

Catalytic Asymmetric Synthesis of Carboranylated Diols Bearing Two Adjacent Stereocenters Located at the α , β -Position of *o*-Carborane Cage Carbon

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Supporting Information

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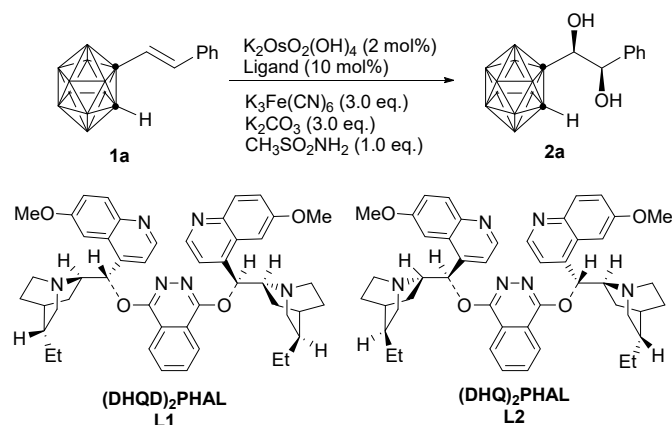
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1. General information

^1H NMR spectra were recorded on a Bruker DPX-300 spectrometer at 300 MHz. ^{13}C $\{^1\text{H}\}$ NMR spectra were recorded on Bruker DRX-300 spectrometers at 75 MHz. ^{19}F NMR spectra were recorded on a Bruker DPX-400 spectrometer at 376 MHz. ^{11}B NMR spectra were recorded on a Bruker DPX-400 spectrometer at 128 MHz. The chemical shifts for ^1H NMR were recorded in ppm (δ) relative to tetramethylsilane (TMS) with the solvent resonance employed as the internal standard (CDCl_3 , d 7.26 ppm). The chemical shifts for ^{13}C NMR were recorded in ppm downfield using the central peak of deuteriochloroform (77.0 ppm) as the internal standard. The ee values determination was carried out using chiral HPLC with Daicel chiral column on Agilent 1200. Flash column chromatography was performed on silica gel (200-300 mesh). TLC analysis was performed using glass-backed plates coated with 0.2 mm silica. The solvents were distilled from appropriate drying agents prior to use, unless otherwise noted.

2. Optimization of reaction conditions

Table S1. Optimization of reaction conditions^a



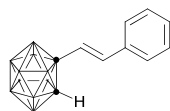
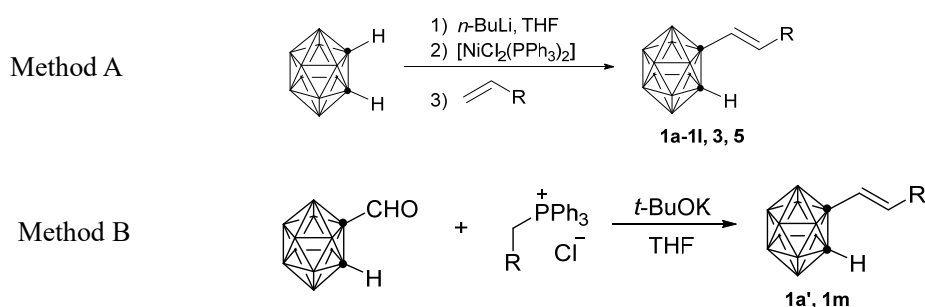
Entry	Ligand	solvent ^b	T/(°C)	C/(mol/l)	Yield(%) ^c	ee(%) ^d
1	AD-mix- β	<i>t</i> -BuOH/H ₂ O=1/1	0	0.1	trace	
2	(DHQD) ₂ PHAL	<i>t</i> -BuOH/H ₂ O=1/1	0	0.1	86	-92
3	(DHQ) ₂ PHAL	<i>t</i> -BuOH/H ₂ O=1/1	0	0.1	89	80
4	(DHQD) ₂ PHAL	<i>t</i> -BuOH/H ₂ O=1/1	15	0.1	91	-96
5	(DHQD) ₂ PHAL	<i>t</i> -BuOH/H ₂ O=1/1	25	0.1	89	-97
6	(DHQD) ₂ PHAL	<i>t</i> -BuOH/H ₂ O=1/1	35	0.1	82	-94
7	(DHQ) ₂ PHAL	<i>t</i> -BuOH/H ₂ O=1/1	25	0.1	92	88
8	(DHQD) ₂ PHAL	Acetone/H ₂ O=1/1	25	0.1	22	-93
9	(DHQ) ₂ PHAL	Acetone/H ₂ O=1/1	25	0.1	17	93
10	(DHQD) ₂ PHAL	DMSO/H ₂ O=1/1	25	0.1	NR	
11	(DHQ) ₂ -PHAL	DMSO/H ₂ O=1/1	25	0.1	NR	
12	(DHQD) ₂ PHAL	MeCN/H ₂ O=1/1	25	0.1	NR	
13	(DHQ) ₂ PHAL	MeCN/H ₂ O=1/1	25	0.1	NR	
14	(DHQD) ₂ PHAL	<i>t</i> -BuOH/H ₂ O=1/3	25	0.1	66	-95
15	(DHQ) ₂ PHAL	<i>t</i> -BuOH/H ₂ O=1/3	25	0.1	71	94
16	(DHQD) ₂ PHAL	<i>t</i> -BuOH/H ₂ O=3/1	25	0.1	57	-94

17	(DHQ) ₂ PHAL	<i>t</i> -BuOH/H ₂ O=3/1	25	0.1	61	90
18	(DHQD) ₂ PHAL	<i>t</i> -BuOH/H ₂ O=1/1	25	0.067	89	-96
19	(DHQ) ₂ PHAL	<i>t</i> -BuOH/H ₂ O=1/1	25	0.067	91	90
20	(DHQD) ₂ PHAL	<i>t</i> -BuOH/H ₂ O=1/1	25	0.2	84	-95
21	(DHQ) ₂ PHAL	<i>t</i> -BuOH/H ₂ O=1/1	25	0.2	91	90

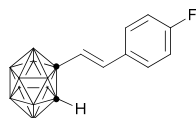
^aUnless indicated otherwise, the reactions were performed with 0.2 mmol of alkenylcarborane **1a** in 2 ml of solvent at indicated temperature for 24 hours. ^bVolume ratio. ^cIsolated yield for syn-1,2-diol isomer and no d.r. value with the anti-1,2-diol isomer undetectable in all cases. ^dDetermined by HPLC using a chiral column. The minus sign indicates the opposite enantiomer.

3. Synthesis of Alkenylcarboranes (**1a-1m**, **3**, **5**).

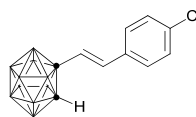
The alkenylcarborane **1a-1l**, **3** and **5** was synthesized according to method A described in the literature ^[1], **1a'**, **1m** was synthesized according to method B in the literature ^[2]



1a: Known compound; ¹H NMR (300 MHz, CDCl₃): δ 7.35 (s, 5H), 6.83 (d, *J* = 16.1 Hz, 1H), 6.27 (d, *J* = 16.1 Hz, 1H), 3.71 (s, 1H).



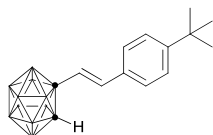
1b: Known compound; ¹H NMR (300 MHz, CDCl₃): δ 7.35 (s, 2H), 7.15 (m, 3H), 6.67 (d, *J* = 15.2 Hz, 1H), 3.68 (s, 1H).



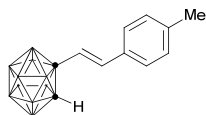
1c: *R*_f = 0.21 (hexane); White solid, 104.6 mg, 37% yield, mp: 106-107 °C. ¹H NMR (300 MHz, CDCl₃) δ 7.41 – 7.26 (m, 4H), 6.81 (d, *J* = 15.7 Hz, 1H), 6.25 (d, *J* = 15.7 Hz, 1H), 3.72 (s, 1H). ¹³C {¹H} NMR (75 MHz, CDCl₃) δ 136.45, 135.36, 132.56, 129.13, 128.14, 123.06, 73.77, 60.82. ¹¹B NMR (128 MHz, CDCl₃) δ -1.80 ((dd, *J* = 148.4, 1.3 Hz, 1B), -4.77 (dd, *J* = 137.3, 4.8 Hz, 1B), -7.04- -115.87 (m, 8B). HRMS (ESI) *m/z* calcd for C₁₀H₁₆B₁₀Cl⁺ (M-H)⁺ 280.1913, found 280.1926.

^[1] Z. Qiu and Z. Xie, *Angew. Chem., Int. Ed.*, 2008, **47**, 6572–6575.

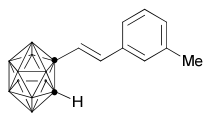
^[2] A. Sousa-Pedrares, C. Vinas and F. Teixidor, *Chem. Commun.*, 2010, **46**, 2998–3000.



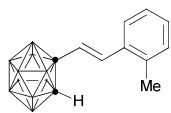
1d: $R_f = 0.27$ (hexane); colorless oil, 123.8mg, 41% yield. ^1H NMR (300 MHz, CDCl_3) δ 7.41 – 7.22 (m, 4H), 6.83 (d, $J = 15.7$ Hz, 1H), 6.23 (d, $J = 15.7$ Hz, 1H), 3.69 (s, 1H), 1.31 (s, 9H). ^{13}C $\{^1\text{H}\}$ NMR (75 MHz, CDCl_3) δ 152.98, 137.44, 131.26, 126.69, 125.83, 121.57, 60.95, 34.74, 31.13. ^{11}B NMR (128 MHz, CDCl_3) δ -1.88 (d, $J = 151.5$ Hz, 1B), -5.03 (d, $J = 141.2$ Hz, 1B), -7.82 - -17.51 (m, 8B). HRMS (ESI) m/z calcd for $\text{C}_{14}\text{H}_{25}\text{B}_{10}^-$ (M-H) $^-$ 301.2965, found 301.2968.



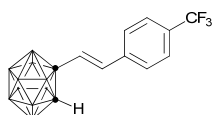
1e: Known compound; ^1H NMR (300 MHz, CDCl_3): δ 7.24 (d, $J = 8.0$ Hz, 2H), 7.14 (d, $J = 8.0$ Hz, 2H), 6.80 (d, $J = 15.8$ Hz, 1H), 6.29 (d, $J = 15.8$ Hz, 1H), 3.70 (s, 1H).



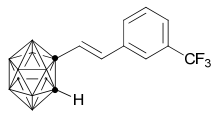
1f: Known compound; ^1H NMR (300 MHz, CDCl_3): δ 7.24 (m, 4H), 7.02 (d, $J = 15.4$ Hz, 1H), 6.41 (d, $J = 15.4$ Hz, 1H), 3.73 (s, 1H), 2.34 (s, 3H).



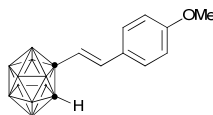
1g: $R_f = 0.24$ (hexane); White solid, 376.4 mg, 64% yield, mp: 82-84 °C. ^1H NMR (300 MHz, CDCl_3) δ 7.51 – 6.95 (m, 5H), 6.16 (d, $J = 15.6$ Hz, 1H), 3.72 (s, 1H), 2.35 (s, 3H). ^{13}C $\{^1\text{H}\}$ NMR (75 MHz, CDCl_3) δ 136.34, 135.89, 133.24, 130.66, 129.30, 126.34, 125.53, 123.78, 74.32, 60.87, 19.59. ^{11}B NMR (128 MHz, CDCl_3) δ -1.82 (d, $J = 150.7$ Hz, 1B), -4.94 (d, $J = 153.5$ Hz, 1B), -7.75 - -15.94 (m, 8H). HRMS (ESI) m/z calcd for $\text{C}_{11}\text{H}_{19}\text{B}_{10}^-$ (M-H) $^-$ 260.2459, found 260.2462.



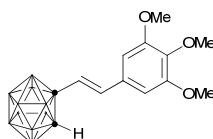
1h: Known compound; ^1H NMR (300 MHz, CDCl_3): δ 7.61 (d, $J = 8.1$ Hz, 2H), 7.45 (d, $J = 8.1$ Hz, 2H), 6.88 (d, $J = 15.9$ Hz, 1H), 6.22 (d, $J = 15.9$ Hz, 1H), 3.74 (s, 1H).



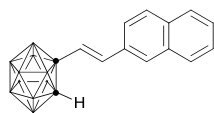
1i: Known compound; ^1H NMR (300 MHz, CDCl_3): δ 7.48 (m, 4H), 6.89 (d, $J = 15.8$ Hz, 1H), 6.34 (d, $J = 15.8$ Hz, 1H), 3.74 (s, 1H).



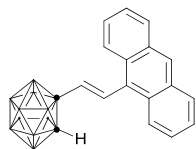
1j: Known compound; ^1H NMR (300 MHz, CDCl_3): δ 7.35 – 7.21 (m, 2H), 6.91 – 6.84 (m, 2H), 6.79 (d, $J = 15.7$ Hz, 1H), 6.14 (d, $J = 15.7$ Hz, 1H), 3.82 (s, 3H), 3.70 (s, 1H).



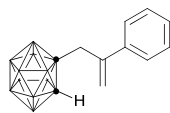
1k: Known compound; ^1H NMR (300 MHz, CDCl_3): δ 7.61 (d, $J = 8.1$ Hz, 2H), 7.45 (d, $J = 8.1$ Hz, 2H), 6.88 (d, $J = 15.9$ Hz, 1H), 6.22 (d, $J = 15.9$ Hz, 1H), 3.74 (s, 1H).



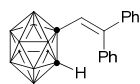
11: Rf = 0.16 (hexane); White solid, 85.6mg, 29% yield, mp: 112-114 °C. ^1H NMR (300 MHz, CDCl_3) δ 7.90 – 7.71 (m, 4H), 7.58 – 7.43 (m, 3H), 7.02 (d, J = 15.7 Hz, 1H), 6.40 (d, J = 15.7 Hz, 1H), 3.76 (s, 1H). ^{13}C {1H} NMR (75 MHz, CDCl_3) δ 137.83, 133.69, 133.26, 131.49, 128.72, 128.28, 128.25, 127.75, 126.95, 126.79, 122.73, 122.59, 74.24, 60.99. ^{11}B NMR (128 MHz, CDCl_3) δ -1.80 (d, J = 153.1 Hz, 1B), -4.85 (d, J = 143.0 Hz, 1B), -8.50- 12.17 (m, 8B). HRMS (ESI) m/z calcd for $\text{C}_{14}\text{H}_{19}\text{B}_{10}^-$ (M-H) $^-$ 296.2459, found 296.2462.



1m: Known compound; ^1H NMR (300 MHz, CDCl_3): 8.43 (s, 1H), 8.00 (m, 4H), 7.74 (m, 1H), 7.51 (m, 4H), 6.18 (d, J = 15.9 Hz, 1H), 3.88 (br, 1H).

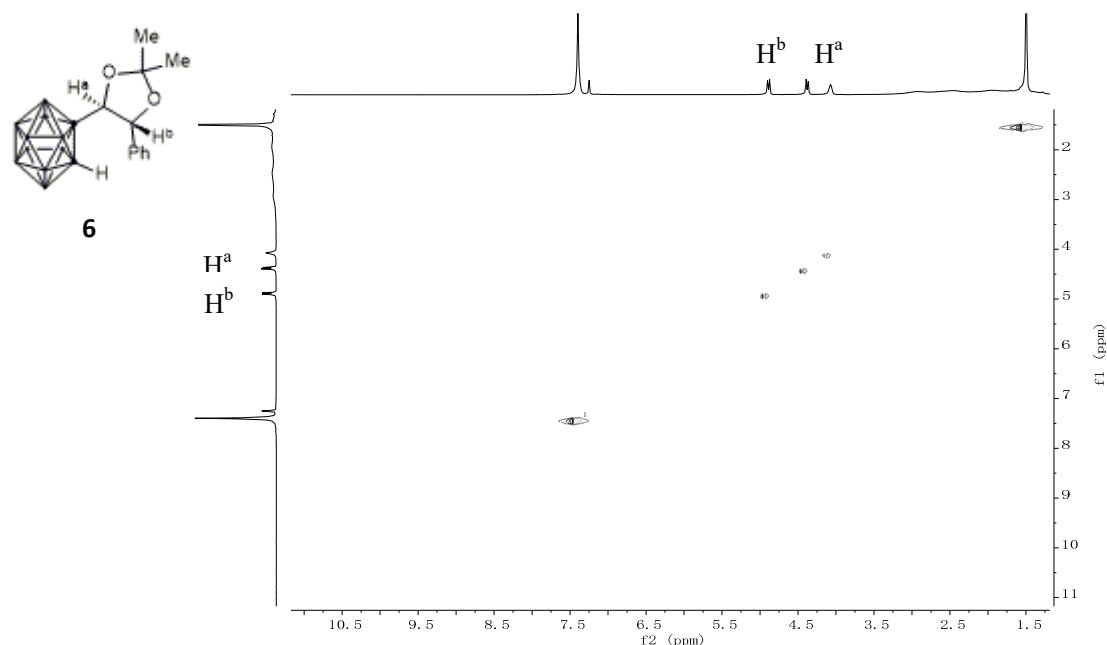


3: Known compound; ^1H NMR (300 MHz, CDCl_3): 7.36 (m, 5H), 5.48 (s, 1H), 5.20 (s, 1H), 3.49 (s, 2H), 3.37 (br, 1H).



5: Known compound; ^1H NMR (300 MHz, CDCl_3): δ 7.43 (m, 3H), 7.45 (m, 3H), 7.15 (m, 4H), 6.25 (s, 1H), 2.99 (s, 1H).

4. 2D-NOESY NMR of compound 6



Scheme S1 2D-NOESY NMR of the compound **6**

The relative stereochemistry of compound **6** was determined by 2D-NOESY NMR (**Scheme S1**). No NOE effect was observed for between H^a and H^b .

5. X-ray structure for compound 2c

A single crystal of the compound **2c** (CCDC 2067838) was grown from its solution in dichloromethane and hexane, which is suitable for X-ray diffraction analysis. The correctness of the X-ray data and the structure had been checked by using the CheckCIF utility on the submission Web site: <http://checkcif.iucr.org>

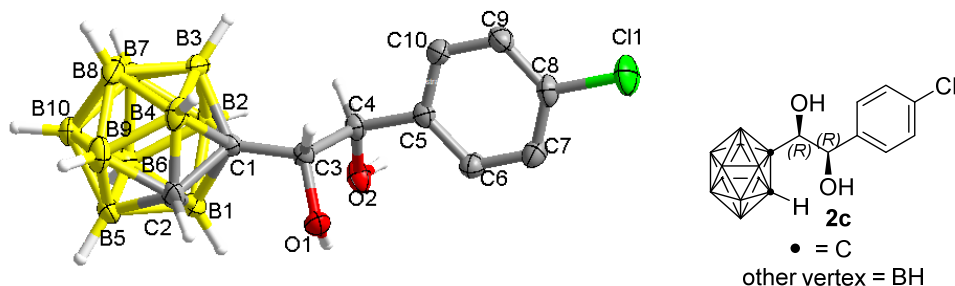


Table S2. Crystal data and structure refinement for 2c

Identification code	20210108
Empirical formula	C ₁₀ H ₁₉ B ₁₀ ClO ₂
Formula weight	314.80
Temperature/K	293(2)
Crystal system	orthorhombic
Space group	P2 ₁ 2 ₁ 2 ₁
a/Å	9.4651(9)
b/Å	12.7542(6)
c/Å	13.7835(5)
α/°	90
β/°	90
γ/°	90
Volume/Å ³	1663.95(18)
Z	4
ρ _{calc} /cm ³	1.257
μ/mm ⁻¹	1.965
F(000)	648.0
Crystal size/mm ³	0.16 × 0.12 × 0.1
Radiation	CuKα (λ = 1.54184)
2θ range for data collection/°	9.448 to 142.078
Index ranges	-7 ≤ h ≤ 11, -15 ≤ k ≤ 15, -15 ≤ l ≤ 16
Reflections collected	6530
Independent reflections	3145 [R _{int} = 0.0317, R _{sigma} = 0.0434]
Data/restraints/parameters	3145/2/215
Goodness-of-fit on F ²	1.027
Final R indexes [I > 2σ (I)]	R ₁ = 0.0456, wR ₂ = 0.1191
Final R indexes [all data]	R ₁ = 0.0527, wR ₂ = 0.1265
Largest diff. peak/hole / e Å ⁻³	0.16/-0.25
Flack parameter	0.000(15)

Table S3. Bond Lengths for 2c

Atom	Atom	Length/Å	Atom	Atom	Length/Å
C1	C8	1.742 (3)	B1	B2	1.770 (6)
O1	C3	1.418 (4)	B1	B5	1.781 (6)
O2	C4	1.415 (4)	B1	B6	1.767 (6)
C1	C2	1.640 (4)	B2	B3	1.774 (6)
C1	C3	1.538 (4)	B2	B6	1.775 (5)
C1	B1	1.718 (5)	B2	B7	1.769 (6)
C1	B2	1.712 (5)	B3	B4	1.765 (7)
C1	B3	1.702 (4)	B3	B7	1.775 (6)
C1	B4	1.738 (5)	B3	B8	1.774 (6)
C2	B1	1.708 (6)	B4	B8	1.754 (7)
C2	B4	1.709 (6)	B4	B9	1.761 (7)
C2	B5	1.703 (6)	B5	B6	1.771 (6)
C2	B9	1.709 (6)	B5	B9	1.779 (8)
C3	C4	1.538 (4)	B5	B10	1.762 (6)
C4	C5	1.517 (4)	B6	B7	1.781 (6)
C5	C6	1.389 (5)	B6	B10	1.773 (6)
C5	C10	1.385 (5)	B7	B8	1.771 (8)
C6	C7	1.377 (5)	B7	B10	1.776 (6)
C7	C8	1.374 (5)	B8	B9	1.767 (8)
C8	C9	1.375 (5)	B8	B10	1.794 (7)
C9	C10	1.393 (5)	B9	B10	1.768 (7)

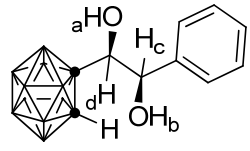
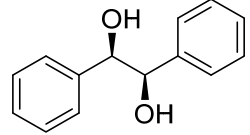
Table S4. Bond Angles for 2c

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C2	C1	B1	61.1(2)	C1	B4	B3	58.1(2)	C9	C8	C11	119.2(3)	B8	B7	B10	60.8(3)
C2	C1	B2	109.9(3)	C1	B4	B8	105.2(3)	C8	C9	C10	118.7(3)	B10	B7	B6	59.8(3)
C2	C1	B3	109.7(3)	C1	B4	B9	105.2(3)	C5	C10	C9	120.8(3)	B3	B8	B10	107.6(3)
C2	C1	B4	60.7(2)	C2	B4	C1	56.8(2)	C1	B1	B2	58.78(19)	B4	B8	B3	60.0(2)
C3	C1	C2	117.0(2)	C2	B4	B3	103.7(3)	C1	B1	B5	105.1(3)	B4	B8	B7	108.2(3)
C3	C1	B1	119.4(3)	C2	B4	B8	104.9(3)	C1	B1	B6	105.4(3)	B4	B8	B9	60.0(3)
C3	C1	B2	124.9(2)	C2	B4	B9	59.0(3)	C2	B1	C1	57.2(2)	B4	B8	B10	107.7(3)
C3	C1	B3	120.9(3)	B8	B4	B3	60.6(3)	C2	B1	B2	104.2(3)	B7	B8	B3	60.1(2)
C3	C1	B4	114.1(3)	B8	B4	B9	60.3(3)	C2	B1	B5	58.4(2)	B7	B8	B10	59.8(3)
B1	C1	B4	113.2(3)	B9	B4	B3	108.4(3)	C2	B1	B6	104.3(3)	B9	B8	B3	107.8(3)
B2	C1	B1	62.1(2)	C2	B5	B1	58.7(2)	B2	B1	B5	107.9(3)	B9	B8	B7	107.5(3)
B2	C1	B4	113.1(3)	C2	B5	B6	104.3(3)	B6	B1	B2	60.3(2)	B9	B8	B10	59.5(3)
B3	C1	B1	113.7(3)	C2	B5	B9	58.7(3)	B6	B1	B5	59.9(2)	C2	B9	B4	59.0(2)
B3	C1	B2	62.6(2)	C2	B5	B10	104.6(3)	C1	B2	B1	59.1(2)	C2	B9	B5	58.4(3)
B3	C1	B4	61.7(2)	B6	B5	B1	59.7(2)	C1	B2	B3	58.4(2)	C2	B9	B8	104.4(3)
C1	C2	B1	61.7(2)	B6	B5	B9	108.0(3)	C1	B2	B6	105.3(3)	C2	B9	B10	104.1(3)
C1	C2	B4	62.5(2)	B9	B5	B1	108.1(3)	C1	B2	B7	105.0(3)	B4	B9	B5	108.4(3)
C1	C2	B5	112.4(3)	B10	B5	B1	108.0(3)	B1	B2	B3	107.8(3)	B4	B9	B8	59.6(3)
C1	C2	B9	112.2(3)	B10	B5	B6	60.2(3)	B1	B2	B6	59.8(2)	B4	B9	B10	108.5(4)
B1	C2	B4	115.3(3)	B10	B5	B9	59.9(3)	B3	B2	B6	108.4(3)	B8	B9	B5	108.5(4)
B1	C2	B9	115.0(3)	B1	B6	B2	60.0(2)	B7	B2	B1	108.0(3)	B8	B9	B10	61.0(3)
B5	C2	B1	62.9(3)	B1	B6	B5	60.4(2)	B7	B2	B3	60.1(2)	B10	B9	B5	59.6(3)
B5	C2	B4	114.6(3)	B1	B6	B7	107.6(3)	B7	B2	B6	60.3(2)	B5	B10	B6	60.1(3)
B5	C2	B9	62.9(3)	B1	B6	B10	108.2(3)	C1	B3	B2	59.0(2)	B5	B10	B7	108.0(3)
B9	C2	B4	62.0(3)	B2	B6	B7	59.6(2)	C1	B3	B4	60.1(2)	B5	B10	B8	108.0(3)
O1	C3	C1	110.7(3)	B5	B6	B2	108.1(3)	C1	B3	B7	105.1(3)	B5	B10	B9	60.5(3)
O1	C3	C4	109.6(2)	B5	B6	B7	107.4(3)	C1	B3	B8	105.9(3)	B6	B10	B7	60.2(3)
C1	C3	C4	112.8(2)	B5	B6	B10	59.6(3)	B2	B3	B7	59.8(2)	B6	B10	B8	108.0(3)
O2	C4	C3	104.5(3)	B10	B6	B2	107.9(3)	B4	B3	B2	108.8(3)	B7	B10	B8	59.5(3)
O2	C4	C5	112.5(3)	B10	B6	B7	60.0(3)	B4	B3	B7	107.4(3)	B9	B10	B6	108.4(3)
C5	C4	C3	111.7(3)	B2	B7	B3	60.1(2)	B4	B3	B8	59.4(3)	B9	B10	B7	107.2(3)
C6	C5	C4	121.6(3)	B2	B7	B6	60.0(2)	B8	B3	B2	108.1(3)	B9	B10	B8	59.5(3)
C10	C5	C4	119.7(3)	B2	B7	B8	108.5(3)								
C10	C5	C6	118.8(3)	B2	B7	B10	108.1(3)								
C7	C6	C5	120.9(3)	B3	B7	B6	108.0(3)								
C8	C7	C6	119.3(3)	B3	B7	B10	108.4(3)								
C7	C8	C11	119.2(3)	B8	B7	B3	60.0(3)								
C7	C8	C9	121.6(3)	B8	B7	B6	108.6(3)								

6. Comparison of NMR data of 2a and 1,2-diphenylethane-1,2-diol.

The chemical shift data of ^1H NMR and ^{13}C NMR of **2a** and diphenylethylene glycol^[3] are shown below for comparison with different structural characterization. The results shows that obvious difference between the carborane and benzene ring moiety.

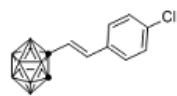
^[3]E. N. Jacobsen, I. Markó, W. S. Mungall, G. Schröder and K. B. Sharpless, *J. Am. Chem. Soc.*, 1988, **110**, 1968–1970.

compounds	^1H NMR chemical shift (ppm)		^{13}C NMR chemical shift (ppm)
	H_a, H_b	H_c, H_d	$\text{CH}(\text{OH})$
	3.28, 2.34	4.99, 4.17	77.6, 75.5
	2.88	4.73	79.1

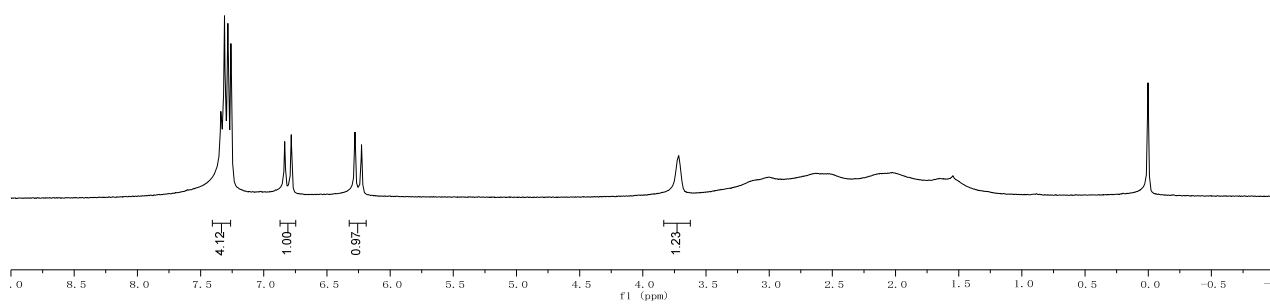
LHN-4-36 ¹H NMR in CDCl₃ 300M

7.3395
7.3113
7.2843
7.2596
6.8345
6.77821
6.2784
6.2280

3.77167



1c

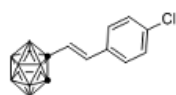


LHN-4-36 ¹³C NMR in CDCl₃ 75M

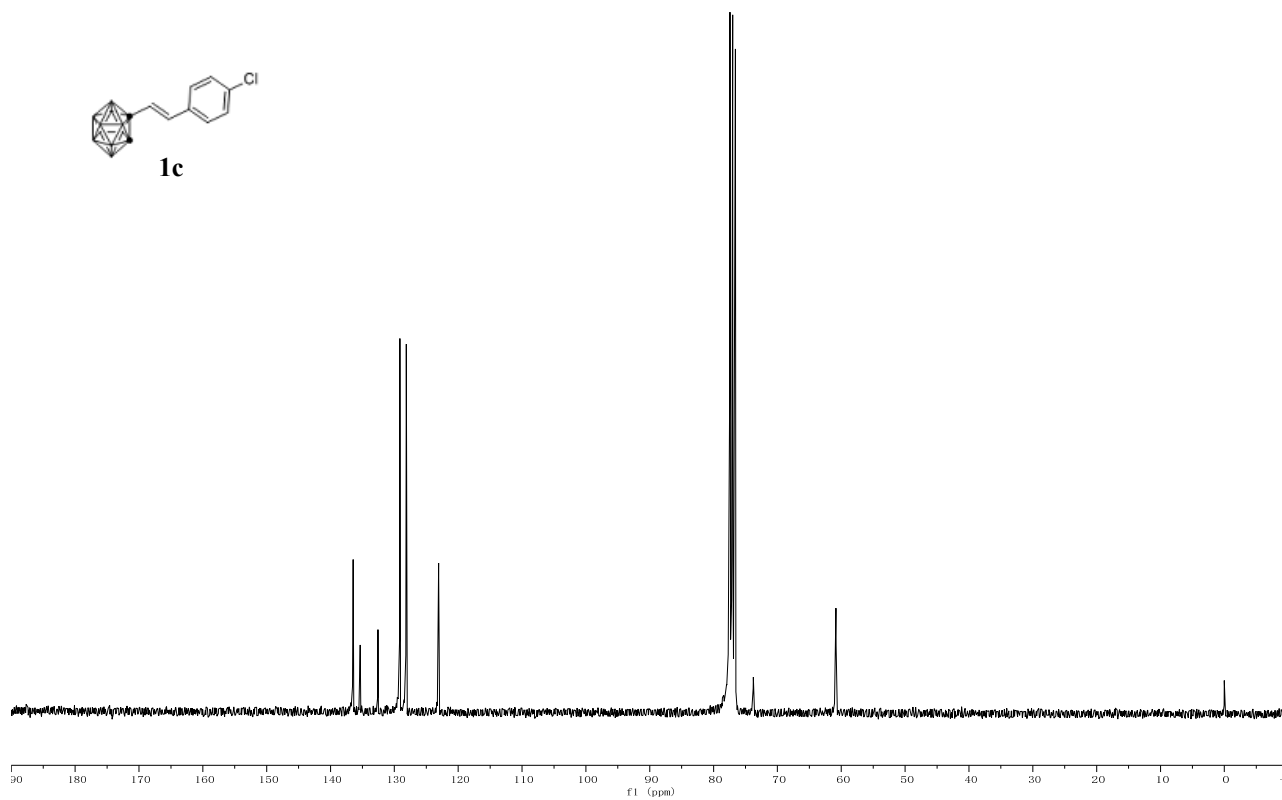
136.4467
132.5593
132.5546
128.1327
128.1369
123.0633

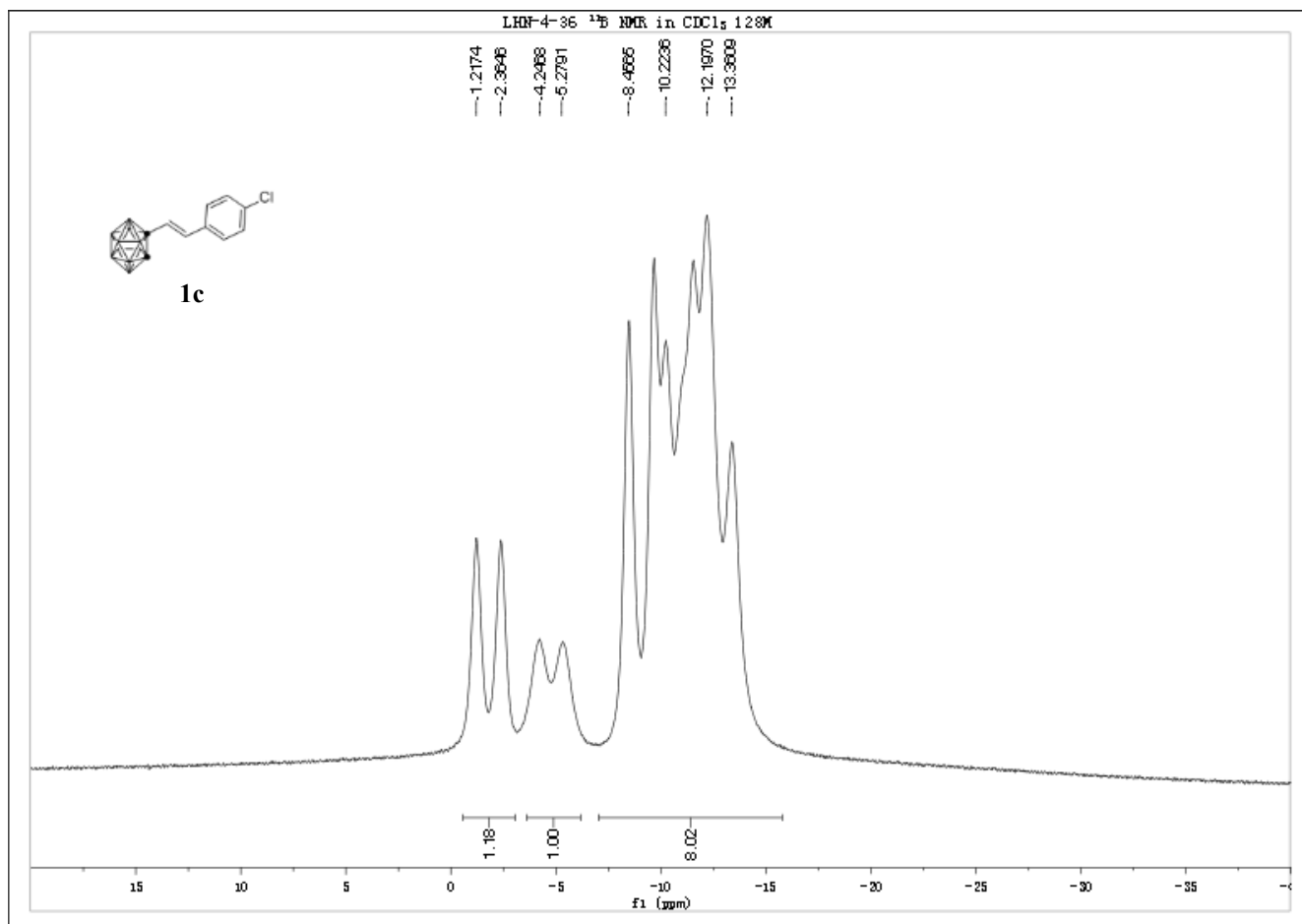
77.4392
77.0157
76.8924
73.7693

60.8244



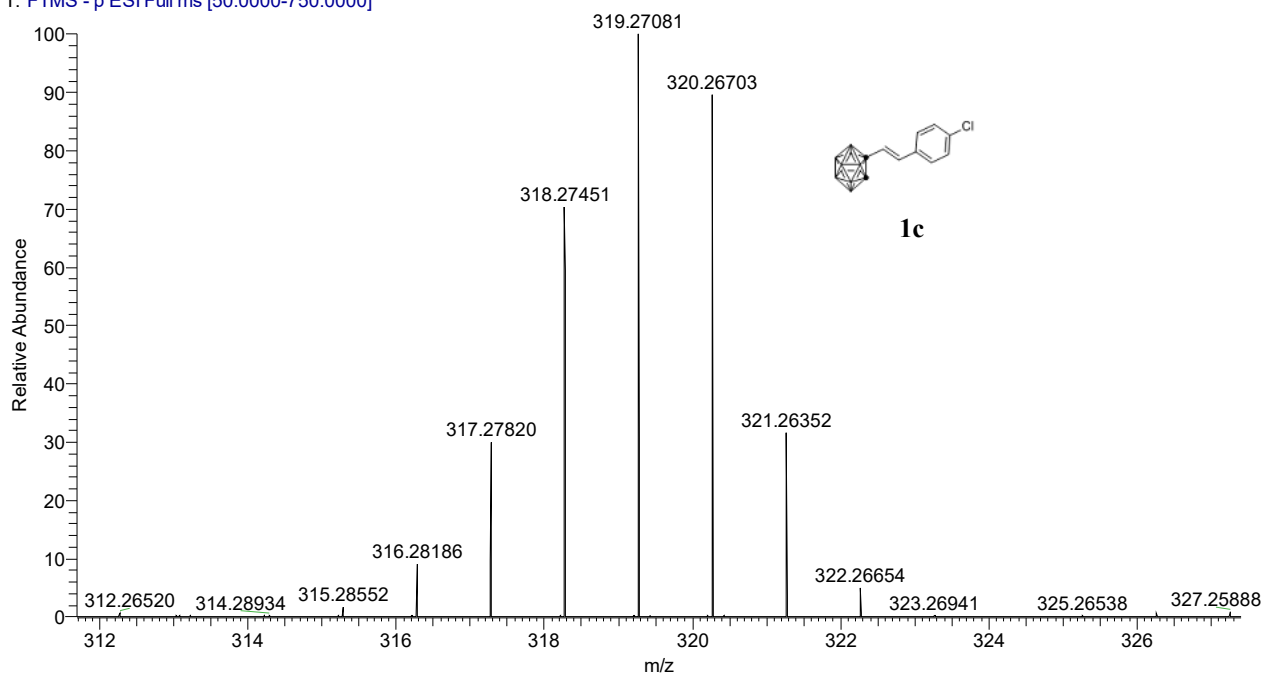
1c



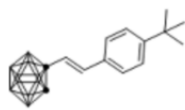
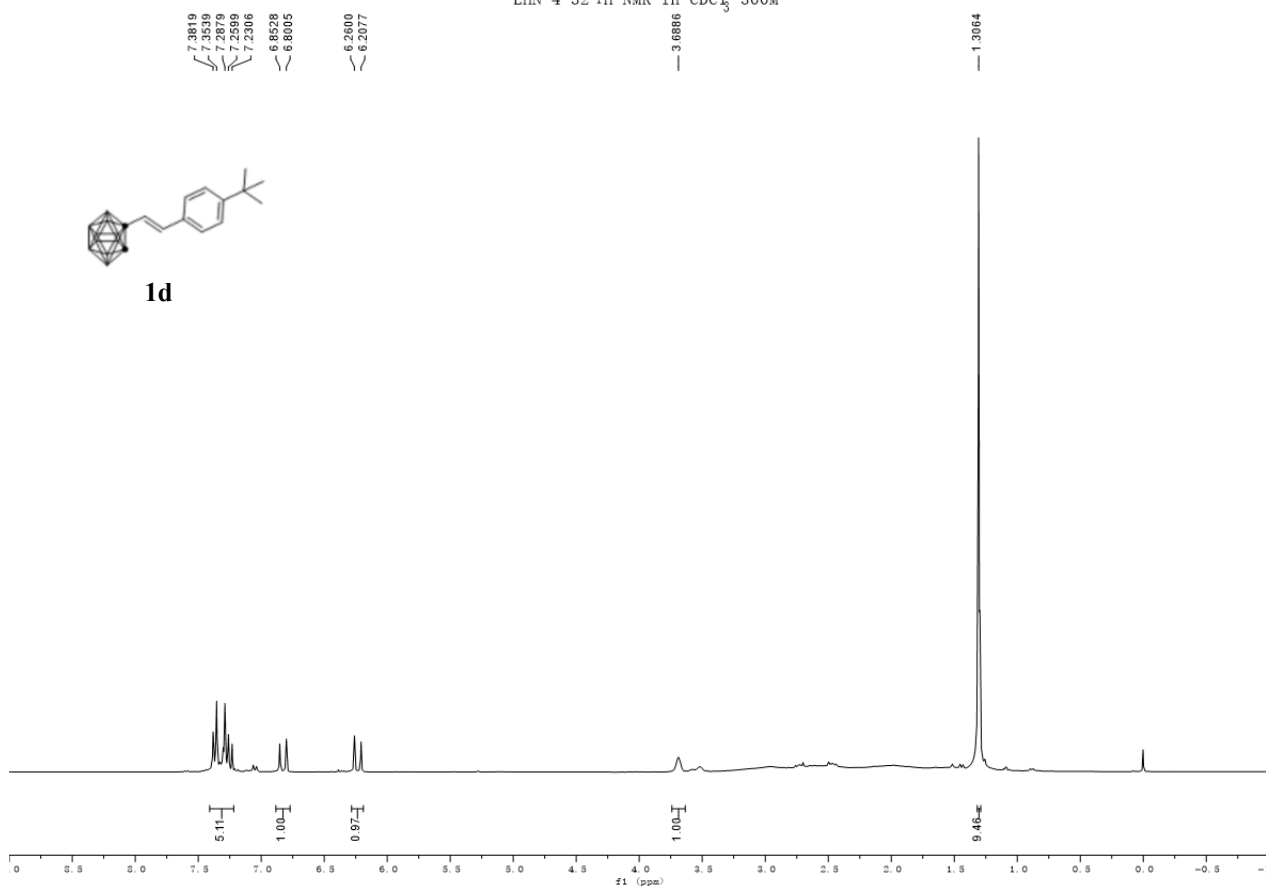


LHN-4-36. HRMS (ESI) m/z calcd for $\text{C}_{10}\text{H}_{16}\text{B}_{10}\text{Cl}^-$ (M-H) 280.19129, found 280.19263.

LHN-4-29 #10 RT: 0.11 AV: 1 NL: 1.15E7
T: FTMS - p ESI Full ms [50.0000-750.0000]

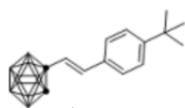
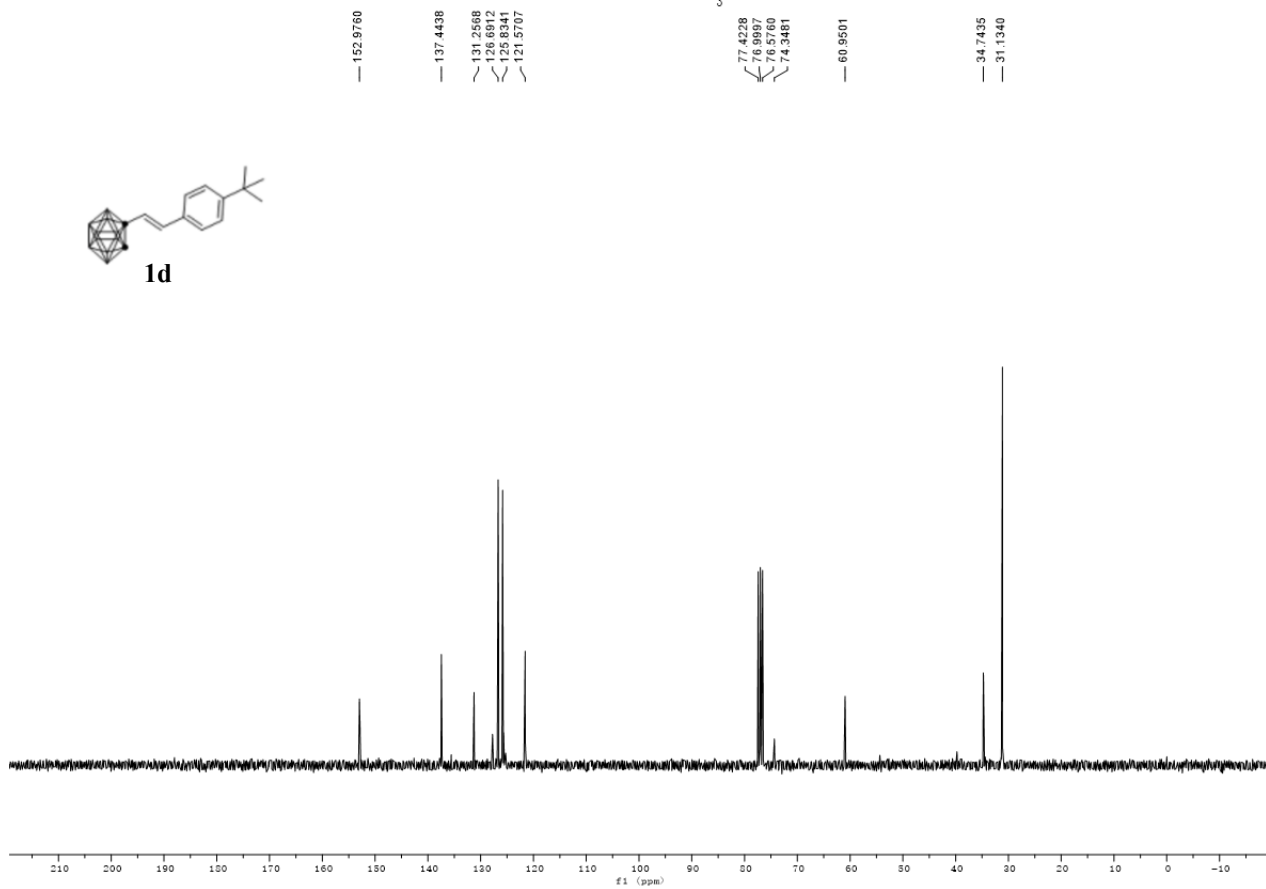


LHN-4-32 1H NMR in CDCl₃ 300M

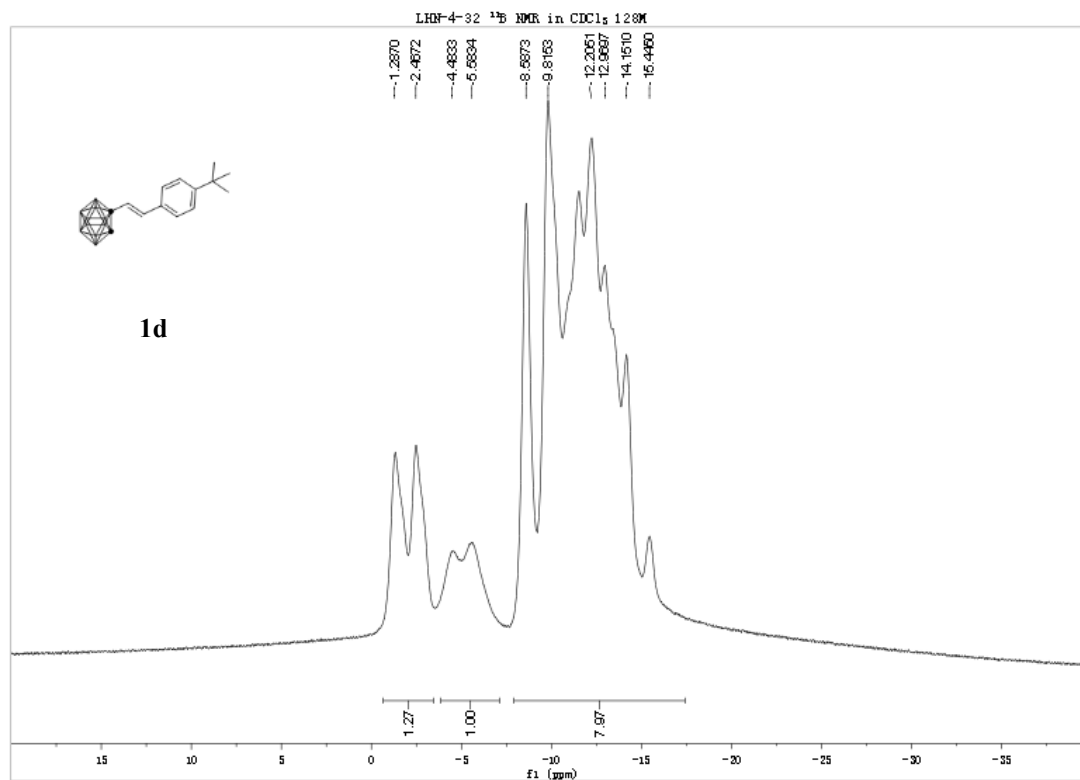


1d

LHN-4-32 13C NMR in CDCl₃ 75M

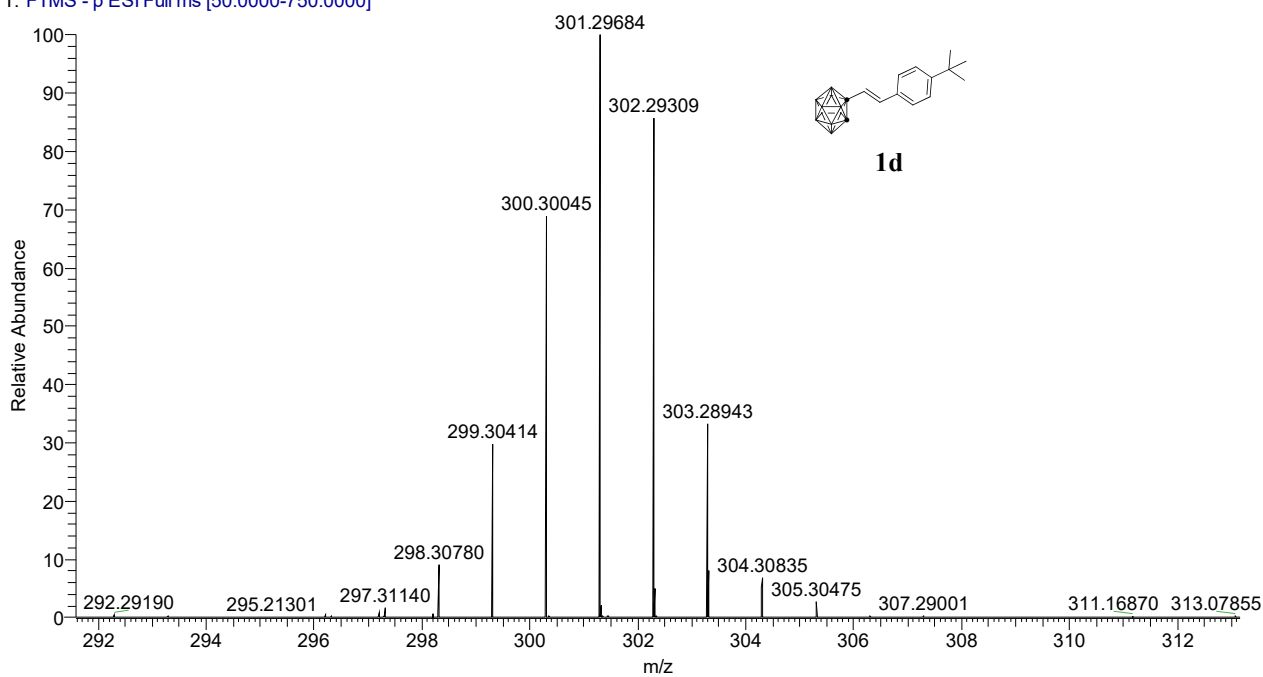


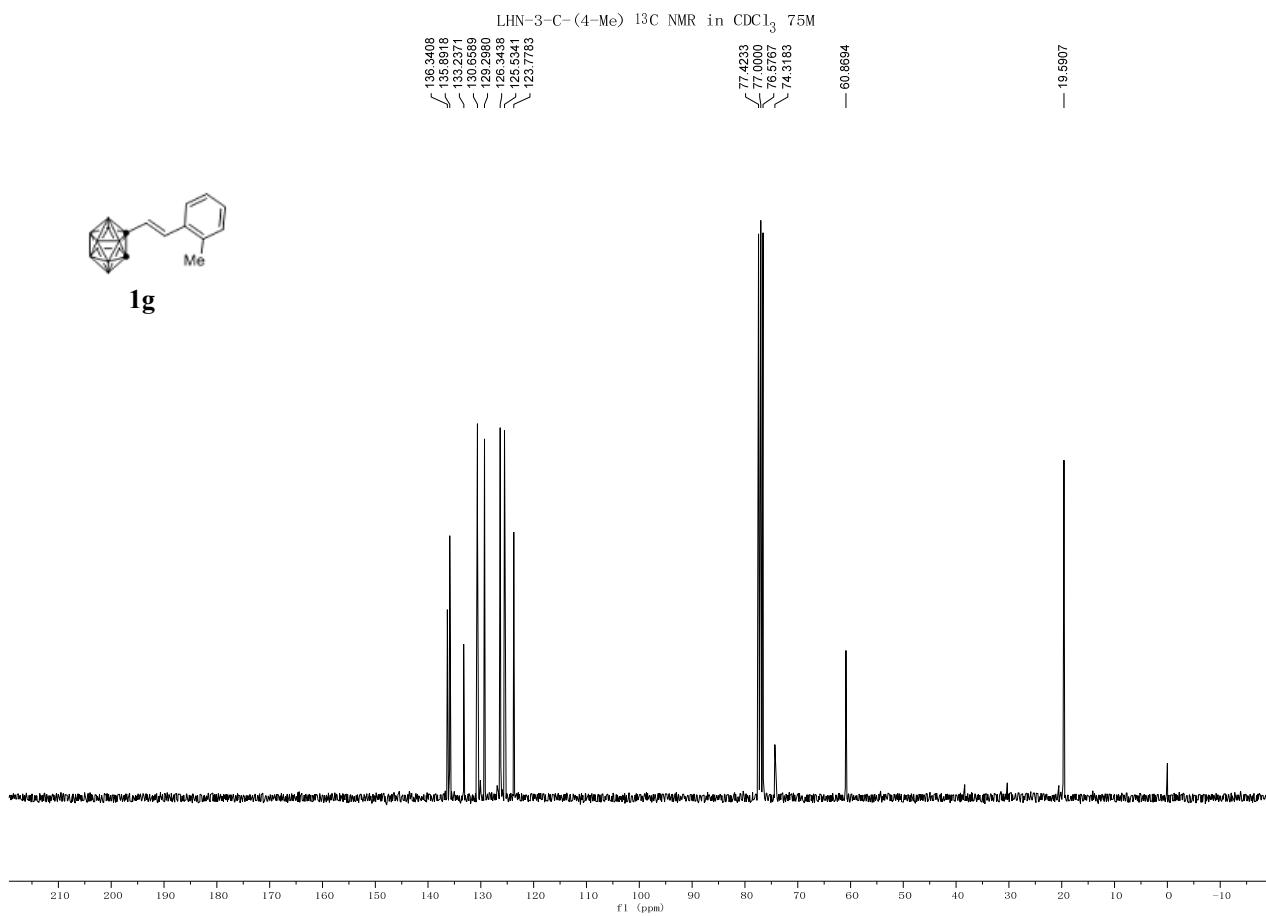
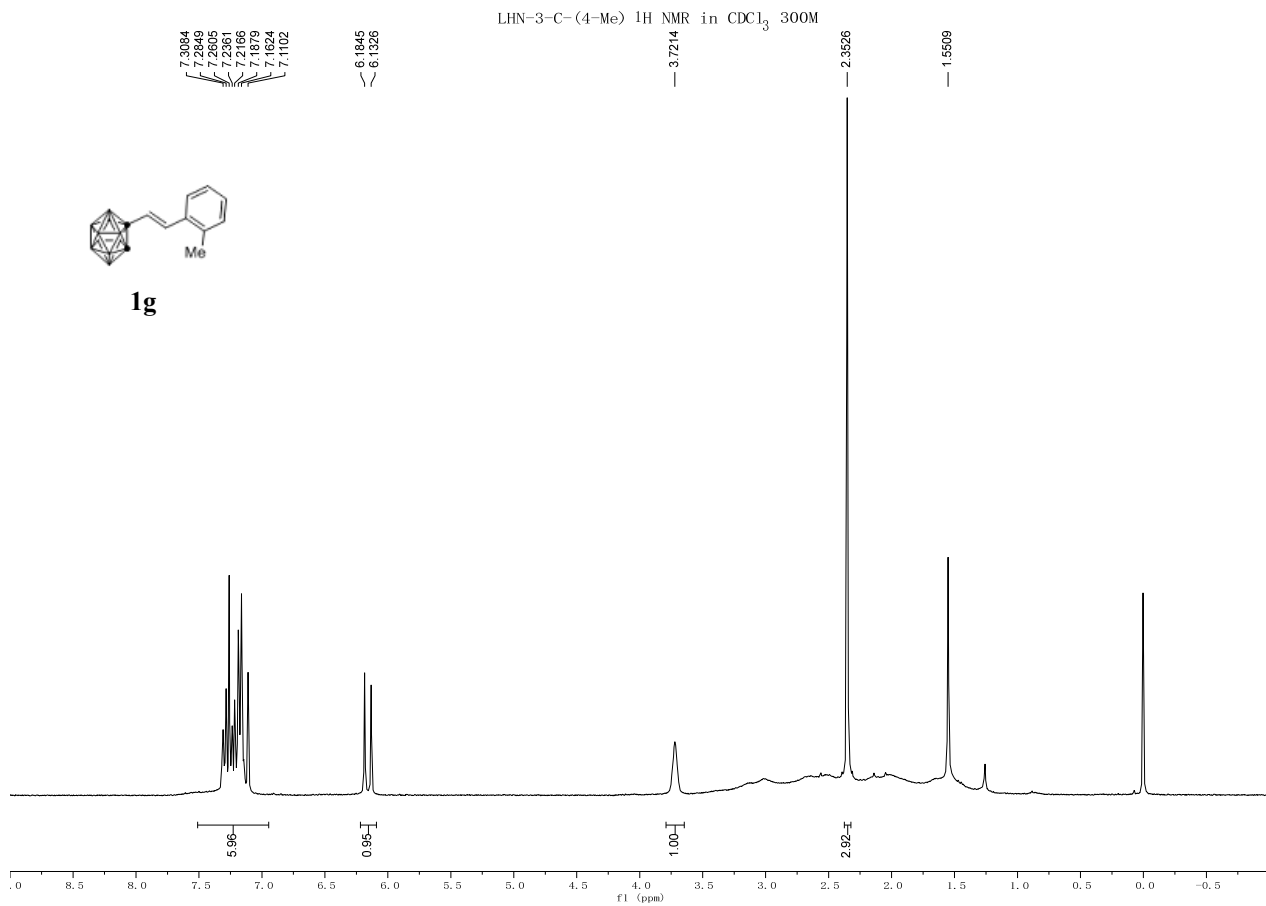
1d

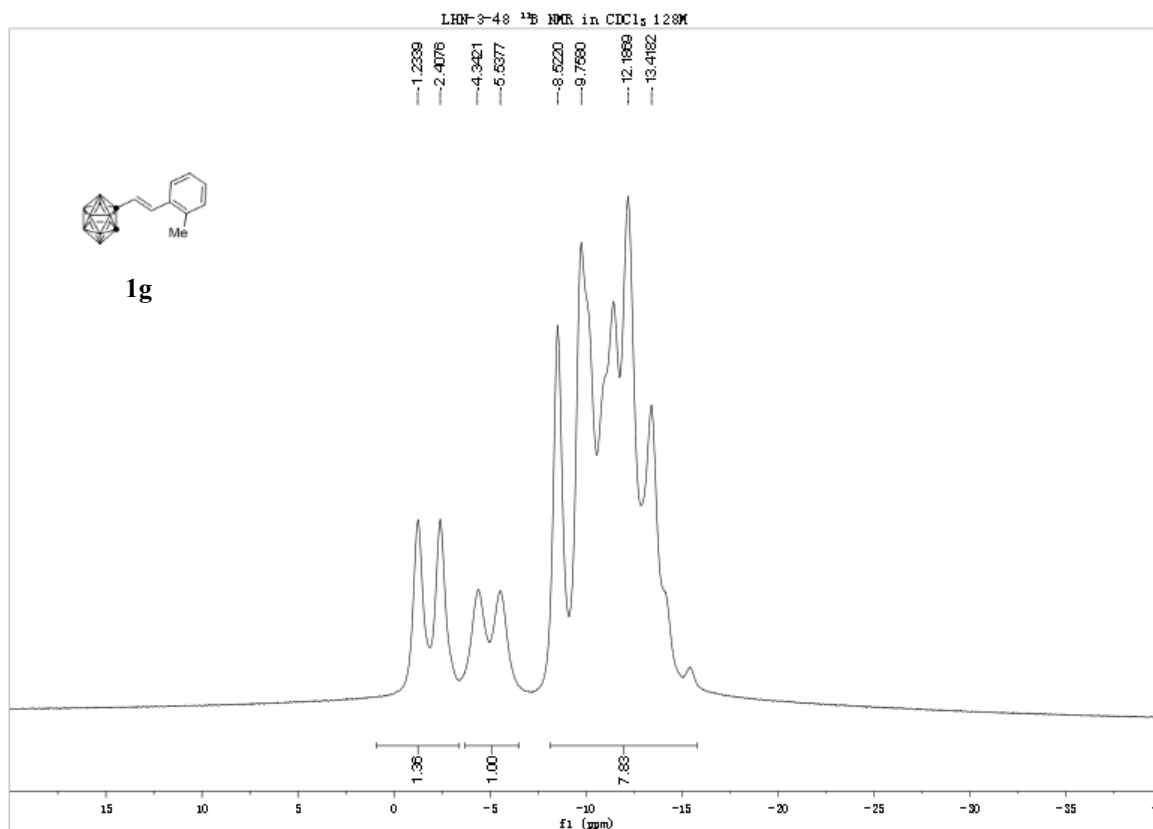


LHN-4-32. HRMS (ESI) m/z calcd for $C_{14}H_{25}B_{10}^-$ (M-H)⁻ 301.29649, found 301.29684.

LHN-4-32 #8 RT: 0.09 AV: 1 NL: 1.40E7
T: FTMS - p ESI Full ms [50.0000-750.0000]

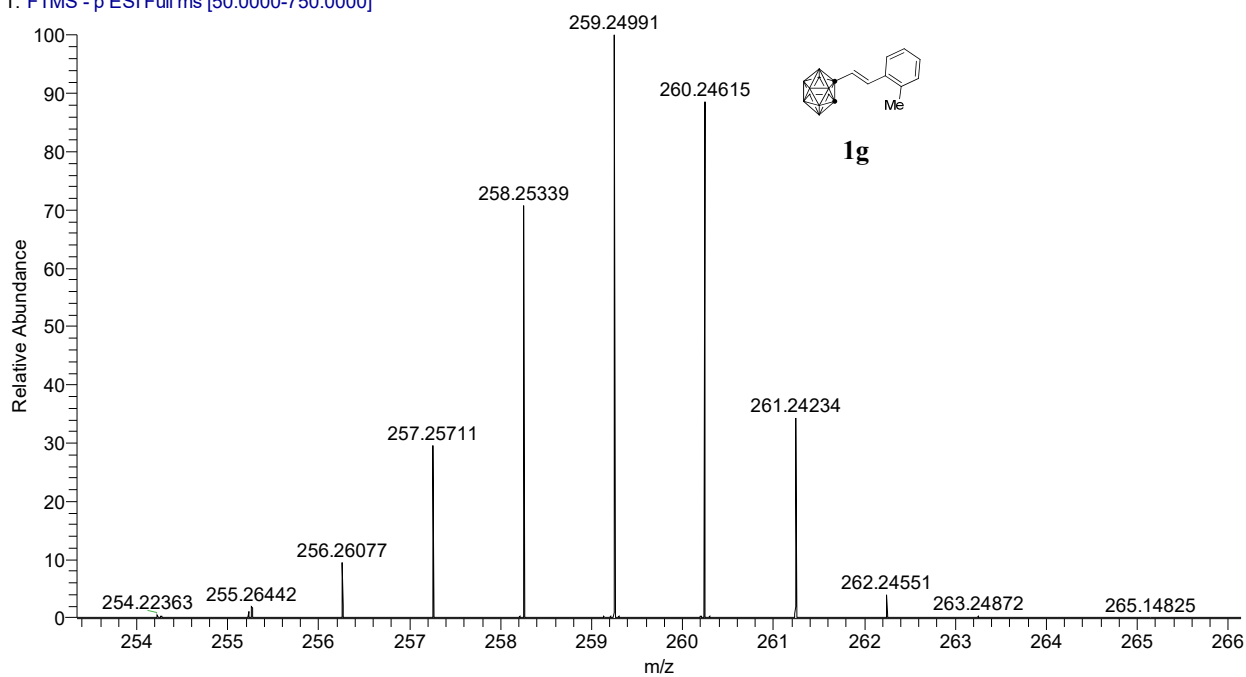


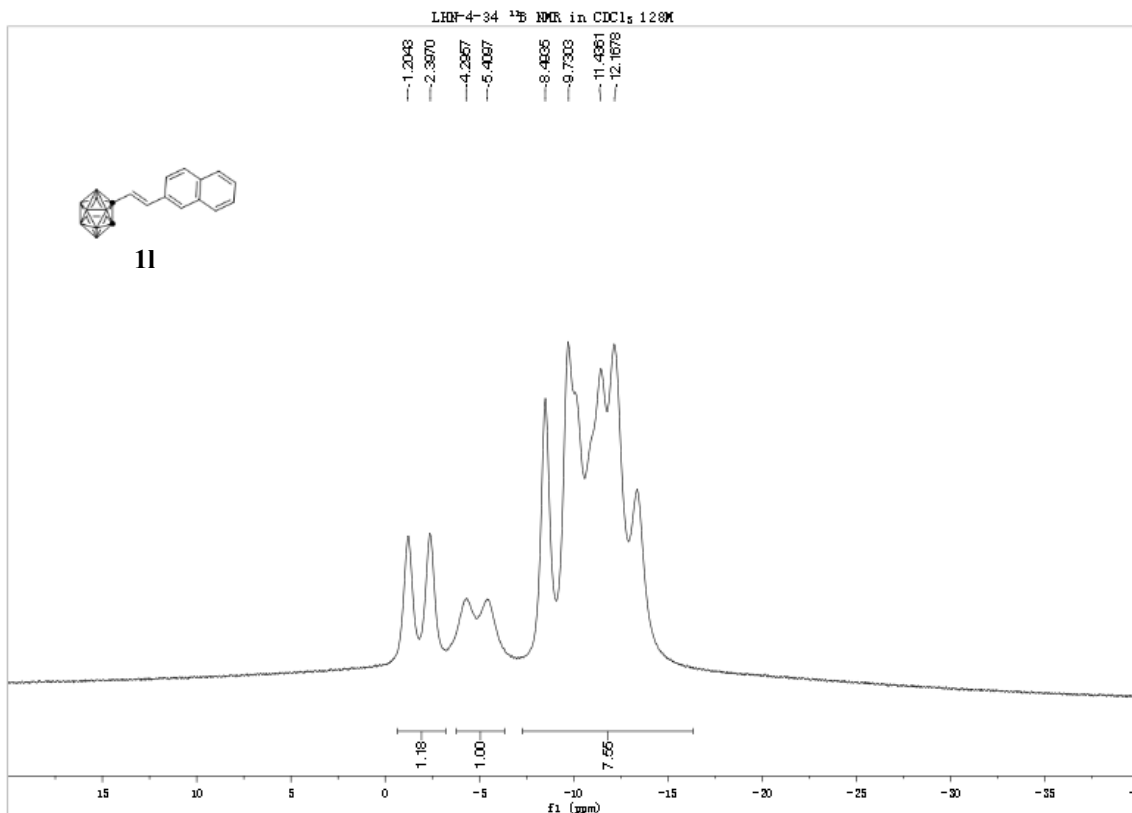




LHN-3-48. HRMS (ESI) m/z calcd for C₁₁H₁₉B₁₀⁻ (M-H)⁻ 260.24591, found 260.24615.

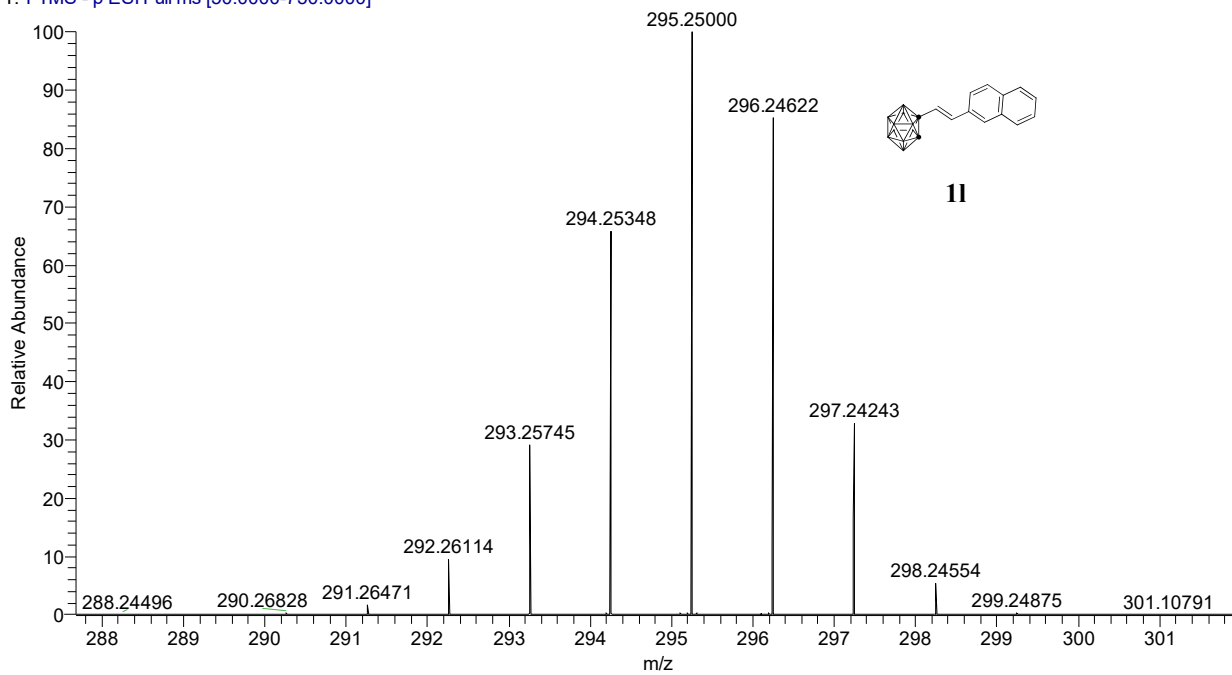
LHN-3-48 #8 RT: 0.09 AV: 1 NL: 2.95E7
T: FTMS - p ESI Full ms [50.0000-750.0000]





LHN-4-34. HRMS (ESI) m/z calcd for $\text{C}_{14}\text{H}_{19}\text{B}_{10}^-$ (M-H) $^-$ 296.24591, found 296.24622.

LHN-4-34 #8 RT: 0.09 AV: 1 NL: 1.96E7
T: FTMS - p ESI Full ms [50.0000-750.0000]



7.4279
7.4196
7.3899
7.3740
7.3488
7.3228
7.2605

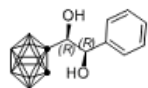
LHN-2-59A 1H NMR in CDCl₃ 300M

4.9998
4.8673

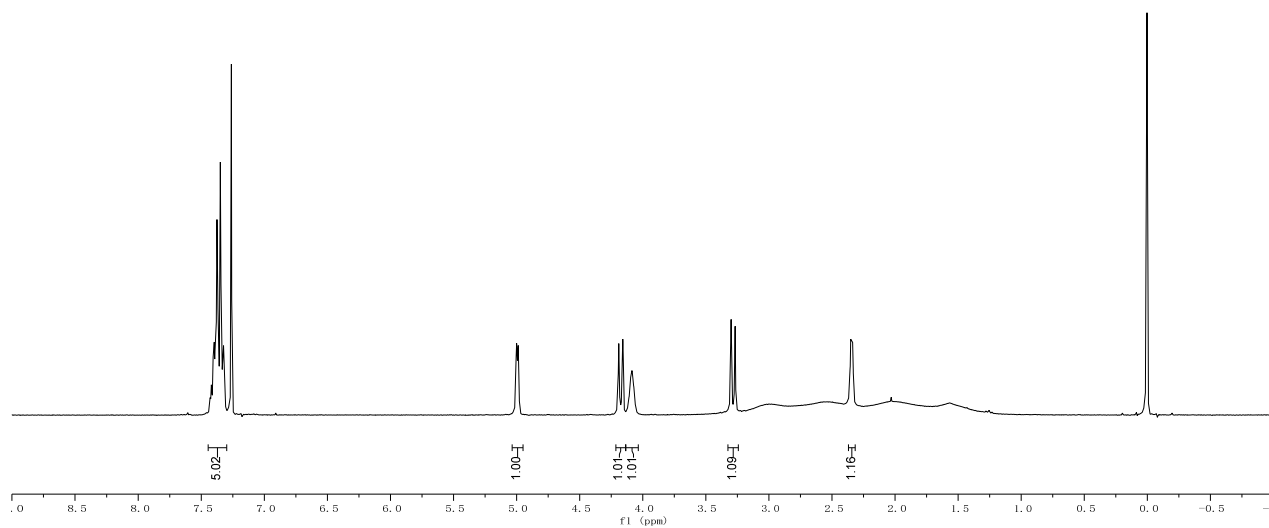
4.1869
4.1584
4.0862

3.2986
3.2680

2.3510
2.3366



2a



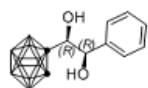
LHN-2-59A 13C NMR in CDCl₃ 75M

140.1676

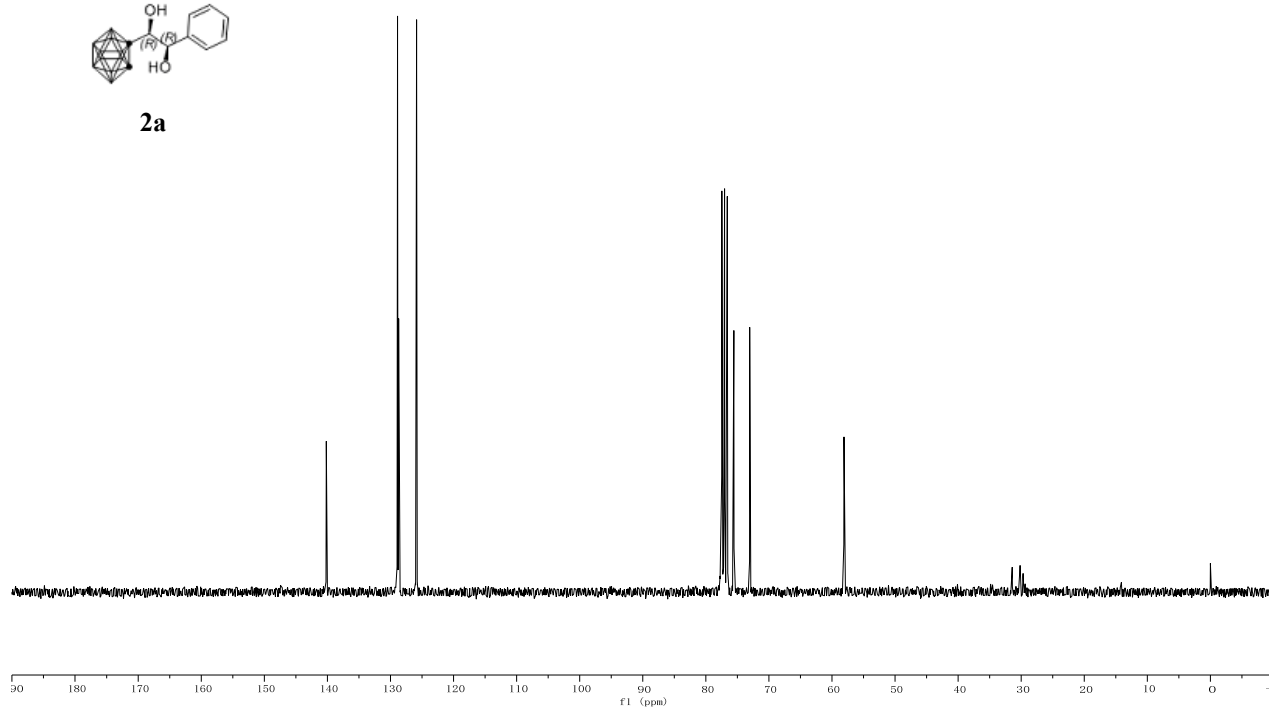
128.8702
128.8500
125.8459

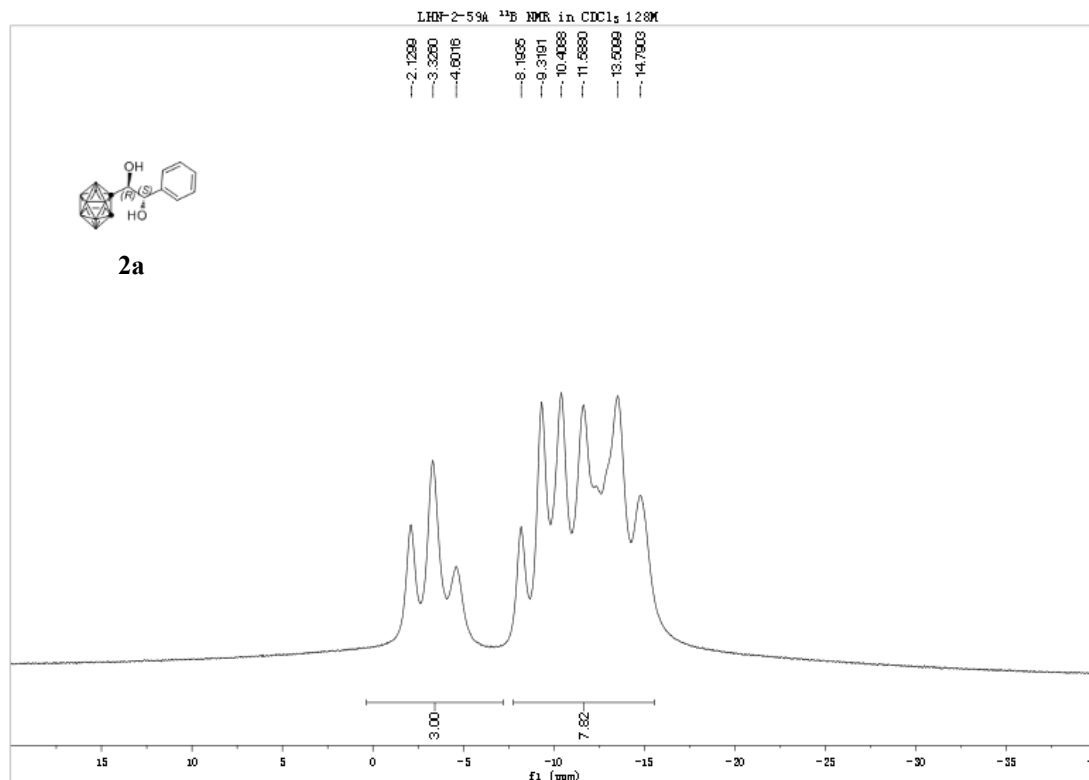
77.6414
77.4475
77.0242
76.6010
73.8508
73.0292

58.0830



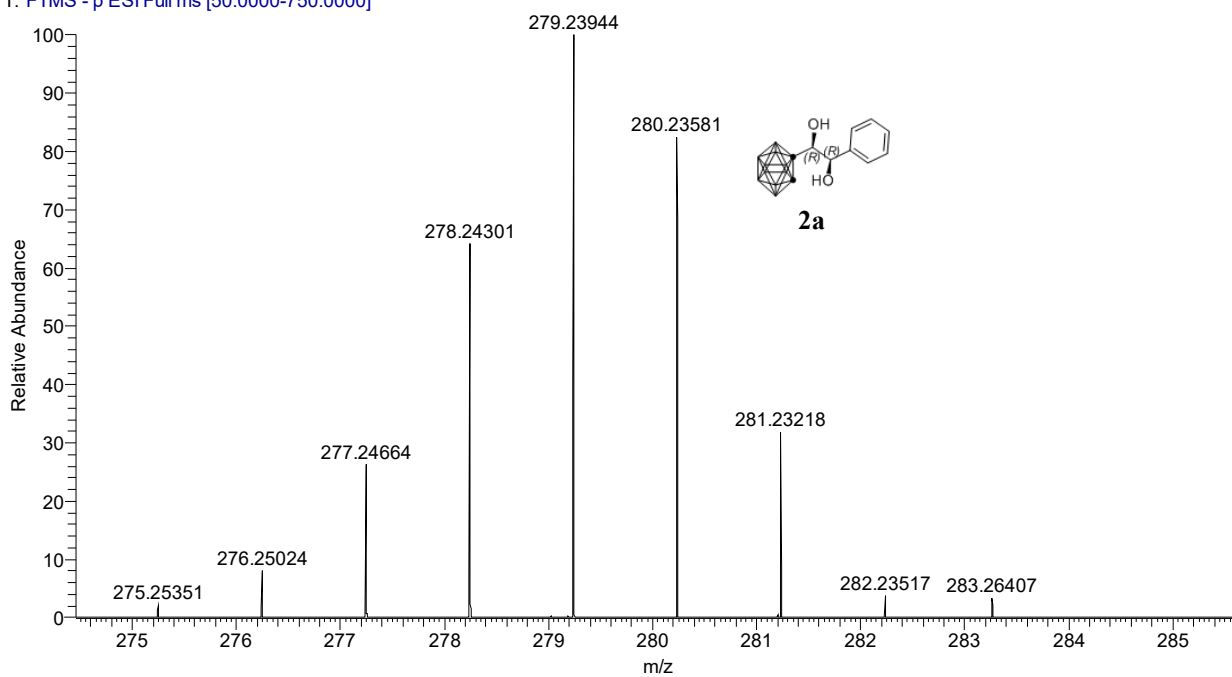
2a





LHN-2-59A. HRMS (ESI) m/z calcd for $C_{10}H_{19}B_{10}O_2^-$ (M-H)⁻ 280.23574, found 280.23581.

LHN-2-59A #8 RT: 0.09 AV: 1 NL: 1.68E6
T: FTMS - p ESI Full ms [50.0000-750.0000]



LHN-3-48H 1H NMR in CDCl₃ 300M

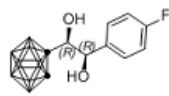
7.3398
7.3320
7.3114
7.2937
7.2696
7.1996
7.0721
7.0434

4.9728

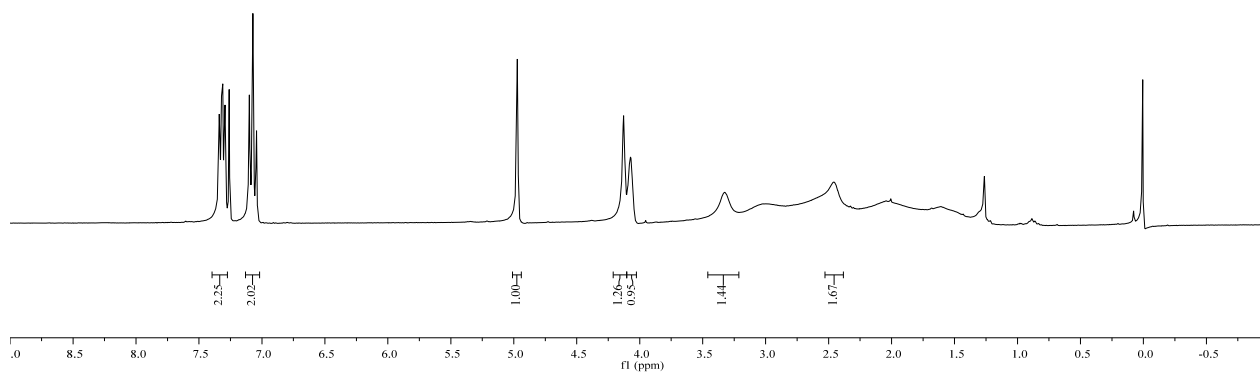
4.1277
4.0730

3.3387

2.4875



2b



LHN-3-48H ¹³C NMR in CDCl₃ 75M

164.3502
161.0671

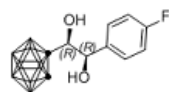
135.9224
135.8798

127.7614
127.6518

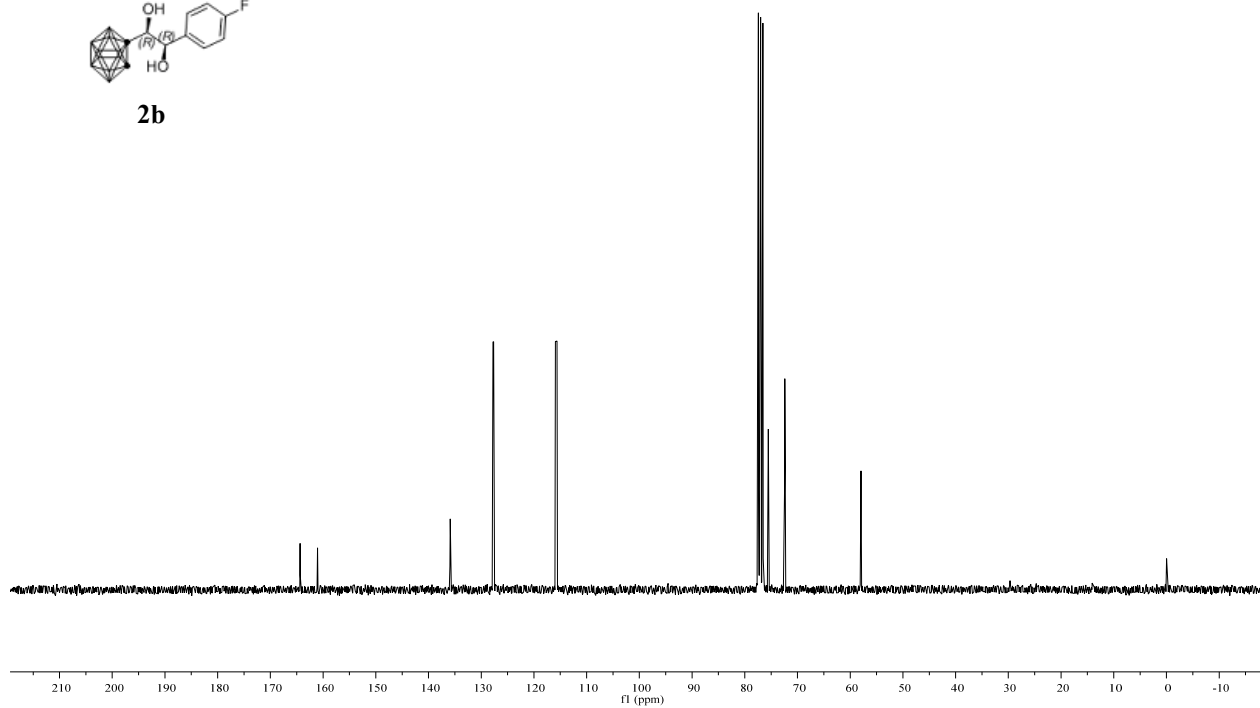
115.9148
115.6278

77.4233
76.9995
76.5762
75.5213
74.4014

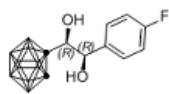
57.9655



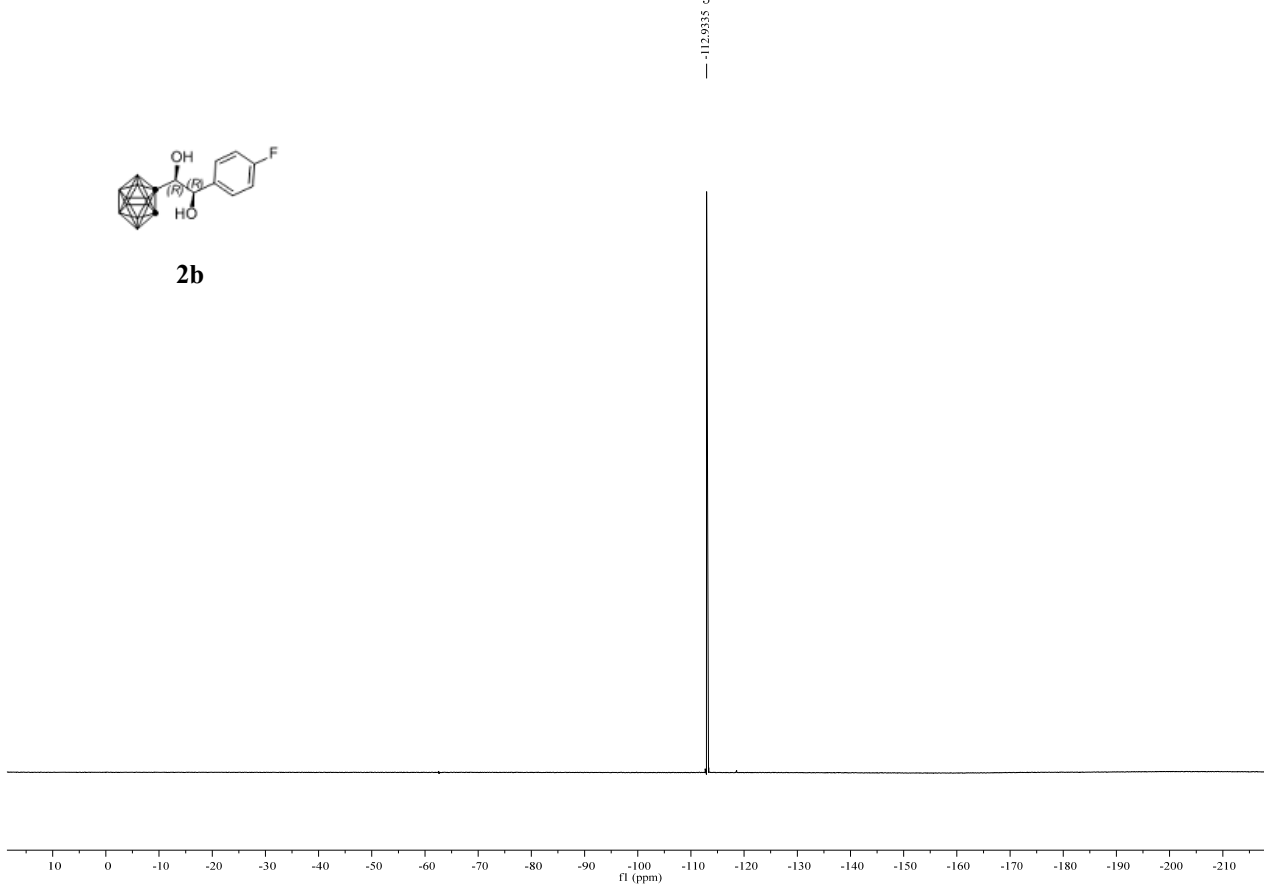
2b



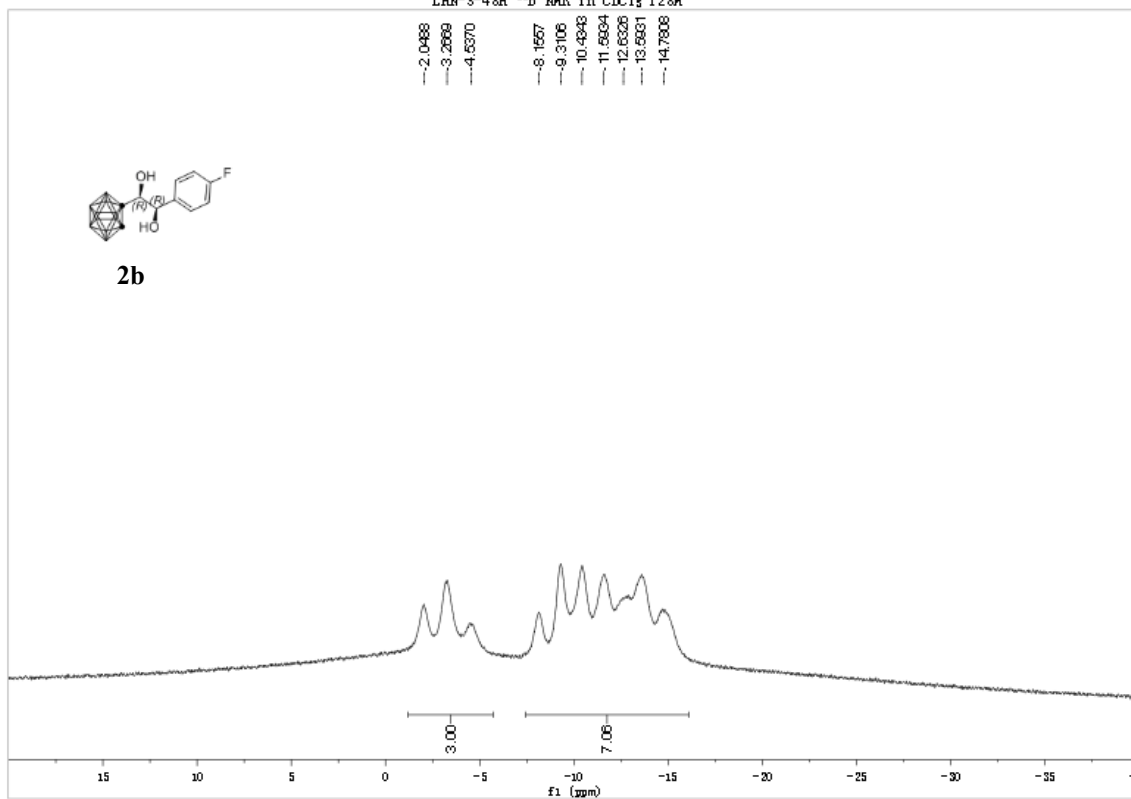
LHN-3-48H 19F NMR in CDCl₃ 376M



2b

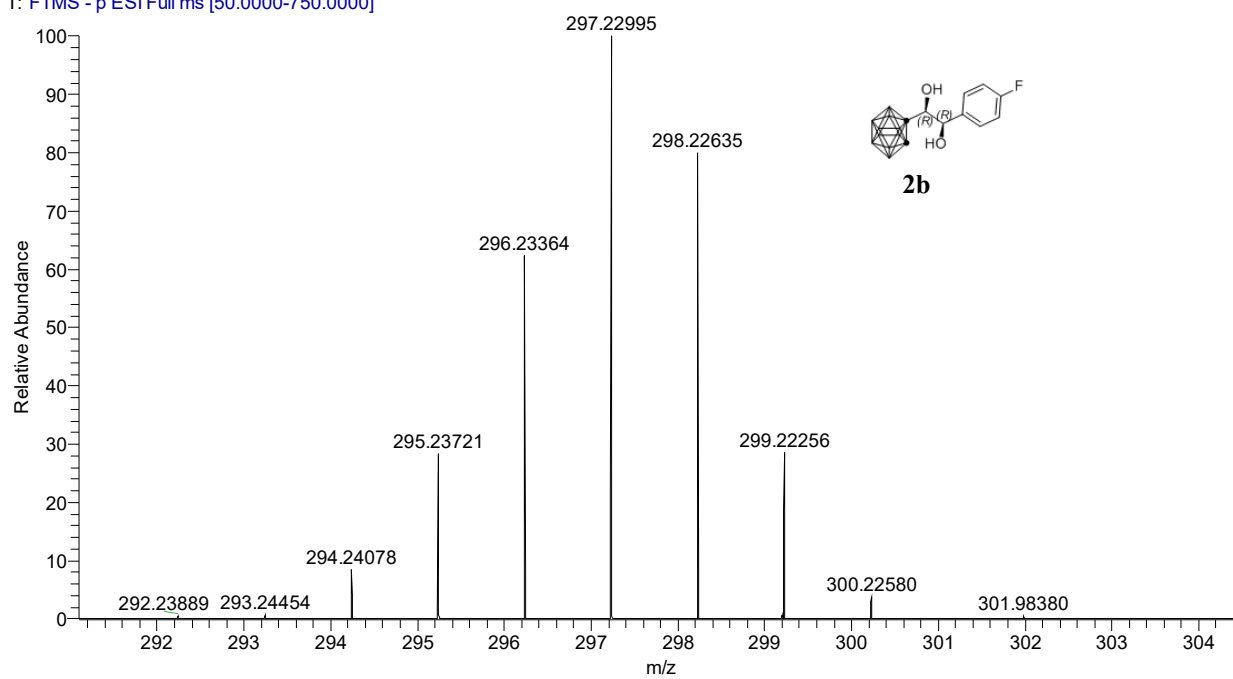


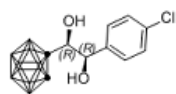
LHN-3-48H ¹³C NMR in CDCl₃ 128M



LHN-3-48H. HRMS (ESI) m/z calcd for $C_{10}H_{18}B_{10}FO_2^-$ (M-H) $^-$ 298.22632, found 298.22635.

LHN-3-48H #8 RT: 0.09 AV: 1 NL: 1.57E6
T: FTMS - p ESI Full ms [50.0000-750.0000]





2c

7.3770
7.3489
7.2918
7.2597

LHN-4-44 ¹H NMR in CDCl₃ 300M

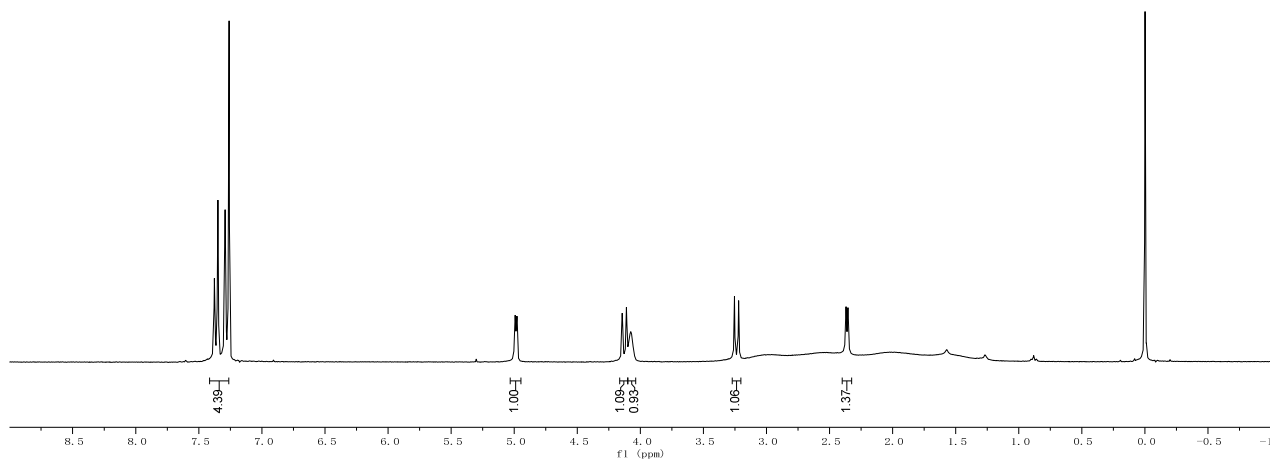
4.9923
4.9782

4.1430
4.1103
4.0755

3.2538
3.2210

2.3693
2.3537

— 1.5716

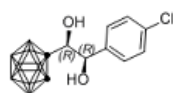


LHN-4-44 ¹³C NMR in CDCl₃ 75M

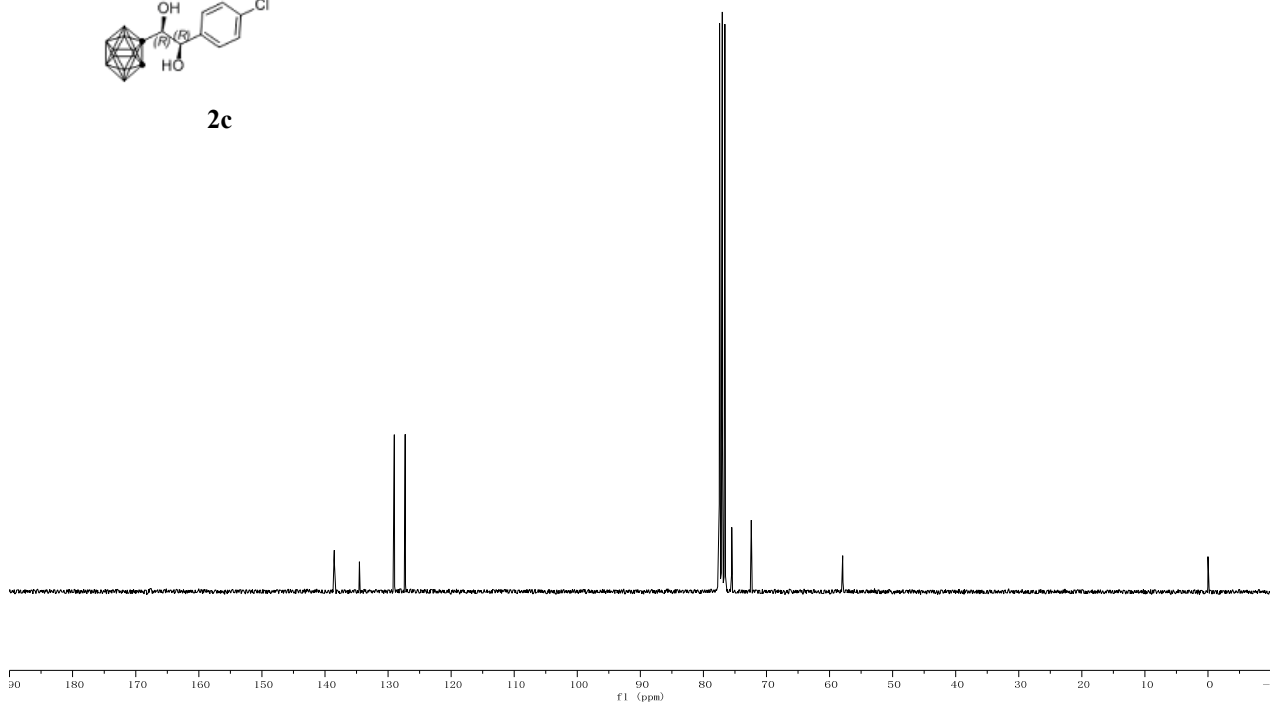
138.5151
134.5430
129.0116
127.2801

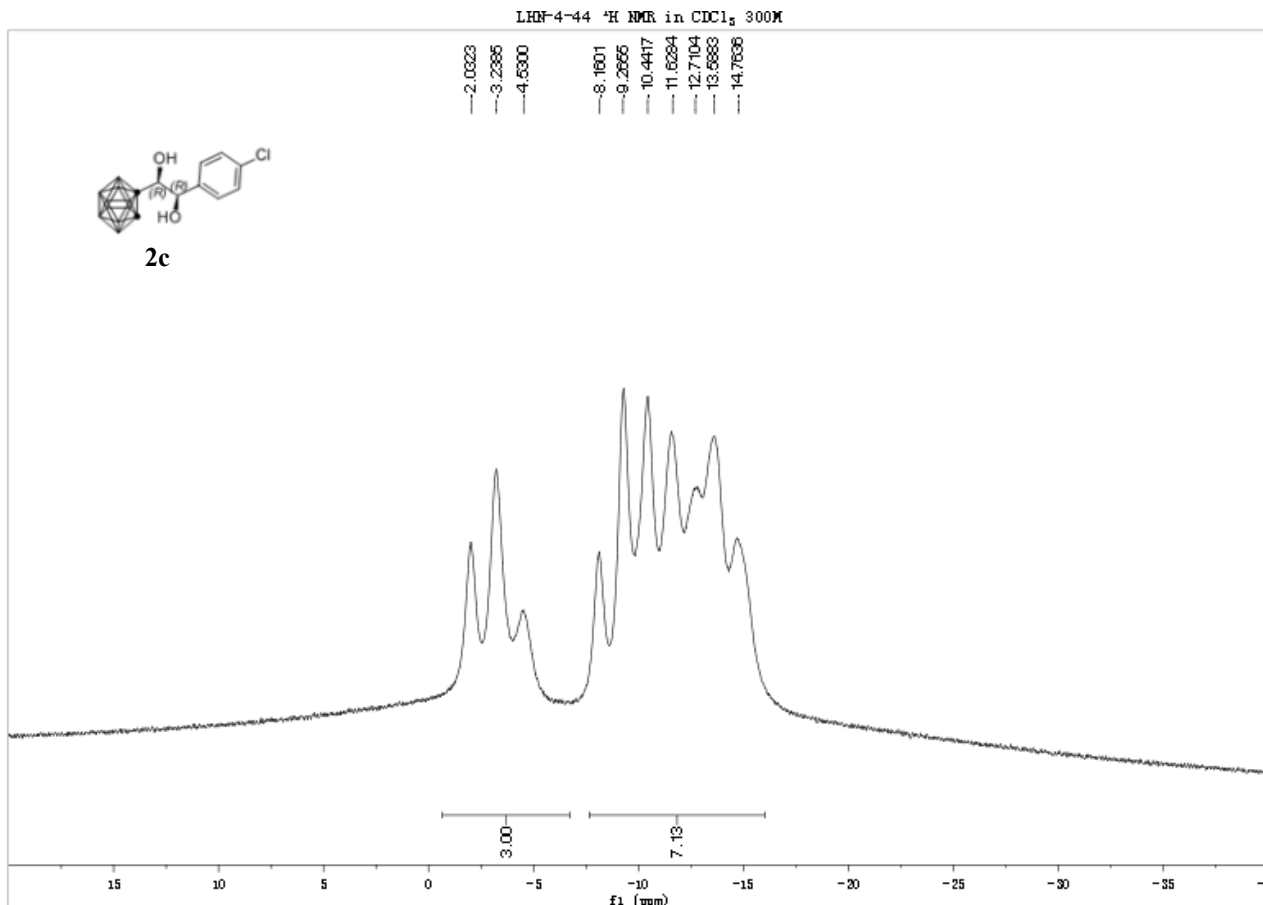
77.4356
77.0124
76.5891
75.5018
72.4042

— 57.9086



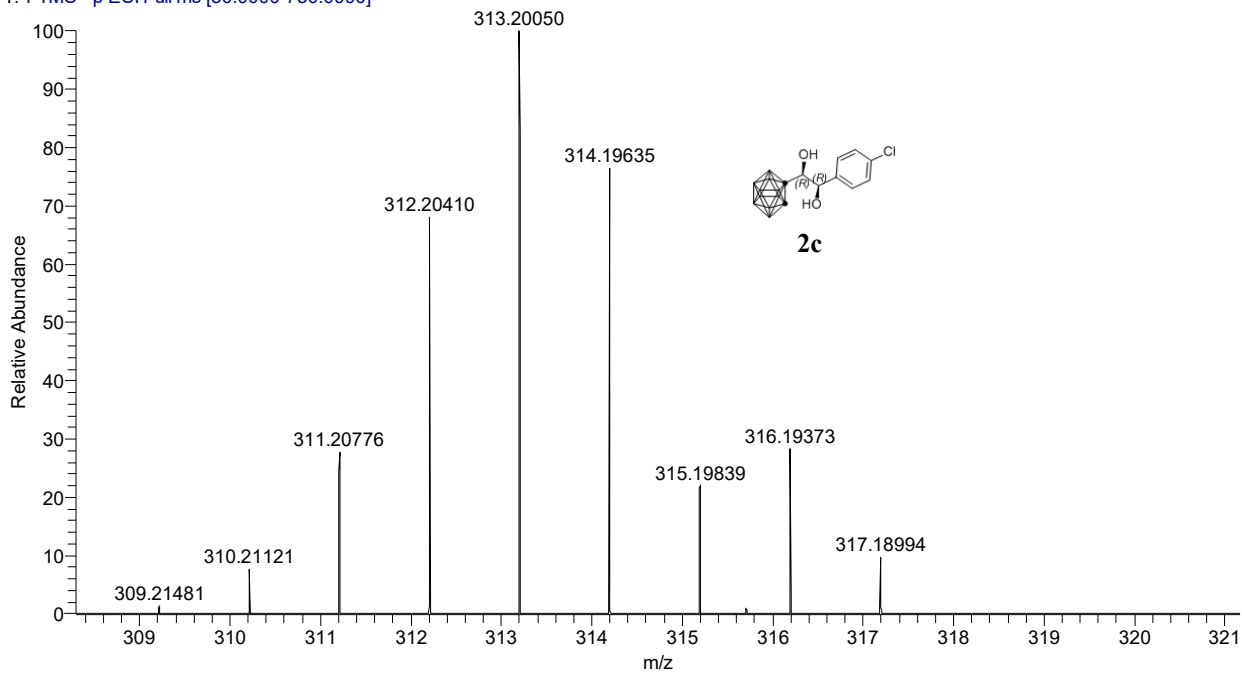
2c

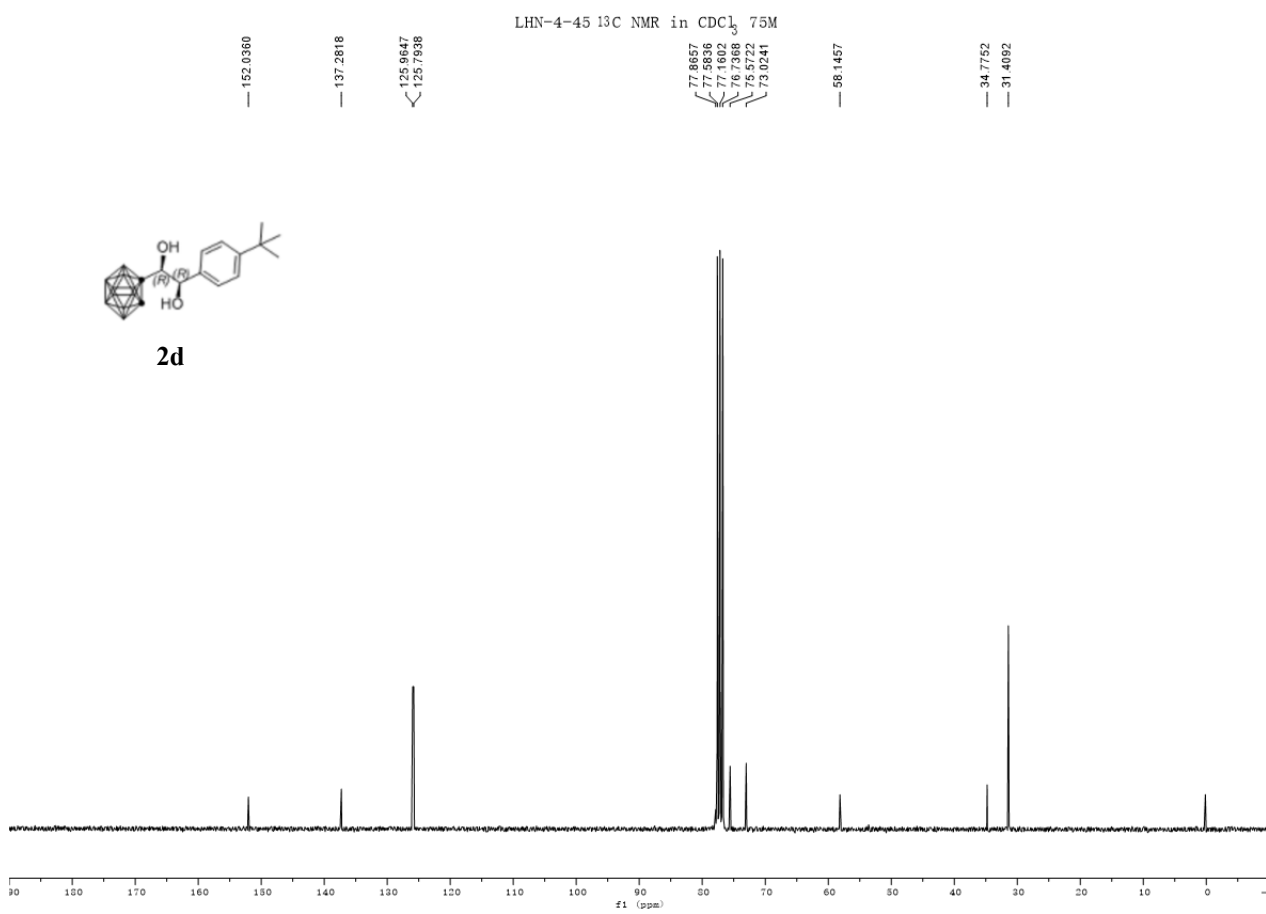
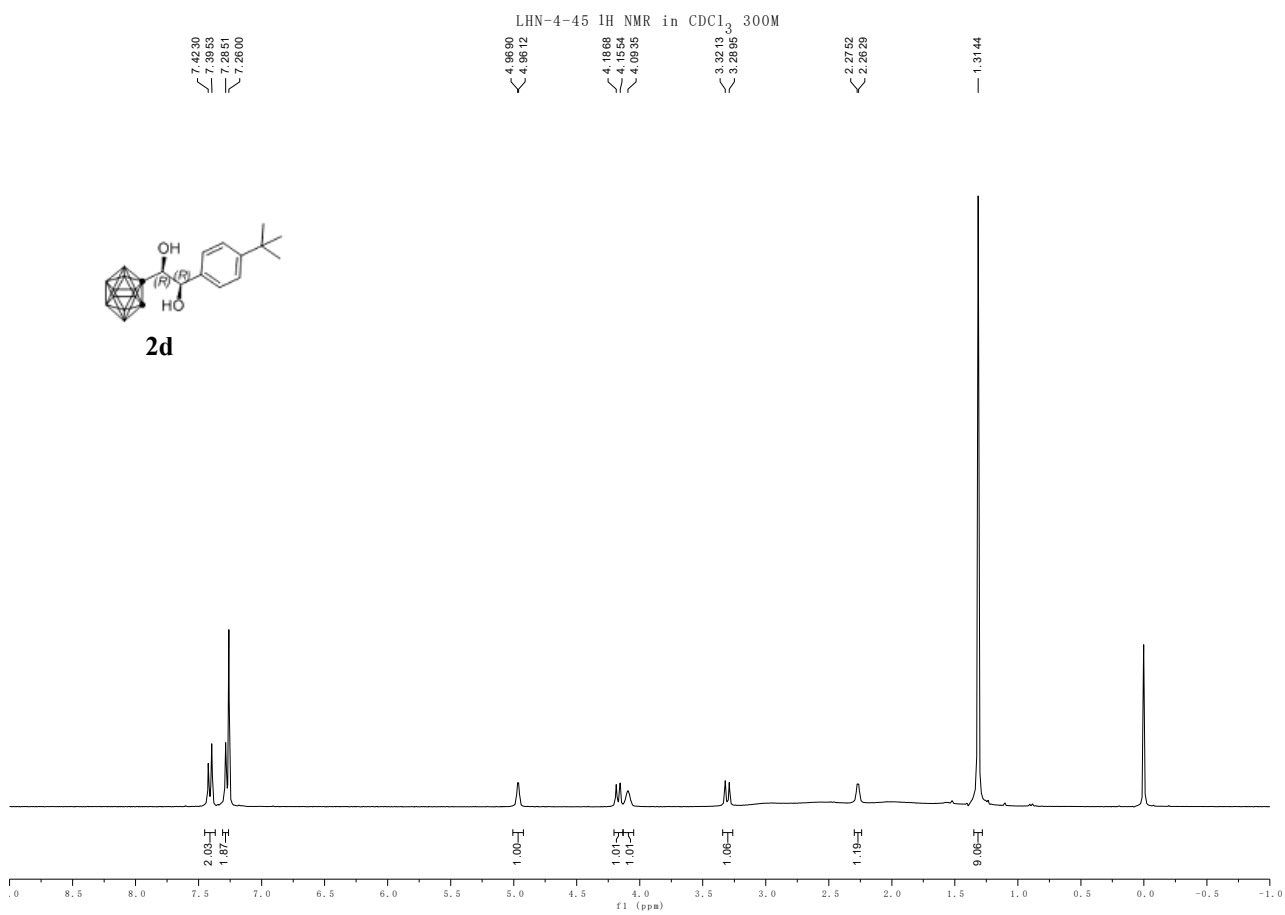


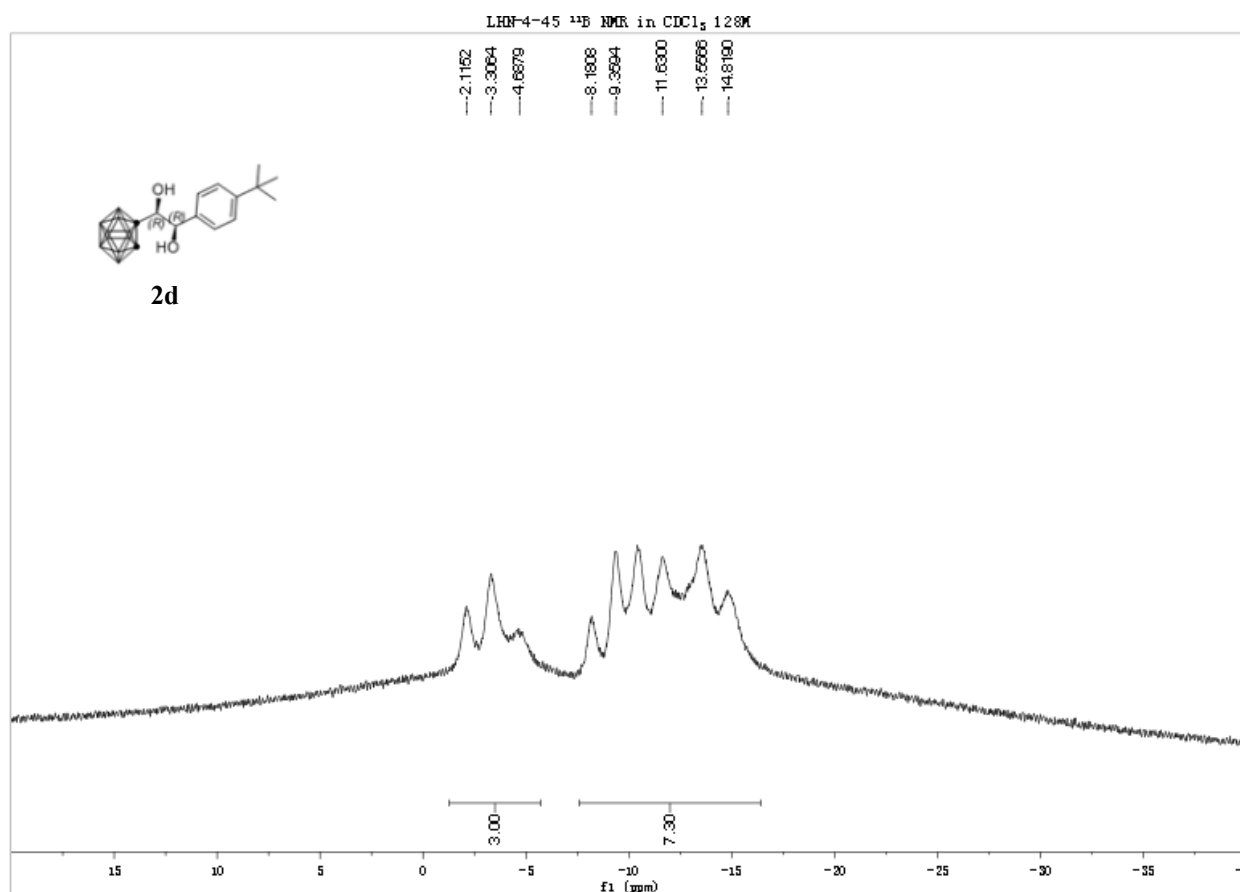


LHN-4-44. HRMS (ESI) m/z calcd for $\text{C}_{10}\text{H}_{18}\text{B}_{10}\text{ClO}_2^-$ (M-H)⁻ 313.20040, found 313.20050.

LHN-4-44 #8 RT: 0.09 AV: 1 NL: 5.86E5
 T: FTMS - p ESI Full ms [50.0000-750.0000]

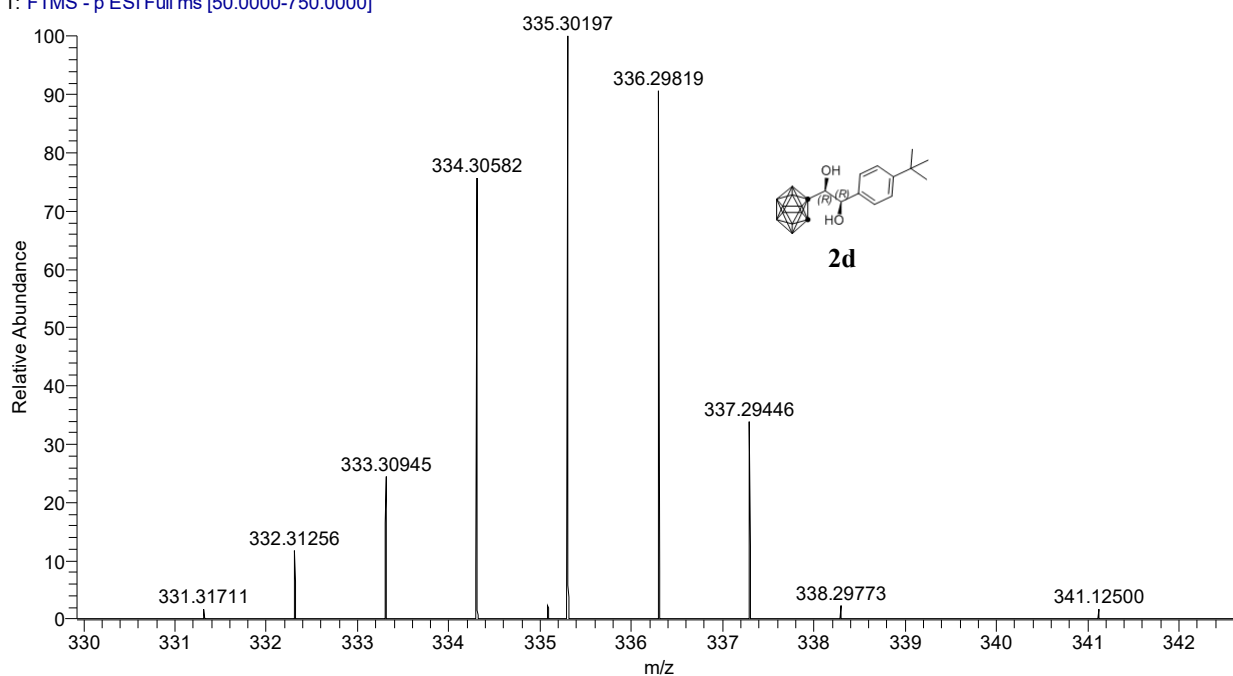






LHN-4-45. HRMS (ESI) m/z calcd for $C_{14}H_{27}B_{10}O_2^-$ (M-H)⁻ 336.29834, found 336.29819.

LHN-4-4S #8 RT: 0.09 AV: 1 NL: 3.09E5
T: FTMS - p ESI Full ms [50.0000-750.0000]



LHN-3-48A ¹H NMR in CDCl₃ 300M

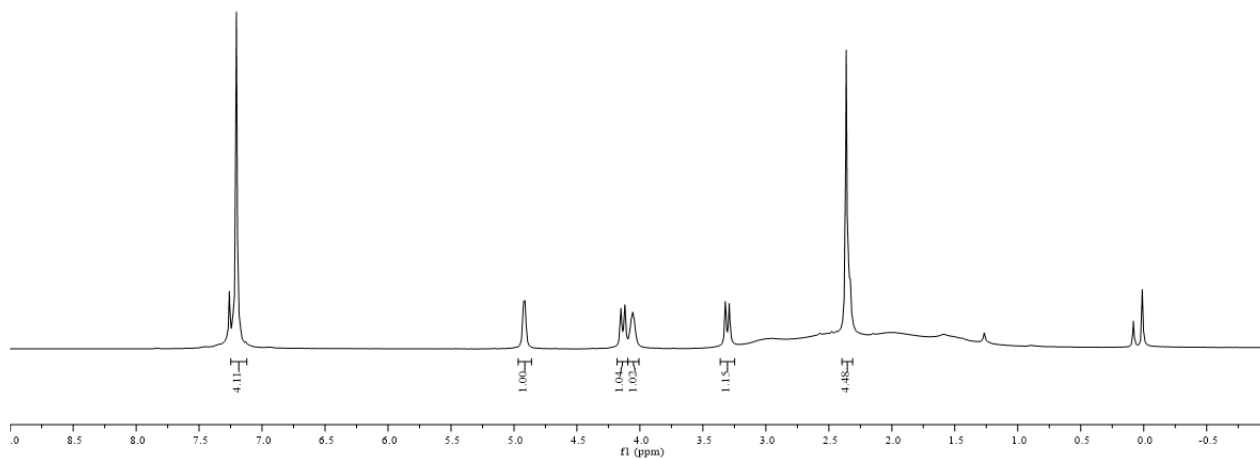
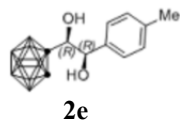
7.2605
7.2040

4.9245
4.9109

4.1510
4.1204
4.0573

3.3231
3.2811

2.3622
2.3441
2.3301



LHN-3-48A ¹³C NMR in CDCl₃ 75M

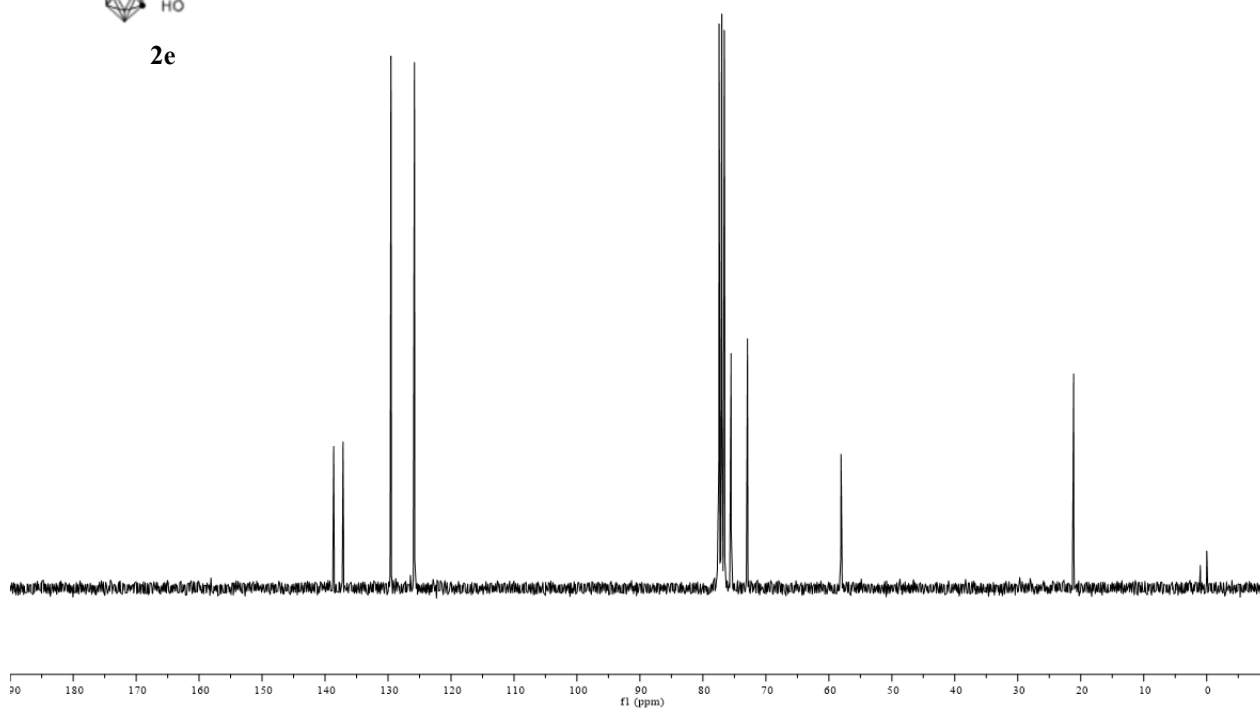
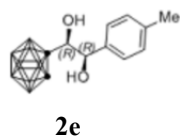
138.6362
137.1487

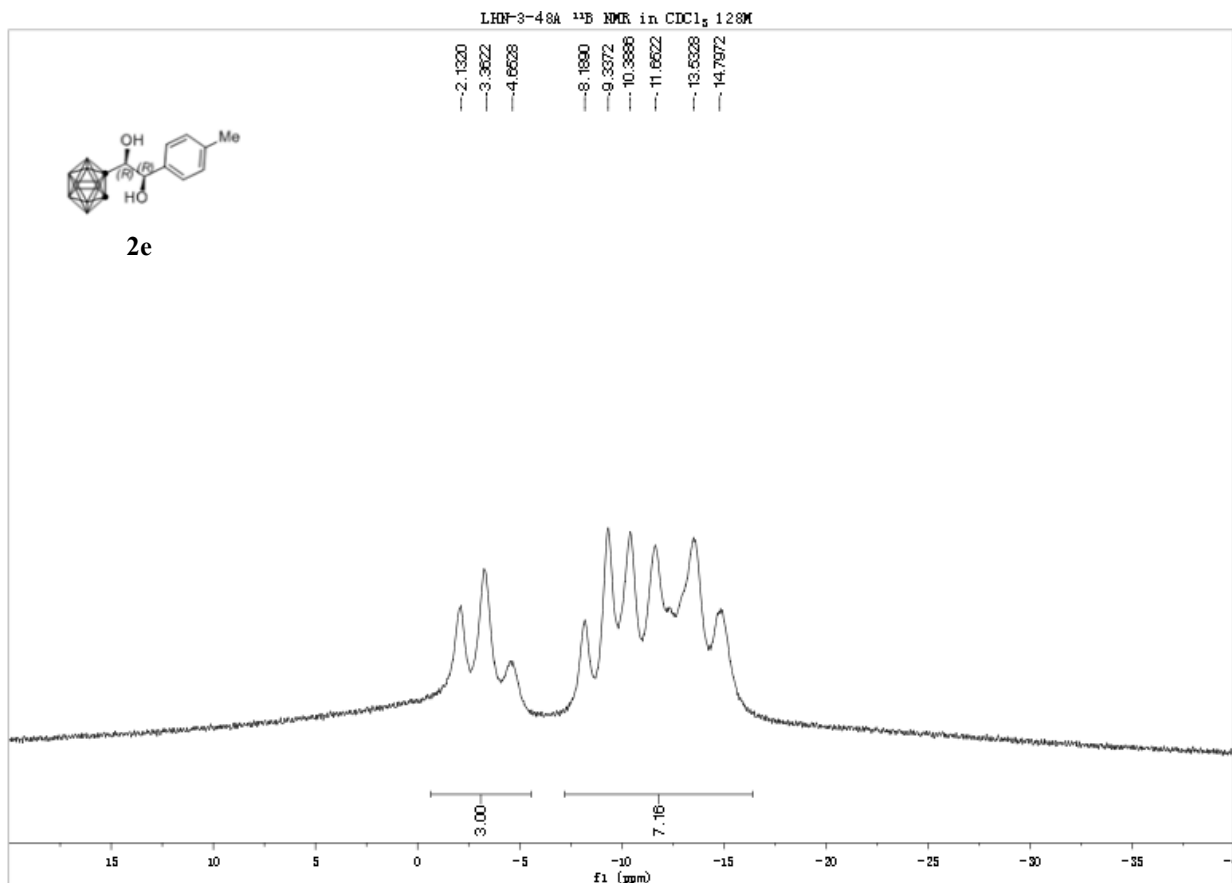
129.8222
125.7920

77.6287
77.4234
76.9999
76.5766
76.1533
75.9223

58.0571

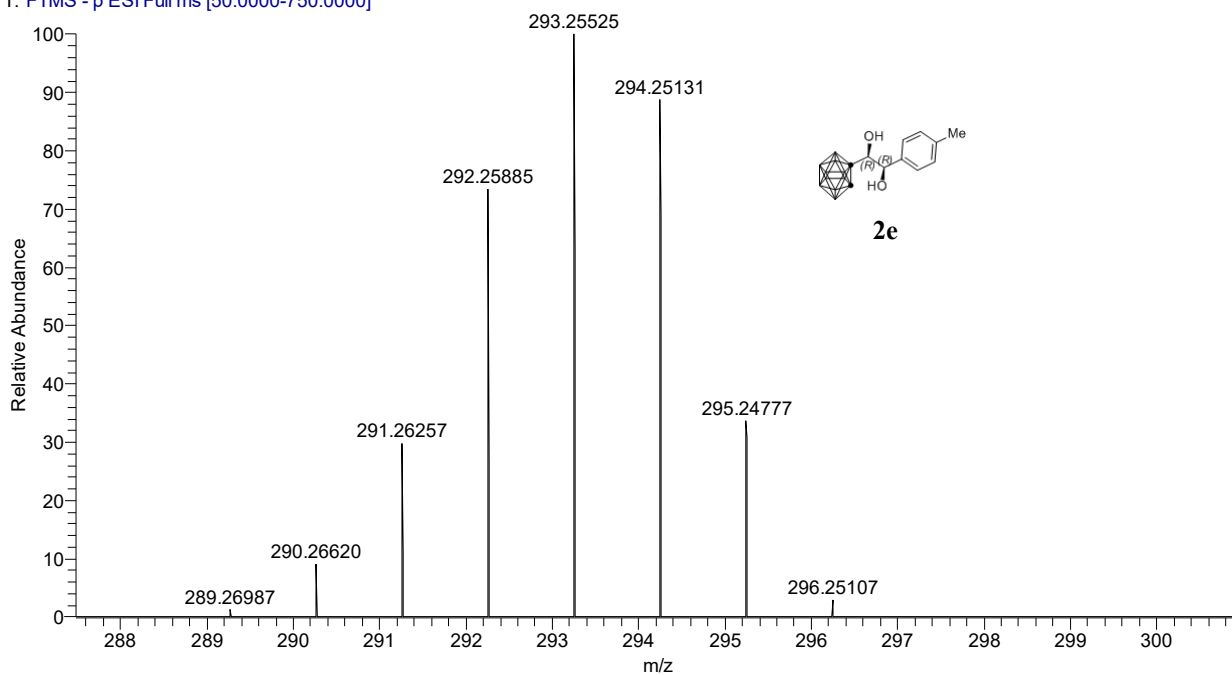
21.1290





LHN-3-48A. HRMS (ESI) m/z calcd for $\text{C}_{11}\text{H}_{21}\text{B}_{10}\text{O}_2^-$ (M-H) $^-$ 294.25139, found 294.25131.

LHN-3-48A #8 RT: 0.09 AV: 1 NL: 8.64E5
T: FTMS - p ESI Full ms [50.0000-750.0000]



LHN-3-48B ¹H NMR in CDCl₃ 300M

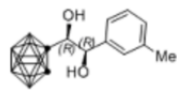
7.2644
7.2588
7.2312
7.1554
7.1293
7.1071
7.0821

4.9075

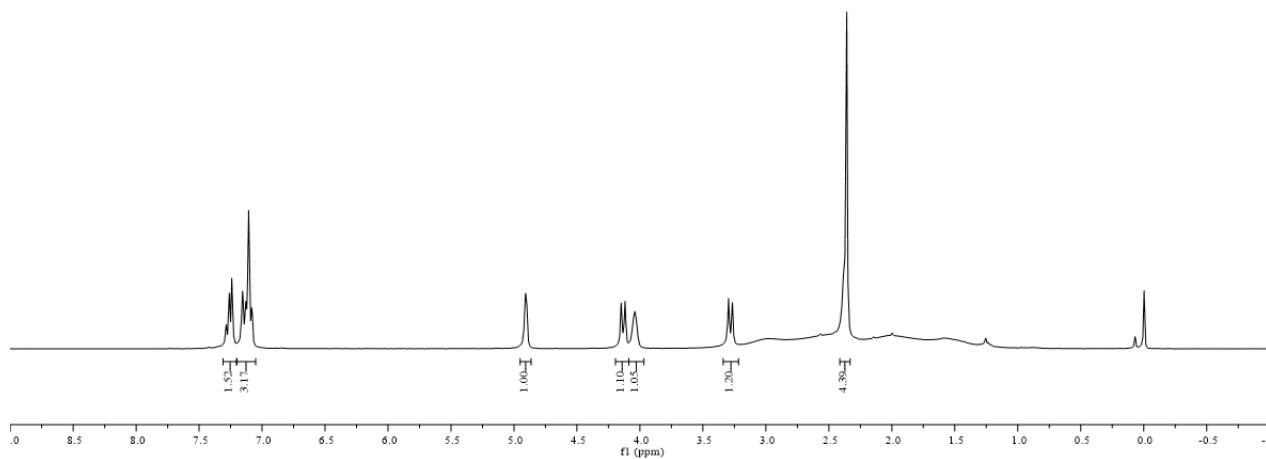
4.1487
4.1182
4.0468

3.2666
3.2653

2.3827
2.3882



2f



LHN-3-48B ¹³C NMR in CDCl₃ 75M

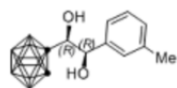
140.0967
138.6969

129.4264
128.7678
128.4473
122.8327

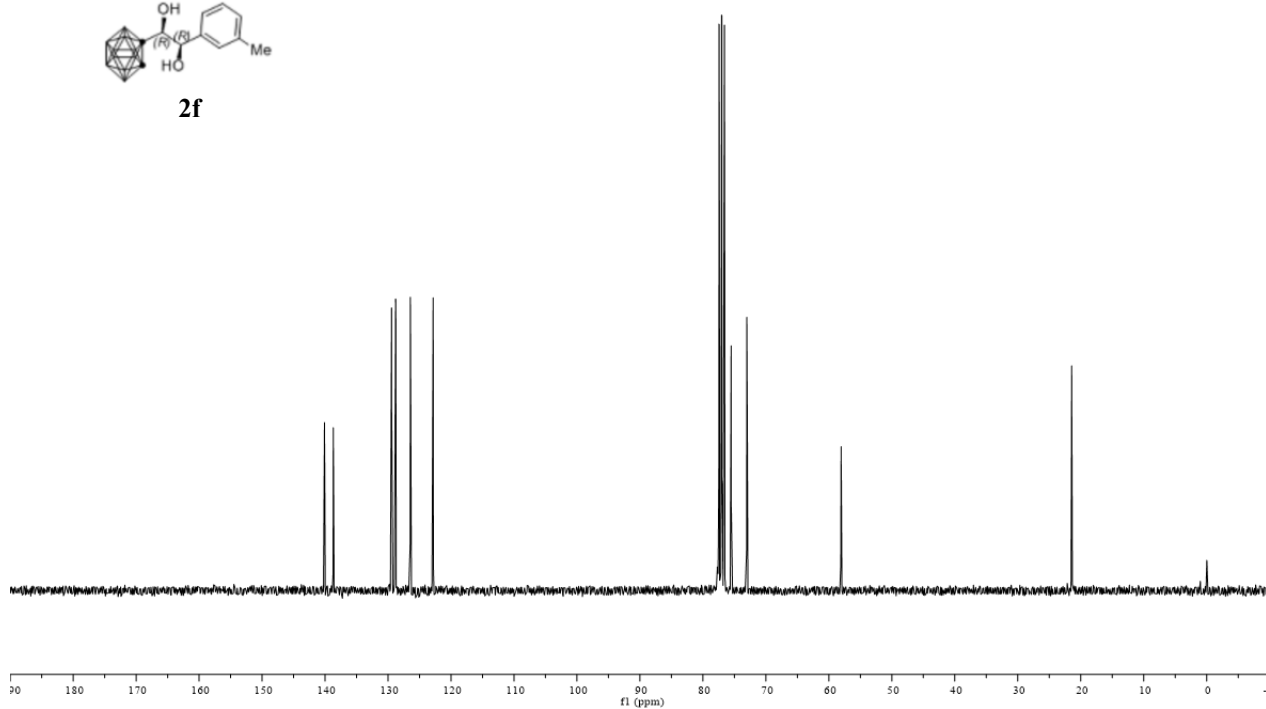
77.6565
77.4236
77.0002
76.5769
76.3416
73.0184

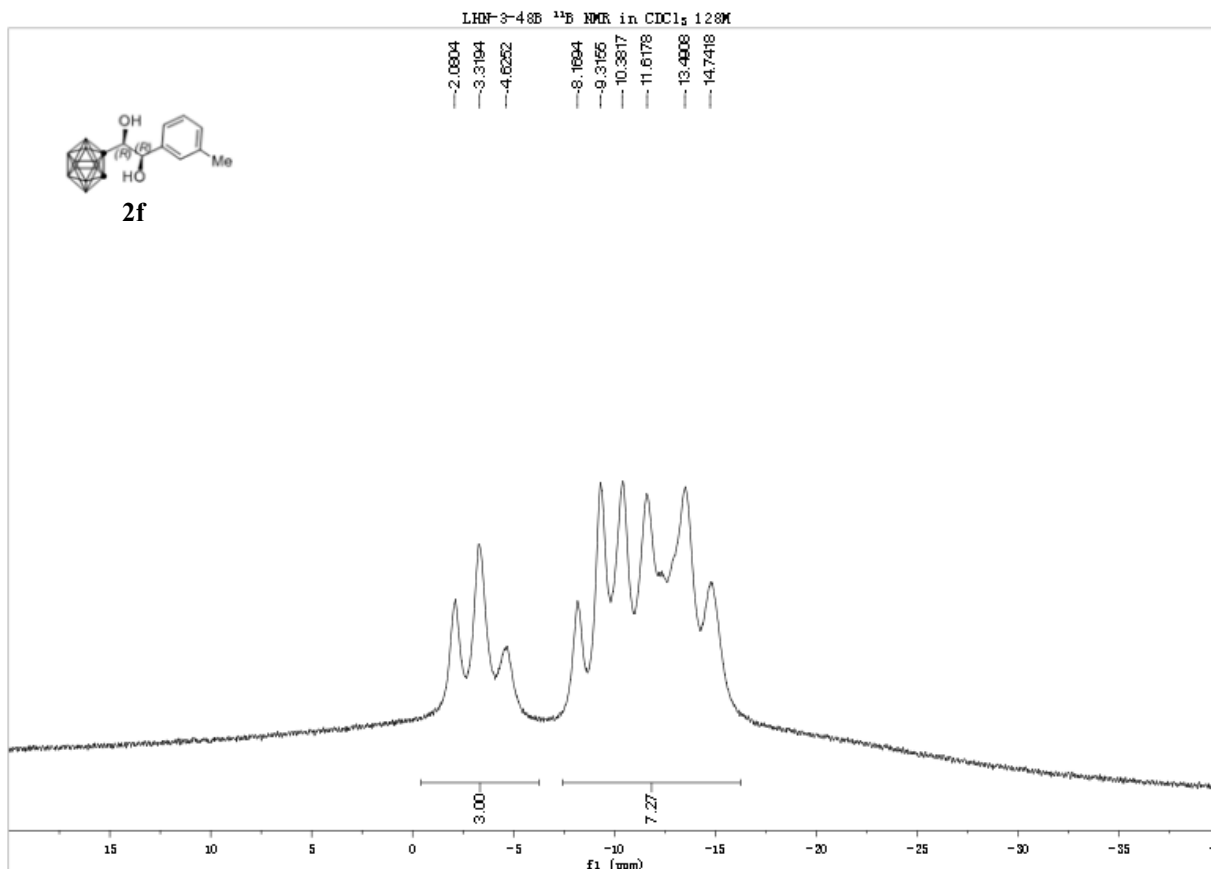
58.0534

21.4719



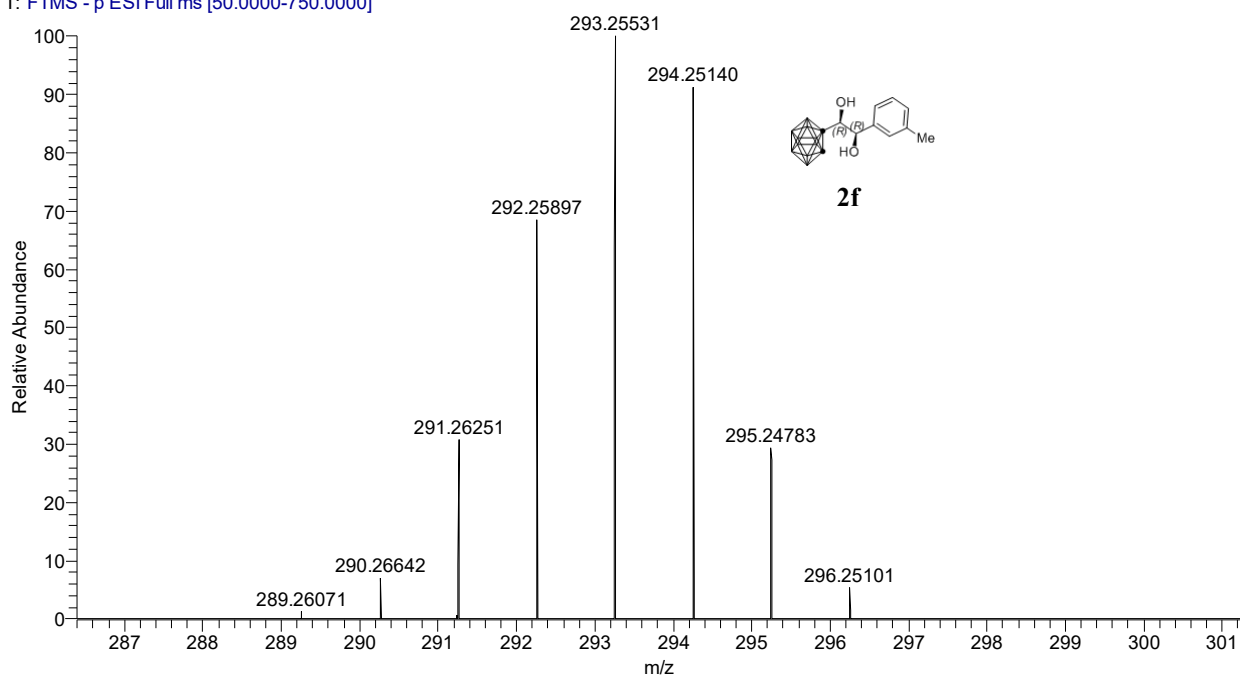
2f





LHN-3-48B. HRMS (ESI) m/z calcd for $C_{11}H_{21}B_{10}O_2^-$ (M-H)⁻ 294.25139, found 294.25140.

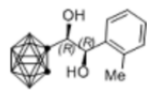
LHN-3-48B #8 RT: 0.09 AV: 1 NL: 6.30E5
T: FTMS - p ESI Full ms [50.0000-750.0000]



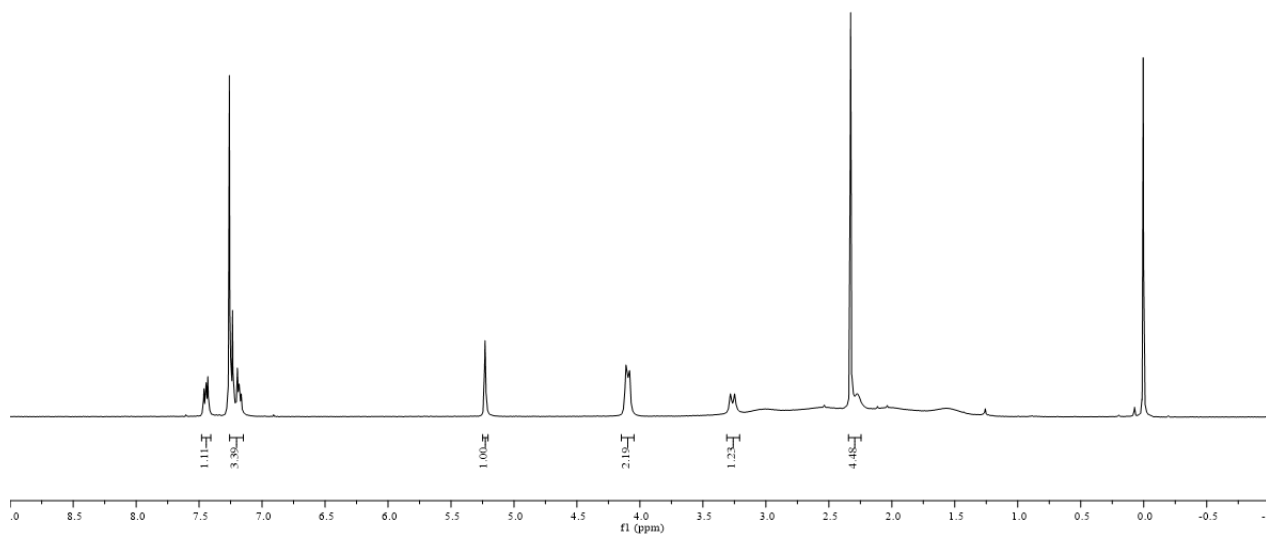
LHN-3-48C ¹H NMR in CDCl₃ 300M

7.4747
7.4618
7.4499
7.4438
7.4311
7.4166
7.2650
7.2599
7.2532
7.2452
7.2345
7.2214
7.1885
7.1882
7.1772
7.1659

5.2299
4.1104
4.0830
2.2811
2.2855
2.2725
2.2714



2g



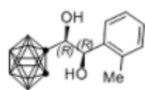
LHN-3-48C ¹³C NMR in CDCl₃ 75M

138.0743
137.8967
130.8967
128.4503
126.4515
125.4124

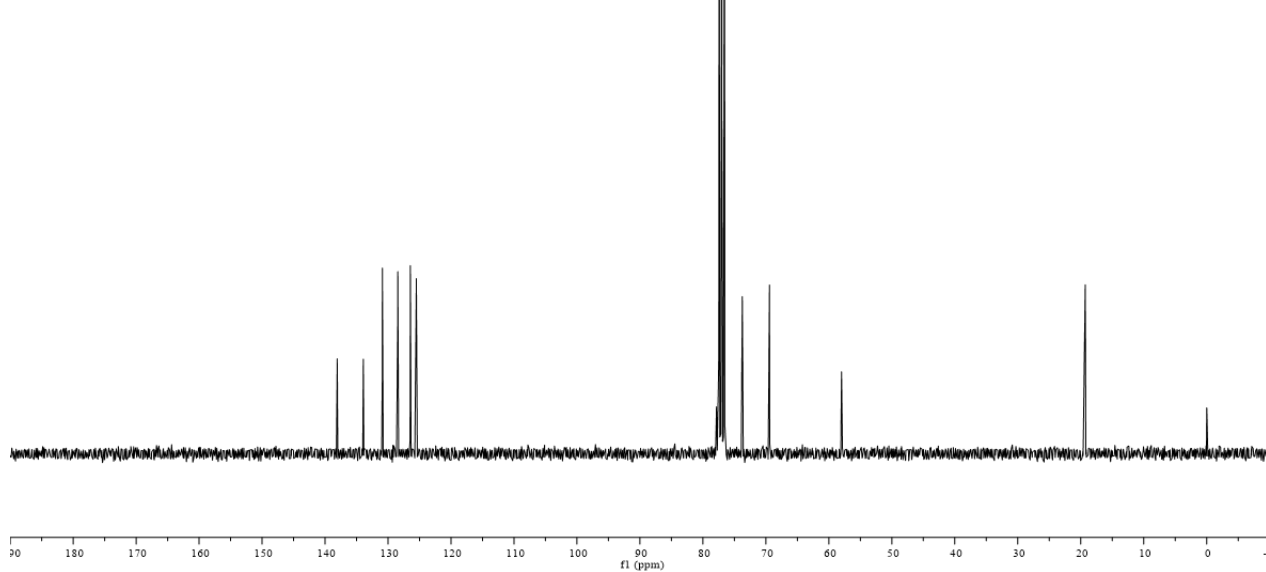
77.8467
77.4235
77.0003
76.5769
73.7367
69.4330

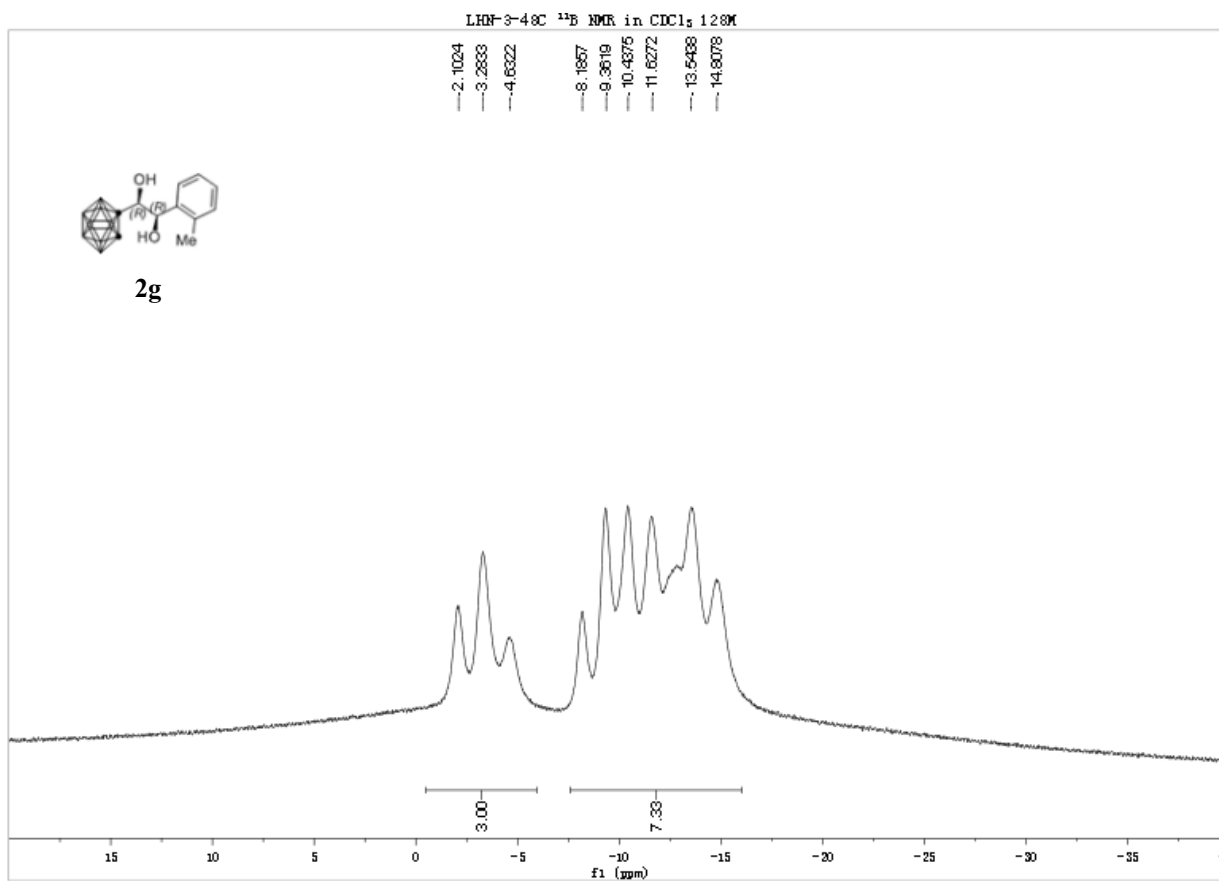
57.9888

19.2834



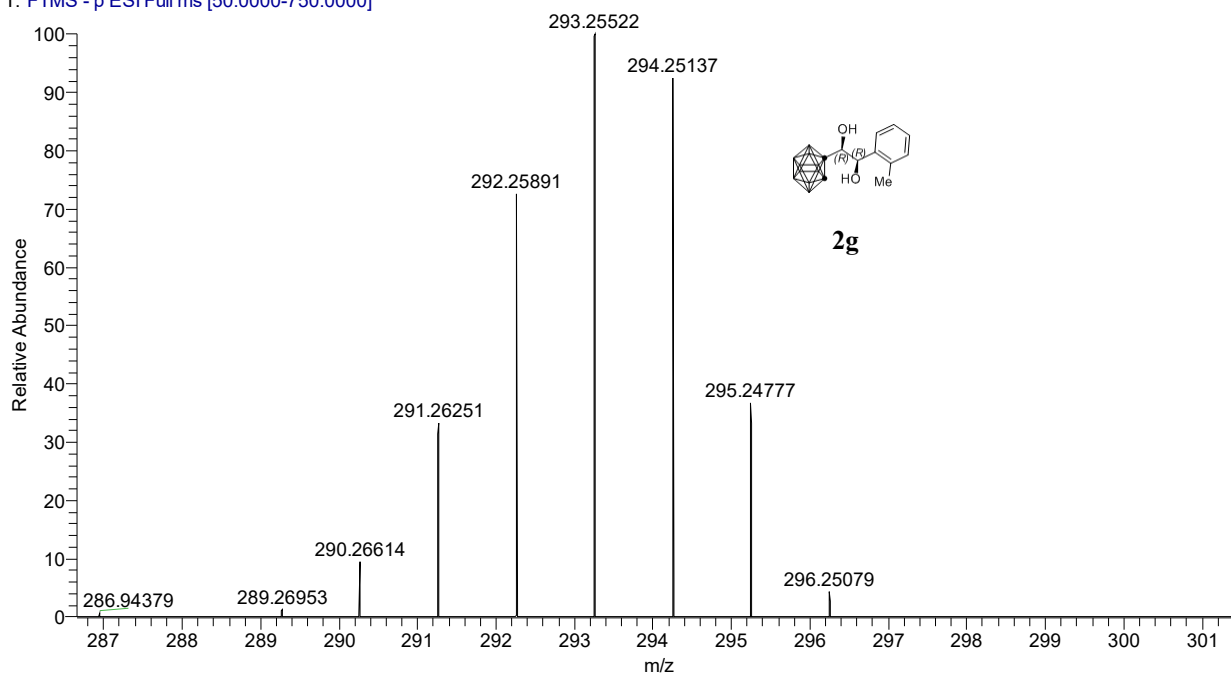
2g





LHN-3-48C. HRMS (ESI) m/z calcd for $\text{C}_{11}\text{H}_{21}\text{B}_{10}\text{O}_2^-$ (M-H) $^-$ 294.25139, found 294.25137.

LHN-3-48C #10 RT: 0.11 AV: 1 NL: 1.01E6
T: FTMS - p ESI Full ms [50.0000-750.0000]



LHN-3-48F 1H NMR in CDCl₃ 300M

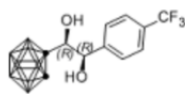
7.6642
7.6370
7.4753
7.4479
7.2959

5.0899
5.0727

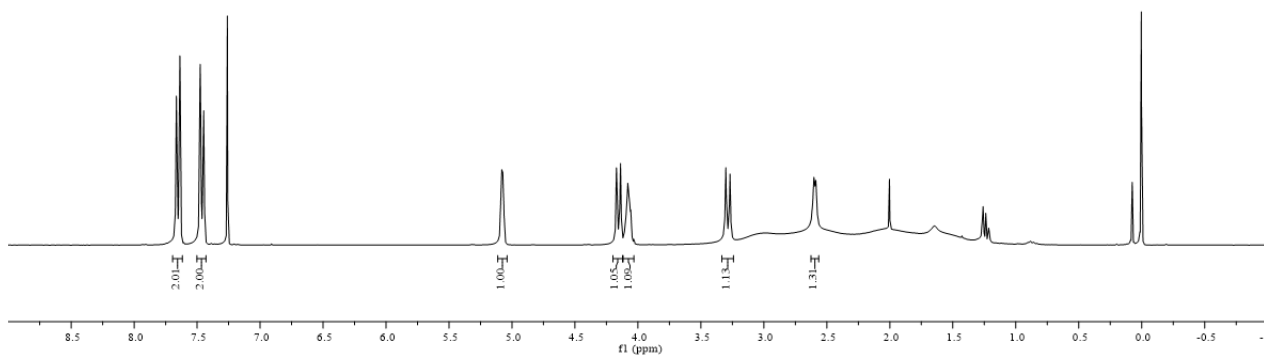
4.1705
4.1380
4.0805

3.3022
3.2889

2.6029
2.5879



2h



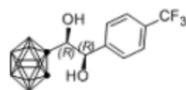
LHN-3-48F 13C NMR in CDCl₃ 75M

143.6671
143.9512
131.4642
131.0313
130.9591
129.8466
129.2346
126.2282
125.8344
125.7853
125.7354
125.6856
125.6220
122.9150
118.4080

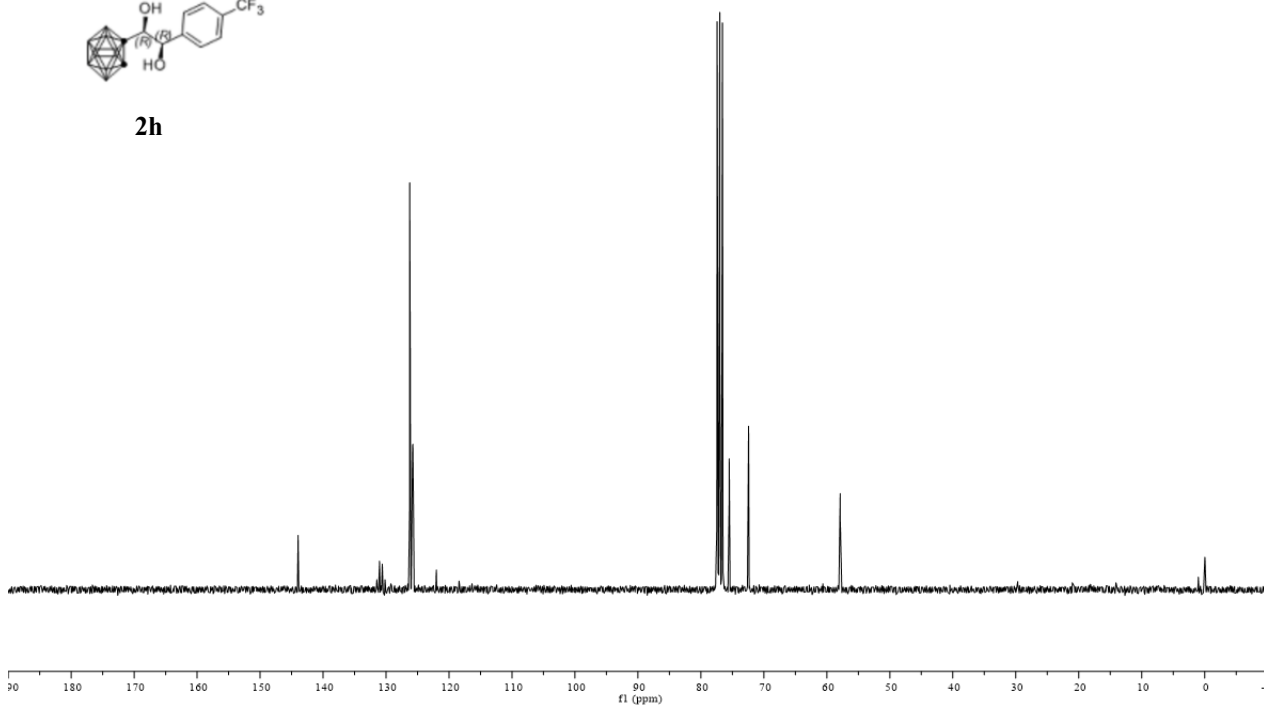
77.4236
77.3129
77.1994
77.0902
76.5768
75.5025
72.4280

57.8774

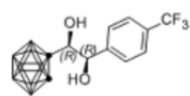
¹³C NMR (75 MHz, Chloroform-d) δ 125.76 (q, J = 3.7 Hz).



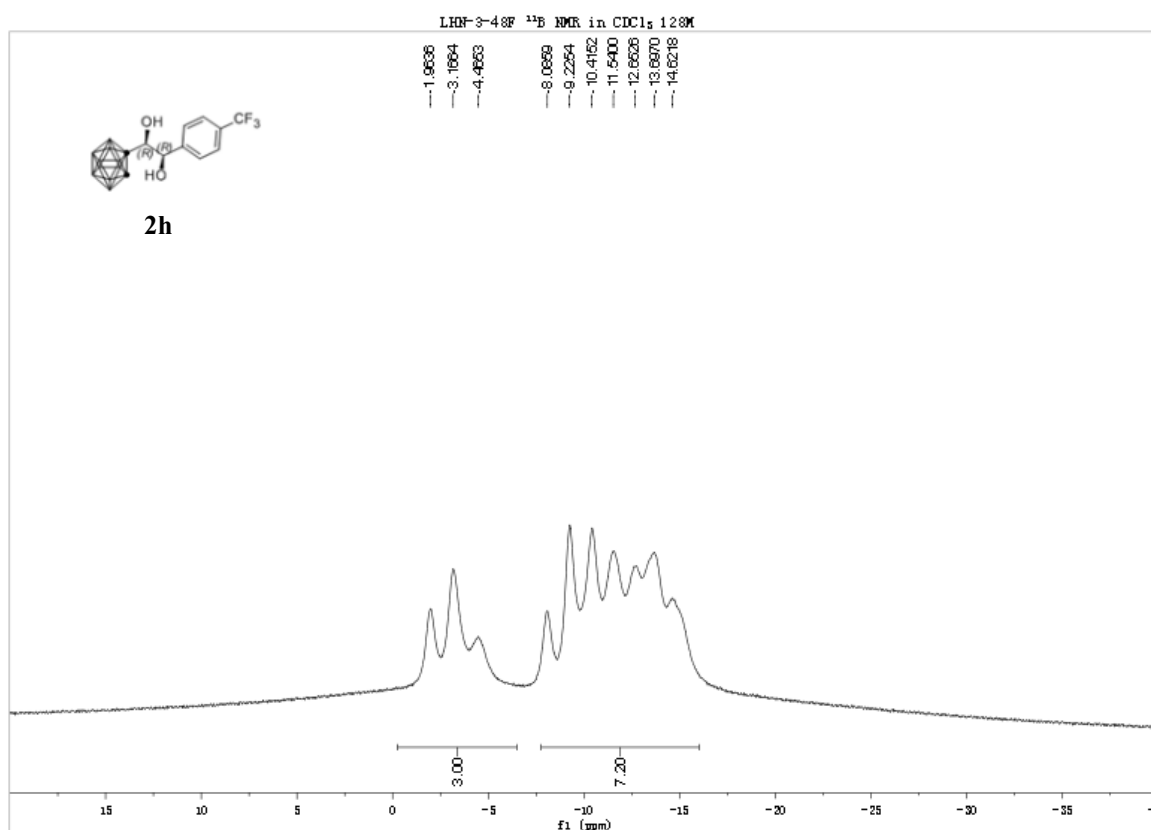
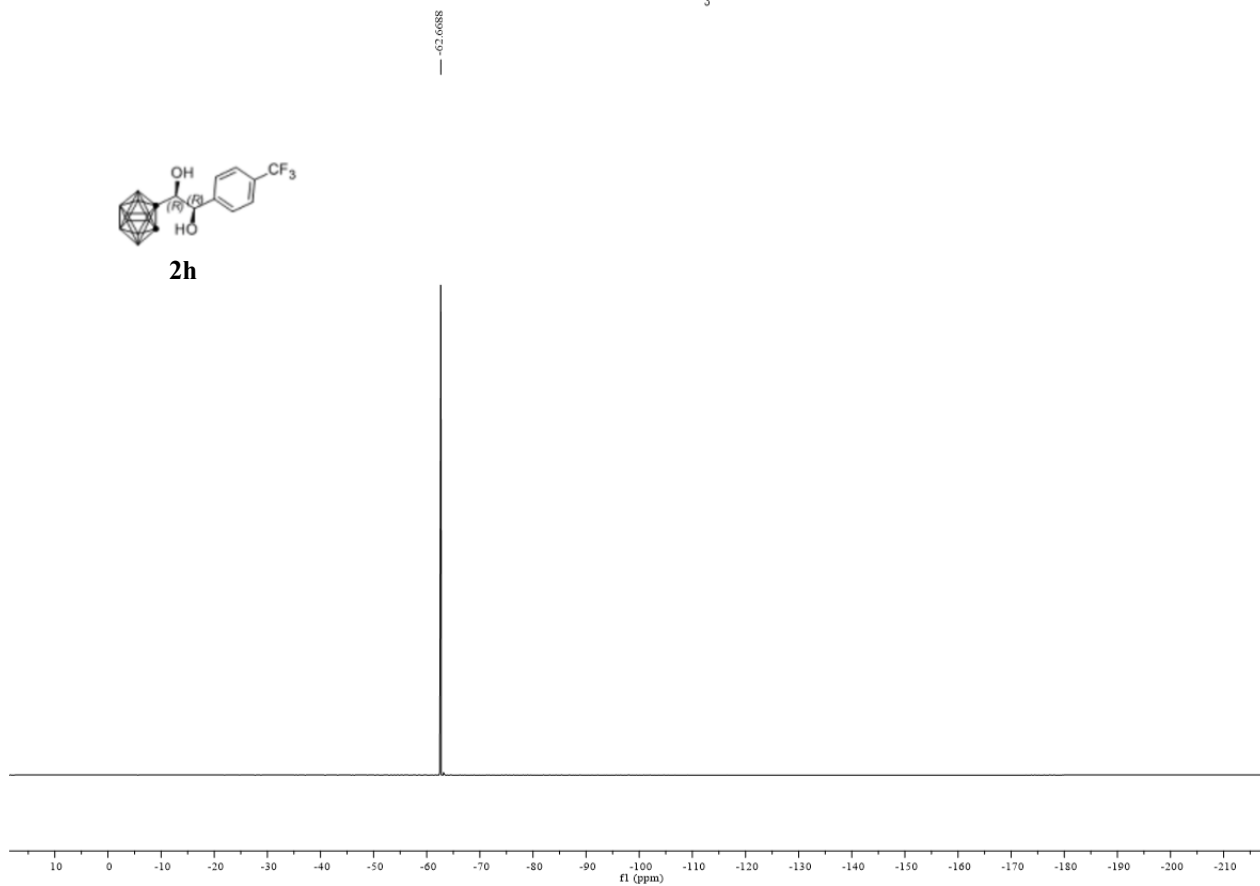
2h



LHN-3-48F 19F NMR in CDCl₃ 376M

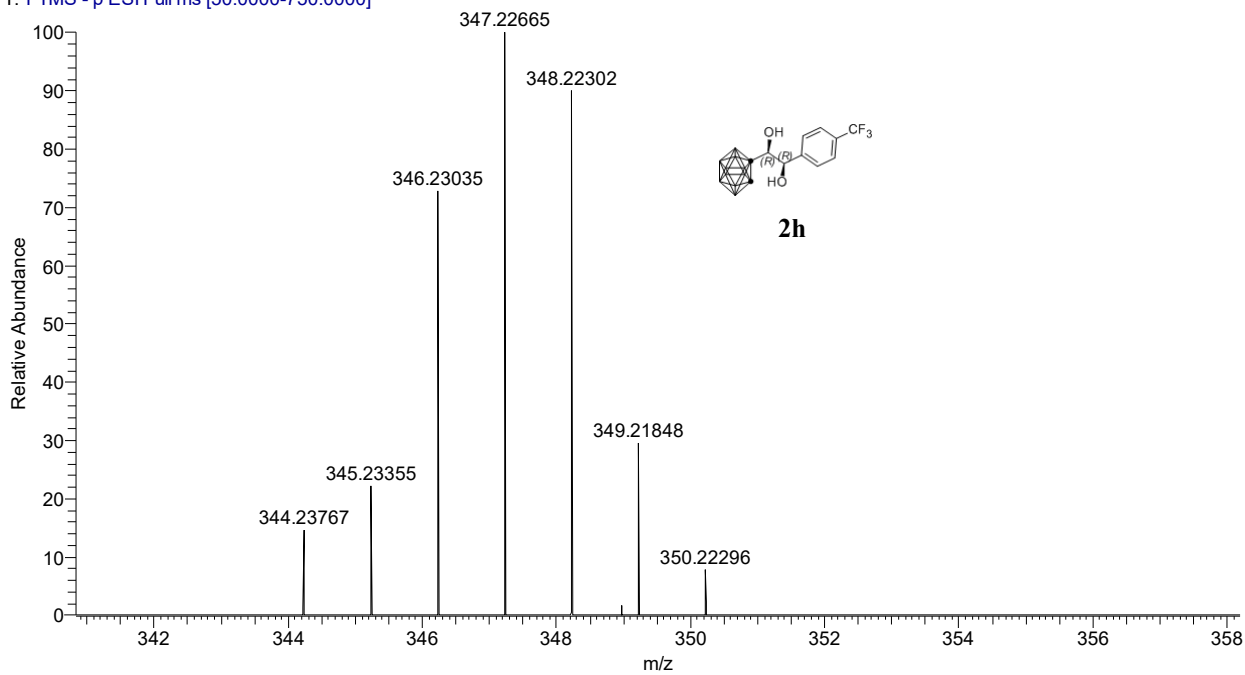


2h



LHN-3-48F. HRMS (ESI) m/z calcd for C₁₁H₁₈B₁₀F₃O₂⁻ (M-H)⁻ 348.22312, found 348.22302.

LHN-3-48F #12 RT: 0.13 AV: 1 NL: 2.82E5
T: FTMS - p ESI Full ms [50.0000-750.0000]



LHN-3-48G 1H NMR in CDCl₃ 300M

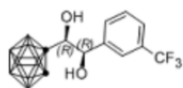
7.62660
7.6152
7.6011
7.5948
7.5886
7.5800
7.5303
7.5262
7.5200
7.5159
7.5097
7.5000

5.0805
5.0705

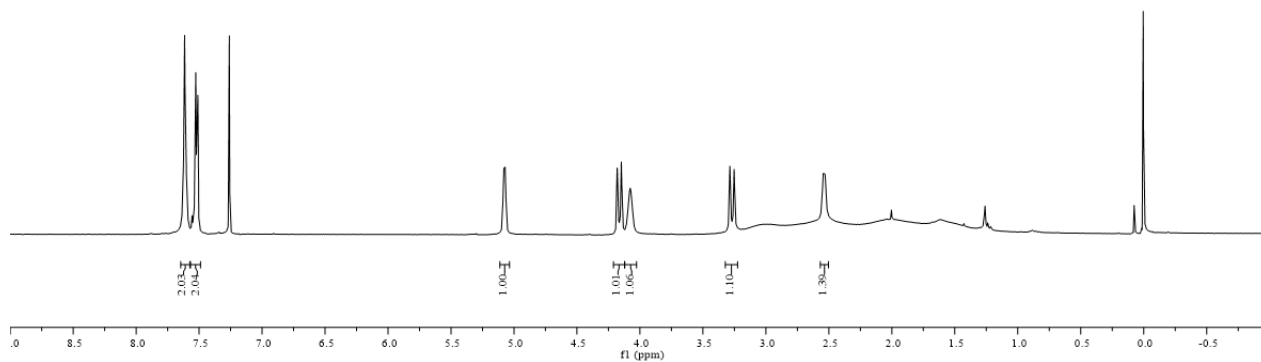
4.1894
4.1876
4.0771

3.2857
3.2524

2.5443
2.5366



2i

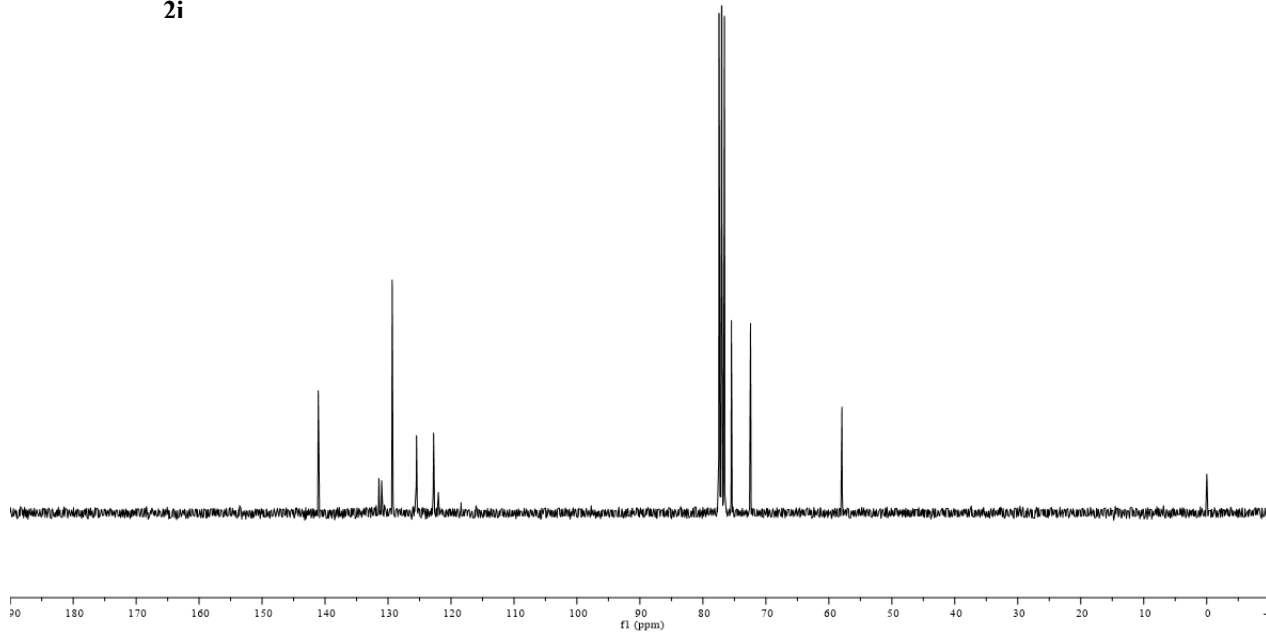
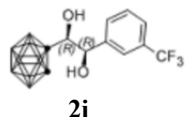


LHN-3-48G ¹³C NMR in CDCl₃ 75M

141.0819
131.8823
131.4516
131.0205
80.5887
80.5887
129.2800
129.1937
125.6280
125.5257
125.4770
125.4271
125.3814
122.8184
122.7679
122.7178
122.6680
122.0171
118.4076

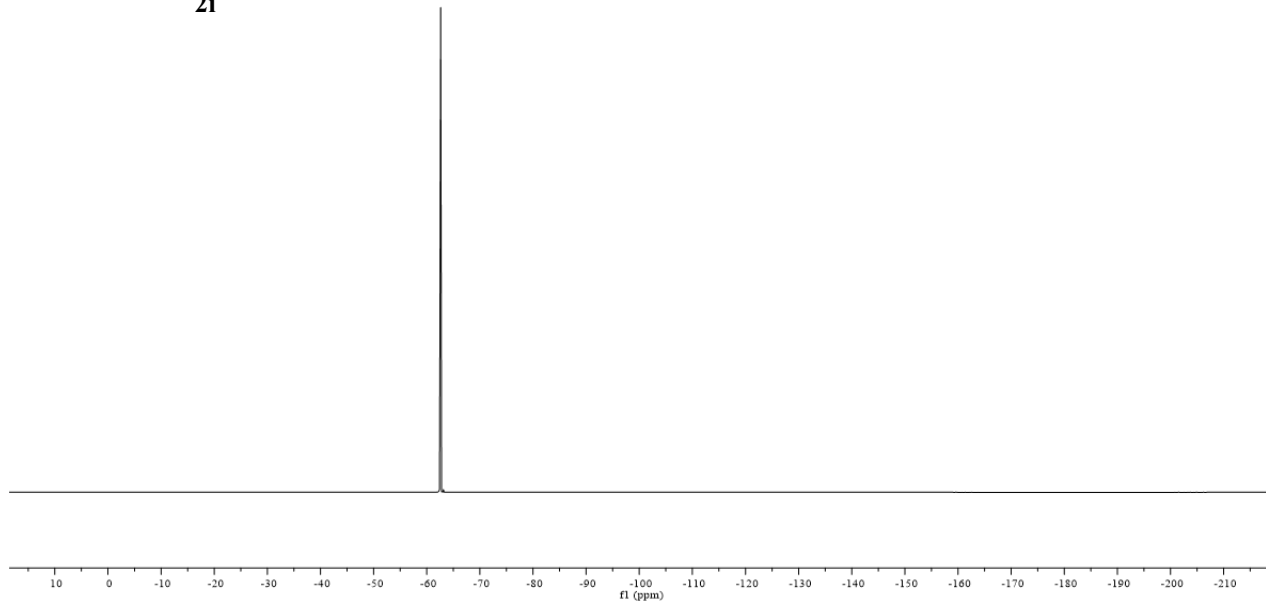
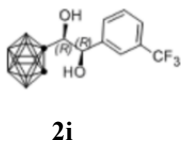
77.4235
77.3298
77.2361
77.0000
76.5767
75.4722
72.4376

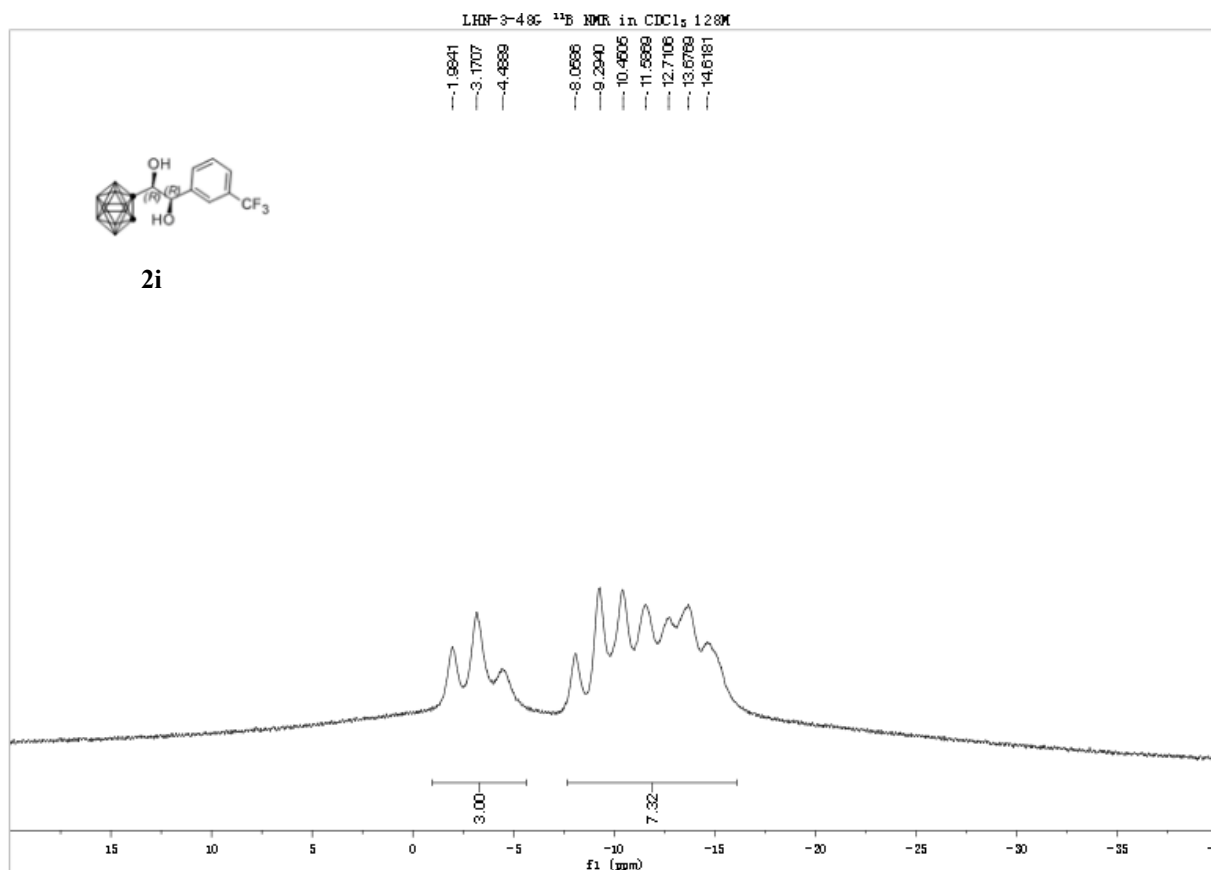
57.9168



LHN-3-48G ¹⁹F NMR in CDCl₃ 376M

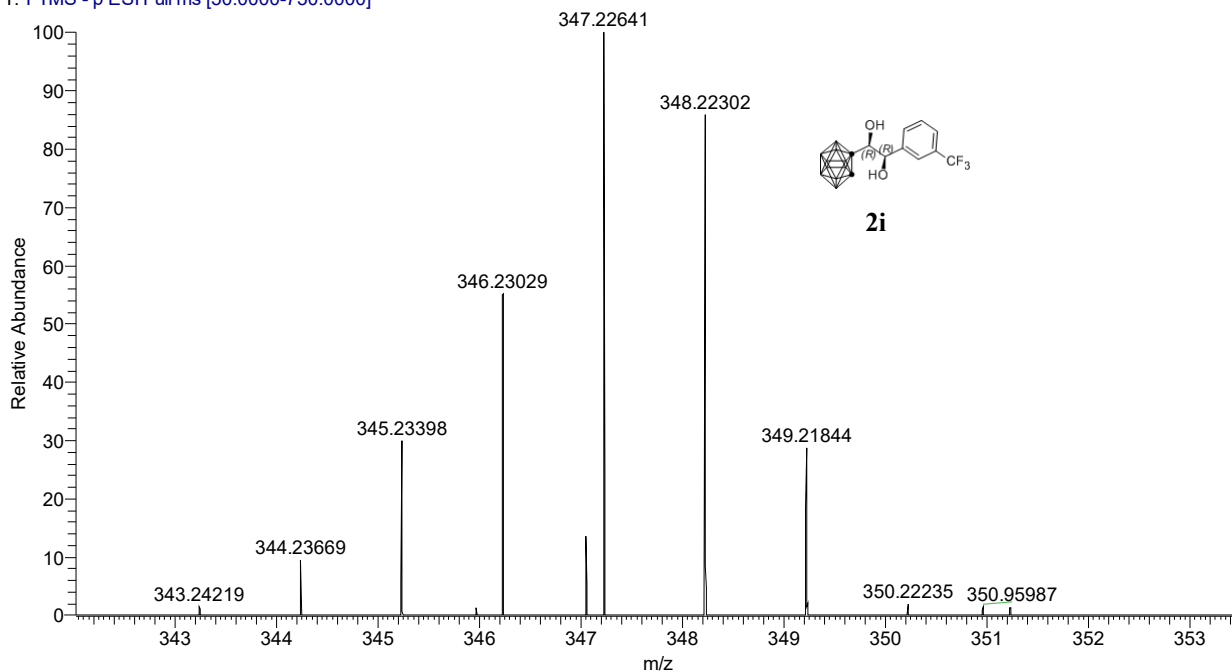
-62.6373





LHN-3-48G. HRMS (ESI) m/z calcd for C₁₁H₁₈B₁₀F₃O₂⁻ (M-H)⁻ 348.22312, found 348.22302.

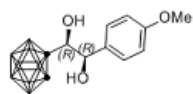
LHN-3-48G #10 RT: 0.11 AV: 1 NL: 3.71E5
T: FTMS - p ESI Full ms [50.0000-750.0000]



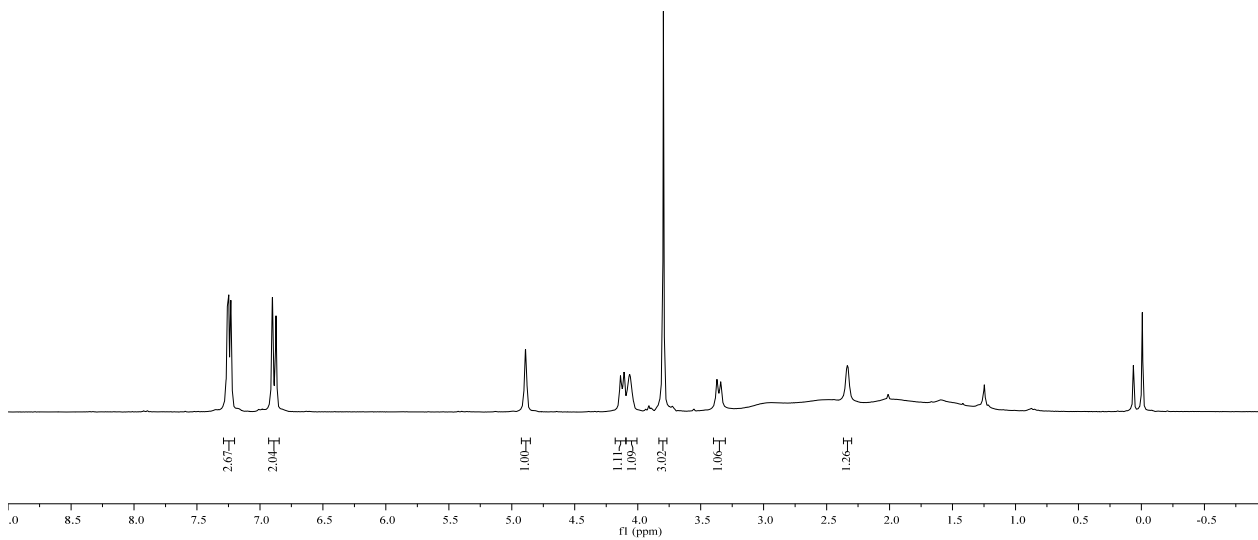
LHN-3-48D 1H NMR in CDCl₃ 300M

7.2896
7.2482
7.2312
6.9010
6.8723

4.8902
4.1566
4.1091
4.0641
3.7958
3.3704
3.3405
2.3364



2j



LHN-3-48D 13C NMR in CDCl₃ 75M

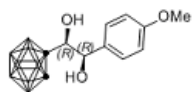
159.8177

132.2251
127.3010

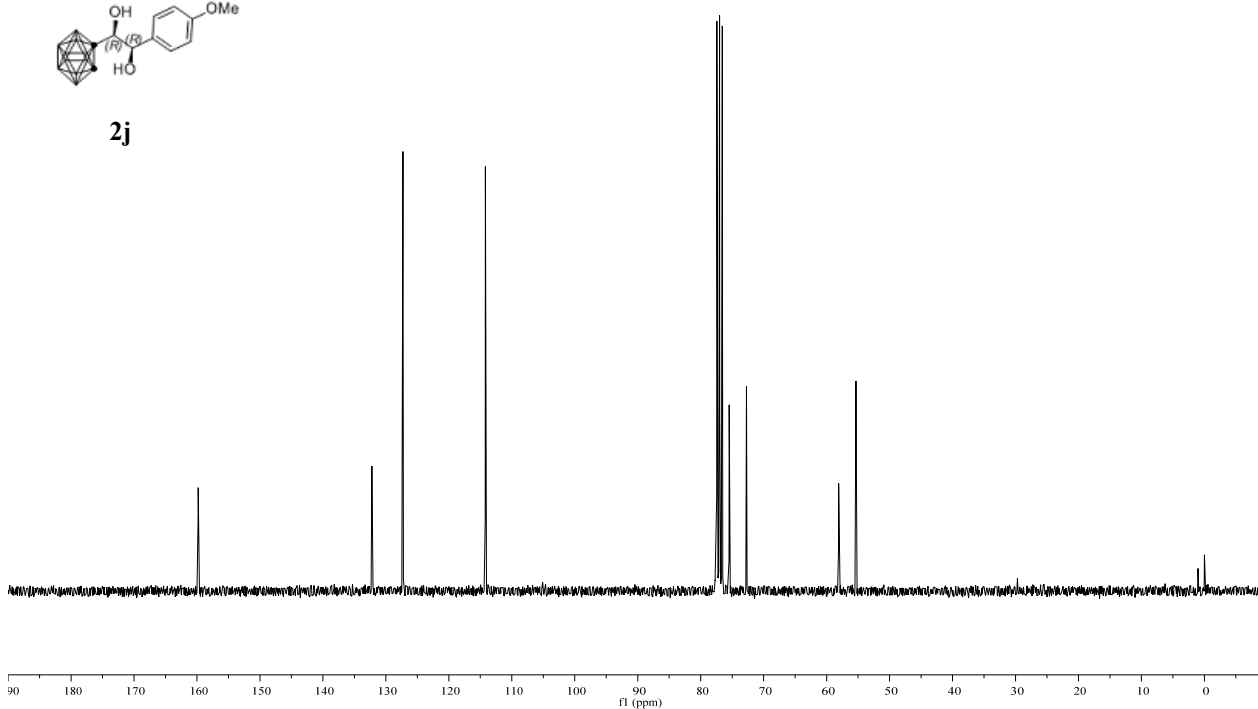
114.2065

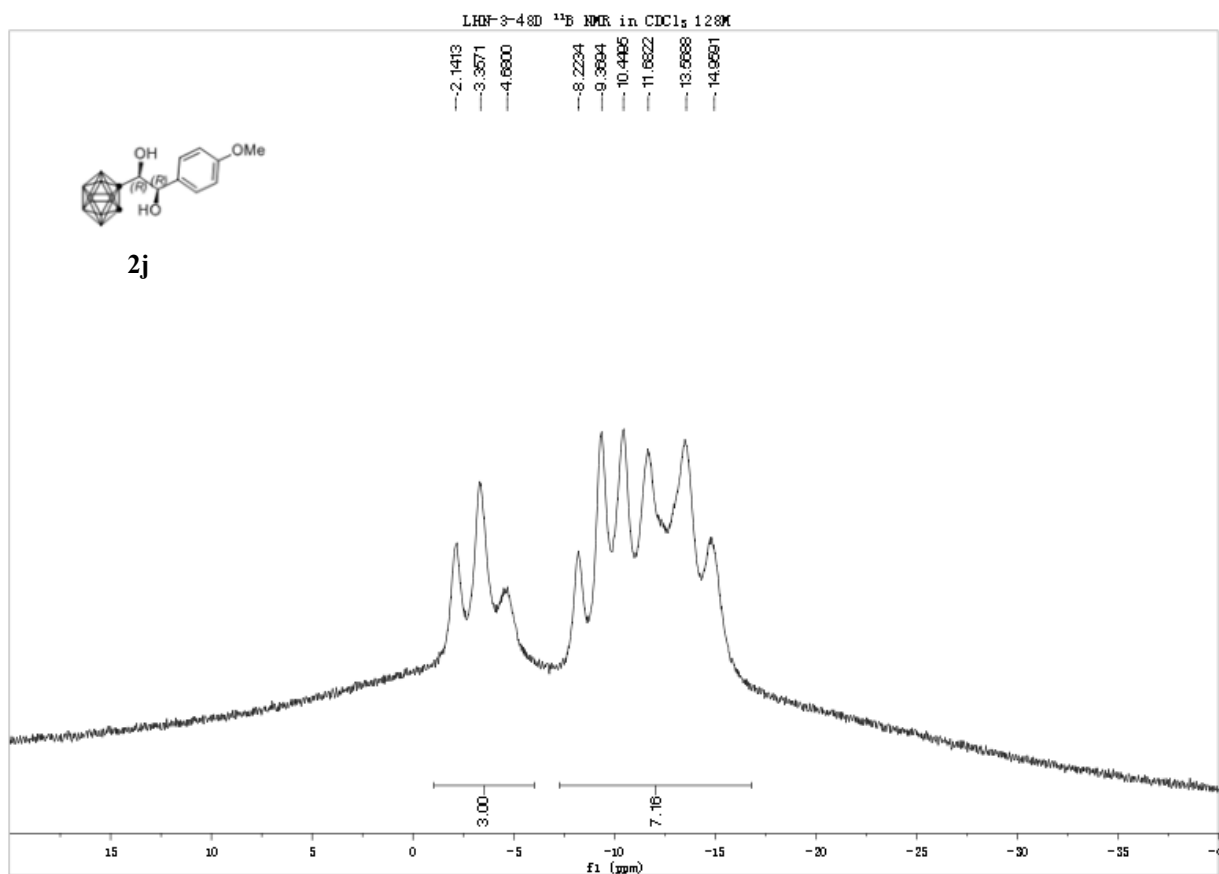
77.6486
77.4236
77.0003
76.5769
75.4470
72.7387

58.0795
55.3447



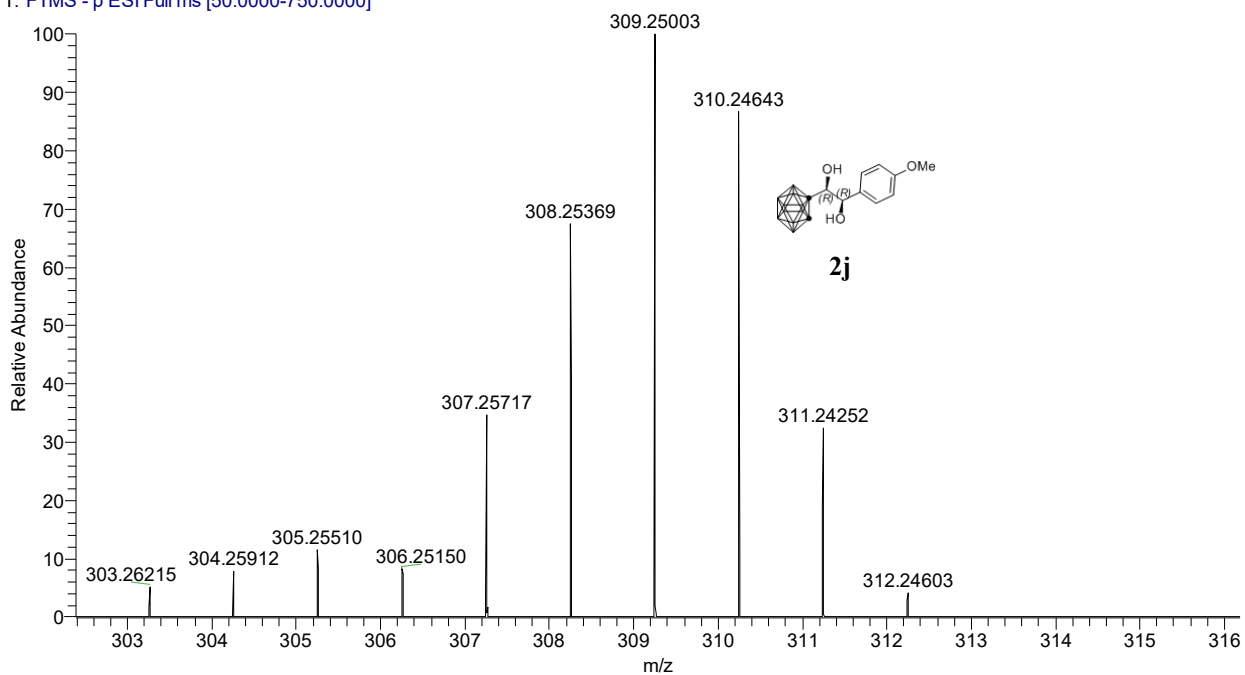
2j

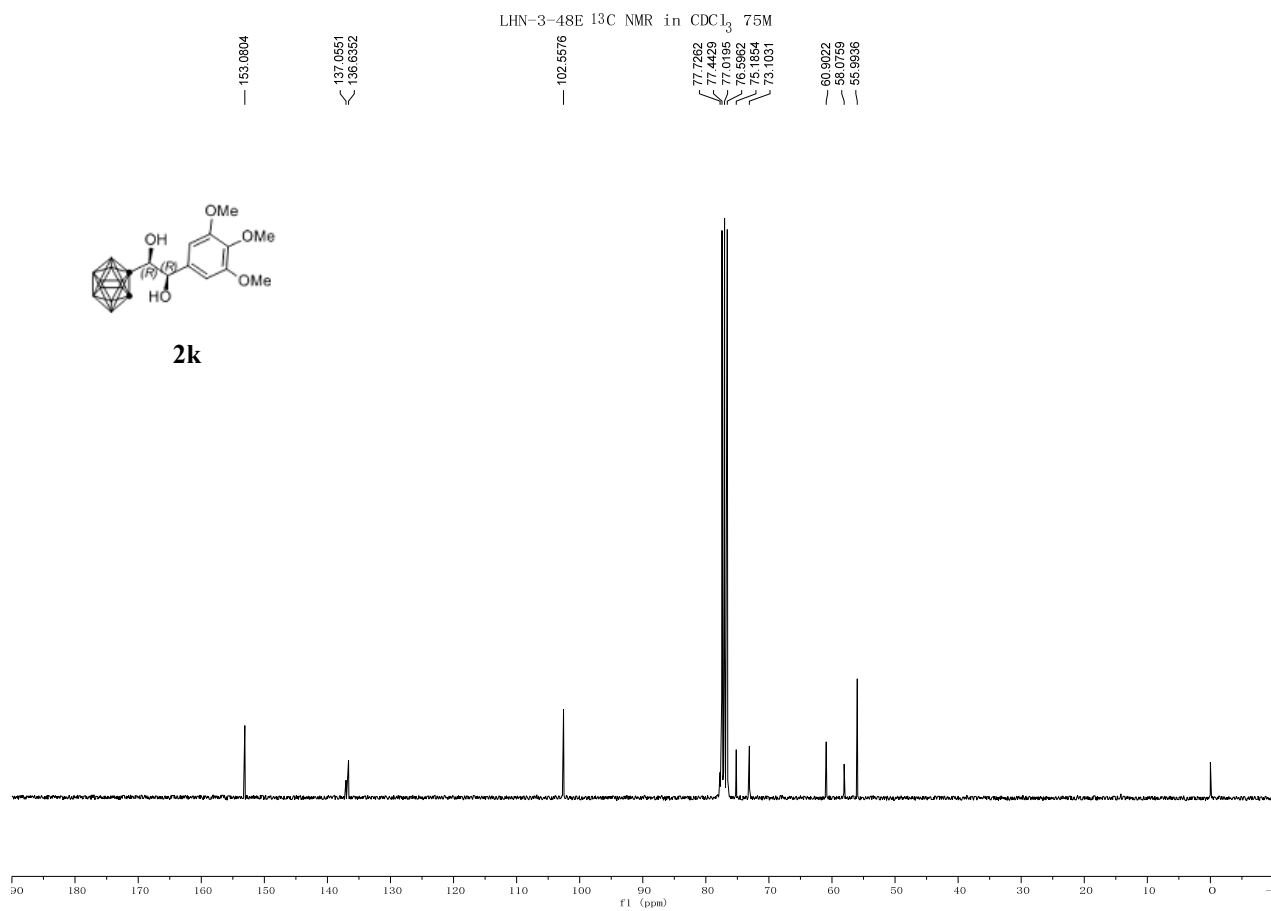
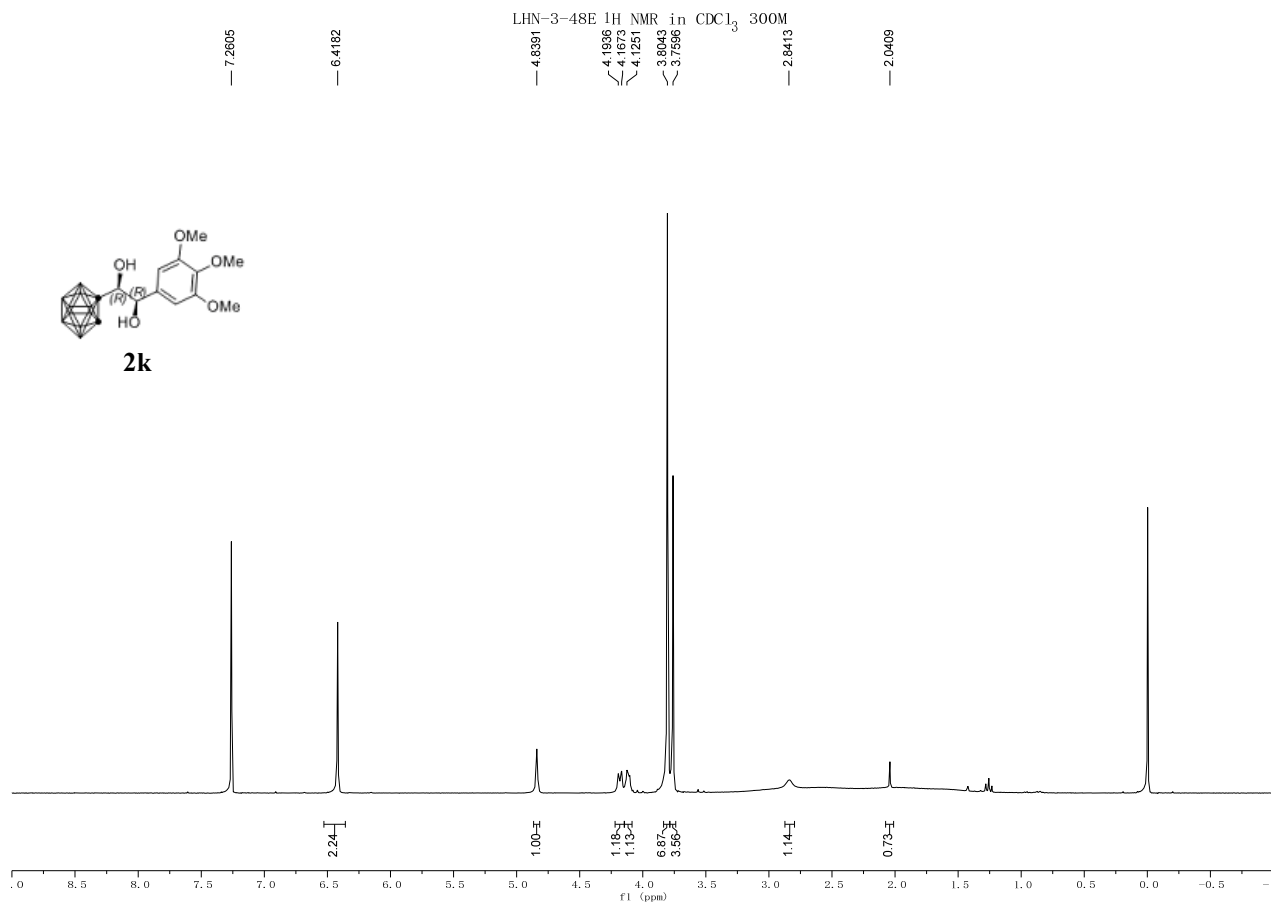


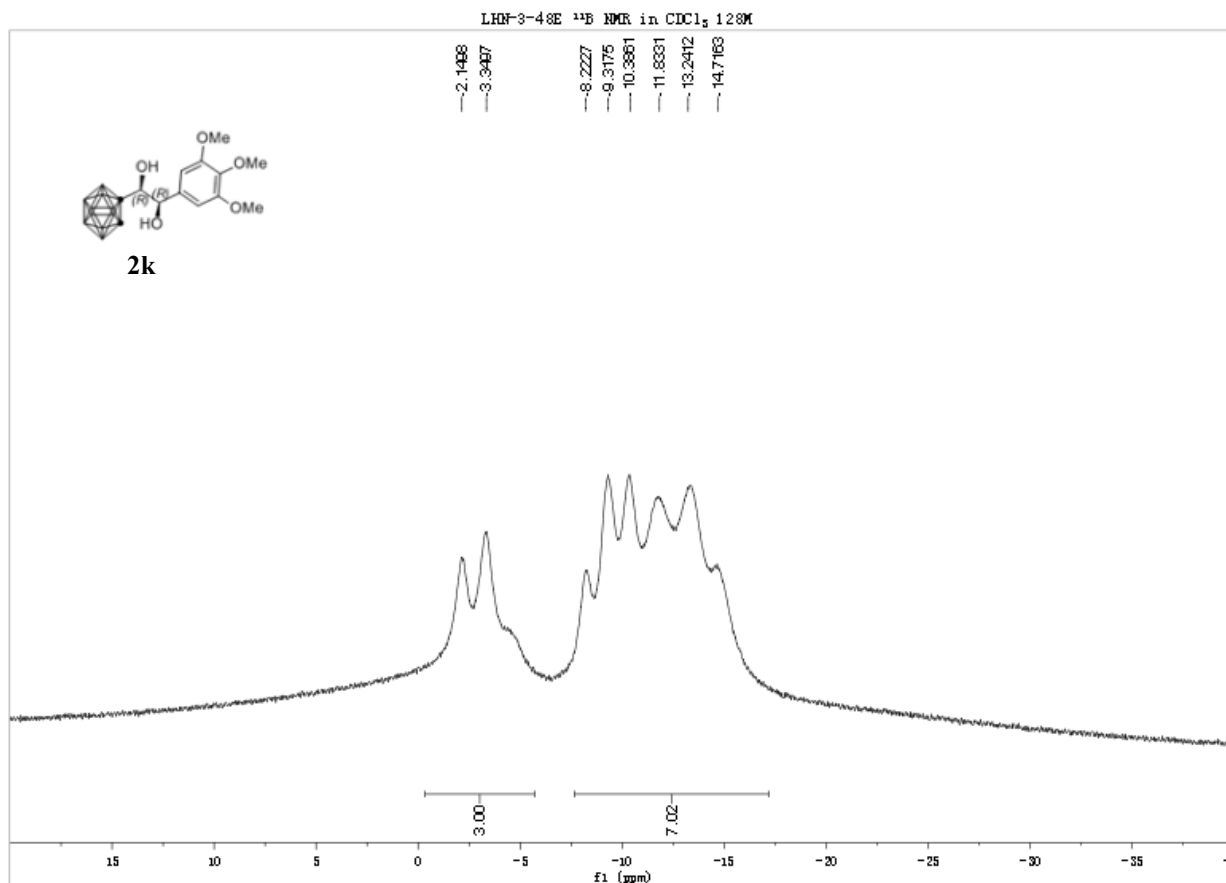


LHN-3-48D. HRMS (ESI) m/z calcd for C₁₁H₂₁B₁₀O₃⁻ (M-H)⁻ 310.24630, found 310.24643.

LHN-3-48D #8 RT: 0.09 AV: 1 NL: 8.13E5
T: FTMS - p ESI Full ms [50.0000-750.0000]

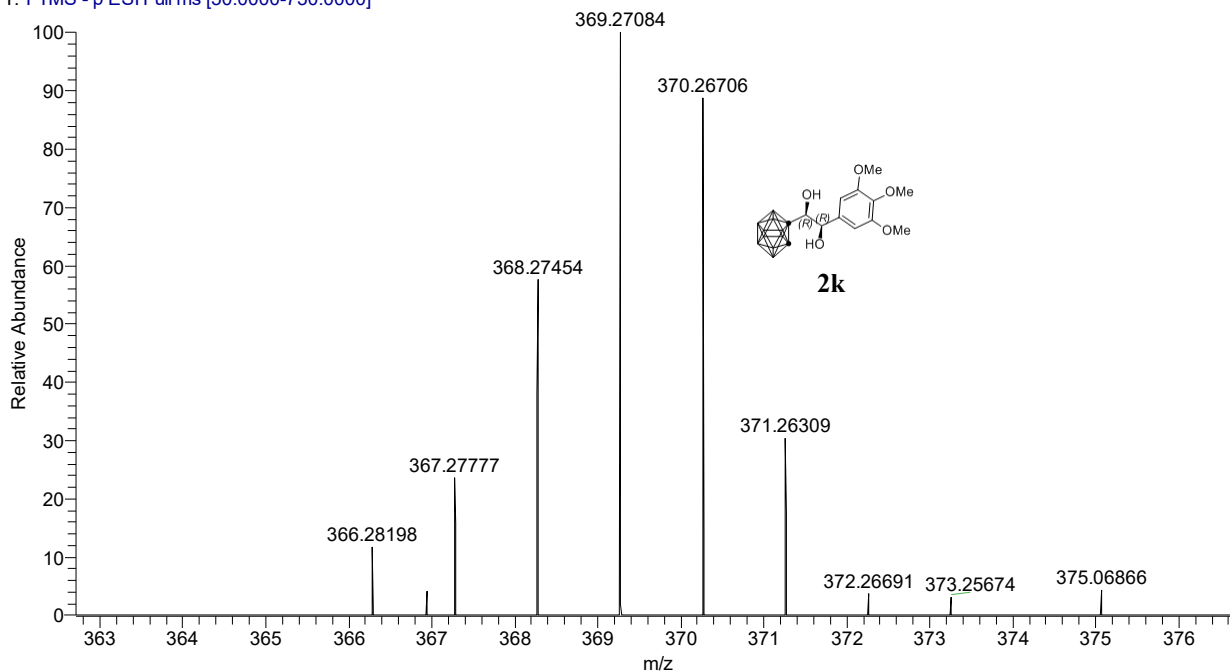






LHN-3-48E. HRMS (ESI) m/z calcd for C₁₃H₂₅B₁₀O₅⁻ (M-H)⁻ 370.26743, found 370.26706.

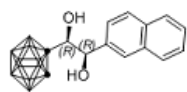
LHN-3-48E #16 RT: 0.18 AV: 1 NL: 7.65E4
T: FTMS - p ESI Full ms [50.0000-750.0000]



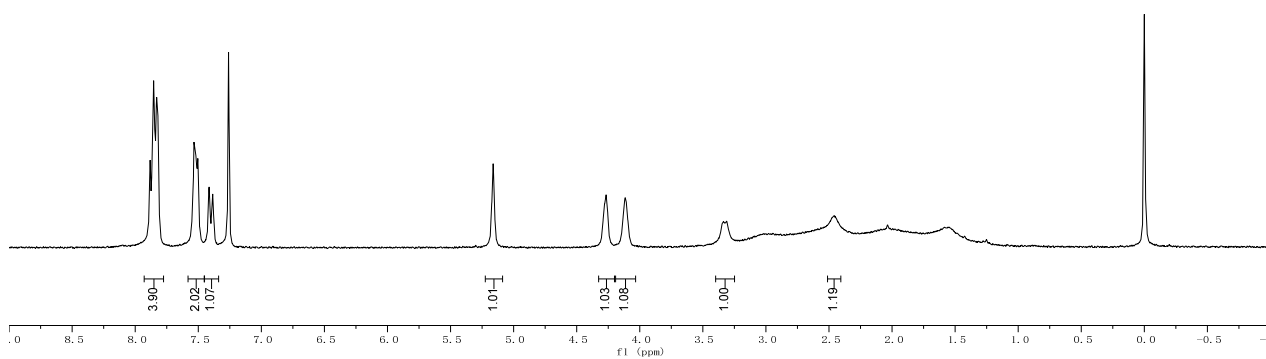
7.8825
7.8541
7.8305
7.8242
7.5340
7.5199
7.4146
7.3880
7.2800

LHN-4-41 ¹H NMR in CDCl₃ 300M

5.1628
4.2665
4.1154
3.3347
2.4777



2l

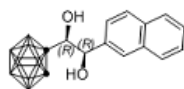


LHN-4-41 ¹³C NMR in CDCl₃ 75M

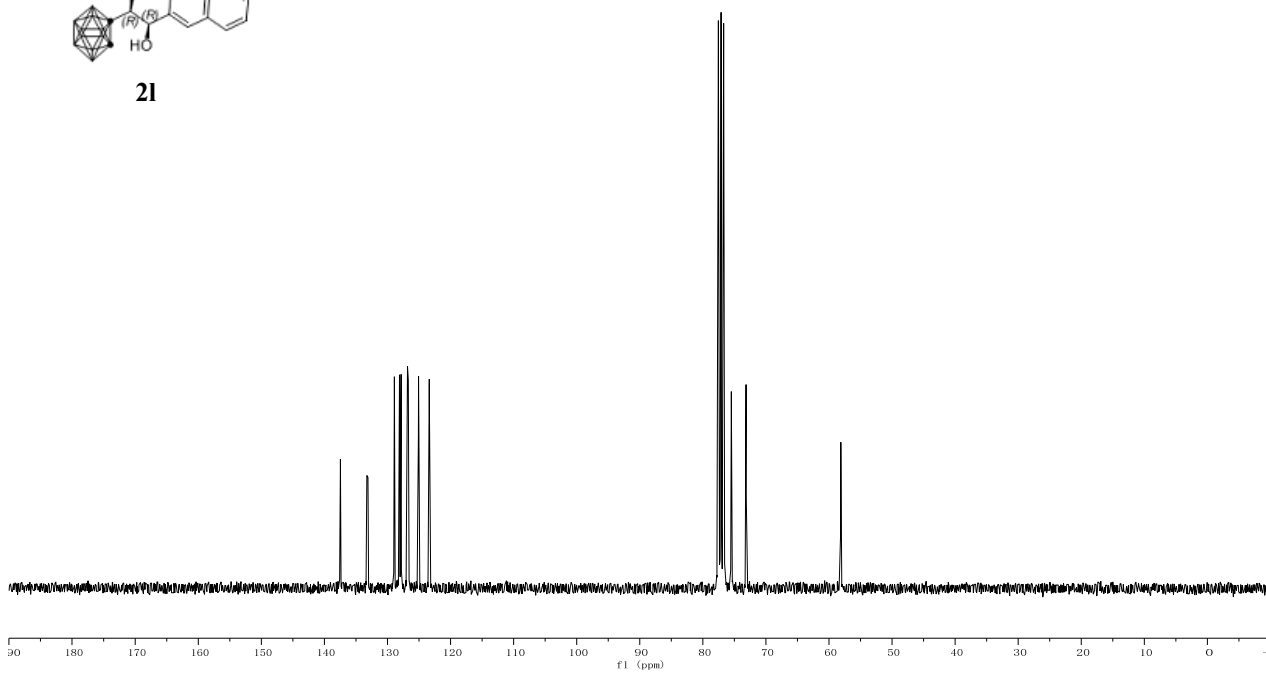
137.4657
133.2665
133.0836
128.9043
128.0949
127.8400
126.8118
126.6954
123.5846
123.3846

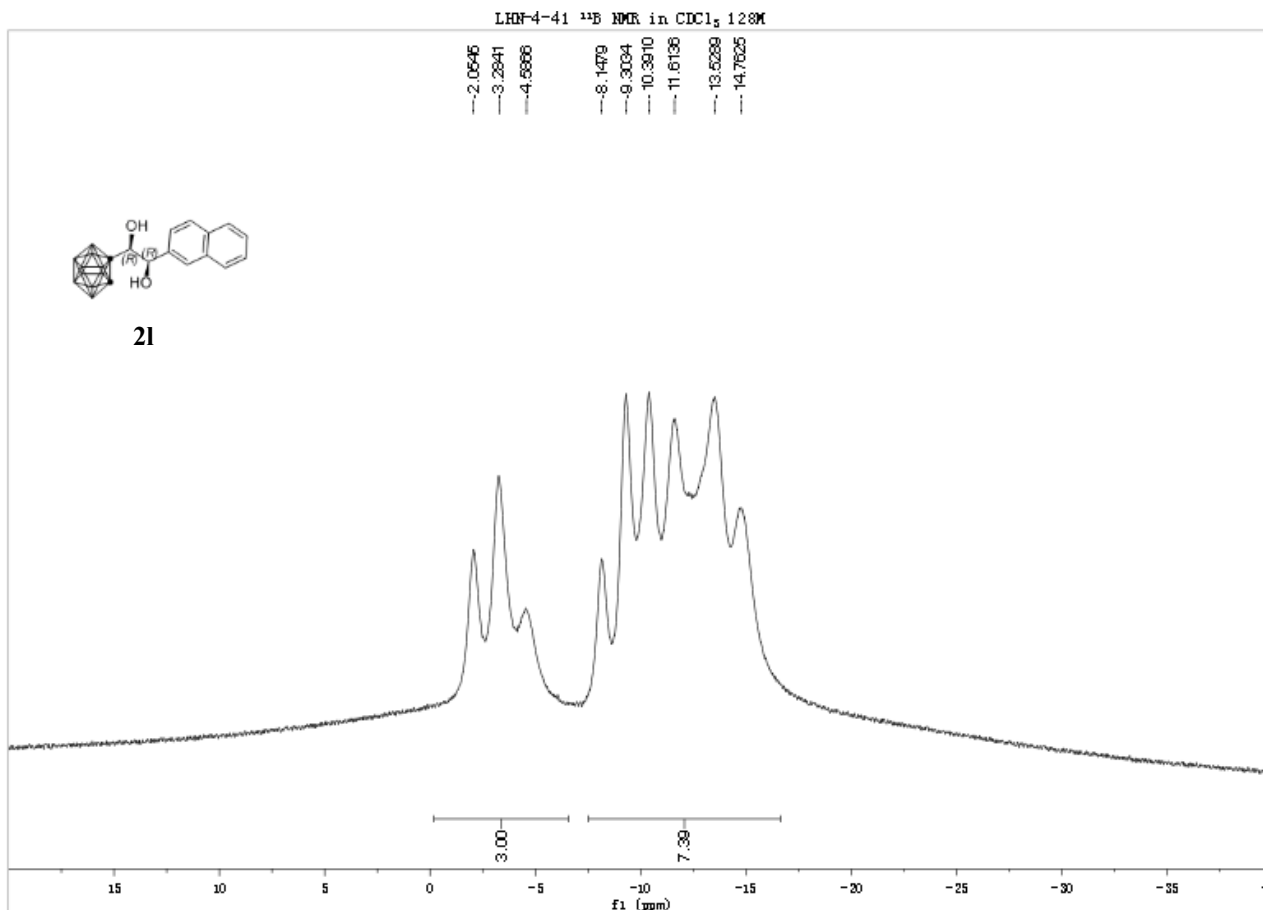
77.6294
77.5302
77.1066
76.6835
75.4912
73.1362

58.1237



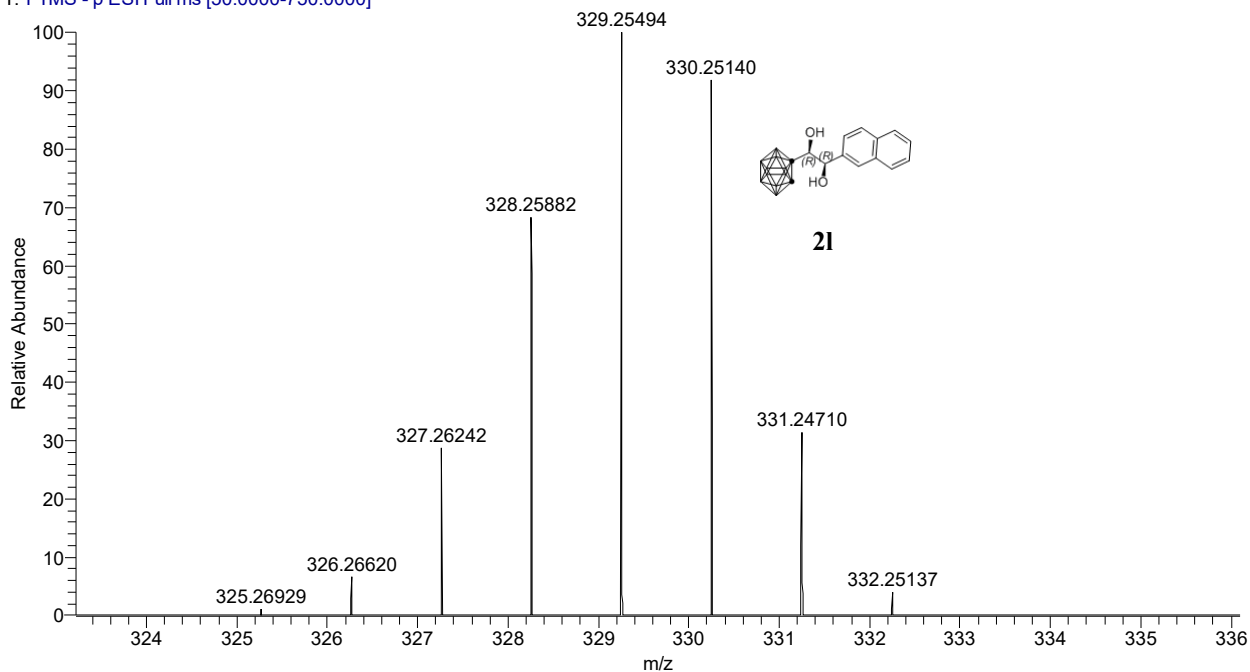
2l



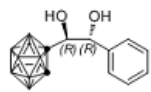


LHN-4-41. HRMS (ESI) m/z calcd for C₁₄H₂₁B₁₀O₂⁻ (M-H)⁻ 330.25139, found 330.25140.

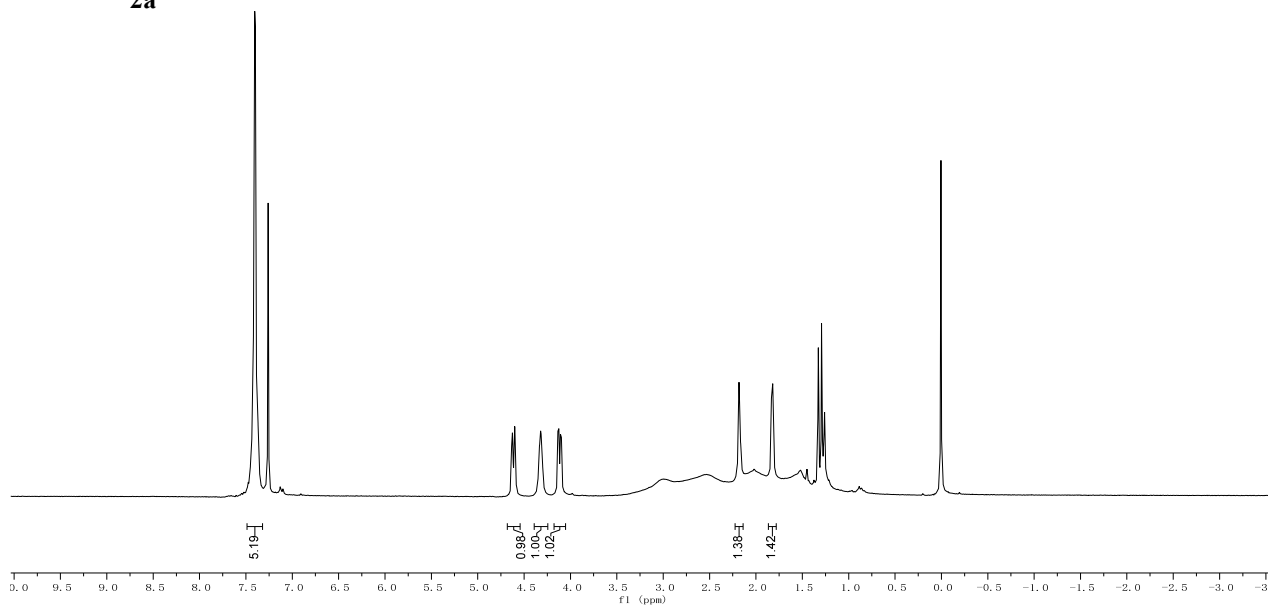
LHN-4-41 #12 RT: 0.13 AV: 1 NL: 4.30E5
 T: FTMS - p ESI Full ms [50.0000-750.0000]



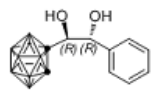
LHN-3748A 1H NMR in CDCl₃ 300M



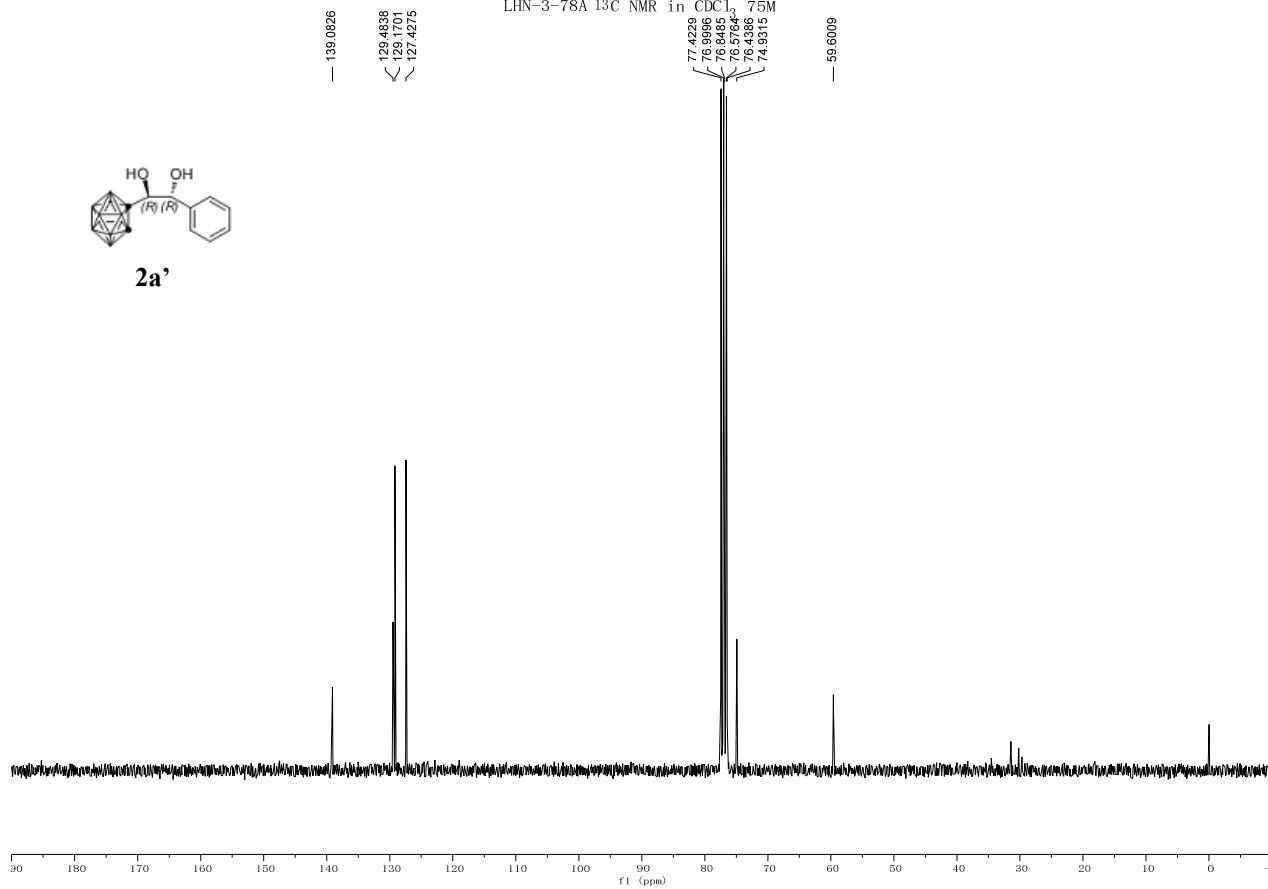
2a'

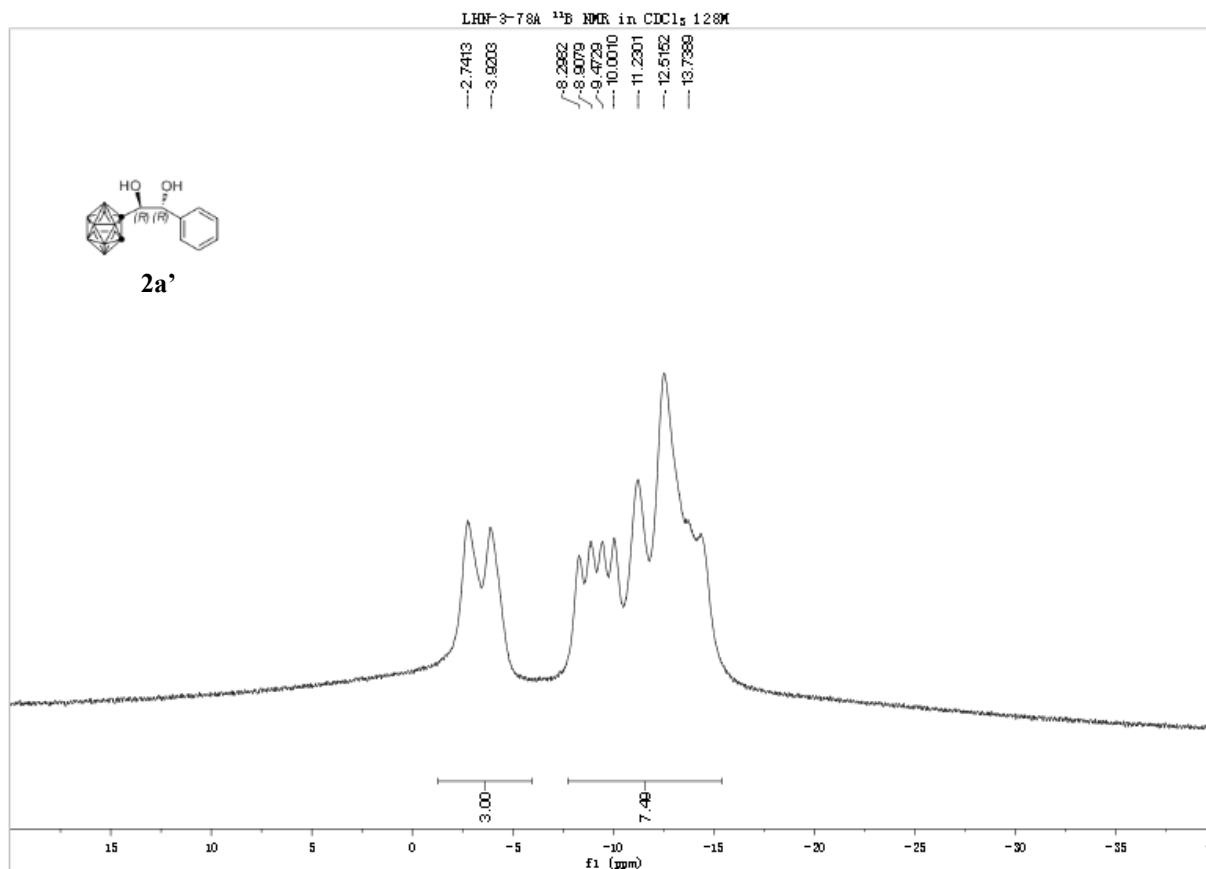


LHN-3-78A 13C NMR in CDCl₃ 75M



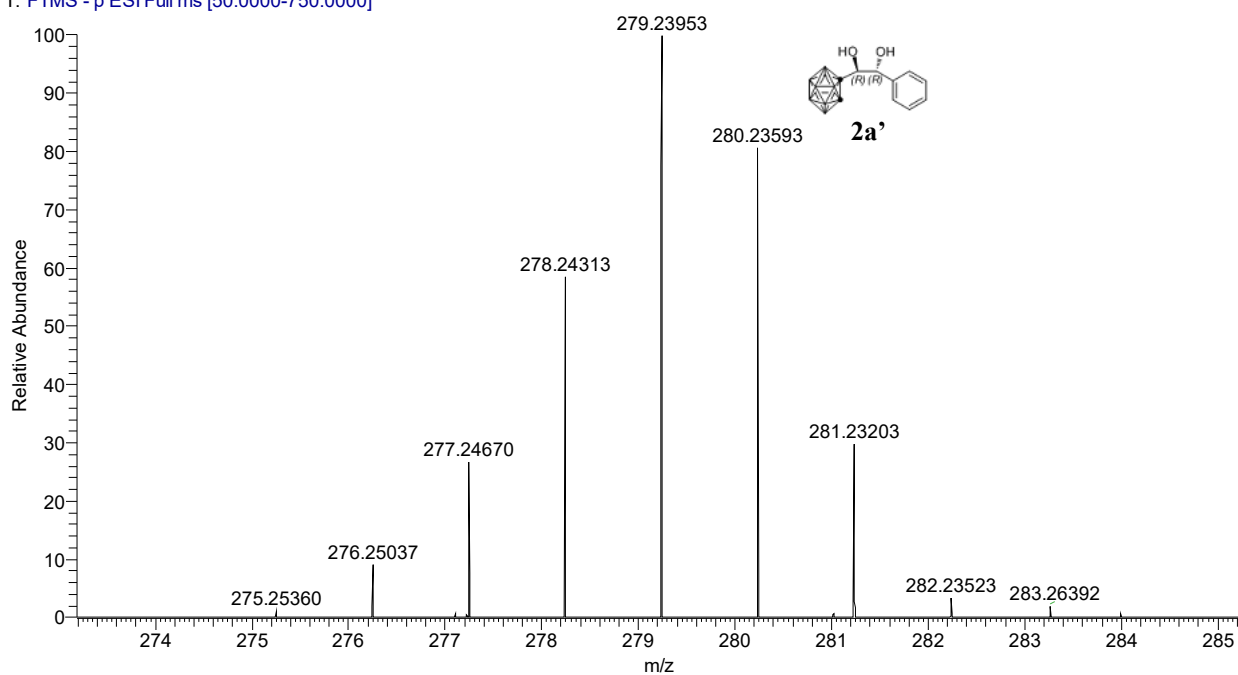
2a'

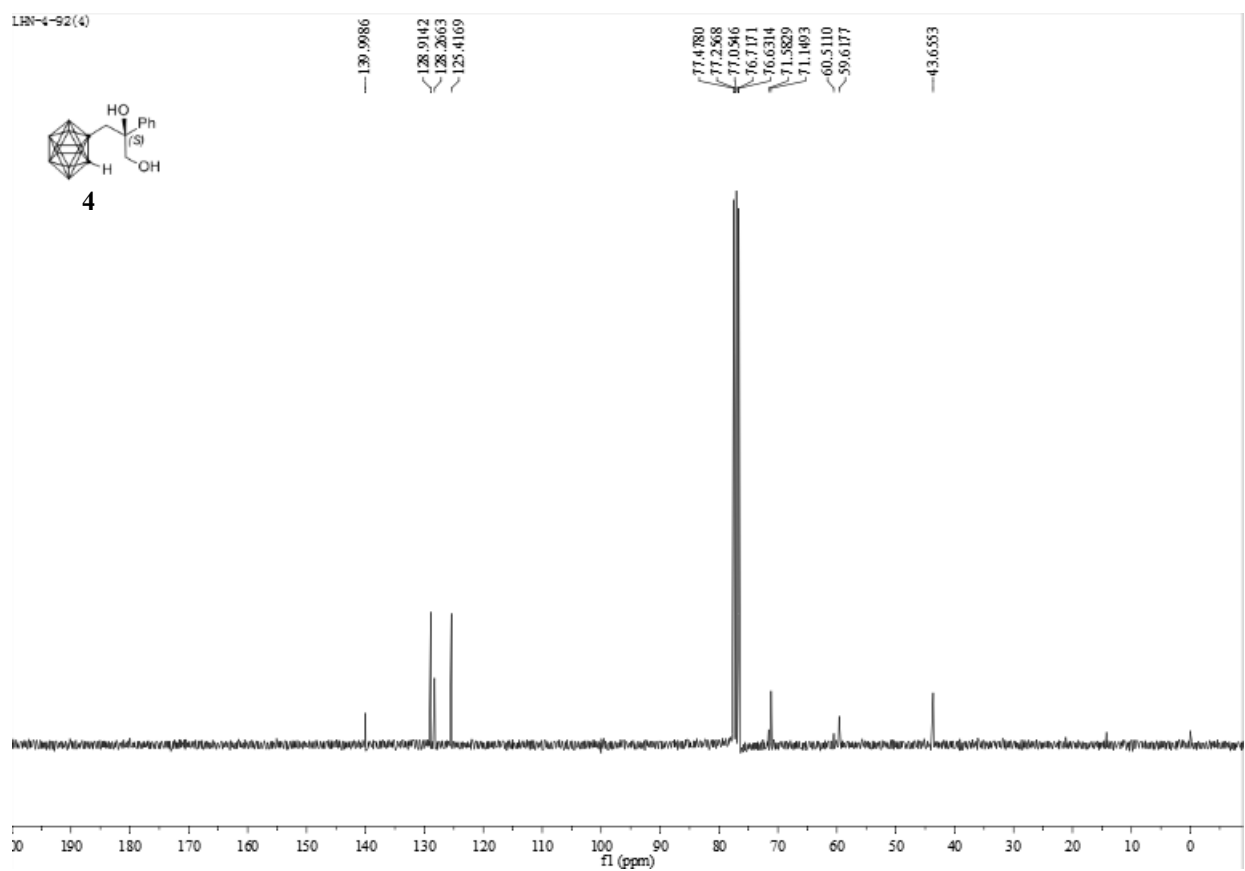
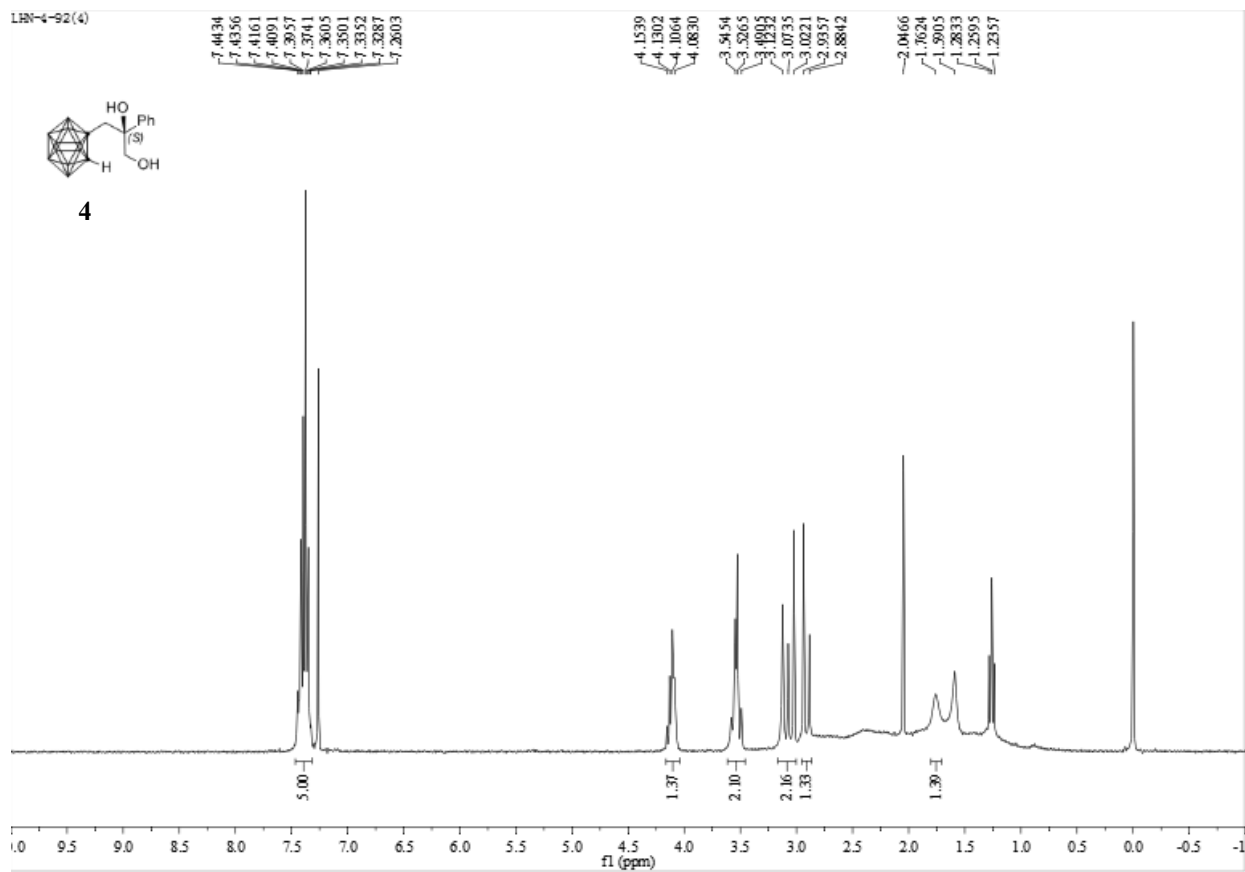


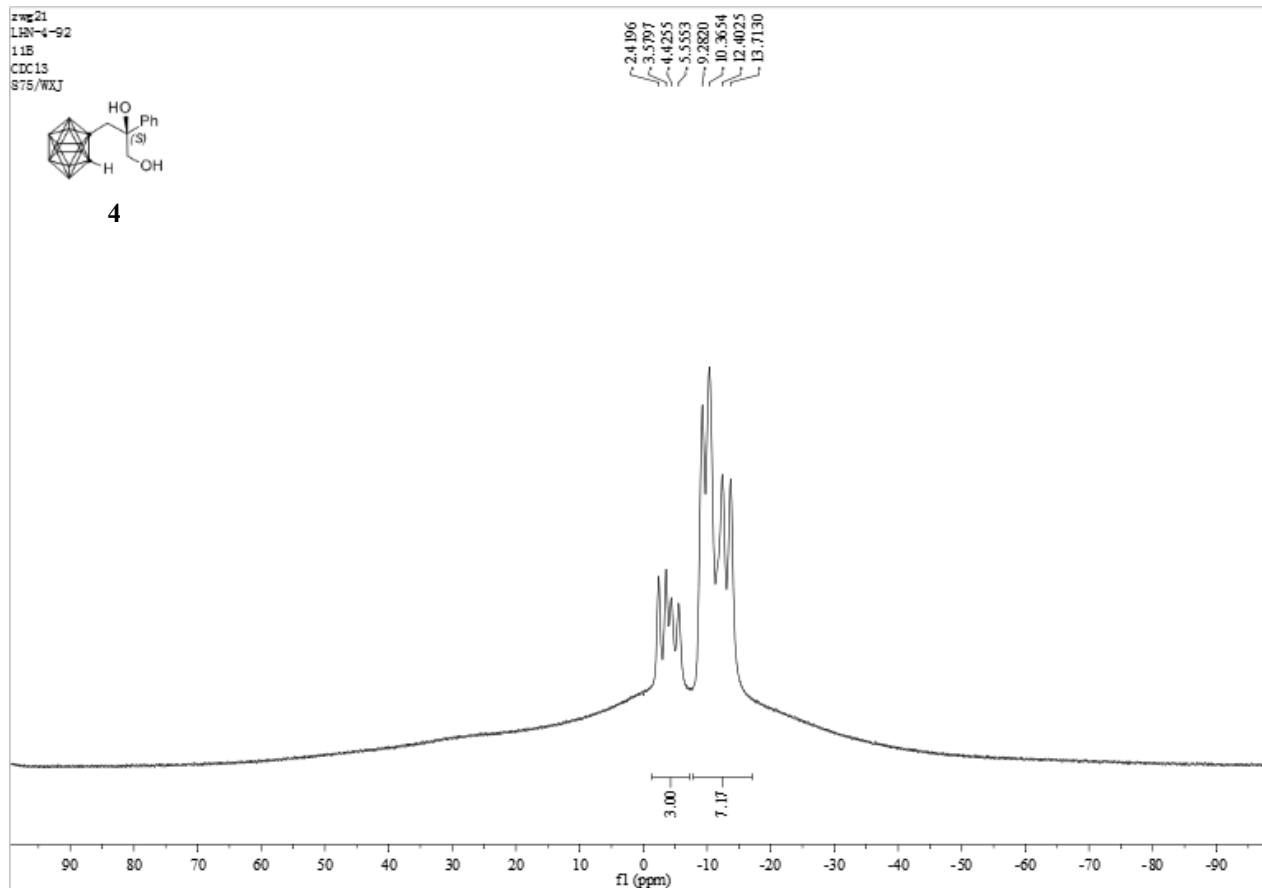


LHN-3-78A. HRMS (ESI) m/z calcd for $C_{10}H_{19}B_{10}O_2^-$ (M-H)⁻ 280.23574, found 280.23593.

LHN-3-78A #12 RT: 0.13 AV: 1 NL: 1.46E6
T: FTMS - p ESI Full ms [50.0000-750.0000]

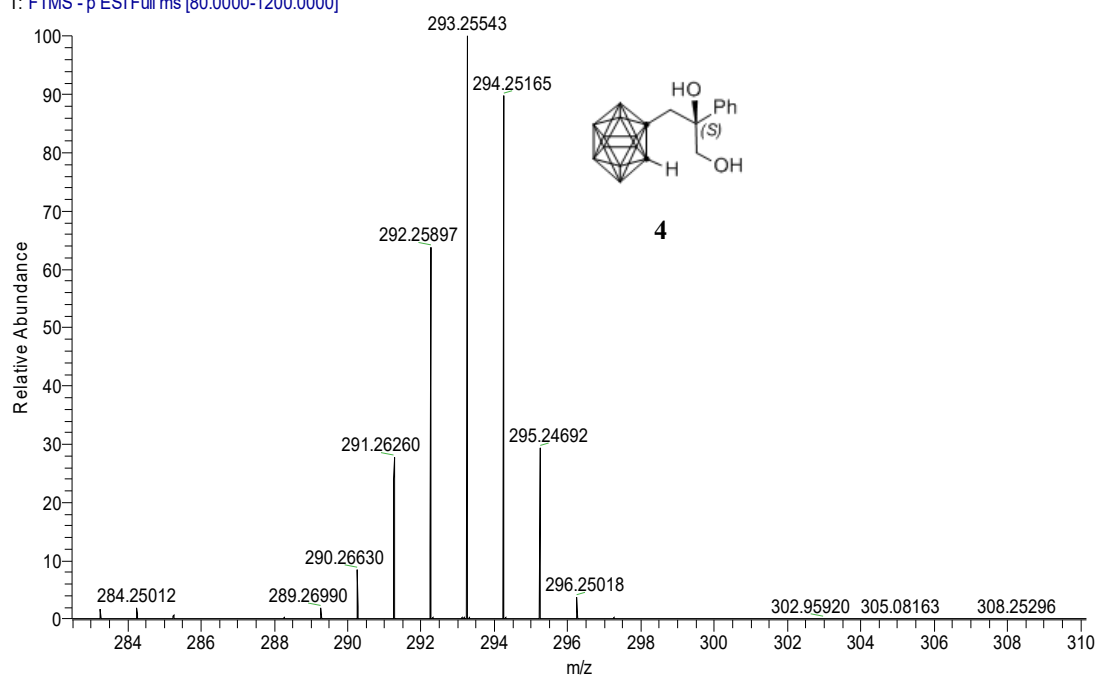






4. HRMS (ESI) m/z calcd for $C_{11}H_{21}B_{10}O_2^-$ (M-H)⁻ 294.25139, found 294.25165.

5-LHN-4-92 #12 RT: 0.09 AV: 1 NL: 1.39E8
 T: FTMS - p ESI Full ms [80.0000-1200.0000]

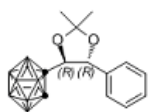


LHN-4-29 1H NMR in CDCl₃ 300M

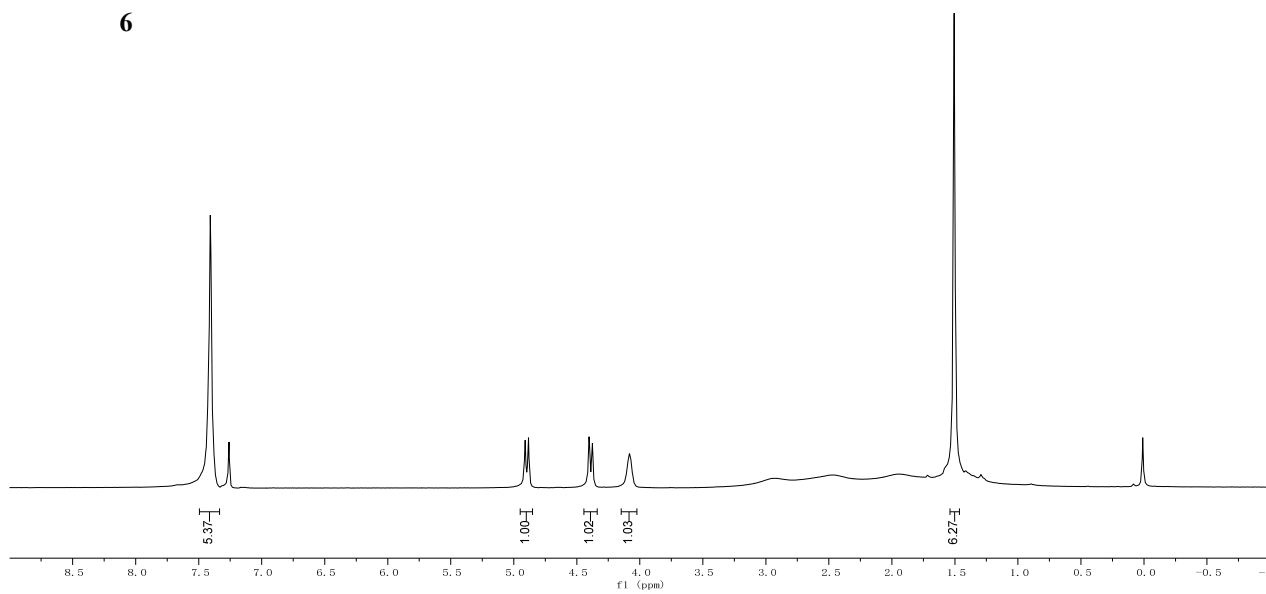
7.4073
7.2699

4.9103
4.8834
4.4028
4.3760
4.0817

1.5054



6



LHN-4-29 13C NMR in CDCl₃ 75M

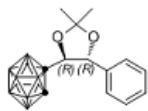
135.0143
128.3291
128.7881
128.2031

110.6305

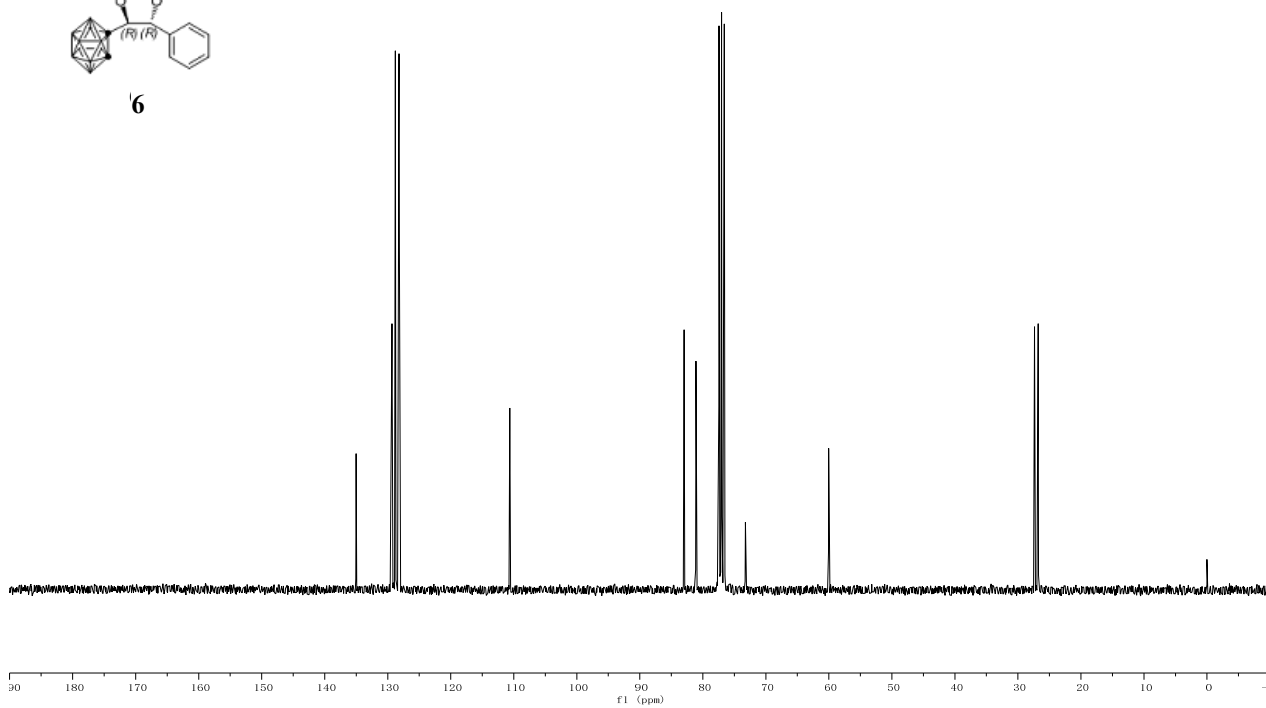
82.9803
81.0986
77.4401
76.0673
73.2513

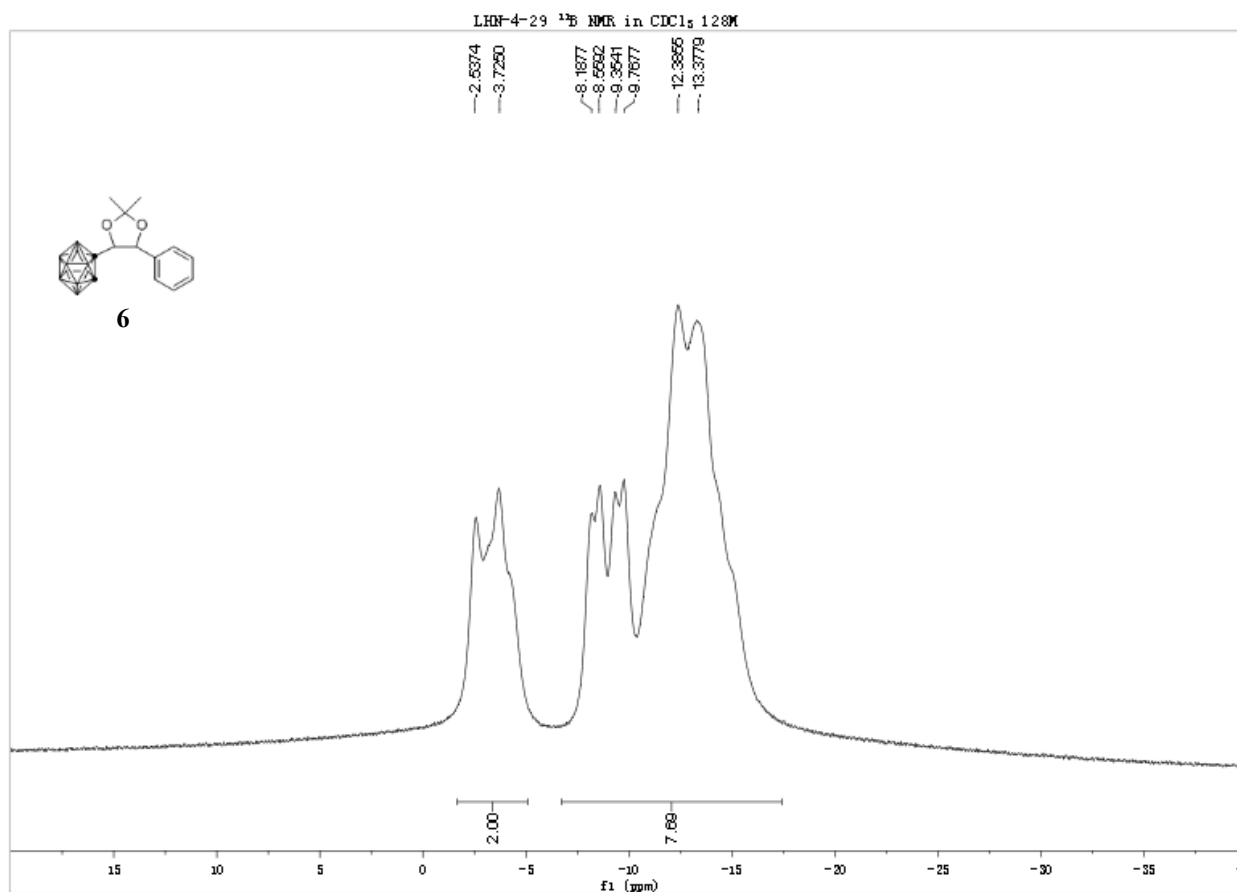
60.0278

27.3563
26.7834



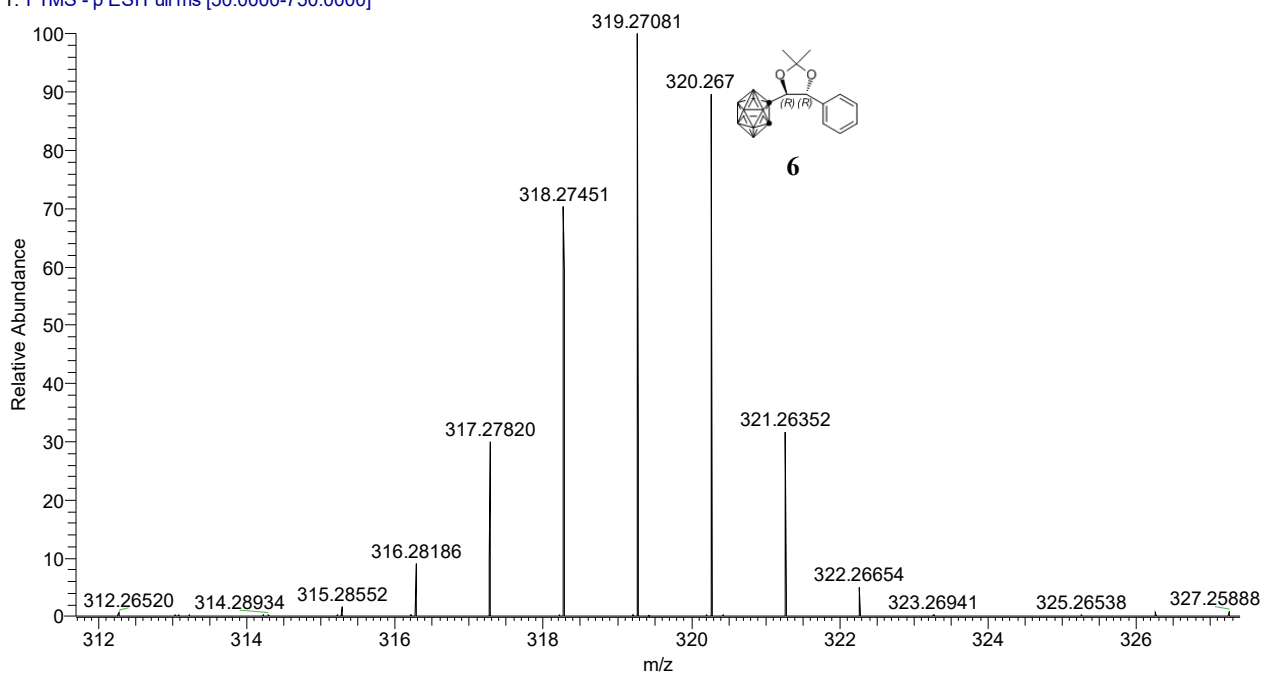
6





LHN-4-29. HRMS (ESI) m/z calcd for $\text{C}_{13}\text{H}_{23}\text{B}_{10}\text{O}_2^-$ (M-H) $^-$ 321.26341, found 321.26352.

LHN-4-29 #10 RT: 0.11 AV: 1 NL: 1.15E7
T: FTMS - p ESI Full ms [50.0000-750.0000]



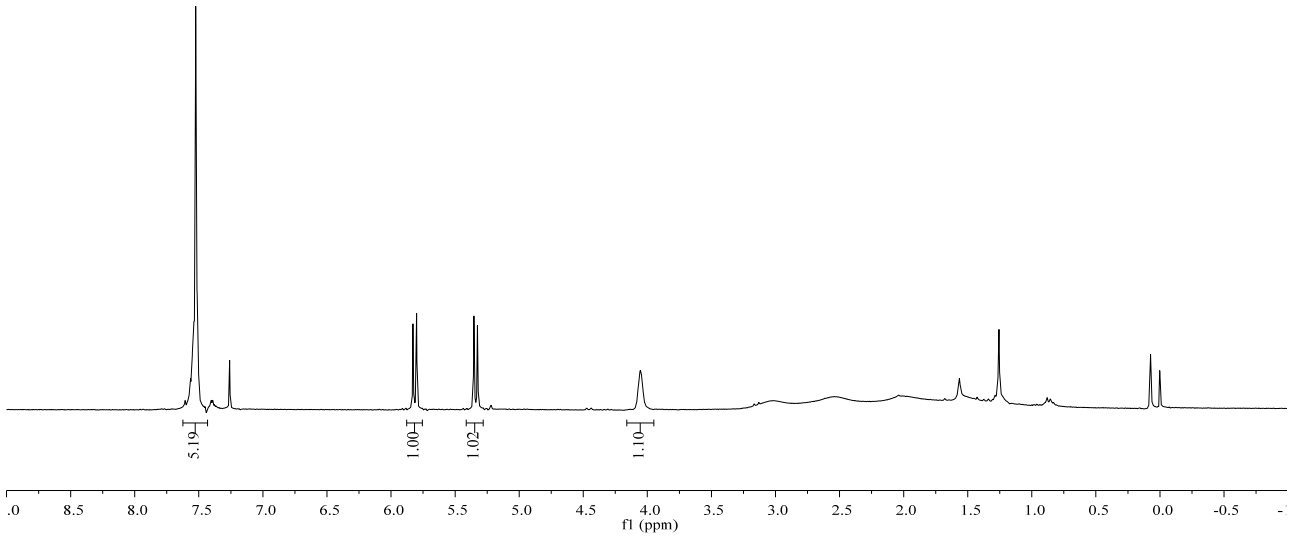
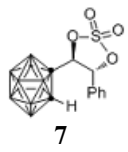
DHX-6-8. 1. fid

7.5469
7.5374
7.5240
7.5127
7.5052

5.8287
5.8010
5.3532
5.3255

DHX-6-8 1H NMR in CDCl₃ 300M

4.0535



DHX-6-8-C. 1. fid

131.8063
129.9070
129.7030
128.6397

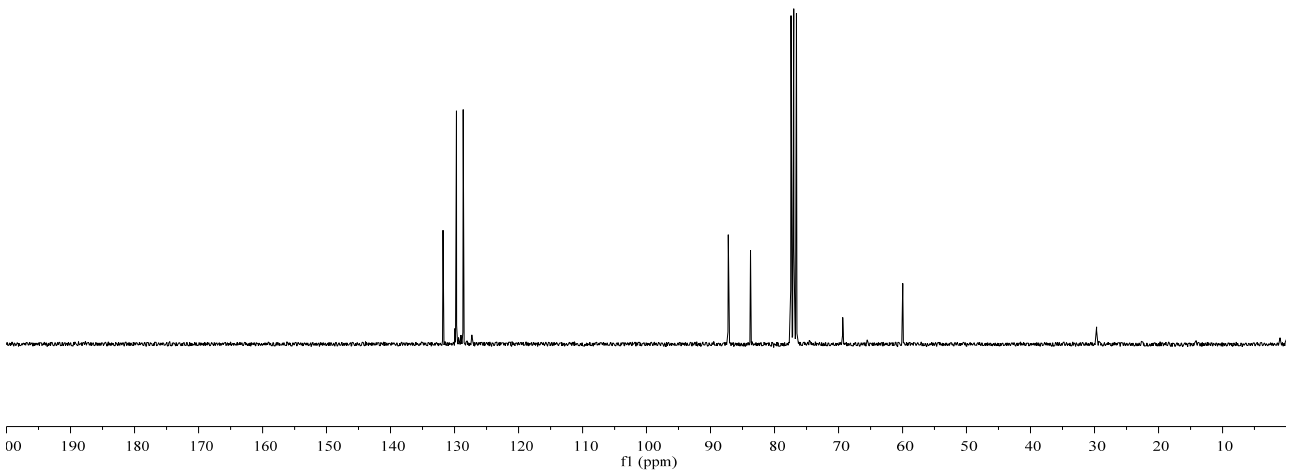
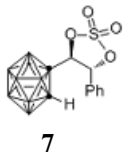
DHX-6-8 13C NMR in CDCl₃ 75M

87.2359
83.7510

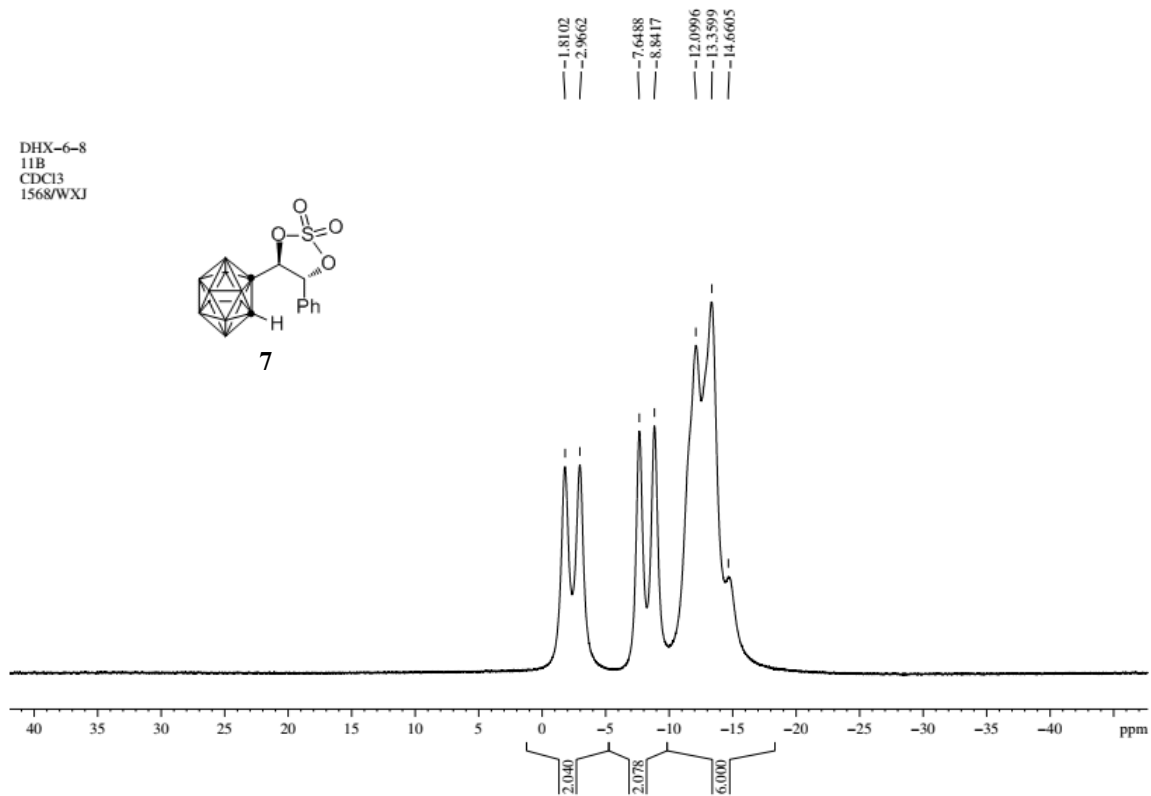
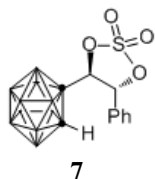
69.3529

59.9746

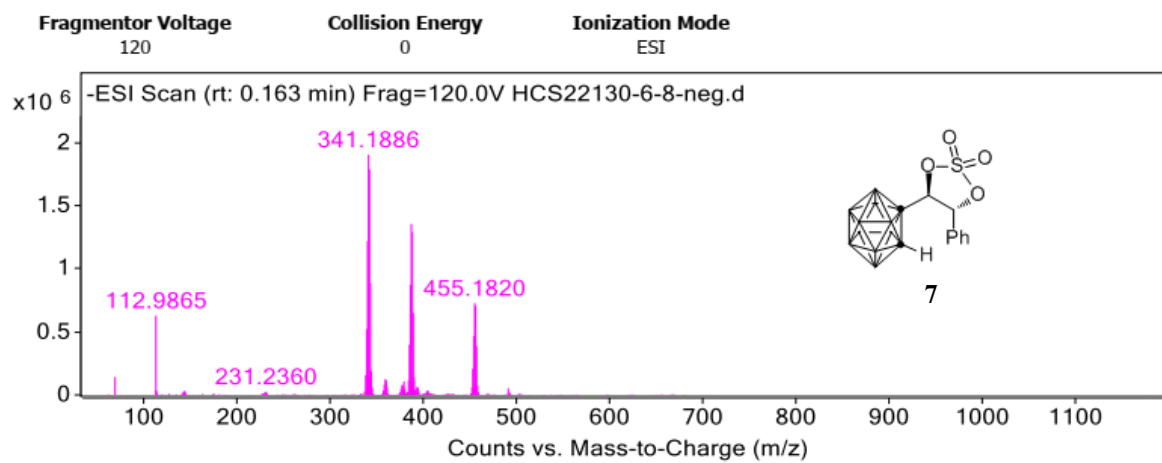
29.6775



DHX-6-8
11B
CDCl3
1568/WXJ



DHX-6-8. HRMS (ESI) m/z calcd for $C_{10}H_{17}B_{10}O_4S^-$ (M-H)⁻ 342.1820, found 342.1854.

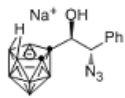


Peak List

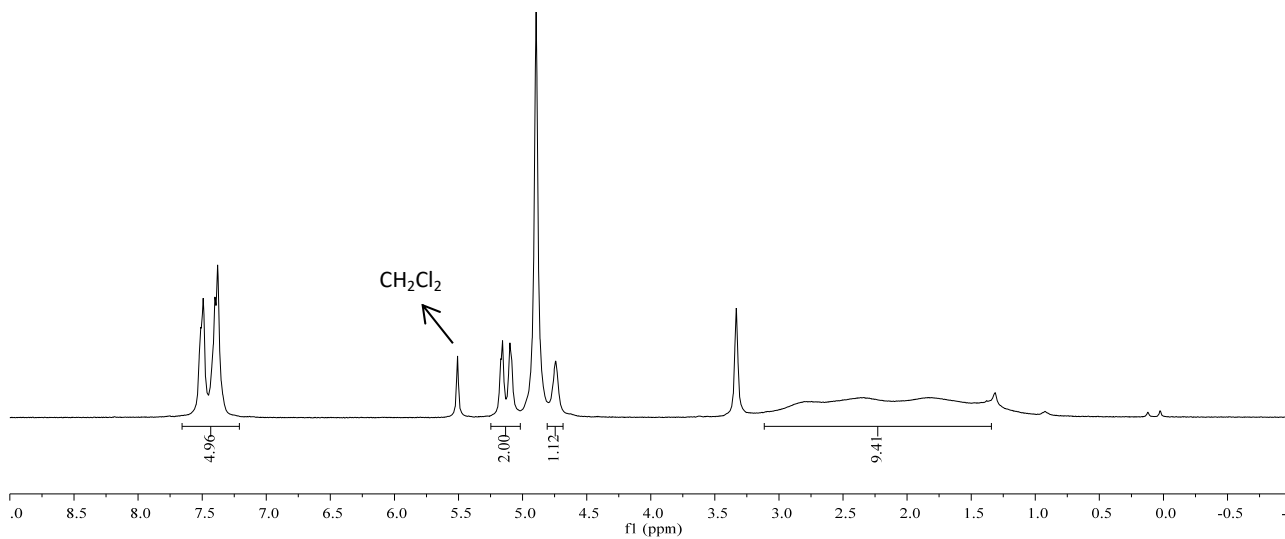
m/z	z	Abund
112.9865		629575.38
339.1957		522686.28
340.1918		1220399.75
341.1886		1906339.88
342.1854		1790748.75
343.183	1	886873.75

DHX-6-10-MEOD. 1. f3
7.5138
7.4908
7.4307
7.4213
7.4012
7.3785
7.3583

DHX-6-10 1H NMR in MeOD-d₄ 300M
5.1716
5.1552
5.1000
5.0834
4.7426



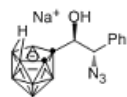
8



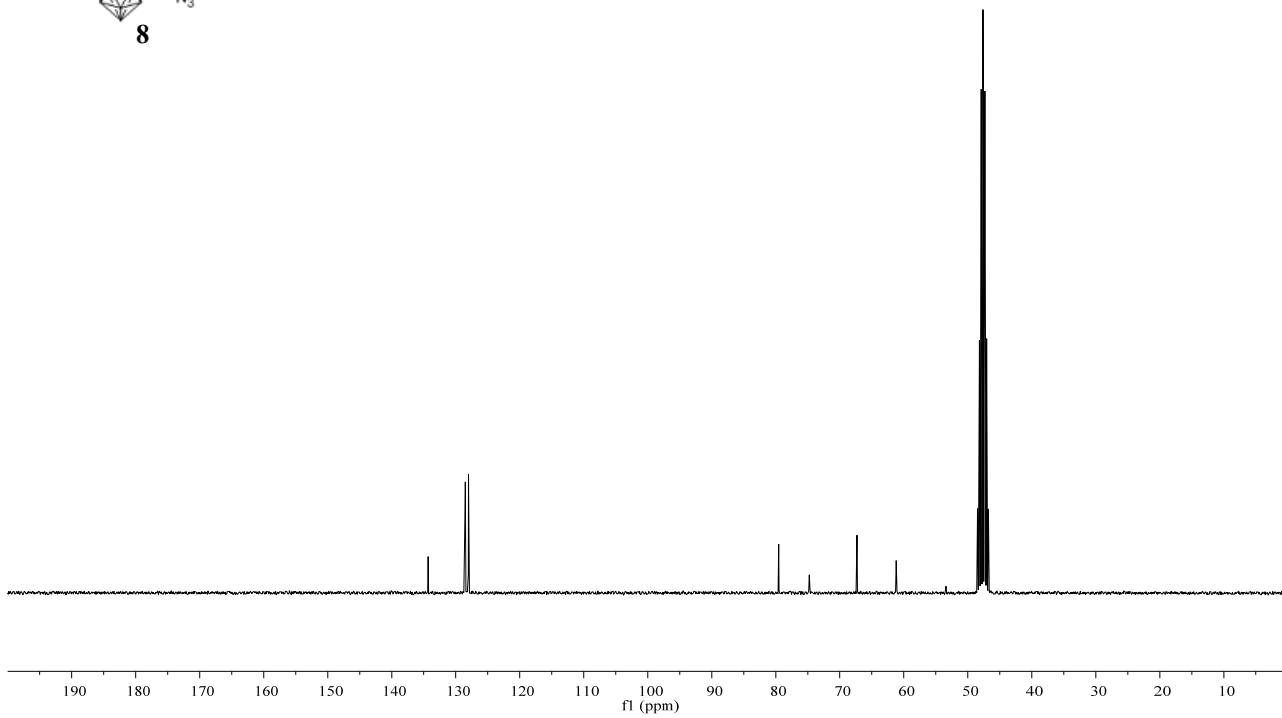
DHX-6-10-MEOD-C. 2. fid

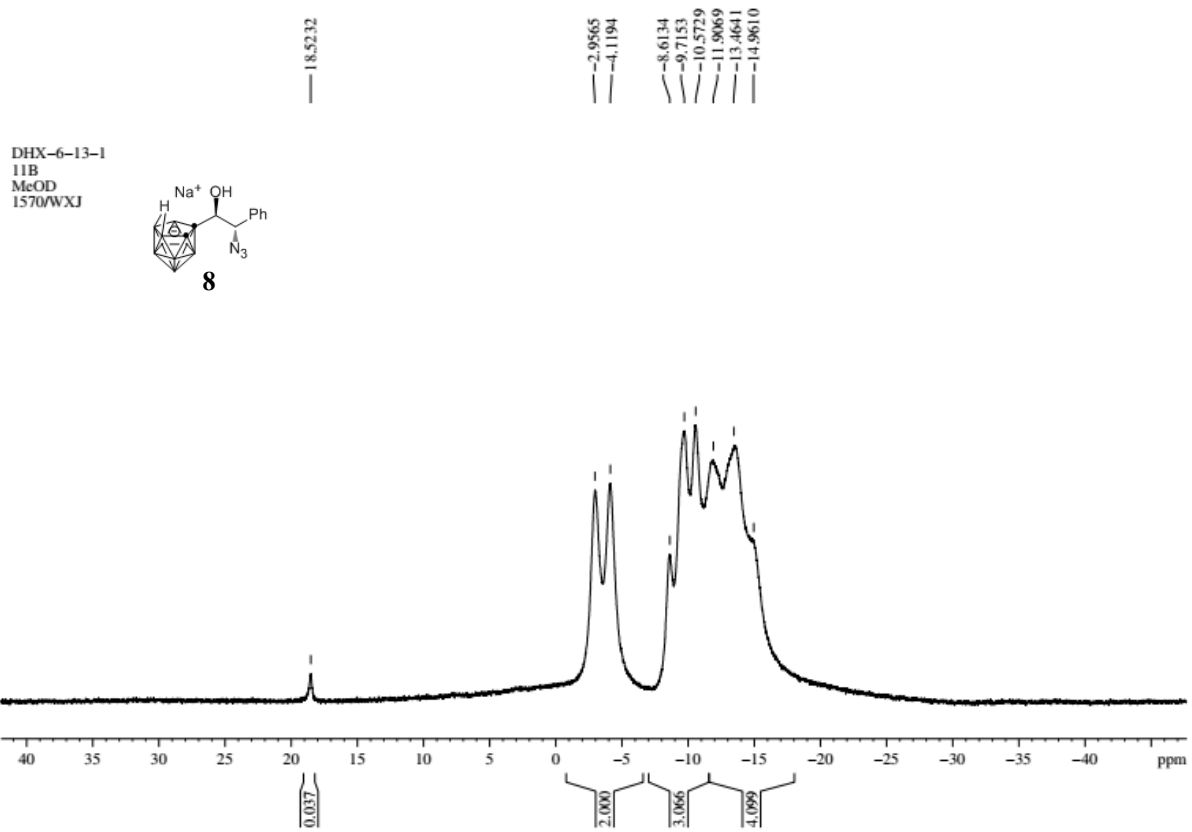
134.3099
128.5086
128.2802
128.0011

79.5386
74.7702
67.3028
61.1953



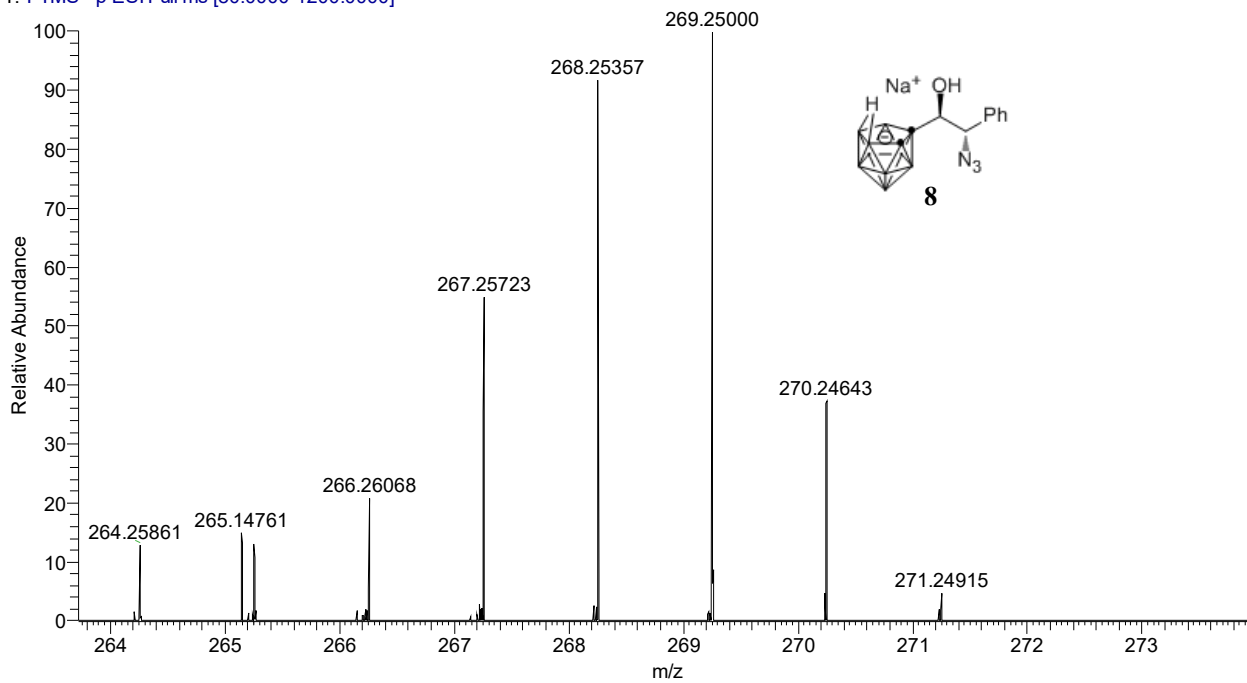
8





DHX-6-10 HRMS (ESI) m/z calcd for $C_{10}H_{19}B_9N_3ONa$ (M-Na)⁻ 295.24074, found 295.24011.

119-3 #14 RT: 0.10 AV: 1 NL: 1.42E6
T: FTMS - p ESI Full ms [80.0000-1200.0000]



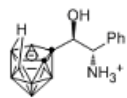
6-16-HCL-6.3.fid

DHX-6-16 1H NMR in MeOD-d₄ 300M

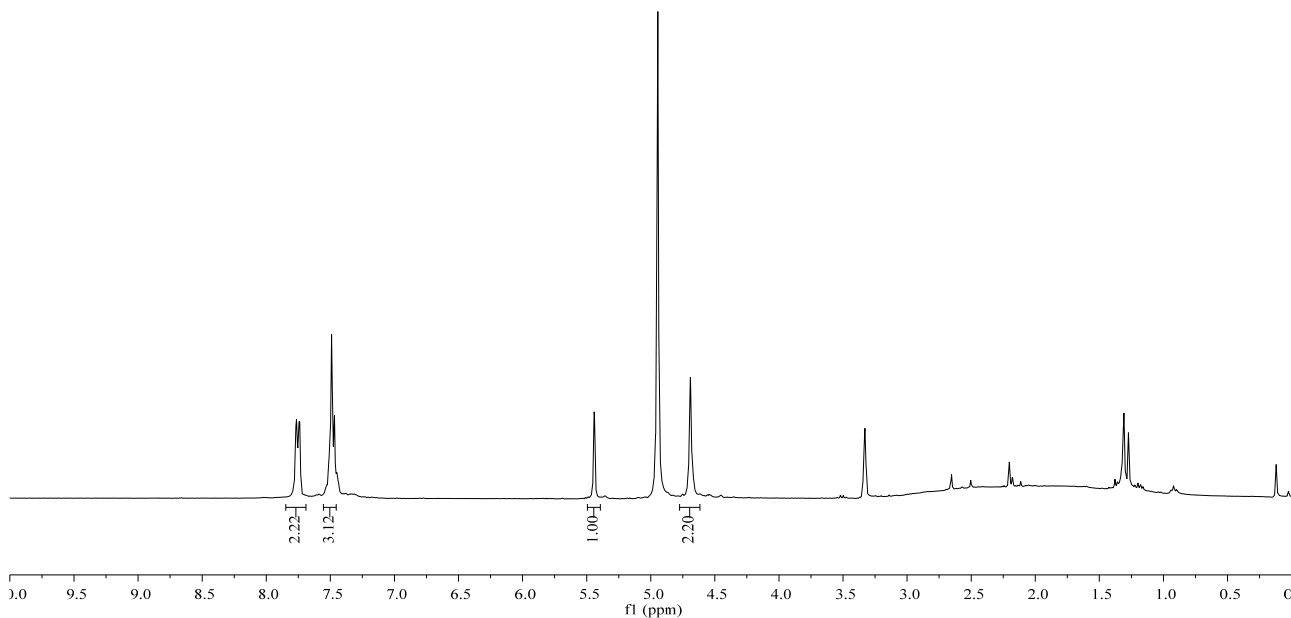
7.7688
7.7629
7.7451
7.7373
7.4904
7.4676

5.4392

4.6951
4.6884



9



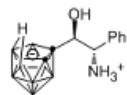
DHX-6-16-HCL-2-C/3h

DHX-6-16 13C NMR in MeOD-d₄ 75M

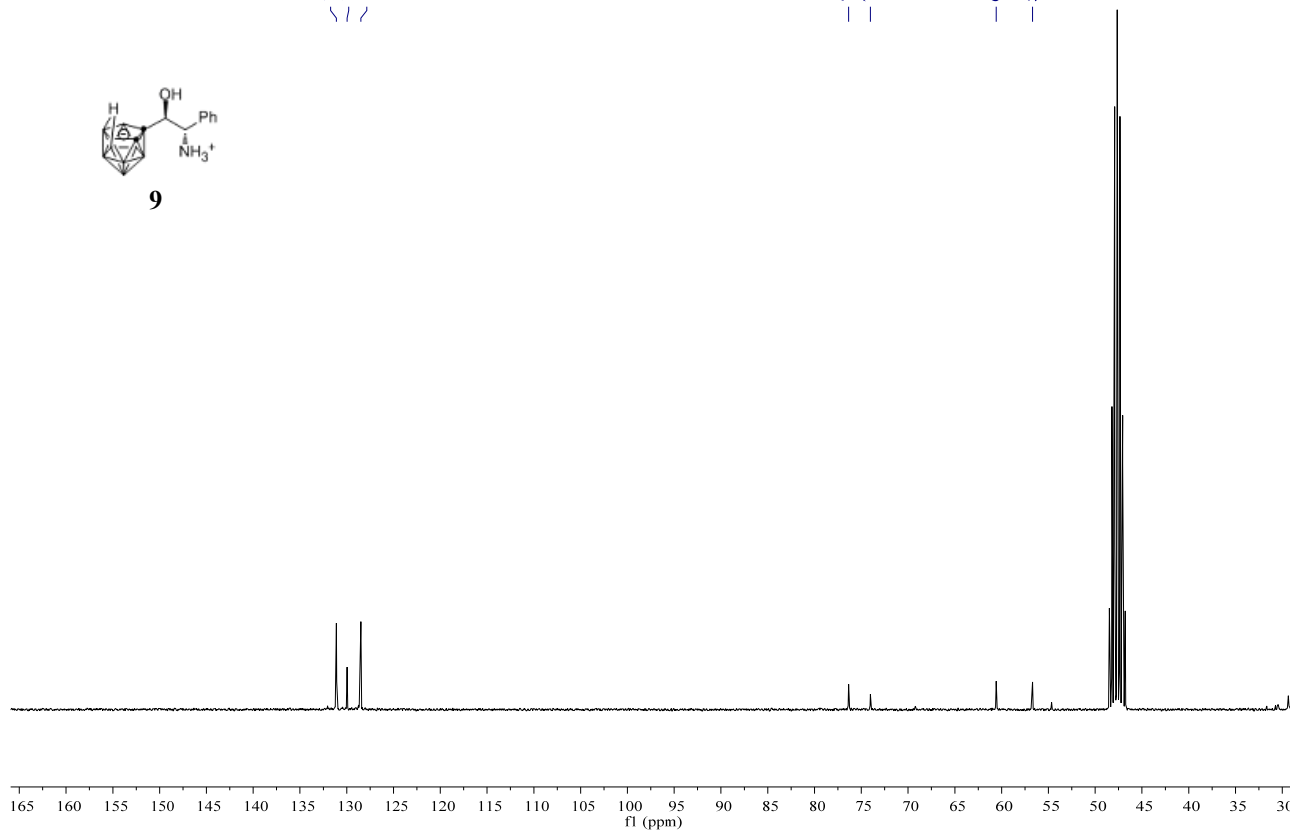
131.1038
129.9555
128.4842

76.3559
74.0285

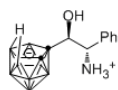
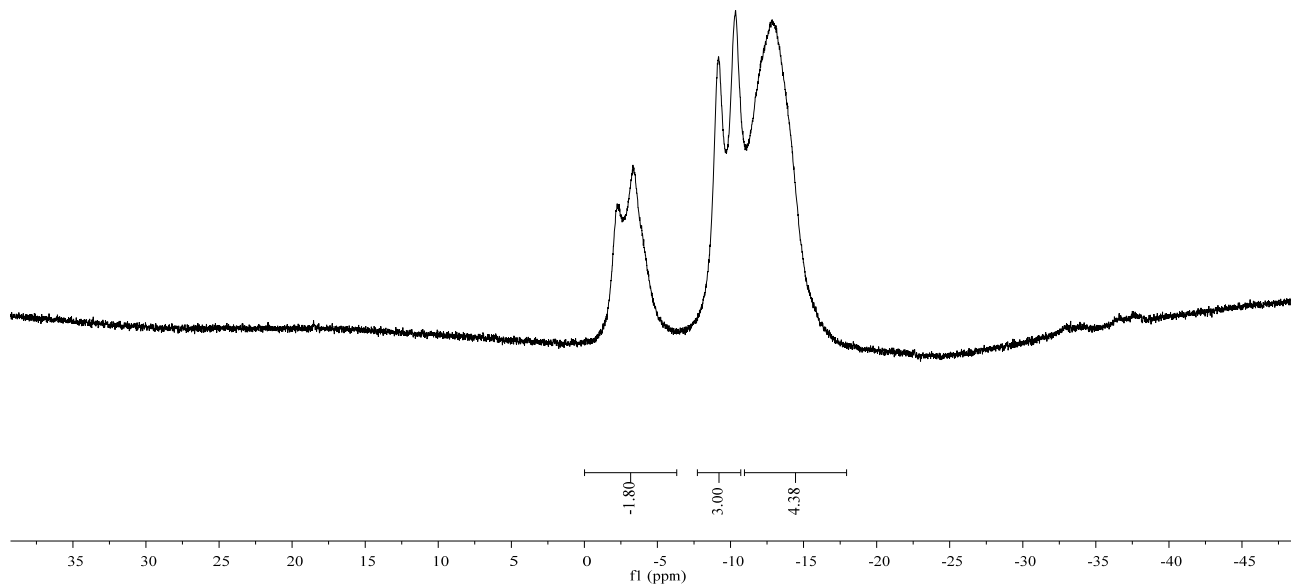
60.5793
56.6985



9

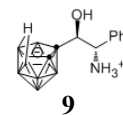
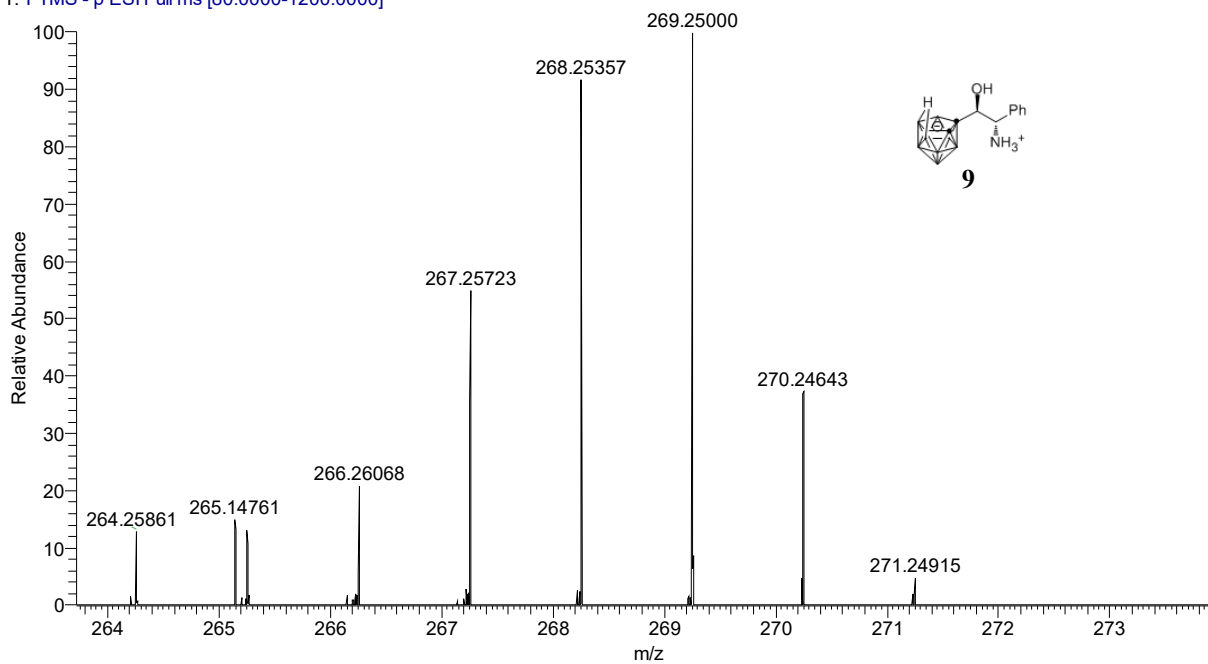


-2.2393
 -3.4143
 -9.1650
 -10.3353
 -12.8098
 -14.5299

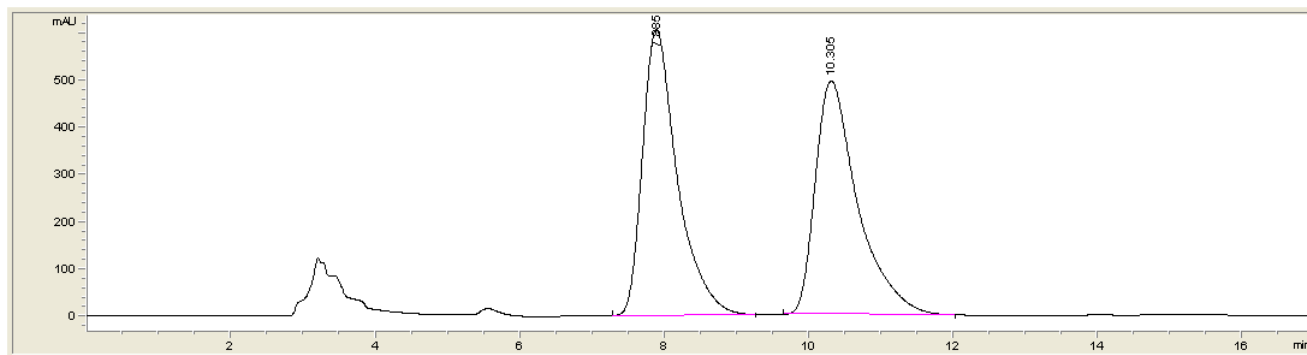
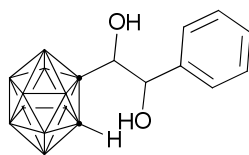
**9**

DHX-6-15-1. HRMS (ESI) m/z calcd for $C_{10}H_{21}B_9NO^+$ (M) 269.25024, found 269.25000.

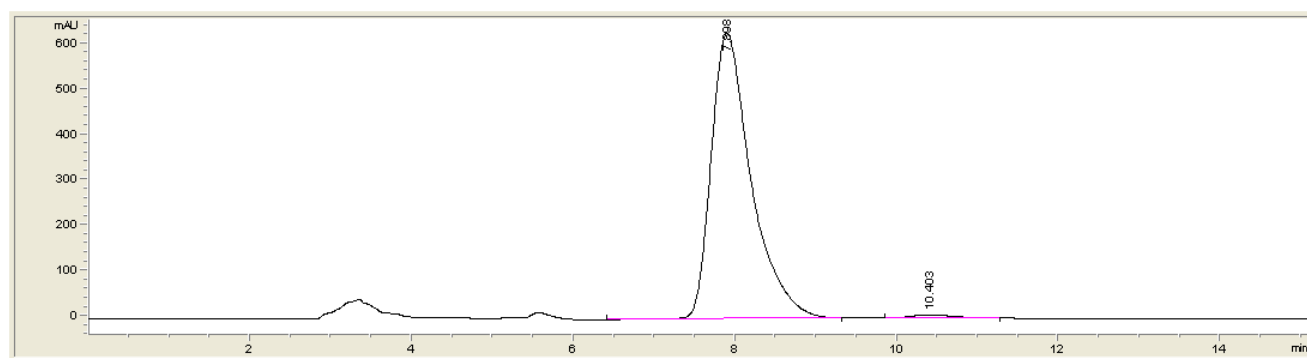
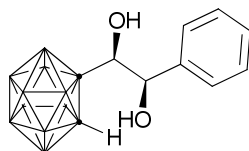
119-3 #14 RT: 0.10 AV: 1 NL: 1.42E6
 T: FTMS - p ESI Full ms [80.0000-1200.0000]

**9**

HPLC for racemic and pure enantioenriched sample 2a

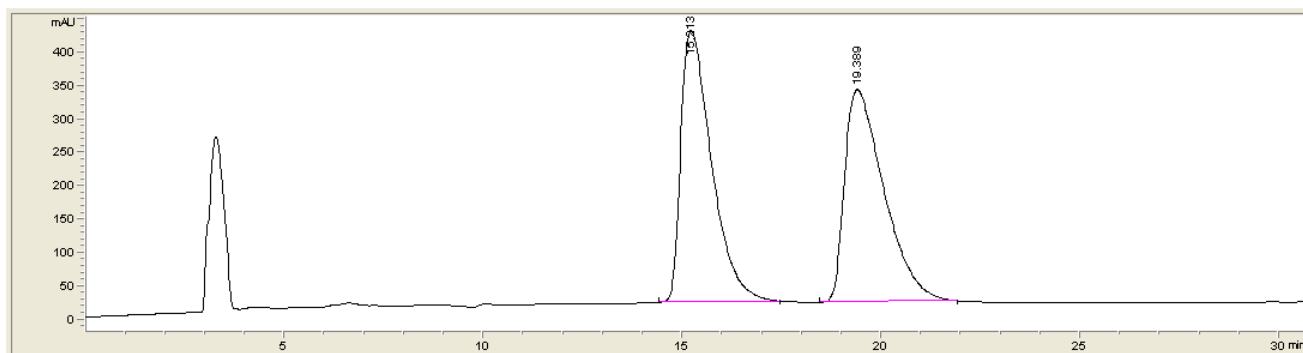
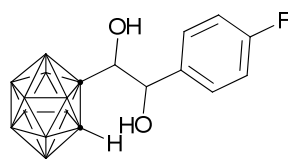


峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	7.885	BB	0.5036	2.03316e4	605.79352	50.1314
2	10.305	BB	0.6090	2.02250e4	494.71295	49.8686

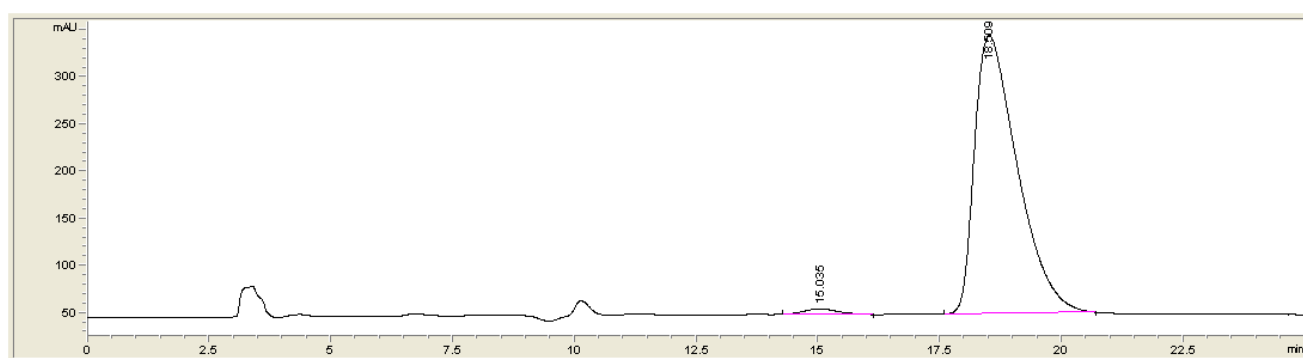
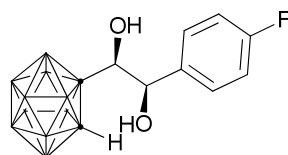


峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	7.898	BB	0.5170	2.17079e4	628.43134	98.7762
2	10.403	BB	0.5495	268.94867	7.37392	1.2238

HPLC for racemic and pure enantioenriched sample **2b**

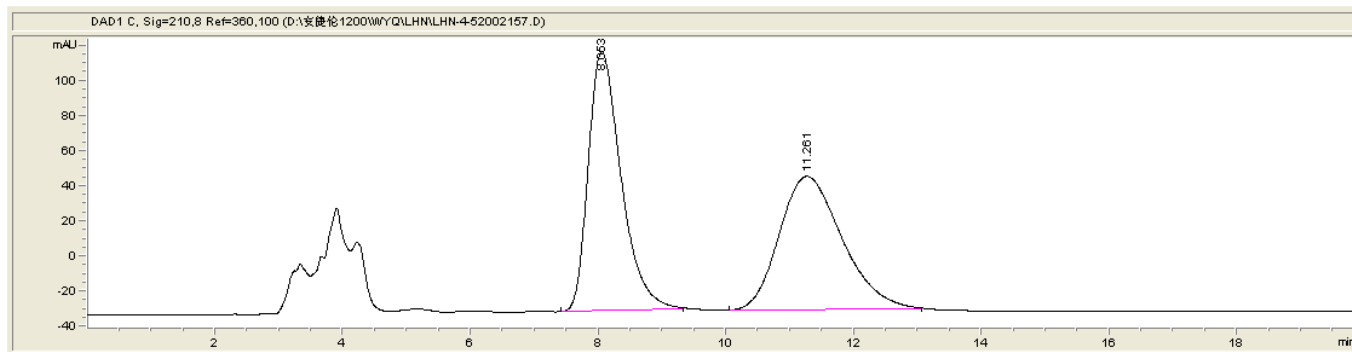
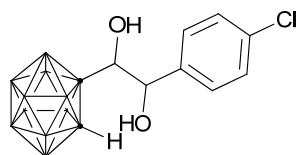


峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	15.213	BB	0.8156	2.18395e4	407.29001	49.9054
2	19.389	BB	1.0548	2.19223e4	318.60016	50.0946

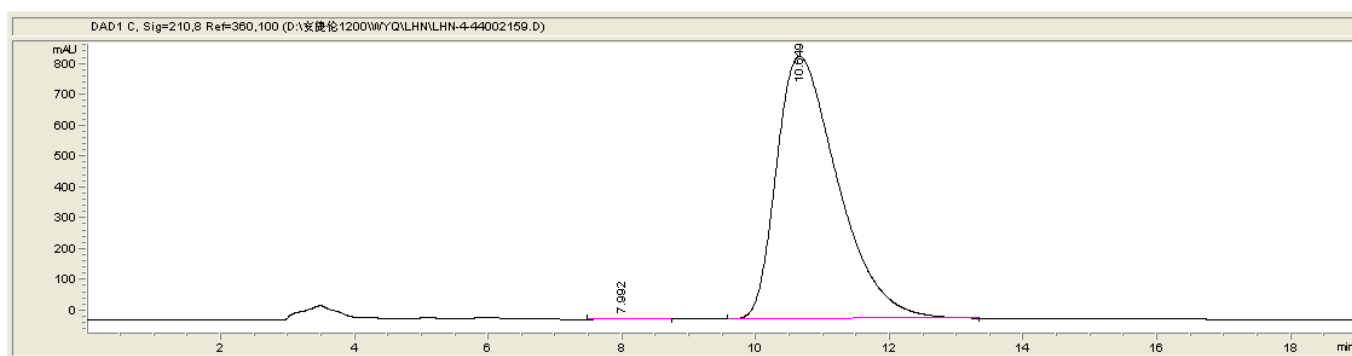
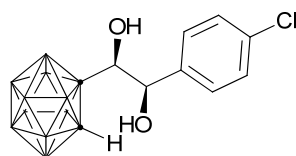


峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	15.035	BB	0.6986	294.74872	5.94304	1.6004
2	18.509	BB	0.9177	1.81229e4	295.40921	98.3996

HPLC for racemic and pure enantioenriched sample 2c

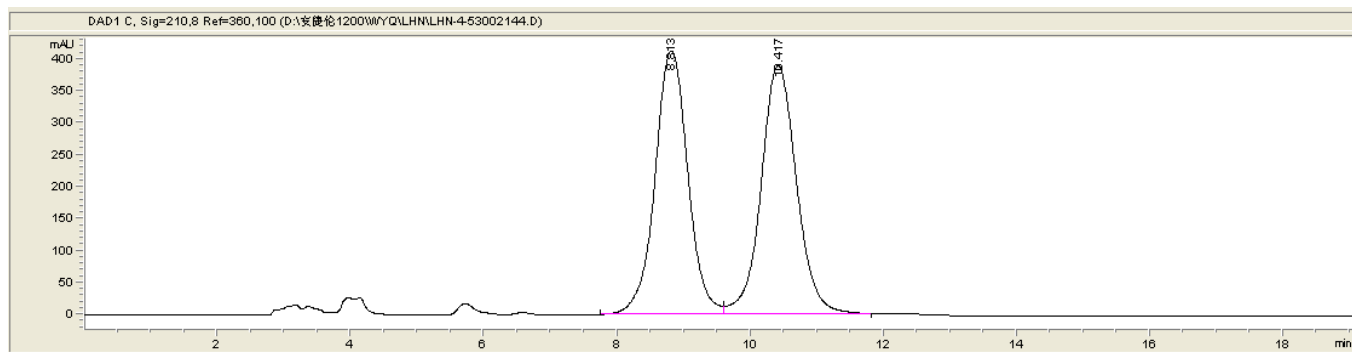
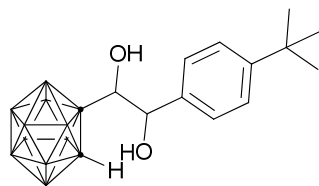


峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	8.053	BB	0.5446	5274.15186	147.70303	50.3873
2	11.261	BB	1.0439	5193.07520	75.92722	49.6127

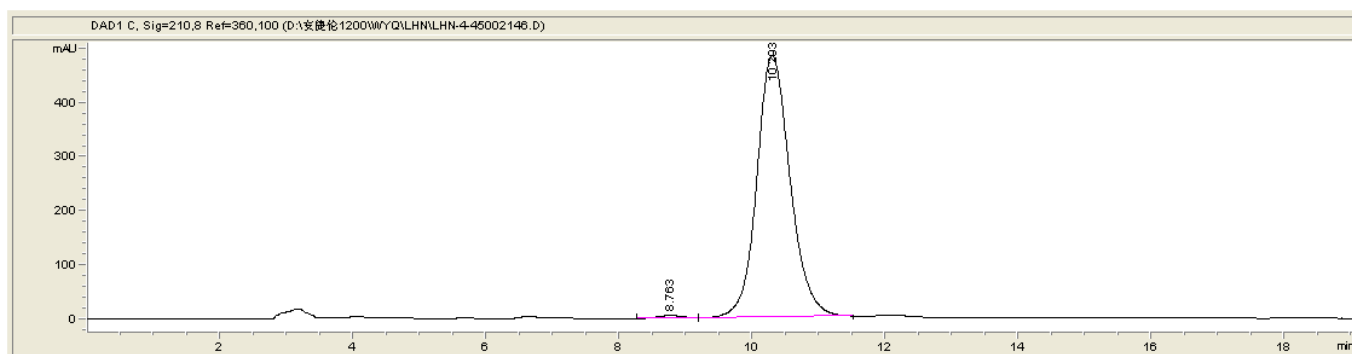
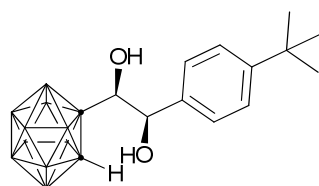


峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	7.992	BB	0.4492	104.77180	3.27511	0.1923
2	10.649	BB	0.9753	5.43894e4	851.42664	99.8077

HPLC for racemic and pure enantioenriched sample 2d

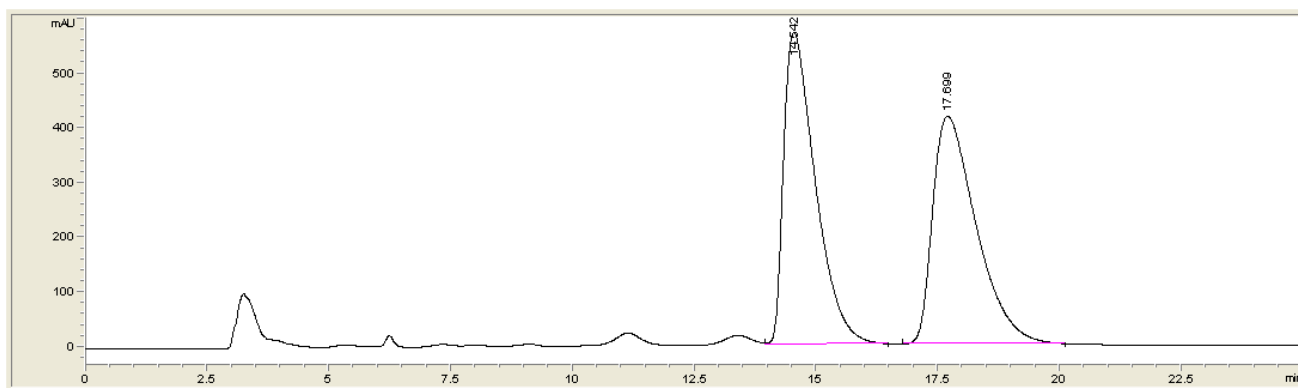
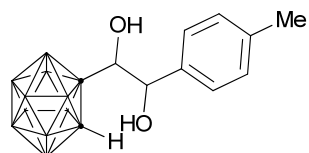


峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	8.813	BV	0.5330	1.41680e4	412.16479	49.5783
2	10.417	VB	0.5698	1.44091e4	389.31464	50.4217

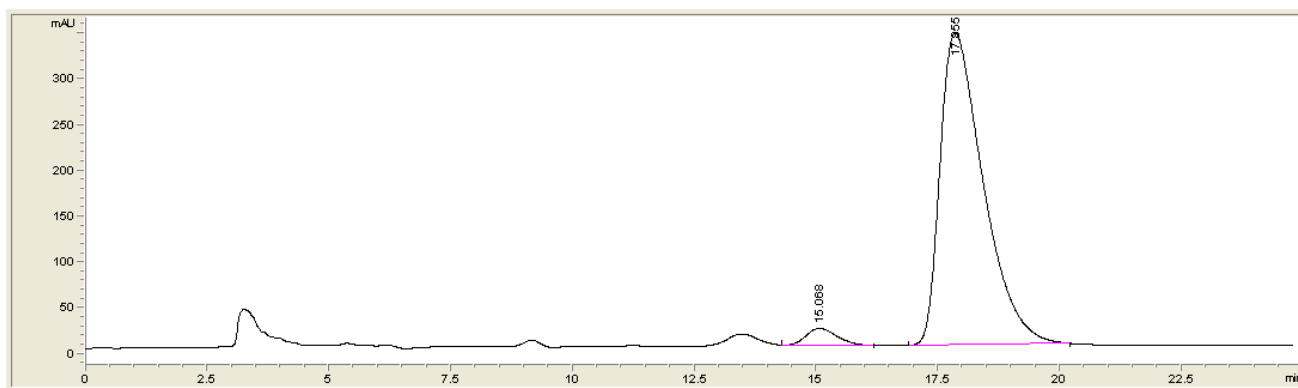
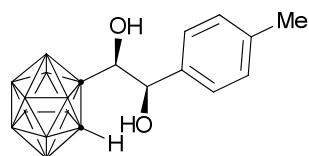


峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	8.763	BV	0.3838	116.29890	4.68217	0.6858
2	10.293	VB	0.5344	1.68429e4	483.54950	99.3142

HPLC for racemic and pure enantioenriched sample 2e

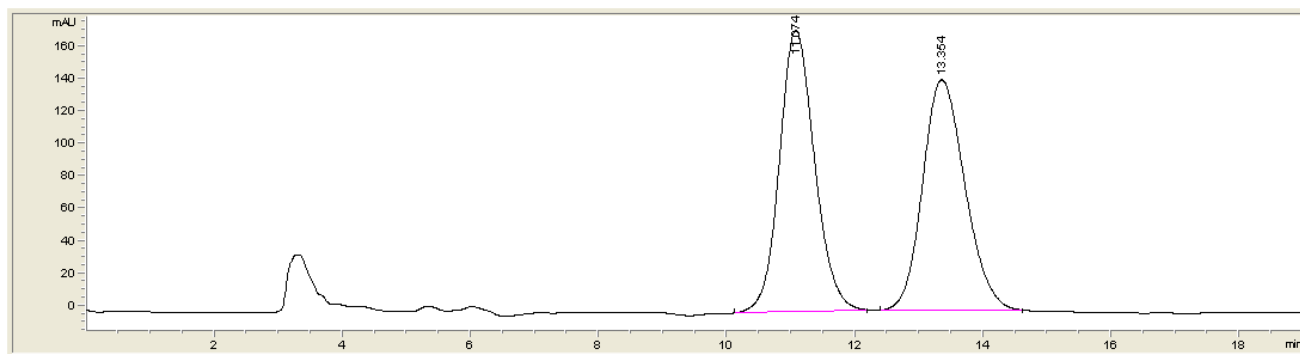
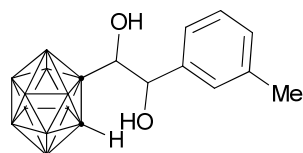


峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	14.542	VB	0.6910	2.59691e4	570.52899	50.0712
2	17.699	BB	0.9512	2.58952e4	416.59033	49.9288

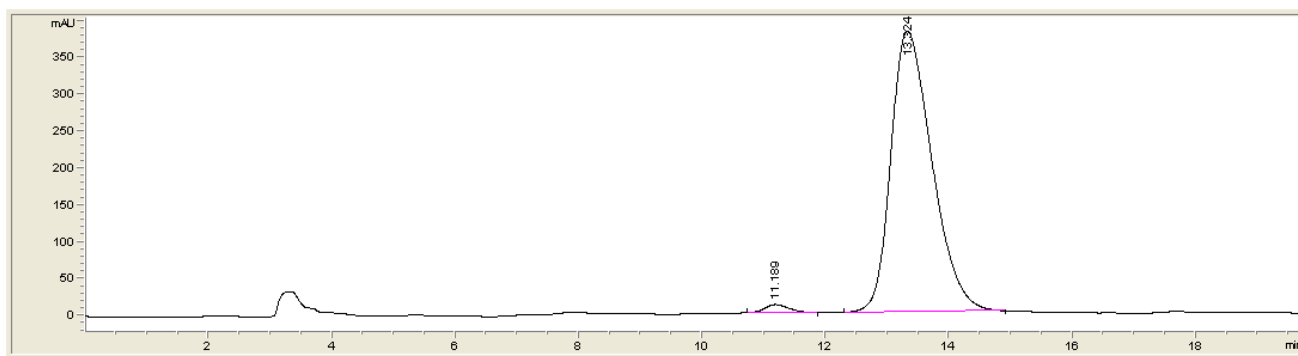
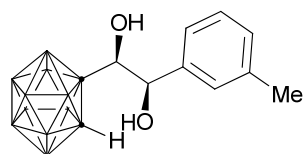


峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	15.068	VB	0.6903	844.27185	18.85989	3.8551
2	17.855	BB	0.9383	2.10558e4	341.03125	96.1449

HPLC for racemic and pure enantioenriched sample 2f

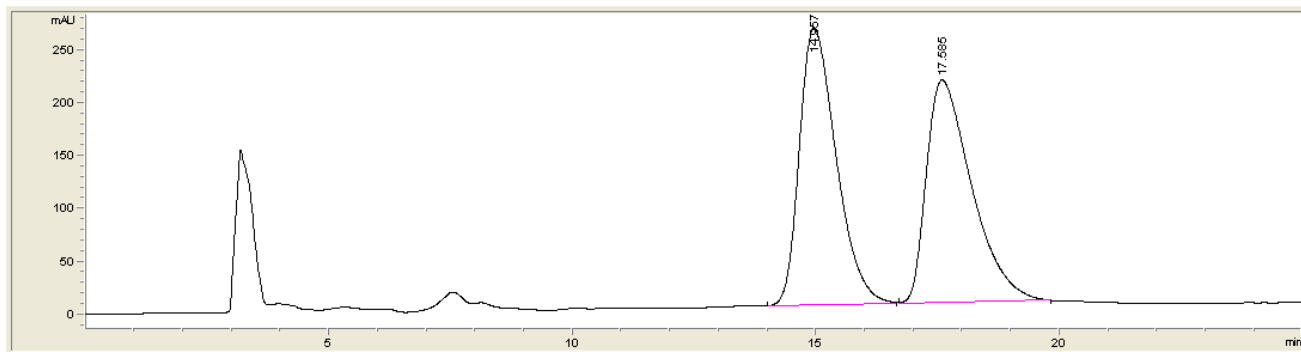
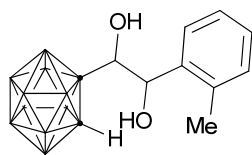


峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	11.074	BB	0.5855	6631.85449	173.68483	50.3293
2	13.354	BB	0.7090	6545.06982	142.18535	49.6707

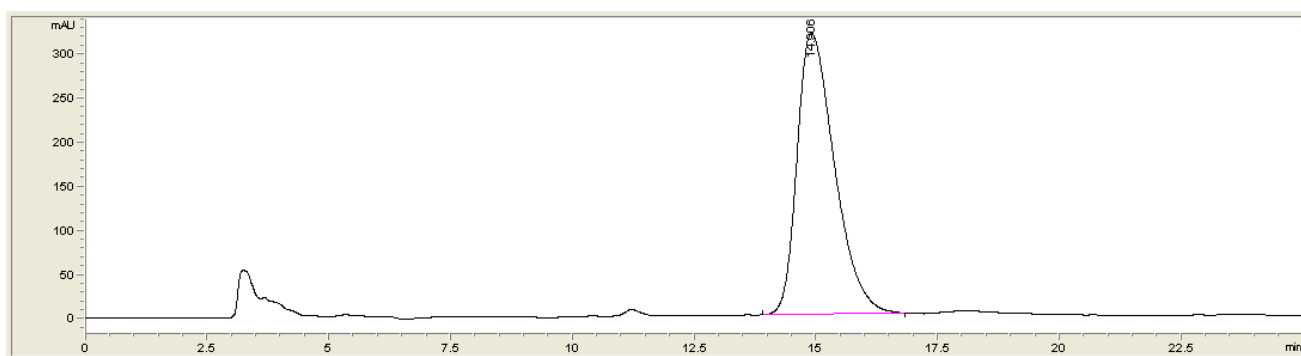
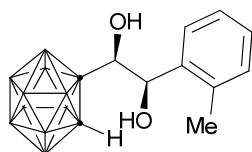


峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	11.189	BB	0.4168	308.29636	11.21220	1.7138
2	13.324	BB	0.7176	1.76811e4	380.84375	98.2862

HPLC for racemic and pure enantioenriched sample 2g

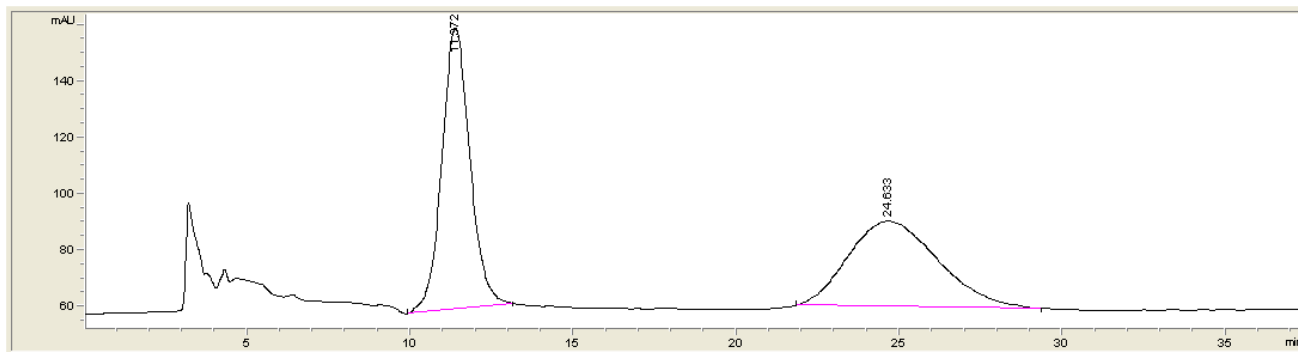
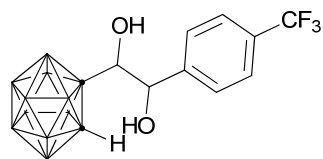


峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	14.957	BB	0.8141	1.38389e4	262.06754	50.3090
2	17.585	BB	0.9763	1.36689e4	210.84578	49.6910

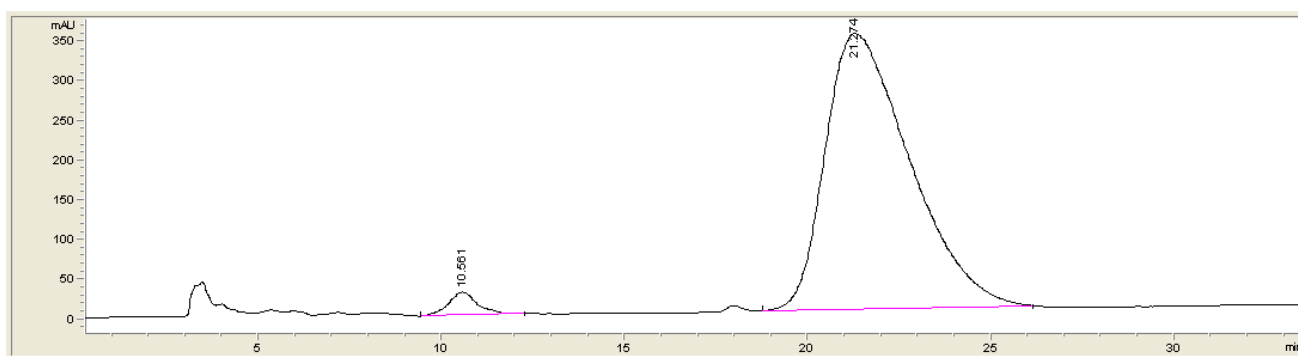
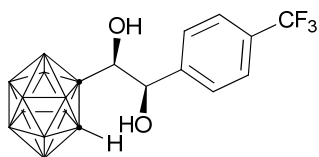


峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	14.906	BB	0.8260	1.71037e4	318.78015	100.0000

HPLC for racemic and pure enantioenriched sample 2h

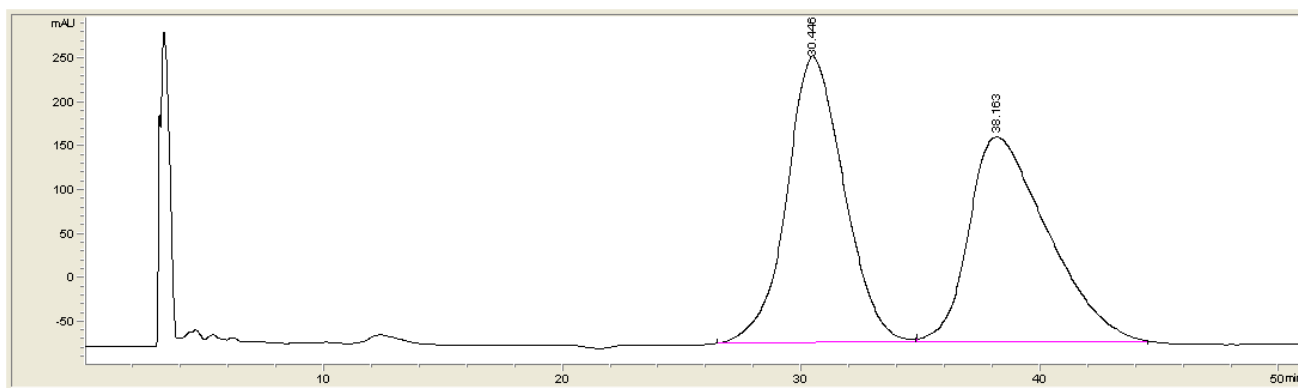
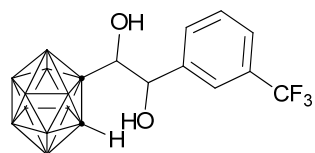


峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	11.372	BB	0.9147	5990.68604	99.73912	50.9016
2	24.633	BB	2.2563	5778.47021	30.25425	49.0984

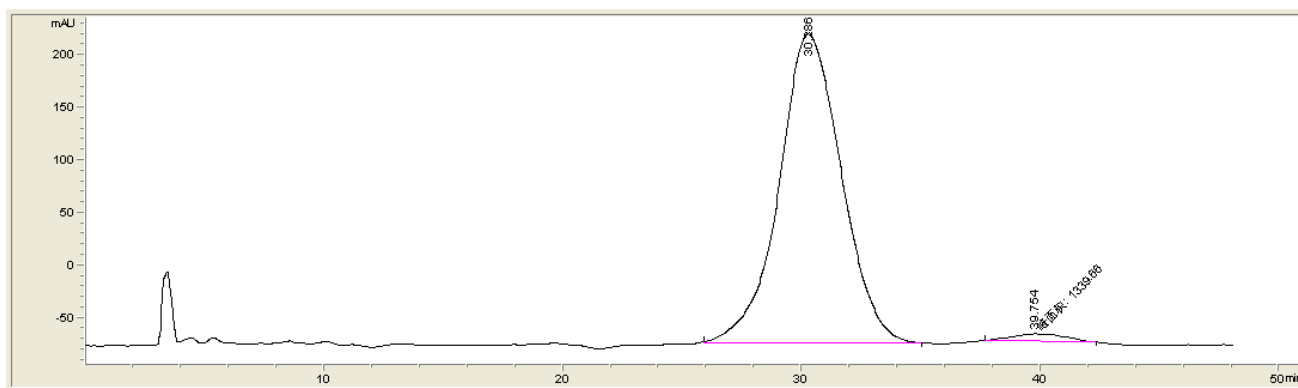
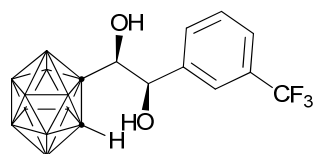


峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	10.561	BB	0.8063	1566.56543	28.72444	2.7265
2	21.274	BB	2.1212	5.58908e4	348.09738	97.2735

HPLC for racemic and pure enantioenriched sample 2i

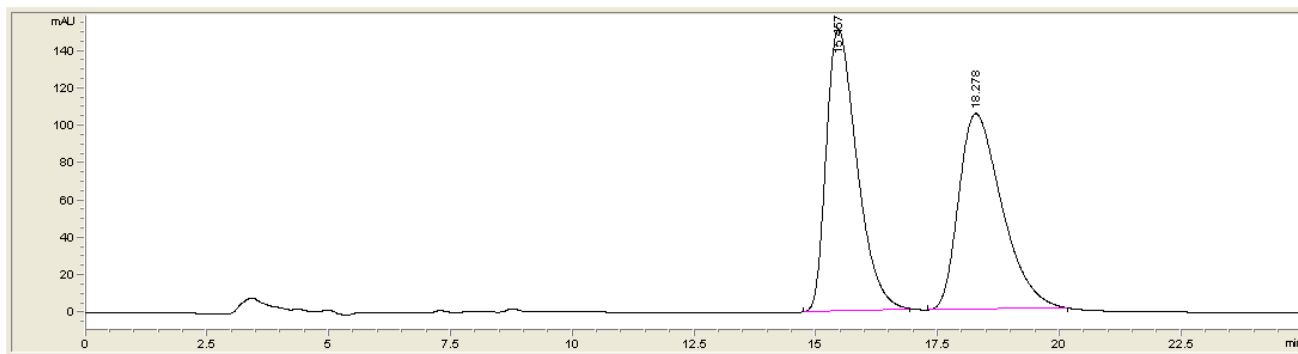
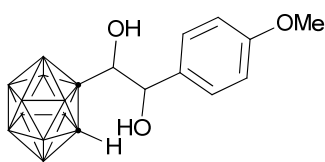


峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	30.446	BB	2.3268	5.46414e4	327.45657	50.4037
2	38.163	BB	2.7996	5.37661e4	234.09047	49.5963

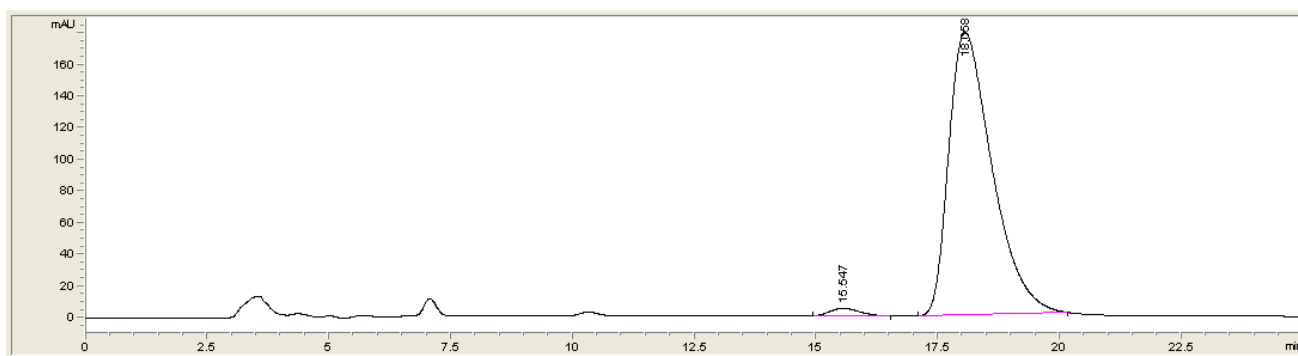
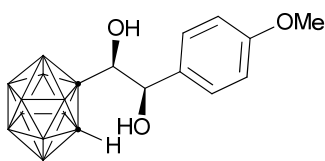


峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	30.286	BB	2.4466	5.35593e4	295.21786	97.5598
2	39.754	MM	2.8032	1339.65540	7.96504	2.4402

HPLC for racemic and pure enantioenriched sample 2j

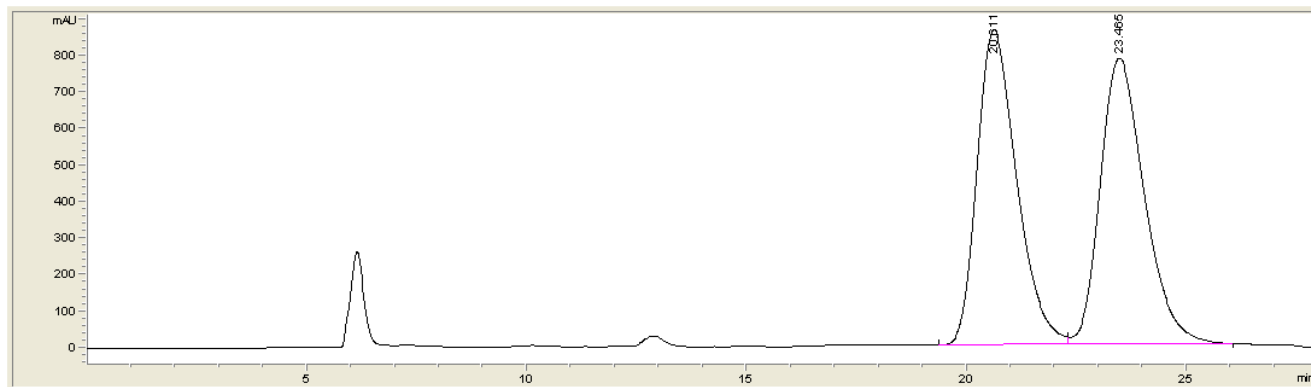
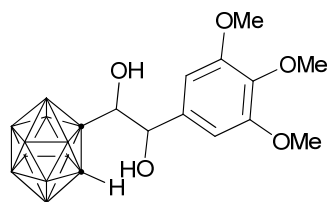


峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	15.457	BB	0.6744	6628.87549	150.94138	50.5158
2	18.278	BB	0.9463	6493.51611	104.88640	49.4842

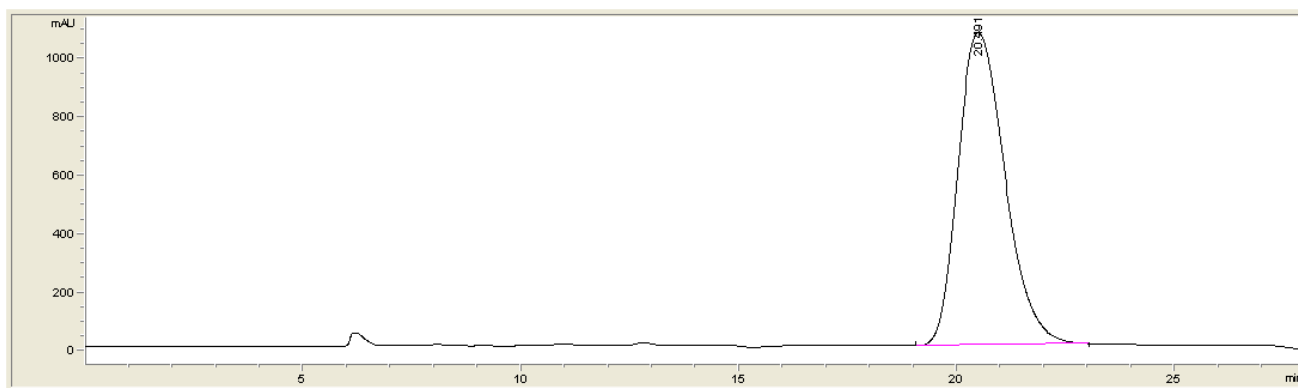
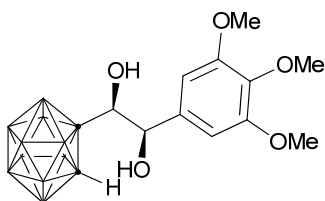


峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	15.547	BB	0.6242	211.78210	4.93942	1.8699
2	18.058	BB	0.9586	1.11141e4	178.94246	98.1301

HPLC for racemic and pure enantioenriched sample 2k

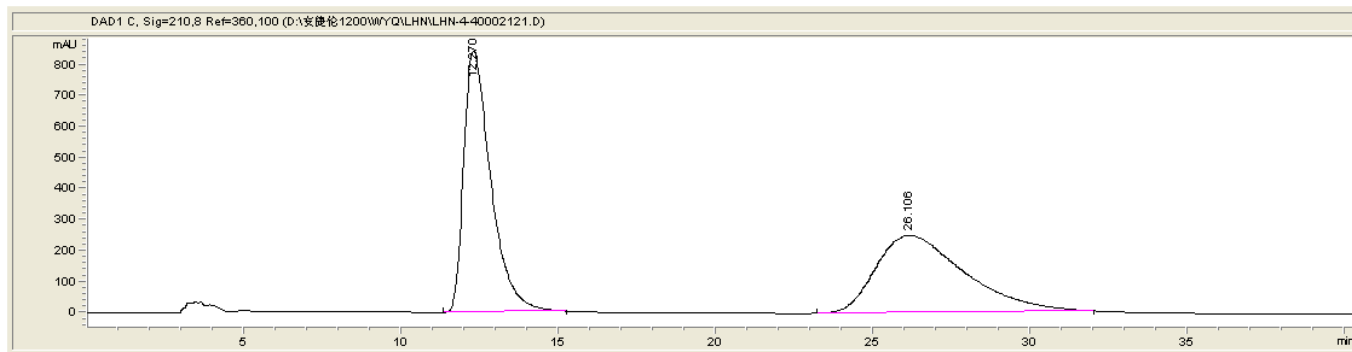
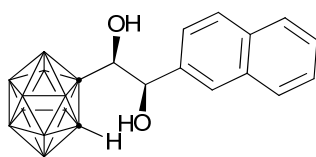


峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	20.611	BV	0.9660	5.41040e4	862.30707	49.7314
2	23.465	VB	1.0716	5.46884e4	784.22723	50.2686

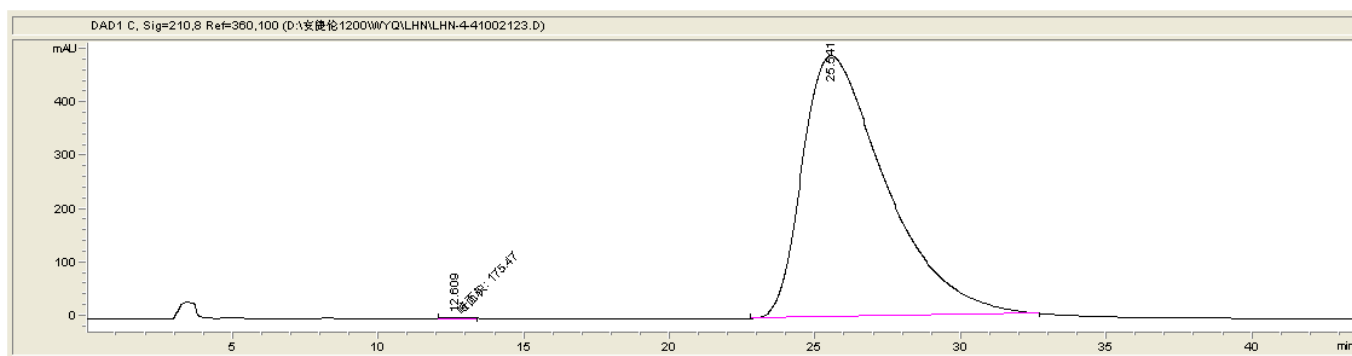
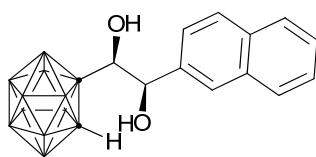


峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	20.491	BB	1.1679	7.99131e4	1066.83972	100.0000

HPLC for racemic and pure enantioenriched sample 21

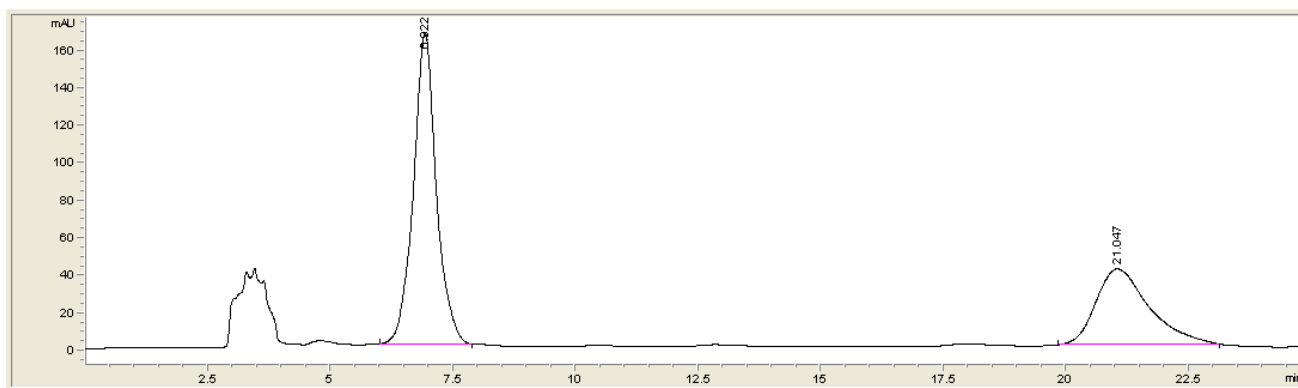
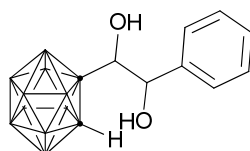


峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	12.270	BB	0.9062	5.06228e4	841.11206	50.9287
2	26.106	BB	2.7403	4.87765e4	248.90213	49.0713

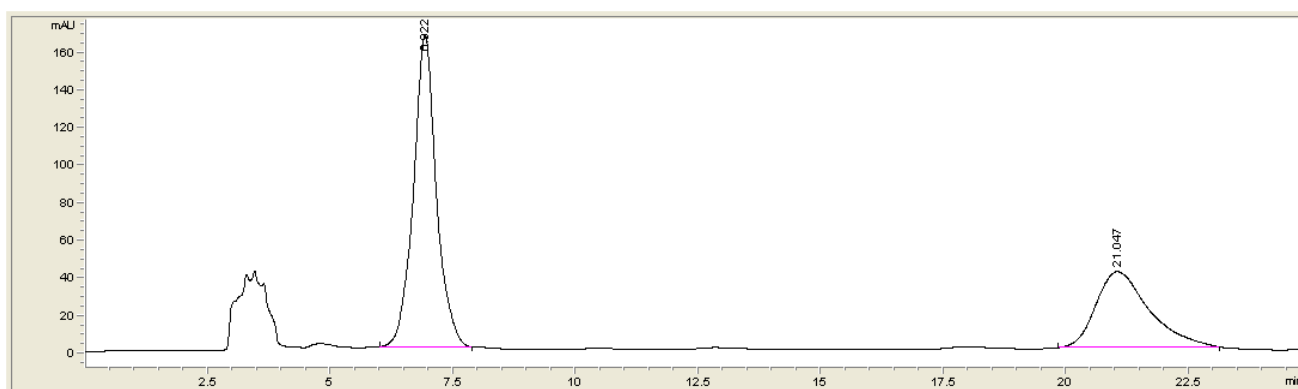
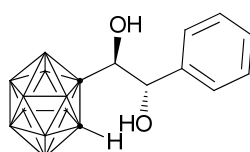


峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	12.609	MM	0.9693	175.46973	3.01703	0.1791
2	25.541	BB	2.8452	9.78019e4	490.71027	99.8209

HPLC for racemic and pure enantioenriched sample 2a'

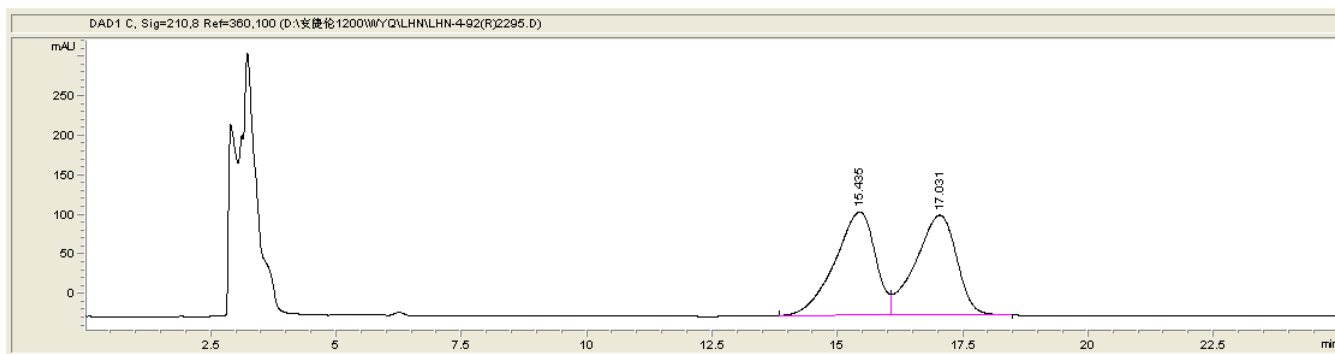
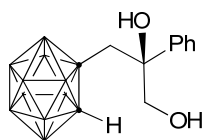


峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	6.967	VB	0.4907	1.61468e4	487.13208	51.2696
2	21.124	BB	1.1707	1.53471e4	193.22076	48.7304

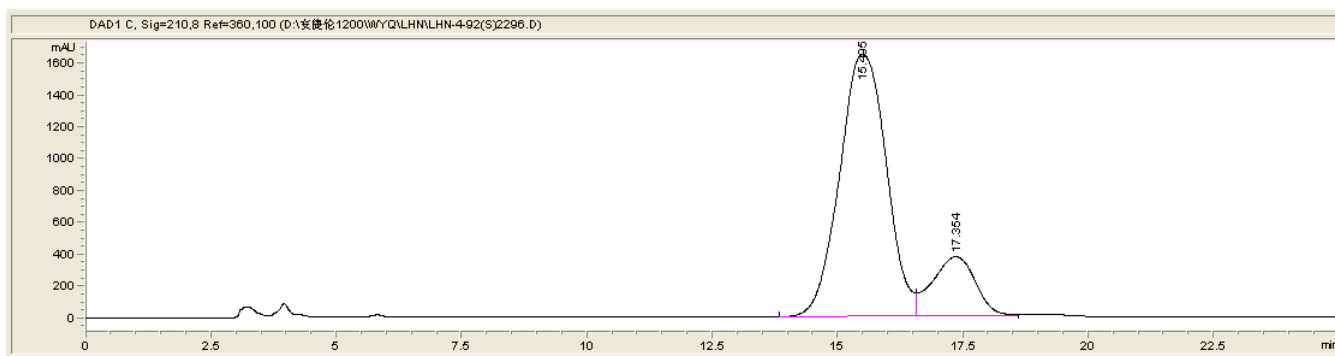
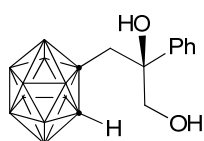


峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	6.922	BB	0.4780	5411.22754	166.13103	63.6937
2	21.047	BB	1.0900	3084.47412	40.52200	36.3063

HPLC for racemic and pure enantioenriched sample 4



峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	15.435	BV	0.8486	7435.73291	130.91412	50.6754
2	17.031	VB	0.8688	7237.52246	126.63398	49.3246



峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	15.495	BV	1.0100	1.07043e5	1647.53174	82.4574
2	17.354	VV	0.9222	2.27730e4	376.20502	17.5426