1 -2.989848 -0.651885 2.132913
1 -1.730637 -1.888938 2.221963
1 -1.336665 -0.223010 2.634445
6 3.499122 -1.198203 -1.666315
1 3.881520 -0.179314 -1.757692
1 4.352146 -1.878347 -1.745952
1 2.831419 -1.398420 -2.507960
6 3.714133 -0.826578 1.374607
1 4.680928 -1.336575 1.390532
1 3.899163 0.243461 1.246392
1 3.233521 -0.976307 2.344655
6 2.281512 -3.308205 0.205949
1 1.795363 -3.508204 1.163916
1 1.646579 -3.697064 -0.594150
1 3.220525 -3.867693 0.185641

Name - **Me_A4**
Zero-point correction= 0.429735 (Hartree/Particle)
Thermal correction to Energy= 0.453220
Thermal correction to Enthalpy= 0.454164
Thermal correction to Gibbs Free Energy= 0.377919
Sum of electronic and zero-point Energies= -1067.309186
Sum of electronic and thermal Energies= -1067.285702
Sum of electronic and thermal Enthalpies= -1067.284758
Sum of electronic and thermal Free Energies= -1067.361003

Charge = 1 Multiplicity = 1
6 -0.045041 -1.159112 0.371949
6 -1.456318 -0.648094 0.511828
6 -1.585479 0.849183 0.076886
1 0.041358 -2.240590 0.472133
6 1.077372 -0.437784 0.147934
6 -2.312571 -1.592408 -0.353913

1	-1.963770	-1.581586	-1.395179
1	-2.184985	-2.616220	0.026632
8	-3.669109	-1.228122	-0.295038
6	-4.482683	-2.097387	-1.058926
1	-4.410426	-3.125432	-0.686729
1	-5.509612	-1.749442	-0.963667
1	-4.188723	-2.078509	-2.114637
6	0.928364	0.999173	0.055745
6	-0.290689	1.610878	0.629930
6	1.871672	1.805372	-0.575251
6	-0.393855	3.077540	0.524729
1	-0.291670	1.388169	1.710676
6	1.672701	3.173042	-0.667055
1	2.754080	1.368957	-1.023845
6	0.547631	3.825118	-0.099253
1	-1.248254	3.555897	0.988629
1	2.412541	3.772030	-1.187818
1	0.460537	4.901271	-0.165602
14	2.763480	-1.330789	-0.021582
6	-1.620949	0.987709	-1.450386
1	-0.815456	0.432892	-1.937618
1	-2.575135	0.612194	-1.825602
1	-1.539049	2.038611	-1.738399
6	-2.832077	1.515124	0.671876
1	-3.016492	2.476666	0.189774
1	-3.696780	0.878519	0.491528
1	-2.738605	1.679366	1.747925
6	-1.849954	-0.864398	1.991562
1	-2.917632	-0.688547	2.120809
1	-1.636320	-1.894814	2.283148
1	-1.299679	-0.207679	2.668842
6	3.991370	-0.493825	1.120452
1	4.961729	-0.991982	1.044150
1	4.139864	0.561803	0.882859
1	3.658036	-0.564027	2.158947
6	3.349062	-1.293894	-1.805066
1	3.696500	-0.312717	-2.133741
1	4.186092	-1.989483	-1.914886
1	2.553838	-1.619519	-2.480098
6	2.502682	-3.107240	0.506694
1	2.086538	-3.176482	1.514701
1	1.848180	-3.650353	-0.179508
1	3.470013	-3.616962	0.510627

Name - **Me_A_TS1**

Zero-point correction= 0.426215 (Hartree/Particle)
Thermal correction to Energy= 0.450582
Thermal correction to Enthalpy= 0.451526
Thermal correction to Gibbs Free Energy= 0.373312

Sum of electronic and zero-point Energies= -1067.295479
Sum of electronic and thermal Energies= -1067.271112
Sum of electronic and thermal Enthalpies= -1067.270168
Sum of electronic and thermal Free Energies= -1067.348382
1 imaginary frequency.
Charge = 1 Multiplicity = 1

6	-0.049952	-1.374972	-0.148842
6	-1.611042	-1.282362	-0.103770
6	-1.717263	-0.900852	1.310535
1	0.261058	-2.416604	-0.187751
6	0.894604	-0.424585	-0.139146
6	-2.188906	-0.265196	-1.084711
1	-1.712184	0.713885	-0.997012
1	-2.015348	-0.631331	-2.105024
8	-3.566233	-0.166872	-0.808547
6	-4.210156	0.786822	-1.634449
1	-4.112744	0.514196	-2.690395
1	-5.262674	0.795815	-1.358771
1	-3.783440	1.784180	-1.479971
6	0.698224	1.039611	0.032614
6	0.828408	1.605886	1.304101
6	0.494412	1.877586	-1.068153
6	0.696825	2.979447	1.480499
1	1.024106	0.963372	2.157159
6	0.360745	3.250318	-0.889072
1	0.431291	1.447909	-2.062470
6	0.454545	3.803821	0.385586
1	0.786470	3.404438	2.473093
1	0.188576	3.888303	-1.747649
1	0.352357	4.873495	0.522160
14	2.729686	-0.940726	-0.361557
6	-2.099219	0.450385	1.727121
1	-3.194461	0.335917	1.845224
1	-1.691201	0.728471	2.696460
1	-1.951135	1.223309	0.978511
6	-1.547327	-1.911710	2.370624
1	-1.228378	-1.467352	3.311139
1	-2.555393	-2.331500	2.525469
1	-0.902776	-2.739089	2.083023
6	-2.186845	-2.675658	-0.410375
1	-3.272190	-2.653779	-0.318517
1	-1.924878	-2.930530	-1.438224
1	-1.784973	-3.447874	0.243216
6	3.379488	0.014369	-1.835369
1	3.332960	1.091496	-1.657789
1	4.423254	-0.253439	-2.019962
1	2.806978	-0.210441	-2.738556
6	3.642653	-0.451545	1.200285
1	4.690423	-0.754241	1.121142
1	3.615001	0.629749	1.353281
1	3.216078	-0.937110	2.081419

6 2.825568 -2.788095 -0.650610
1 2.453309 -3.357495 0.204585
1 2.265213 -3.087628 -1.539697
1 3.870397 -3.070595 -0.805121

Name - **Me_A_TS2**
Zero-point correction= 0.426454 (Hartree/Particle)
Thermal correction to Energy= 0.450159
Thermal correction to Enthalpy= 0.451103
Thermal correction to Gibbs Free Energy= 0.375288
Sum of electronic and zero-point Energies= -1067.296470
Sum of electronic and thermal Energies= -1067.272766
Sum of electronic and thermal Enthalpies= -1067.271822
Sum of electronic and thermal Free Energies= -1067.347636
1 imaginary frequency.
Charge = 1 Multiplicity = 1
6 -0.164112 -1.223241 0.375121
6 -1.624745 -0.761493 0.563601
6 -1.794872 0.725638 0.598344
1 -0.113213 -2.302254 0.512542
6 0.942220 -0.544434 0.074168
6 -2.412057 -1.333727 -0.635609
1 -1.984210 -1.006709 -1.590607
1 -2.341342 -2.428013 -0.594923
8 -3.746295 -0.909549 -0.508435
6 -4.567636 -1.390324 -1.558846
1 -4.579870 -2.485065 -1.569321
1 -5.573930 -1.017826 -1.378245
1 -4.210430 -1.023856 -2.527283
6 0.972316 0.926970 -0.093913
6 0.929223 1.766027 1.025053
6 1.082377 1.499080 -1.369559
6 0.926964 3.151887 0.870905
1 0.910080 1.325918 2.016355
6 1.075915 2.877122 -1.521208
1 1.137019 0.851854 -2.238496
6 0.986866 3.708552 -0.400486
1 0.884555 3.790714 1.745233
1 1.137354 3.310617 -2.512320
1 0.982109 4.784706 -0.524311
14 2.616008 -1.448810 -0.069730
6 -2.013341 1.516590 -0.614019
1 -3.109422 1.650465 -0.636950
1 -1.577764 2.513984 -0.517239
1 -1.710309 1.031490 -1.535827
6 -2.026776 1.406591 1.876702
1 -1.913748 2.485493 1.805013
1 -3.087724 1.182023 2.092470
1 -1.460618 0.986555 2.705689

6 -2.142384 -1.429480 1.856393
1 -3.186954 -1.175356 2.037562
1 -2.076451 -2.510734 1.729126
1 -1.542061 -1.160701 2.724936
6 3.307508 -1.166270 -1.790145
1 3.512630 -0.108455 -1.971030
1 4.248786 -1.712076 -1.899560
1 2.618860 -1.522023 -2.560562
6 3.743860 -0.680184 1.215540
1 4.736098 -1.137271 1.174856
1 3.859123 0.392556 1.038478
1 3.345311 -0.819753 2.223613
6 2.359095 -3.276016 0.251972
1 1.957688 -3.457830 1.252069
1 1.683216 -3.724051 -0.480883
1 3.318951 -3.794396 0.179234

Name - **Me_A_TS3**
Zero-point correction= 0.427287 (Hartree/Particle)
Thermal correction to Energy= 0.450664
Thermal correction to Enthalpy= 0.451608
Thermal correction to Gibbs Free Energy= 0.376704
Sum of electronic and zero-point Energies= -1067.299617
Sum of electronic and thermal Energies= -1067.276240
Sum of electronic and thermal Enthalpies= -1067.275296
Sum of electronic and thermal Free Energies= -1067.350200
1 imaginary frequency.
Charge = 1 Multiplicity = 1
6 -0.027223 -1.229234 0.261014
6 -1.452236 -0.742702 0.492603
6 -1.716687 0.692668 0.093899
1 0.057586 -2.312376 0.326407
6 1.065815 -0.483055 0.066239
6 -2.356233 -1.599169 -0.445334
1 -2.007372 -1.530404 -1.482667
1 -2.263447 -2.642774 -0.116811
8 -3.684512 -1.158775 -0.336430
6 -4.576604 -1.939078 -1.114618
1 -4.565955 -2.982567 -0.783491
1 -5.572470 -1.523476 -0.975464
1 -4.306390 -1.894093 -2.175002
6 0.934272 0.983403 0.025752
6 0.200248 1.638655 1.034316
6 1.444516 1.740490 -1.035987
6 -0.003702 3.031372 0.979667
1 -0.039436 1.101940 1.944330
6 1.207124 3.103235 -1.096982
1 1.986533 1.247407 -1.833813
6 0.476036 3.756121 -0.089674

1 -0.538485 3.525431 1.782507
1 1.585737 3.674418 -1.936658
1 0.311083 4.824522 -0.148074
14 2.794486 -1.287482 -0.019892
6 -1.623177 1.066833 -1.337323
1 -0.935392 0.448995 -1.909753
1 -2.641622 0.936640 -1.731947
1 -1.379330 2.125980 -1.449723
6 -2.682943 1.484897 0.894427
1 -2.768990 2.507117 0.531684
1 -3.638571 0.963225 0.724699
1 -2.490827 1.463638 1.964946
6 -1.842926 -1.060617 1.946585
1 -2.912727 -0.918665 2.103179
1 -1.605645 -2.105199 2.154042
1 -1.291876 -0.449667 2.662731
6 3.813725 -0.465139 1.320524
1 4.829478 -0.868460 1.335165
1 3.881502 0.612620 1.148398
1 3.368517 -0.625848 2.305628
6 3.585326 -1.004775 -1.699421
1 3.915660 0.027786 -1.830583
1 4.469260 -1.643656 -1.784625
1 2.905851 -1.262167 -2.515504
6 2.600002 -3.122062 0.298724
1 2.125030 -3.316355 1.263350
1 2.014657 -3.611908 -0.483422
1 3.588931 -3.588210 0.313925

Name - **Me_B2**
Zero-point correction= 0.425389 (Hartree/Particle)
Thermal correction to Energy= 0.449987
Thermal correction to Enthalpy= 0.450932
Thermal correction to Gibbs Free Energy= 0.373157
Sum of electronic and zero-point Energies= -1067.299841
Sum of electronic and thermal Energies= -1067.275242
Sum of electronic and thermal Enthalpies= -1067.274298
Sum of electronic and thermal Free Energies= -1067.352072

Charge = 1 Multiplicity = 1
6 0.884017 -1.507073 0.208952
6 -1.529366 -1.251568 -0.354037
6 -0.557234 -1.937040 0.534068
1 1.586883 -2.336502 0.162029
6 1.304872 -0.246821 0.072943
6 -2.701164 -0.569960 0.211000
1 -3.194102 -1.298388 0.884873
1 -2.337907 0.233374 0.881075
8 -3.559718 -0.098538 -0.769214

6	-4.624032	0.676884	-0.231961
1	-4.229496	1.553948	0.290595
1	-5.234817	0.994635	-1.073355
1	-5.229159	0.079004	0.455844
6	0.341583	0.883081	0.152868
6	0.065937	1.498440	1.381301
6	-0.307472	1.348833	-0.997078
6	-0.900179	2.491993	1.466913
1	0.600493	1.177253	2.268902
6	-1.275835	2.347737	-0.910705
1	-0.045936	0.926300	-1.961063
6	-1.587259	2.906392	0.322805
1	-1.121302	2.946243	2.425501
1	-1.785279	2.682032	-1.806634
1	-2.344229	3.678214	0.396777
14	3.136120	0.179065	-0.214794
6	-0.827160	-1.778512	2.037475
1	-0.862000	-0.732995	2.343336
1	-1.758395	-2.269955	2.329592
1	-0.014425	-2.259363	2.583359
6	-0.697148	-3.452295	0.169673
1	-0.054959	-3.999699	0.860853
1	-1.723073	-3.799880	0.302528
1	-0.370693	-3.655874	-0.849161
6	3.676953	1.304188	1.183794
1	4.725773	1.585660	1.057575
1	3.082850	2.221658	1.200546
1	3.572411	0.809875	2.152955
6	4.133624	-1.405637	-0.241405
1	4.063004	-1.939411	0.709618
1	3.804013	-2.074949	-1.039948
1	5.187066	-1.171794	-0.416304
6	3.244437	1.079650	-1.855940
1	2.651506	1.997923	-1.840613
1	4.281254	1.352868	-2.070332
1	2.883720	0.451731	-2.674593
6	-1.475669	-1.436940	-1.804791
1	-2.175567	-2.273798	-1.987266
1	-1.908155	-0.587970	-2.330653
1	-0.490857	-1.716850	-2.170463

Name - **Me_B3**

Zero-point correction= 0.426014 (Hartree/Particle)
Thermal correction to Energy= 0.450408
Thermal correction to Enthalpy= 0.451352
Thermal correction to Gibbs Free Energy= 0.374043
Sum of electronic and zero-point Energies= -1067.296765
Sum of electronic and thermal Energies= -1067.272371
Sum of electronic and thermal Enthalpies= -1067.271427

Sum of electronic and thermal Free Energies= -1067.348736

Charge = 1 Multiplicity = 1

6	-0.803685	1.485017	-0.109118
6	1.658010	0.914179	-0.458390
6	0.658949	1.930386	-0.054374
1	-1.465821	2.347810	-0.161769
6	-1.322084	0.256039	-0.011776
6	2.924926	0.820302	0.294742
1	3.370745	1.833701	0.205843
1	2.719542	0.690349	1.366607
8	3.763729	-0.155928	-0.217069
6	4.956366	-0.300002	0.544300
1	4.720719	-0.581843	1.575200
1	5.534789	-1.090255	0.072485
1	5.532876	0.629899	0.541296
6	-0.457248	-0.944780	0.077994
6	0.501549	-1.073807	1.092423
6	-0.542080	-1.946168	-0.896133
6	1.394972	-2.147588	1.095655
1	0.518889	-0.352398	1.902534
6	0.345889	-3.013020	-0.890690
1	-1.274163	-1.856882	-1.690171
6	1.327473	-3.110401	0.098143
1	2.134907	-2.230204	1.883701
1	0.281781	-3.768291	-1.665108
1	2.022111	-3.941308	0.094291
14	-3.209459	0.030373	0.140483
6	0.917326	2.571600	1.317621
1	0.869186	1.838820	2.124260
1	1.880830	3.084711	1.354781
1	0.141843	3.315548	1.503433
6	0.851092	3.036471	-1.157403
1	0.207485	3.869274	-0.871133
1	1.882093	3.393523	-1.192906
1	0.551863	2.677024	-2.140612
6	-3.502833	-0.688132	1.847924
1	-4.568900	-0.862990	2.014809
1	-2.982757	-1.643431	1.959523
1	-3.142093	-0.010101	2.625443
6	-4.037579	1.700913	-0.046024
1	-3.720540	2.403717	0.728095
1	-3.833171	2.145087	-1.023583
1	-5.120142	1.575080	0.042350
6	-3.857279	-1.154020	-1.164096
1	-3.504997	-2.174137	-0.996400
1	-4.949851	-1.168889	-1.114103
1	-3.572274	-0.846911	-2.173326
6	1.594861	0.226045	-1.744538
1	2.396425	0.670187	-2.357284
1	1.906506	-0.816932	-1.615148

1 0.632959 0.313842 -2.240866

Name - **Me_B4**

Zero-point correction= 0.429924 (Hartree/Particle)
Thermal correction to Energy= 0.453510
Thermal correction to Enthalpy= 0.454455
Thermal correction to Gibbs Free Energy= 0.378031
Sum of electronic and zero-point Energies= -1067.309680
Sum of electronic and thermal Energies= -1067.286094
Sum of electronic and thermal Enthalpies= -1067.285150
Sum of electronic and thermal Free Energies= -1067.361573

Charge = 1 Multiplicity = 1

6	0.794722	-1.475778	0.065422
6	-1.535296	-0.520200	-0.205186
6	-0.678436	-1.796325	0.075874
1	1.430944	-2.359556	0.045492
6	1.371566	-0.252008	0.075936
6	-2.982630	-0.736134	0.248583
1	-3.314551	-1.730955	-0.078186
1	-3.062427	-0.705082	1.344798
8	-3.814931	0.244037	-0.322854
6	-5.158980	0.114122	0.102408
1	-5.237978	0.233720	1.189305
1	-5.731487	0.896869	-0.391382
1	-5.562458	-0.864800	-0.178366
6	0.485260	0.892655	0.138120
6	-0.890703	0.674495	0.643602
6	0.861119	2.157004	-0.296775
6	-1.758565	1.863789	0.722581
1	-0.815598	0.275821	1.666701
6	-0.043864	3.208406	-0.252798
1	1.850419	2.327414	-0.700391
6	-1.351341	3.078459	0.275755
1	-2.737086	1.742968	1.169451
1	0.271204	4.177243	-0.626512
1	-1.996209	3.944997	0.331286
14	3.277815	-0.092438	0.025122
6	-0.971045	-2.405307	1.467874
1	-0.857496	-1.686843	2.282857
1	-1.983535	-2.813082	1.501877
1	-0.278424	-3.227410	1.656888
6	-0.921324	-2.891962	-0.979579
1	-0.373605	-3.792589	-0.694637
1	-1.978924	-3.154399	-1.045955
1	-0.578144	-2.586061	-1.968203
6	3.801067	1.084809	1.386678
1	4.890857	1.169765	1.404151
1	3.391152	2.088508	1.252827

1 3.476103 0.712539 2.361571
6 3.982670 -1.798695 0.337922
1 3.618762 -2.224878 1.276156
1 3.752668 -2.493784 -0.473274
1 5.071388 -1.721507 0.406513
6 3.846320 0.516209 -1.657772
1 3.624190 1.569776 -1.838441
1 4.931076 0.394450 -1.728788
1 3.390016 -0.071807 -2.457865
6 -1.516199 -0.145593 -1.693832
1 -2.146653 -0.834295 -2.258276
1 -1.915038 0.857997 -1.844191
1 -0.505162 -0.190856 -2.103156

Name - **Me_B_TS1**
Zero-point correction= 0.425513 (Hartree/Particle)
Thermal correction to Energy= 0.449544
Thermal correction to Enthalpy= 0.450488
Thermal correction to Gibbs Free Energy= 0.374067
Sum of electronic and zero-point Energies= -1067.293836
Sum of electronic and thermal Energies= -1067.269805
Sum of electronic and thermal Enthalpies= -1067.268861
Sum of electronic and thermal Free Energies= -1067.345282
1 imaginary frequency.
Charge = 1 Multiplicity = 1
6 -0.575271 1.502439 0.315926
6 1.583199 1.589655 -0.226097
6 0.784125 2.011965 0.923217
1 -1.187816 2.346528 0.006292
6 -1.044938 0.261400 0.132286
6 2.559600 0.495334 -0.075781
1 3.359621 1.006636 0.510537
1 2.192166 -0.308113 0.573722
8 3.028852 0.031476 -1.293842
6 4.063180 -0.933283 -1.142446
1 3.709541 -1.786821 -0.555503
1 4.333250 -1.263103 -2.142652
1 4.934619 -0.487129 -0.653856
6 -0.301573 -1.009471 0.341299
6 -0.294833 -1.657146 1.579787
6 0.332860 -1.613970 -0.749584
6 0.390442 -2.857680 1.738224
1 -0.812723 -1.208958 2.421213
6 1.012059 -2.817038 -0.589008
1 0.308774 -1.128332 -1.719839
6 1.050609 -3.436757 0.656965
1 0.405481 -3.342587 2.706997
1 1.510343 -3.269239 -1.438695
1 1.580471 -4.373187 0.782955

14 -2.851836 0.025603 -0.467849
6 1.135354 1.386914 2.272897
1 1.156740 0.300682 2.260212
1 2.106446 1.756355 2.612083
1 0.383720 1.696794 2.999694
6 0.687735 3.539799 1.079441
1 -0.080230 3.754776 1.823857
1 1.639902 3.934320 1.436901
1 0.418846 4.048785 0.155728
6 -3.721919 -0.964136 0.863285
1 -4.762404 -1.140285 0.577796
1 -3.242169 -1.935403 1.007417
1 -3.716850 -0.432363 1.817939
6 -3.648427 1.702838 -0.708954
1 -3.660049 2.283533 0.216554
1 -3.138514 2.285347 -1.480497
1 -4.684680 1.565224 -1.028798
6 -2.790632 -0.933399 -2.076576
1 -2.339194 -1.917766 -1.932469
1 -3.806009 -1.079099 -2.455339
1 -2.219128 -0.399166 -2.839649
6 1.536152 2.265246 -1.529560
1 2.505080 2.779108 -1.633956
1 1.522691 1.522500 -2.330095
1 0.730623 2.984456 -1.629852

Name - **Me_B_TS2**
Zero-point correction= 0.425202 (Hartree/Particle)
Thermal correction to Energy= 0.449092
Thermal correction to Enthalpy= 0.450036
Thermal correction to Gibbs Free Energy= 0.373352
Sum of electronic and zero-point Energies= -1067.296015
Sum of electronic and thermal Energies= -1067.272125
Sum of electronic and thermal Enthalpies= -1067.271181
Sum of electronic and thermal Free Energies= -1067.347865
1 imaginary frequency.
Charge = 1 Multiplicity = 1
6 -0.841557 1.536277 0.052398
6 1.583995 1.146137 -0.460503
6 0.600199 2.036860 0.190713
1 -1.556164 2.357137 0.040491
6 -1.271442 0.271386 0.022865
6 2.821538 0.782158 0.245946
1 3.329113 1.752555 0.439591
1 2.567863 0.386998 1.240274
8 3.609373 -0.085629 -0.492814
6 4.688226 -0.618409 0.265907
1 4.306273 -1.191695 1.116551
1 5.243261 -1.276189 -0.398265

1	5.342953	0.181388	0.623791
6	-0.339561	-0.887095	0.084604
6	0.333694	-1.198828	1.272411
6	-0.157584	-1.721658	-1.027115
6	1.217148	-2.274864	1.328579
1	0.145050	-0.605877	2.160709
6	0.722100	-2.794302	-0.970676
1	-0.689032	-1.504019	-1.947899
6	1.420811	-3.067825	0.205289
1	1.734682	-2.497464	2.254514
1	0.866386	-3.418189	-1.844744
1	2.108217	-3.904164	0.246272
14	-3.136141	-0.117898	0.014404
6	0.894408	2.361489	1.662170
1	0.899683	1.466932	2.285268
1	1.846854	2.884668	1.777273
1	0.108649	3.019827	2.034300
6	0.716781	3.365868	-0.637891
1	0.069042	4.093096	-0.146640
1	1.738361	3.748944	-0.629501
1	0.383062	3.229332	-1.665345
6	-3.481483	-1.089710	1.580083
1	-4.536831	-1.370289	1.631936
1	-2.886516	-2.006845	1.605292
1	-3.240575	-0.501597	2.469256
6	-4.092360	1.493449	-0.012361
1	-3.873914	2.106183	0.865967
1	-3.869086	2.079445	-0.907649
1	-5.164722	1.280814	-0.011970
6	-3.551547	-1.158800	-1.491043
1	-3.065691	-2.136424	-1.446598
1	-4.631755	-1.324743	-1.530702
1	-3.251911	-0.664181	-2.418344
6	1.488174	0.803558	-1.875998
1	2.219533	1.472981	-2.365314
1	1.878353	-0.200012	-2.050571
1	0.500615	0.962852	-2.299348

Name - **Me_B_TS3**

Zero-point correction= 0.426484 (Hartree/Particle)
Thermal correction to Energy= 0.449873
Thermal correction to Enthalpy= 0.450817
Thermal correction to Gibbs Free Energy= 0.376057
Sum of electronic and zero-point Energies= -1067.295778
Sum of electronic and thermal Energies= -1067.272390
Sum of electronic and thermal Enthalpies= -1067.271445
Sum of electronic and thermal Free Energies= -1067.346206
1 imaginary frequency.
Charge = 1 Multiplicity = 1

6	0.842732	-1.476515	-0.103675
6	-1.603735	-0.823211	-0.423652
6	-0.622922	-1.903898	-0.086362
1	1.506599	-2.337938	-0.146944
6	1.351328	-0.243634	-0.002830
6	-2.906414	-0.817471	0.290116
1	-3.336845	-1.809995	0.035761
1	-2.774827	-0.820098	1.378552
8	-3.730057	0.209214	-0.148804
6	-4.974387	0.235115	0.537886
1	-4.818575	0.392318	1.610007
1	-5.543545	1.064924	0.126010
1	-5.522538	-0.699173	0.382513
6	0.446025	0.920958	0.082317
6	-0.606455	0.927857	1.017250
6	0.550272	1.986031	-0.816777
6	-1.542896	1.972121	1.032969
1	-0.612491	0.187882	1.808793
6	-0.387269	3.009478	-0.803174
1	1.339270	1.985862	-1.558840
6	-1.442989	3.002834	0.115572
1	-2.336503	1.972459	1.771118
1	-0.304952	3.818183	-1.519982
1	-2.167259	3.807733	0.115433
14	3.235810	0.002874	0.153326
6	-0.898668	-2.606021	1.253956
1	-0.830518	-1.923132	2.102018
1	-1.877598	-3.090720	1.263942
1	-0.147766	-3.383720	1.398823
6	-0.812608	-2.956913	-1.229405
1	-0.173651	-3.807517	-0.987820
1	-1.845016	-3.308335	-1.280389
1	-0.513628	-2.557701	-2.197523
6	3.527134	0.748457	1.848864
1	4.592654	0.931639	2.010264
1	3.002475	1.702743	1.947263
1	3.172333	0.080405	2.637511
6	4.066956	-1.668378	-0.008478
1	3.746950	-2.362705	0.771974
1	3.868585	-2.124193	-0.981898
1	5.148808	-1.539573	0.084124
6	3.883242	1.166001	-1.170867
1	3.568845	2.197445	-0.997462
1	4.976670	1.147244	-1.148830
1	3.563722	0.865215	-2.171542
6	-1.578158	-0.156000	-1.733811
1	-2.351621	-0.658493	-2.335127
1	-1.923036	0.877937	-1.642362
1	-0.614544	-0.223505	-2.230925

5.2.3 Geometries for the Scheme SI4 (R = Ph)

Name - **Ph_A1**
Zero-point correction= 0.481339 (Hartree/Particle)
Thermal correction to Energy= 0.508796
Thermal correction to Enthalpy= 0.509740
Thermal correction to Gibbs Free Energy= 0.424918
Sum of electronic and zero-point Energies= -1258.952800
Sum of electronic and thermal Energies= -1258.925344
Sum of electronic and thermal Enthalpies= -1258.924400
Sum of electronic and thermal Free Energies= -1259.009221

Charge = 1 Multiplicity = 1

6	0.216861	-0.180872	1.169695
6	1.142397	-1.041158	0.072277
6	0.737286	-1.669926	1.331946
1	0.879254	0.508889	1.678668
6	-0.926246	0.382404	0.619124
6	0.483817	-1.398479	-1.237814
1	1.167078	-2.098200	-1.741620
1	-0.479531	-1.900184	-1.112864
8	0.324683	-0.221896	-1.987464
6	-0.091701	-0.484097	-3.318032
1	-1.022471	-1.063070	-3.327361
1	-0.258816	0.480131	-3.795939
1	0.681460	-1.033450	-3.863533
6	-2.090758	-0.344122	0.114166
6	-2.772171	-1.198415	0.993122
6	-2.648557	-0.063587	-1.143683
6	-3.972233	-1.782905	0.607983
1	-2.376861	-1.368035	1.987209
6	-3.818727	-0.692753	-1.539007
1	-2.136448	0.610991	-1.818273
6	-4.485770	-1.548461	-0.663019
1	-4.500555	-2.426555	1.300426
1	-4.222236	-0.504050	-2.526411
1	-5.411099	-2.021492	-0.968785
14	-1.098022	2.321937	0.639706
6	-0.176700	-2.882267	1.336342
1	-0.924197	-2.897566	0.550977
1	0.460959	-3.762621	1.219298
1	-0.680197	-2.963198	2.300305
6	1.731201	-1.726436	2.481923
1	1.181403	-1.757761	3.423885
1	2.325220	-2.639679	2.404560
1	2.410639	-0.875373	2.495042

6	2.498437	-0.423741	-0.100080
6	3.612614	-1.260093	-0.012864
6	2.666596	0.920913	-0.423158
6	4.886349	-0.747569	-0.235036
1	3.482055	-2.310606	0.224049
6	3.941550	1.434131	-0.631808
1	1.797644	1.562274	-0.514731
6	5.052613	0.600819	-0.536679
1	5.747224	-1.401544	-0.166971
1	4.066479	2.482604	-0.873670
1	6.045873	1.001773	-0.699111
6	-2.826171	2.656364	1.264597
1	-2.996257	3.734577	1.320634
1	-3.572406	2.225400	0.592693
1	-2.974367	2.235629	2.262069
6	-0.847114	2.907266	-1.125802
1	-1.780478	2.878195	-1.691016
1	-0.504296	3.945435	-1.100112
1	-0.101776	2.308262	-1.653441
6	0.201618	3.008685	1.795838
1	0.122560	2.572486	2.794680
1	1.221097	2.865057	1.430780
1	0.036743	4.085530	1.892213

Name - **Ph_A2**

Zero-point correction= 0.479238 (Hartree/Particle)
Thermal correction to Energy= 0.507158
Thermal correction to Enthalpy= 0.508102
Thermal correction to Gibbs Free Energy= 0.421684
Sum of electronic and zero-point Energies= -1258.948910
Sum of electronic and thermal Energies= -1258.920989
Sum of electronic and thermal Enthalpies= -1258.920045
Sum of electronic and thermal Free Energies= -1259.006463

Charge = 1 Multiplicity = 1

6	0.013038	0.891262	0.396346
6	-1.118498	-0.149460	0.273236
6	-0.842352	-1.132205	-0.825118
1	-0.342194	1.830501	0.811352
6	1.314600	0.697171	0.180857
6	-1.192293	-0.778336	1.680661
1	-0.203954	-1.185254	1.932831
1	-1.412032	0.027596	2.392809
8	-2.163374	-1.789106	1.761893
6	-2.191856	-2.392246	3.044348
1	-2.405551	-1.647530	3.818013

1	-2.981990	-3.140255	3.031140
1	-1.233916	-2.876052	3.266178
6	1.850650	-0.594512	-0.321169
6	2.079188	-0.794393	-1.689011
6	2.204164	-1.610911	0.578894
6	2.572663	-2.009256	-2.153086
1	1.859617	0.006684	-2.386804
6	2.694148	-2.824009	0.114479
1	2.090471	-1.442432	1.644568
6	2.866220	-3.031112	-1.254217
1	2.730046	-2.156574	-3.214956
1	2.945937	-3.608377	0.818050
1	3.246641	-3.978953	-1.615805
14	2.583613	2.067021	0.562488
6	-0.682969	-2.567790	-0.593999
1	-1.674069	-2.996542	-0.828629
1	0.015159	-2.996848	-1.318460
1	-0.436442	-2.837069	0.426812
6	-0.946118	-0.684457	-2.227644
1	-0.371254	-1.319787	-2.897367
1	-2.010021	-0.801254	-2.487230
1	-0.706188	0.370709	-2.352898
6	-2.438300	0.552085	-0.149911
6	-3.663172	-0.112228	-0.020440
6	-2.419598	1.820192	-0.739467
6	-4.842275	0.500707	-0.432395
1	-3.700030	-1.102995	0.408865
6	-3.601150	2.426991	-1.151033
1	-1.485858	2.347618	-0.892130
6	-4.817862	1.771734	-0.994608
1	-5.782703	-0.024188	-0.315043
1	-3.564688	3.413471	-1.597177
1	-5.737675	2.245667	-1.315537
6	3.542852	2.400516	-1.012954
1	4.271164	3.198796	-0.846690
1	4.089822	1.509663	-1.332886
1	2.881312	2.708847	-1.826187
6	3.728887	1.403791	1.889810
1	4.238296	0.498608	1.548881
1	4.492440	2.147011	2.134869
1	3.180109	1.165718	2.804323
6	1.668931	3.593669	1.143432
1	0.961284	3.950897	0.390676
1	1.123552	3.407023	2.071811
1	2.385745	4.396644	1.334582

Name - **Ph_A3**

Zero-point correction= 0.479916 (Hartree/Particle)
Thermal correction to Energy= 0.507449
Thermal correction to Enthalpy= 0.508394
Thermal correction to Gibbs Free Energy= 0.423480
Sum of electronic and zero-point Energies= -1258.951851
Sum of electronic and thermal Energies= -1258.924317
Sum of electronic and thermal Enthalpies= -1258.923373
Sum of electronic and thermal Free Energies= -1259.008287

Charge = 1 Multiplicity = 1

6	0.170897	0.693117	0.807866
6	-1.134913	-0.065554	0.544818
6	-0.970661	-1.499739	0.143433
1	-0.020843	1.594108	1.387915
6	1.404864	0.439563	0.363309
6	-1.804538	-0.176935	1.966758
1	-1.038326	-0.436586	2.706281
1	-2.207663	0.815247	2.202947
8	-2.816226	-1.151188	1.948854
6	-3.491009	-1.245114	3.195388
1	-3.978627	-0.295668	3.438294
1	-4.241359	-2.026031	3.094049
1	-2.789758	-1.508972	3.993534
6	1.711378	-0.750947	-0.464044
6	1.025035	-1.003688	-1.659084
6	2.668636	-1.677538	-0.028516
6	1.256414	-2.180720	-2.375999
1	0.332271	-0.266844	-2.051102
6	2.889877	-2.848123	-0.737352
1	3.203178	-1.497013	0.896699
6	2.175459	-3.109446	-1.911028
1	0.717423	-2.361702	-3.298522
1	3.615191	-3.566869	-0.374670
1	2.352468	-4.025552	-2.460984
14	2.794052	1.712629	0.670875
6	-0.243252	-2.436682	1.011720
1	-1.033773	-3.006010	1.525789
1	0.313372	-3.158661	0.406944
1	0.399248	-1.956943	1.744987
6	-1.806358	-2.078046	-0.911222
1	-1.477572	-3.071108	-1.208319
1	-2.790132	-2.166382	-0.412454
1	-1.956471	-1.411108	-1.758687
6	-2.015453	0.757374	-0.412512
6	-3.411458	0.662124	-0.368166
6	-1.437732	1.624852	-1.342553
6	-4.200479	1.399592	-1.243494

1	-3.887391	0.005752	0.349434
6	-2.229617	2.360261	-2.221055
1	-0.362413	1.752028	-1.376476
6	-3.613388	2.247620	-2.177649
1	-5.279050	1.309941	-1.192030
1	-1.758567	3.028346	-2.932071
1	-4.230450	2.822471	-2.857666
6	3.346168	2.272716	-1.031630
1	4.174421	2.981870	-0.954818
1	3.683833	1.420798	-1.628035
1	2.528104	2.761855	-1.567059
6	4.232380	0.937813	1.593847
1	4.779370	0.226427	0.971652
1	4.930936	1.727214	1.885489
1	3.904254	0.428222	2.503218
6	2.088457	3.140429	1.656766
1	1.263431	3.628184	1.131440
1	1.733561	2.819608	2.639564
1	2.870184	3.888506	1.813958

Name - **Ph_A4**

Zero-point correction= 0.482661 (Hartree/Particle)
Thermal correction to Energy= 0.509444
Thermal correction to Enthalpy= 0.510388
Thermal correction to Gibbs Free Energy= 0.426241
Sum of electronic and zero-point Energies= -1258.961390
Sum of electronic and thermal Energies= -1258.934608
Sum of electronic and thermal Enthalpies= -1258.933664
Sum of electronic and thermal Free Energies= -1259.017810

Charge = 1 Multiplicity = 1

6	-0.240912	-0.845929	0.631626
6	1.068734	-0.093835	0.543221
6	0.834849	1.429188	0.226853
1	-0.143666	-1.835982	1.075199
6	-1.460196	-0.428238	0.225405
6	1.688416	-0.303259	1.946974
1	0.925545	-0.078878	2.705641
1	1.957123	-1.364167	2.048942
8	2.816631	0.506595	2.170998
6	3.287505	0.390698	3.501135
1	3.553202	-0.646672	3.732518
1	4.171594	1.019572	3.587394
1	2.525267	0.732105	4.211009
6	-1.539191	0.877155	-0.403263
6	-0.290623	1.499157	-0.898560

6	-2.741556	1.565389	-0.524402
6	-0.424759	2.830873	-1.513833
1	0.101475	0.853449	-1.707263
6	-2.773037	2.828389	-1.095632
1	-3.659674	1.136181	-0.146499
6	-1.618297	3.465626	-1.612837
1	0.470154	3.286355	-1.920873
1	-3.723693	3.348394	-1.152923
1	-1.703275	4.438847	-2.077165
14	-2.977672	-1.573323	0.464264
6	0.323141	2.184643	1.462966
1	-0.516279	1.677818	1.944718
1	1.129193	2.287289	2.190296
1	-0.001981	3.188165	1.177187
6	2.103408	2.110055	-0.296914
1	1.979130	3.194391	-0.295560
1	2.937962	1.869764	0.358850
1	2.355490	1.785381	-1.309048
6	1.905943	-0.783809	-0.553284
6	3.300803	-0.851022	-0.457058
6	1.296506	-1.350817	-1.677891
6	4.055885	-1.447792	-1.460474
1	3.799533	-0.427007	0.404417
6	2.053265	-1.942401	-2.686400
1	0.215174	-1.358084	-1.772552
6	3.437639	-1.990895	-2.582892
1	5.134481	-1.486778	-1.362225
1	1.554224	-2.374219	-3.545753
1	4.028498	-2.454925	-3.363513
6	-2.322214	-3.256118	0.957383
1	-1.615032	-3.651145	0.223524
1	-1.835469	-3.238052	1.935557
1	-3.161175	-3.954411	1.021214
6	-3.885109	-1.698701	-1.171543
1	-4.701114	-2.420900	-1.080585
1	-4.316848	-0.750335	-1.497896
1	-3.210304	-2.052767	-1.955244
6	-4.083825	-0.914670	1.828820
1	-4.575096	0.028951	1.583946
1	-4.867663	-1.649454	2.034371
1	-3.510658	-0.771258	2.748229

Name - **Ph_A_TS1**

Zero-point correction= 0.478648 (Hartree/Particle)

Thermal correction to Energy= 0.505988

Thermal correction to Enthalpy= 0.506932

Thermal correction to Gibbs Free Energy= 0.421943
Sum of electronic and zero-point Energies= -1258.946572
Sum of electronic and thermal Energies= -1258.919233
Sum of electronic and thermal Enthalpies= -1258.918289
Sum of electronic and thermal Free Energies= -1259.003277
1 imaginary frequency.
Charge = 1 Multiplicity = 1

6	0.046474	0.878395	-0.018993
6	1.146504	-0.226569	0.014493
6	0.806789	-0.970058	1.251839
1	0.462636	1.878154	0.027781
6	-1.282914	0.738040	-0.080964
6	1.110210	-1.067781	-1.269646
1	0.120992	-1.509943	-1.421859
1	1.318305	-0.401996	-2.116702
8	2.086301	-2.071950	-1.162525
6	2.118314	-2.907791	-2.306256
1	2.360792	-2.327175	-3.202296
1	2.890960	-3.655433	-2.139070
1	1.152802	-3.405852	-2.449975
6	-2.016366	-0.552400	0.010669
6	-2.465101	-0.991663	1.261241
6	-2.331150	-1.305598	-1.125310
6	-3.142205	-2.200934	1.384410
1	-2.285127	-0.378942	2.139195
6	-3.000297	-2.518034	-0.999305
1	-2.037114	-0.944942	-2.105387
6	-3.395347	-2.975164	0.256734
1	-3.472077	-2.535874	2.360640
1	-3.219882	-3.104027	-1.883856
1	-3.915860	-3.920438	0.351271
14	-2.383198	2.293631	-0.253096
6	0.420824	-2.377126	1.239850
1	1.404568	-2.878360	1.138944
1	-0.051112	-2.700130	2.164572
1	-0.140880	-2.678275	0.354611
6	0.923644	-0.303244	2.557403
1	-0.047429	-0.366924	3.061112
1	1.598519	-0.904123	3.181191
1	1.270920	0.724371	2.501059
6	2.544650	0.408699	0.131746
6	3.556270	-0.227087	0.851808
6	2.850925	1.562671	-0.589284
6	4.839705	0.305417	0.891052
1	3.362595	-1.158547	1.373254
6	4.138138	2.089980	-0.558644
1	2.099326	2.052953	-1.197646
6	5.132509	1.470747	0.190713

1 5.611340 -0.198434 1.460284
1 4.361028 2.986080 -1.125061
1 6.132415 1.886258 0.218672
6 -3.519458 2.341726 1.237052
1 -4.156628 3.229107 1.193311
1 -4.167037 1.461799 1.264254
1 -2.949552 2.379395 2.169038
6 -3.367971 2.078633 -1.831464
1 -3.972692 1.168887 -1.797242
1 -4.043590 2.926684 -1.970515
1 -2.710439 2.022590 -2.702534
6 -1.292273 3.814780 -0.327493
1 -0.717987 3.947687 0.592908
1 -0.596805 3.775617 -1.169881
1 -1.919875 4.700765 -0.456429

Name - **Ph_A_TS2**

Zero-point correction= 0.478298 (Hartree/Particle)
Thermal correction to Energy= 0.505540
Thermal correction to Enthalpy= 0.506484
Thermal correction to Gibbs Free Energy= 0.420696
Sum of electronic and zero-point Energies= -1258.948517
Sum of electronic and thermal Energies= -1258.921275
Sum of electronic and thermal Enthalpies= -1258.920331
Sum of electronic and thermal Free Energies= -1259.006119
1 imaginary frequency.
Charge = 1 Multiplicity = 1
6 -0.005309 0.744680 0.539451
6 -1.177417 -0.253319 0.341700
6 -0.825253 -1.400864 -0.559899
1 -0.393100 1.647745 1.006931
6 1.295460 0.632111 0.281996
6 -1.474003 -0.753791 1.778304
1 -0.535915 -1.040831 2.269841
1 -1.905133 0.084866 2.339397
8 -2.358321 -1.845497 1.741886
6 -2.606973 -2.372456 3.034973
1 -3.049350 -1.611255 3.685783
1 -3.304302 -3.199152 2.916854
1 -1.678095 -2.737886 3.486891
6 1.904193 -0.563481 -0.348101
6 1.862666 -0.741820 -1.735227
6 2.573470 -1.509600 0.441153
6 2.416561 -1.880178 -2.317534
1 1.396535 0.016920 -2.355090
6 3.123528 -2.642391 -0.139905

1	2.633259	-1.359867	1.514138
6	3.035983	-2.836432	-1.520902
1	2.367044	-2.014606	-3.391591
1	3.619995	-3.379666	0.479544
1	3.465322	-3.723309	-1.971035
14	2.472385	2.081224	0.676577
6	-0.351682	-2.688627	-0.052747
1	-1.244824	-3.335671	-0.107343
1	0.383881	-3.123349	-0.735557
1	-0.003105	-2.680717	0.974180
6	-1.168821	-1.344917	-1.986568
1	-0.648668	-2.102248	-2.567876
1	-2.250833	-1.566081	-2.005498
1	-1.071763	-0.348144	-2.414967
6	-2.360444	0.542564	-0.254213
6	-3.680321	0.169266	0.010955
6	-2.125279	1.640169	-1.087431
6	-4.737815	0.887947	-0.539234
1	-3.885857	-0.680998	0.647287
6	-3.184130	2.352174	-1.640323
1	-1.108754	1.947843	-1.310011
6	-4.495574	1.978675	-1.366659
1	-5.755502	0.589405	-0.317171
1	-2.979690	3.200556	-2.282325
1	-5.321495	2.534324	-1.794185
6	3.224837	2.610579	-0.956639
1	3.944315	3.418714	-0.800131
1	3.751788	1.778856	-1.431791
1	2.457257	2.968407	-1.647726
6	3.806909	1.463015	1.837998
1	4.395026	0.665762	1.376552
1	4.487836	2.281691	2.086074
1	3.381128	1.083075	2.770021
6	1.487074	3.469209	1.456842
1	0.694642	3.827087	0.794412
1	1.034950	3.158095	2.402024
1	2.150641	4.312214	1.667263

Name - **Ph_A_TS3**

Zero-point correction= 0.480185 (Hartree/Particle)
Thermal correction to Energy= 0.506821
Thermal correction to Enthalpy= 0.507765
Thermal correction to Gibbs Free Energy= 0.425083
Sum of electronic and zero-point Energies= -1258.950519
Sum of electronic and thermal Energies= -1258.923883
Sum of electronic and thermal Enthalpies= -1258.922939

Sum of electronic and thermal Free Energies= -1259.005621

1 imaginary frequency.

Charge = 1 Multiplicity = 1

6	-0.234997	-0.717357	0.819031
6	1.077708	0.019644	0.561183
6	0.913678	1.456208	0.100229
1	-0.086824	-1.620592	1.407660
6	-1.448122	-0.413845	0.347007
6	1.733492	0.138809	1.982135
1	0.966615	0.446183	2.703361
1	2.091689	-0.862163	2.253212
8	2.786884	1.067902	1.974327
6	3.408320	1.178360	3.245576
1	3.833132	0.216857	3.551396
1	4.202805	1.915367	3.150489
1	2.686519	1.511506	3.998772
6	-1.626974	0.790378	-0.486551
6	-0.741822	1.048107	-1.551182
6	-2.607113	1.743085	-0.179717
6	-0.845395	2.239873	-2.292019
1	-0.083623	0.263334	-1.905247
6	-2.675906	2.928357	-0.892761
1	-3.280097	1.570886	0.651378
6	-1.789073	3.185648	-1.950757
1	-0.176550	2.408300	-3.128031
1	-3.421006	3.669438	-0.627708
1	-1.863337	4.112866	-2.505015
14	-2.907685	-1.614614	0.618294
6	0.241547	2.424235	0.998422
1	-0.453499	1.966245	1.697889
1	1.057084	2.907513	1.554935
1	-0.252515	3.209832	0.420495
6	1.902883	2.035034	-0.837139
1	1.628959	3.042678	-1.142830
1	2.822031	2.088727	-0.230949
1	2.122132	1.398218	-1.691845
6	1.952830	-0.835607	-0.375712
6	3.349892	-0.747317	-0.339728
6	1.370254	-1.731091	-1.276774
6	4.132505	-1.513332	-1.196277
1	3.831146	-0.073969	0.357851
6	2.155139	-2.495435	-2.136913
1	0.293951	-1.855478	-1.305479
6	3.539279	-2.386166	-2.103376
1	5.211603	-1.425718	-1.151909
1	1.678187	-3.182014	-2.826108
1	4.151652	-2.981695	-2.769823
6	-2.274125	-3.080828	1.595336

1 -1.463194 -3.596954 1.075169
1 -1.918731 -2.784076 2.585404
1 -3.087973 -3.797242 1.735558
6 -3.464461 -2.129186 -1.096288
1 -4.315280 -2.812776 -1.036658
1 -3.770961 -1.258870 -1.683005
1 -2.657775 -2.635914 -1.632630
6 -4.316506 -0.785194 1.539933
1 -4.857968 -0.076841 0.909508
1 -5.028026 -1.552779 1.857586
1 -3.965831 -0.263764 2.433891

Name - **Ph_B2**

Zero-point correction= 0.481040 (Hartree/Particle)
Thermal correction to Energy= 0.508509
Thermal correction to Enthalpy= 0.509453
Thermal correction to Gibbs Free Energy= 0.424575
Sum of electronic and zero-point Energies= -1258.949796
Sum of electronic and thermal Energies= -1258.922328
Sum of electronic and thermal Enthalpies= -1258.921383
Sum of electronic and thermal Free Energies= -1259.006261

Charge = 1 Multiplicity = 1
6 -1.005242 0.825318 1.256603
6 1.418945 0.115436 0.895941
6 0.334344 0.435410 1.907529
1 -1.453016 1.711968 1.703658
6 -1.662808 0.150584 0.310096
6 2.009286 -1.243265 1.008257
1 2.464864 -1.295323 2.016625
1 1.163113 -1.949125 1.035993
8 2.915198 -1.607390 0.020884
6 3.289945 -2.974812 0.124677
1 2.412099 -3.620768 0.024745
1 3.984244 -3.171873 -0.688920
1 3.782027 -3.169084 1.082626
6 -1.090814 -1.068624 -0.321270
6 -1.439815 -2.339820 0.151105
6 -0.210314 -0.968219 -1.404694
6 -0.867516 -3.478344 -0.403320
1 -2.148658 -2.427229 0.967904
6 0.359383 -2.111035 -1.962621
1 0.025898 0.008459 -1.812641
6 0.042103 -3.365454 -1.455803
1 -1.131058 -4.455876 -0.016904
1 1.053763 -2.016177 -2.788910

1 0.488311 -4.255007 -1.884547
14 -3.355484 0.740724 -0.320116
6 0.034972 -0.698864 2.908906
1 -0.330210 -1.604994 2.427550
1 0.906356 -0.939308 3.522598
1 -0.751004 -0.346363 3.577802
6 0.864952 1.635532 2.744494
1 0.155488 1.815854 3.553567
1 1.835366 1.397174 3.185015
1 0.962314 2.542118 2.149662
6 1.938720 1.115911 0.017211
6 3.284101 1.046054 -0.429811
6 1.168521 2.251272 -0.359535
6 3.825349 2.065292 -1.194141
1 3.903986 0.212831 -0.141761
6 1.705187 3.234260 -1.159455
1 0.132624 2.326088 -0.061578
6 3.038111 3.146356 -1.575461
1 4.861217 2.010145 -1.502772
1 1.095799 4.076125 -1.461736
1 3.458970 3.927576 -2.197655
6 -4.589785 -0.652300 -0.090682
1 -5.579119 -0.336747 -0.432715
1 -4.300323 -1.534294 -0.667731
1 -4.669880 -0.940451 0.960484
6 -3.146844 1.134409 -2.142515
1 -2.835121 0.246969 -2.699694
1 -4.090267 1.487113 -2.567997
1 -2.394282 1.913470 -2.292055
6 -3.867014 2.265575 0.643257
1 -3.951000 2.056208 1.712639
1 -3.156537 3.084929 0.505831
1 -4.843384 2.610531 0.292877

Name - **Ph_B3**

Zero-point correction= 0.480236 (Hartree/Particle)
Thermal correction to Energy= 0.508070
Thermal correction to Enthalpy= 0.509014
Thermal correction to Gibbs Free Energy= 0.422073
Sum of electronic and zero-point Energies= -1258.948131
Sum of electronic and thermal Energies= -1258.920298
Sum of electronic and thermal Enthalpies= -1258.919354
Sum of electronic and thermal Free Energies= -1259.006295

Charge = 1 Multiplicity = 1
6 1.044945 -1.486040 -0.558058

6	-1.480034	-0.960661	-0.434060
6	-0.395638	-2.003272	-0.623250
1	1.710392	-2.124000	-1.138988
6	1.576582	-0.481737	0.151050
6	-2.631002	-1.459521	0.369658
1	-2.878378	-2.439864	-0.075191
1	-2.250608	-1.688315	1.378487
8	-3.766779	-0.664044	0.426617
6	-4.823853	-1.307966	1.127396
1	-4.529662	-1.520095	2.159771
1	-5.667880	-0.622723	1.120865
1	-5.103560	-2.240387	0.627363
6	0.766960	0.427983	1.003227
6	0.022123	-0.058614	2.082513
6	0.722319	1.800759	0.727993
6	-0.796761	0.789471	2.827225
1	0.104520	-1.103076	2.358686
6	-0.095711	2.645169	1.467010
1	1.294684	2.198893	-0.102188
6	-0.868800	2.141105	2.513522
1	-1.370220	0.390833	3.656297
1	-0.139533	3.699915	1.220491
1	-1.508543	2.801317	3.086692
14	3.457768	-0.196102	0.109573
6	-0.450316	-3.192208	0.367275
1	-0.380896	-2.875286	1.406538
1	-1.341662	-3.807672	0.237108
1	0.411637	-3.827858	0.160324
6	-0.678816	-2.637558	-2.027433
1	0.054015	-3.432709	-2.175936
1	-1.673569	-3.086263	-2.046899
1	-0.605265	-1.931782	-2.850073
6	-1.453918	0.297625	-1.092568
6	-2.326335	1.349340	-0.692615
6	-0.500444	0.580007	-2.116669
6	-2.247480	2.596953	-1.286021
1	-3.031567	1.185395	0.104981
6	-0.456298	1.814712	-2.718135
1	0.199071	-0.172569	-2.442507
6	-1.327971	2.828957	-2.301784
1	-2.904551	3.390008	-0.953212
1	0.259773	2.004012	-3.507485
6	4.044073	-0.138792	1.890267
1	5.119013	0.054502	1.935951
1	3.533187	0.657452	2.438590
1	3.845573	-1.084876	2.400150
6	4.274115	-1.605306	-0.820681
1	4.049192	-2.574353	-0.368574

1 3.969328 -1.632711 -1.870110
1 5.358535 -1.467493 -0.795157
6 3.853865 1.429651 -0.748348
1 3.613466 2.291573 -0.122321
1 4.924659 1.467397 -0.968212
1 3.313040 1.524389 -1.693998
1 -1.278336 3.803770 -2.773458

Name - **Ph_B4**
Zero-point correction= 0.483251 (Hartree/Particle)
Thermal correction to Energy= 0.510014
Thermal correction to Enthalpy= 0.510959
Thermal correction to Gibbs Free Energy= 0.428157
Sum of electronic and zero-point Energies= -1258.949146
Sum of electronic and thermal Energies= -1258.922382
Sum of electronic and thermal Enthalpies= -1258.921438
Sum of electronic and thermal Free Energies= -1259.004240

Charge = 1 Multiplicity = 1
6 1.053678 1.494611 0.503067
6 -1.293700 0.759902 -0.004627
6 -0.380851 1.949216 0.464123
1 1.692999 2.084241 1.158050
6 1.611025 0.503851 -0.238478
6 -2.698632 1.347109 -0.252235
1 -2.978727 1.949352 0.620538
1 -2.655985 2.017151 -1.121917
8 -3.688797 0.373617 -0.475742
6 -4.961496 0.962098 -0.673208
1 -4.958873 1.612167 -1.555510
1 -5.673030 0.152157 -0.821428
1 -5.256346 1.549772 0.202731
6 0.741413 -0.237793 -1.127593
6 -0.656811 0.228950 -1.344106
6 1.177398 -1.372611 -1.807067
6 -1.516070 -0.623116 -2.190944
1 -0.546100 1.126030 -1.989384
6 0.313510 -2.093213 -2.616650
1 2.192448 -1.724985 -1.689257
6 -1.036388 -1.723054 -2.823110
1 -2.541464 -0.302502 -2.332314
1 0.690701 -2.981664 -3.112402
1 -1.665648 -2.317805 -3.471413
14 3.466390 0.107896 0.006701
6 -0.334985 3.146233 -0.532766
1 0.070931 2.893714 -1.514041

1 -1.320189 3.597028 -0.654571
1 0.319156 3.908931 -0.105244
6 -0.843988 2.557370 1.810455
1 0.008330 2.987929 2.341227
1 -1.552867 3.366977 1.632866
1 -1.326512 1.836340 2.466844
6 -1.294731 -0.434850 0.980119
6 -2.048589 -1.577689 0.674802
6 -0.489635 -0.495990 2.125462
6 -2.016362 -2.710781 1.480426
1 -2.686538 -1.588688 -0.196514
6 -0.454941 -1.628648 2.934166
1 0.138610 0.334153 2.417136
6 -1.220771 -2.743527 2.619614
1 -2.617891 -3.570637 1.209673
1 0.181348 -1.631955 3.811398
6 4.368848 0.195004 -1.636135
1 5.435892 0.023934 -1.468298
1 4.026382 -0.542570 -2.364351
1 4.255324 1.187157 -2.080521
6 4.170209 1.403484 1.163338
1 4.054050 2.415657 0.768023
1 3.716157 1.360530 2.156532
1 5.240690 1.215452 1.283167
6 3.629887 -1.581613 0.808475
1 3.325774 -2.406767 0.161935
1 4.673524 -1.748753 1.089541
1 3.025184 -1.626002 1.718452
1 -1.194535 -3.625478 3.248411

Name - **Ph_B_TS1**

Zero-point correction= 0.479218 (Hartree/Particle)
Thermal correction to Energy= 0.506744
Thermal correction to Enthalpy= 0.507688
Thermal correction to Gibbs Free Energy= 0.421386
Sum of electronic and zero-point Energies= -1258.941470
Sum of electronic and thermal Energies= -1258.913944
Sum of electronic and thermal Enthalpies= -1258.912999
Sum of electronic and thermal Free Energies= -1258.999302
1 imaginary frequency.
Charge = 1 Multiplicity = 1
6 -0.083004 0.971855 0.986137
6 1.476750 -0.599129 0.729917
6 0.765545 0.015581 1.879574
1 0.354916 1.964484 0.964751
6 -1.203350 0.779420 0.268714

6	0.986375	-1.921066	0.246769
1	1.530405	-2.660083	0.873210
1	-0.070442	-2.054913	0.485873
8	1.217712	-2.109225	-1.114314
6	0.872585	-3.422962	-1.532723
1	-0.174288	-3.641800	-1.298802
1	1.021826	-3.459840	-2.609354
1	1.516214	-4.163618	-1.046263
6	-2.013911	-0.459978	0.130954
6	-2.963368	-0.776198	1.108925
6	-1.948485	-1.237707	-1.030021
6	-3.801984	-1.872729	0.947957
1	-3.038261	-0.157500	1.996942
6	-2.789439	-2.336185	-1.186051
1	-1.223261	-0.992040	-1.799311
6	-3.715164	-2.658525	-0.198423
1	-4.527587	-2.109057	1.717178
1	-2.723844	-2.936919	-2.085934
1	-4.372188	-3.510408	-0.325061
14	-1.969053	2.279983	-0.653693
6	-0.046050	-0.958998	2.743189
1	-0.792327	-1.535910	2.207306
1	0.635420	-1.645918	3.251078
1	-0.567997	-0.376604	3.503264
6	1.654635	0.840794	2.821558
1	1.013567	1.330566	3.555855
1	2.339624	0.175848	3.351120
1	2.238203	1.604520	2.315451
6	2.662071	-0.055394	0.106374
6	3.641370	-0.982083	-0.320364
6	2.937010	1.321823	-0.033914
6	4.862726	-0.544039	-0.802276
1	3.464382	-2.044000	-0.226463
6	4.135092	1.747291	-0.574233
1	2.193506	2.062124	0.218614
6	5.108375	0.818122	-0.941679
1	5.616268	-1.267694	-1.085225
1	4.315897	2.806302	-0.705897
1	6.055110	1.159645	-1.342949
6	-3.728165	2.456592	-0.036222
1	-4.214343	3.301203	-0.531546
1	-4.309210	1.556297	-0.251330
1	-3.754987	2.633511	1.041870
6	-1.944169	1.888809	-2.487264
1	-2.592848	1.043336	-2.726162
1	-2.302218	2.758212	-3.045889
1	-0.932853	1.658436	-2.831207
6	-0.962094	3.818797	-0.294935

1 -0.921625 4.042514 0.773898
1 0.059177 3.737825 -0.676172
1 -1.431312 4.670967 -0.794418

Name - **Ph_B_TS2**
Zero-point correction= 0.480800 (Hartree/Particle)
Thermal correction to Energy= 0.506718
Thermal correction to Enthalpy= 0.507662
Thermal correction to Gibbs Free Energy= 0.427220
Sum of electronic and zero-point Energies= -1258.946153
Sum of electronic and thermal Energies= -1258.920235
Sum of electronic and thermal Enthalpies= -1258.919291
Sum of electronic and thermal Free Energies= -1258.999733
2 imaginary frequency.
Charge = 1 Multiplicity = 1
6 -1.185231 0.267610 1.484071
6 1.359129 0.054599 1.138121
6 0.201497 0.095393 2.122270
1 -1.884244 0.706637 2.195466
6 -1.630838 -0.124345 0.286282
6 2.224714 -1.151202 1.278140
1 2.709824 -1.033327 2.269422
1 1.564836 -2.019316 1.381256
8 3.160873 -1.381914 0.278096
6 3.721241 -2.684507 0.372943
1 2.939819 -3.443224 0.263462
1 4.438090 -2.778860 -0.439253
1 4.231291 -2.819140 1.331630
6 -0.755578 -0.759532 -0.737114
6 -0.295754 -2.071005 -0.579850
6 -0.403160 -0.061404 -1.900190
6 0.539413 -2.651655 -1.533507
1 -0.612456 -2.645721 0.284622
6 0.437398 -0.635183 -2.844056
1 -0.768011 0.949873 -2.045229
6 0.917301 -1.932065 -2.660471
1 0.884642 -3.670141 -1.397388
1 0.718098 -0.072020 -3.726517
1 1.571923 -2.379595 -3.398656
14 -3.470089 0.065775 -0.159389
6 0.068345 -1.156118 3.019813
1 -0.165478 -2.056099 2.451234
1 0.959887 -1.328145 3.626825
1 -0.764404 -0.983025 3.702618
6 0.491435 1.282389 3.091326
1 -0.277331 1.278882 3.865623

1 1.461535 1.145537 3.574366
1 0.486727 2.248443 2.592354
6 1.670474 1.156142 0.295077
6 2.929184 1.252084 -0.363979
6 0.745236 2.225991 0.104970
6 3.230636 2.341343 -1.160837
1 3.667416 0.480125 -0.226458
6 1.049493 3.293174 -0.705401
1 -0.231160 2.189637 0.563133
6 2.294079 3.353481 -1.343754
1 4.197676 2.401221 -1.642895
1 0.325057 4.084094 -0.850490
6 -4.133554 -1.662133 -0.460445
1 -5.185533 -1.626141 -0.755813
1 -3.574995 -2.158363 -1.258696
1 -4.054022 -2.272727 0.442691
6 -4.368495 0.899531 1.260100
1 -4.313686 0.311842 2.179714
1 -3.964903 1.895489 1.460804
1 -5.424511 1.015253 1.001786
6 -3.631057 1.097689 -1.719259
1 -3.177487 0.598340 -2.578621
1 -4.689368 1.257359 -1.944344
1 -3.160787 2.077755 -1.600708
1 2.530382 4.198138 -1.980747

Name - **Ph_B_TS3**
Zero-point correction= 0.481607 (Hartree/Particle)
Thermal correction to Energy= 0.508257
Thermal correction to Enthalpy= 0.509202
Thermal correction to Gibbs Free Energy= 0.425690
Sum of electronic and zero-point Energies= -1258.940958
Sum of electronic and thermal Energies= -1258.914307
Sum of electronic and thermal Enthalpies= -1258.913363
Sum of electronic and thermal Free Energies= -1258.996875
1 imaginary frequency.
Charge = 1 Multiplicity = 1
6 1.289084 -1.148377 -0.995931
6 -1.222381 -0.792895 -0.457160
6 -0.146273 -1.587071 -1.255926
1 1.989805 -1.562724 -1.718703
6 1.741442 -0.403269 0.021039
6 -2.375609 -1.706962 -0.076243
1 -2.807020 -2.021194 -1.044148
1 -1.984529 -2.607689 0.401393
8 -3.366060 -1.153905 0.736734

6 -4.281802 -2.137700 1.195564
1 -3.765753 -2.888257 1.804085
1 -5.022813 -1.621803 1.802057
1 -4.777480 -2.631919 0.354522
6 0.759407 0.131373 0.972768
6 -0.268405 -0.728501 1.452747
6 0.693557 1.485325 1.282751
6 -1.257728 -0.231408 2.341159
1 -0.084923 -1.795206 1.435066
6 -0.359624 1.972357 2.049457
1 1.425171 2.171534 0.874601
6 -1.328090 1.117316 2.598793
1 -1.954481 -0.919200 2.801449
1 -0.424158 3.037773 2.240826
1 -2.103621 1.518928 3.238164
14 3.600314 -0.031820 0.219269
6 -0.138103 -3.108689 -0.958653
1 0.016684 -3.343087 0.095474
1 -1.051249 -3.595639 -1.305974
1 0.692098 -3.552129 -1.510045
6 -0.470313 -1.473244 -2.771466
1 0.204874 -2.138082 -3.313566
1 -1.492082 -1.804461 -2.969347
1 -0.354064 -0.468624 -3.166898
6 -1.492053 0.614850 -0.825464
6 -2.680249 1.268387 -0.443919
6 -0.548577 1.374972 -1.554513
6 -2.928971 2.587016 -0.814374
1 -3.417345 0.746438 0.142544
6 -0.798343 2.684776 -1.916555
1 0.402282 0.947456 -1.835127
6 -1.997859 3.298732 -1.554415
1 -3.858855 3.052958 -0.512375
1 -0.052985 3.232006 -2.480452
6 4.054036 -0.438438 1.991183
1 5.108201 -0.219252 2.178997
1 3.457098 0.156205 2.688265
1 3.880885 -1.495151 2.208843
6 4.533238 -1.110518 -0.993828
1 4.311763 -2.170236 -0.846652
1 4.305351 -0.848471 -2.030187
1 5.607199 -0.968249 -0.845543
6 3.949045 1.779459 -0.143776
1 3.661253 2.432260 0.683132
1 5.023005 1.910903 -0.304666
1 3.431289 2.111577 -1.047412
1 -2.194089 4.325112 -1.841384

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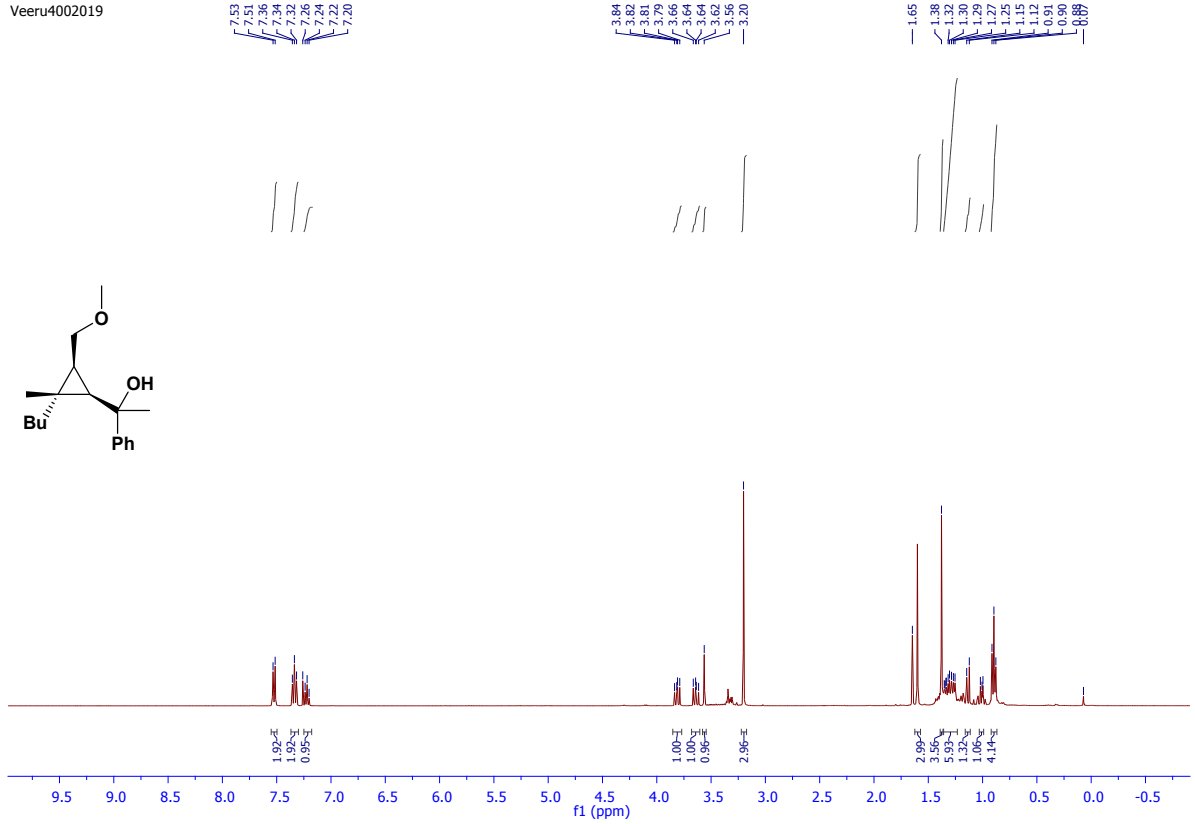
NMR Spectra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3.56
5.93
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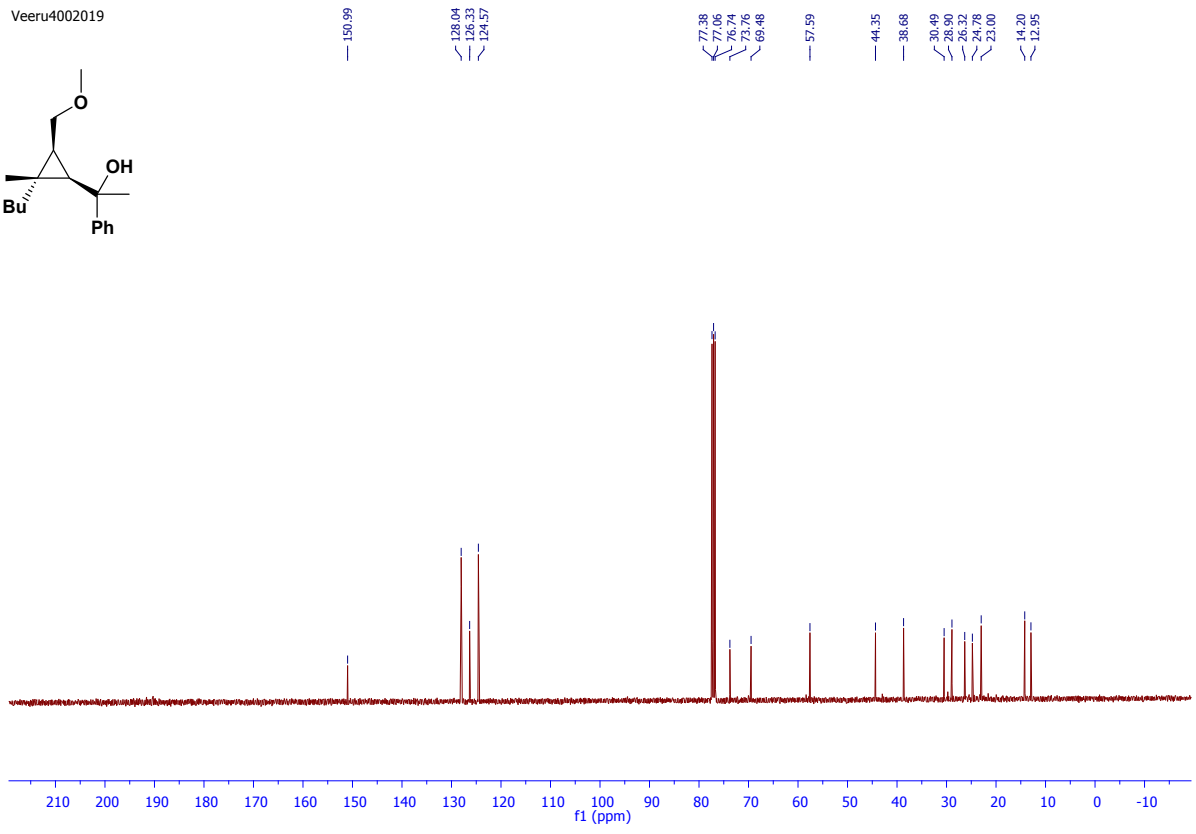
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38.68
30.49
28.90
26.32
24.78
23.00
14.20
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OH
Bu
Ph
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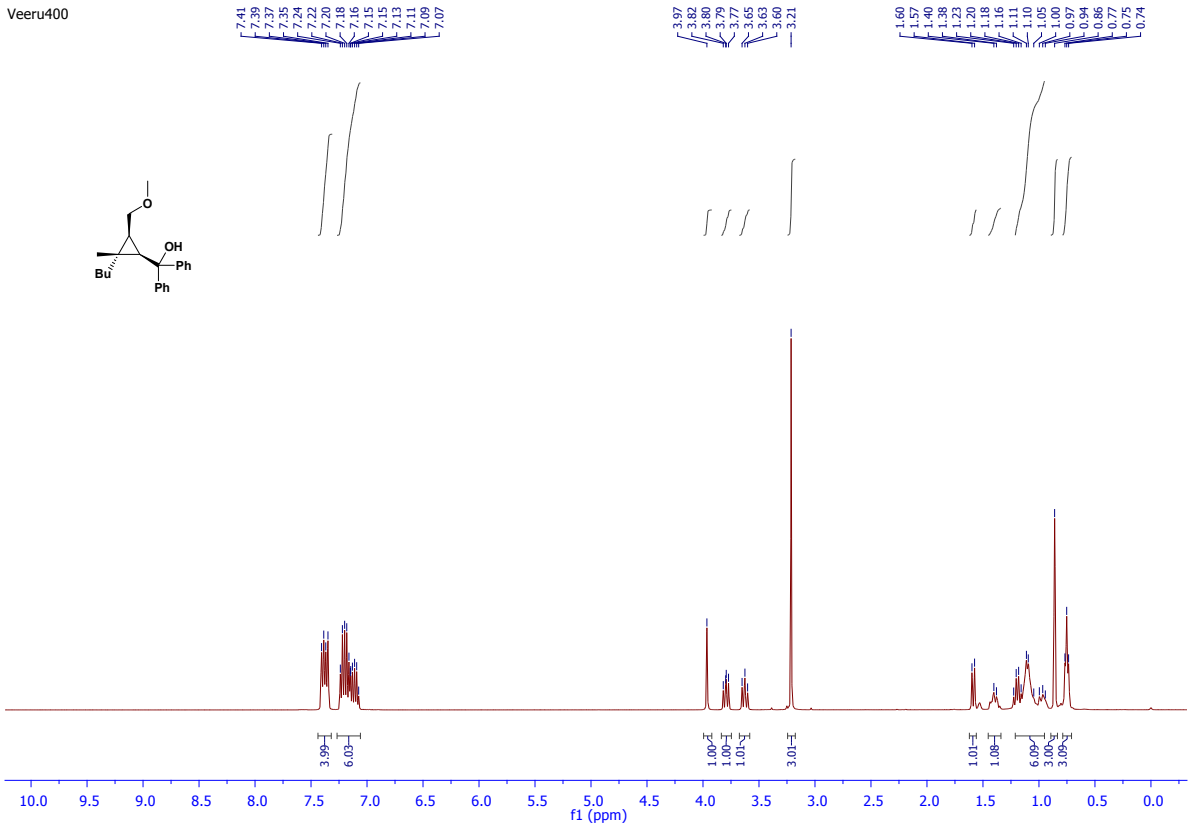
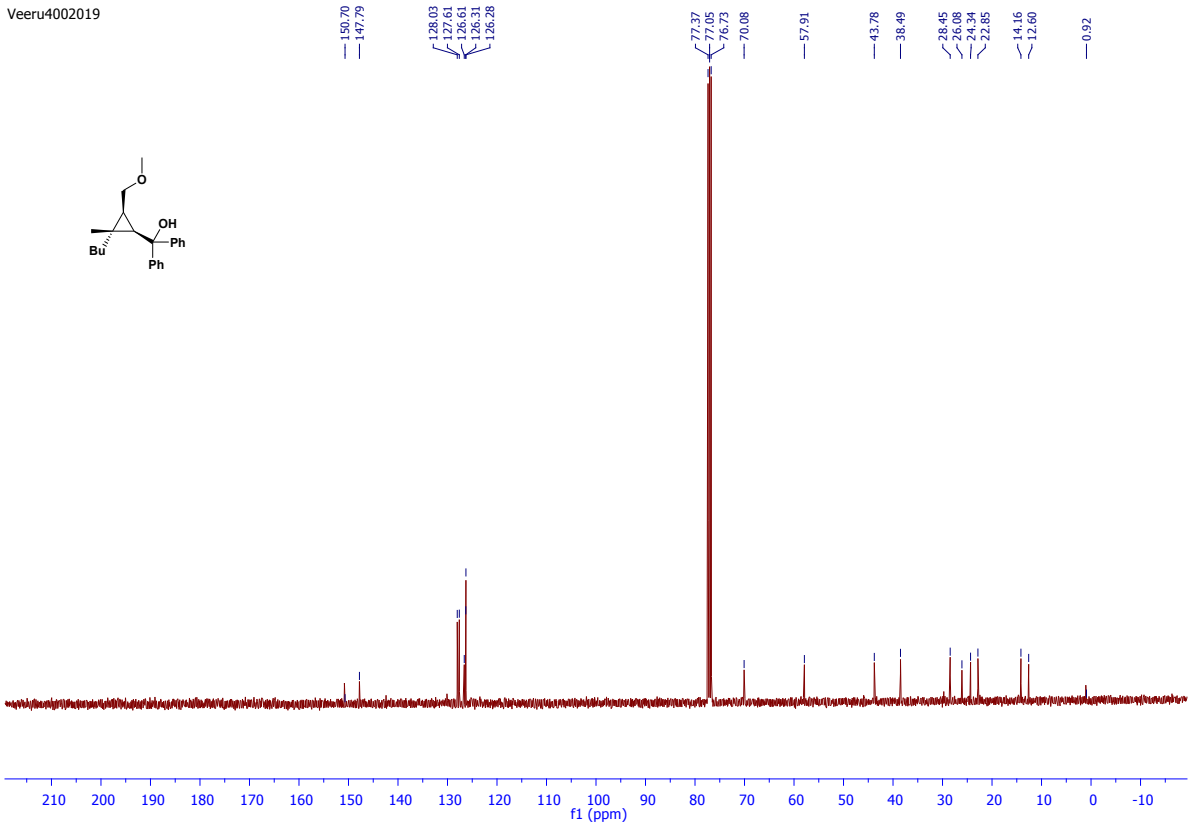
f1 (ppm)

Veeru400



Veeru4002019



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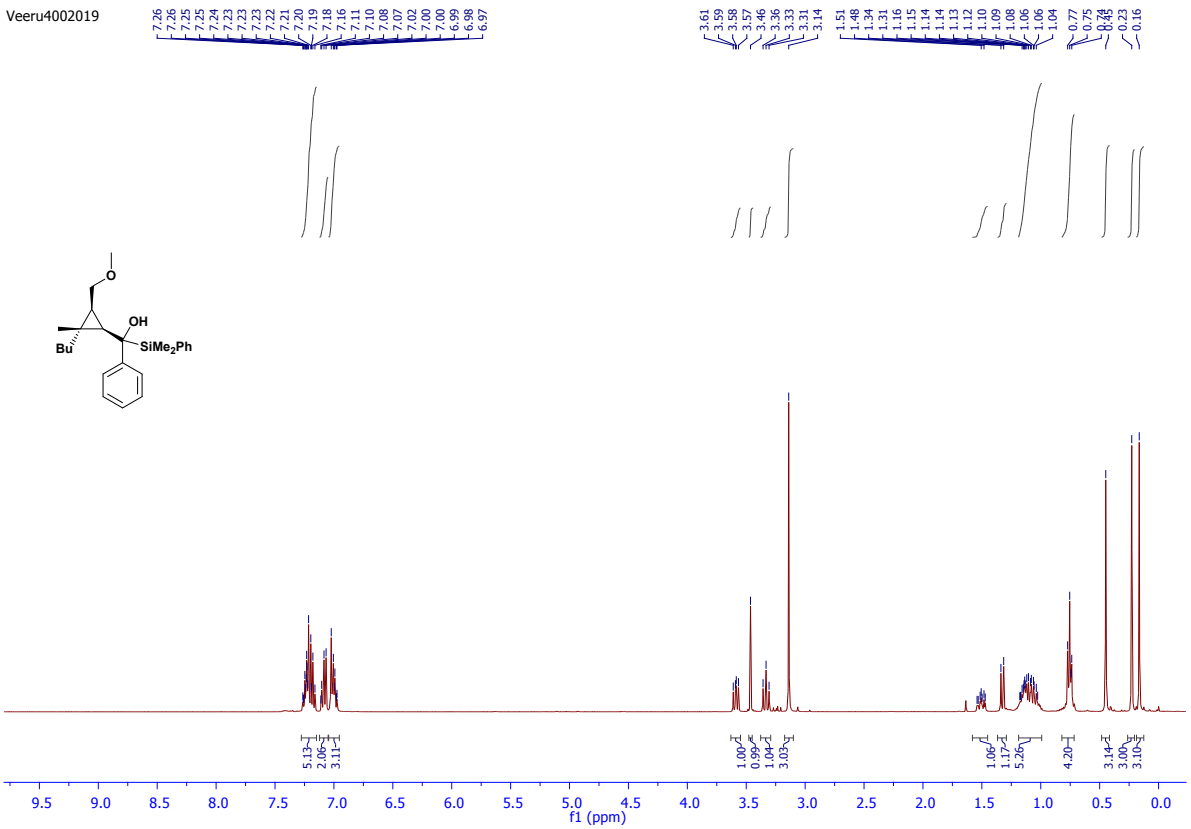

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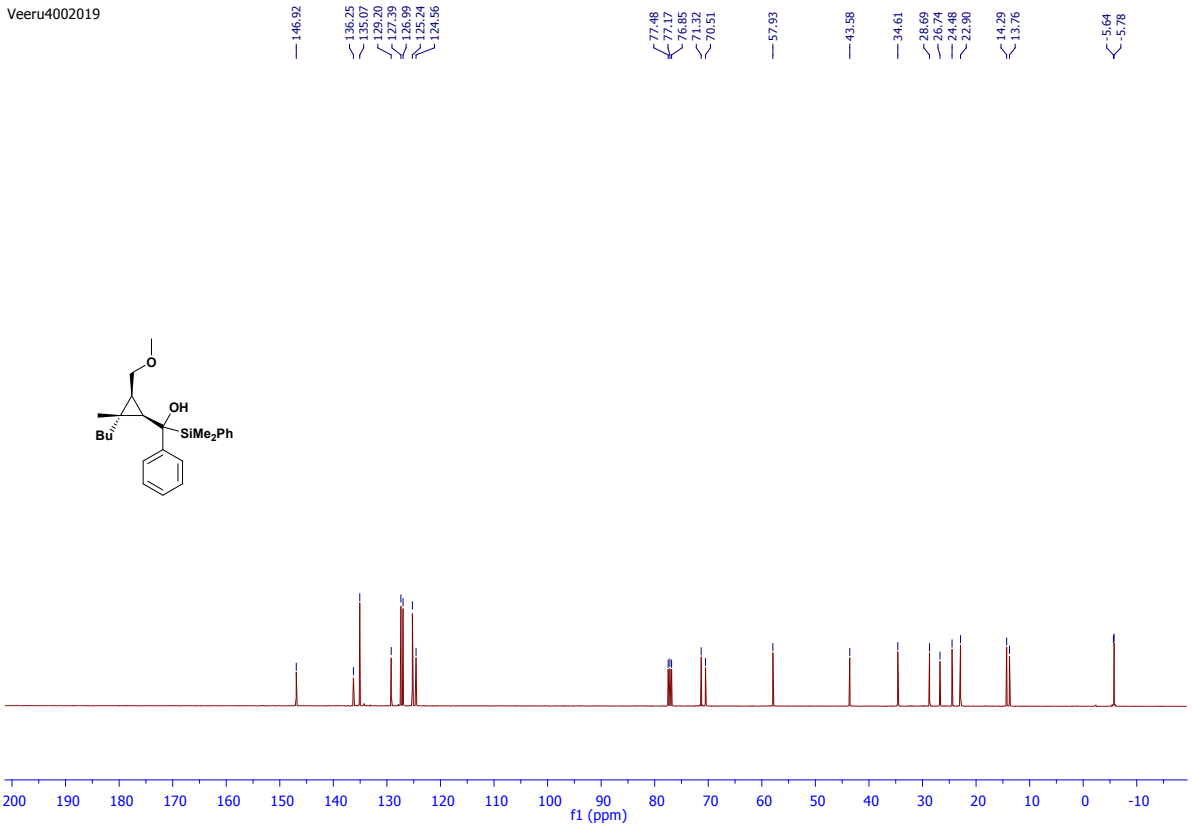

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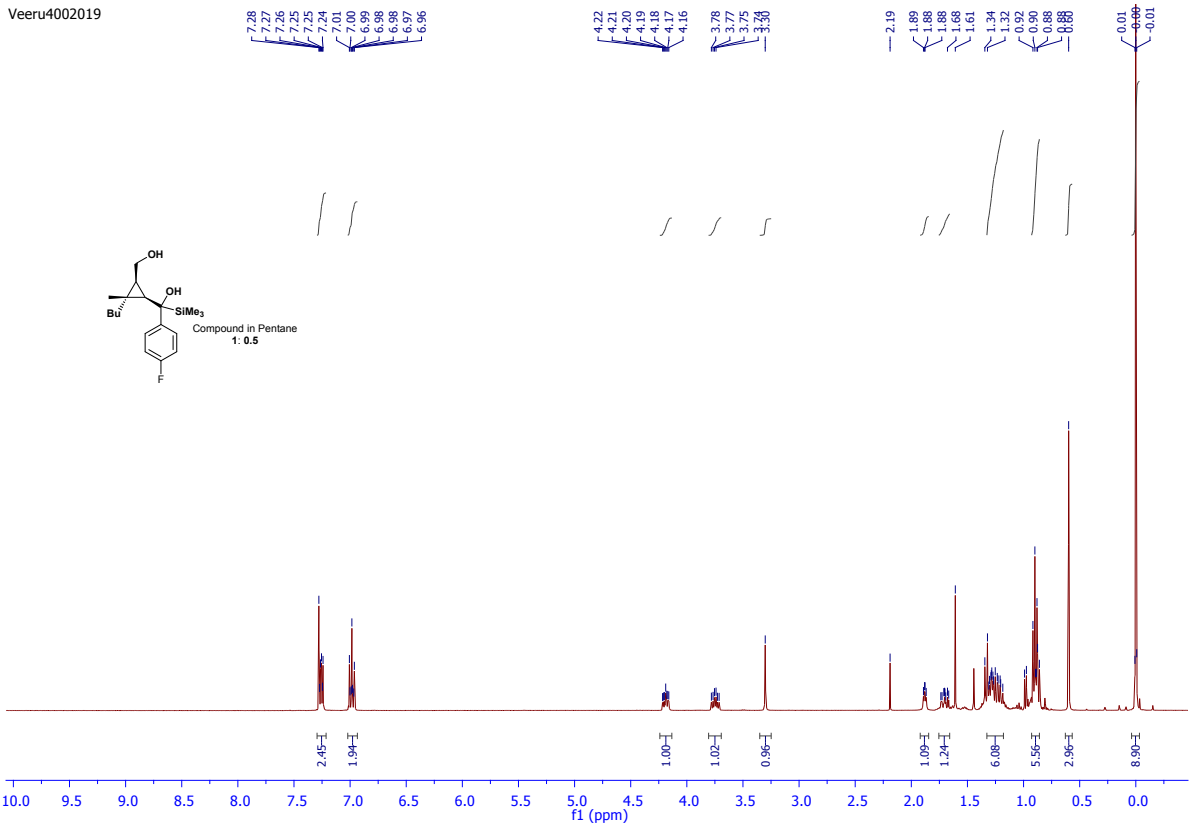

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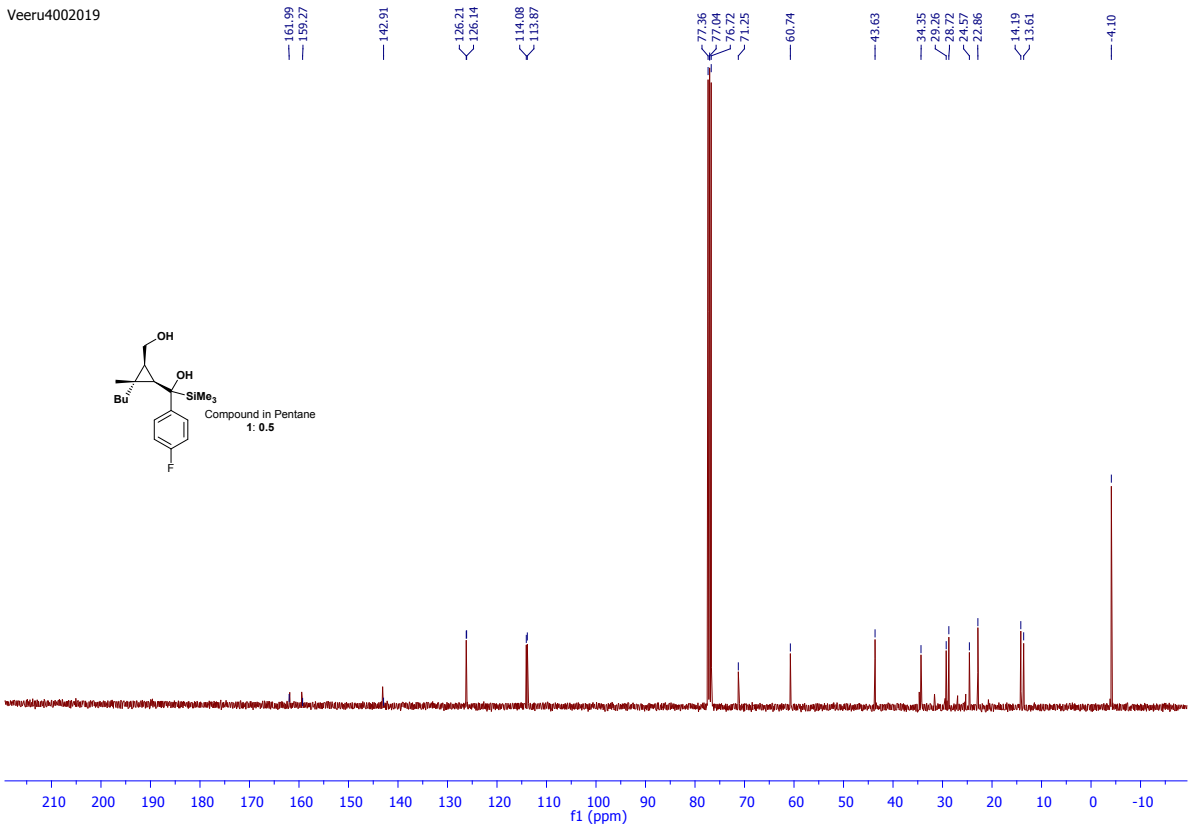

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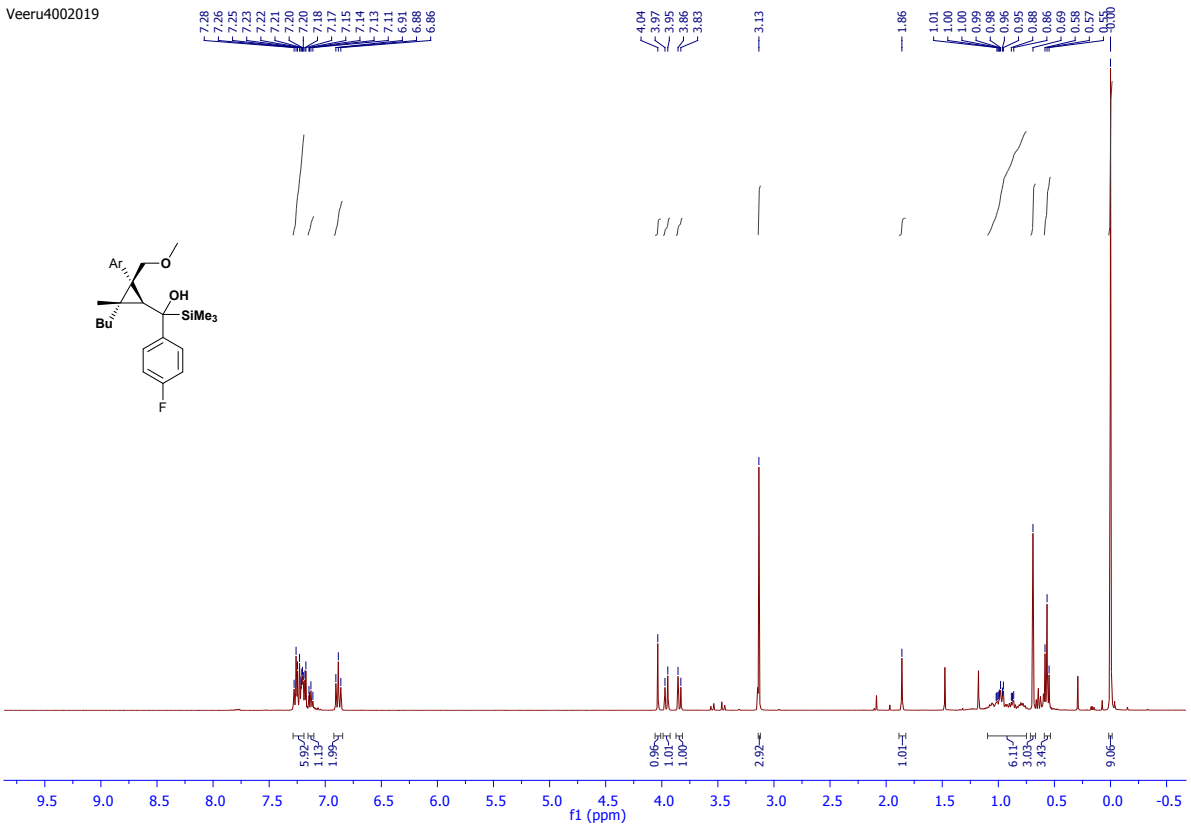

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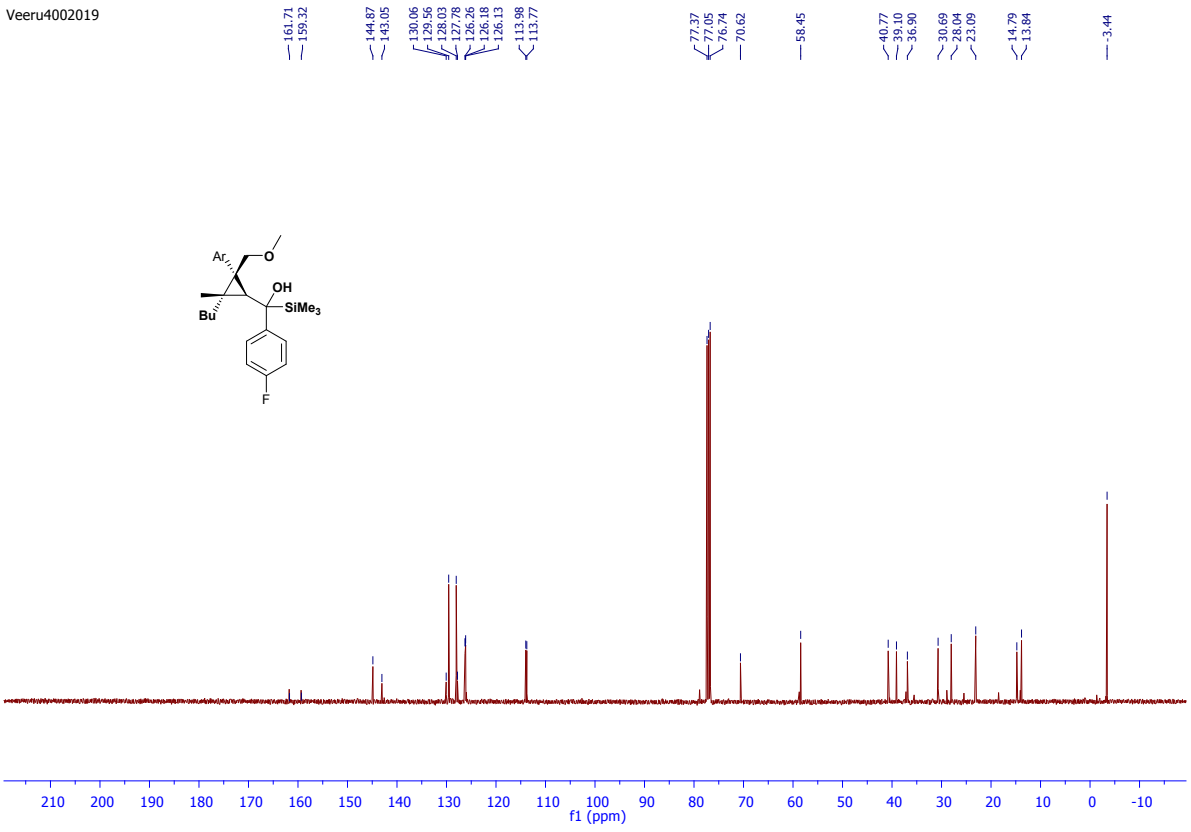

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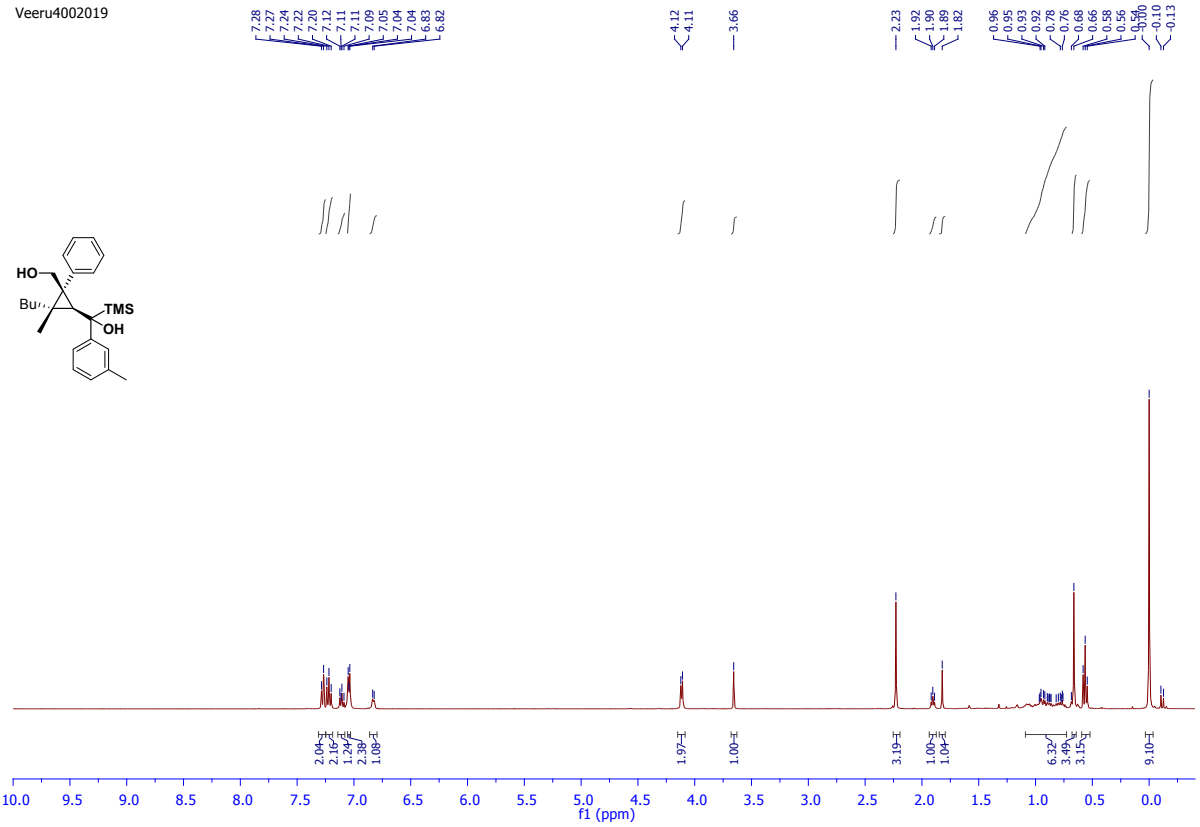

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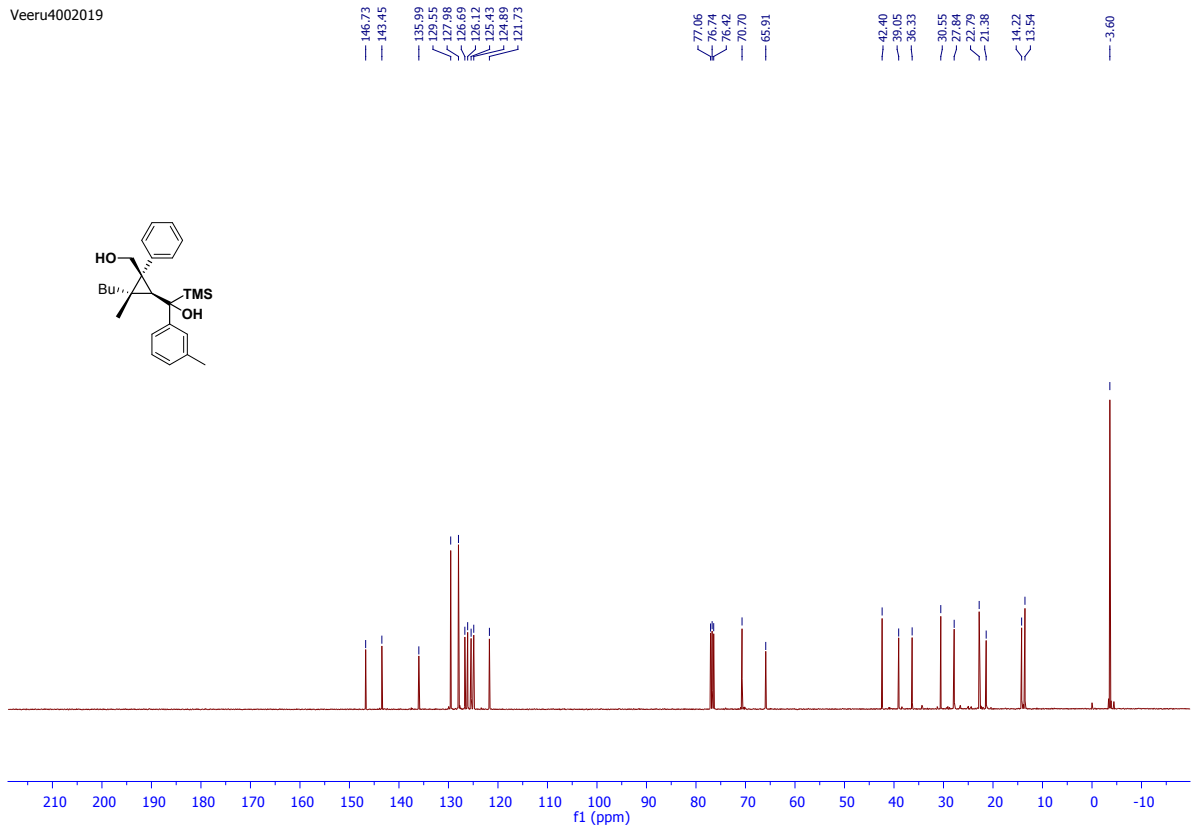

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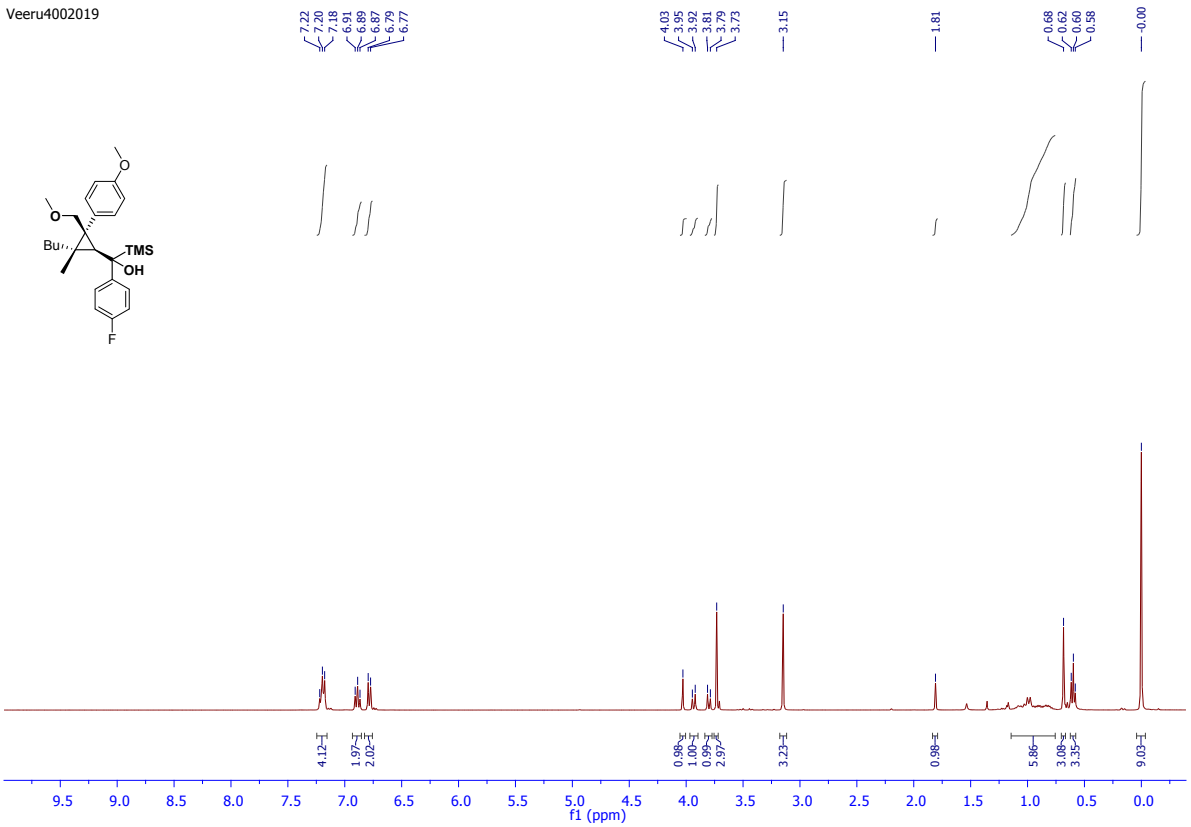

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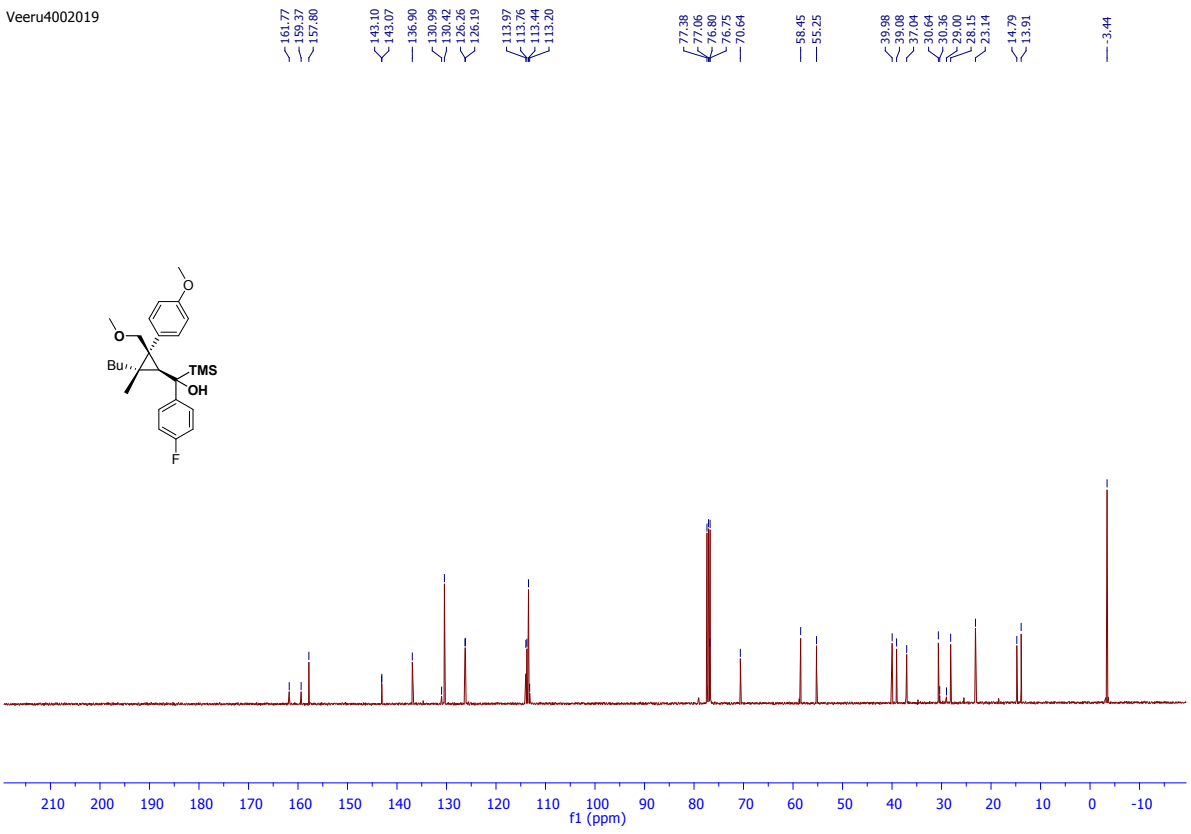

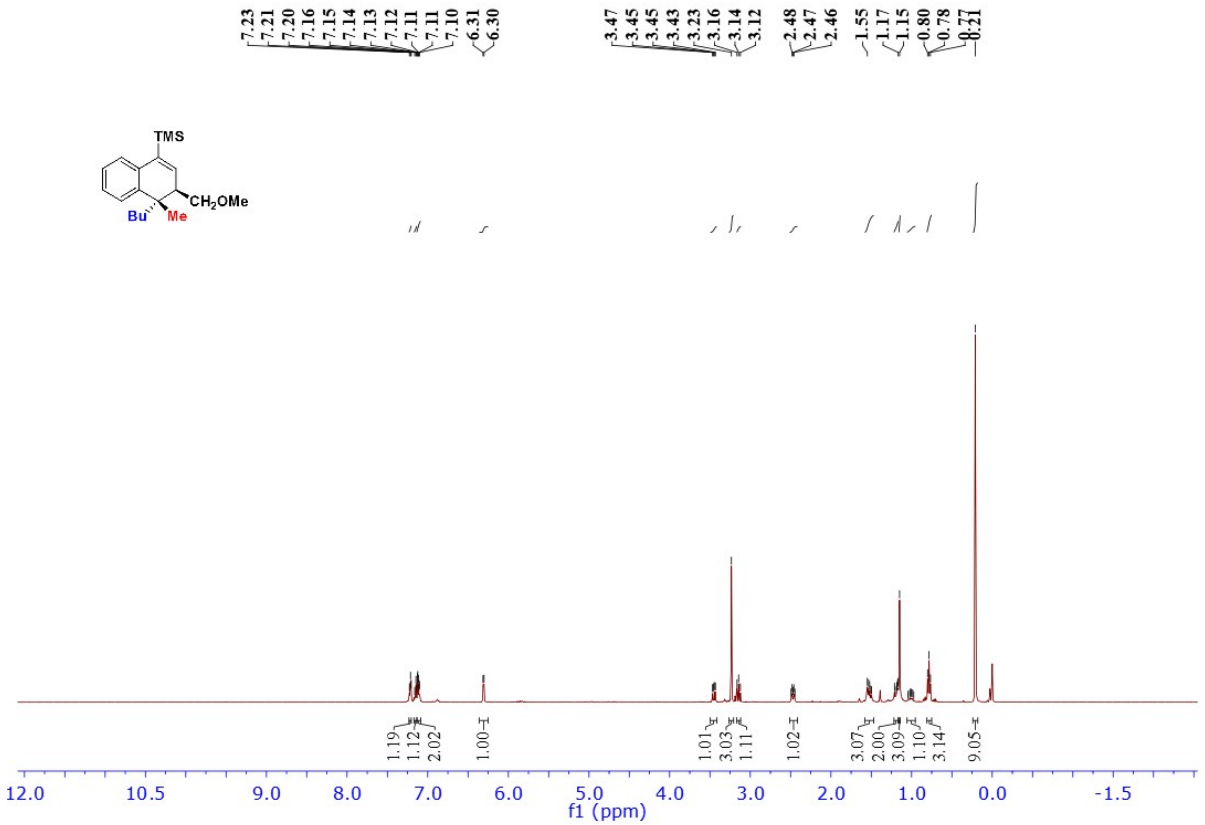
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7.20
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7.14
7.13
7.12
7.11
7.11
7.10
6.31
6.30
3.47
3.45
3.45
3.43
3.23
3.16
3.14
3.12
2.48
2.47
2.46
1.55
1.17
1.15
0.80
0.78
0.77
0.21
TMS
CH2OMe
Bu
Me
1.19
1.12
2.02
1.00
1.01
3.03
1.11
1.02
3.07
2.00
3.09
1.10
3.14
9.05
12.0
10.5
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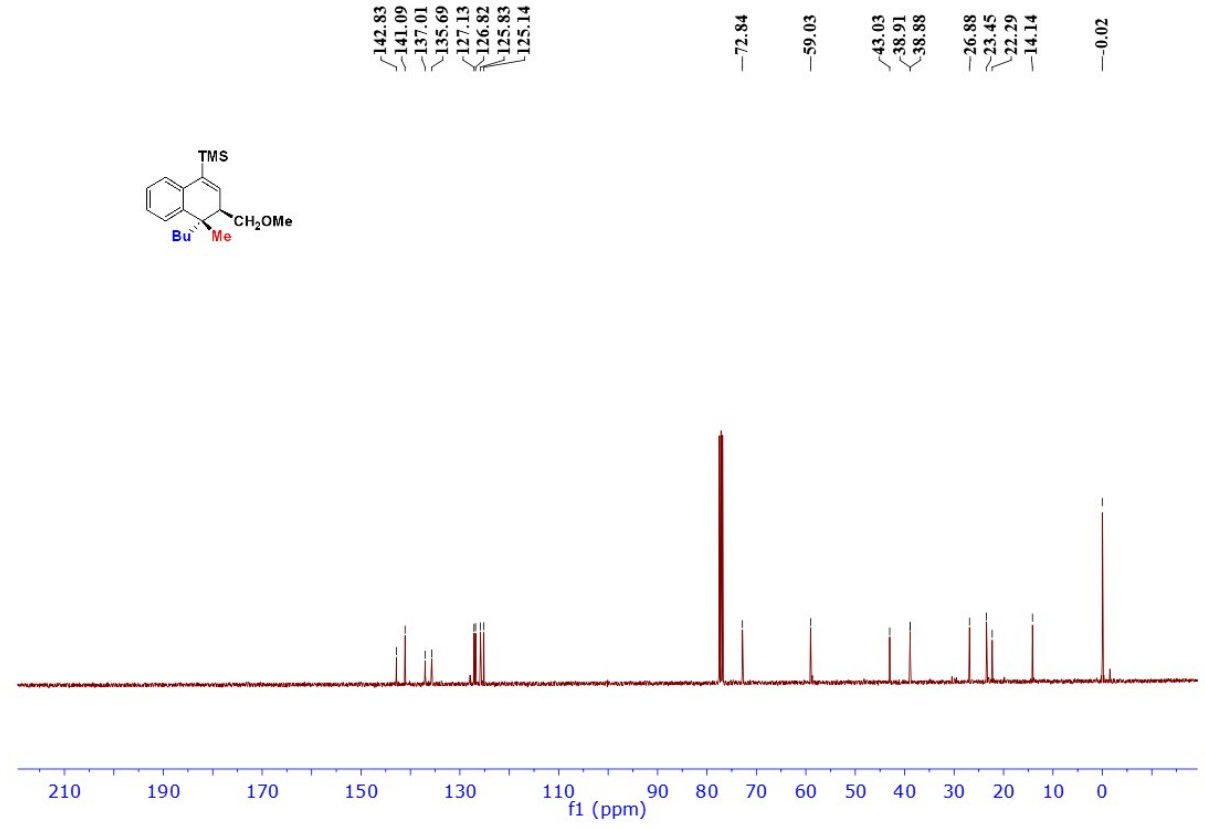
6.0
5.0
4.0
3.0
2.0
1.0
0.0
-1.5
f1 (ppm)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137.01
135.69
127.13
126.82
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125.14
72.84
59.03
43.03
38.91
38.88
26.88
23.45
22.29
14.14
-0.02
TMS
CH2OMe
Bu
Me
210
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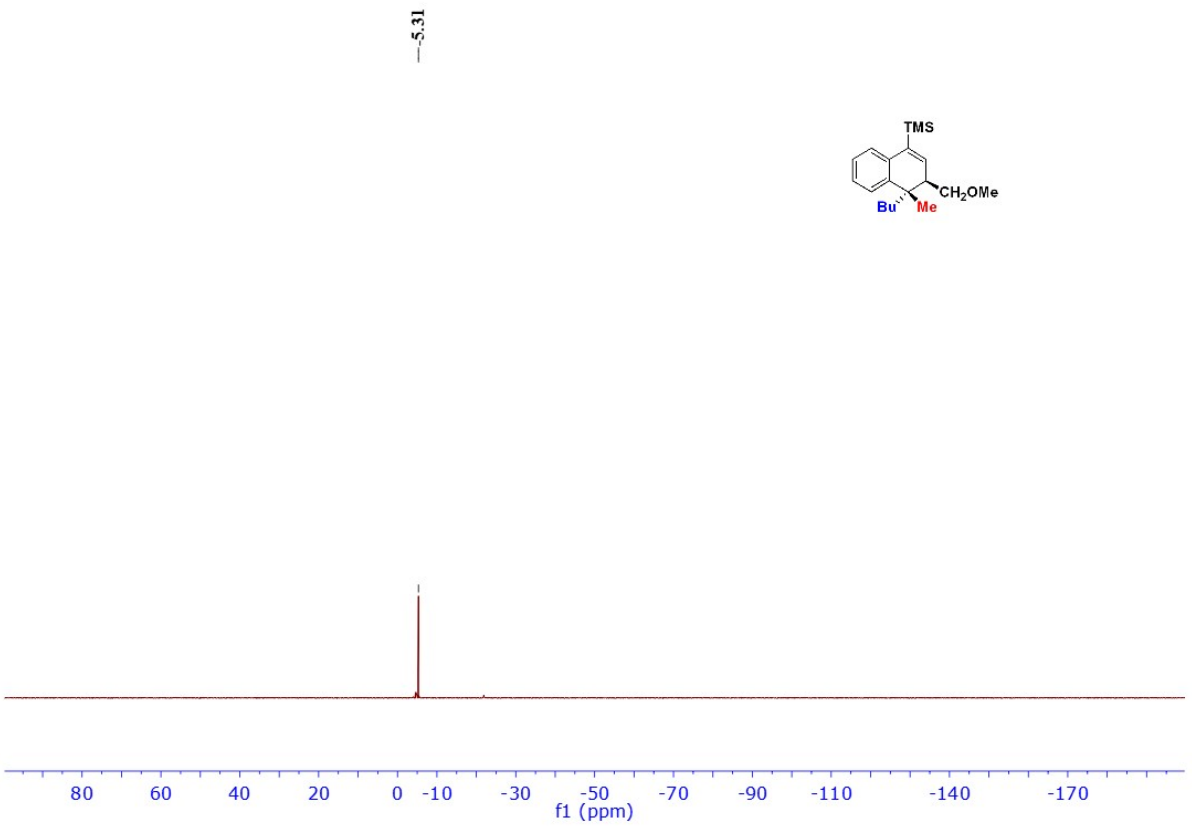
170
150
130
110
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


-5.31
TMS
CH2OMe
Bu
Me
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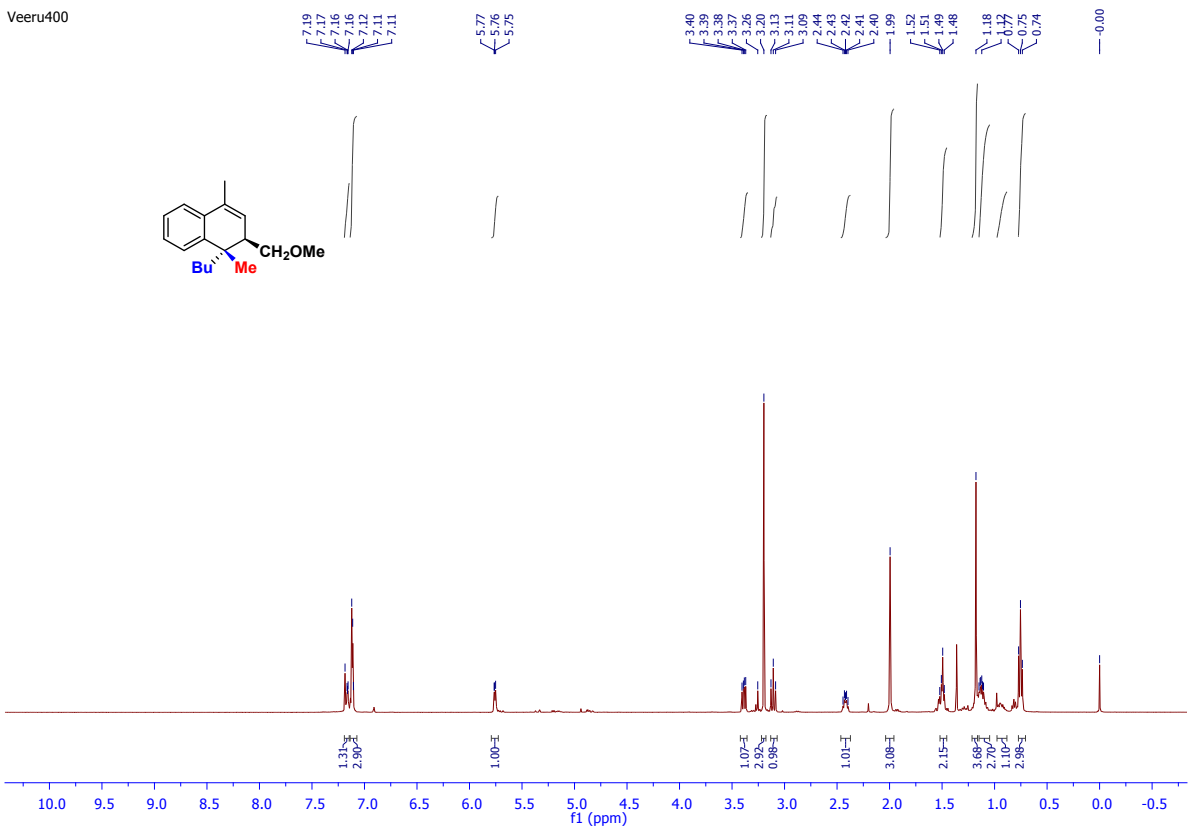
60
40
20
0
-10
-30
-50
-70
-90
-110
-140
-170
f1 (ppm)


Veeru400
7.19
7.17
7.16
7.16
7.12
7.11
7.11
5.77
5.76
5.75
3.40
3.39
3.38
3.37
3.26
3.20
3.13
3.11
3.09
2.44
2.43
2.42
2.41
2.40
1.99
1.52
1.51
1.49
1.48
1.18
0.77
0.75
0.74
0.00
CH2OMe
Bu
Me
1.31
2.90
1.00
1.07
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1.01
3.08
2.15
3.69
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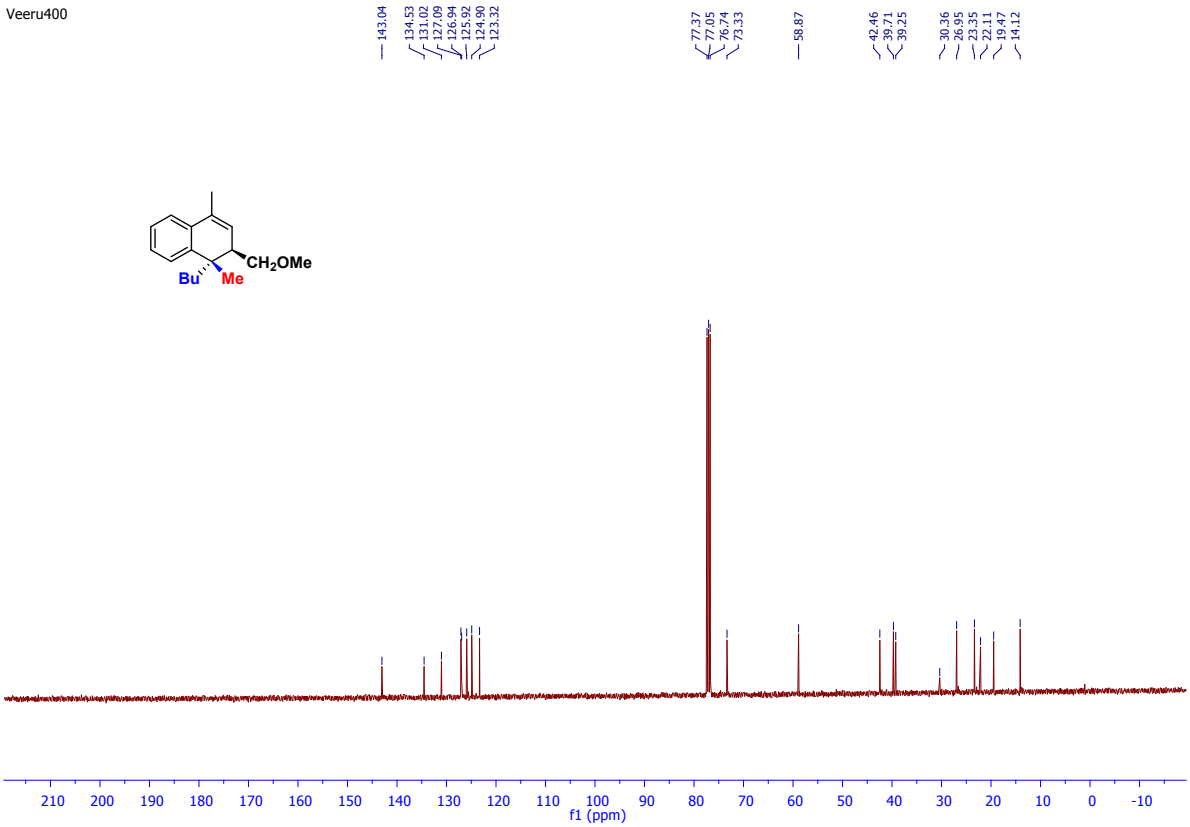
1.19
2.98
f1 (ppm)

Veeru400



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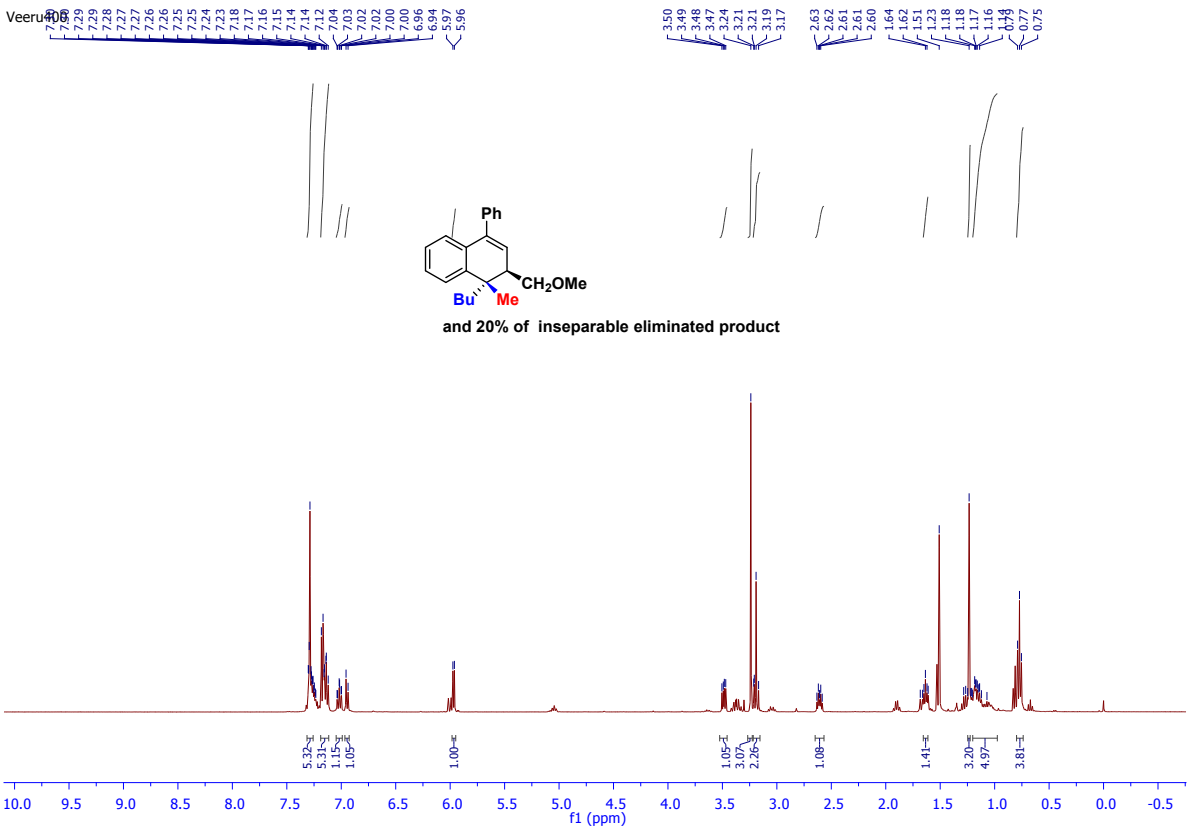
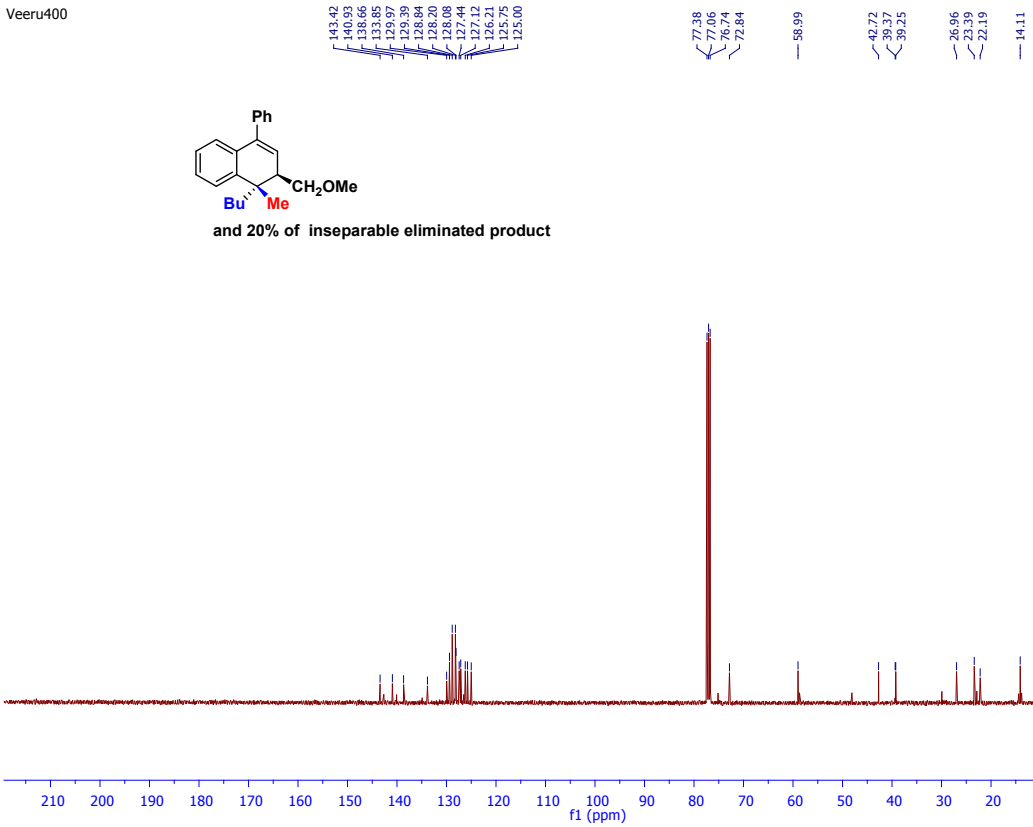


and 20% of inseparable eliminated product

Veeru400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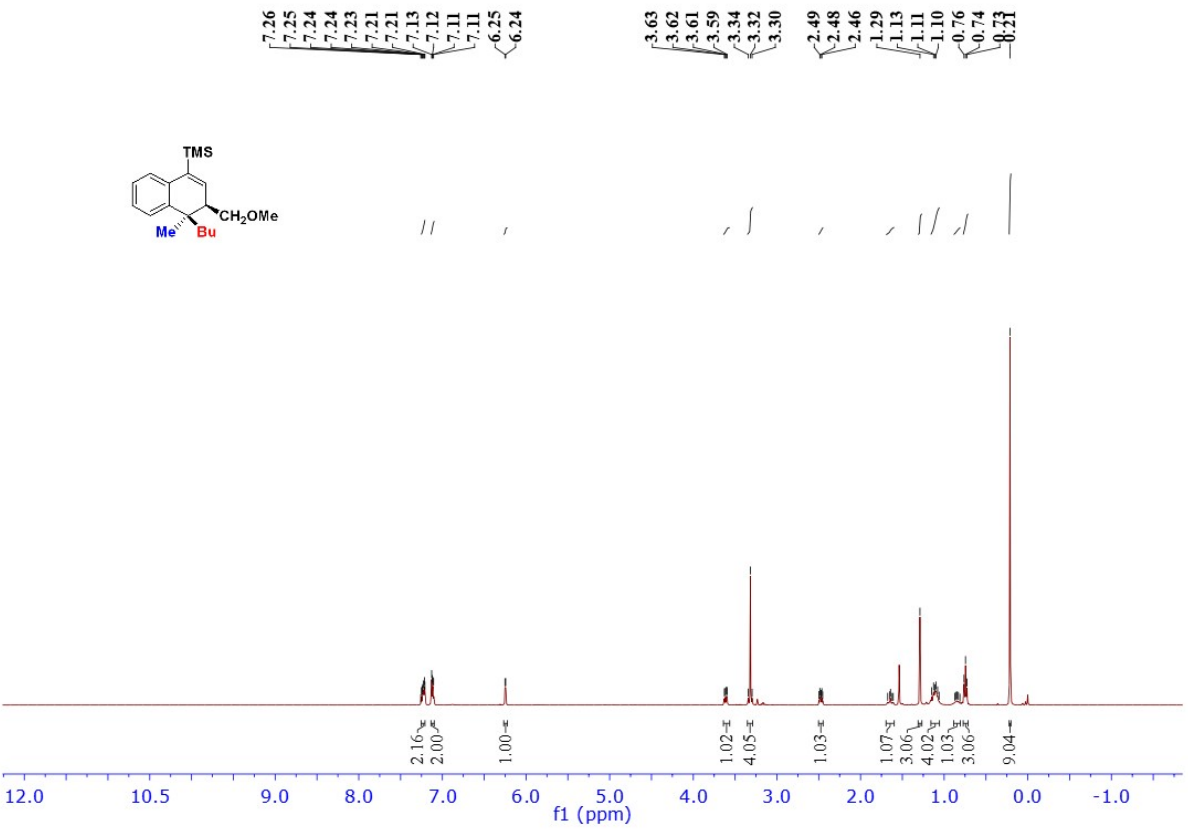
133.85
129.97
129.39
128.84
128.20
128.08
127.44
127.12
126.21
125.75
125.00
77.38
77.06
76.74
72.84
58.99
42.72
39.37
39.25
26.96
23.39
22.19
14.11
Ph
CH2OMe
Bu
Me
and 20% of inseparable eliminated product
f1 (ppm)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7.21
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7.11
6.25
6.24
3.63
3.62
3.61
3.59
3.34
3.32
3.30
2.49
2.48
2.46
1.29
1.13
1.11
1.10
0.76
0.74
0.73
0.21
TMS
CH2OMe
Me
Bu
2.16
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1.00
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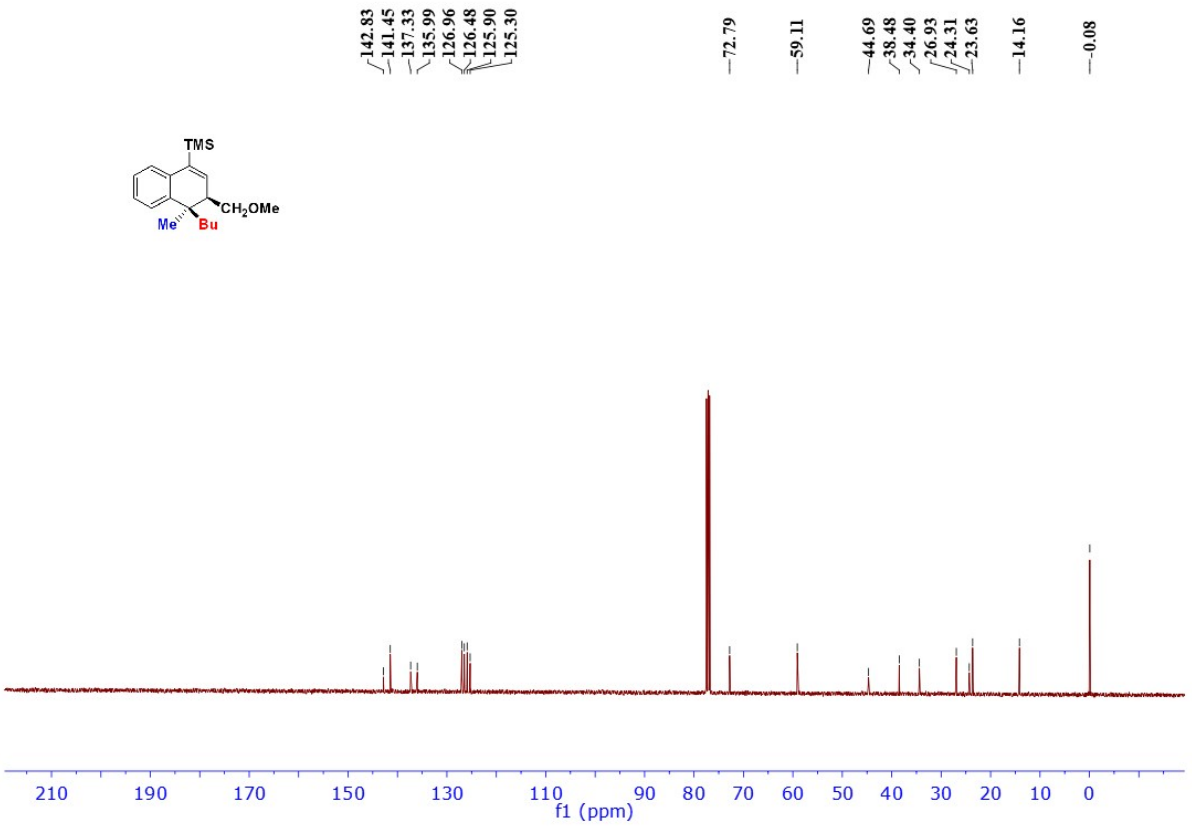
4.05
1.03
1.07
3.06
4.02
1.03
3.06
9.04
f1 (ppm)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125.30
72.79
59.11
44.69
38.48
34.40
26.93
24.31
23.63
14.16
-0.08
TMS
CH2OMe
Me
Bu
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170
150
130
110
90
80
70
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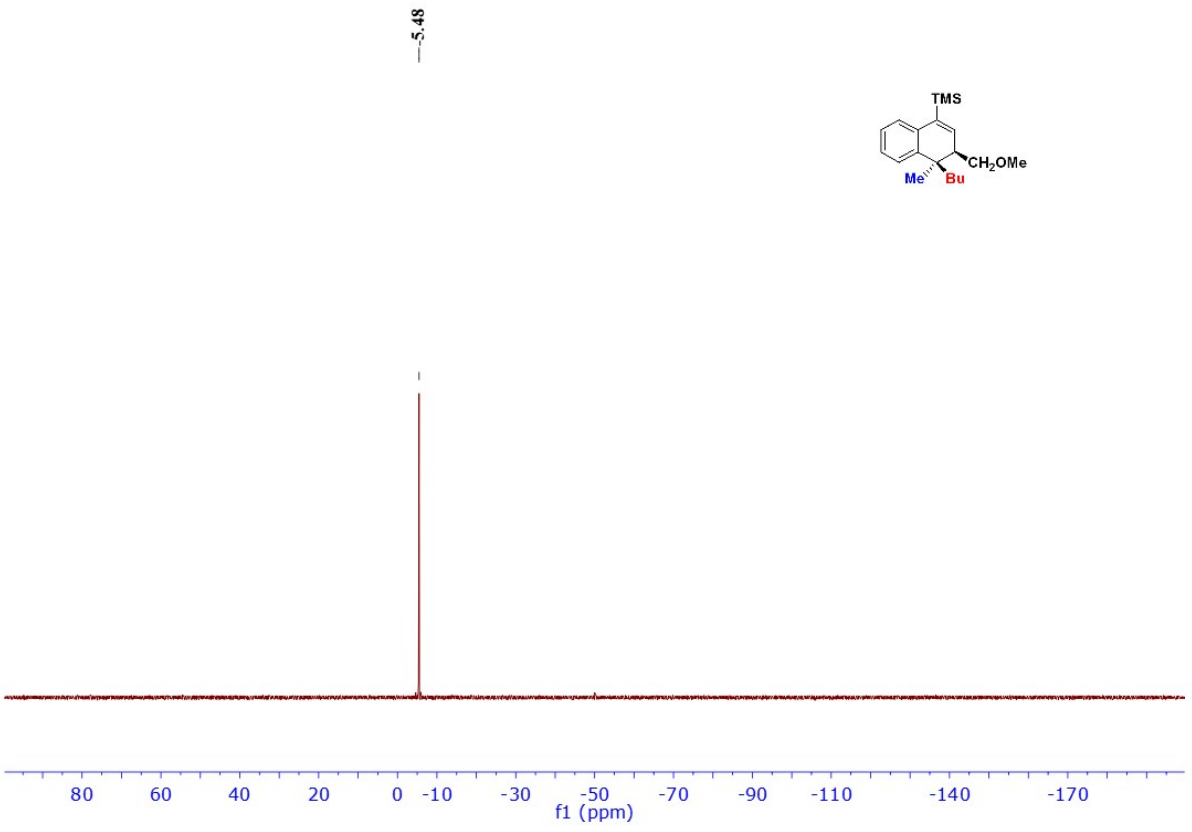
50
40
30
20
10
0
f1 (ppm)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-50
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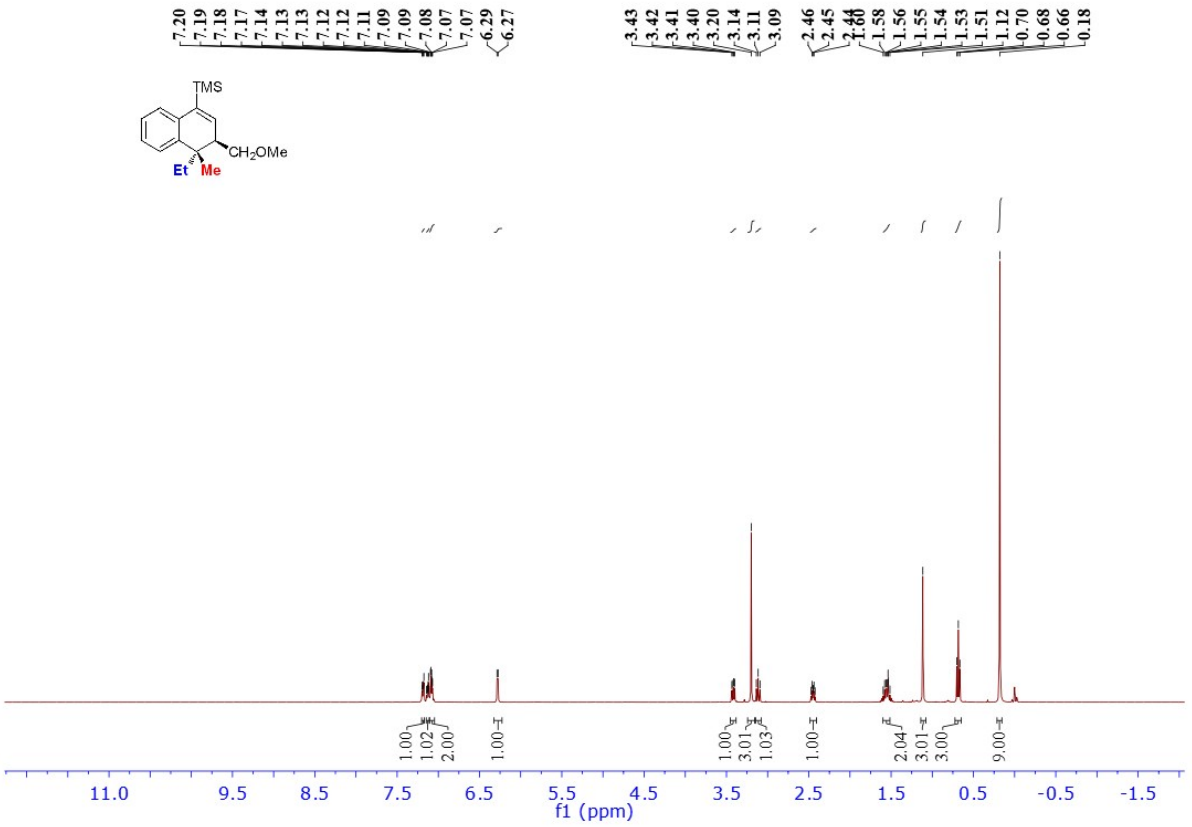
f1 (ppm)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7.11
7.09
7.09
7.08
7.07
7.07
6.29
6.27
3.43
3.42
3.41
3.40
3.20
3.14
3.11
3.09
2.46
2.45
2.44
1.60
1.58
1.56
1.55
1.54
1.53
1.51
1.12
0.70
0.68
0.66
0.18
TMS
CH2OMe
Et
Me
1.00
1.02
2.00
1.00
1.00
3.01
1.03
1.00
2.04
3.01
3.00
9.00
11.0
9.5
8.5
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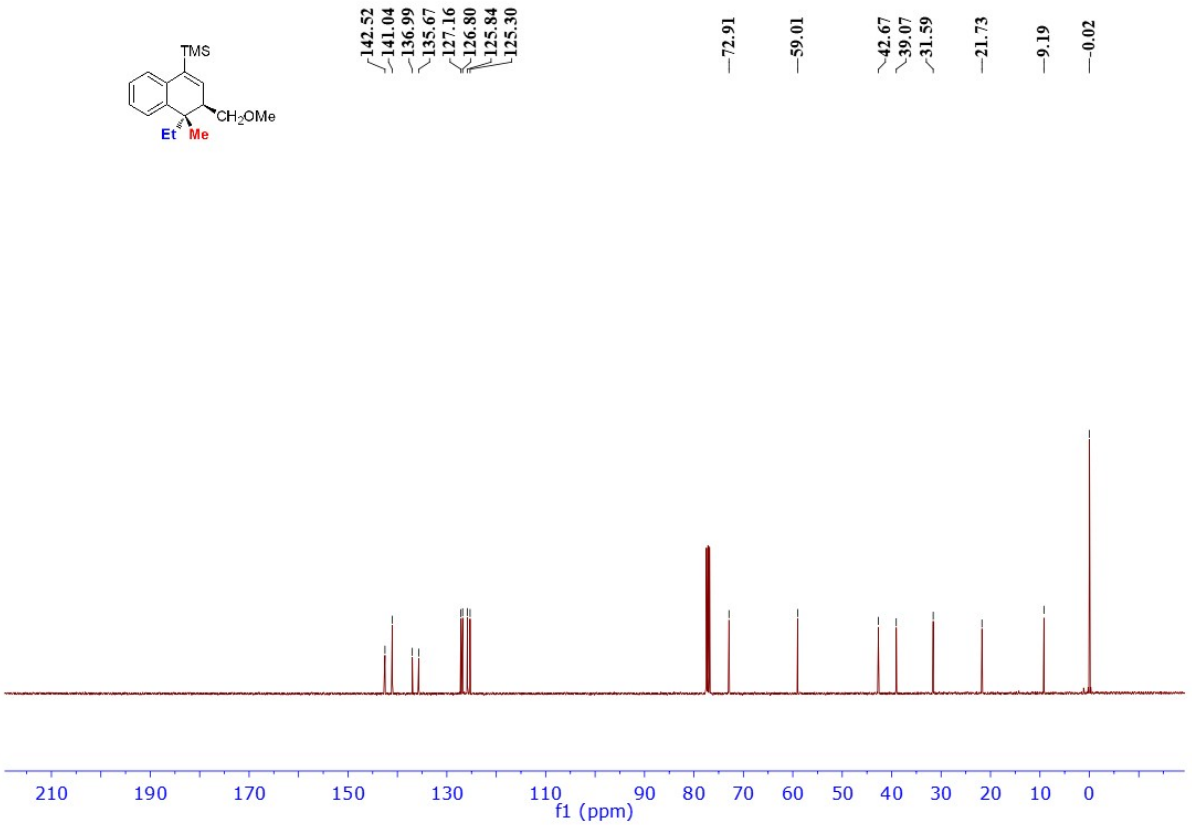
5.5
4.5
3.5
2.5
1.5
0.5
-0.5
-1.5
f1 (ppm)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125.30
72.91
59.01
42.67
39.07
31.59
21.73
9.19
-0.02
TMS
CH2OMe
Et
Me
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170
150
130
110
90
80
70
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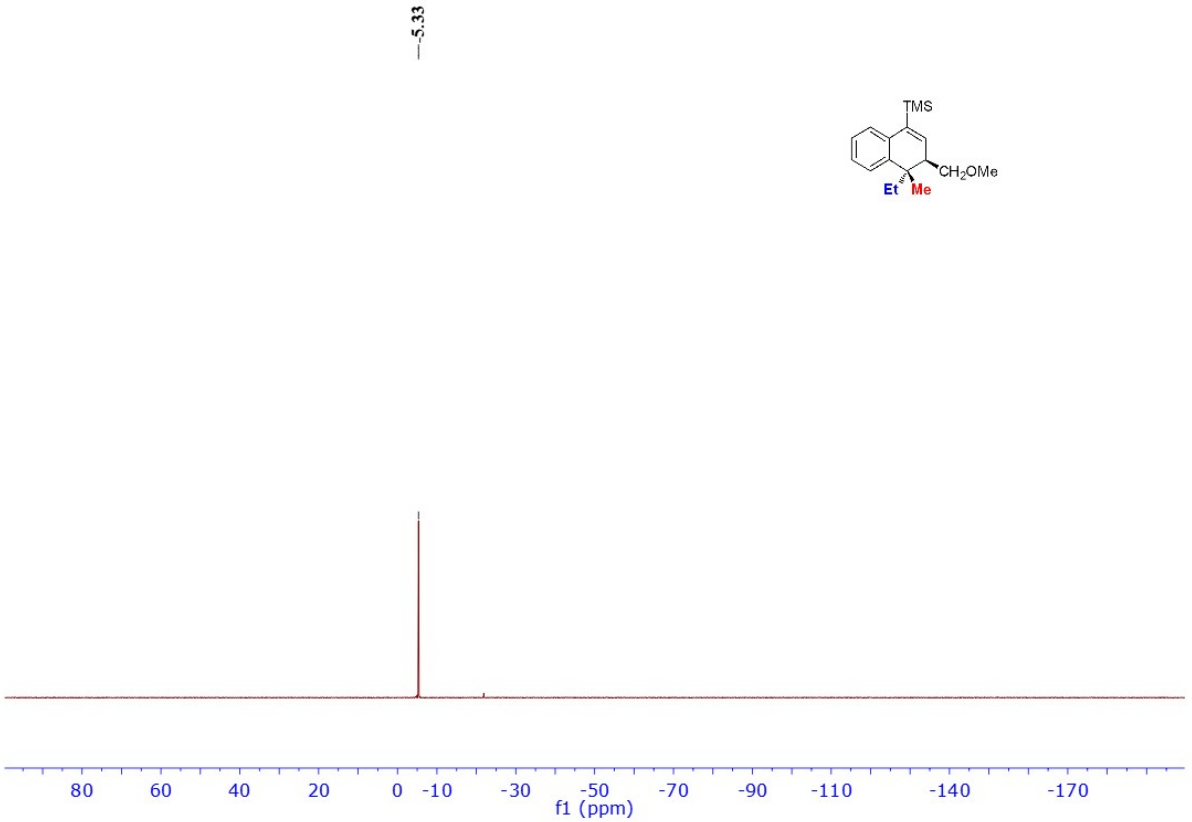
50
40
30
20
10
0
f1 (ppm)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TMS
CH2OMe
Et
Me
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-50
-70
-90
-110
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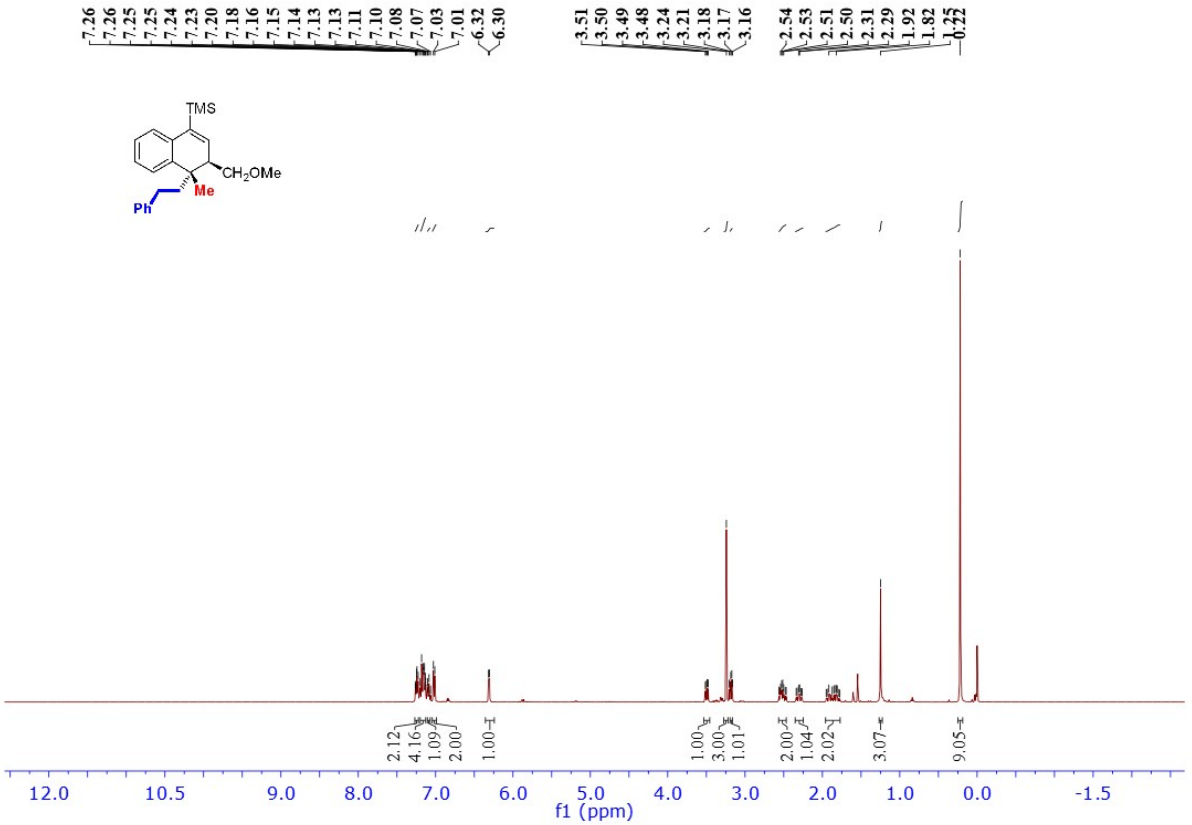
-170
f1 (ppm)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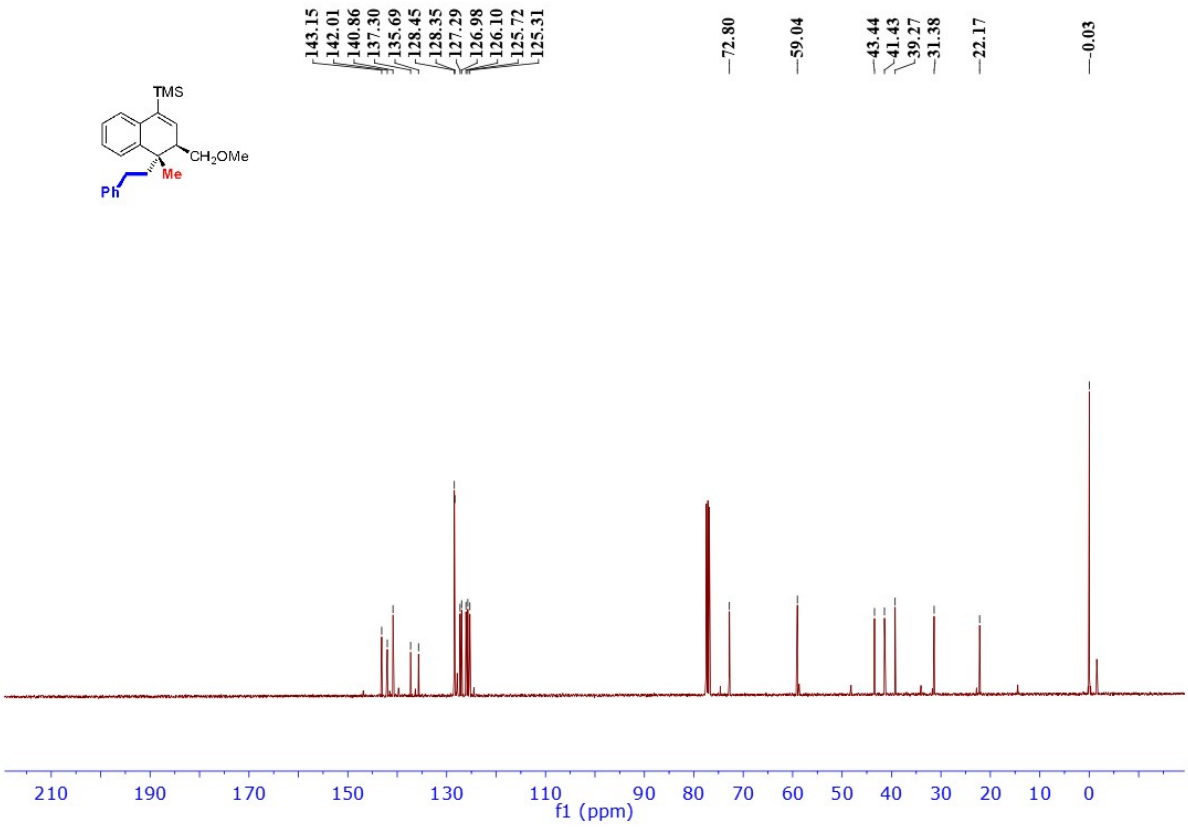
7.13
7.11
7.10
7.08
7.07
7.03
7.01
6.32
6.30
3.51
3.50
3.49
3.48
3.24
3.21
3.18
3.17
3.16
2.54
2.53
2.51
2.50
2.31
2.29
1.92
1.82
1.25
0.22
TMS
CH2OMe
Me
Ph
2.12
4.16
1.09
2.00
1.00
1.00
3.00
1.01
2.00
1.04
2.02
3.07
9.05
12.0
10.5
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
-1.5
f1 (ppm)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127.29
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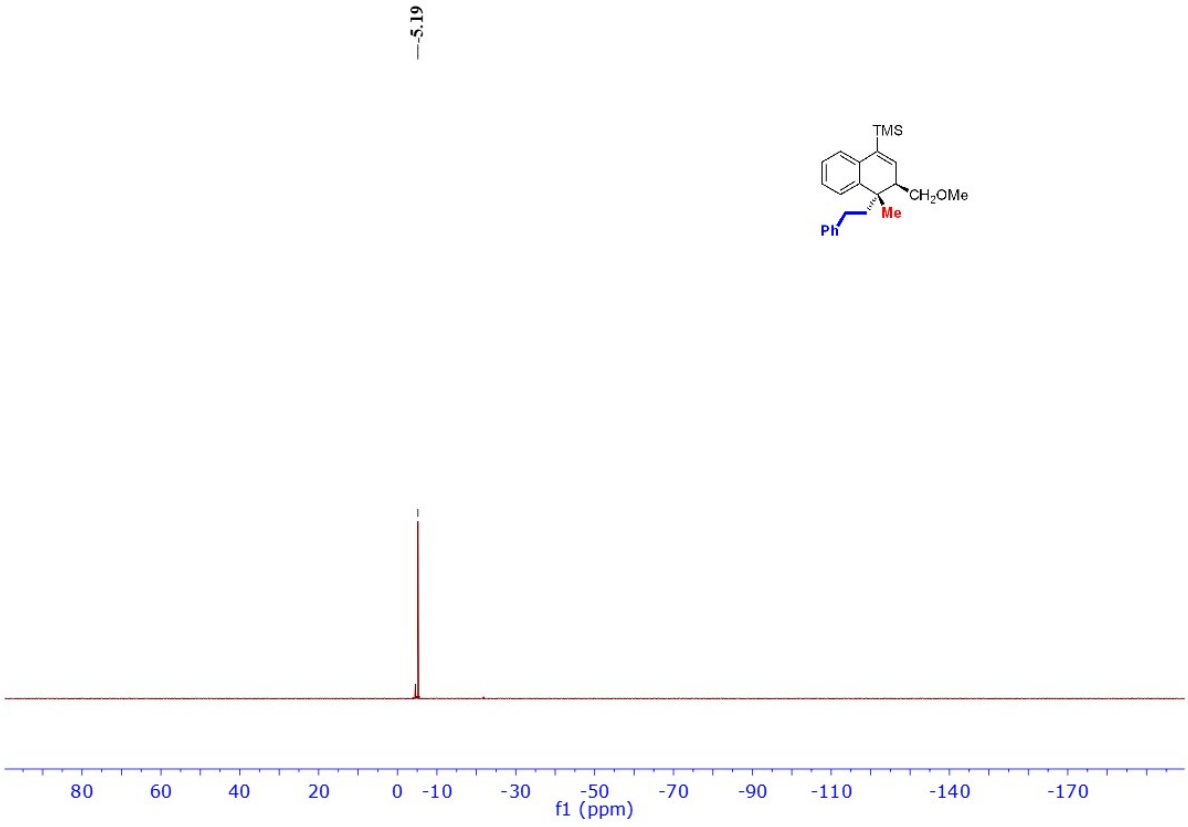
126.10
125.72
125.31
72.80
59.04
43.44
41.43
39.27
31.38
22.17
0.03
TMS
CH2OMe
Me
Ph
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


5.19
TMS
CH2OMe
Me
Ph
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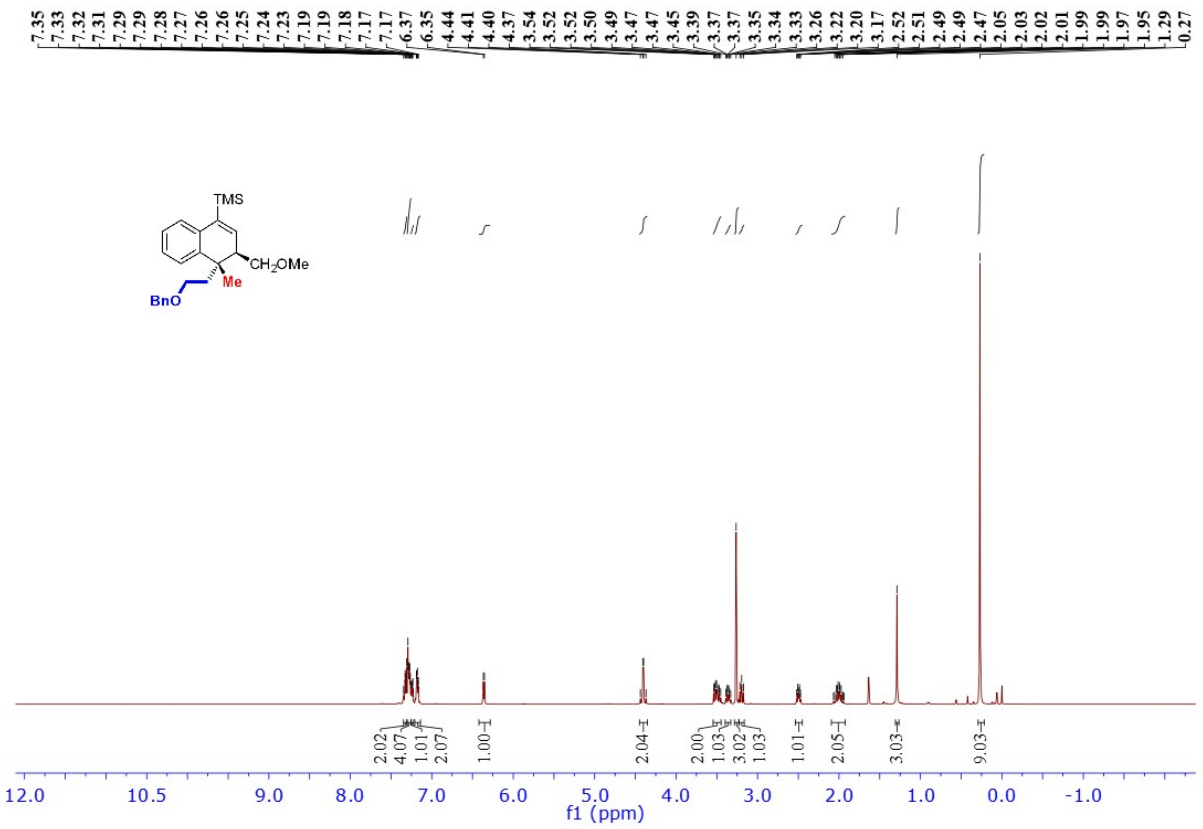
40
20
0
-10
-30
-50
-70
-90
-110
-140
-170
f1 (ppm)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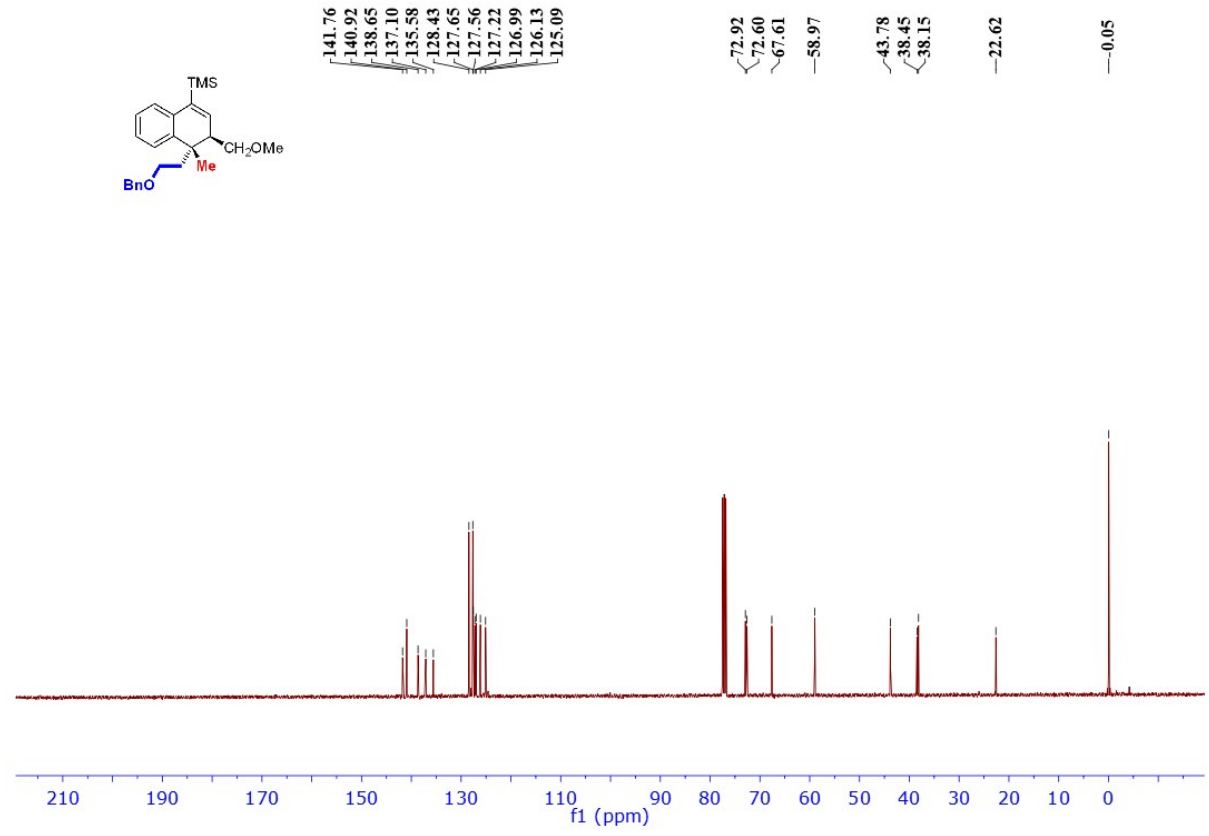
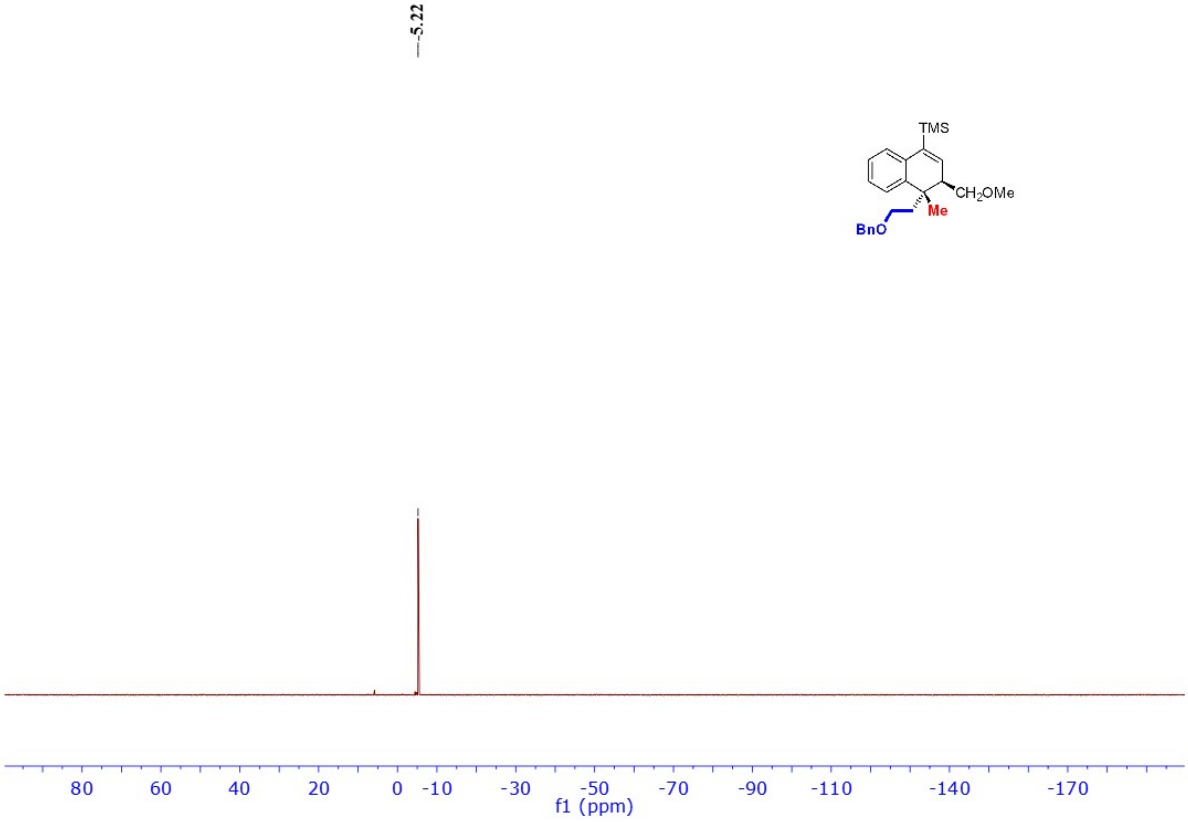
TMS
CH2OMe
Me
BnO
2.02 4.07 1.01 2.07 1.00 2.04 2.00 1.03 3.02 1.03 1.01 2.05 3.03 9.03
12.0 10.5 9.0 8.0 7.0 6.0 5.0 4.0 3.0 2.0 1.0 0.0 -1.0
f1 (ppm)


141.76 140.92 138.65 137.10 135.58 128.43 127.65 127.56 127.22 126.99 126.13 125.09
72.92 72.60 67.61 58.97 43.78 38.45 38.15 22.62 -0.05
TMS
CH2OMe
Me
BnO
210 190 170 150 130 110 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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TMS
CH2OMe
Me
BnO
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40
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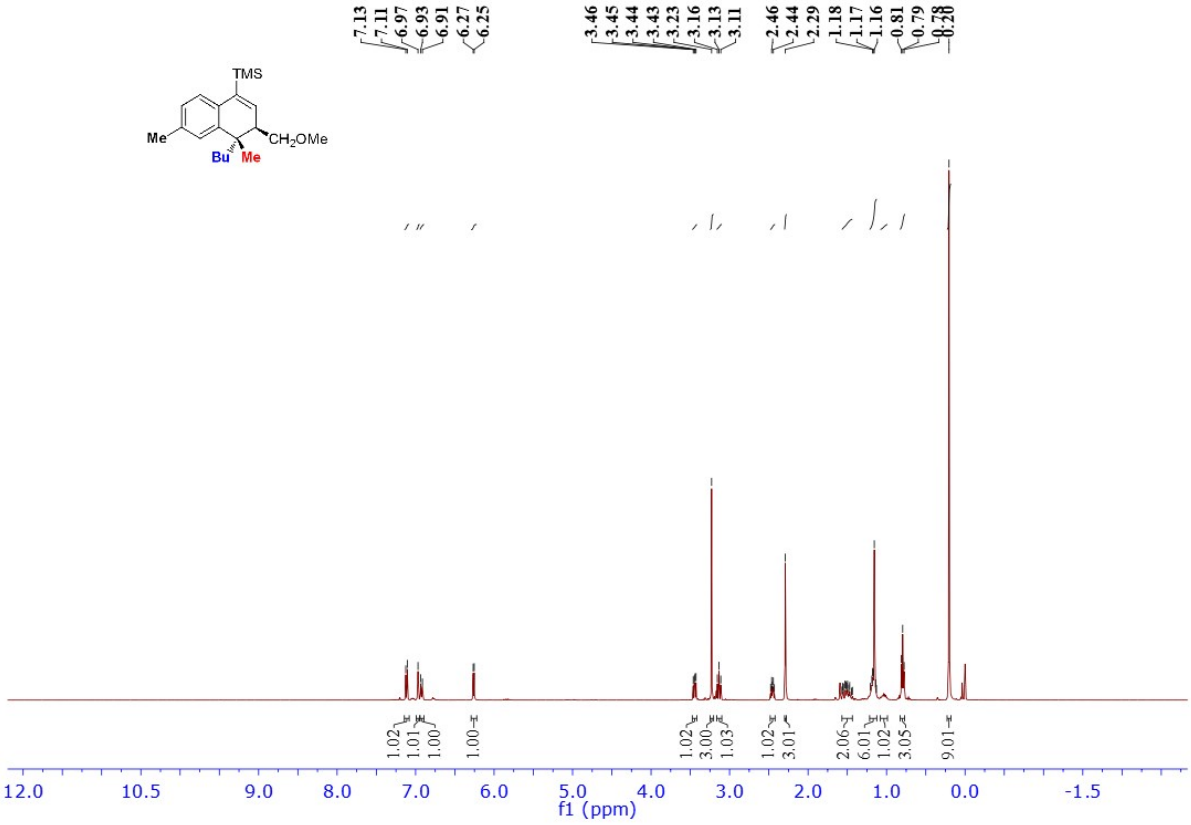
0
-10
-30
-50
-70
-90
-110
-140
-170
f1 (ppm)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6.91
6.27
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3.45
3.44
3.43
3.23
3.16
3.13
3.11
2.46
2.44
2.29
1.18
1.17
1.16
0.81
0.79
TMS
Me
CH2OMe
Bu
Me
1.02
1.01
1.00
1.00
1.02
3.00
1.03
1.02
3.01
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6.01
1.02
3.05
9.01
12.0
10.5
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6.0
5.0
4.0
3.0
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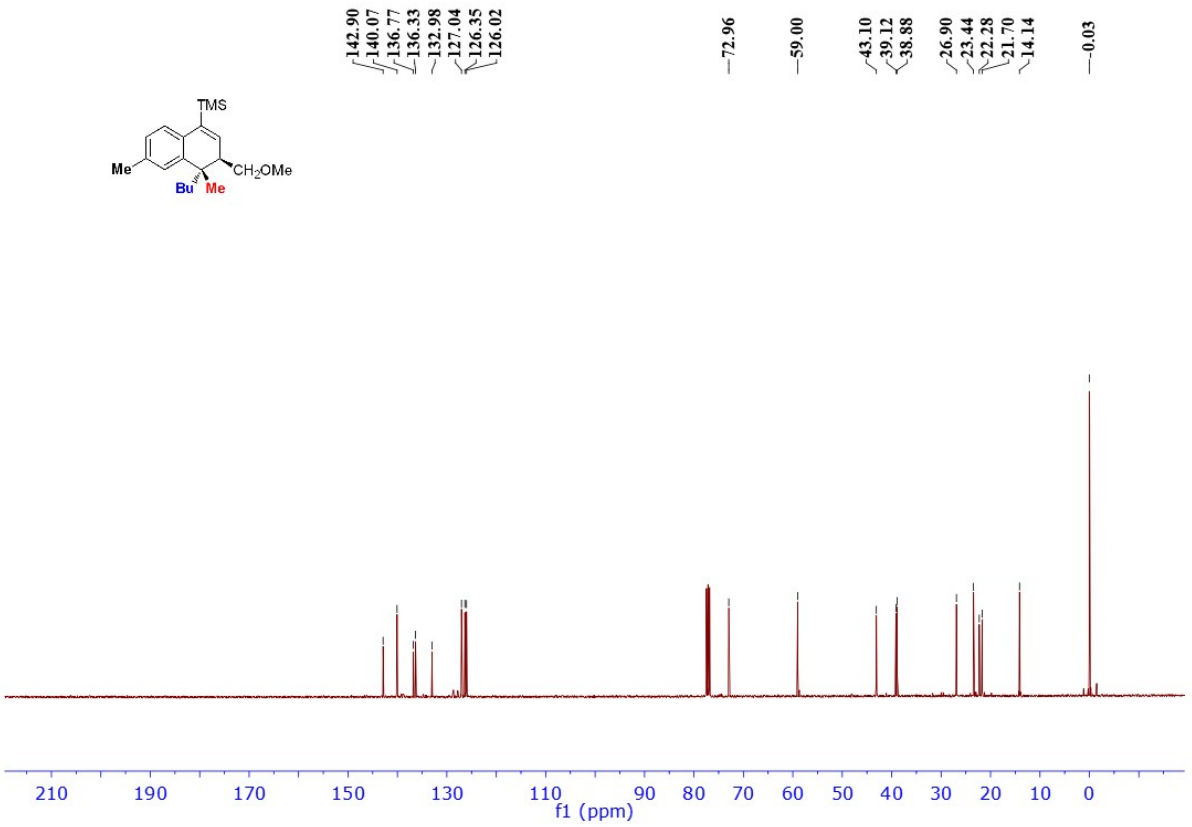
1.0
0.0
-1.5
f1 (ppm)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126.35
126.02
72.96
59.00
43.10
39.12
38.88
26.90
23.44
22.28
21.70
14.14
0.03
TMS
Me
CH2OMe
Bu
Me
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150
130
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90
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50
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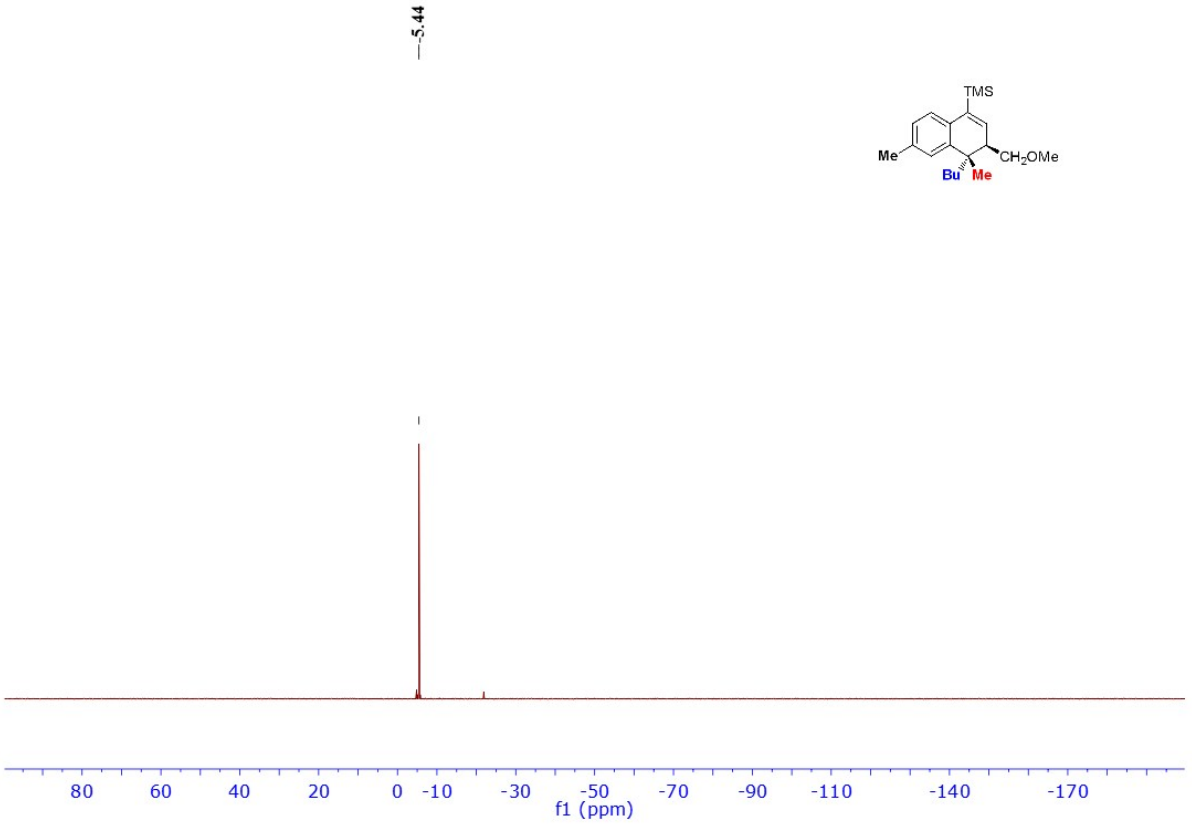
10
0
f1 (ppm)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CH2OMe
Bu
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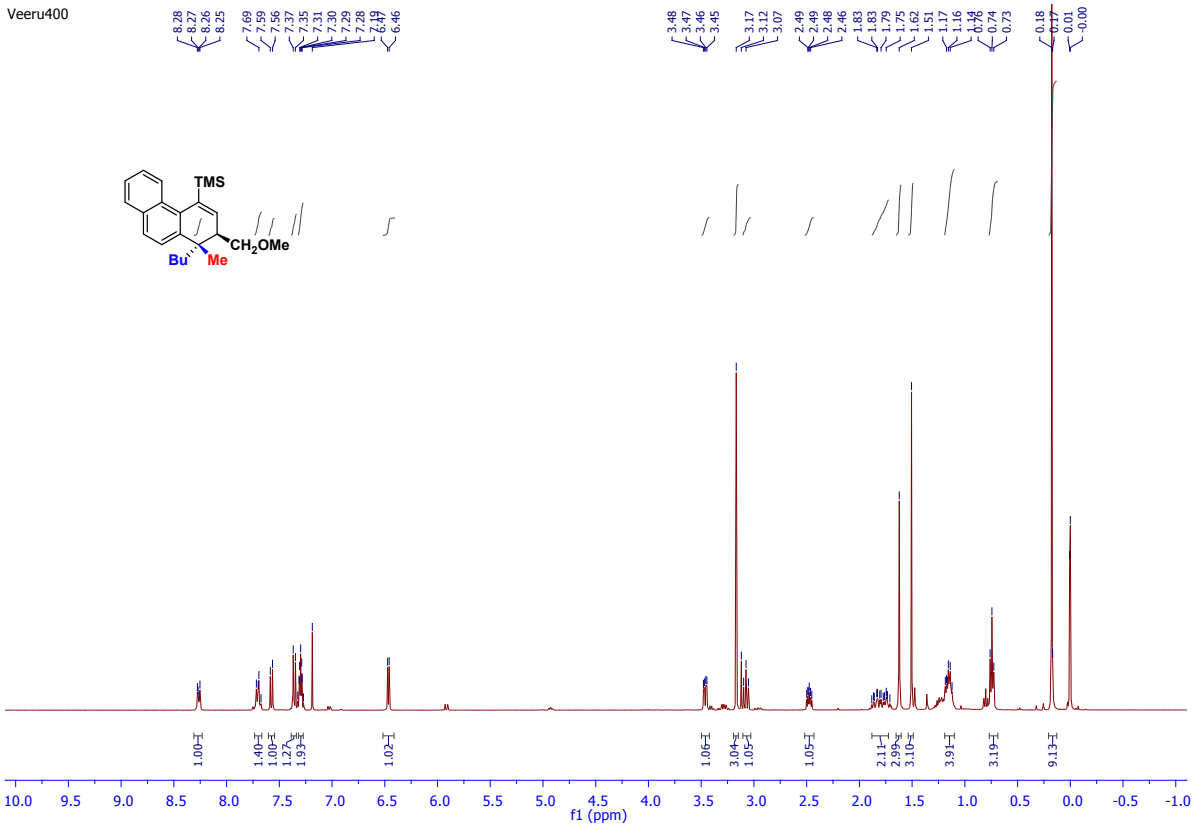
40
20
0
-10
-30
-50
-70
-90
-110
-140
-170
f1 (ppm)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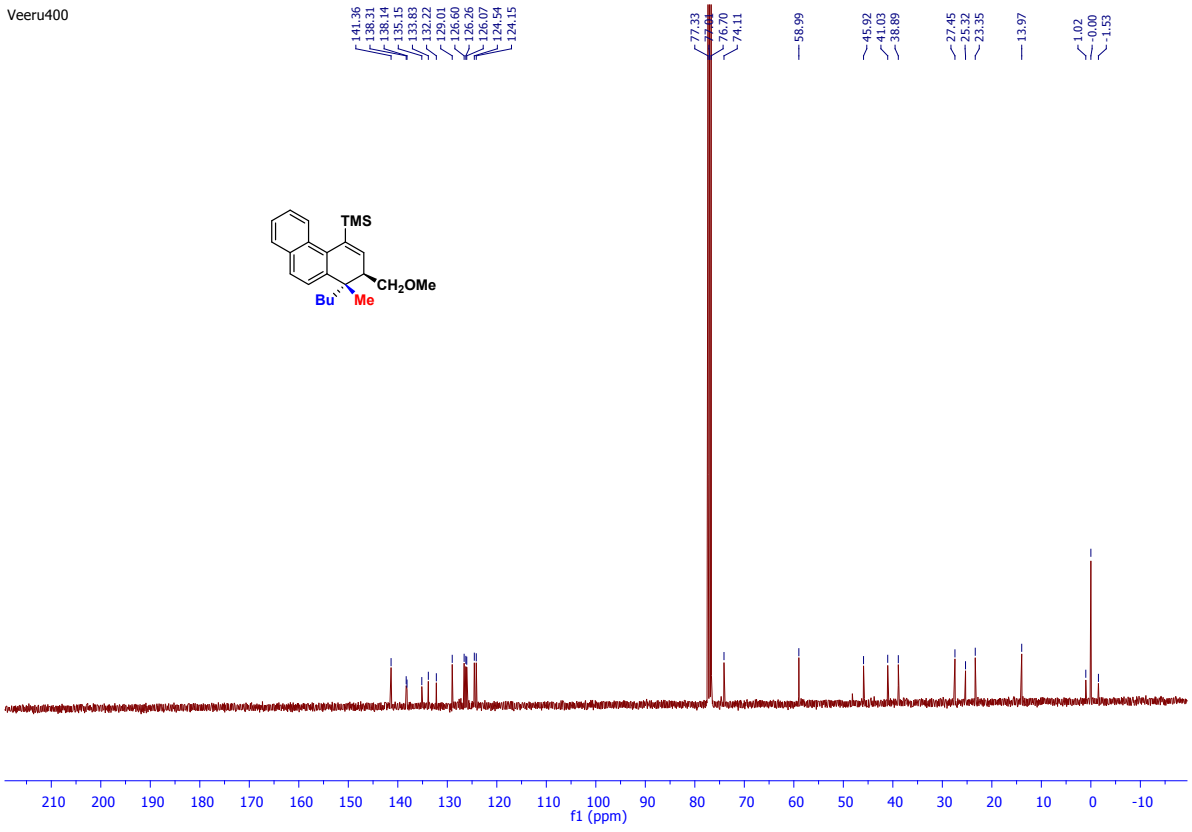
TMS
CH2OMe
Bu
Me
f1 (ppm)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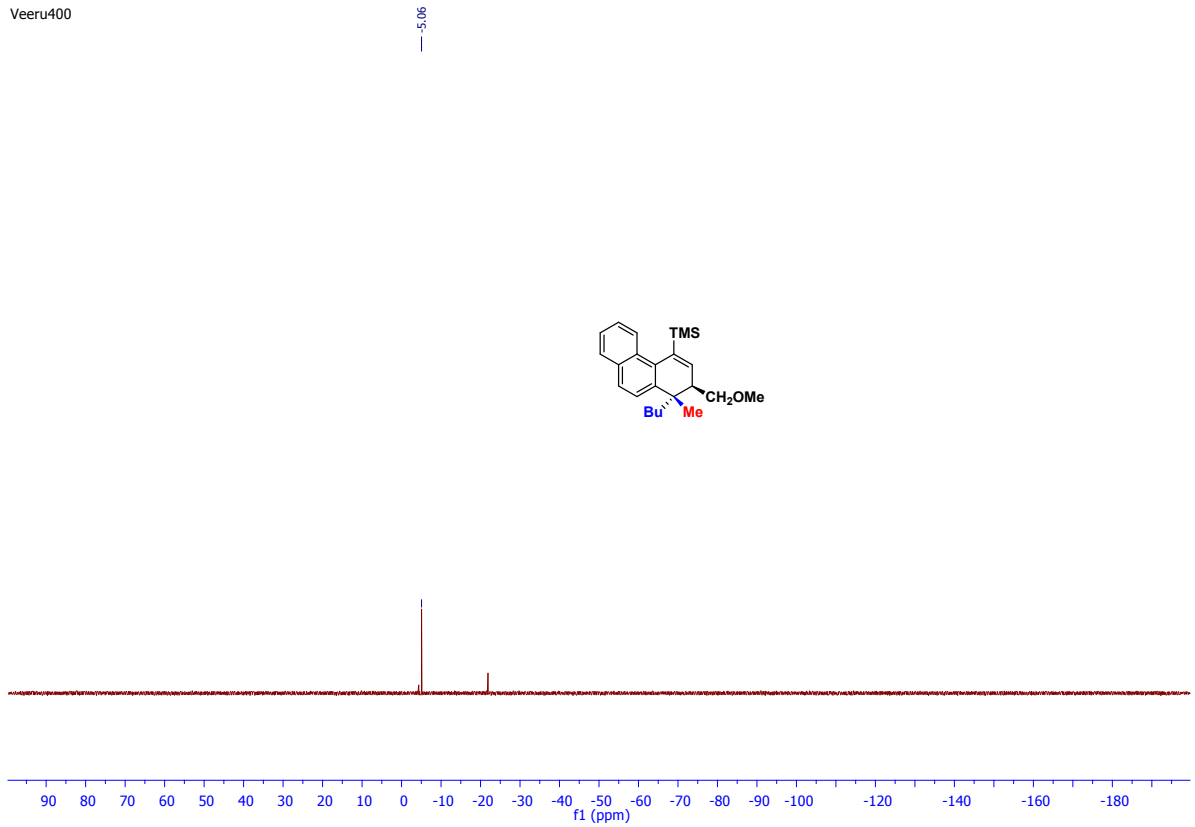
Bu
Me
f1 (ppm)

Veeru400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Me
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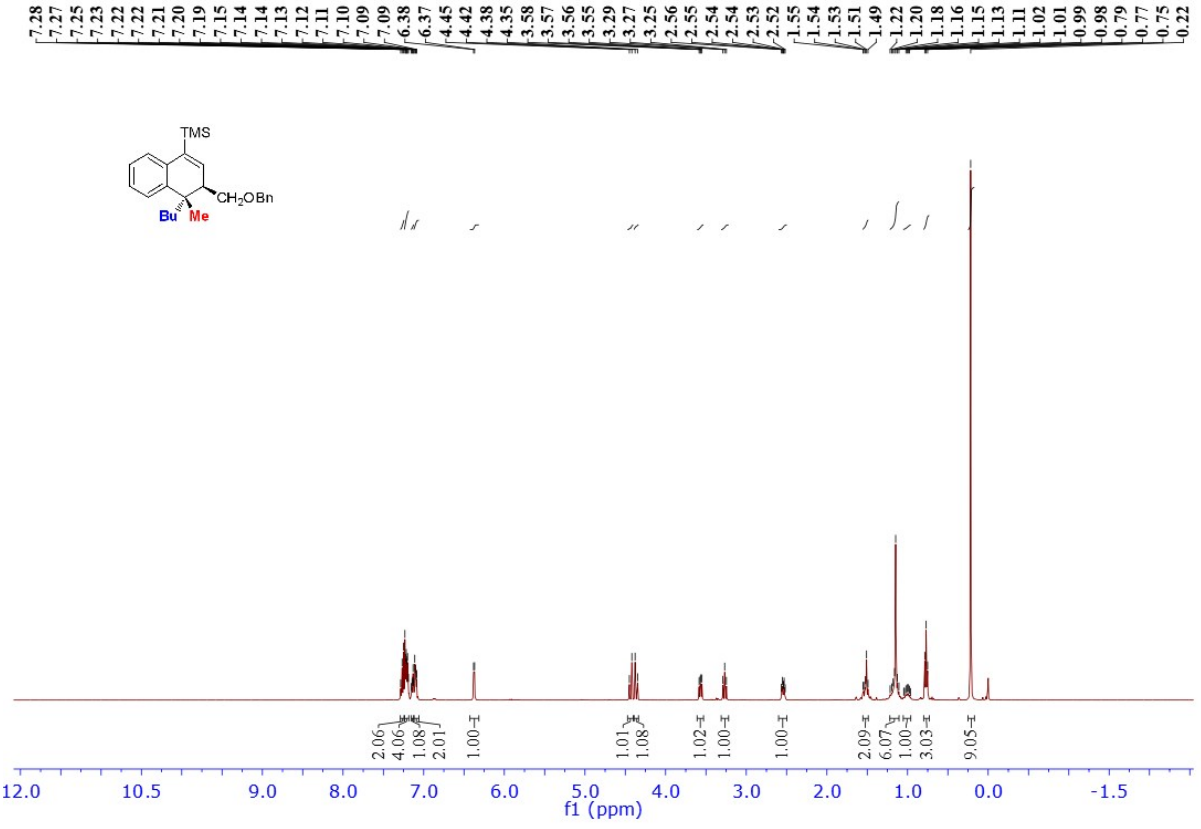
f1 (ppm)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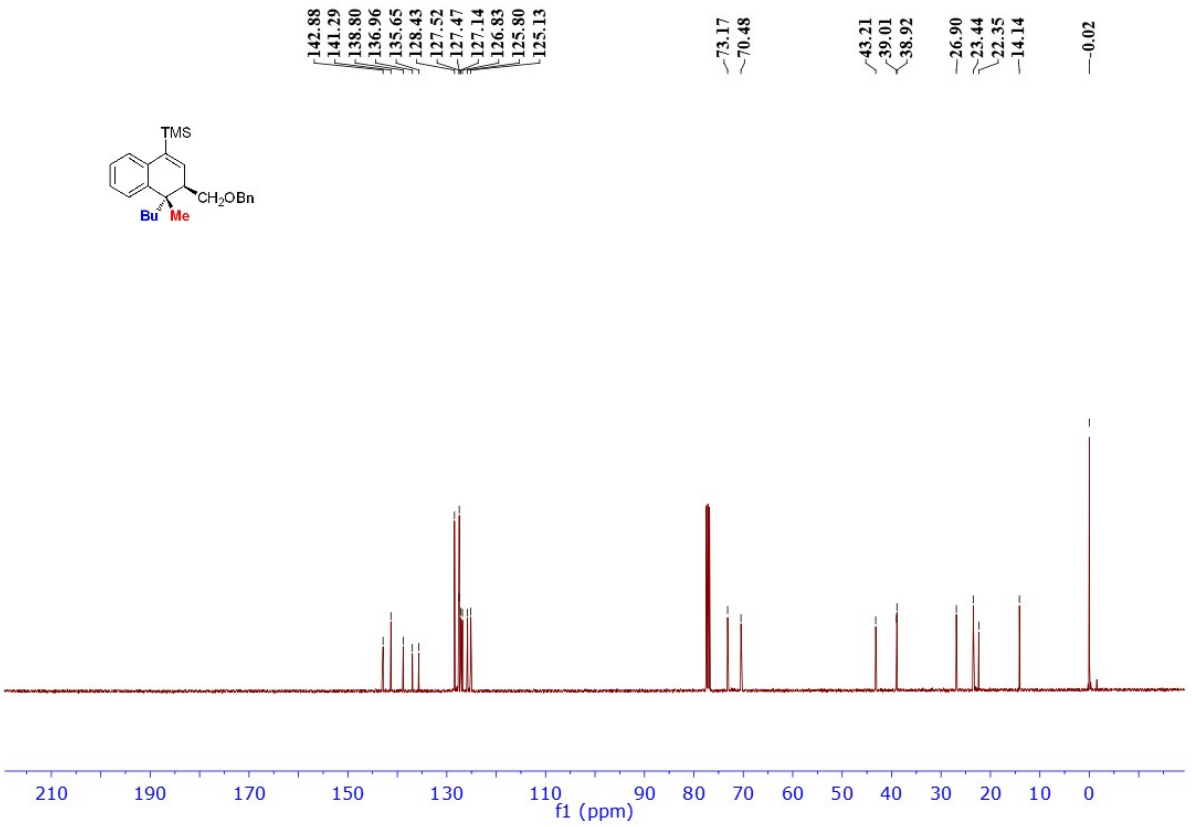
TMS
CH2OBn
Bu
Me
2.06 4.06 1.08 2.01 1.00 1.01 1.08 1.02 1.00 1.00 2.09 6.07 1.00 3.03 9.05
12.0 10.5 9.0 8.0 7.0 6.0 5.0 4.0 3.0 2.0 1.0 0.0 -1.5
f1 (ppm)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126.83
125.80
125.13
73.17
70.48
43.21
39.01
38.92
26.90
23.44
22.35
14.14
0.02
TMS
CH2OBn
Bu
Me
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170
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90
80
70
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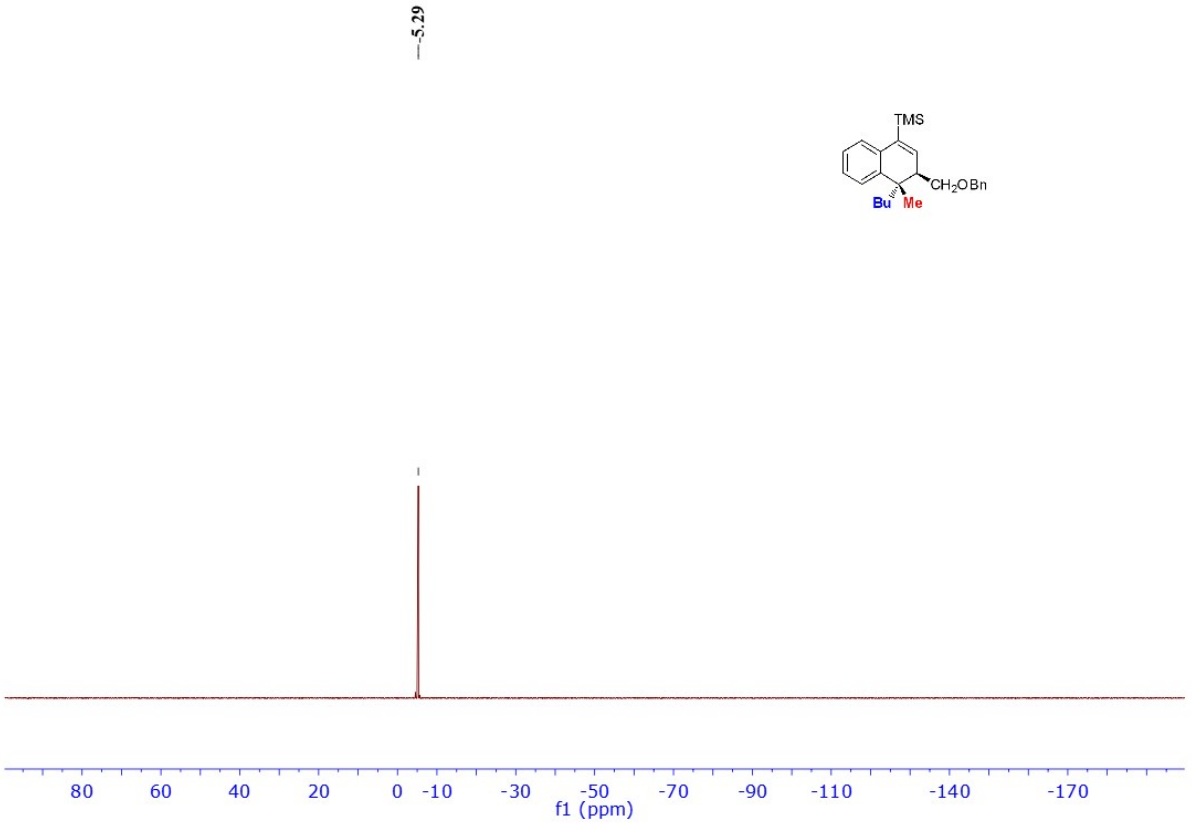
50
40
30
20
10
0
f1 (ppm)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Bu
Me
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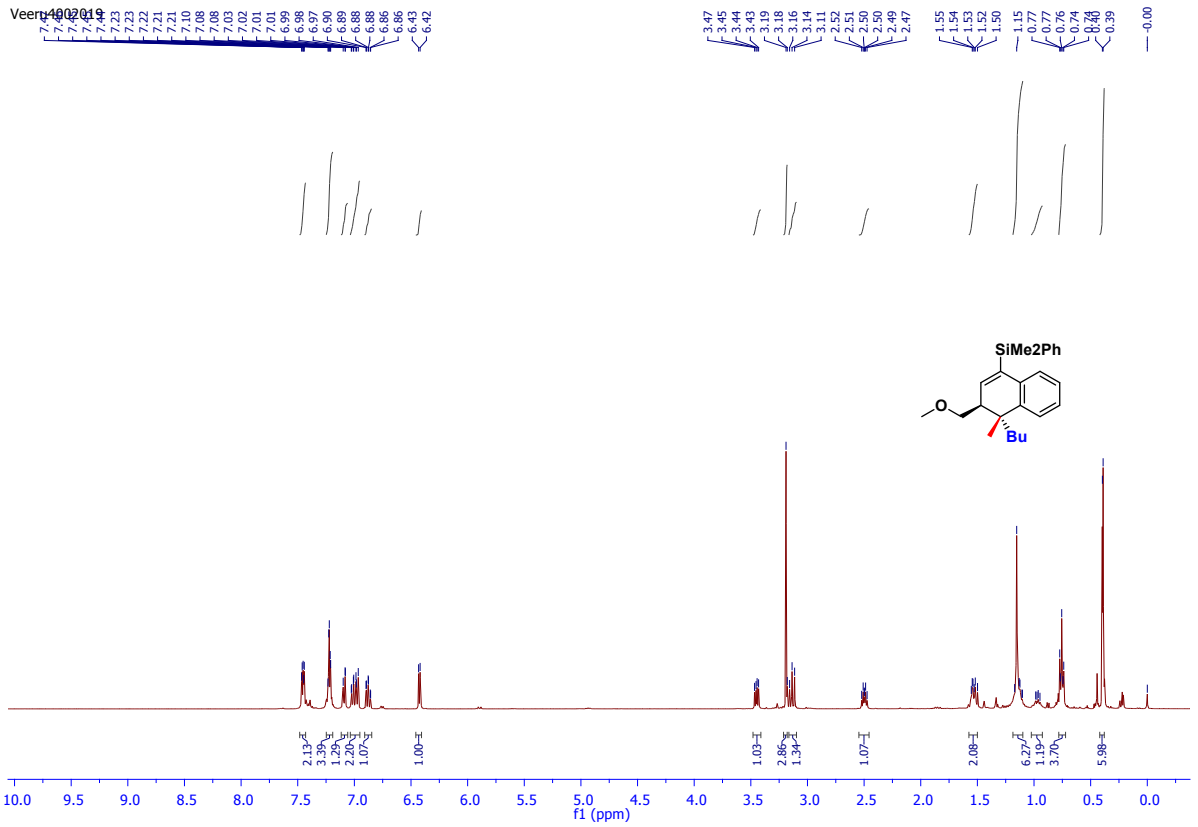
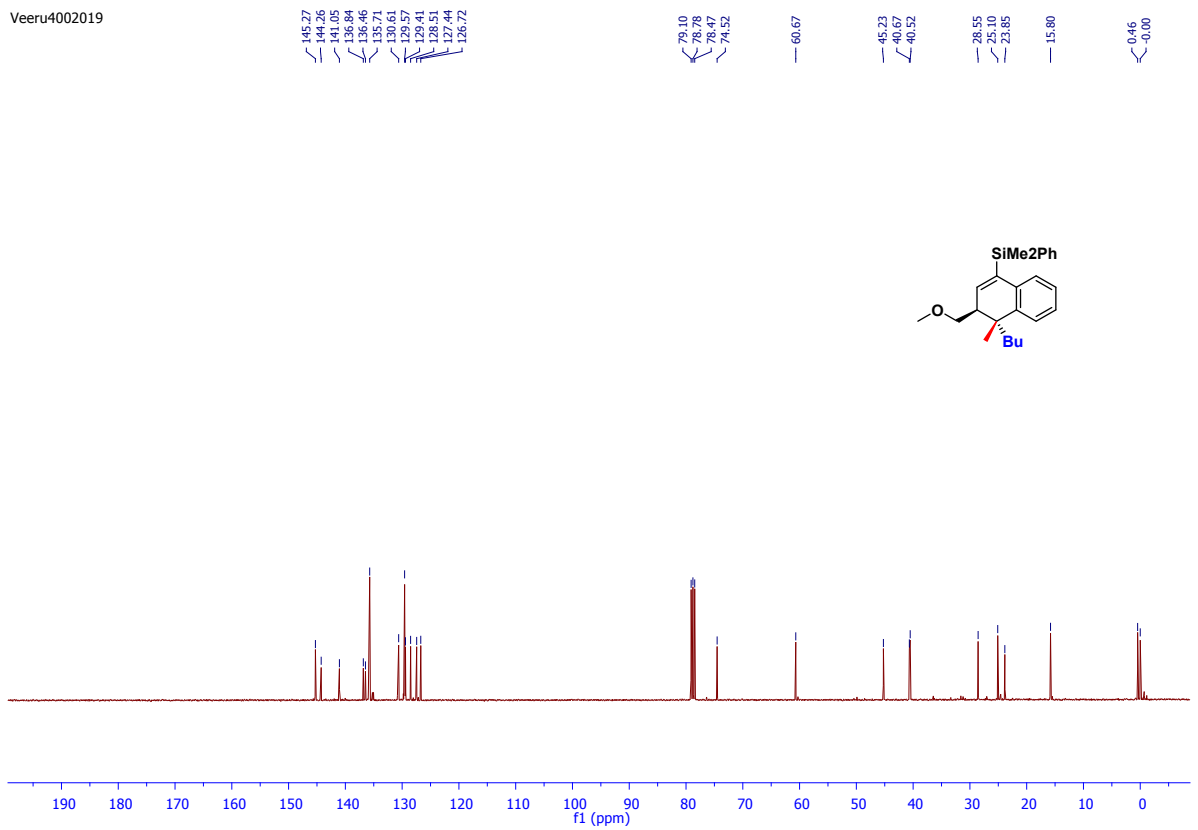
0
-10
-30
-50
-70
-90
-110
-140
-170
f1 (ppm)


Veeru4002019
SiMe2Ph
O
Bu
f1 (ppm)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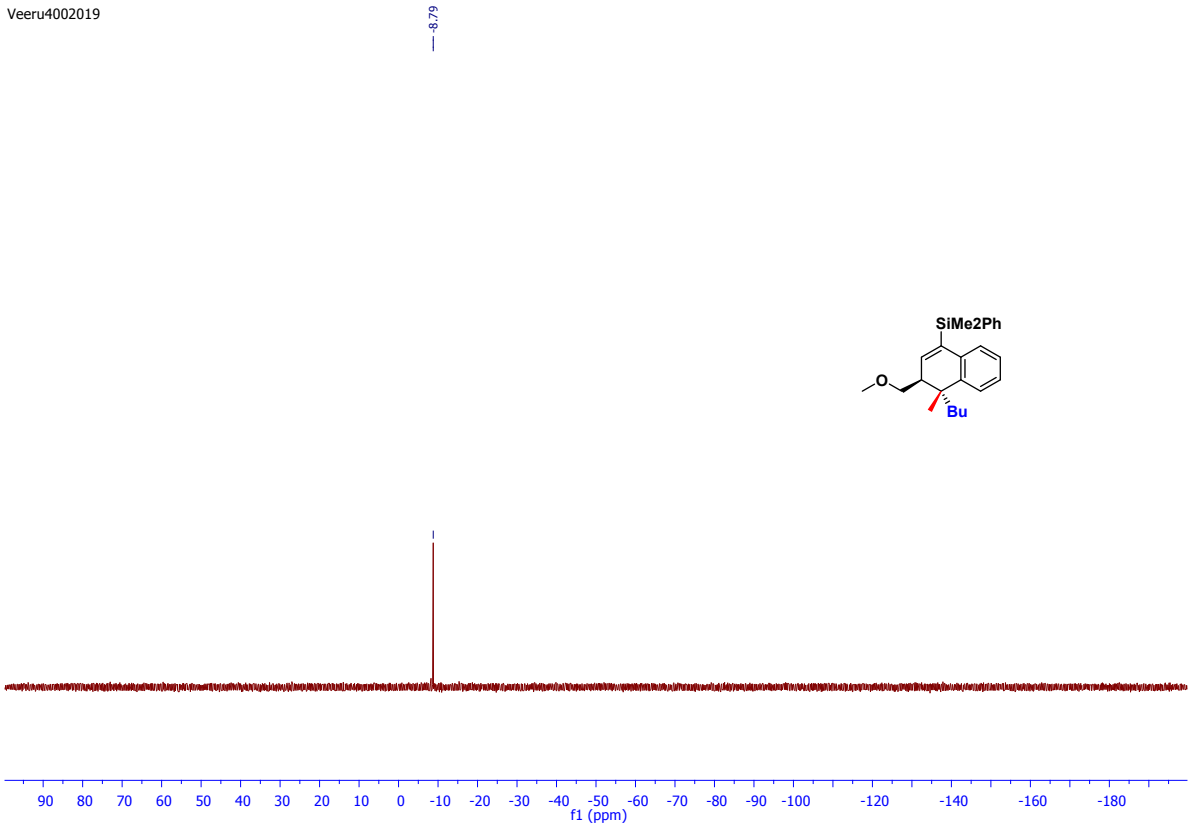
O
Bu
f1 (ppm)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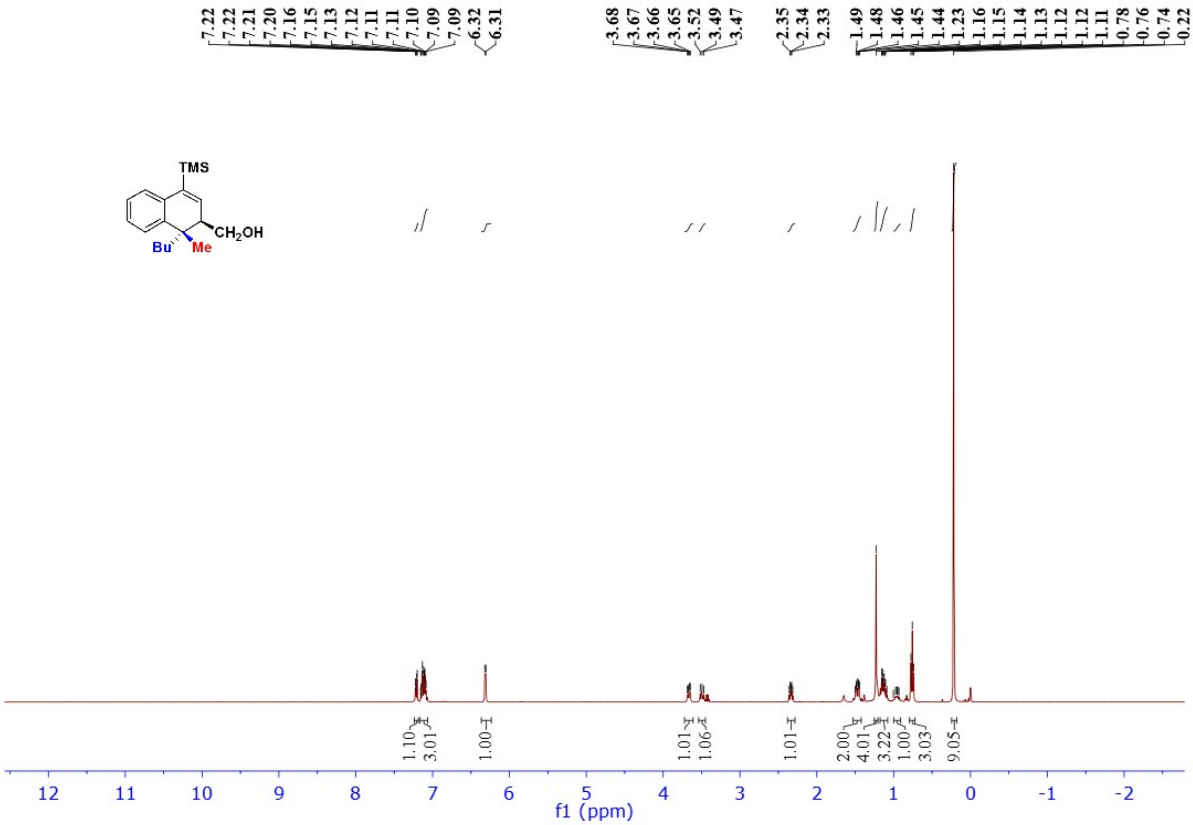
f1 (ppm)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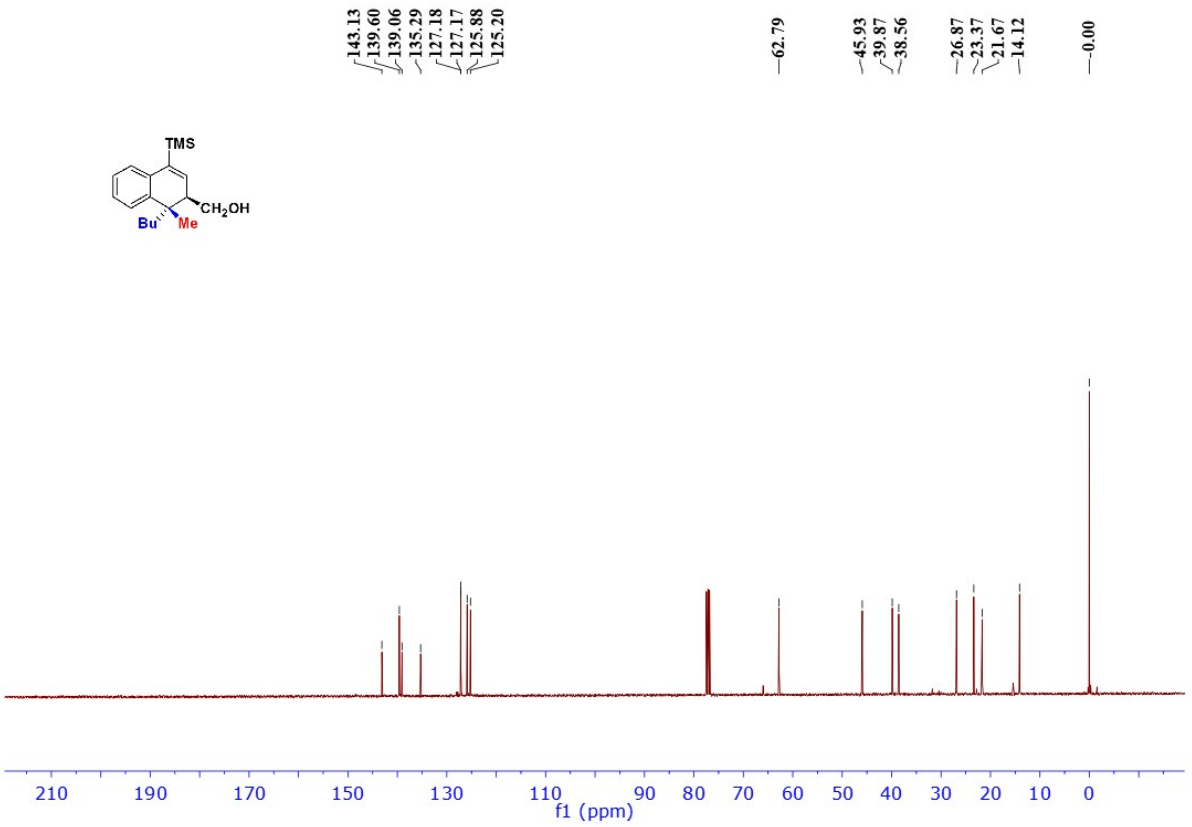
3.68 3.67 3.66 3.65 3.52 3.49 3.47
2.35 2.34 2.33
1.49 1.48 1.46 1.45 1.44 1.23 1.16 1.15 1.14 1.13 1.12 1.12 1.11 0.78 0.76 0.74 0.22
TMS
CH2OH
Bu
Me
1.10 3.01 1.00 1.01 1.06 1.01 2.00 4.01 3.22 1.00 3.03 9.05
12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2
f1 (ppm)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127.17
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125.20
62.79
45.93
39.87
38.56
26.87
23.37
21.67
14.12
0.00
TMS
CH2OH
Bu
Me
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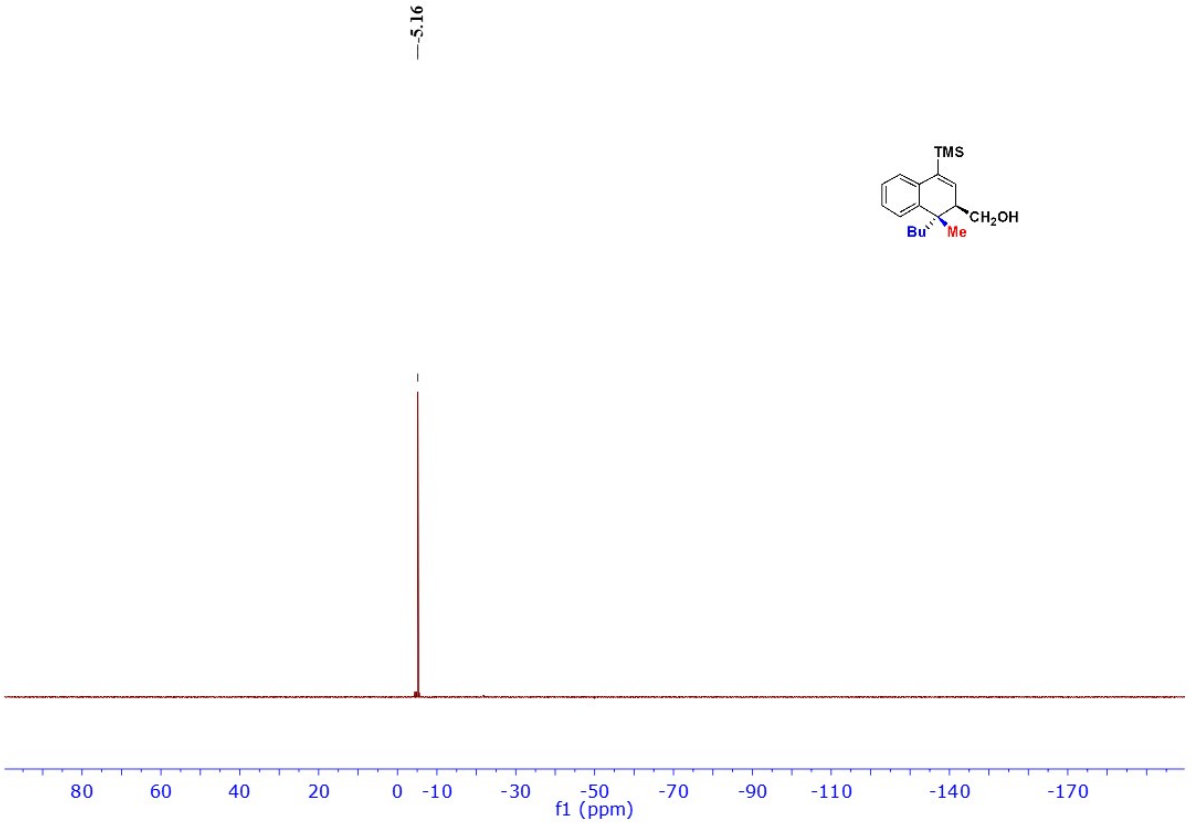
170
150
130
110
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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CH2OH
Bu
Me
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40
20
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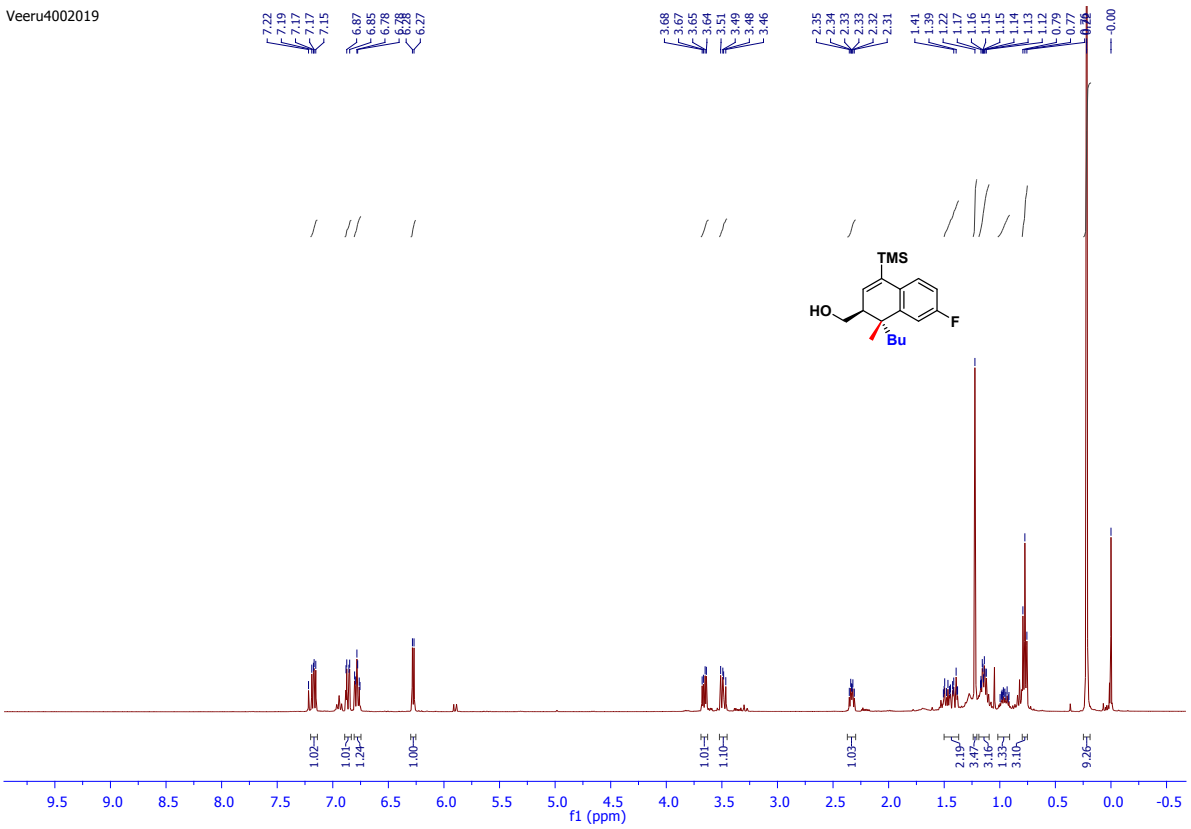
-10
-30
-50
-70
-90
-110
-140
-170
f1 (ppm)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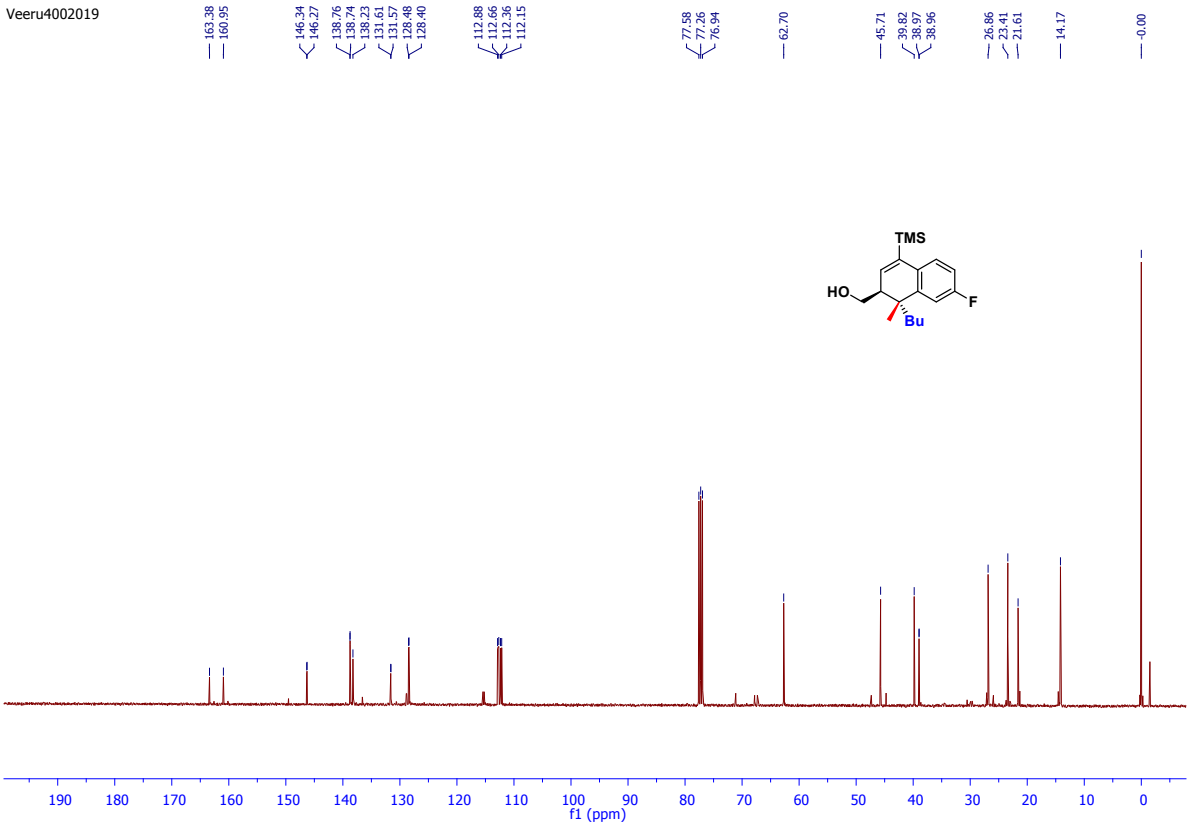
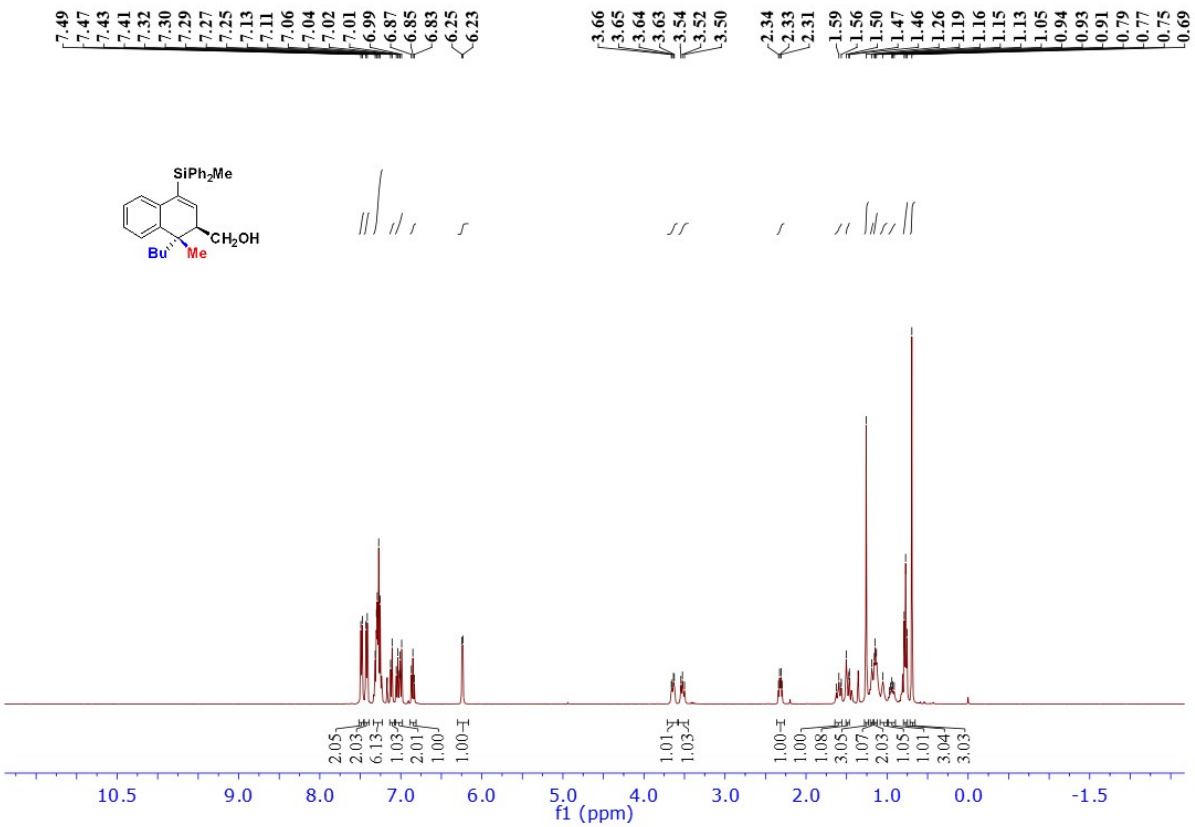
TMS
HO
F
Bu
f1 (ppm)


Veeru4002019
TMS
HO
F
Bu
f1 (ppm)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7.11
7.06
7.04
7.02
7.01
6.99
6.87
6.85
6.83
6.25
6.23
3.66
3.65
3.64
3.63
3.54
3.52
3.50
2.34
2.33
2.31
1.59
1.56
1.50
1.47
1.46
1.26
1.19
1.16
1.15
1.13
1.05
0.94
0.93
0.91
0.79
0.77
0.75
0.69
SiPh2Me
CH2OH
Bu
Me
2.05
2.03
6.13
1.03
2.01
1.00
1.00
1.01
1.03
1.00
1.00
1.08
3.05
1.07
2.03
1.05
1.01
3.04
3.03
10.5
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6.0
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4.0
3.0
2.0
1.0
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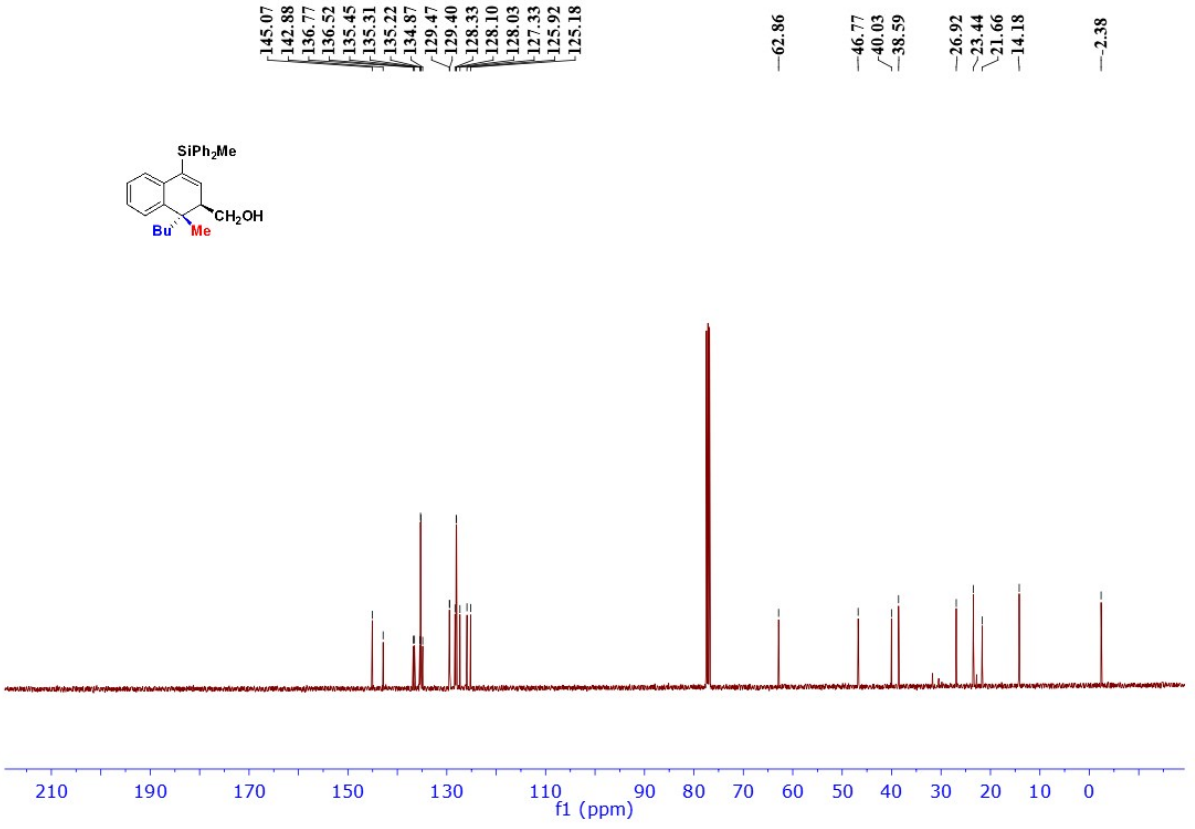
-1.5
f1 (ppm)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134.87
129.47
129.40
128.33
128.10
128.03
127.33
125.92
125.18
62.86
46.77
40.03
38.59
26.92
23.44
21.66
14.18
-2.38
SiPh2Me
CH2OH
Bu
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170
150
130
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90
80
70
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50
40
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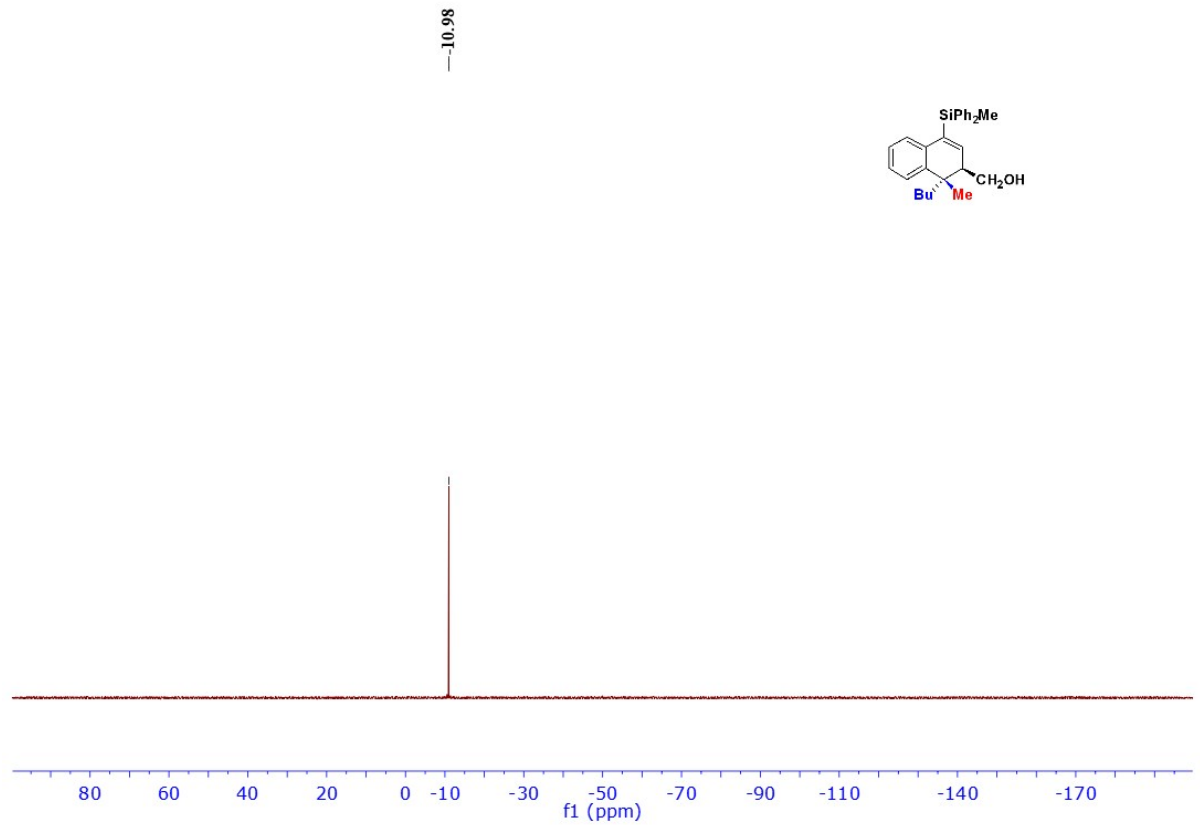
20
10
0
f1 (ppm)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SiPh2Me
CH2OH
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-50
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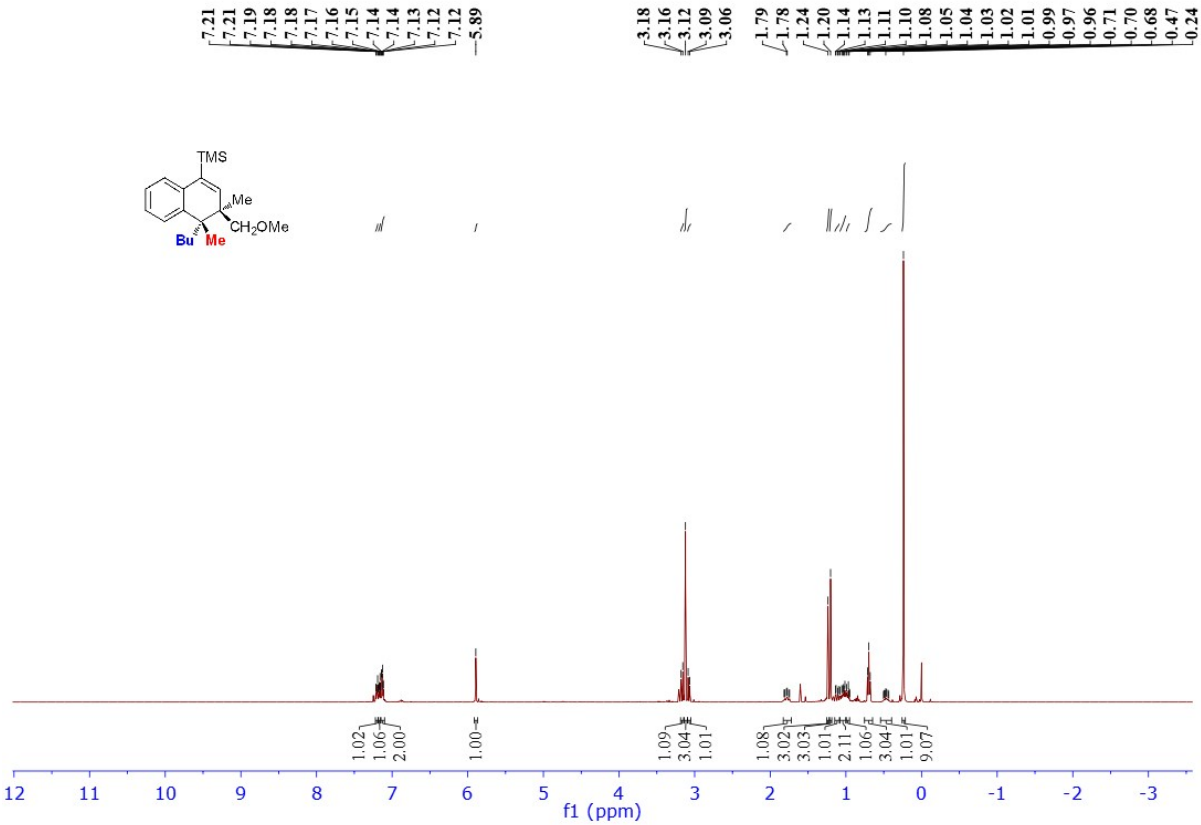
-90
-110
-140
-170
f1 (ppm)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7.15
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7.14
7.13
7.12
7.12
5.89
3.18
3.16
3.12
3.09
3.06
1.79
1.78
1.24
1.20
1.14
1.13
1.11
1.10
1.08
1.05
1.04
1.03
1.02
1.01
0.99
0.97
0.96
0.71
0.70
0.68
0.47
0.24
TMS
Me
CH2OMe
Bu
Me
1.02
1.06
2.00
1.00
1.09
3.04
1.01
1.08
3.02
3.03
1.01
2.11
1.06
3.04
1.01
9.07
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9
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7
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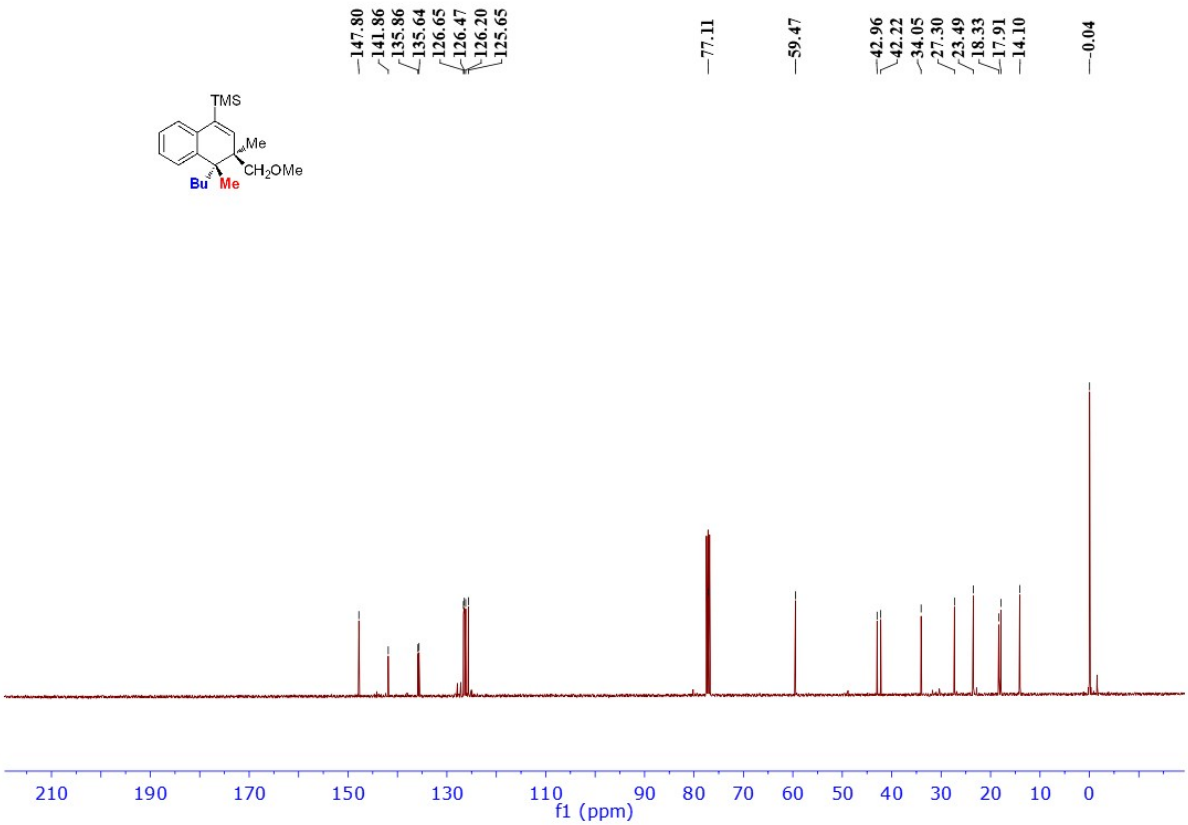
5
4
3
2
1
0
-1
-2
-3
f1 (ppm)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125.65
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59.47
42.96
42.22
34.05
27.30
23.49
18.33
17.91
14.10
0.04
TMS
Me
CH2OMe
Bu
Me
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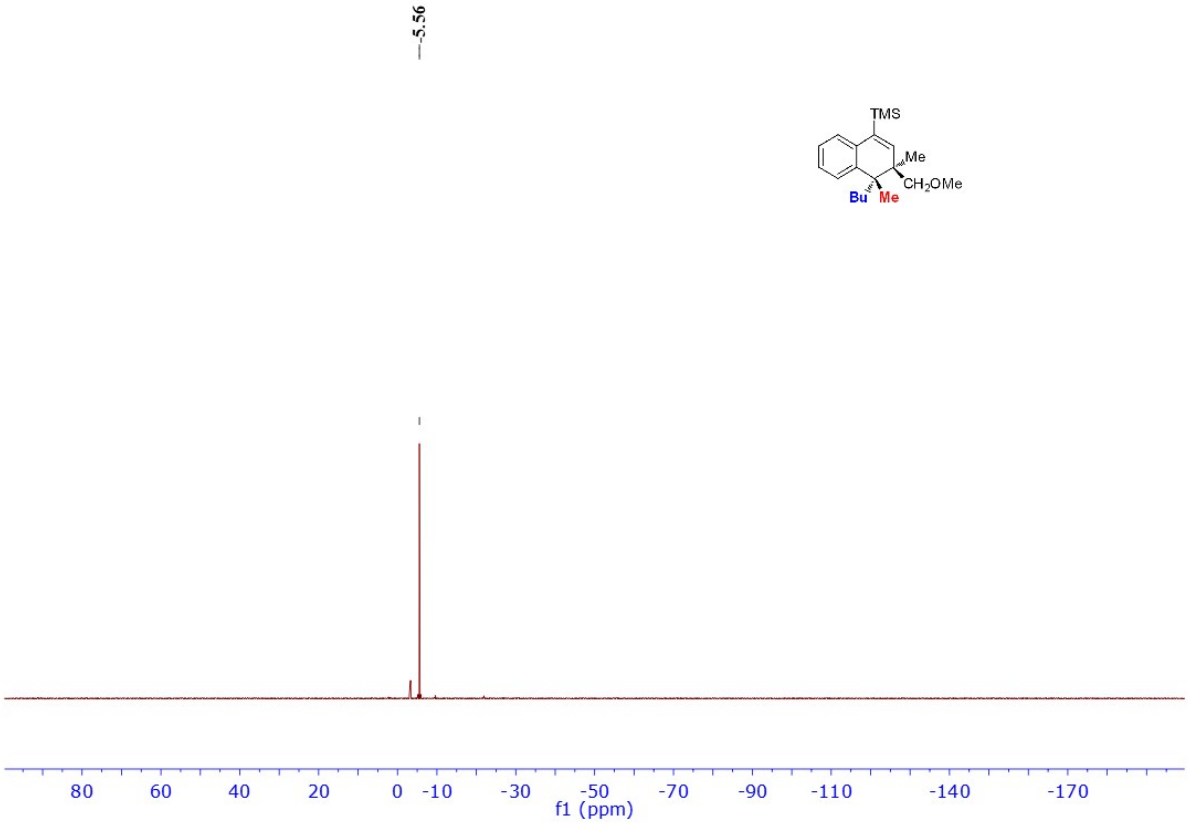
170
150
130
110
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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-10
-30
-50
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-90
-110
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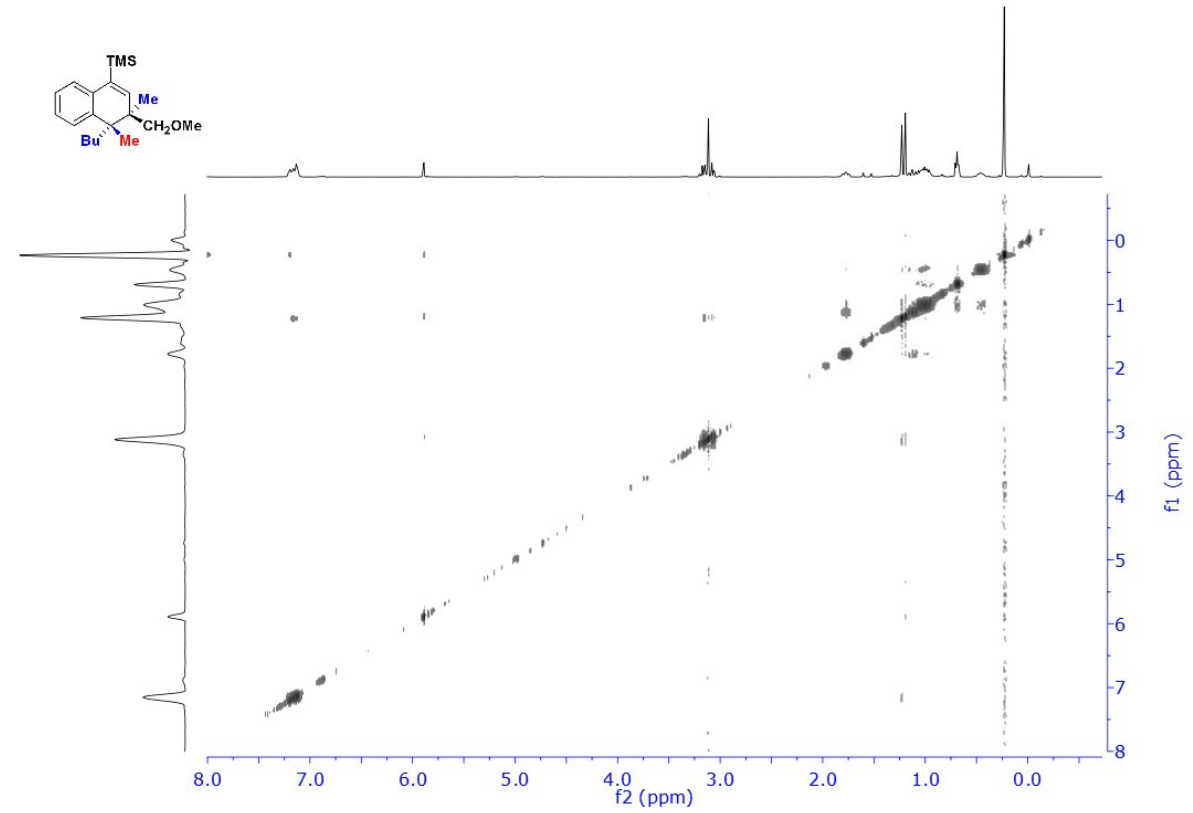
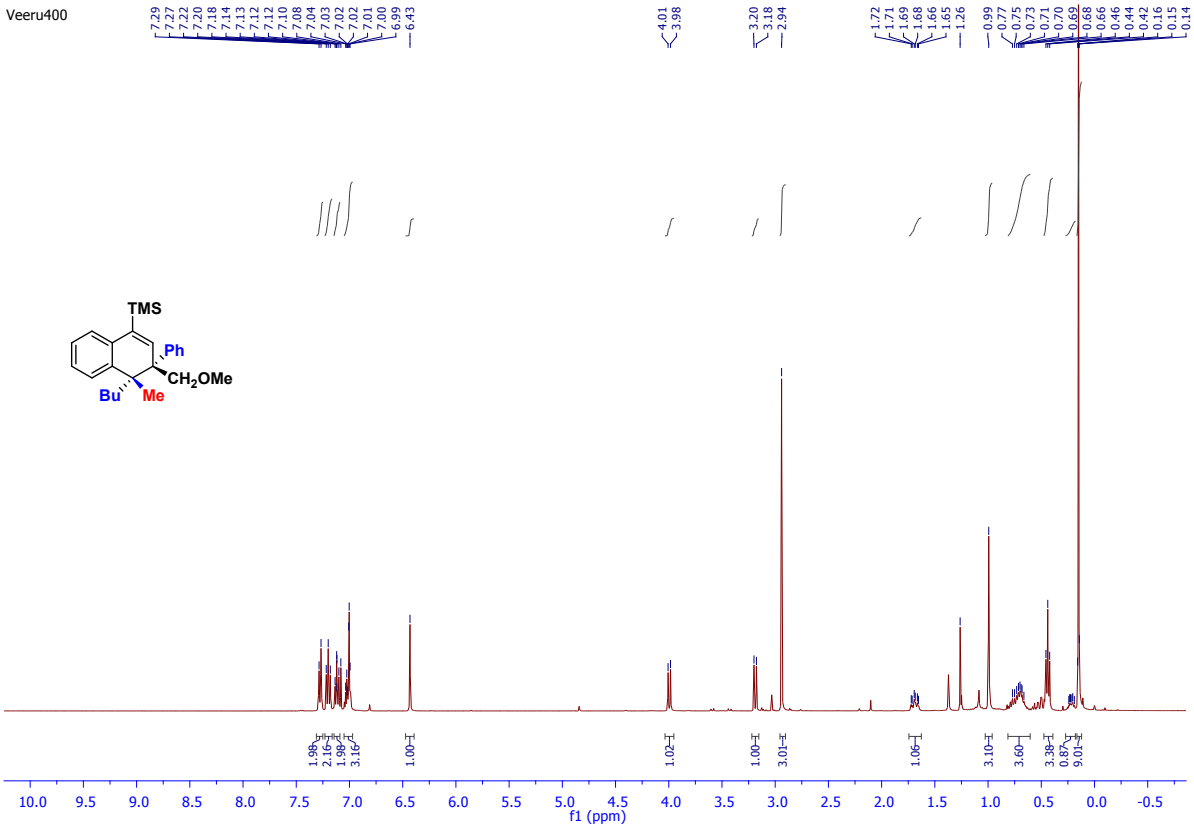
-170
f1 (ppm)


TMS
Me
CH2OMe
Bu
Me
f1 (ppm)
f2 (ppm)


Veeru400
TMS
Ph
CH2OMe
Bu
Me
f1 (ppm)

Veeru400

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140.58
136.45
135.01
130.04
127.39
126.83
126.60
126.44
126.39
125.83

77.38
77.07
76.75
74.57

59.61

52.97

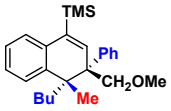
42.40

34.16
30.37
26.29
23.17

17.39

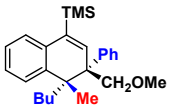
13.95

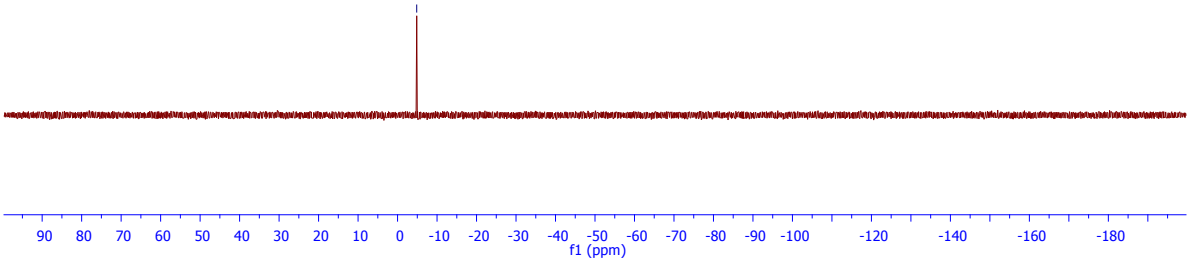
-0.00



Veeru400

-4.85





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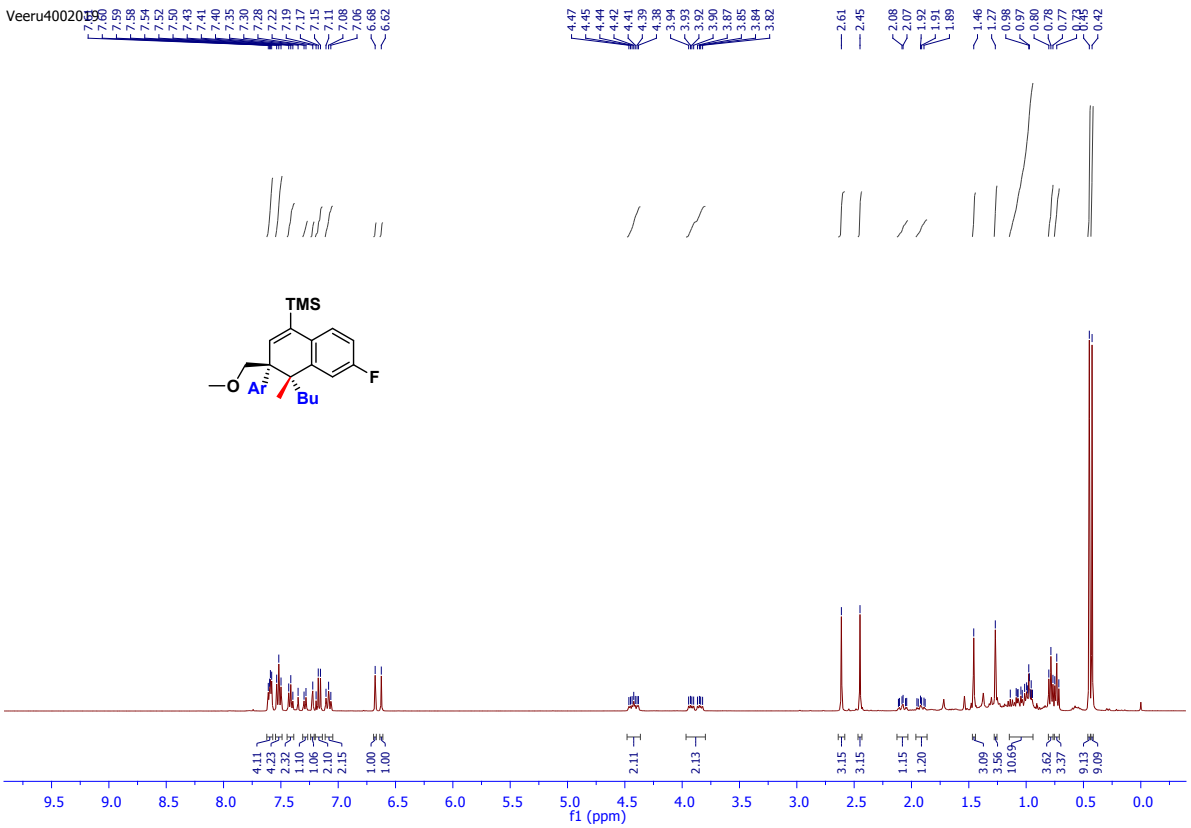

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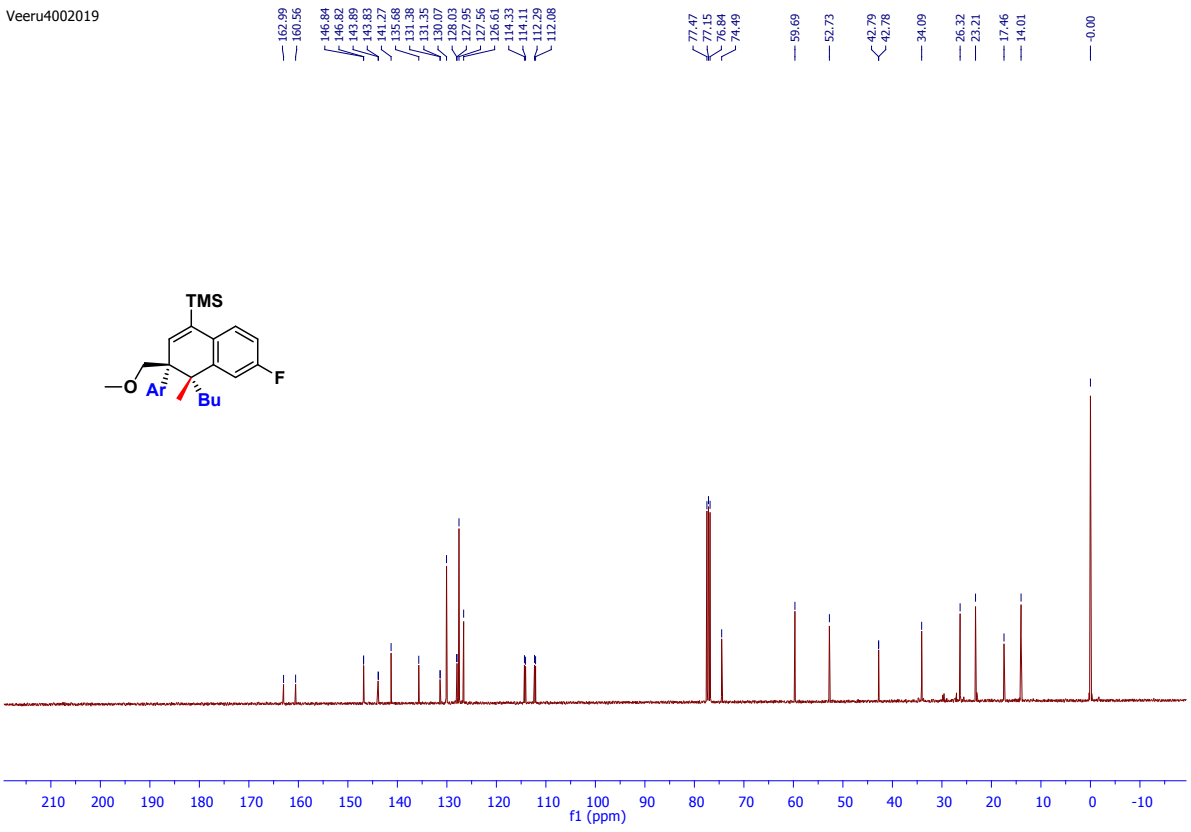

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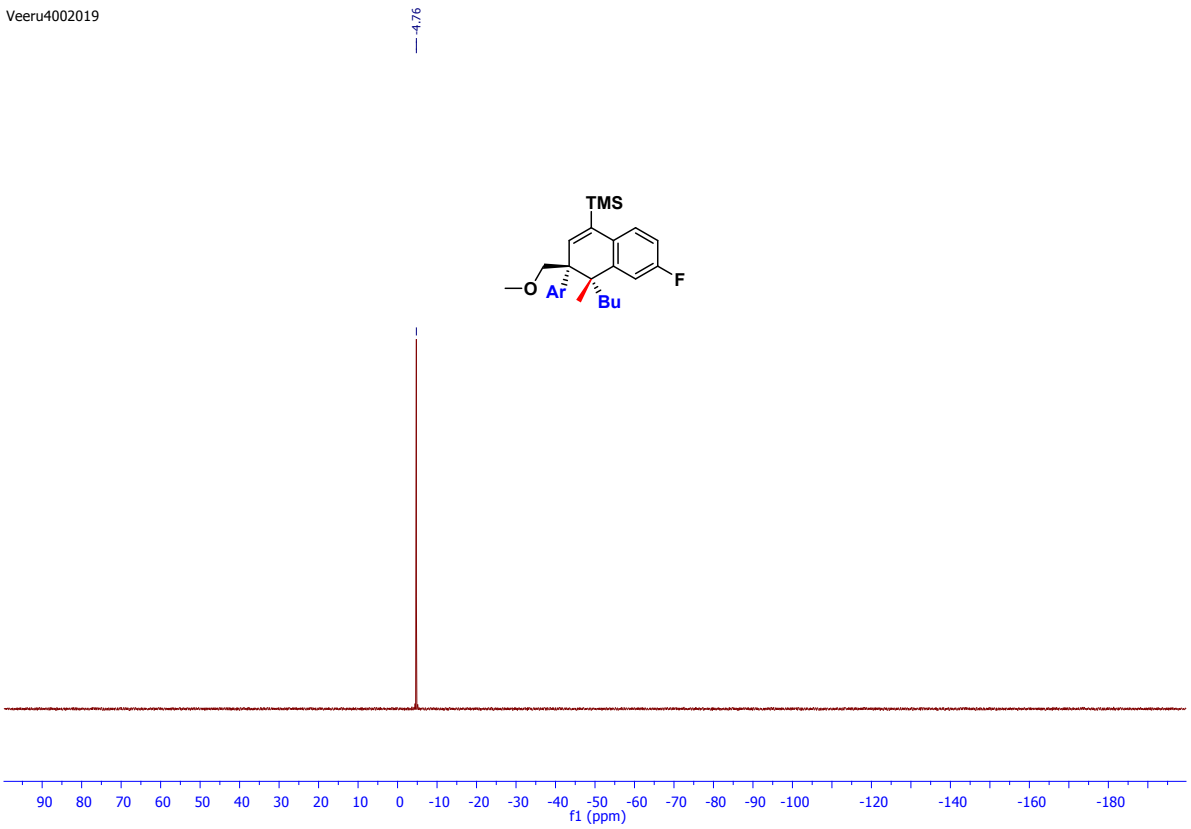

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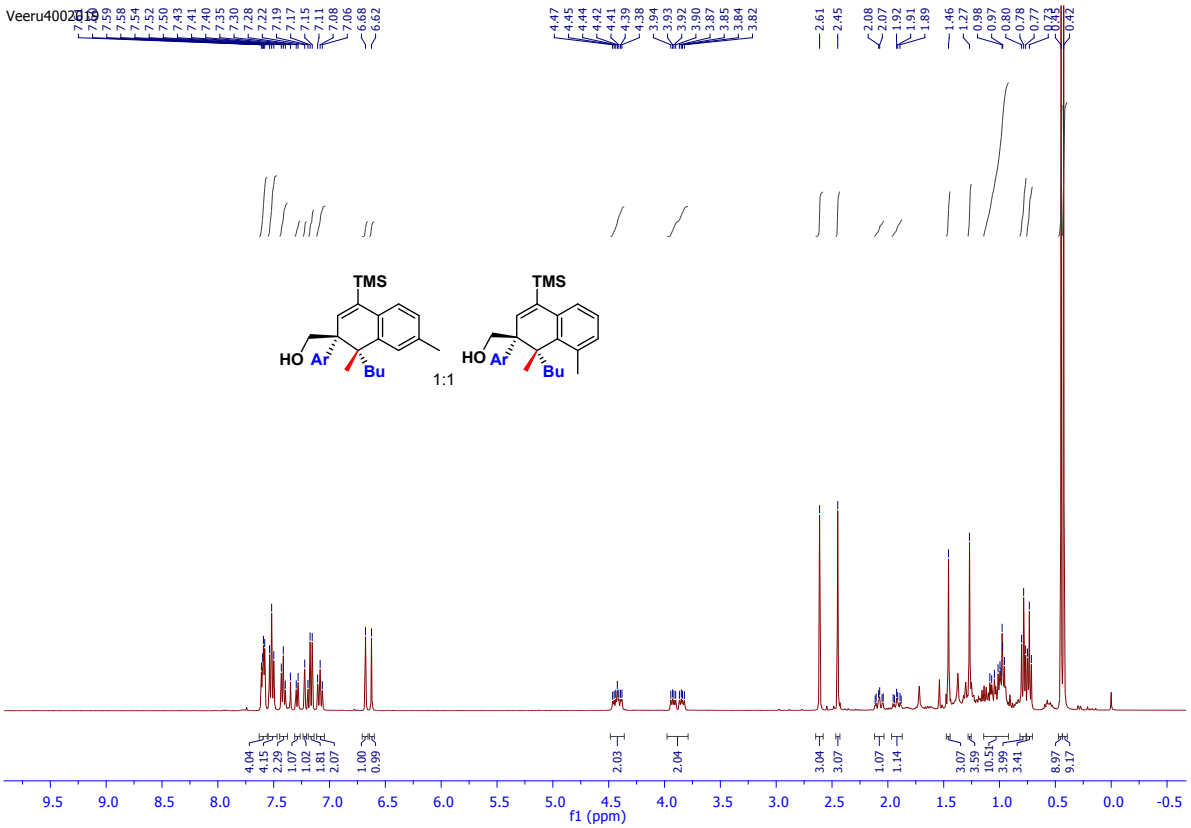

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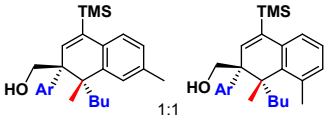

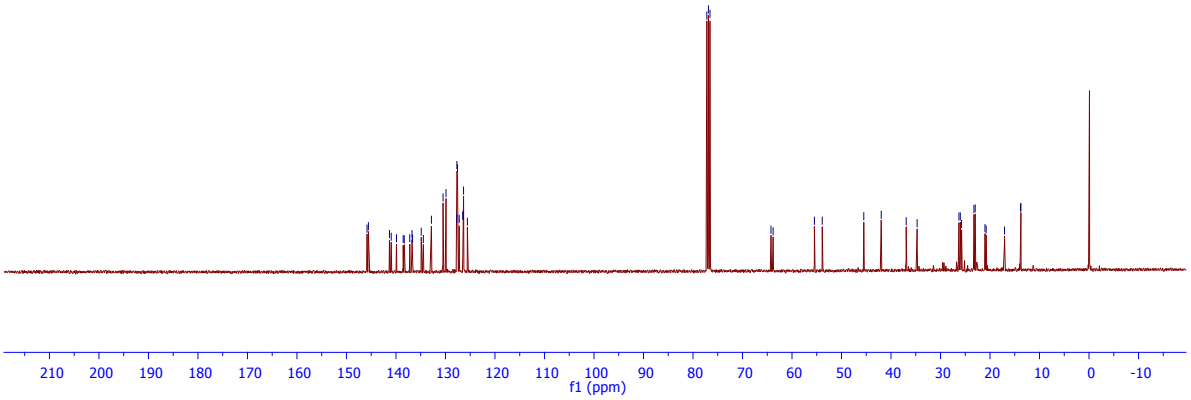

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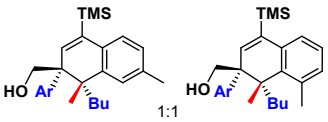

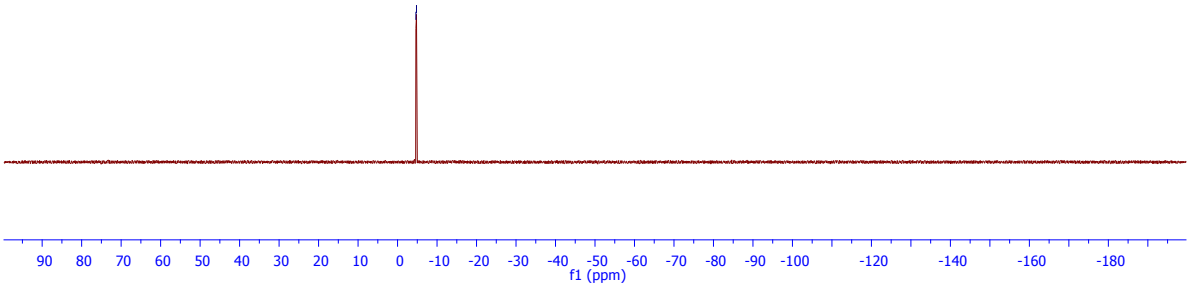

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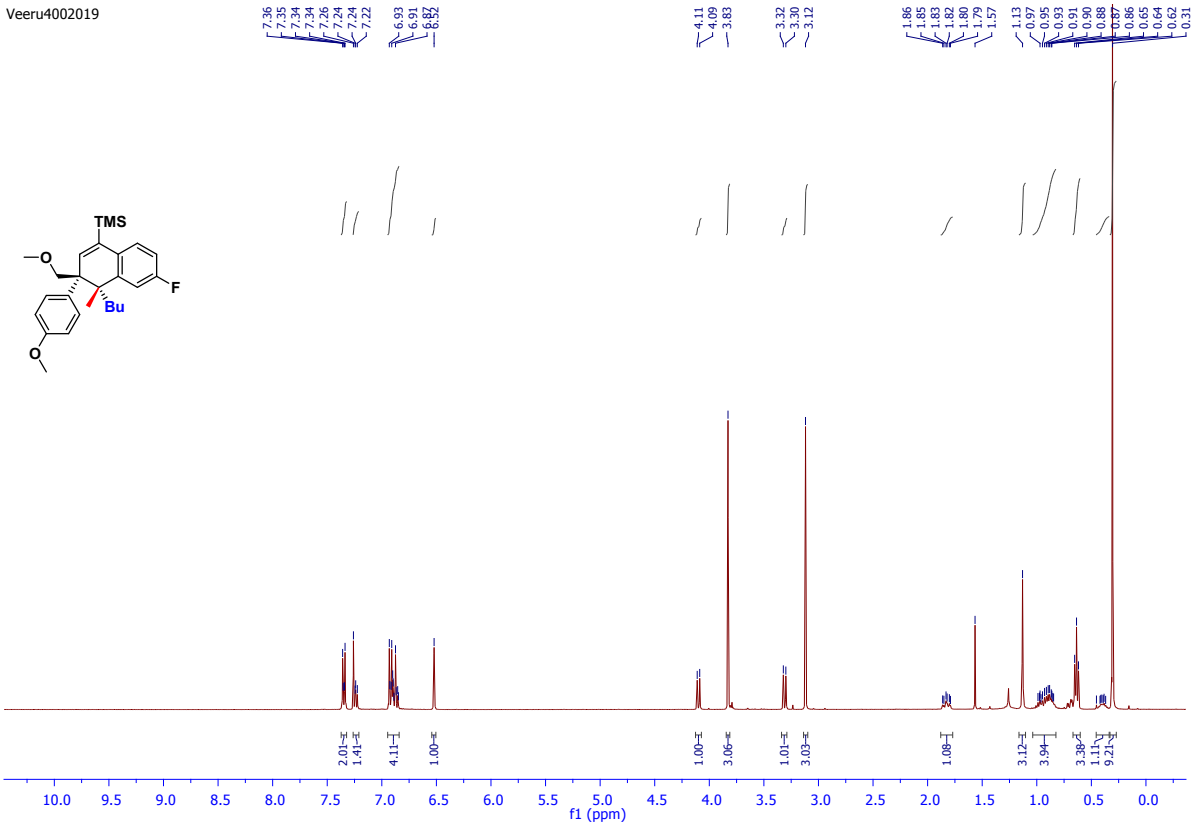

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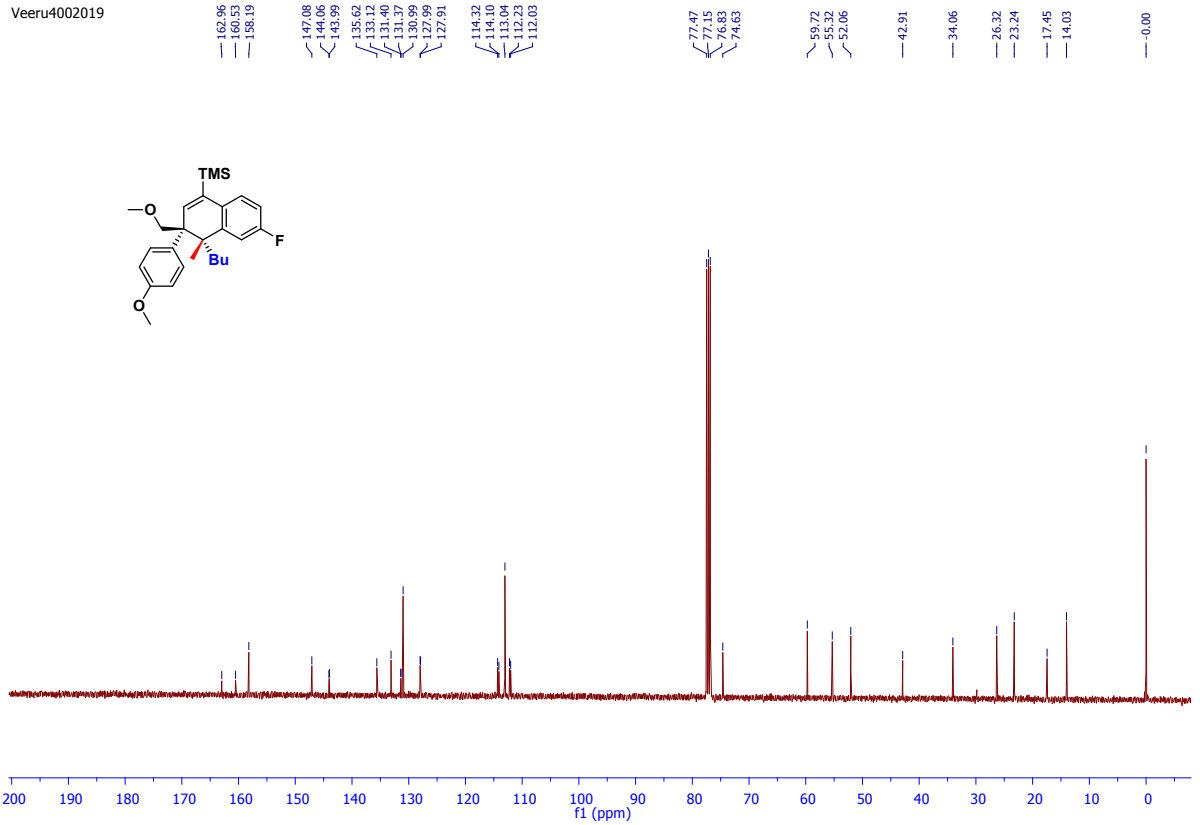

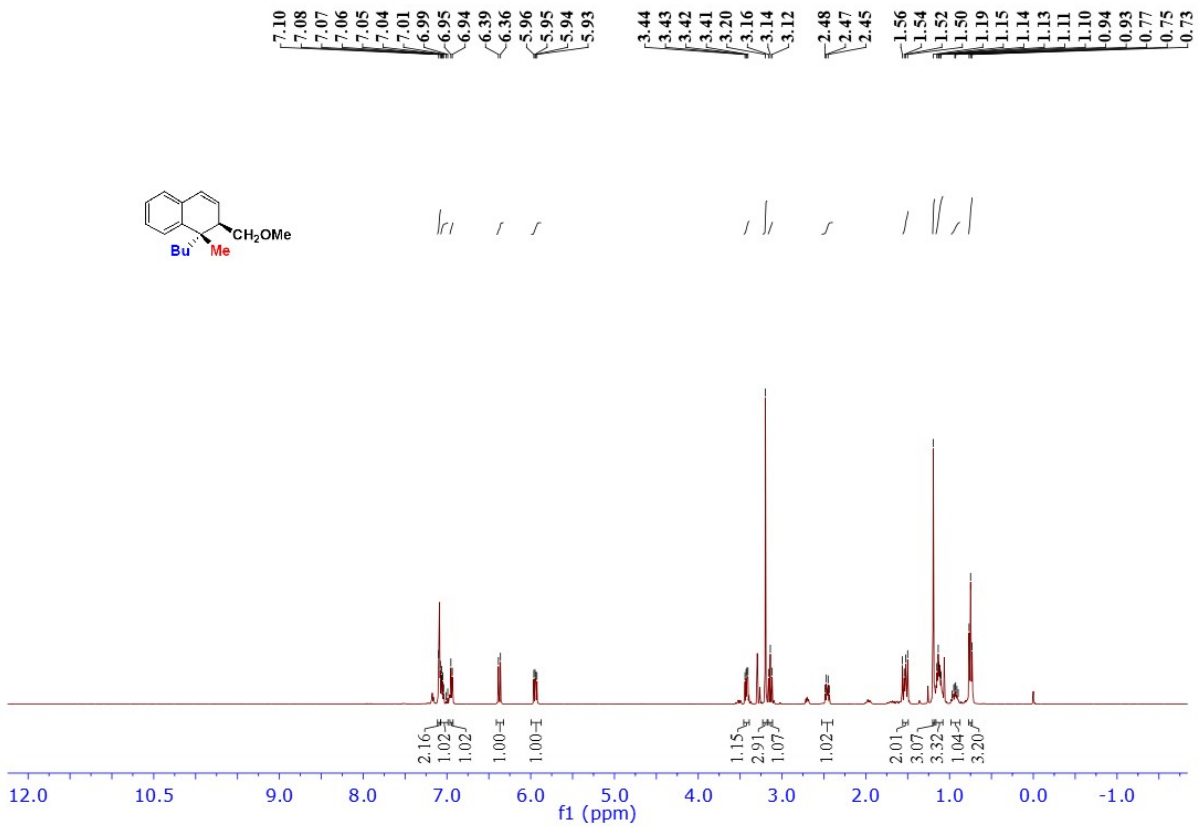
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5.95
5.94
5.93
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3.43
3.42
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3.20
3.16
3.14
3.12
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2.47
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1.14
1.13
1.11
1.10
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0.93
0.77
0.75
0.73
CH2OMe
Bu
Me
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1.02
1.00
1.00
1.15
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1.07
1.02
2.01
3.07
3.32
1.04
3.20
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10.5
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1.0
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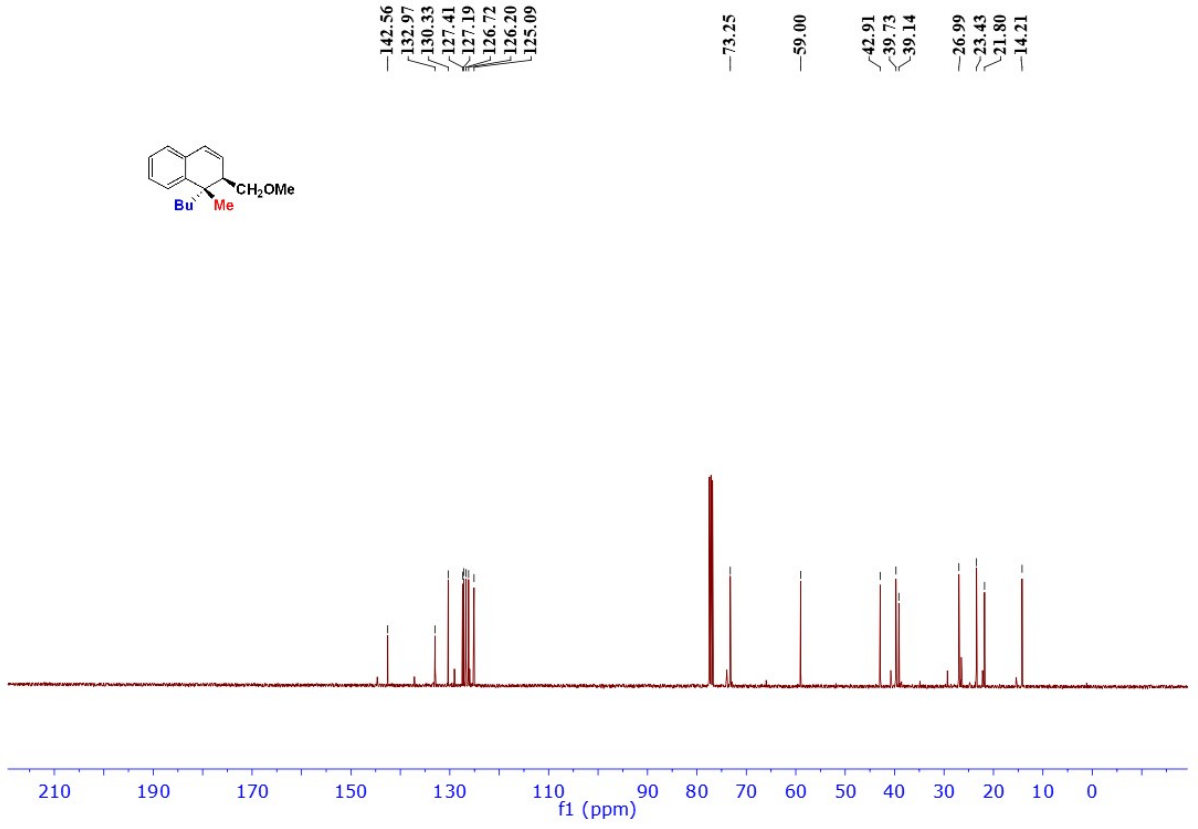
-1.0
f1 (ppm)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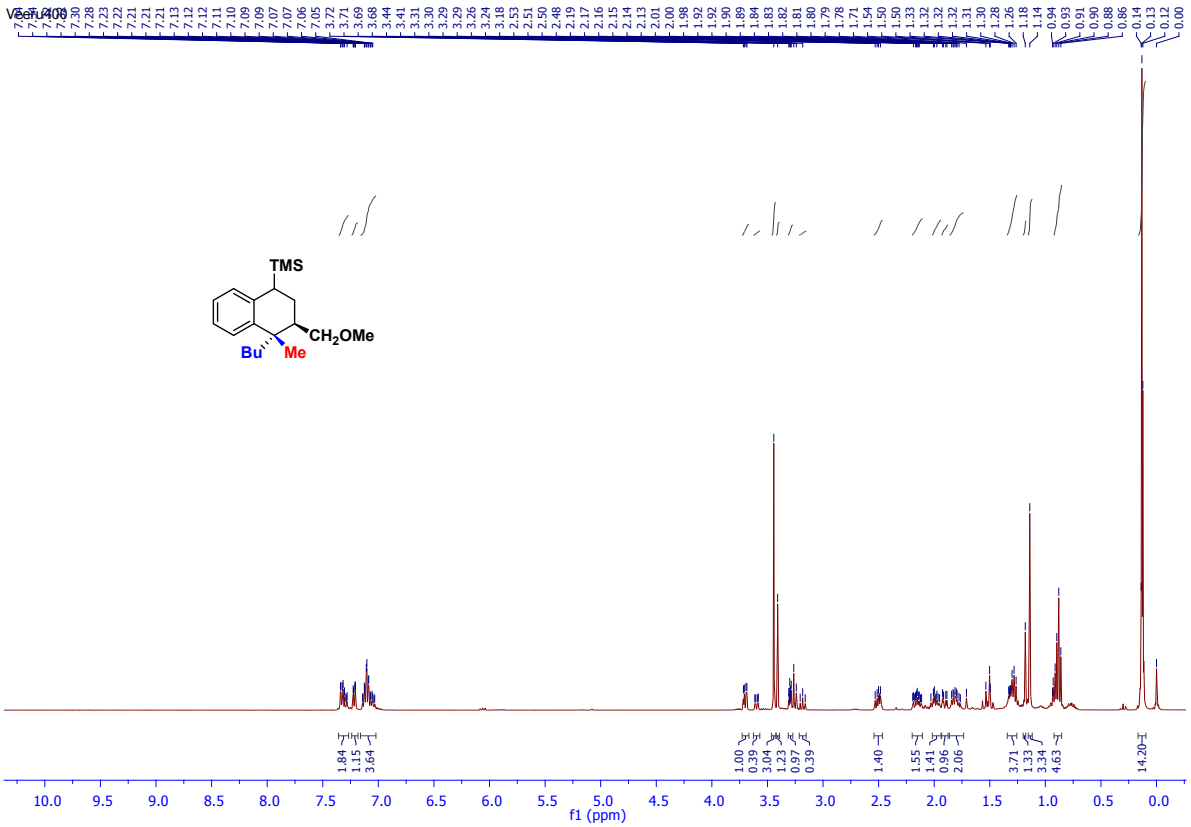
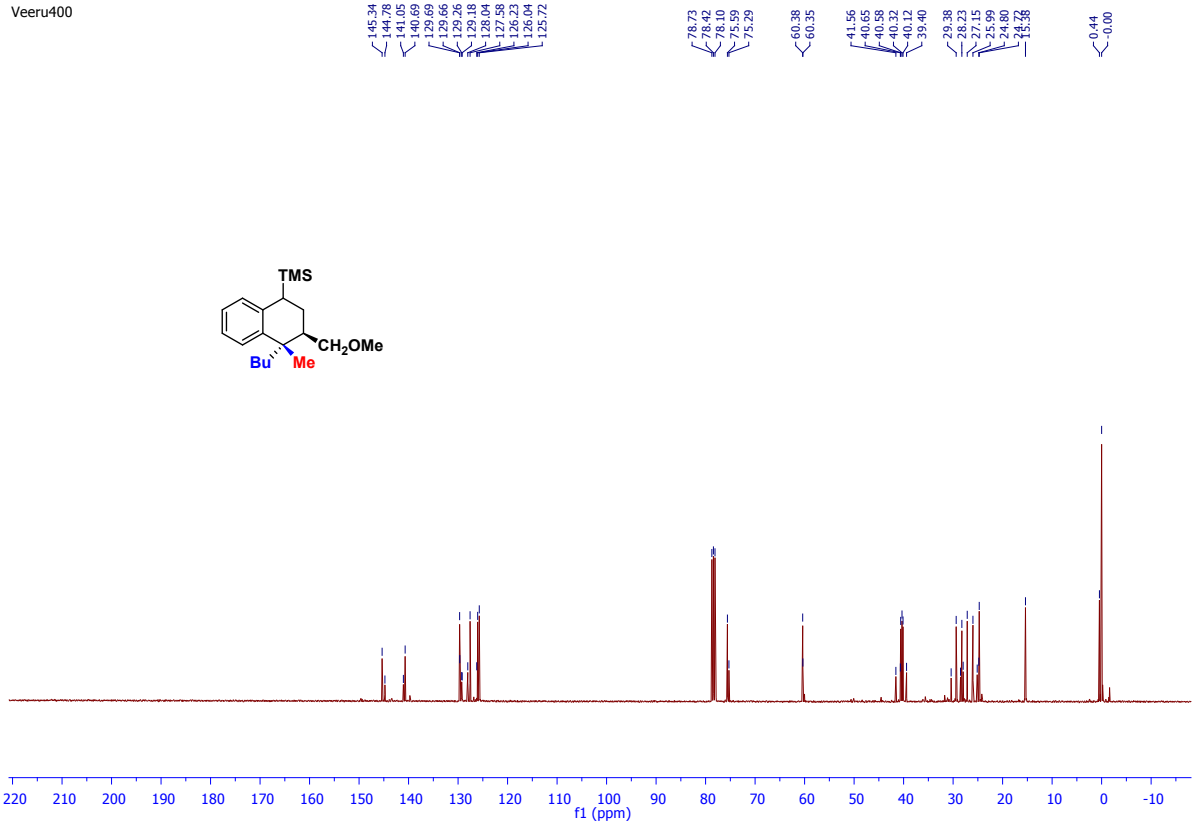
127.19
126.72
126.20
125.09
73.25
59.00
42.91
39.73
39.14
26.99
23.43
21.80
14.21
CH2OMe
Bu
Me
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


Veeru400
TMS
CH2OMe
Bu
Me
f1 (ppm)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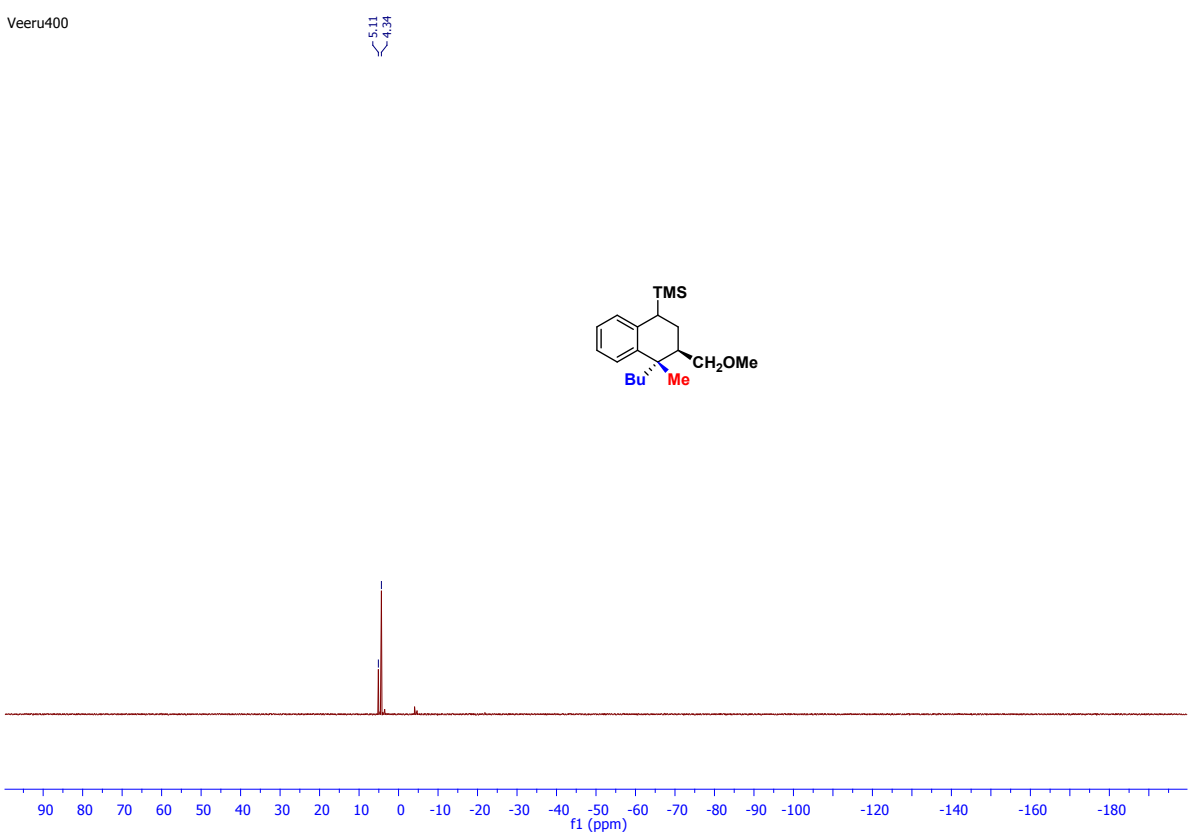
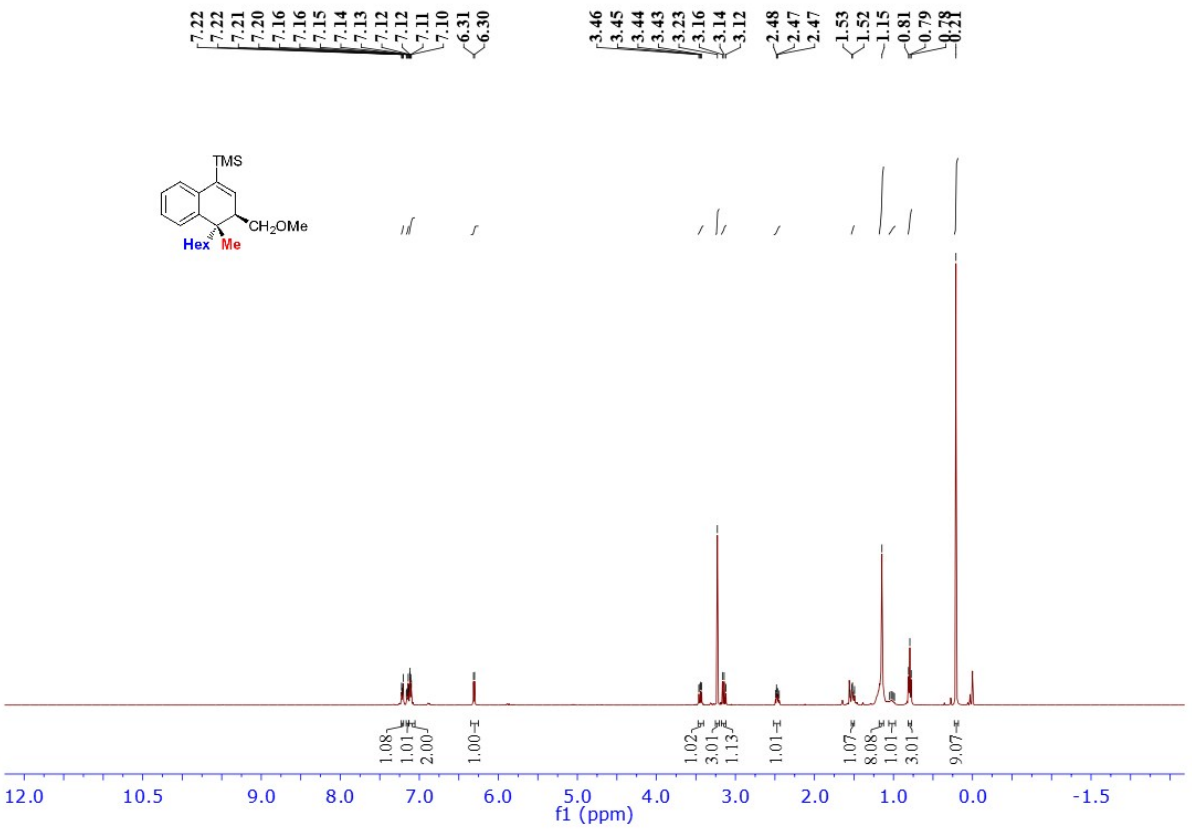
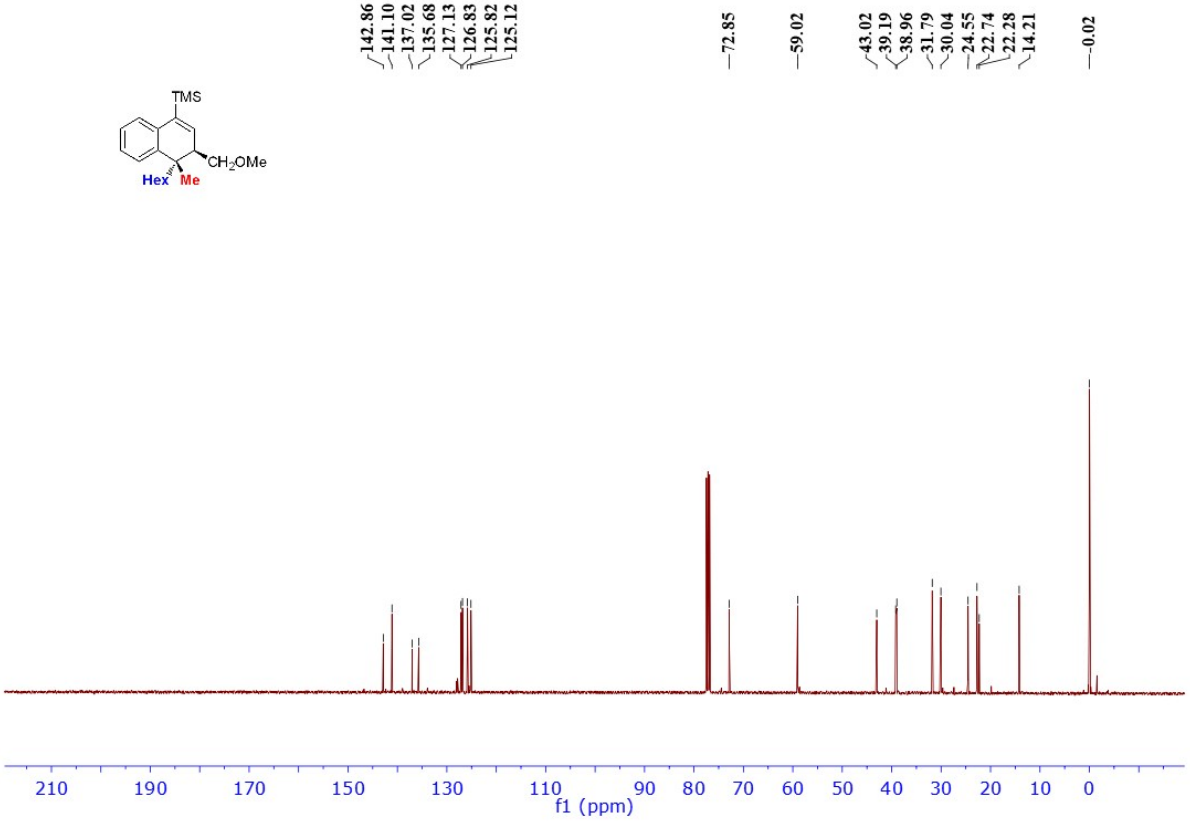
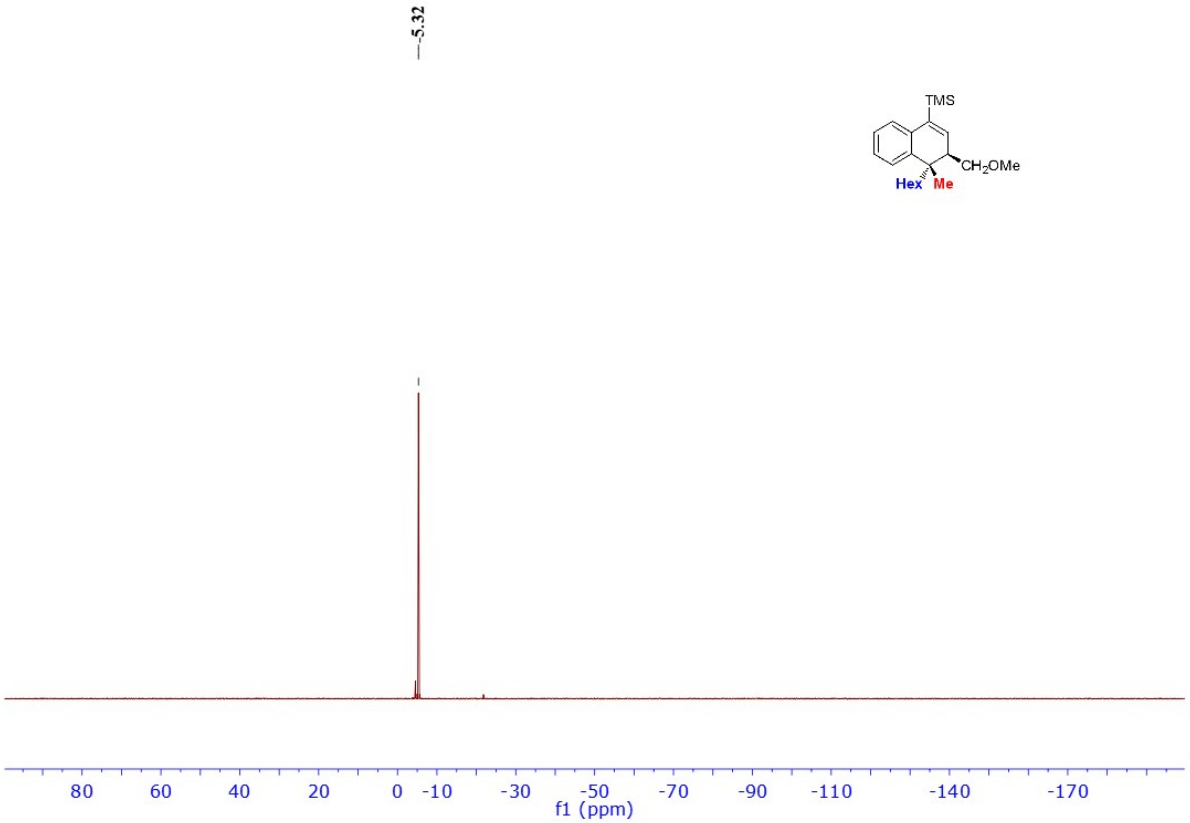
TMS
CH2OMe
Bu
Me
f1 (ppm)

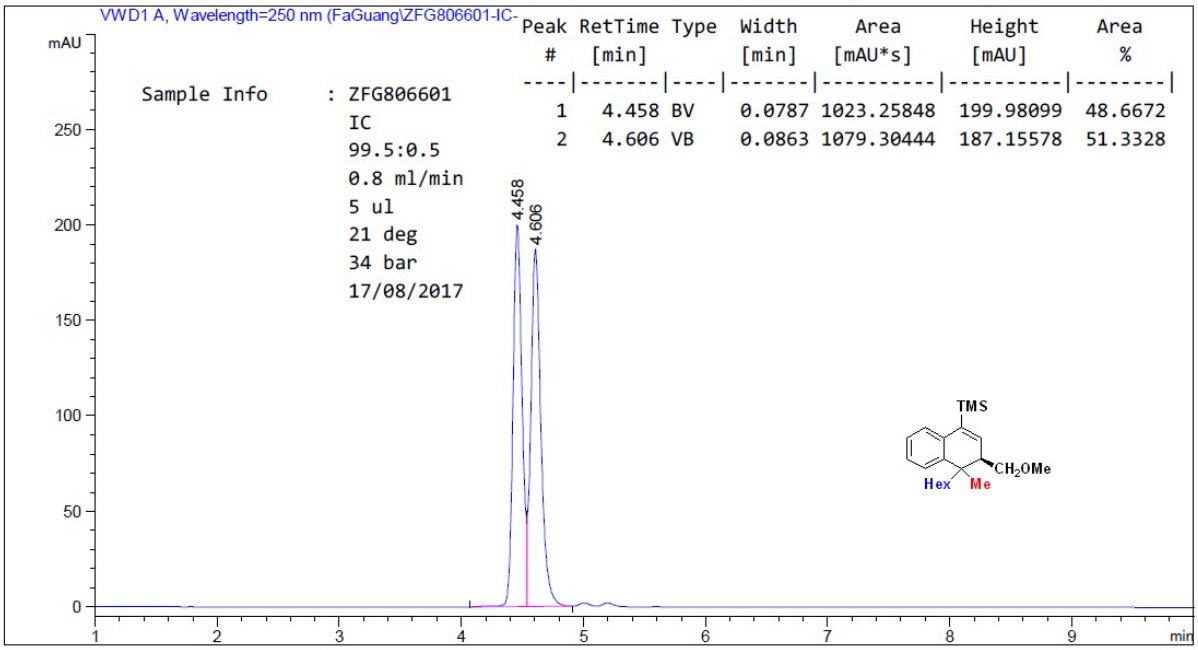
Veeru400


5.11
4.34
TMS
CH2OMe
Bu
Me
f1 (ppm)

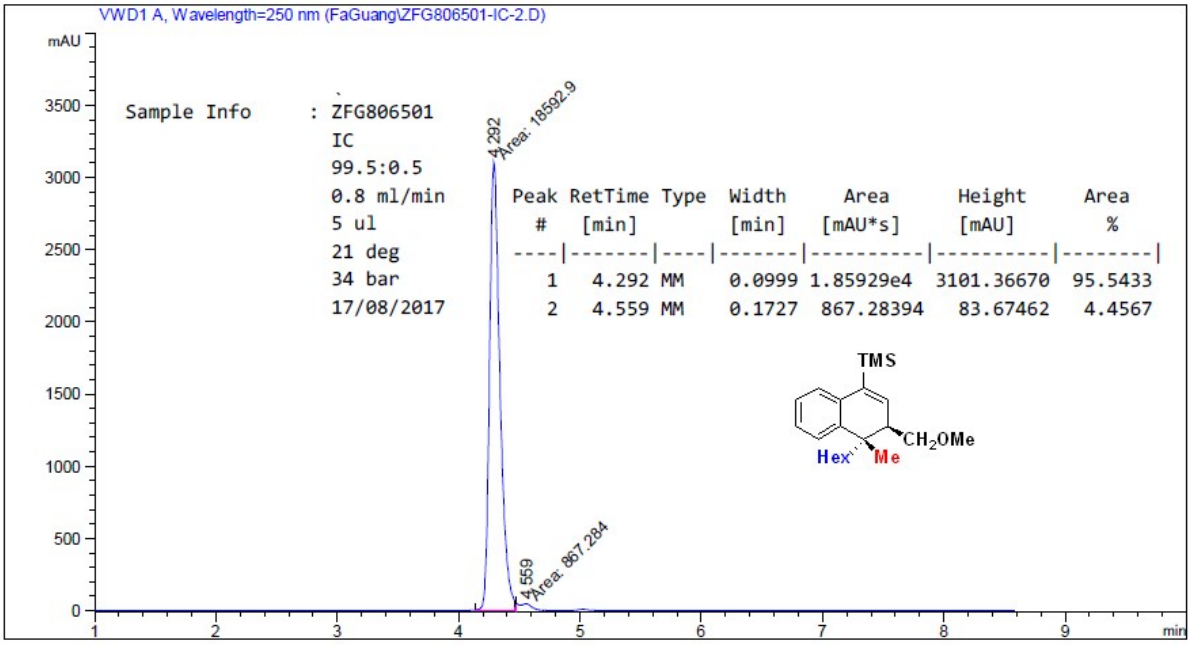

7.22
7.22
7.21
7.20
7.16
7.16
7.15
7.14
7.13
7.12
7.12
7.11
7.10
6.31
6.30
3.46
3.45
3.44
3.43
3.23
3.16
3.14
3.12
2.48
2.47
2.47
1.53
1.52
1.15
0.81
0.79
0.78
0.21
TMS
CH2OMe
Hex
Me
1.08
1.01
2.00
1.00
1.02
3.01
1.13
1.01
1.07
8.08
1.01
3.01
9.07
f1 (ppm)


142.86
141.10
137.02
135.68
127.13
126.83
125.82
125.12
72.85
59.02
43.02
39.19
38.96
31.79
30.04
24.55
22.74
22.28
14.21
0.02
TMS
CH2OMe
Hex
Me
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

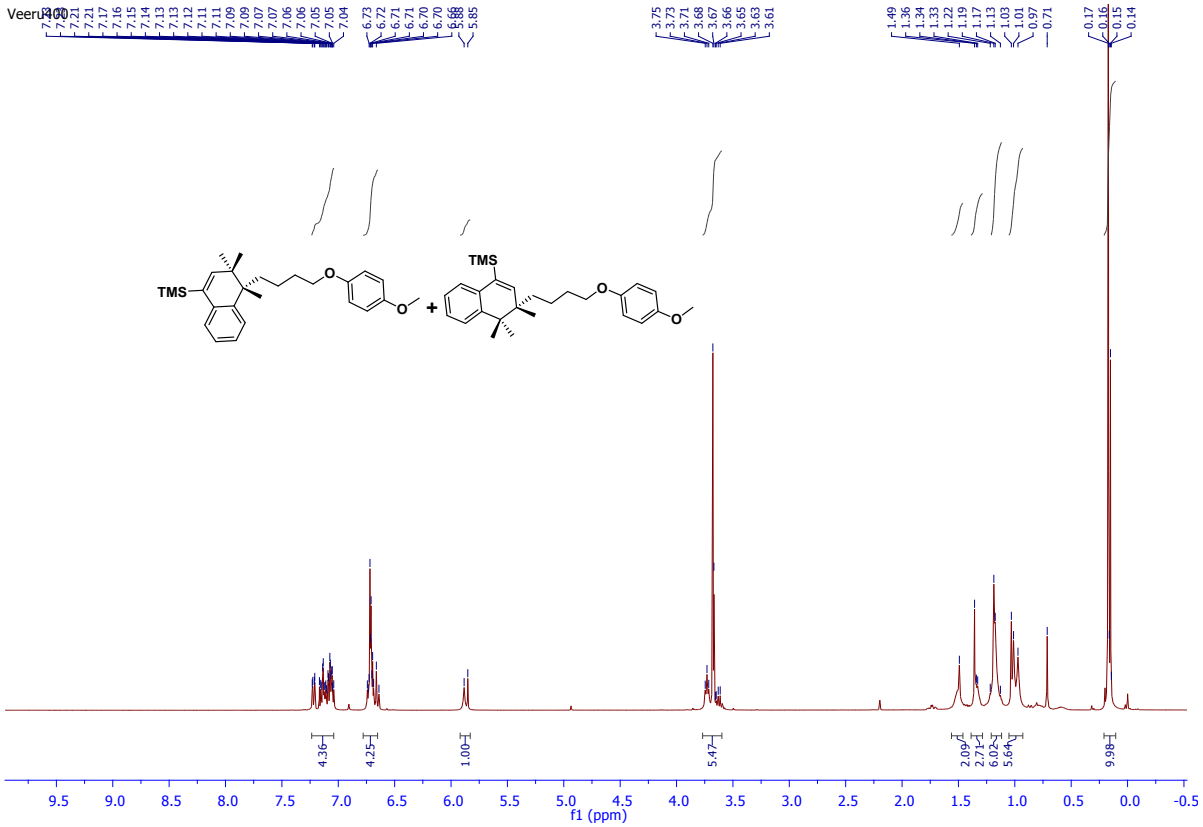

5.32
TMS
CH2OMe
Hex
Me
80
60
40
20
0
-10
-30
-50
-70
-90
-110
-140
-170
f1 (ppm)

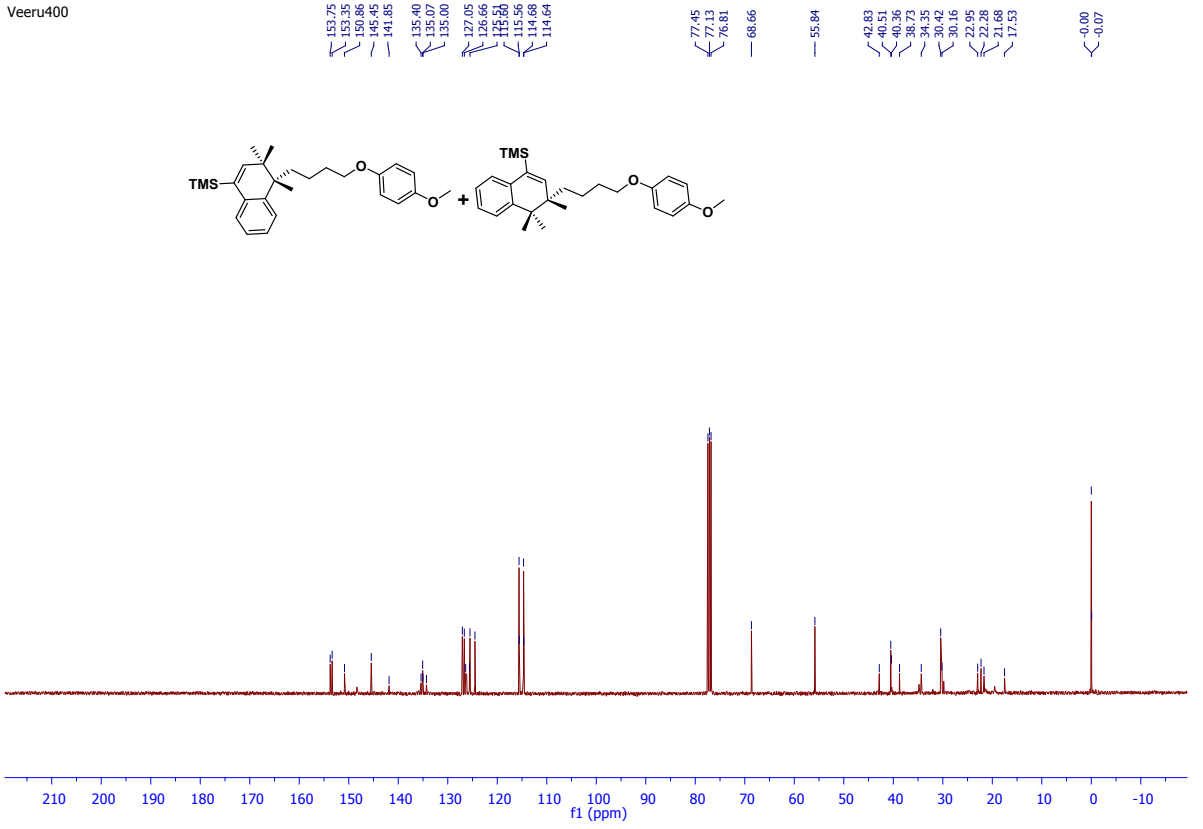


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	4.458	BV	0.0787	1023.25848	199.98099	48.6672
2	4.606	VB	0.0863	1079.30444	187.15578	51.3328

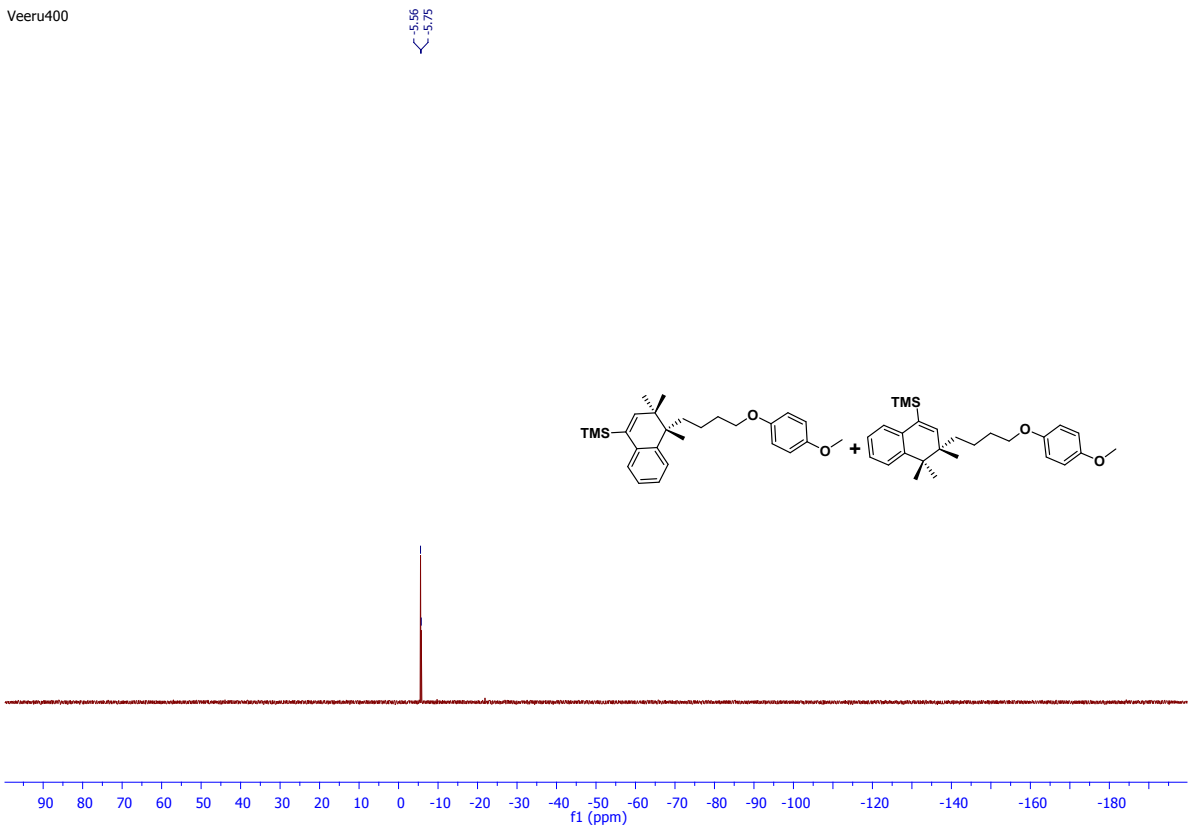


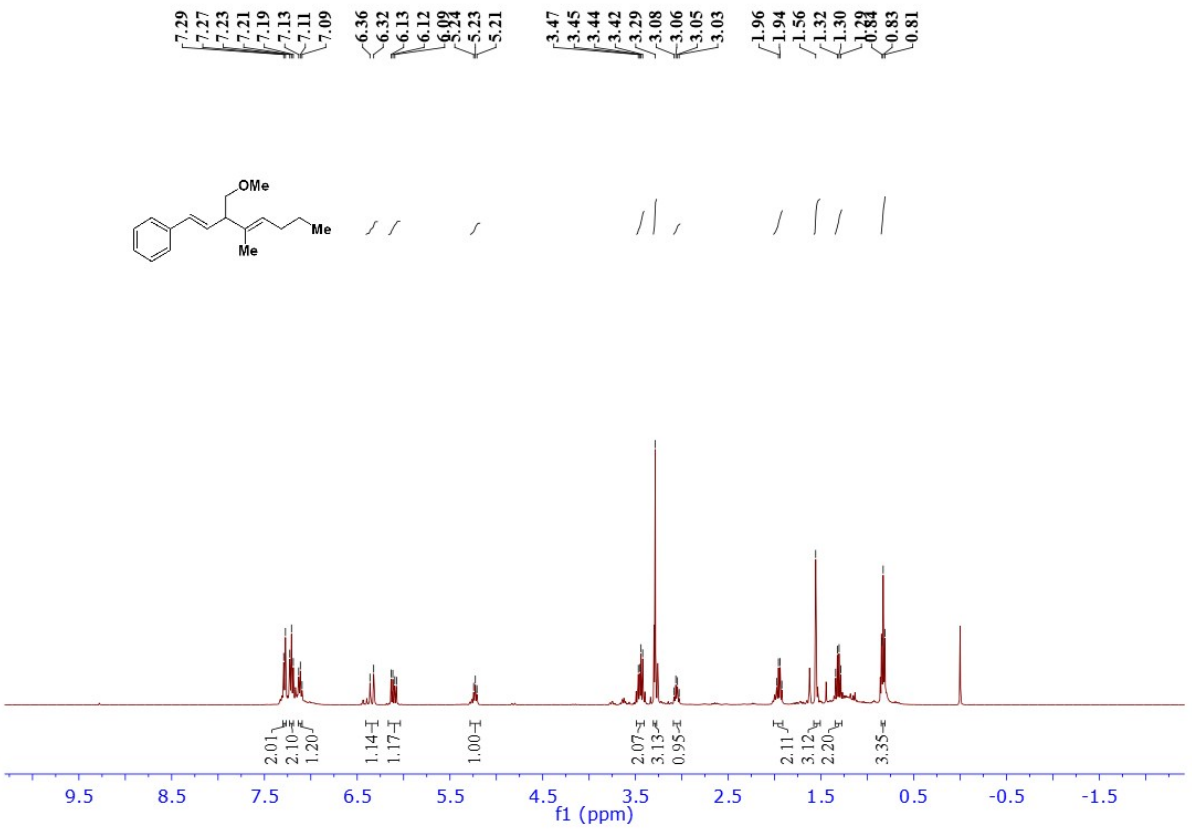
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	4.292	MM	0.0999	1.85929e4	3101.36670	95.5433
2	4.559	MM	0.1727	867.28394	83.67462	4.4567

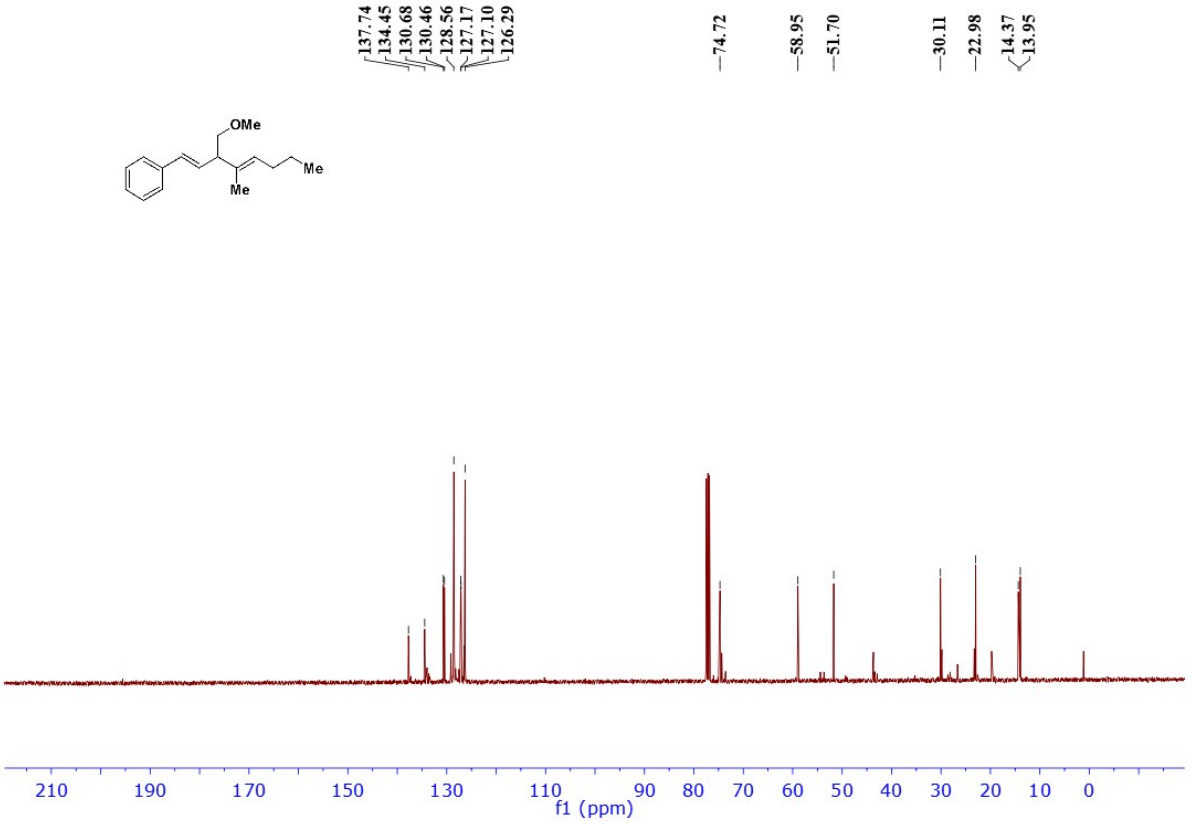

Veeru400
TMS
TMS
f1 (ppm)

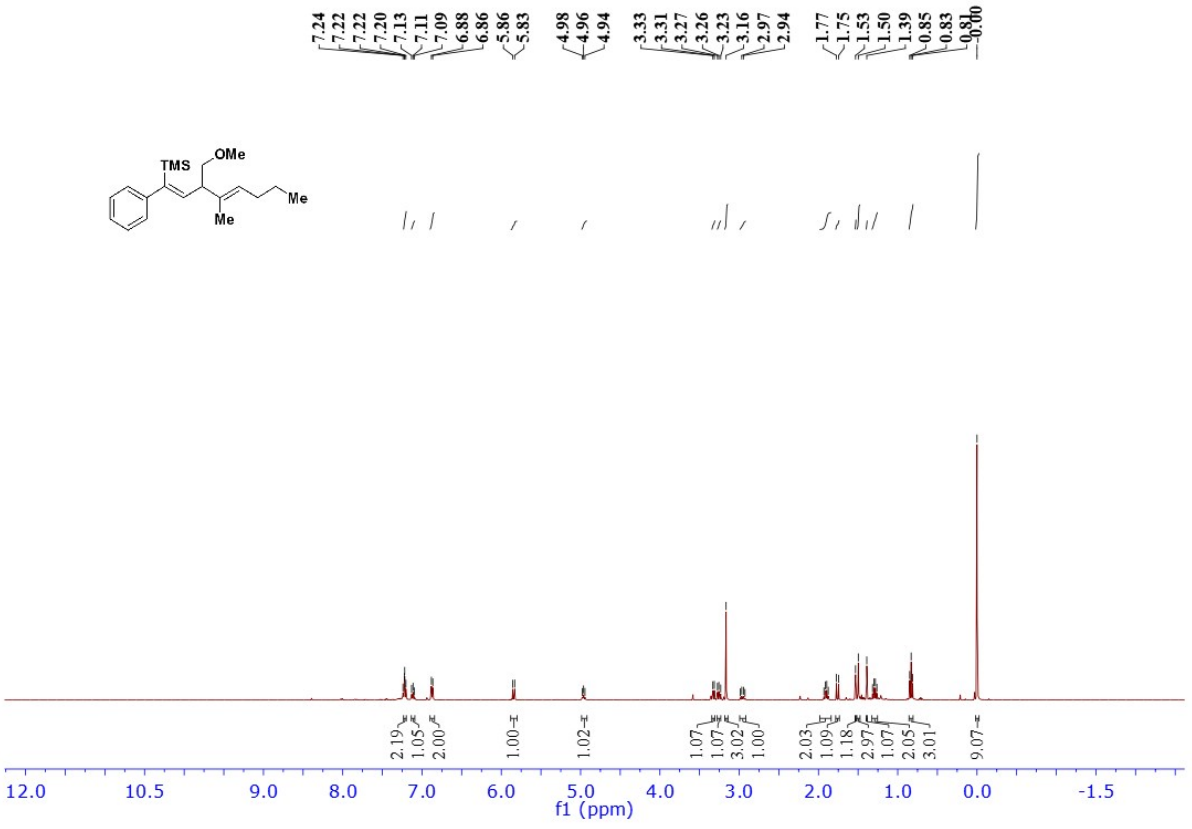

Veeru400
TMS
TMS
f1 (ppm)

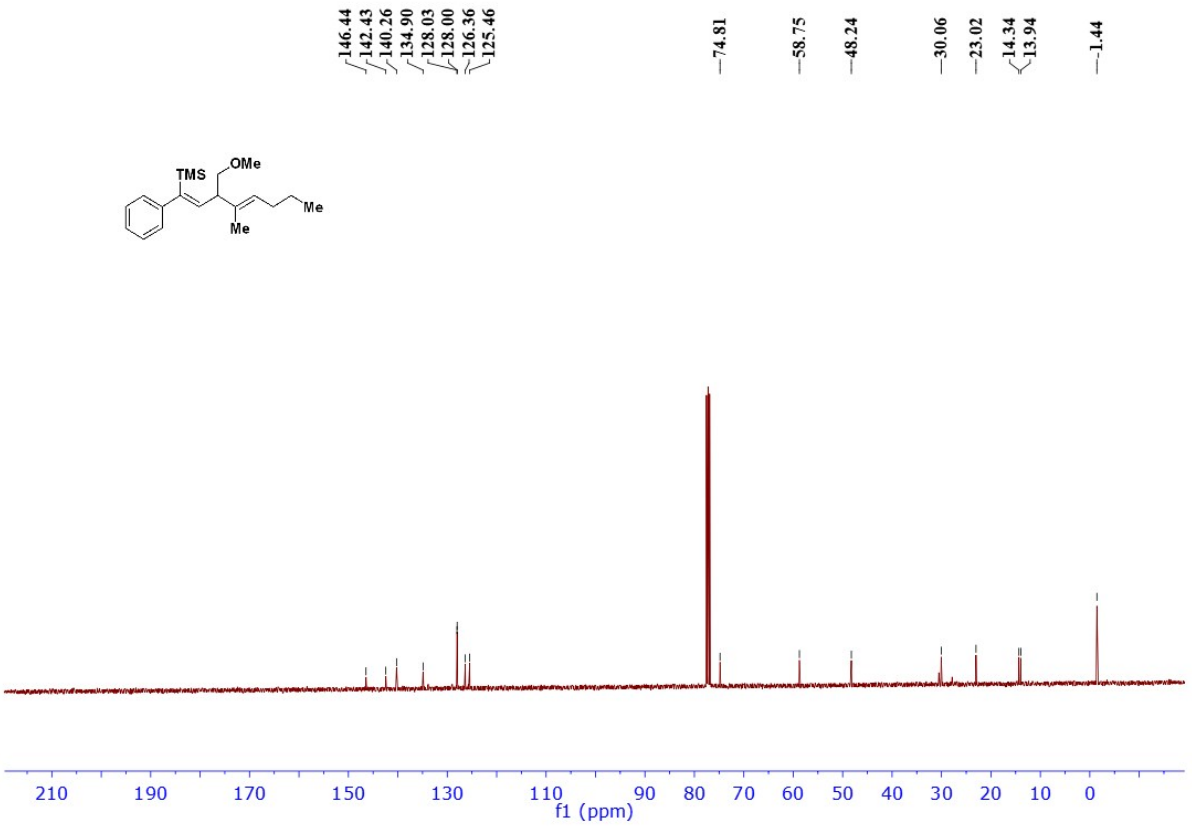
Veeru400

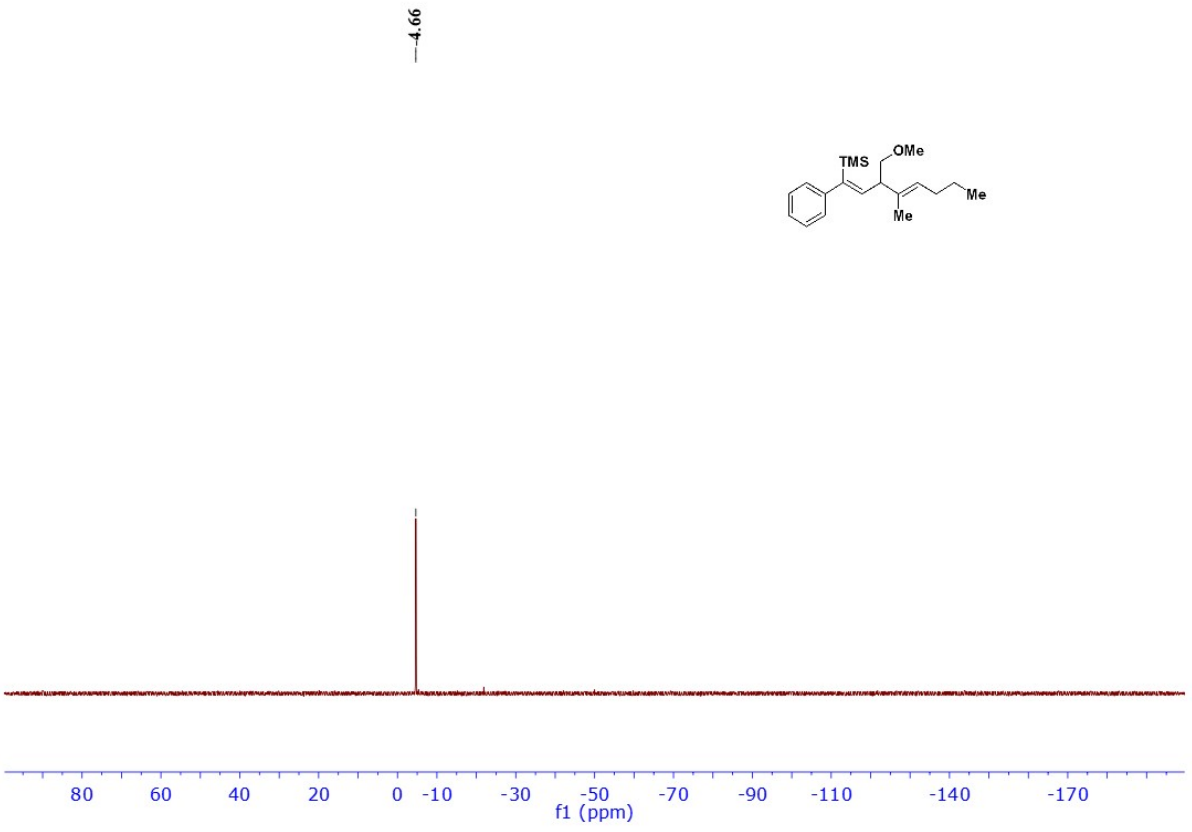

5.56
5.75
TMS
O
O
+
TMS
O
O
90 80 70 60 50 40 30 20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -120 -140 -160 -180
f1 (ppm)


7.29
7.27
7.23
7.21
7.19
7.13
7.11
7.09
6.36
6.32
6.13
6.12
5.24
5.23
5.21
3.47
3.45
3.44
3.42
3.29
3.08
3.06
3.05
3.03
1.96
1.94
1.56
1.32
1.30
0.83
0.81
OMe
Me
Me
2.01
2.10
1.20
1.14
1.17
1.00
2.07
3.13
0.95
2.11
3.12
2.20
3.35
9.5 8.5 7.5 6.5 5.5 4.5 3.5 2.5 1.5 0.5 -0.5 -1.5
f1 (ppm)

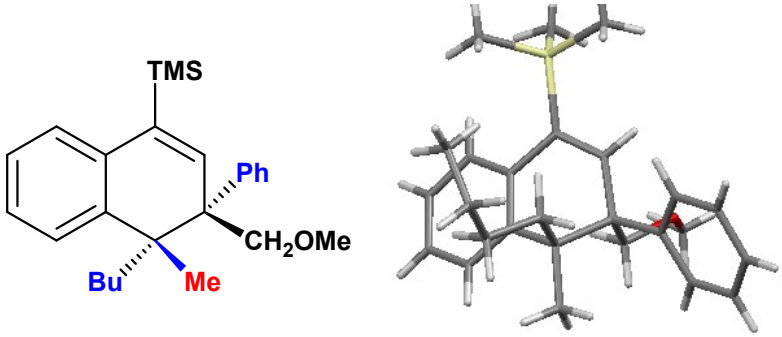

137.74
134.45
130.68
130.46
128.56
127.17
127.10
126.29
74.72
58.95
51.70
30.11
22.98
14.37
13.95
OMe
Me
Me
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


7.24
7.22
7.22
7.20
7.13
7.11
7.09
6.88
6.86
5.86
5.83
4.98
4.96
4.94
3.33
3.31
3.27
3.26
3.23
3.16
2.97
2.94
1.77
1.75
1.53
1.50
1.39
0.85
0.83
0.81
0.00
TMS
OMe
Me
Me
2.19
1.05
2.00
1.00
1.02
1.07
1.07
3.02
1.00
2.03
1.09
1.18
2.97
1.07
2.05
3.01
9.07
12.0
10.5
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
-1.5
f1 (ppm)


146.44
142.43
140.26
134.90
128.03
128.00
126.36
125.46
74.81
58.75
48.24
30.06
23.02
14.34
13.94
1.44
TMS
OMe
Me
Me
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


4.66
TMS
OMe
Me
Me
80
60
40
20
0
-10
-30
-50
-70
-90
-110
-140
-170
f1 (ppm)

Single X- Ray Crystal Structure of **4q**



Single X- Ray Crystal Structure of **4t**