Supplementary Information for

Discovery and bioinspired total syntheses of unprecedented sesquiterpenoid dimers unveiled bifurcating [4 + 2] cycloaddition and target differentiation of enantiomers

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1. Experimental Procedures and Characterization Data

1.1 Extraction and Isolation

The stems and leaves of *Schisandra henryi* were obtained from Nujiang City, Yunnan Province, China, in September 2017, and the plant species was identified by Prof. Heng Li from the Kunming Institute of Botany. A voucher specimen (KIB 2017092501) has been deposited in the Herbarium of the Kunming Institute of Botany, Chinese Academy of Sciences.

As previously described[1], the air-dried powder of stems and leaves of *S. henryi* (19 Kg) was extracted with 70% aqueous acetone (3 × 100 L, 3 days each) at room temperature to give a crude extract (1.2 kg), which was dissolved in H_2O and partitioned with EtOAc. EtOAc fraction (635 g) was chromatographed on a silica gel column eluted with $CHCl_3$/acetone (1:0, 9:1, 7:3, 3:2, 1:1, and 0:1) to afford fractions A–F. Fr. C (137 g) was decolorized on MCI gel with MeOH/H_2O (90:10, 100:0) and the obtained fraction (90:10) was further purified by RP-18 with MeOH/H_2O (30:70 to 100:0) to give seven subfractions C_1–C_7. Fr. C_3 (24 g) were chromatographed on silica gel column eluted with petroleum ether/acetone in gradient system to afford seven major subfractions (C_{3A}–C_{3G}). Fr. C_{3C} (9.4 g) was separated by RP-18, Sephadex LH-20 and further purified by semi-preparative HPLC to afford compound **1** (3.1 mg). Fr. B (247 g) passaged over an MCI gel column with MeOH/H_2O (90:10, 100:0) and the obtained fraction (90:10) was further purified by RP-18 with MeOH/H_2O (30:70 to 100:0) to give six subfractions B_1–B_6. Fr. B_5 (20 g) was chromatographed over silica gel, RP-18, Sephadex LH-20 gel and semi-preparative HPLC to afford compounds **2** (26.2 mg), **3** (56.1 mg), **4** (3.5 mg), and **5** (68.3 mg), respectively.

Henryinin A (**1**): colorless massive crystals (MeOH/H_2O), $[\alpha]_D^{19}$ = −68.3 (*c* 0.086, MeOH), m.p. 255–257 °C, UV (MeOH) λ_{max} (log ε) 289 (4.31) nm. IR (KBr) ν_{max} 3425, 2928, 1720, 1664, 1632, 1446, 1375, 1142, 1103, 1,46, 907, 872 cm^{-1}. HRESIMS *m/z* 533.2304 $[M + K]^+$ (calcd for $C_{30}H_{38}O_6K$ 533.2300). ^1H NMR (pyridine-d_5, 500 MHz) and ^{13}C NMR (pyridine-d_5, 125 MHz), see **Table S1**.

Henryinin B (**2**): colorless massive crystals (MeOH/H_2O), $[\alpha]_D^{24}$ = −6.8 (*c* 0.13, MeOH). m.p. 298–300 °C, UV (MeOH) λ_{max} (log ε) 205 (4.50) nm. IR (KBr) ν_{max} 3363, 2928, 1727, 1655, 1625, 1442, 1196, 1141, 923 cm^{-1}. HRESIMS *m/z* 459.2541 $[M + H]^+$ (calcd for $C_{30}H_{35}O_4$ 459.2530). ^1H NMR (pyridine-d_5, 500 MHz) and ^{13}C NMR (pyridine-d_5, 125 MHz), see **Table S2**.

Henryinin C (**3**): colorless massive crystals, $[\alpha]_D^{24}$ = +44.4 (*c* 0.94, MeOH). colorless crystals (MeOH/H_2O), m.p. 260–262 °C, UV (MeOH) λ_{max} (log ε) 289 (4.20) nm. IR (KBr) ν_{max} 3445, 2927, 2865, 1723, 1666, 1632, 1442, 1370, 1138,

903, 869 cm^{-1}. HRESIMS *m/z* 485.2675 $[M + Na]^+$ (calcd for $C_{30}H_{38}O_4Na$ 485.2662). ^1H NMR (pyridine-d_5, 500 MHz) and ^{13}C NMR (pyridine-d_5, 125 MHz), see **Table S3**.

Henryinin D (**4**): colorless massive crystals (MeOH/H_2O), $[\alpha]_D^{24}$ = −49.8 (*c* 0.13, MeOH). m.p. 268–270 °C, UV (MeOH) λ_{max} (log ε) 289 (3.96) nm. IR (KBr) ν_{max} 3444, 3075, 2923, 2852, 1720, 1667, 1632, 1588, 1443, 1371, 1256, 1141, 1114, 1078, 906, 870 cm^{-1}. HRESIMS *m/z* 485.2671 $[M + Na]^+$ (calcd for $C_{30}H_{38}O_4Na$ 485.2662). ^1H NMR (pyridine-d_5, 500 MHz) and ^{13}C NMR (pyridine-d_5, 125 MHz), see **Table S4**.

Henryinin E (**5**): colorless massive crystals (MeOH/H_2O), $[\alpha]_D^{22}$ = –78.4 (*c* 0.11, MeOH), m.p. 280–282 °C, UV (MeOH) λ_{max} (log ε) 203 (4.28) nm. IR (KBr) ν_{max} 3480, 3356, 2945, 2929, 1712, 1661, 1368, 1172, 909 cm^{-1}. HRESIMS *m/z* 487.2814 $[M + Na]^+$ (calcd for $C_{30}H_{40}O_4Na$ 487.2819). ^1H NMR (pyridine-d_5, 500 MHz) and ^{13}C NMR (pyridine-d_5, 125 MHz), see **Table S5**.

1.2 Comparison of NMR Data for Natural and Synthetic Henryinins A–E (1–5)

Table S1. NMR data of natural and synthetic henryinin A (**1**) in pyridine-d_5

position	**1** (natural)		**1** (synthetic)	
	δ_C, type[a]	δ_H (multi., *J* in Hz)[b]	δ_C, type[a]	δ_H (multi., *J* in Hz)[b]
1	153.4, s		153.5, s	
2	123.2, d	6.30 (s)	123.3, d,	6.30 (s)
3	203.1, s		203.2, s	
4	75.0, s		75.1, s	
5	46.5, d	3.91 (d, 2.3)	46.7, d	3.91 (d, 2.3)
6	49.1, s		49.3, s	
7	48.7, d	3.55 (d, 5.3)	48.8, d	3.55 (d, 5.1)
8a	28.3, t	3.06 (d, 19.8)	28.4, t	3.06 (d, 19.8)
8b		2.00 (dd, 19.8, 5.3)		2.00 (dd, 19.8, 5.3)
9	133.4, d	5.61 (d, 5.3)	133.5, d	5.61 (d, 5.0)
10	131.9, s		132.0, s	
11	147.2, s		147.4, s	
12a	117.8, t	5.39 (brs)	118.0, t	5.39 (brs)
12b		4.90 (brs)		4.91 (brs)
13	22.6, q	1.60 (brs)	22.7, q	1.60 (brs)
14	20.1, q	1.81 (s)	20.2, q	1.81 (s)
15	33.9, q	1.51 (s)	34.0, q	1.50 (s)
1'	138.2, s		138.4, s	
2'	60.5, d	4.16 (s)	60.6, d	4.16 (s)
3'	212.9, s		213.0, s	
4'	71.8, s		71.9, s	
5'	48.7, d	4.08 (d, 2.3)	48.8, d	4.08 (d, 2.3)
6'	141.5, s		141.6, s	
7'	44.1, d	3.96 (d, 6.8)	44.2, d	3.96 (d, 6.8)
8'a	32.8, t	2.25 (m)	32.9, t	2.24 (m)
8'b		2.17 (dd, 13.5, 3.8)		2.17 (dd, 13.4, 3.5)
9'	73.9, d	4.59 (dd, 12.5, 3.8)	74.1, d	4.58 (dd, 12.5, 3.5)
10'	73.8, s		73.9, s	
11'	147.2, s		147.4, s	
12'a	115.6, t	5.41 (d, 2.2)	115.7, t	5.41 (d, 2.2)
12'b		4.90 (d, 2.2)		4.91 (d, 2.2)
13'	22.0, q	1.81 (s)	22.1, q	1.81 (s)
14'	19.9, q	1.50 (s)	20.0, q	1.50 (s)
15'	26.6, q	1.54 (s)	26.7, q	1.53 (s)

[a]Recorded at 125 MHz, [b]Recorded at 500 MHz

Table S2. NMR comparison data of natural and synthetic henryinin B (**2**) in $CDCl_3$

position	**2** (natural)		**2** (synthetic)	
	δ_C, type[a]	δ_H (multi., *J* in Hz)[b]	δ_C, type[b]	δ_H (multi., *J* in Hz)[a]
1	152.4, s		152.4, s	
2	120.2, d	5.66 (s)	120.2, d	5.67 (s)
3	200.4, s		200.5, s	
4	73.7, s		73.7, s	
5	43.8, d	3.46 (d, 2.5)	43.8, d	3.46 (d, 2.5)
6	47.9, s		47.9, s	
7	48.2, d	2.98 (d, 5.5)	48.2, d	2.97 (d, 5.5)
8a	27.9, t	3.07 (m)	27.9, t	3.08 (m)
8b		2.25 (dd, 20.2, 5.5)		2.26 (dd, 20.2, 5.5)
9	132.9, d	6.09 (d, 4.5)	132.9, d	6.10 (d, 4.4)
10	131.4, s		131.4, s	
11	145.2, s		145.2, s	
12a	118.3, t	5.05 (d, 2.3)	118.3, t	5.05 (d, 2.3)
12b		4.89 (d, 2.3)		4.90 (d, 2.3)
13	21.8, q	1.57 (brs)	21.8, q	1.57 (brs)
14	19.9, q	1.81 (s)	19.9, q	1.82 (s)
15	32.3, q	1.16 (s)	32.3, q	1.16 (s)
1'	132.1, s		132.1, s	
2'	59.0, d	4.01 (s)	59.0, d	4.01 (s)
3'	213.0, s		212.9, s	
4'	72.7, s		72.8, s	
5'	46.4, d	4.25 (d, 2.5)	46.3, d	4.25 (d, 2.5)
6'	135.2, s		135.2, s	
7'	140.0, s		140.1, s	
8'	128.2, d	6.97 (d, 7.9)	128.2, d	6.97 (d, 7.9)
9'	129.6, d	7.00 (d, 7.9)	129.6, d	7.00 (d, 7.9)
10'	135.2, s		135.3, s	
11'	145.2, s		145.2, s	
12'a	116.3, t	5.25 (brs)	116.4, t	5.26 (brs)
12'b		5.10 (brs)		5.10 (brs)
13'	24.8, q	2.19 (brs)	24.8, q	2.19 (brs)
14'	18.2, q	1.98 (s)	18.2, q	1.98 (s)
15'	26.1, q	1.20 (s)	26.2, q	1.20 (s)

[a]Recorded at 125 MHz in, [b]Recorded at 500 MHz

Table S3. NMR comparison data of natural and synthetic henryinin C (**3**) in $CDCl_3$

position	**3** (natural)		**3** (synthetic)	
	δ_C, type[a]	δ_H (multi., *J* in Hz)[b]	δ_C, type[a]	δ_H (multi., *J* in Hz)[b]
1	154.9, s		155.0, s	
2	120.0, d	6.05 (s)	120.0, d	6.08 (s)
3	201.7, s		201.8, s	
4	73.7, s		73.7, s	
5	44.8, d	3.25 (d, 2.4)	44.8, d	3.26 (d, 2.4)
6	49.2, s		49.2, s	
7	47.6, d	2.82 (overlap)	47.4, d	2.84 (overlap)
8a	27.7, t	2.82 (overlap)	27.7, t	2.84 (overlap)
8b		2.15 (dd, 20.1, 4.6)		2.18 (dd, 20.1, 4.6)
9	133.4, d	6.03 (d, 4.4)	133.4, d	6.06 (d, 4.3)
10	131.1, s		131.2, s	
11	145.5, s		145.5, s	
12a	117.8, t	4.95 (brs)	117.8, t	4.97 (brs)
12b		4.80 (brs)		4.83 (brs)
13	21.7, q	1.53 (overlap)	22.4, q	1.55 (overlap)
14	19.9, q	1.84 (s)	20.0, q	1.87 (s)
15	33.2, q	1.20 (s)	33.3, q	1.22 (brs)
1'	138.0, s		138.1, s	
2'	62.6, d	3.12 (s)	62.6, d	3.14 (s)
3'	212.5, s		212.3, s	
4'	71.8, s		72.0, s	
5'	47.6, d	3.36 (d, 2.4)	47.4, d	3.39 (d, 2.4)
6'	139.8, s		139.8, s	
7'	43.5, d	2.82 (overlap)	43.5, d	2.84 (overlap)
8'a	23.7, t	1.53 (overlap)	23.7, t	1.55 (overlap)
8'b		1.43 (overlap)		1.45 (overlap)
9'a	28.3, t	1.53 (overlap)	28.4, t	1.55 (overlap)
9'b		1.31 (m)		1.34 (m)
10'	33.0, d	1.43 (overlap)	33.1, d	1.45 (overlap)
11'	145.5, s		145.5, s	
12'a	115.0, d	4.89 (brs, 2H)	115.1, d	4.93 (brs, 2H)
12'b				
13'	22.3, q	1.66 (s)	22.4, q	1.69 (s)
14'	18.9, q	0.82 (d, 7.0)	19.0, q	0.85 (d, 7.0)
15'	25.7, q	1.15 (s)	25.9, q	1.17 (s)

[a]Recorded at 125 MHz, [b]Recorded at 500 MHz

Table S4. NMR comparison data of natural and synthetic henryinin D (**4**) in $CDCl_3$

position	**4** (natural)		**4** (synthetic)	
	δ_C, type[a]	δ_H (multi., *J* in Hz)[b]	δ_C, type[a]	δ_H (multi., *J* in Hz)[b]
1	154.5, s		154.5, s	
2	121.0, d	6.07 (s)	120.9, d	6.06 (s)
3	202.2, s		202.2, s	
4	73.9, s		73.9, d	
5	44.4, d	3.30 (d, 2.7)	44.3, s	3.30 (d, 2.7)
6	48.5, s		48.3, d	
7	47.7, d	2.91 (overlap)	47.7, d	2.91 (overlap)
8a	27.6, t	2.91 (overlap)	27.6, t	2.91 (overlap)
8b		2.15 (dd, 20.7, 4.9)		2.15 (dd, 20.7, 4.9)
9	133.7, d	6.09 (d, 4.9)	133.7, d	6.09 (d, 4.9)
10	131.7, s		131.6, s	
11	146.1, s		146.0, s	
12a	117.8, t	5.00 (brs)	117.8, t	4.99 (brs)
12b		4.86 (brs)		4.85 (brs)
13	22.6, q	1.57 (overlap)	22.6, q	1.57 (overlap)
14	20.0, q	1.87 (s)	20.0, q	1.86 (s)
15	33.2, q	1.23 (s)	33.2, q	1.22 (s)
1'	135.9, s		135.9, s	
2'	62.0, d	3.26 (s)	62.0, d	3.26 (s)
3'	212.1, s		212.2, s	
4'	71.7, s		71.7, s	
5'	47.1, d	3.44 (d, 2.7)	47.1, d	3.44 (d, 2.7)
6'	141.8, s		141.8, s	
7'	43.3, d	2.91 (overlap)	43.3, d	2.91 (overlap)
8'a	24.7, t	1.57 (overlap)	24.5, t	1.57 (overlap)
8'b		1.57 (overlap)		1.57 (overlap)
9'a	29.1, t	1.71 (m)	29.0, t	1.71 (m)
9'b		1.25 (m)		1.25 (m)
10'	31.6, d	1.98 (m)	31.5, d	1.97 (m)
11'	146.1, s		146.0, s	
12'a	115.3, t	4.96 (brs)	115.3, t	4.96 (brs)
12'b		4.91 (brs)		4.91 (brs)
13'	22.6, q	1.71 (s)	22.6, q	1.71 (s)
14'	17.4, q	0.70 (d, 7.3)	17.4, q	0.69 (d, 7.3)
15'	26.5, q	1.20 (s)	26.4, q	1.20 (s)

[a]Recorded at 125 MHz, [b]Recorded at 500 MHz

Table S5. NMR comparison data of natural and synthetic henryinin E (**5**) in $CDCl_3$

position	**5** (natural)		**5** (synthetic)	
	δ_C, type[a]	δ_H (multi., *J* in Hz)[b]	δ_H (multi., *J* in Hz)[a]	δ_C, type[b]
1	166.1, s		166.2, s	
2	122.8, d	6.09 (s)	122.8, d	6.11 (s)
3	201.6, s		201.7, s	
4	73.2, s		73.2, s	
5	60.8, d	3.77 (d, 2.3)	60.7, d	3.77 (d, 2.3)
6	52.8, s		52.8, s	
7	49.9, d	2.71 (brs)	49.9, d	2.71 (brs)
8a	24.1, t	2.35 (overlap)	24.1, t	2.36 (brs)
8b		1.55 (overlap)		1.55 (overlap)
9a	30.0, t	1.85 (m)	30.1, t	1.85 (m)
9b		1.80 (m)		1.85 (m)
10	32.8, d	2.66 (m)	32.8, d	2.67 (m)
11	146.3, s		146.3, s	
12a	117.9, t	4.90 (brs)	117.9, t	4.89 (brs)
12b		4.90 (brs)		4.89 (brs)
13	25.7, q	1.75 (s)	25.8, q	1.76 (s)
14	19.1, q	1.13 (d, 6.9)	19.1, q	1.16 (d, 6.9)
15	33.2, q	1.29 (s)	33.2, q	1.31 (brs)
1'	137.5, s		137.5, s	
2'	60.8, d	3.75 (s)	60.7, d	3.77(overlap)
3'	212.1, s		212.1, s	
4'	71.5, s		71.5, s	
5'	47.6, d	3.38 (d, 2.3)	47.5, d	3.40 (d, 2.3)
6'	139.9, s		139.8, s	
7'	43.3, d	2.85 (t, 6.4)	43.3, d	2.86 (t, 6.4)
8'a	24.1, t	1.55 (overlap)	24.1, t	1.55 (overlap)
8'b		1.42 (m)		1.43 (m)
9'a	28.5, t	1.55 (overlap)	28.5, t	1.55 (overlap)
9'b		1.33 (m)		1.34 (m)
10'	32.5, d	1.55 (overlap)	32.5, d	1.55 (overlap)
11'	145.6, s		145.6, s	
12'a	114.9, t	4.90 (brs)	115.0, t	4.89 (brs)
12'b		4.90 (brs)		4.89 (brs)
13'	22.3, q	1.66 (s)	22.3, q	1.67 (s)
14'	19.1, q	0.92 (d, 6.9)	19.2, q	0.93 (d, 6.9)
15'	25.7, q	1.15 (s)	25.8, q	1.16 (s)

[a] Recorded at 125 MHz, [b]Recorded at 500 MHz

1.3 Structural Elucidation of Compounds 1–5

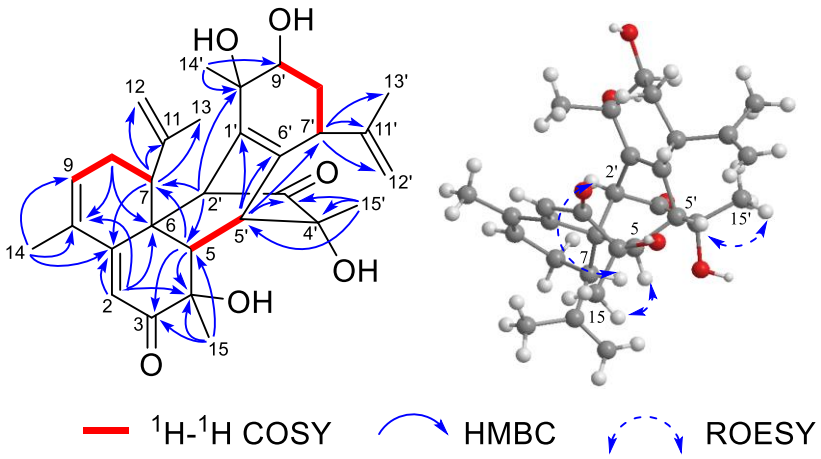


Figure S1. Selected ^{1}H–^{1}H COSY, HMBC and ROESY correlations of henryinin A (**1**)

Henryinin B (**2**) was obtained as a colorless crystal. Its molecular formula of $C_{30}H_{34}O_4$ was established by HRESIMS ($[M + H]^+$ *m/z* 459.2541, calcd 459.2530), requiring 14 degrees of unsaturation. By detailed comparison of the 1D NMR spectra of **2** with those of **1**, it was obvious that the signals for **1** at C-7′ (δ_C 44.1), C-8′ (δ_C 32.8), C-9′ (δ_C 73.9), and C-10′ (δ_C 73.8) together with H-7′ (δ_H 3.96, d, *J* = 6.8 Hz), H-8′ (δ_H 2.17, dd, *J* = 13.5, 3.8 Hz; 2.25, m), and H-9′ (δ_H 4.59, dd, *J* = 12.5, 3.8 HZ) were absent in **2**. Instead, additional four aromatic carbons at δ_C 140.0, 128.2, 129.6, and 135.2 together with two aromatic protons (δ_H 6.97, d, *J* = 7.9 Hz; 7.00, d, *J* = 7.9 Hz) were observed, which suggested that the E ring in **2** was aromatic. This speculation was further confirmed by the HMBC correlations of H_2-8′ with C-6′, C-10′ and C-11′, of H-9′ with C-1′, C-7′ and C-14′, together with the ^{1}H–^{1}H COSY correlations of H_2-8′/H-9′ (Figure S2). In order to further confirm the structure of **2** and its absolute configuration, **2** was crystallized in methanol to afford single crystals. The X-ray diffraction analysis was performed using an anomalous dispersion with copper radiation resulted in a Flack parameter of 0.12(7), assigning its absolute stereochemistry to be 4*R*,5*R*,6*R*,7*R*,2′*S*,4′*R*,5′*R* (Figure 1, CCDC no. 2212936).

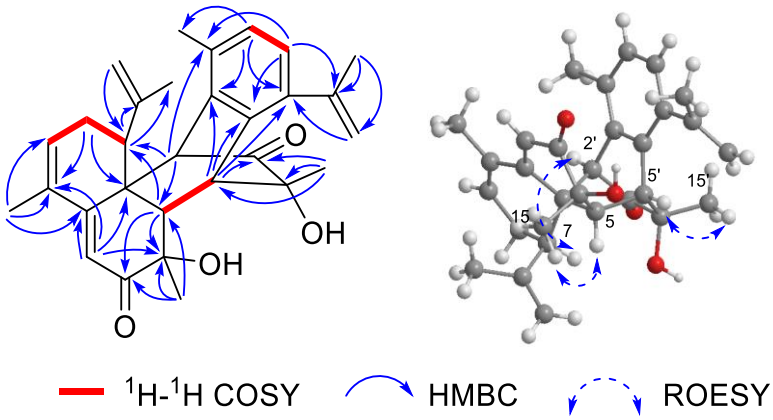


Figure S2. Selected ^{1}H–^{1}H COSY, HMBC and ROESY correlations of henryinin B (**2**)

Henryinin C (**3**) was obtained as colorless crystals. The HRESIMS ([M + Na]$^+$ *m/z* 485.2675, calcd 485.2662) indicated a molecular formula of $C_{30}H_{38}O_4$, of which the numbers of oxygen atoms were two less than those of **1**. The 1D NMR spectroscopic data of **3** was also closely similar to those of **1**. The main difference was the replacement of an oxygenated methine ($\delta_{C\text{-}9'}$ 73.9) and a quaternary carbon ($\delta_{C\text{-}10'}$ 73.8) in **1** by a methylene (δ_C 28.3) and a methine (δ_C 33.0) in **3**, which was verified by the HMBC correlations from H_3-14′ to C-1′, C-9′ and C-10′, as well as the ^{1}H–^{1}H COSY correlations of H-7′/H_2-8′/H_2-9′/H-10′/H_3-14′ (Figure S3). In addition, the single-crystal X-ray diffraction analysis of **3** using Cu K*α* radiation [Flack parameter = –0.03(5)] confirmed its structure and defined the absolute configuration to be 4*R*,5*R*,6*R*,7*R*,2′*S*,4′*R*,5′*R*,7′*R*,10′*R* (Figure 1, CCDC no. 2212937).

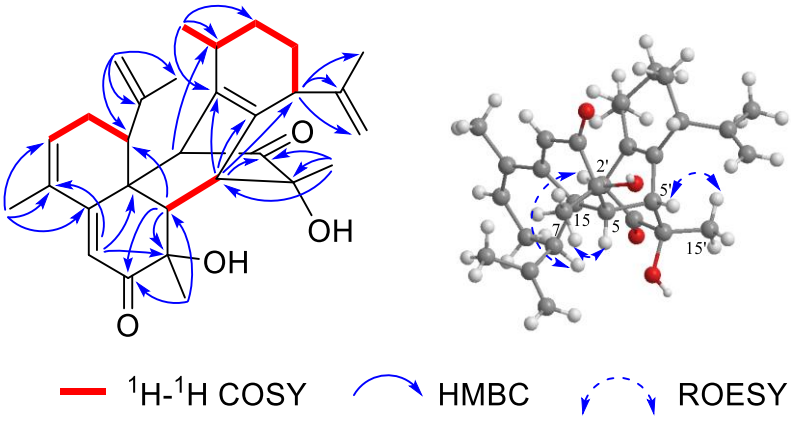


Figure S3. Selected ^{1}H–^{1}H COSY, HMBC and ROESY correlations of henryinin C (**3**)

Henryinin D (**4**) was obtained as colorless crystals. The HRESIMS ([M + Na]$^+$ *m/z* 485.2671, calcd 485.2662) indicated a molecular formula of $C_{30}H_{38}O_4$, which was identical to that of **3**. The 1D NMR spectrum of **4** was also closely similar to those of **3** except for the chemical shifts of the E ring moiety. The proton signals of 14′-methyl and 10′-methine in **4** were shifted from δ_H 0.82 to 0.70 (H_3-14′) and from δ_H 1.43 to 1.98 (H-10′) compared with those in the spectrum of **3** (Tables S3 and S4). In addition, the chemical shifts of C-14′, C-10′, C-9′ and C-1′ were shifted from δ_C 18.9 to 17.4, from δ_C 33.0 to 31.6, from δ_C 28.3 to 29.1 and from δ_C 138.0 to 135.9, respectively, suggesting that **4** should be a C-10′ epimer of **3**. The planar structure of **4** was confirmed by the 2D NMR data (Figure S4). Furthermore, the single-crystal X-ray diffraction analysis of **4** using Cu K*α* radiation [Flack parameter = –0.01(4)] established its absolute configuration as 4*R*,5*R*,6*R*,7*R*,2′*S*,4′*R*,5′*R*,7′*R*,10′*S* (Figure 1, CCDC no. 2212938).

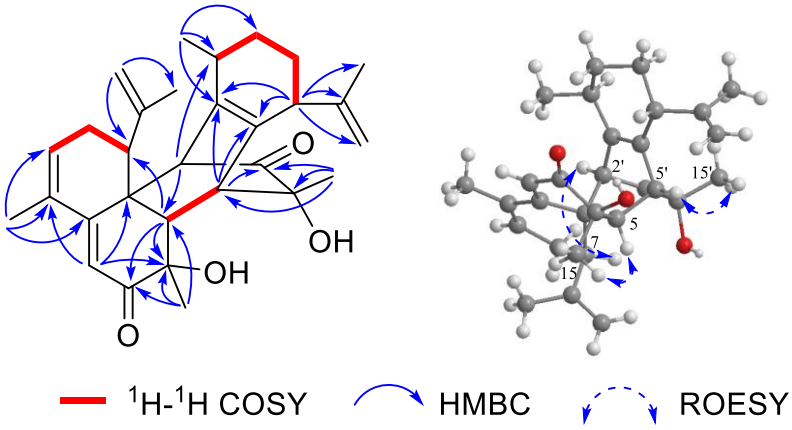


Figure S4. Selected ^{1}H–^{1}H COSY, HMBC and ROESY correlations of henryinin D (**4**)

Henryinin E (**5**) was obtained as a colorless crystal. The HRESIMS ([M + Na]$^+$ *m/z* 487.2814, calcd 487.2819) indicated a molecular formula of $C_{30}H_{40}O_4$, requiring 11 degrees of unsaturation. The 1D NMR spectrum of **5** was closely similar to those of **3**. Further comparison of the 1D NMR data between **5** and **3** revealed that one double bond ($\delta_{C\text{-}9}$ 133.4; $\delta_{C\text{-}10}$ 131.1; $\delta_{H\text{-}9}$ 6.03, d, J = 4.4 Hz) was absent in **5**, which was replaced by one methylene group (δ_C 30.0; δ_H 1.85, m; 1.80, m) and one methine group (δ_C 32.8; δ_H 2.66, m). This deduction was supported by 2D NMR data (Figure S5). Furthermore, its planar structure and absolute configuration (4*R*,5*R*,6*R*,7*R*,2′*S*,4′*R*,5′*R*,7′*R*,10′*R*) was verified by the single-crystal X-ray diffraction analysis of **5** using Cu Kα radiation [Flack parameter = 0.07(7)] (Figure 1, CCDC no. 2212942).

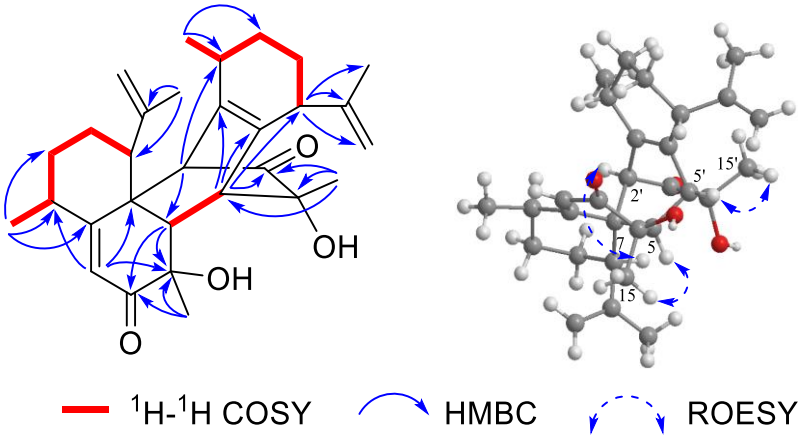


Figure S5. Selected ^{1}H–^{1}H COSY, HMBC and ROESY correlations of henryinin E (**5**)

1.4 More Detailed Results from the Studies of Hydrogenation, Aromatization and Dearomatization Reactions

Detailed results from the studies of hydrogenation. The selective hydrogenation of compound **19** was performed. As shown in Table S6, treatment of **19** with 10% Pd/C (5% mol) in benzyl alcohol at room temperature or 100 °C failed to react (Table S6, entry 1)[2]. When the H_2 balloon was given and hexane was used as solvent, the undesired product (all carbon–carbon double bonds were hydrogenated) was obtained (Table S6, entry 2)[3]. In addition, the reactions

similarly afforded the same undesired product by using $NiCl_2 \cdot 6H_2O$ and $NaBH_4$ in methanol (Table S6, entry 3)[4]. Finally, different solvents for the reaction were investigated using 5% $Pd/CaCO_3$ as catalyst (Table S6, entries 4–7) and the methanol was found to be optimal solvent (Table S6, entry 6)[2].

Table S6. Optimizations of the hydrogenation of compound **19**.

entry	conditions	yield
1	10% Pd/C (5% mol), Benzyl Alcohol, RT or 100 °C	NR
2	10% Pd/C (2% mol), H_2, Hexane, RT	Undesired products
3	$NiCl_2 \cdot 6H_2O$, $NaBH_4$, Methanol	Undesired products
4	5% $Pd/CaCO_3$ (5% mol), H_2, Hexane, RT	Trace
5	5% $Pd/CaCO_3$ (5% mol), H_2, EtOAc, RT	40% (incomplete reaction)
6	5% $Pd/CaCO_3$ (5% mol), H_2, Methanol, RT	91%
7	5% $Pd/CaCO_3$ (5% mol), H_2, Water, RT	Undesired products

Detailed results from the studies of aromatization. The optimized reaction conditions proved that the $Pd(OAc)_2$ can catalyzes the dehydrogenation of **19** to afford phenol derivative **18b, c**. Inspired by Saegusa−Ito oxidation, we further began optimizing the reaction. $Pd(OAc)_2$ catalysts under various reaction conditions. Treatment of **19** with 0.5 equiv of $Pd(OAc)_2$ cat. under a variety of conditions only only yield a small amount of the desired product **18a** (Table S7, entries 1–4)[5], which suggested oxidation procedure fail to improve the yield of reaction using catalytic amounts of palladium salts. Thus we examine the yield of reaction by use different amounts of $Pd(OAc)_2$ and the relatively high yields of desired product **18a** were obtained in the presence of 2 equiv of $Pd(OAc)_2$ (Table S7, entries 5 and 6). Similarly, we optimizing the reaction by using the same way in acetonitrile solvent and results were similar with DMSO (Table S7, entries 7–10)[6].

Table S7. Optimizations of the aromatization of compound **19**.

entry	conditions	yield
1	$Pd(OAc)_2$ (0.5 equiv), DMSO, air, 23 °C	11%
2	$Pd(OAc)_2$ (0.5 equiv), DMSO, O_2, 23 °C	9%
3	$Pd(OAc)_2$ (0.5 equiv), DMSO, air, 65 °C	25%
4	$Pd(OAc)_2$ (0.5 equiv), DMSO, air, 100 °C	23%
5	$Pd(OAc)_2$ (1 equiv), DMSO, air, 65 °C	34%
6	$Pd(OAc)_2$ (2 equiv), DMSO, air, 65 °C	52%
7	$Pd(OAc)_2$ (0.5 equiv), CH_3CN, O_2, 65 °C	12%
8	$Pd(OAc)_2$ (1 equiv), CH_3CN, air, 65 °C	36%
9	$Pd(OAc)_2$ (1 equiv), CH_3CN, air, 100 °C	32%
10	$Pd(OAc)_2$ (2 equiv), CH_3CN, air, 65 °C	54%

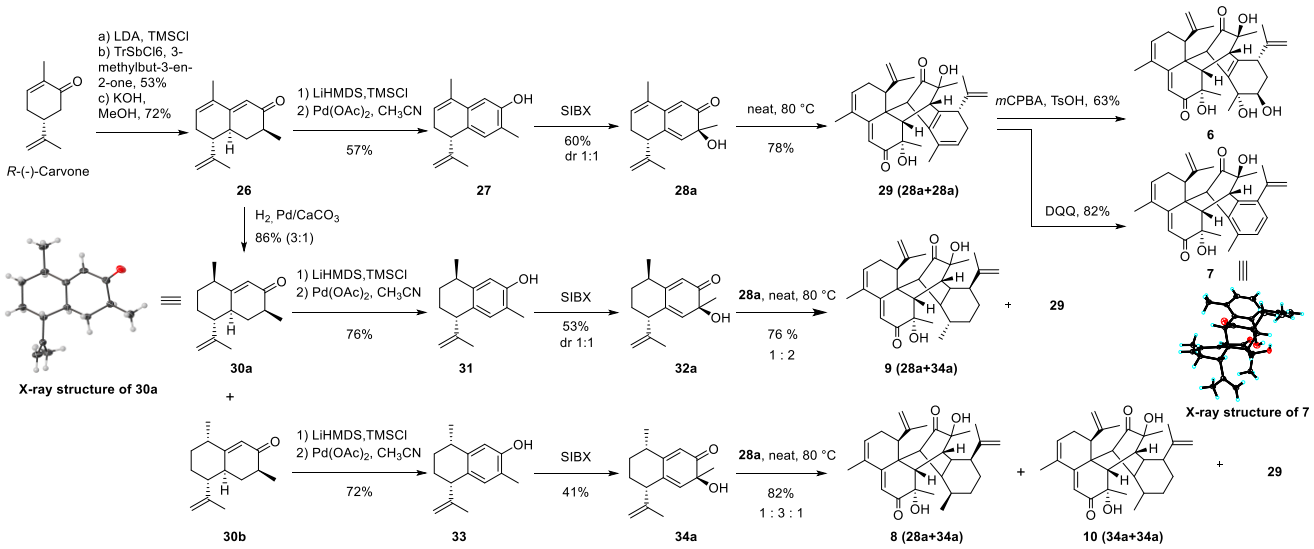
Detailed results from the studies of dearomatization. The dearomatization of phenol derivatives have found widespread use in the synthesis of cyclohexadienones. First, the oxidative dearomatization **18a** was performed by using the system Oxone/$NaHCO_3$/acetone and no product could be detected (Table S8, entry 1)[7]. A similar outcome was observed with $[Cu(CH_3CN)_4]PF_6$ in dichloromethane (Table S8, entry 2)[8]. Treatment of **18a** with hypervalent iodine reagents such as $PhI(OAc)_2$ and $PhI(OCOCF_3)_2$ afforded miscellaneous products (Table S8, entries 3 and 4)[9-10]. Treatment of **18a** with $Pb(OAc)_4$ can undergo oxidative dearomatization to furnish acetylated desired product (Table S8, entry 5). Unfortunately, the obtained products failed to undergo the Diels–Alder cycloaddition and was broken via deacetylation with virous bases. Finally, treatment of **18a** with SIBX afforded the desired product in 91% yield (Table S8, entry 6).

Table S8. Optimizations of dearomatization of **18a**.

entry	conditions	yield
1	Oxone (4 equiv), $NaHCO_3$, Acetone/H_2O, 23 °C	NR
2	$[Cu(CH_3CN)_4]PF_6$, CH_2Cl_2, 23 °C	NR
3	$PhI(OAc)_2$ (1 equiv), CH_2Cl_2, –40 °C	miscellaneous products
4	$PhI(OCOCF_3)_2$ (1 equiv), CH_2Cl_2, 23 °C	miscellaneous products
5	$Pb(OAc)_4$, CH2Cl2, 23 °C	Undesired products
6	SIBX (1.1 equiv), DMSO, Toluene, 23 °C	63%

1.5 The Synthetic Routes of Enantiomers 6–10

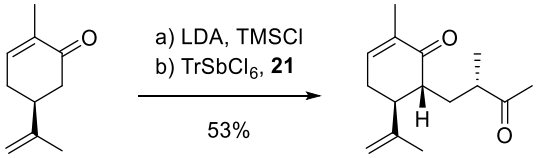
Scheme S1. Total syntheses of enantiomers **6**–**10**.



To further explore whether the isopropenyl group located at C-7 affected the Diels−Alder reaction of our intermediates and biological activities of enantiomeric natural products **6–10**, the total synthesis of their enantiomers was completed

using *R*-(–)-carvone as starting material (Scheme S1). In our synthesis process, Diels−Alder reaction also exhibited extremely regio- and stereo-selectivities. Thus, the isopropenyl group located at C-7 affected the Diels−Alder reaction.

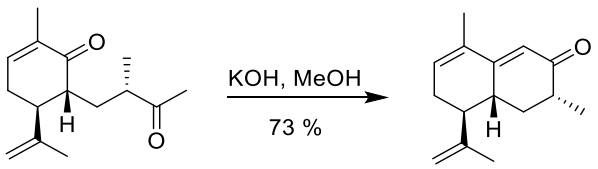
1.6 Total Synthetic Procedures of Henryinins A–E (1–5) and Their Enantiomers (6–10)



22 **20**

Synthesis of compound 20: The methyl isopropenyl ketone (**21**) was prepared according to a literature-reported procedure[11]. ^{1}H NMR (500 MHz, $CDCl_3$) δ 1.72 (s, 3H), 2.20 (s, 3H), 5.68 (s, 1H), 5.85 (s, 1H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$) δ 199.8, 144.7, 125.6, 25.4, 17.1 ppm. To a solution of LDA (1 M, 10 mL, 1.5 equiv) was added to a stirred solution of **22** [*S*-(+)-carvone] (1 mL, 6.4 mmol) in dry THF (5 mL) at –78 °C. After 30 min TMSCl (1 mL, 7.89 mmol, 1.2 equiv) was added and the resultant was allowed to warm to room temperature for 1 h. The resultant mixture was then poured into a cold saturated solution of $NaHCO_3$ and brine (1:1). The water phase was extracted with petroleum ether. The solvent was removed under vacuum and the crude TMS enol ethers were used without further purification. To a solution of the crude product and **21** were added trityl antimonium hexachloride (184.6 mg, 0.32 mmol, 0.05 eq) at –40 °C for 5 mins before the reaction was quenched with pyridine. The 2 M HCl (10 mL) in THF (20 mL) was added to the resultant mixture, warmed to room temperature and stirred for 30 min. Then the water phase was extracted with petroleum ether, washed subsequently with 2 M solution of HCl, a saturated solution of $NaHCO_3$. The extracts were dried over Na_2SO_4 and the organic solvent was removed under vacuum. The crude product was purified by silica gel column eluted with petroleum ether/EtOAc (100:1 to 30:1, v/v) to afford **20** (824.9 mg, 53%).

20: R_f = 0.43 (silica, EtOAc/PE 1:6); $[\alpha]_D^{27}$ = +3.2 (*c* 0.161, MeOH), ^{1}H NMR (500 MHz, $CDCl_3$) δ 0.93 (d, *J* = 6.9, 3H), 1.16 (m, 1H), 1.58 (s, 3H), 1.64 (brs, 3H), 1.88 (m, 1H), 2.10 (s, 3H), 2.25 (m, 2H), 2.34 (m, 1H), 2.75 (m, 1H), 4.66 (s, 1H), 4.71 (s, 1H), 6.54 (m, 1H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$) δ 212.5, 201.7, 145.1, 142.9, 134.7, 113.8, 48.9, 46.8, 45.3, 31.1, 30.7, 28.0, 18.7, 15.9, 15.6 ppm. HRMS (ESI) *m/z* 257.1513 $[M + Na]^+$ (calcd for $C_{15}H_{22}O_2Na$ 257.1512).

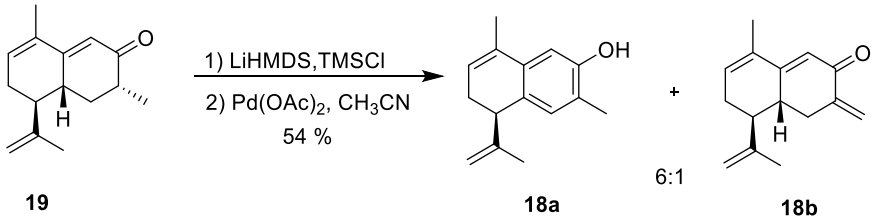


20 **19**

Synthesis of compound 19: The ketones **20** (445.1 mg, 1.90 mmol) were dissolved in a 3 M solution of KOH in methanol (2 mL). The resulting solution was stirred at room temperature for more than 3 h until only optically pure

compound **19** was observed by thin layer. The reaction mixture was then poured into a 2 M solution of HCl (3 mL). The organic solvent was removed under vacuum and the residue extracted with EtOAc. The extracts were dried over Na_2SO_4 and purified by a flash column chromatography on silica gel eluted with petroleum ether/EtOAc (80:1, v/v) to afford compound **19** (297 mg, 73%).

19: R_f = 0.46 (silica, EtOAc/PE 1:12); $[\alpha]_D^{27}$ = +61.8 (*c* 0.175, MeOH), ^{1}H NMR (500 MHz, $CDCl_3$) δ 1.04 (d, *J* = 6.8, 3H), 1.18 (m, 1H), 1.62 (brs, 3H), 1.74 (brs, 3H), 1.89 (m, 1H), 2.09 (m, 2H), 2.23 (m, 2H), 2.40 (m, 1H), 4.73 (brs, 1H), 4.75 (brs, 1H), 5.83 (d, *J* = 2.0, 1H), 6.02 (d, *J* = 4.7, 1H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$) δ 202.4, 158.1, 145.6, 136.0, 131.4, 121.7, 113.4, 48.6, 41.4, 38.4, 36.2, 31.6, 19.2, 18.0, 15.0 ppm. HRMS (ESI) *m/z* 217.1589 $[M + H]^+$ (calcd for $C_{15}H_{21}O$ 217.1587).



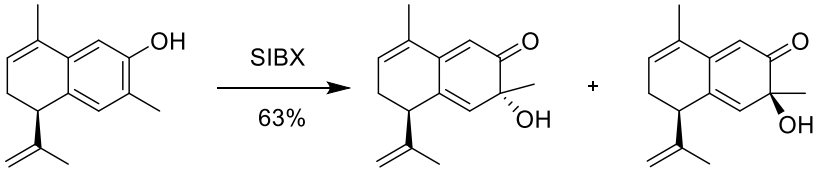
19 **18a** **18b**

Synthesis of compounds 18a and 18b: To a solution of LiHMDS (1 M, 5 mL, 1.8 equiv) was added to a stirred solution of **19** (594.6 mg, 2.75 mmol) in dry THF (3 mL) at –78 °C. After 30 min TMSCl (0.42 mL, 3.3 mmol, 1.2 equiv) was added and the resultant was allowed to warm to room temperature for 1 h. The resultant mixture was then poured into a cold saturated solution of $NaHCO_3$. The water phase was extracted with petroleum ether. The organic extracts were combined and dried over Na_2SO_4. The solvent was removed under vacuum and the crude TMS enol ethers were used without further purification. To a solution of the silyl enol ether obtained above in freshly distilled acetonitrile was added palladium(II) acetate, freshly prepared according to the reported procedure and other additive[6]. The reaction mixture was stirred for 20 min, and filtered through a short silica gel column with EtOAc. The filtrate was concentrated in vacuo and the residue was purified by column chromatography on silica gel to give **18a** (274.9 mg, 47%) and **18b** (45.6 mg, 8%).

18a: R_f = 0.38 (silica, EtOAc/PE 1:12); $[\alpha]_D^{28}$ = –118.4 (*c* 0.087, MeOH), ^{1}H NMR (500 MHz, $CDCl_3$) δ 1.73 (s, 3H), 2.00 (brs, 1H), 2.22 (s, 3H), 2.35 (m, 2H), 3.43 (t, 8.3, 1H), 4.54 (s, 1H), 4.69 (s, 1H), 4.85 (s, 1H), 5.76 (s, 1H), 6.71 (s, 1H), 6.84 (s, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 152.4, 147.6, 135.0, 131.4, 129.9, 129.6, 123.9, 121.8, 112.9, 110.2, 45.3, 28.4, 20.0, 19.5, 15.7 ppm. HRMS (ESI) *m/z* 213.1287 $[M - H]^-$ (calcd for $C_{15}H_{19}O$ 213.1285).

18b: R_f = 0.38 (silica, EtOAc/PE 1:12); $[\alpha]_D^{28}$ = –12.9 (*c* 0.157, MeOH), ^{1}H NMR (500 MHz, $CDCl_3$) δ 1.67 (s, 3H), 1.82 (brs, 3H), 2.21 (m, 4H), 2.47 (m, 1H), 2.68 (dd, 14.3, 4.4, 1H), 4.80 (s, 1H), 4.83 (s, 1H), 5.19 (s, 1H), 5.90 (s, 1H), 6.04

(s, 1H), 6.14 (d, J = 4.6, 1H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$) δ 189.5, 158.7, 145.6, 142.6, 137.2, 131.7, 122.7, 119.1, 113.7, 48.7, 38.3, 36.2, 31.6, 19.3, 18.1. ppm. HRMS (ESI) *m/z* 215.1428 $[M + H]^+$ (calcd for $C_{15}H_{19}O$ 215.1430).

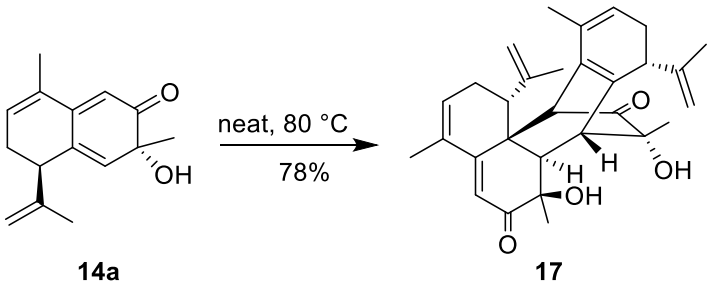


18a **14a** 1:1 **14b**

Synthesis of compounds 14a and **14b:** To a stirred solution of phenol **18a** (120.3 mg, 560 *μ*mol) in dry toluene and dimethyl sulfoxide (4 mL, 3:1) was added SIBX (215 mg, 80 wt. %, 1.1 equiv.) in one portion and stirred for 15 hours at room temperature, after which time it was filtered. The filtrate was then diluted with EtOAc (15 mL), and washed with sat. aq. $NaHCO_3$ (3 × 4 mL) and brine (2 × 4 mL). The organic layer was dried over Na_2SO_4, filtered and concentrated under vacuum. The residue was purified by silica gel preparation lamella chromatography to give diastereomeric mixture **14a** and **14b** (81 mg, ratio of 1:1 analyzed by HPLC) in 63 % yield. The mixture of **14a** and **14b** was further purified by semi-preparative HPLC.

14a: R_f = 0.42 (silica, EtOAc/PE 1:6); $[\alpha]_D^{21}$ = +73.8 (*c* 0.539, MeOH), ^{1}H NMR (500 MHz, $CDCl_3$) δ 1.40 (s, 3H), 1.74 (s, 3H), 1.94 (d, 2.3, 3H), 2.37 (overlap, 2H), 3.17 (m, 1H), 3.22 (s, 1H), 4.83 (s, 1H), 4.98 (s, 1H), 5.98 (s, 1H), 6.14 (d, 2.3, 1H), 6.26 (s, 1H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$) δ 206.1, 149.5, 144.8, 137.7, 137.3, 131.8, 131.7, 115.2, 114.9, 75.1, 45.7, 29.5, 29.3, 19.7, 19.2. ppm. HRMS (ESI) *m/z* 253.1197 $[M + Na]^+$ (calcd for $C_{15}H_{18}O_2Na$ 253.1199).

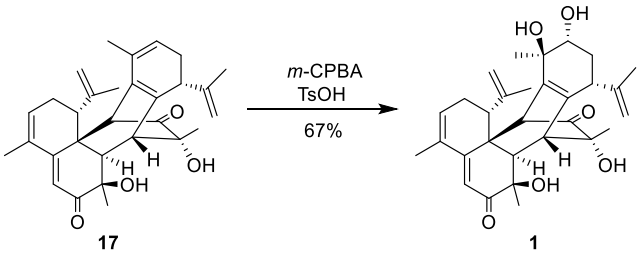
14b: R_f = 0.42 (silica, EtOAc/PE 1:6); $[\alpha]_D^{20}$ = –7.2 (*c* 0.075, MeOH), ^{1}H NMR (500 MHz, $CDCl_3$) δ 1.39 (s, 3H), 1.69 (s, 3H), 1.94 (d, 1.7, 3H), 2.42 (overlap, 2H), 3.19 (overlap, 2H), 4.77 (s, 1H), 4.89 (s, 1H), 5.99 (s, 1H), 6.15 (d, 1.7, 1H), 6.23 (s, 1H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$) δ 206.0, 149.3, 145.2, 137.9, 136.5, 131.8, 131.6, 115.2, 114.2, 75.2, 45.5, 29.3, 29.2, 20.1, 19.2 ppm. HRMS (ESI) *m/z* 253.1202 $[M + Na]^+$ (calcd for $C_{15}H_{18}O_2Na$ 253.1199).



14a **17**

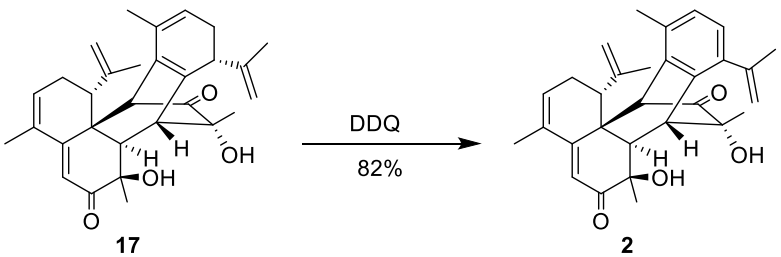
Synthesis of compound 17: To a stirred solution of **14a** (13 mg, 56 *μ*mol) was added in DCM (0.5 mL) at room temperature. After removal of the solvent under argon bubbling, the residue was heated at 80 °C for 12 h before it was cooled to room temperature. The residue was directly purified by semi-preparative HPLC to give **17** (10 mg, 78%) as a white powder.

17: R_f = 0.44 (silica, EtOAc/PE 1:6); $[\alpha]_D^{27}$ = +6.3 (*c* 0.067, MeOH), ^{1}H NMR (500 MHz, $CDCl_3$) δ 1.20 (s, 3H), 1.23 (brs, 3H), 1.42 (m, 3H), 1.57 (overlap, 6H), 1.85 (brs, 3H), 1.96 (m, 1H), 2.17 (s, 1H), 2.52 (m, 1H), 2.94 (overlap, 2H), 3.05 (dd, 10.9, 3.0, 1H), 3.34 (s, 1H), 3.41 (d, 2.5, 1H), 3.53 (s, 1H), 3.96 (s, 1H), 4.56 (s, 1H), 4.84 (s, 1H), 4.86 (d, 2.0, 1H), 4.99 (d, J = 2.2, 1H), 5.34 (m, 1H), 6.06 (d, J = 4.3, 1H), 6.09 (s, 1H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$) δ 211.7, 202.9, 154.6, 147.2, 137.9, 133.2, 131.6, 131.5, 128.1, 122.5, 120.4, 117.8, 112.6, 73.7, 71.4, 58.5, 49.4, 48.8, 47.6, 44.2, 42.8, 33.2, 31.1, 28.0, 27.3, 25.6, 21.5, 19.9, 19.7, 18.5 ppm. HRMS (ESI) *m/z* 461.2693 $[M + H]^+$ (calcd for $C_{30}H_{37}O_4$ 461.2686).



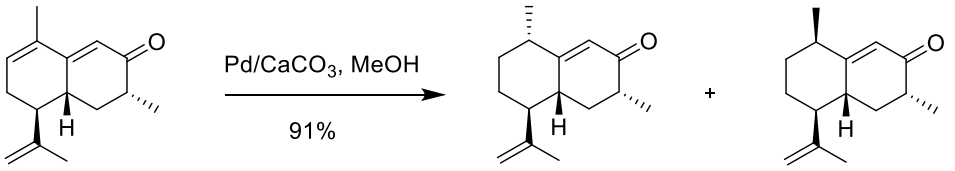
Synthesis of 1: To a stirred solution of diene **17** (10.1 mg, 21.7 μmol, 1.0 equiv.) in a mixed solution of CH_2Cl_2/HFIP/H_2O (2.4 mL, 8:3:1) at 0 °C was added *p*-TsOH (3.74 mg, 21.7 μmol, 1.0 equiv) and *m*-CPBA (5.84 mg, ca. 70%, 26 μmol, 1.2 equiv) and the resulting mixture was stirred for 2 h. The resultant mixture was then poured into saturated solution of $Na_2S_2O_3$ and $NaHCO_3$. The organic phase was separated and the aqueous phase was extracted with EtOAc. The combined organic extracts were dried over Na_2SO_4 and concentrated under reduced pressure. The residue was directly purified by semi-preparative HPLC to give **1** (7.21 mg, 67%) as a white powder.

1: R_f = 0.32 (silica, EtOAc/PE 1:6); $[\alpha]_D^{22}$ = –66.4 (*c* 0.081, MeOH), ^{1}H NMR (600 MHz, $CDCl_3$) δ 1.50 (overlap, 6H), 1.53 (s, 3H), 1.60 (brs, 3H), 1.81 (overlap, 6H), 2.00 (dd, 19.7, 5.4, 1H), 2.18 (dd, 13.4, 3.5, 1H), 2.24 (m, 1H), 3.06 (d, 19.7, 1H), 3.55 (d, 5.1, 1H), 3.91 (brs, 1H), 3.96 (d, 6.8, 1H), 4.08 (d, 2.6, 1H), 4.16 (s, 1H), 4.58 (dd, 12.5, 3.5, 1H), 4.91 (brs, 1H), 5.39 (brs, 1H), 5.41 (d, 2.2, 1H), 5.61 (d, 4.6, 1H), 6.30 (s, 1H), 6.49 (s, 1H), 7.67 (s, 1H) ppm; ^{13}C NMR (150 MHz, $CDCl_3$) δ 213.0, 203.2, 153.5, 147.4, 141.6, 138.4, 133.5, 132.0, 123.3, 118.0, 115.7, 75.1, 74.1, 73.9, 71.9, 60.6, 49.3, 48.9, 48.8, 46.7, 44.2, 34.0, 32.9, 28.4, 26.7, 22.7, 22.1, 20.2, 20.0. ppm. HRMS (ESI) *m/z* 495.2736 $[M + H]^+$ (calcd for $C_{30}H_{39}O_6$ 495.2741).



Synthesis of compound 2: To a stirred solution of diene **17** (10.8 mg, 21.7 μmol, 1.0 equiv) in CH_2Cl_2 (2 mL) at 0 °C was added DDQ (1.5 mg, 6.5 μmol, 0.3 equiv) and the resulting mixture was stirred for 12 h. The resultant mixture was then poured into saturated solution of $Na_2S_2O_3$ and $NaHCO_3$. The organic phase was separated and the aqueous phase was extracted with EtOAc. The combined organic extracts were dried over Na_2SO_4 and concentrated under reduced pressure. The residue was directly purified by semi-preparative HPLC to give **2** (8.2 mg, 82%) as a white powder.

2: R_f = 0.44 (silica, EtOAc/PE 1:6); $[\alpha]_D^{20}$ = –9.0 (*c* 0.082, MeOH), ^{1}H NMR (500 MHz, $CDCl_3$) δ 1.16 (s, 3H), 1.20 (s, 3H), 1.57 (brs, 3H), 1.81 (m, 3H), 1.98 (s, 3H), 2.19 (brs, 3H), 2.26 (dd, 20.2, 5.1, 1H), 2.97 (d, 5.7, 1H), 3.08 (m, 1H), 3.46 (d, 2.1, 1H), 4.01 (s), 4.25 (d, 2.7, 1H), 4.90 (brs, 1H), 5.05 (d, 2.3), 5.10 (brs, 1H), 5.26 (brs, 1H), 5.67 (s, 1H), 6.10 (d, 4.4), 6.97 (d, 7.9, 1H), 7.00 (d, 7.9, 1H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$) δ 212.9, 200.5, 152.4, 145.2, 140.1, 135.3, 135.2, 132.9, 132.1, 131.4, 129.6, 128.2, 120.2, 118.3, 116.4, 73.7, 72.8, 59.0, 48.2, 47.9, 46.3, 43.8, 32.3, 27.9, 26.2, 24.8, 21.8, 19.9, 18.2. ppm. HRMS (ESI) *m/z* 459.2526 $[M + H]^+$ (calcd for $C_{30}H_{35}O_4$ 459.2530).

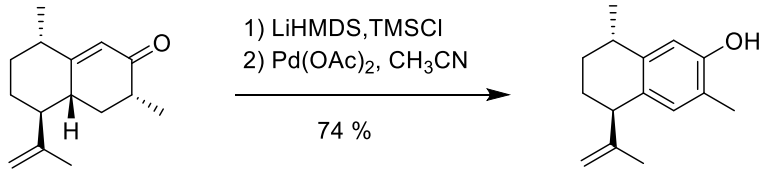


19 **25a** 1:3 **25b**

Synthesis of compounds 25a and **25b**: To a stirred solution of compound **19** (200.7 mg, 0.926 mmol) in MeOH (3 mL) at room temperature was added a catalytic amount of palladium (5 % on $CaCO_3$; 10 mg, 0.5% equiv). The reaction mixture was hydrogenated under an atmosphere of H_2 for 30 min and detected by HPLC, then it was filtered through a pad of Celite. The filter cake was washed with EtOAc (20 mL), the filtrates were combined, and the solvent was removed on the rotary evaporator to give the mixture of **25a** and **25b** (184 mg, 1:3, 91%).

25a: R_f = 0.52 (silica, EtOAc/PE 1:14); $[\alpha]_D^{27}$ = –2.3 (*c* 0.114, MeOH), ^{1}H NMR (500 MHz, $CDCl_3$) δ 1.03 (d, 6.7, 3H), 1.07 (d, 6.7, 3H), 1.17 (m, 2H), 1.61 (m, 2H), 1.67 (s, 3H), 1.83 (m, 2H), 1.95 (m, 1H), 2.23 (m, 3H), 4.71 (s, 1H), 4.75 (s, 1H), 5.83 (brs, 1H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$) δ 202.6, 168.2, 146.4, 122.3, 112.3, 54.6, 40.4, 40.1, 37.7, 35.7, 34.6, 31.4, 18.5, 18.1, 14.6 ppm. HRMS (ESI) *m/z* 219.1746 $[M + H]^+$ (calcd for $C_{15}H_{23}O$ 219.1743).

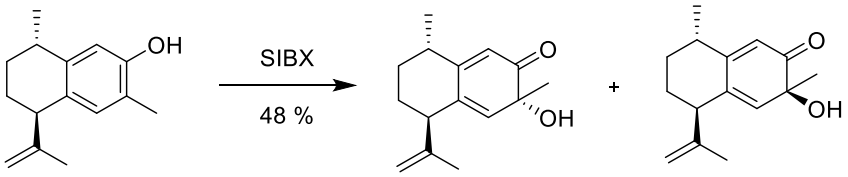
25b: R_f = 0.52 (silica, EtOAc/PE 1:14); $[\alpha]_D^{27}$ = +26.4 (*c* 0.178, MeOH), ^{1}H NMR (500 MHz, $CDCl_3$) δ 1.00 (d, 6.7, 3H), 112 (d, 7.4, 3H), 1.09 (m, 1H), 1.42 (m, 1H), 1.65 (s, 3H), 1.69 (m, 4H), 1.92 (m, 1H), 2.17 (m, 1H), 2.47 (m, 1H), 2.58 (m, 1H), 4.69 (s, 1H), 4.72 (s, 1H), 5.78 (d, 2.3, 1H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$) δ 202.2, 169.5, 146.3, 124.5, 112.2, 53.9, 40.5, 37.5, 36.4, 35.9, 31.3, 25.7, 20.9, 18.5, 14.5 ppm. HRMS (ESI) *m/z* 219.1746 $[M + H]^+$ (calcd for $C_{15}H_{23}O$ 219.1743).



25a **23**

Synthesis of compound 23: To a solution of LiHMDS (1 M, 1.1 mL, 1.8 equiv) was added to a stirred solution of **25a** (133.4 mg, 609 *μ*mol) in dry THF (2 mL) at –78 °C. After 30 min TMSCl (93 *μ*L, 730 *μ*mol, 1.2 equiv) was added and the resultant was allowed to warm to room temperature for 1 h. The resultant mixture was then poured into a cold saturated solution of $NaHCO_3$. The water phase was extracted with petroleum ether. The organic extracts were combined and dried over Na_2SO_4. The solvent was removed under vacuum and the crude TMS enol ethers were used without further purification. To a solution of the silyl enol ether obtained above in freshly distilled acetonitrile was added palladium(II) acetate, freshly prepared according to the reported procedure and other additive[6]. The reaction mixture was stirred for 20 min, and filtered through a short silica gel column with EtOAc. The filtrate was concentrated in vacuo and the residue was purified by column chromatography on silica gel to give **23** (96.4 mg, 74%).

23: R_f = 0.40 (silica, EtOAc/PE 1:16); $[\alpha]_D^{27}$ = +5.8 (*c* 0.072, MeOH), ^{1}H NMR (500 MHz, $CDCl_3$) *δ* 1.26 (d, 6.9 Hz, 3H), 1.41 (m, 1H), 1.63 (s, 3H), 1.71 (m, 1H), 1.93 (m, 1H), 2.19 (s, 3H), 2.81 (m, 1H), 3.45 (m, 1H), 4.68 (s, 1H), 4.76 (s, 1H), 4.89 (s, 1H), 6.67 (s, 1H), 6.84 (s, 1H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$) *δ* 152.0, 149.6, 141.6, 131.4, 130.1, 121.2, 113.5, 113.3, 47.4, 32.8, 30.4, 26.9, 22.6, 19.5, 15.5 ppm. HRMS (ESI) *m/z* 215.1439 $[M - H]^-$ (calcd for $C_{15}H_{19}O$ 215.1441).

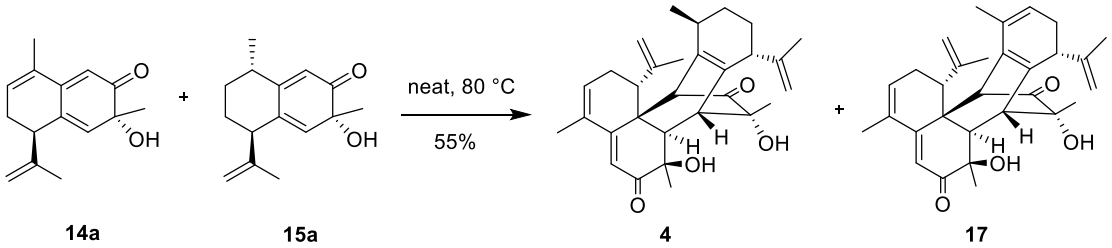


23 **15a** 1:1 **15b**

Synthesis of compounds 15a and **15b**: To a stirred solution of phenol **23** (28.1 mg, 130 *μ*mol) in dry toluene and dimethyl sulfoxide (1.8 mL, 2:1) was added SIBX (68 mg, 80 wt. %, 1.50 equiv) in one portion and stirred for 15 hours at room temperature, after which time it was filtered. The filtrate was then diluted with EtOAc (15 mL), and washed with sat. aq. $NaHCO_3$ (3 × 4 mL) and brine (2 × 4 mL). The organic layer was dried over Na_2SO_4, filtered and concentrated under vacuum to give diastereomeric mixture **15a** and **15b** (14.4 mg, 48 %). The mixture of **15a** and **15b** was further purified by semipreparative HPLC.

15a: R_f = 0.42 (silica, EtOAc/PE 1:6); $[\alpha]_D^{26}$ = –14.8 (*c* 1.65, MeOH), ^{1}H NMR (600 MHz, $CDCl_3$) δ 1.22 (d, 6.6, 3H), 1.35 (m, 1H), 1.39 (s, 3H), 1.70 (s, 3H), 1.76 (m, 2H), 1.91 (m, 1H), 2.56 (m, 1H), 3.08 (m, 1H), 3.19 (s, 1H), 4.82 (s, 1H), 4.92 (s, 1H), 6.00 (s, 1H), 6.21 (s, 1H) ppm; ^{13}C NMR (150 MHz, $CDCl_3$) δ 206.1, 161.8, 146.6, 139.9, 132.6, 118.5, 114.2, 75.6, 48.0, 35.0, 30.4, 29.0, 27.1, 19.4, 19.0 ppm. HRMS (ESI) *m/z* 255.1359 $[M + Na]^+$ (calcd for $C_{15}H_{20}O_2Na$ 255.1356).

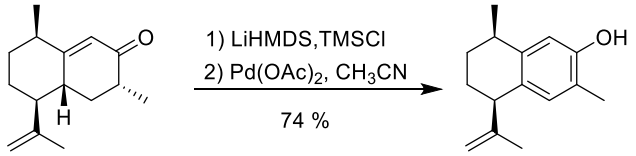
15b: R_f = 0.42 (silica, EtOAc/PE 1:6); $[\alpha]_D^{22}$ = –64.0 (*c* 0.091, MeOH), ^{1}H NMR (600 MHz, $CDCl_3$) δ 1.23 (d, 6.9, 3H), 1.30 (m, 1H), 1.36 (s, 3H), 1.65 (s, 3H), 1.79 (m, 1H), 1.91 (m, 1H), 2.65 (m, 1H), 3.11 (m, 1H), 3.16 (s, 1H), 4.80 (s, 1H), 4.89 (s, 1H), 6.00 (d, 1.7, 1H), 6.22 (d, 1.9, 1H) ppm; ^{13}C NMR (150 MHz, $CDCl_3$) δ 206.1, 162.4, 146.7, 140.6, 132.3, 120.1, 114.2, 75.7, 47.7, 34.7, 29.5, 29.1, 26.4, 21.5, 19.0. ppm. HRMS (ESI) *m/z* 255.1360 $[M + Na]^+$ (calcd for $C_{15}H_{20}O_2Na$ 255.1356).



14a **15a** **4** **17**

Synthesis of compounds 4 and **17**: To a stirred solution of **14a** (30.1 mg, 129 *μ*mol, 1.0 equiv) and **15a** (10 mg, 43 *μ*mol) was added in dichloromethane (0.5 mL) at room temperature. After removal of the solvent under argon bubbling, the residue was heated at 80 °C for 12 h before it was cooled to room temperature. The residue was directly purified by semi-preparative HPLC to give **4** (13 mg, 55% yield based on **15a**) and **17** (17 mg, 86% yield based on **14a**).

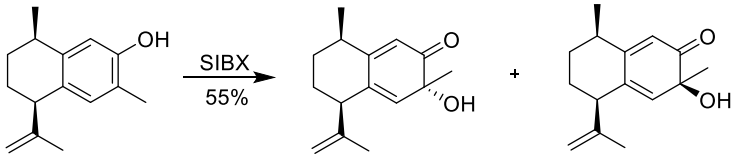
4: R_f = 0.44 (silica, EtOAc/PE 1:6); $[\alpha]_D^{20}$ = −50.2 (*c* 0.164, MeOH), ^{1}H NMR (500 MHz, $CDCl_3$) δ 0.69 (d, 7.3, 3H), 1.20 (s, 3H), 1.22 (brs, 3H), 1.25 (m, 1H), 1.57 (overlap, 6H), 1.71 (overlap, 4H), 1.86 (s, 3H), 1.97 (m, 1H), 2.15 (dd, 20.7, 4.8, 1H), 2.91 (overlap, 3H), 3.26 (s, 1H), 3.30 (brs, 1H), 3.44 (d, 2.7, 1H), 3.83 (s, 1H), 4.85 (s, 1H), 4.91 (brs, 1H), 4.96 (brs, 1H), 4.99 (d, 2.3, 1H), 6.06 (s, 1H), 6.09 (d, 4.9, 1H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$) δ 212.2, 202.2, 154.5, 146.0, 146.0, 141.8, 135.9, 133.7, 131.6, 120.9, 117.8, 115.3, 73.9, 71.7, 62.0, 48.3, 47.7, 47.1, 44.3, 43.3, 33.2, 31.5, 29.0, 27.6, 26.4, 24.5, 22.6, 22.6, 20.0, 17.4 ppm. HRMS (ESI) *m/z* 463.2850 $[M + H]^+$ (calcd for $C_{30}H_{39}O_4$ 463.2843).



25b **24**

Synthesis of compound 24: To a solution of LiHMDS (1 M, 1.3 mL, 1.8 equiv) was added to a stirred solution of **25b** (160.5 mg, 734 *μ*mol) in dry THF (2 mL) at -78 °C. After 30 min TMSCl (112 *μ*L, 880 *μ*mol, 1.2 equiv) was added and the resultant was allowed to warm to room temperature for 1 h. The resultant mixture was then poured into a cold saturated solution of $NaHCO_3$. The water phase was extracted with petroleum ether. The organic extracts were combined and dried over Na_2SO_4. The solvent was removed under vacuum and the crude TMS enol ethers were used without further purification. To a solution of the silyl enol ether obtained above in freshly distilled acetonitrile was added palladium(II) acetate, freshly prepared according to the reported procedure and other additive[6]. The reaction mixture was stirred for 20 min, and filtered through a short silica gel column with EtOAc. The filtrate was concentrated in vacuo and the residue was purified by column chromatography on silica gel to give **24** (117 mg, 74%).

24: R_f = 0.40 (silica, EtOAc/PE 1:16); $[\alpha]_D^{27}$ = +4.0 (*c* 0.147, MeOH), ^{1}H NMR (500 MHz, $CDCl_3$) *δ* 1.27 (d, 7.1 Hz, 3H), 1.64 (m, 1H), 1.68 (s, 3H), 1.73 (m, 1H), 1.87 (m, 2H), 2.20 (s, 3H), 2.22 (s, 1H), 2.83 (m, 1H), 3.42 (m, 1H), 4.68 (s, 1H), 4.89 (s, 1H), 4.93 (s, 1H), 6.61 (s, 1H), 6.85 (s, 1H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$) *δ* 152.0, 149.5, 141.7, 131.4, 129.9, 121.4, 114.3, 113.6, 47.2, 32.6, 28.8, 24.8, 23.4, 19.7, 15.5 ppm. HRMS (ESI) *m/z* 215.1445 $[M - H]^-$ (calcd for $C_{15}H_{19}O$ 215.1441).



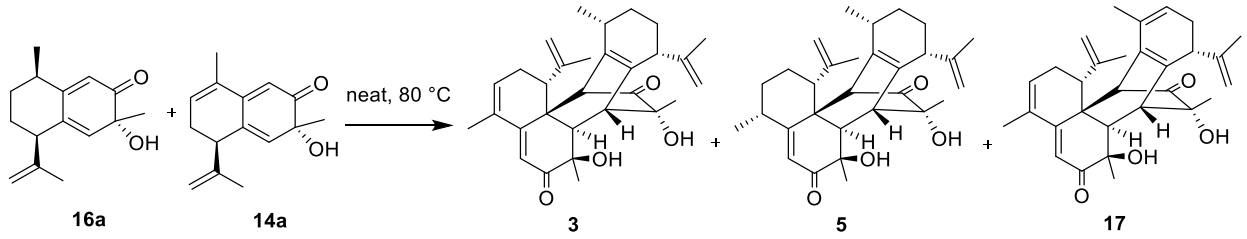
24 **16a** **16b**

Synthesis of compounds 16a and **16b**: To a stirred solution of phenol **24** (10.1 mg, 46 *μ*mol) in dry toluene and dimethyl sulfoxide (1.2 mL, 2:1) was added SIBX (24 mg, 80 wt. %, 1.5 equiv) in one portion and stirred for 15 hours at room temperature, after which time it was filtered. The filtrate was then diluted with EtOAc (15 mL), and washed with sat. aq. $NaHCO_3$ (3 × 4 mL) and brine (2 × 4 mL). The organic layer was dried over Na_2SO_4, filtered and concentrated under vacuum to give the residue which was composed of **16a** and **16b** by HPLC analysis. The mixture purified by silica gel preparation lamella chromatography to give diastereomeric mixture (5.84 mg, 55%) of **16a** and **16b** (ratio = 1:3, detected by NMR). The mixture of **16a** and **16b** was further purified by semi-preparative HPLC to give **16b** (2.1 mg) and **16a** undergo partly spontaneous [4 + 2] cyclodimerizations to give **5**.

16a: R_f = 0.42 (silica, EtOAc/PE 1:6); ^{1}H NMR (500 MHz, $CDCl_3$) *δ* 1.21 (d, 5.6, 3H), 1.36 (s, 3H), 1.43 (m, 1H), 1.70 (m, 1H), 1.71 (s, 3H), 1.75 (m, 2H), 1.87 (m, 1H), 2.74 (m, 1H), 3.08 (m, 1H), 4.79 (s, 1H), 4.90 (s, 1H), 5.92 (s, 1H),

6.18 (s, 1H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$) δ 206.0, 162.7, 146.1, 138.6, 132.6, 119.7, 114.7, 75.8, 46.3, 34.0, 29.2, 28.0, 24.1, 21.3, 19.4 ppm. HRMS (ESI) *m/z* 233.1538 $[M + H]^+$ (calcd for $C_{15}H_{21}O_2$ 233.1536).

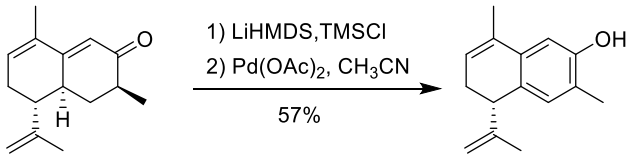
16b: R_f = 0.42 (silica, EtOAc/PE 1:6); ^{1}H NMR (500 MHz, $CDCl_3$) δ 1.20 (d, J = 6.7, 3H), 1.37 (s, 3H), 1.50 (m, 1H), 1.72 (s, 3H), 1.73 (m, 2H), 1.87 (m, 1H), 2.68 (d, 6.8, 1H), 3.17 (s, 2H), 4.78 (s, 1H), 4.96 (s, 1H), 5.96 (s, 1H), 6.11 (s, 1H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$) δ 206.1, 162.7, 145.8, 138.6, 133.6, 118.6, 114.6, 75.8, 45.4, 33.3, 28.9, 28.1, 24.7, 20.0, 19.4 ppm. HRMS (ESI) *m/z* 233.1535 $[M + H]^+$ (calcd for $C_{15}H_{21}O_2$ 233.1536).



Synthesis of compounds 3, 5, and 17: To a stirred solution of **16** (a mixture of **16a** and **16b**, 1:3, 50.1 mg, 71.9 μmol) and **14a** (40 mg, 174 μmol) was added in DCM (0.5 mL) at room temperature. After removal of the solvent under argon bubbling, the residue was heated at 80 °C for 12 h before it was cooled to room temperature. The residue was directly purified by semi-preparative HPLC to give **3** (2.4 mg, 7% yield based on **16a**), **5** (4.8 mg, 28% yield based on **16a**) and **17** (13 mg, 32% yield based on **14a**) as a white powder.

3: R_f = 0.44 (silica, EtOAc/PE 1:6); $[\alpha]_D^{25}$ = +52.6 (*c* 0.151, MeOH), ^{1}H NMR (500 MHz, $CDCl_3$) δ 0.85 (d, 6.9, 3H), 1.17 (s, 3H), 1.22 (brs, 3H), 1.34 (m, 1H), 1.45 (overlap, 2H), 1.55 (overlap, 5H), 1.69 (s, 3H), 1.87 (s, 3H), 2.18 (dd, 20.1, 4.6, 1H), 2.84 (overlap, 3H), 3.14 (s, 1H), 3.26 (brs, 1H), 3.39 (d, 2.5, 1H), 3.82 (s, 1H), 4.83 (s, 1H), 4.93 (overlap, 2H), 4.97 (brs, 1H), 6.06 (d, 4.3, 1H), 6.08 (s, 1H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$) δ 212.3, 201.8, 155.0, 145.5, 145.5, 139.8, 138.1, 133.4, 131.2, 120.0, 117.8, 115.1, 73.7, 72.0, 62.6, 49.2, 47.4, 47.4, 44.8, 43.5, 33.3, 33.1, 28.4, 27.7, 25.9, 23.7, 22.4, 22.4, 20.0, 19.0 ppm. HRMS (ESI) *m/z* 463.2851 $[M + H]^+$ (calcd for $C_{30}H_{39}O_4$ 463.2843).

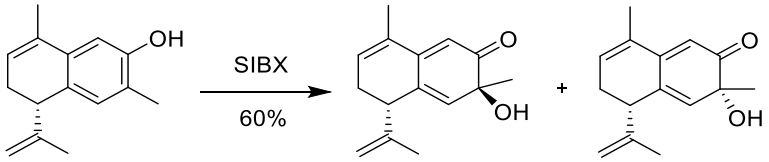
5: R_f = 0.44 (silica, EtOAc/PE 1:6); $[\alpha]_D^{22}$ = –77.6 (*c* 0.116, MeOH), ^{1}H NMR (500 MHz, $CDCl_3$) δ 0.93 (d, 6.8, 3H), 1.16 (overlap, 6H), 1.31 (brs, 3H),1.34 (m, 1H), 1.43 (m, 1H), 1.55 (overlap, 4H), 1.67 (s, 3H), 1.76 (s, 3H),1.85 (overlap, 2H), 2.36 (brs, 1H), 2.67 (m, 1H), 2.71 (brs, 1H), 2.86 (s, 1H), 3.40 (d, 2.3, 1H), 3.77 (overlap, 2H), 4.89 (overlap, 4H), 6.11 (d, 2.1, 1H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$) δ 212.1, 201.7, 166.2, 146.3, 145.6, 139.8, 137.5, 122.8, 117.9, 115.0, 73.2, 71.5, 60.7, 52.8, 49.9, 47.5, 43.3, 33.2, 32.8, 32.5, 30.1, 28.5, 25.8, 25.8, 24.1, 24.1, 22.3, 19.2, 19.1 ppm. HRMS (ESI) *m/z* 487.2817 $[M + Na]^+$ (calcd for $C_{30}H_{40}O_4Na$ 487.2819).



26 **27**

Synthesis of compound 27: To a solution of LiHMDS (1 M, 4 mL, 1.8 equiv) was added to a stirred solution of **26** (500.4 mg, 2.31 mmol) in dry THF (3 mL) at –78 °C. After 30 min TMSCl (0.35 mL, 2.77 mmol, 1.2 equiv) was added and the resultant was allowed to warm to room temperature for 1 h. The resultant mixture was then poured into a cold saturated solution of $NaHCO_3$. The water phase was extracted with PE. The organic extracts were combined and dried over Na_2SO_4. The solvent was removed under vacuum and the crude TMS enol ethers were used without further purification. To a solution of the silyl enol ether obtained above in freshly distilled acetonitrile was added palladium(II) acetate, freshly prepared according to the reported procedure and other additive[6]. The reaction mixture was stirred for 20 min, and filtered through a short silica gel column with EtOAc. The filtrate was concentrated in vacuo and the residue was purified by column chromatography on silica gel and HPLC to give **27** (280.6 mg, 4:1, 57 %).

27: R_f = 0.38 (silica, EtOAc/PE 1:12); $[\alpha]_D^{25}$ = +125.3 (*c* 0.129, MeOH), ^{1}H NMR (500 MHz, $CDCl_3$) δ 1.73 (s, 3H), 2.00 (brs, 1H), 2.22 (s, 3H), 2.35 (m, 2H), 3.43 (t, 8.3, 1H), 4.63 (brs, 1H), 4.69 (s, 1H), 4.85 (s, 1H), 5.76 (s, 1H), 6.70 (s, 1H), 6.84 (s, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 152.4, 147.6, 135.0, 131.5, 129.9, 129.6, 123.9, 121.8, 112.9, 110.2, 45.3, 28.5, 20.0, 19.5, 15.7 ppm. HRMS (ESI) *m/z* 213.1287 $[M - H]^-$ (calcd for $C_{15}H_{17}O$ 213.1285).



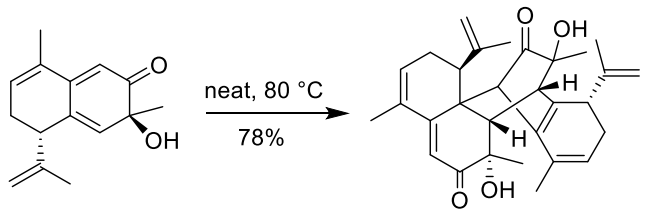
27a **28a** 1:1 **28b**

Synthesis of compounds 28a and **28b**: To a stirred solution of phenol **27a** (62.2 mg, 290 μmol) in dry toluene and dimethyl sulfoxide (4 mL, 3:1) was added SIBX (112 mg, 80 wt. %, 1.1 equiv) in one portion and stirred for 15 hours at room temperature, after which time it was filtered. The filtrate was then diluted with EtOAc (15 mL), and washed with sat. aq. $NaHCO_3$ (3 × 4 mL) and brine (2 × 4 mL). The organic layer was dried over Na_2SO_4, filtered and concentrated under vacuum. The residue was purified by silica gel preparation lamella chromatography to give diastereomeric mixture of **28a** and **28b** (40 mg ratio of 1:1) in 60 % yield. The mixture of **28a** and **28b** was further purified by semipreparative HPLC.

28a: R_f = 0.42 (silica, EtOAc/PE 1:6); $[\alpha]_D^{28}$ = –77.0 (*c* 0.121, MeOH), ^{1}H NMR (500 MHz, $CDCl_3$) δ 1.40 (s, 3H), 1.74 (s, 3H), 1.94 (d, 2.3, 3H), 2.36 (overlap, 2H), 3.17 (m, 1H), 3.23 (s, 1H), 4.82 (s, 1H), 4.97 (s, 1H), 5.98 (s, 1H), 6.14 (d,

2.3, 1H), 6.27 (s, 1H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$) δ 206.1, 149.5, 144.8, 137.7, 137.3, 131.8, 131.7, 115.2, 114.9, 75.1, 45.7, 29.5, 29.3, 19.6, 19.2. ppm. HRMS (ESI) *m/z* 231.1381 $[M + H]^+$ (calcd for $C_{15}H_{19}O_2$ 231.1380).

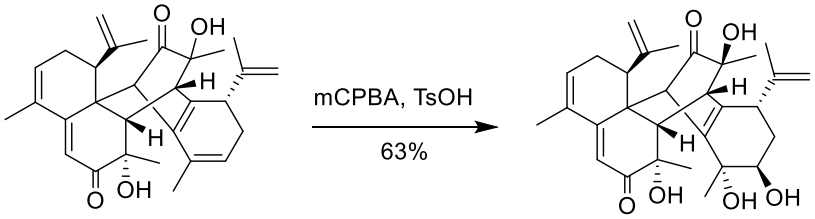
28b: R_f = 0.42 (silica, EtOAc/PE 1:6); $[\alpha]_D^{28}$ = +15.2 (*c* 0.122, MeOH), ^{1}H NMR (500 MHz, $CDCl_3$) δ 1.38 (s, 3H), 1.69 (s, 3H), 1.94 (d, 1.7, 3H), 2.41 (overlap, 2H), 3.19 (overlap, 2H), 4.77 (s, 1H), 4.88 (s, 1H), 5.98 (s, 1H), 6.15 (d, 1.7, 1H), 6.23 (s, 1H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$) δ 206.1, 149.4, 145.2, 137.9, 136.6, 131.9, 131.7, 115.3, 114.2, 75.2, 45.6, 29.4, 29.3, 20.1, 19.3 ppm. HRMS (ESI) *m/z* 231.1376 $[M + H]^+$ (calcd for $C_{15}H_{19}O_2$ 231.1380).



28a **29**

Synthesis of compound 29: To a stirred solution of **28a** (10.1 mg, 43.4 μmol) was added in DCM (0.5 mL) at room temperature. After removal of the solvent under argon bubbling, the residue was heated at 80 °C for 12 h before it was cooled to room temperature. The residue was directly purified by semi-preparative HPLC to give **29** (7.8 mg, 78%) as a white powder.

29: R_f = 0.44 (silica, EtOAc/PE 1:6); $[\alpha]_D^{22}$ = –20.9 (*c* 0.042, MeOH), ^{1}H NMR (500 MHz, $CDCl_3$) δ 1.20 (s, 3H), 1.23 (brs, 3H), 1.42 (m, 3H), 1.57 (overlap, 6H), 1.85 (brs, 3H), 1.96 (m, 1H), 2.12 (s, 1H), 2.20 (m, 1H), 2.52 (m, 1H), 2.94 (overlap, 2H), 3.05 (dd, J = 10.9, 3.0, 1H), 3.34 (s, 1H), 3.41 (d, J = 2.5, 1H), 3.53 (s, 1H), 3.96 (s, 1H), 4.56 (s, 1H), 4.84 (s, 1H), 4.87 (brs, 1H), 4.99 (d, J = 2.2, 1H), 5.35 (m, 1H), 6.07 (d, J = 4.3, 1H), 6.09 (s, 1H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$) δ 211.7, 202.9, 154.6, 147.2, 137.9, 133.2, 131.6, 131.5, 128.1, 122.5, 120.4, 117.9, 112.6, 73.7, 71.4, 58.5, 49.3, 48.9, 47.5, 44.2, 42.8, 33.2, 31.1, 28.0, 27.3, 25.6, 21.3, 19.9, 19.7, 18.5 ppm. HRMS (ESI) *m/z* 483.2511 $[M + Na]^+$ (calcd for $C_{30}H_{36}O_4Na$ 483.2506).

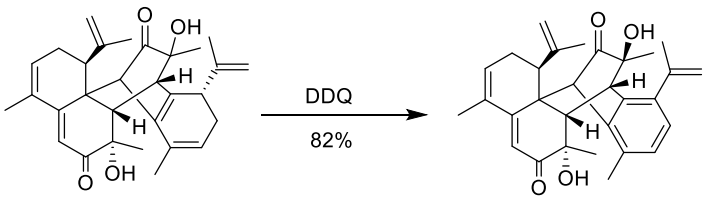


29 **6**

Synthesis of compound 6: To a stirred solution of diene **29** (8.0 mg, 17.4 μmol, 1.0 equiv.) in a mixed solution of CH_2Cl_2/HFIP/H_2O (2.4 mL, 8:3:1) at 0 °C was added *p*TsOH (3.2 mg, 17.4 μmol, 1.0 equiv) and *m*-CPBA (3.6 mg, 20.9 μmol, 1.2 equiv) and the resulting mixture was stirred for 2 h. The resultant mixture was then poured into saturated solution of $Na_2S_2O_3$ and $NaHCO_3$. The organic phase was separated and the aqueous phase was extracted with EtOAc.

The combined organic extracts were dried over Na_2SO_4 and concentrated under reduced pressure. The residue was directly purified by semi-preparative HPLC to give **6** (5.4 mg, 63%) as a white powder.

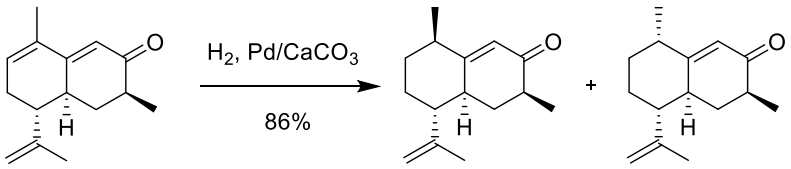
6: R_f = 0.32 (silica, EtOAc/PE 1:6); $[\alpha]_D^{20}$ = +57.8 (*c* 0.072, MeOH), ^{1}H NMR (500 MHz, pyridine-d_5) δ 1.50 (overlap, 6H), 1.54 (s, 3H), 1.60 (brs, 3H), 1.81 (overlap, 6H), 2.00 (dd, J = 19.7, 5.4, 1H), 2.18 (dd, 13.4, 3.5, 1H), 3.06 (d, 19.7, 1H), 3.55 (d, 5.1, 1H), 3.91 (brs, 1H), 3.96 (d, 6.8, 1H), 4.08 (d, 2.6, 1H), 4.16 (s, 1H), 4.58 (dd, 12.5, 3.5, 1H), 4.91 (brs, 2H), 5.39 (brs, 1H), 5.41 (d, 2.2, 1H), 5.61 (d, 4.6, 1H), 6.30 (s, 1H), 6.47 (s, 1H), 7.66 (s, 1H) ppm; ^{13}C NMR (125 MHz, pyridine-d_5) δ 213.0, 203.2, 153.5, 147.4, 141.6, 138.4, 133.5, 132.0, 123.3, 118.0, 115.7, 75.1, 74.1, 73.9, 71.9, 60.7, 49.2, 48.9, 48.9, 46.7, 44.2, 34.0, 32.9, 28.5, 26.7, 22.7, 22.1, 20.2, 20.0. ppm. HRMS (ESI) *m/z* 495.2748 $[M + H]^+$ (calcd for $C_{30}H_{39}O_6$ 495.2741).



29 **7**

Synthesis of compound 7: To a stirred solution of diene **29** (8.1 mg, 17.4 μmol, 1.0 equiv.) in CH_2Cl_2 (2 mL) at 0 °C was added DDQ (2 mg, 8.7 μmol, 0.5 equiv) and the resulting mixture was stirred for 12 h. The resultant mixture was then poured into saturated solution of $Na_2S_2O_3$ and $NaHCO_3$. The organic phase was separated and the aqueous phase was extracted with EtOAc. The combined organic extracts were dried over Na_2SO_4 and concentrated under reduced pressure. The residue was directly purified by semipreparative HPLC to give **7** (6.5 mg, 82 %) as a white powder.

7: R_f = 0.44 (silica, EtOAc/PE 1:6); $[\alpha]_D^{27}$ = +4.4 (*c* 0.121, MeOH), ^{1}H NMR (500 MHz, $CDCl_3$) δ 1.16 (s, 3H), 1.20 (s, 3H), 1.57 (brs, 3H), 1.82 (m, 3H), 1.98 (s, 3H), 2.19 (brs, 3H), 2.26 (dd, 20.2, 5.1, 1H), 2.42 (s, 1H), 2.97 (d, 5.7, 1H), 3.08 (m, 1H), 3.45 (d, 2.1, 1H), 3.65 (s, 1H), 4.01 (s), 4.25 (d, 2.7, 1H), 4.90 (brs, 1H), 5.05 (d, 2.3), 5.10 (brs, 1H), 5.26 (brs, 1H), 5.67 (s, 1H), 6.10 (d, 4.4), 6.97 (d, 7.9, 1H), 7.00 (d, 7.9, 1H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$) δ 212.9, 200.5, 152.4, 145.2, 140.1, 135.2, 135.2, 132.9, 132.1, 131.4, 129.6, 128.2, 120.2, 118.5, 116.4, 73.7, 72.8, 59.0, 48.3, 47.9, 46.3, 43.8, 32.3, 27.7, 26.2, 24.8, 21.8, 19.9, 18.2. ppm. HRMS (ESI) *m/z* 459.2529 $[M + H]^+$ (calcd for $C_{30}H_{35}O_4$ 459.2530).

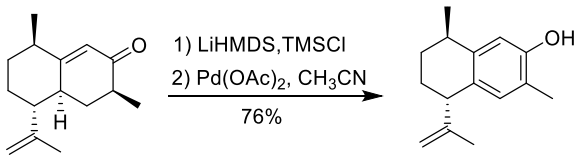


26 **30a** 3:1 **30b**

Synthesis of compounds 30a and **30b**: To a stirred solution of compound **26** (1.01 g, 4.62 mmol) in MeOH (10 mL) at room temperature was added a catalytic amount of palladium (5 % on $CaCO_3$; 50 mg, 0.005 equiv). The reaction mixture was hydrogenated under an atmosphere of H_2 for 30 min and detected by HPLC, then it was filtered through a pad of Celite. The filter cake was washed with EtOAc (100 mL), the filtrates were combined, and the solvent was removed on the rotary evaporator to give the mixture of **30a** and **30b** (863 mg, 3:1, 86%).

30a: R_f = 0.52 (silica, EtOAc/PE 1:14); $[\alpha]_D^{27}$ = +6.1 (*c* 0.108, MeOH), ^{1}H NMR (500 MHz, $CDCl_3$) δ 1.02 (d, 6.7, 3H), 1.06 (d, 6.7, 3H), 1.17 (m, 2H), 1.61 (m, 2H), 1.65 (s, 3H), 1.85 (m, 2H), 1.94 (m, 1H), 2.23 (m, 3H), 4.70 (s, 1H), 4.73 (s, 1H), 5.82 (brs, 1H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$) δ 202.4, 168.0, 146.4, 122.3, 112.3, 54.6, 40.4, 40.0, 37.7, 35.7, 34.6, 31.4, 18.4, 18.1, 14.5 ppm. HRMS (ESI) *m/z* 241.1565 $[M + Na]^+$ (calcd for $C_{15}H_{22}ONa$ 241.1563).

30b: R_f = 0.52 (silica, EtOAc/PE 1:14); $[\alpha]_D^{27}$ = –9.8 (*c* 0.135, MeOH), ^{1}H NMR (500 MHz, $CDCl_3$) δ 1.07 (d, J = 6.7, 3H), 1.18 (d, J = 7.3, 3H), 1.13 (m, 1H), 1.48 (m, 1H), 1.72 (s, 3H), 174 (m, 4H), 1.98 (m, 1H), 2.24 (m, 1H), 2.51 (m, 1H), 2.64 (m, 1H), 4.75 (s, 1H), 4.79 (s, 1H), 5.86 (d, 2.3, 1H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$) δ 202.7, 169.9, 146.6, 124.7, 112.3, 54.0, 40.7, 37.6, 36.5, 36.0, 31.4, 25.8, 21.1, 18.6, 14.7 ppm. HRMS (ESI) *m/z* 241.1565 $[M + Na]^+$ (calcd for $C_{15}H_{22}ONa$ 241.1563).

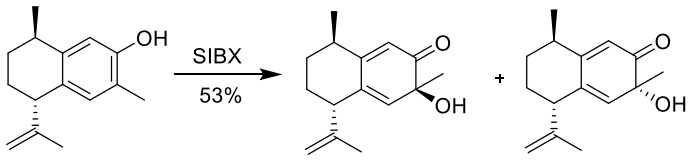


30a **31**

Synthesis of compound 31: To a solution of LiHMDS (1 M, 2.3 mL, 1.8 equiv) was added to a stirred solution of **30a** (275.3 mg, 1.26 mmol) in dry THF (4 mL) at –78 °C. After 30 min TMSCl (192 μL, 1.51 mmol, 1.2 equiv) was added and the resultant was allowed to warm to room temperature for 1 h. The resultant mixture was then poured into a cold saturated solution of $NaHCO_3$. The water phase was extracted with PE. The organic extracts were combined and dried over Na_2SO_4. The solvent was removed under vacuum and the crude TMS enol ethers were used without further purification. To a solution of the silyl enol ether obtained above in freshly distilled acetonitrile was added palladium(II) acetate, freshly prepared according to the reported procedure and other additive[6]. The reaction mixture was stirred for 20 min, and filtered through a short silica gel column with EtOAc. The filtrate was concentrated in vacuo and the residue was purified by column chromatography on silica gel to give **31** (206.12 mg, 76%).

31: R_f = 0.40 (silica, EtOAc/PE 1:16); $[\alpha]_D^{27}$ = +26.9 (*c* 0.151, MeOH), ^{1}H NMR (500 MHz, $CDCl_3$) δ 1.26 (d, 6.9 Hz, 3H), 1.41 (m, 1H), 1.63 (s, 3H), 1.72 (m, 1H), 1.89 (m, 1H), 1.96 (m, 1H), 2.19 (s, 3H), 2.81 (m, 1H), 3.45 (m, 1H), 4.68 (m, 1H), 4.72 (s, 1H), 4.89 (m, 1H), 6.67 (s, 1H), 6.85 (s, 1H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$) δ 152.0, 149.5, 141.5,

131.3, 130.0, 121.2, 113.4, 113.3, 47.4, 32.7, 30.3, 26.9, 22.6, 19.5, 15.5 ppm. HRMS (ESI) *m/z* 215.1437 $[M - H]^-$ (calcd for $C_{15}H_{19}O$ 215.1441).

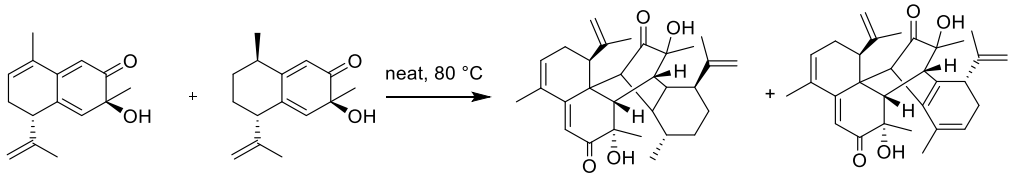


31 **32a** **32b**

Synthesis of compounds 32a and **32b**: To a stirred solution of phenol **31** (60.2 mg, 278 *μ*mol) in dry toluene and dimethyl sulfoxide (5 mL, 2:1) was added SIBX (145 mg, 80 wt, %, 1.50 equiv) in one portion and stirred for 15 hours at room temperature, after which time it was filtered. The filtrate was then diluted with EtOAc (30 mL), and washed with sat. aq. $NaHCO_3$ (3 × 10 mL) and brine (2 × 10 mL). The organic layer was dried over Na_2SO_4, filtered and concentrated under vacuum to give the residue which was composed of **32a** and **32b** by HPLC analysis. The mixture purified by silica gel preparation lamella chromatography to give diastereomeric mixture **32a** and **32b** (34.1 mg, ratio of 1:1) in 53 % yield. The mixture of **32a** and **32b** was further purified by semi-preparative HPLC.

32a: R_f = 0.42 (silica, EtOAc/PE 1:6); $[\alpha]_D^{25}$ = +9.5 (*c* 0.168, MeOH), ^{1}H NMR (800 MHz, $CDCl_3$) *δ* 1.22 (d, 6.6, 3H), 1.35 (m, 1H), 1.39 (s, 3H), 1.70 (s, 3H), 1.76 (m, 2H), 1.91 (m, 1H), 2.56 (m, 1H), 3.08 (m, 1H), 3.19 (s, 1H), 4.82 (s, 1H), 4.92 (s, 1H), 6.00 (s, 1H), 6.21 (s, 1H) ppm; ^{13}C NMR (200 MHz, $CDCl_3$) *δ* 206.0, 161.7, 146.5, 139.7, 132.4, 118.3, 114.1, 75.5, 47.8, 34.9, 30.2, 28.8, 27.0, 19.2, 18.8 ppm. HRMS (ESI) *m/z* 255.1357 $[M + Na]^+$ (calcd for $C_{15}H_{20}O_2Na$ 255.1356).

32b: R_f = 0.42 (silica, EtOAc/PE 1:6); $[\alpha]_D^{25}$ = +120.5 (*c* 0.210, MeOH), ^{1}H NMR (800 MHz, $CDCl_3$) *δ* 1.23 (d, 6.9, 3H), 1.31 (m, 1H), 1.37 (s, 3H), 1.65 (s, 3H), 1.79 (m, 1H), 1.91 (m, 1H), 2.65 (m, 1H), 3.11 (m, 1H), 3.15 (s, 1H), 4.80 (s, 1H), 4.89 (s, 1H), 6.00 (d, 1.7, 1H), 6.22 (d, 1.9, 1H) ppm; ^{13}C NMR (200 MHz, $CDCl_3$) *δ* 206.1, 162.4, 146.7, 140.6, 132.3, 120.1, 114.2, 75.7, 47.7, 34.7, 29.5, 29.1, 26.4, 21.5, 19.0. ppm. HRMS (ESI) *m/z* 255.1351 $[M + Na]^+$ (calcd for $C_{15}H_{20}O_2Na$ 255.1356).

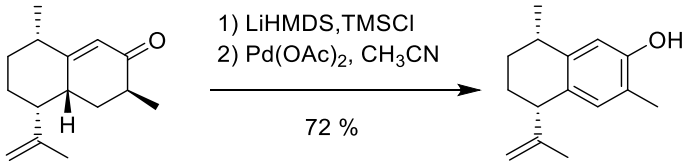


28a **32a** **9** **29**

Synthesis of compounds 9 and 29: To a stirred solution of **32** (the mixture of **32a** and **32b**, 30 mg, 129 *μ*mol) and **28** (the mixture of **28a** and **28b**, 60 mg, 261 *μ*mol) was added in DCM (0.5 mL) at room temperature. After removal of

the solvent under argon bubbling, the residue was heated at 80 °C for 12 h before it was cooled to room temperature. The residue was directly purified by semi-preparative HPLC to give **9** (5.2 mg, 35%) and **29** (12.3 mg, 41%).

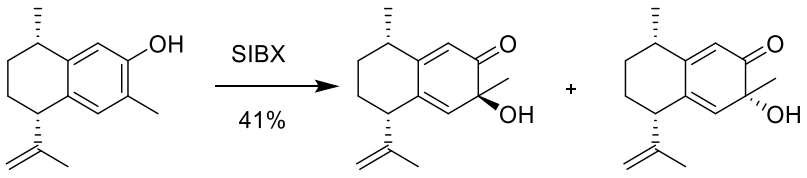
9: R_f = 0.44 (silica, EtOAc/PE 1:6); $[\alpha]_D^{27}$ = +54.8 (*c* 0.115, MeOH), ^{1}H NMR (500 MHz, $CDCl_3$) δ 0.70 (d, 7.3, 3H), 1.20 (s, 3H), 1.22 (brs, 3H), 1.25 (m, 1H), 1.57 (overlap, 6H), 1.71 (overlap, 4H), 1.86 (s, 3H), 1.97 (m, 1H), 2.17 (m, 1H), 2.90 (overlap, 3H), 3.26 (s, 1H), 3.31 (brs, 1H), 3.44 (d, 2.7, 1H), 3.83 (s, 1H), 4.85 (s, 1H), 4.91 (brs, 1H), 4.96 (brs, 1H), 4.99 (d, 2.3, 1H), 6.06 (s, 1H), 6.08 (d, 4.9, 1H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$) δ 212.2, 202.2, 154.5, 146.1, 146.1, 141.8, 135.9, 133.7, 131.7, 121.0, 117.9, 115.3, 73.9, 71.7, 62.0, 48.4, 47.7, 47.1, 44.4, 43.3, 33.2, 31.5, 29.1, 27.7, 26.5, 24.6, 22.6, 22.6, 20.0, 17.4 ppm. HRMS (ESI) *m/z* 463.2839 $[M + H]^+$ (calcd for $C_{30}H_{39}O_4$ 463.2843).



30b **33**

Synthesis of compound 33: To a solution of LiHMDS (1 M, 1.9 mL, 1.8 equiv) was added to a stirred solution of **30b** (230.4 mg, 1.1 mmol) in dry THF (2 mL) at -78 °C. After 30 min TMSCl (170 μL, 1.3 mmol, 1.2 equiv) was added and the resultant was allowed to warm to room temperature for 1 h. The resultant mixture was then poured into a cold saturated solution of $NaHCO_3$. The water phase was extracted with PE. The organic extracts were combined and dried over Na_2SO_4. The solvent was removed under vacuum and the crude TMS enol ethers were used without further purification. To a solution of the silyl enol ether obtained above in freshly distilled acetonitrile was added palladium(II) acetate, freshly prepared according to the reported procedure and other additive[6]. The reaction mixture was stirred for 20 min, and filtered through a short silica gel column with EtOAc. The filtrate was concentrated in vacuo and the residue was purified by column chromatography on silica gel to give **33** (172 mg, 72%).

33: R_f = 0.40 (silica, EtOAc/PE 1:16); $[\alpha]_D^{20}$ = –4.3 (*c* 0.152, MeOH), ^{1}H NMR (500 MHz, $CDCl_3$) δ 1.25 (d, 7.1 Hz, 3H), 1.64 (m, 1H), 1.68 (s, 3H), 1.73 (m, 1H), 1.87 (m, 2H), 2.18 (s, 3H), 2.82 (m, 1H), 3.40 (m, 1H), 4.56 (brs, 1H), 4.66 (m, 1H), 4.91 (s, 1H), 6.59 (s, 1H), 6.83 (s, 1H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$) δ 152.0, 149.5, 141.7, 131.4, 129.9, 121.3, 114.2, 113.6, 47.2, 32.6, 28.8, 24.8, 23.4, 19.7, 15.5 ppm. HRMS (ESI) *m/z* 215.1442 $[M - H]^-$ (calcd for $C_{15}H_{19}O$ 215.1441).

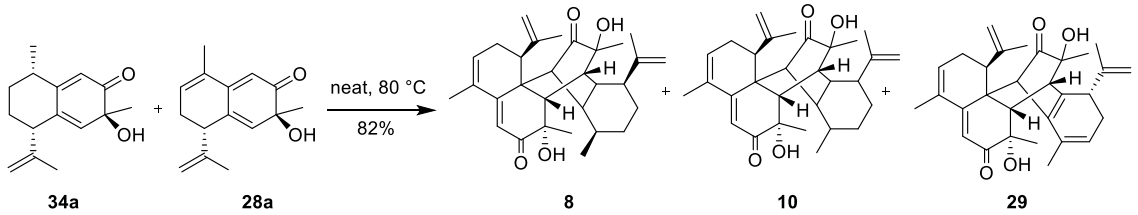


33 **34a** **34b**

Synthesis of compounds 34a and **34b**: To a stirred solution of phenol **33** (30.1 mg, 139 *μ*mol) in dry toluene and dimethyl sulphoxide (1.2 mL, 2:1) was added SIBX (73.2 mg, 80 wt. %, 1.5 equiv) in one portion and stirred for 15 hours at room temperature, after which time it was filtered. The filtrate was then diluted with EtOAc (15 mL), and washed with sat. aq. $NaHCO_3$ (3 × 4 mL) and brine (2 × 4 mL). The organic layer was dried over Na_2SO_4, filtered and concentrated under vacuum to give the residue which was composed of **34a** and **34b** by HPLC analysis. The mixture purified by silica gel preparation lamella chromatography to give diastereomeric mixture **34a** and **34b** (13.2 mg, 41%).

34a: R_f = 0.42 (silica, EtOAc/PE 1:6); ^{1}H NMR (800 MHz, $CDCl_3$) *δ* 1.21 (d, 5.6, 3H), 1.37 (s, 3H), 1.43 (m, 1H), 1.69 (m, 1H), 1.71 (s, 3H), 1.75 (m, 2H), 1.87 (m, 1H), 2.75 (m, 1H), 3.09 (m, 1H), 4.79 (s, 1H), 4.90 (s, 1H), 5.93 (s, 1H), 6.18 (s, 1H) ppm; ^{13}C NMR (200 MHz, $CDCl_3$) *δ* 206.1, 162.7, 146.1, 138.6, 132.6, 119.7, 114.6, 75.8, 46.4, 34.0, 29.2, 28.0, 24.1, 21.3, 19.4 ppm. HRMS (ESI) *m/z* 233.1534 $[M + H]^+$ (calcd for $C_{15}H_{21}O_2$ 233.1536).

34b: R_f = 0.42 (silica, EtOAc/PE 1:6); ^{1}H NMR (800 MHz, $CDCl_3$) *δ* 1.20 (d, 6.7, 3H), 1.37 (s, 3H), 1.50 (m, 1H), 1.72 (s, 3H), 1.73 (m, 2H), 1.87 (m, 1H), 2.68 (d, 6.8, 1H), 3.17 (s, 2H), 4.77 (s, 1H), 4.95 (s, 1H), 5.95 (s, 1H), 6.10 (s, 1H) ppm; ^{13}C NMR (200 MHz, $CDCl_3$) *δ* 206.1, 162.7, 145.7, 138.6, 133.6, 118.6, 114.6, 75.8, 45.4, 33.3, 28.9, 28.0, 24.7, 20.0, 19.4 ppm. HRMS (ESI) *m/z* 233.1539 $[M + H]^+$ (calcd for $C_{15}H_{21}O_2$ 233.1536).



Synthesis of compounds 8, 10, and 29: To a stirred solution of **34** (the mixture of **34a** and **34b**, 40 mg, 174 *μ*mol) and **28** (the mixture of **28a** and **28b**, 100 mg, 431 *μ*mol) was added in DCM (0.5 mL) at room temperature. After removal of the solvent under argon bubbling, the residue was heated at 80 °C for 12 h before it was cooled to room temperature. The residue was directly purified by semi-preparative HPLC to give **8** (5.2 mg, 10% yield based on **28a**), **10** (6.1 mg, 30% based on **34a**) and **29** (21 mg, 42% based on **34a**) as a white powder.

8: R_f = 0.44 (silica, EtOAc/PE 1:6); $[\alpha]_D^{22}$ = +59.7 (*c* 0.190, MeOH), ^{1}H NMR (500 MHz, $CDCl_3$) *δ* 0.85 (d, 6.9, 3H), 1.18 (s, 3H), 1.23 (brs, 3H), 1.34 (m, 1H), 1.47 (overlap, 2H), 1.55 (overlap, 5H), 1.69 (s, 3H), 1.87 (s, 3H), 2.14 (dd, 20.1, 4.6, 1H), 2.84 (overlap, 3H), 3.15 (s, 1H), 3.26 (brs, 1H), 3.39 (d, 2.5, 1H), 3.81 (s, 1H), 4.83 (s, 1H), 4.93 (overlap, 2H), 4.97 (brs, 1H), 6.05 (d, J = 4.3, 1H), 6.08 (s, 1H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$) *δ* 212.3, 201.8, 155.0, 145.5, 145.5, 139.9, 138.1, 133.4, 131.2, 120.0, 117.8, 115.1, 73.7, 72.0, 62.6, 49.2, 47.5, 47.5, 44.8, 43.6, 33.3, 33.1, 28.4, 27.8, 25.9, 23.7, 22.4, 22.4, 20.0, 19.0 ppm. HRMS (ESI) *m/z* 463.2842 $[M + H]^+$ (calcd for $C_{30}H_{39}O_4$ 463.2843).

10: R_f = 0.44 (silica, EtOAc/PE 1:6); $[\alpha]_D^{22}$ = +78.0 (*c* 0.080, MeOH), ^{1}H NMR (500 MHz, $CDCl_3$) δ 0.93 (d, J = 6.8, 3H), 1.16 (overlap, 6H), 1.31 (brs, 3H), 1.34 (m, 1H), 1.43 (m, 1H), 1.55 (overlap, 4H), 1.68 (s, 3H), 1.76 (s, 3H), 1.85 (overlap, 2H), 2.08 (s, 1H), 2.36 (brs, 1H), 2.67 (m, 1H), 2.71 (brs, 1H), 2.87 (s, 1H), 3.40 (d, 2.3, 1H), 3.77 (overlap, 2H), 4.89 (overlap, 3H), 4.95 (s, 1H), 6.11 (d, 2.1, 1H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$) δ 212.1, 201.7, 166.1, 146.3, 145.6, 139.9, 137.5, 122.9, 117.4, 115.0, 73.2, 71.5, 60.8, 52.8, 49.8, 47.6, 43.3, 33.3, 32.9, 32.5, 30.0, 28.6, 25.8, 25.8, 24.2, 24.1, 22.3, 19.2, 19.1 ppm. HRMS (ESI) *m/z* 487.2814 $[M + Na]^+$ (calcd for $C_{30}H_{40}O_4Na$ 487.2819).

1.7 X-ray Crystallographic Analysis for 1−5, 25a, 7, and 30a

X-ray crystal data for **1**: $2(C_{30}H_{38}O_6)\bullet CH_4O$, *M* = 1021.25, *a* = 8.6927(9) Å, *b* = 29.467(3) Å, *c* = 11.3135(12) Å, α = 90°, β = 112.393(3)°, γ = 90°, *V* = 2679.4(5) Å^3, *T* = 130(2) K, space group *P*21, *Z* = 2, μ(CuKα) = 0.708 mm^{-1}, 33070 reflections measured, 10338 independent reflections (R_{int} = 0.0432). The final R_1 values were 0.0428 ($I > 2\sigma(I)$). The final $wR(F^2)$ values were 0.1162 ($I > 2\sigma(I)$). The final R_1 values were 0.0430 (all data). The final $wR(F^2)$ values were 0.1165 (all data). The goodness of fit on F^2 was 1.015. Flack parameter = 0.09(4) and the Cambridge Crystallographic Data Centre (CCDC) number was 2212935.

X-ray crystal data for **2**: $C_{30}H_{34}O_4$, *M* = 458.57, *a* = 8.7346(3) Å, *b* = 9.9202(3) Å, *c* = 28.6562(8) Å, α = 90°, β = 90°, γ = 90°, *V* = 2483.03(13) Å^3, *T* = 100(2) K, space group *P*212121, *Z* = 4, μ(CuKα) = 0.634 mm^{-1}, 12892 reflections measured, 4364 independent reflections (R_{int} = 0.0539). The final R_1 values were 0.0511 ($I > 2\sigma(I)$). The final $wR(F^2)$ values were 0.1454 ($I > 2\sigma(I)$). The final R_1 values were 0.0514 (all data). The final $wR(F^2)$ values were 0.1463 (all data). The goodness of fit on F^2 was 1.085. Flack parameter = 0.12(7) and the Cambridge Crystallographic Data Centre (CCDC) number was 2212936.

X-ray crystal data for **3**: $C_{30}H_{38}O_4$, *M* = 462.60, *a* = 8.8971(2) Å, *b* = 15.2326(3) Å, *c* = 18.8392(3) Å, α = 90°, β = 90°, γ = 90°, *V* = 2553.20(9) Å^3, *T* = 100(2) K, space group *P*212121, *Z* = 4, μ(CuKα) = 0.617 mm^{-1}, 15802 reflections measured, 4650 independent reflections (R_{int} = 0.0374). The final R_1 values were 0.0344 ($I > 2\sigma(I)$). The final $wR(F^2)$ values were 0.0889 ($I > 2\sigma(I)$). The final R_1 values were 0.0345 (all data). The final $wR(F^2)$ values were 0.0890 (all data). The goodness of fit on F^2 was 1.068. Flack parameter = -0.03(5) and the Cambridge Crystallographic Data Centre (CCDC) number was 2212937.

X-ray crystal data for **4**: $C_{30}H_{38}O_4\bullet H_2O$, *M* = 480.62, *a* = 8.7065(2) Å, *b* = 13.1797(2) Å, *c* = 22.9727(4) Å, α = 90°, β = 90°, γ = 90°, *V* = 2636.10(9) Å^3, *T* = 100.(2) K, space group *P*212121, *Z* = 4, μ(Cu Kα) = 0.644 mm^{-1}, 20914 reflections measured, 5192 independent reflections (R_{int} = 0.0305). The final R_1 values were 0.0307 ($I > 2\sigma(I)$). The final $wR(F^2)$

values were 0.0794 ($I > 2\sigma(I)$). The final R_1 values were 0.0318 (all data). The final $wR(F^2)$ values were 0.0806 (all data). The goodness of fit on F^2 was 1.048. Flack parameter = -0.01(4) and the Cambridge Crystallographic Data Centre (CCDC) number was 2212938.

X-ray crystal data for **5**: $C_{30}H_{40}O_4$, M = 464.62, a = 8.6842(2) Å, b = 15.4286(3) Å, c = 19.2929(4) Å, α = 90°, β = 90°, γ = 90°, V = 2584.96(9) Å^3, T = 100(2) K, space group $P212121$, Z = 4, μ(CuKα) = 0.610 mm^{-1}, 14778 reflections measured, 4472 independent reflections (R_{int} = 0.0521). The final R_1 values were 0.0438 ($I > 2\sigma(I)$). The final $wR(F^2)$ values were 0.1145 ($I > 2\sigma(I)$). The final R_1 values were 0.0440 (all data). The final $wR(F^2)$ values were 0.1147 (all data). The goodness of fit on F^2 was 1.045. Flack parameter = 0.07(7) and the Cambridge Crystallographic Data Centre (CCDC) number was 2212942.

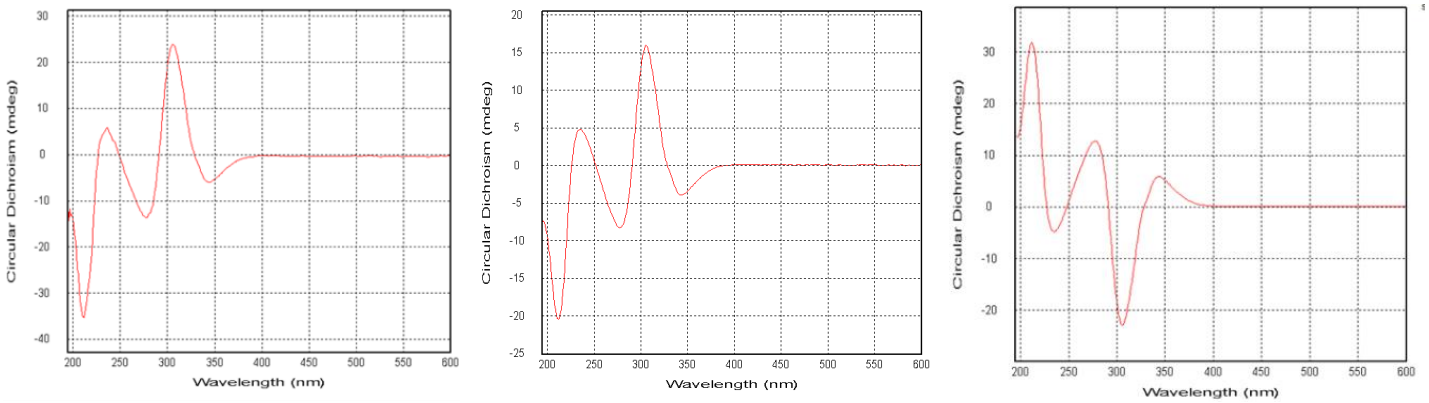
X-ray crystal data for **25a**: $C_{15}H_{22}O$, M = 218.32, a = 8.2056(2) Å, b = 9.4771(2) Å, c = 16.4429(3) Å, α = 90°, β = 90°, γ = 90°, V = 1278.69(5) Å^3, T = 100.(2) K, space group $P212121$, Z = 4, μ(Cu Kα) = 0.521 mm^{-1}, 11438 reflections measured, 2511 independent reflections (R_{int} = 0.0429). The final R_1 values were 0.0302 ($I > 2\sigma(I)$). The final $wR(F^2)$ values were 0.0802 ($I > 2\sigma(I)$). The final R_1 values were 0.0312 (all data). The final $wR(F^2)$ values were 0.0813 (all data). The goodness of fit on F^2 was 1.101. Flack parameter = -0.02(11) and the Cambridge Crystallographic Data Centre (CCDC) number was 2212947.

X-ray crystal data for **7**: $C_{30}H_{34}O_4$, M = 458.57, a = 8.7330(5) Å, b = 9.9169(6) Å, c = 28.6719(17) Å, α = 90°, β = 90°, γ = 90°, V = 2483.1(3) Å^3, T = 101. (2) K, space group $P212121$, Z = 4, μ(Cu Kα) = 0.634 mm^{-1}, 26362 reflections measured, 4890 independent reflections (R_{int} = 0.0617). The final R_1 values were 0.0376 ($I > 2\sigma(I)$). The final $wR(F^2)$ values were 0.0978 ($I > 2\sigma(I)$). The final R_1 values were 0.0396 (all data). The final $wR(F^2)$ values were 0.0997 (all data). The goodness of fit on F^2 was 1.043. Flack parameter = 0.12(6) and the Cambridge Crystallographic Data Centre (CCDC) number was 2212943.

X-ray crystal data for **30a**: $C_{15}H_{22}O$, M = 218.32, a = 8.2085(3) Å, b = 9.4732(3) Å, c = 16.4463(6) Å, α = 90°, β = 90°, γ = 90°, V = 1278.88(8) Å^3, T = 100. (2) K, space group $P212121$, Z = 4, μ(Cu Kα) = 0.521 mm^{-1}, 31500 reflections measured, 2518 independent reflections (R_{int} = 0.0653). The final R_1 values were 0.0306 ($I > 2\sigma(I)$). The final $wR(F^2)$ values were 0.0789 ($I > 2\sigma(I)$). The final R_1 values were 0.0309 (all data). The final $wR(F^2)$ values were 0.0791 (all data). The goodness of fit on F^2 was 1.061. Flack parameter = 0.18(9) and the Cambridge Crystallographic Data Centre (CCDC) number was 2212950.

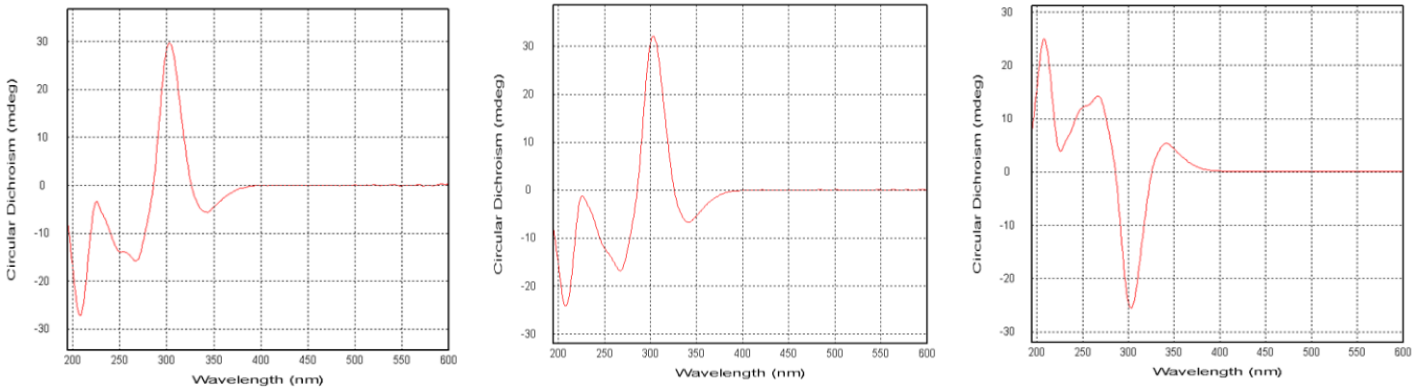
1.8 Comparison of the Circular Dichroism Spectra of Natural and Synthetic Compounds

Figure S6. Circular dichroism spectra of natural and synthetic **1** as well as enantiomer **6**



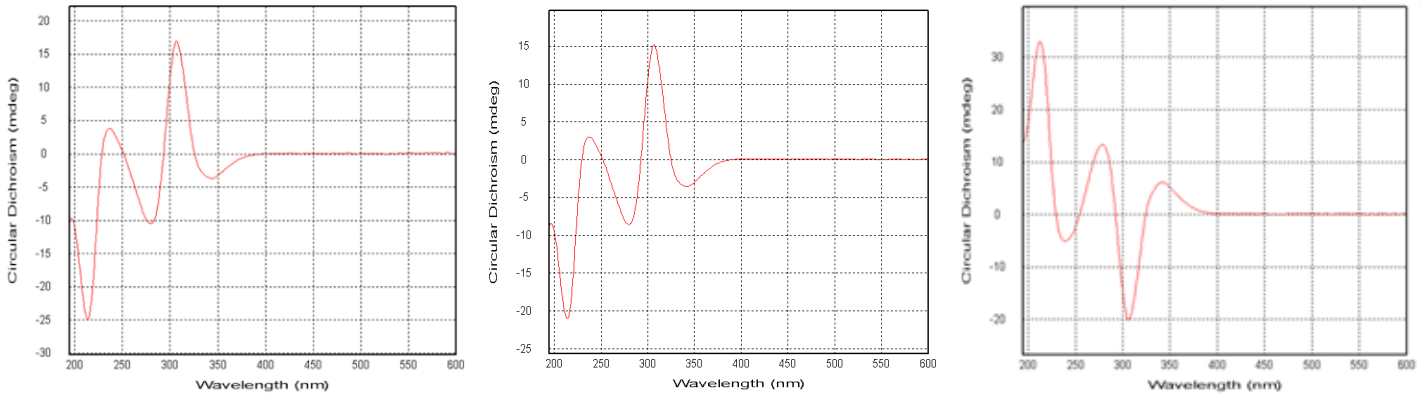
(A) natural **1** (0.17 mg/mL) (B) synthetic **1** (0.20 mg/mL) (C) enantiomer **6** (0.43 mg/mL)

Figure S7. Circular dichroism spectra of natural and synthetic **2** as well as enantiomer **7**



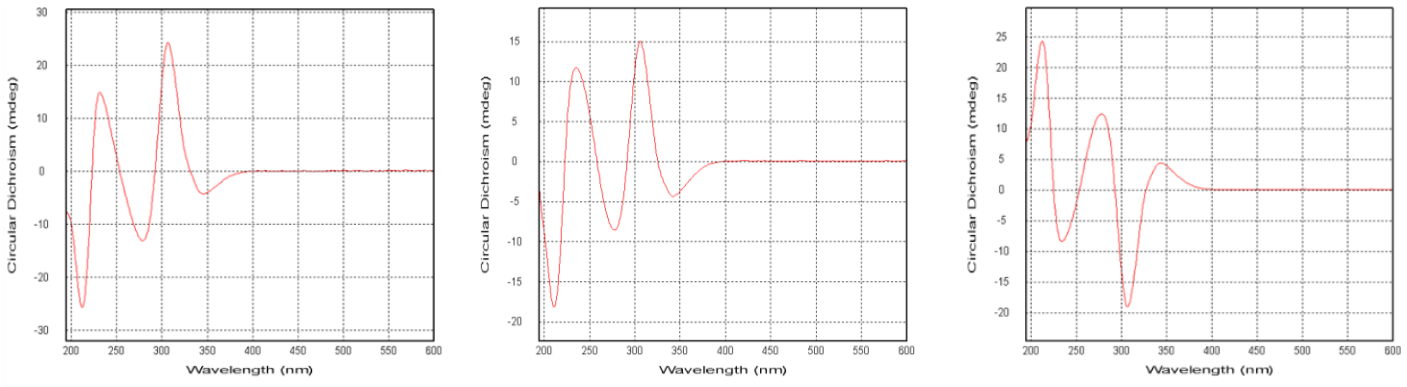
(A) natural **2** (0.12 mg/mL) (B) synthetic **2** (0.20 mg/mL) (C) enantiomer **7** (0.10 mg/mL)

Figure S8. Circular dichroism spectra of natural and synthetic **3** as well as enantiomer **8**



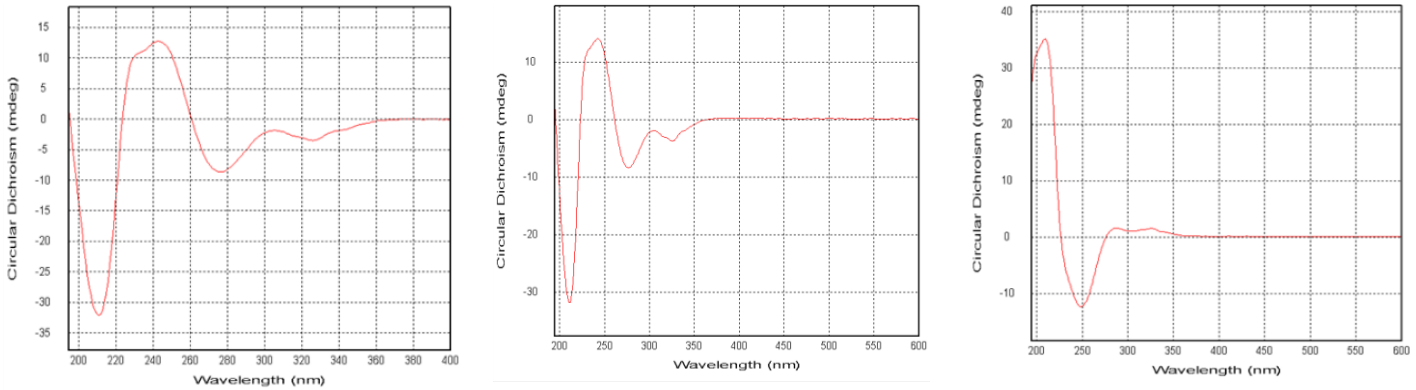
(A) natural **3** (0.14 mg/mL) (B) synthetic **3** (0.24 mg/mL) (C) enantiomer **8** (0.14 mg/mL)

Figure S9. Circular dichroism spectra of natural and synthetic **4** as well as enantiomer **9**



(A) natural **4** (0.20 mg/mL) (B) synthetic **4** (0.20 mg/mL) (C) enantiomer **9** (0.28 mg/mL)

Figure S10. Circular dichroism spectra of natural and synthetic **5** as well as enantiomer **10**



(A) natural **5** (0.13 mg/mL) (B) synthetic **5** (0.20 mg/mL) (C) enantiomer **10** (0.21 mg/mL)

2. Mechanistic Study on Diels-Alder Reaction

2.1 Computational Details

Density functional theory (DFT) calculations were performed with Gaussian 16 Rev. A.03 package[12]. Geometry optimizations were conducted at the theoretical level of ωB97X-D/def2-SVP[13,14]. Frequency analyses at the same level verified there are zero/one imaginary frequency for the obtained intermediates/transition states, respectively. Single-point energies were calculated at the ωB97X-D/def2-TZVPP level. Entropy and enthalpy were corrected by Grimme's quasi-harmonic approximation[15] and Head-Gordon's method[16], respectively, implemented in Paton's GoodVibes[17]. Conformation search was realized by Crest.[18,19] Distortion/interaction analyses[20,21] along the intrinsic reaction coordinate (IRC) derived from the key transition state help in revealing the origin of selectivity. The quasi-classical direct molecular dynamics simulation[22] was performed with the python version of Progdyn[23], an in-house code. 3D representations of molecular structures were generated by CYLview.[24]

Figure S11. Two pairs of truncated transition states where the (a) Me and (b) OH attached to C3 of **14** are replaced by H.

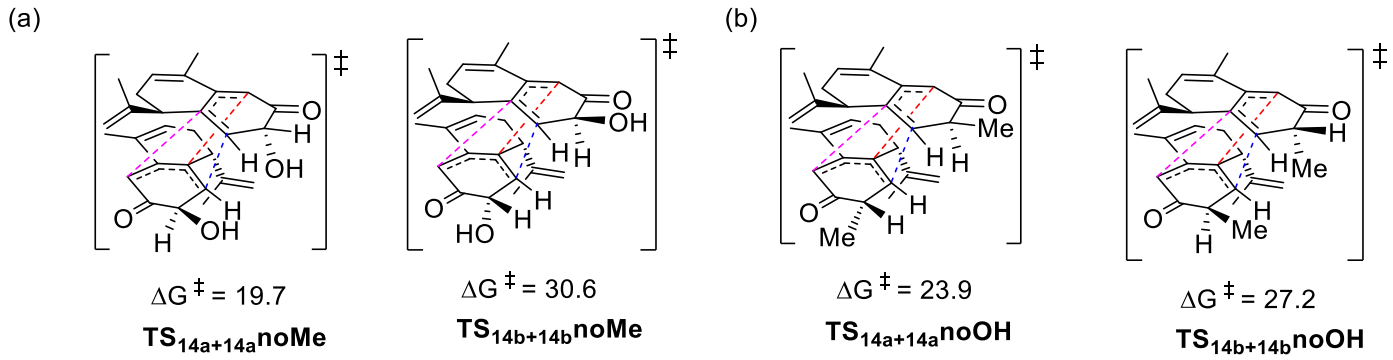


Figure S12. Distortion/interaction activation analyses (DIAS) along the intrinsic reaction coordinates derived from $TS_{14a+14a}$ and $TS_{14b+14b}$. For the sake of space, absolute value of interaction energy is plotted.

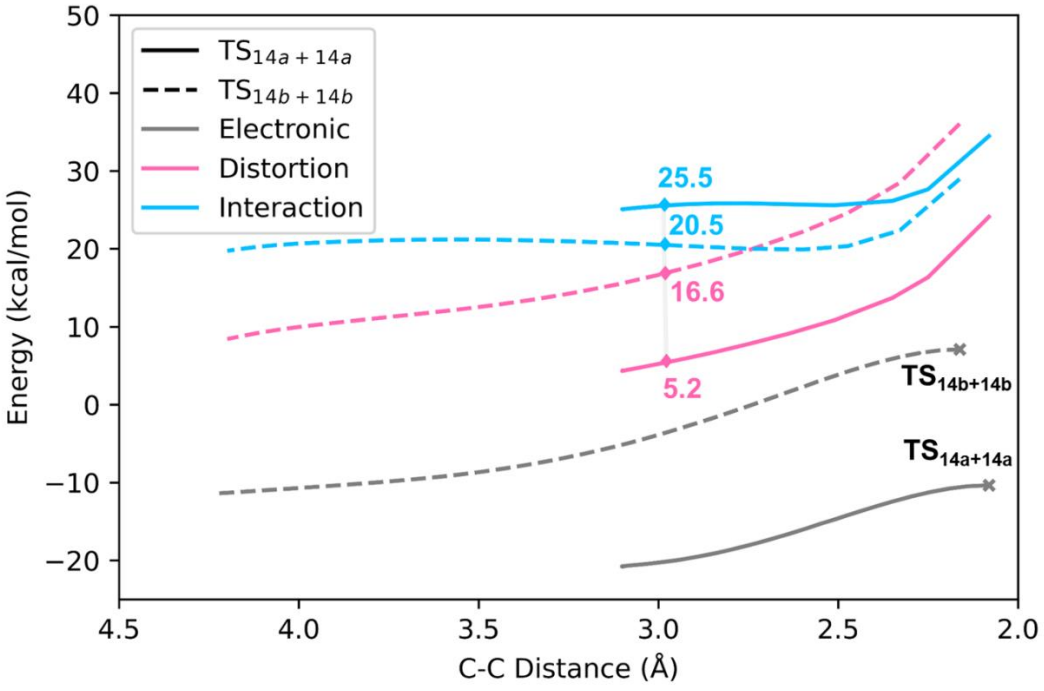
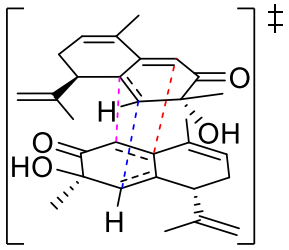
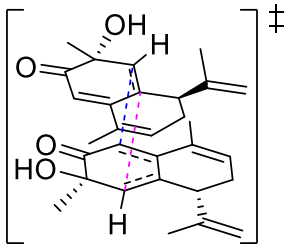


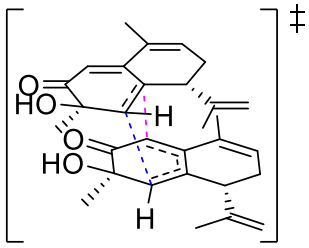
Figure S13. Free energy barriers for the formation of other stereoisomers and regiomers from **14b**



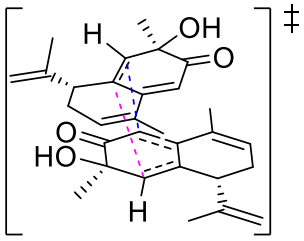
$TS_{14a+14a}$
$\Delta G^{\ddagger}$ = 19.4
ΔG = -10.5



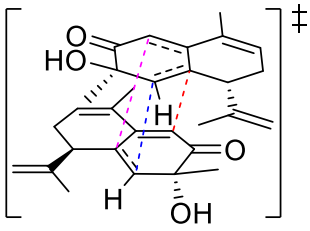
II
$\Delta G^{\ddagger}$ = 36.0
ΔG = -1.8



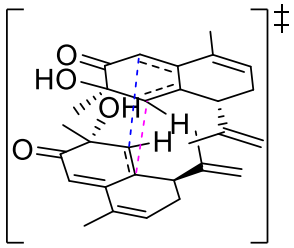
III
$\Delta G^{\ddagger}$ = 45.5
ΔG = 2.3



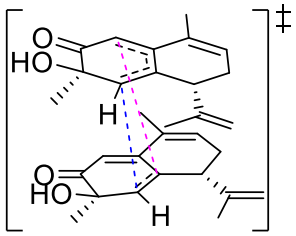
IV
$\Delta G^{\ddagger}$ = 45.3
ΔG = 5.2



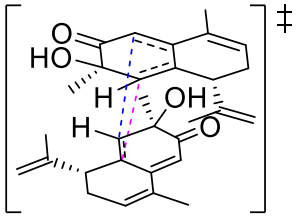
V
$\Delta G^{\ddagger}$ = 45.4
ΔG = -1.9



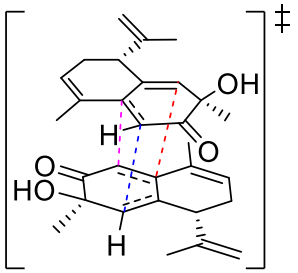
VI
$\Delta G^{\ddagger}$ = 61.0
ΔG = 12.4



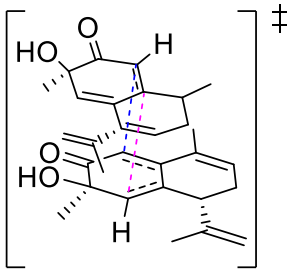
VII
$\Delta G^{\ddagger}$ = 41.0
ΔG = -0.2



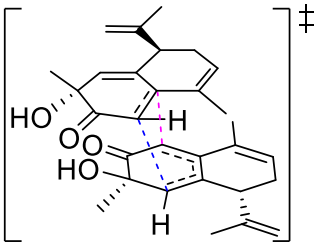
VIII
$\Delta G^{\ddagger}$ = 36.1
ΔG = 2.6



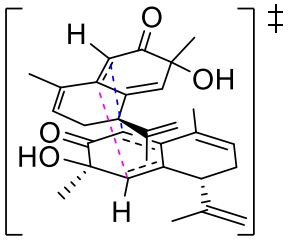
A = VIII
$\Delta G^{\ddagger}$ = 36.1
ΔG = 9.8



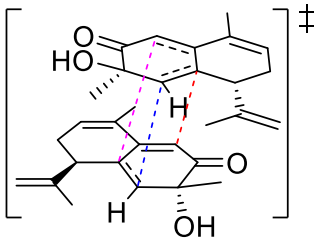
B
$\Delta G^{\ddagger}$ = 49.8
ΔG = 8.1



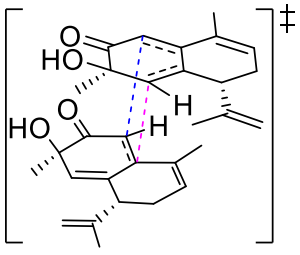
C
$\Delta G^{\ddagger}$ = 33.4
ΔG = 0.2



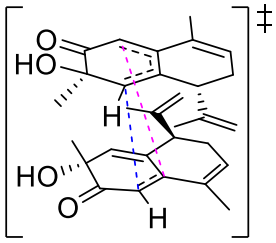
D
$\Delta G^{\ddagger}$ = 41.6
ΔG = 7.1



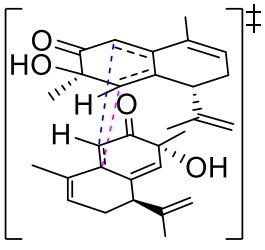
E = IV
$\Delta G^{\ddagger}$ = 45.3
ΔG = 4.4



F
$\Delta G^{\ddagger}$ = 51.6
ΔG = 5.3



G
$\Delta G^{\ddagger}$ = 55.6
ΔG = 9.7



H
$\Delta G^{\ddagger}$ = 60.0
ΔG = 16.0

Figure S14. Structures of transition states that appears in **Figure S13**

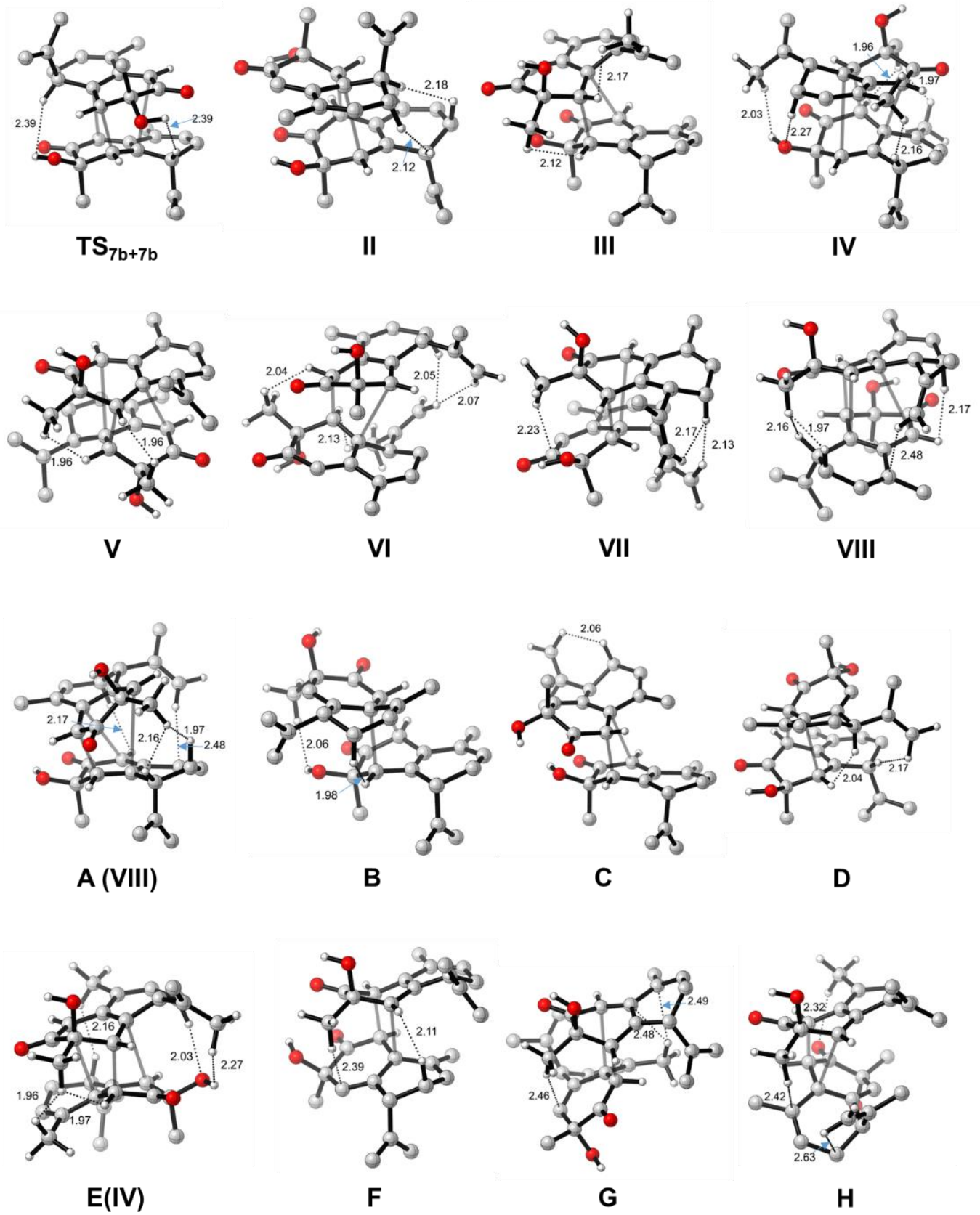


Figure S15. Free energy barriers and reaction energies for the homo-dimerization reaction of (a) **16a** and (b) **16b**.

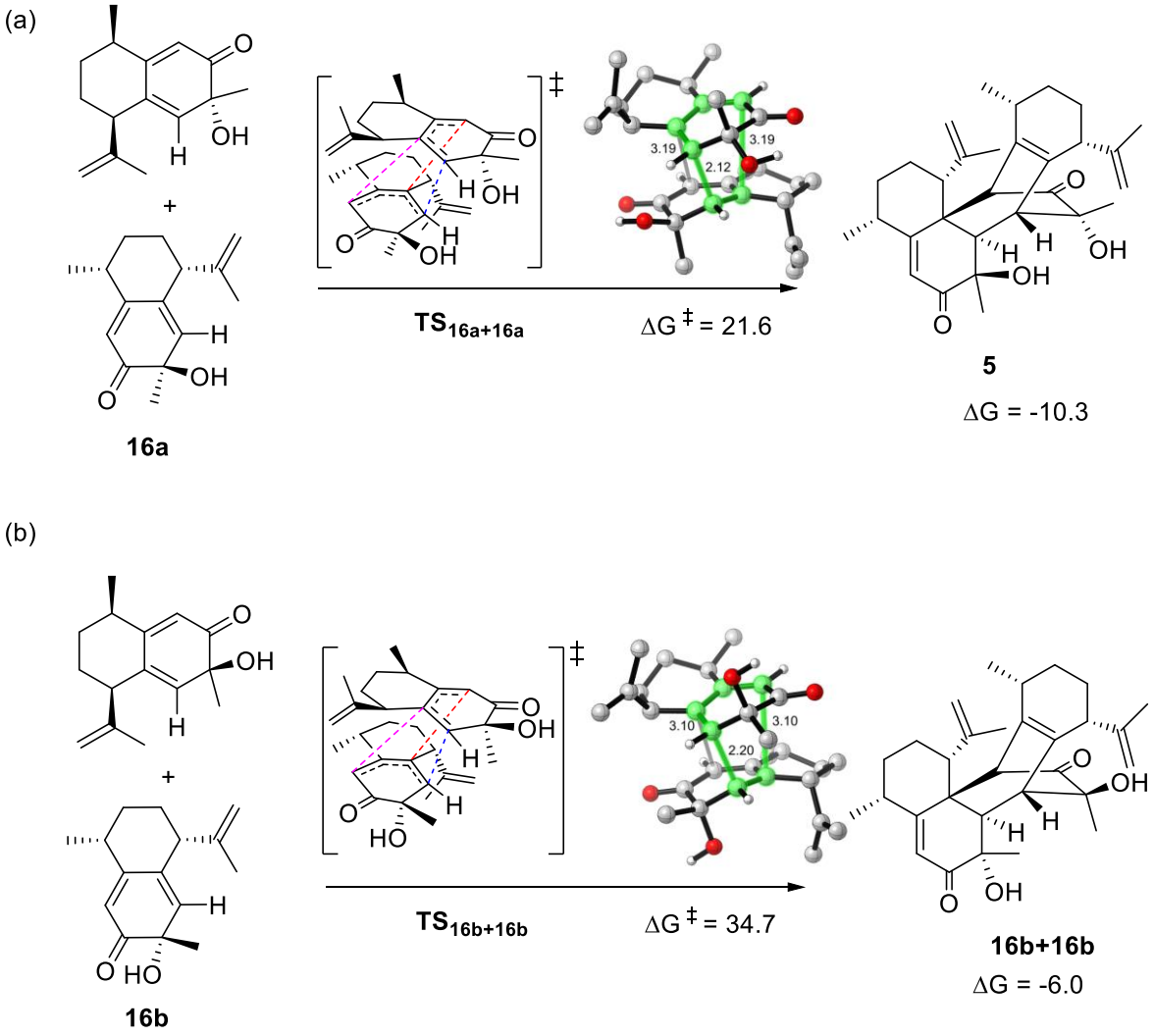


Figure S16. Homo-dimerization reaction of (a) **15a** and (b) **15b**.

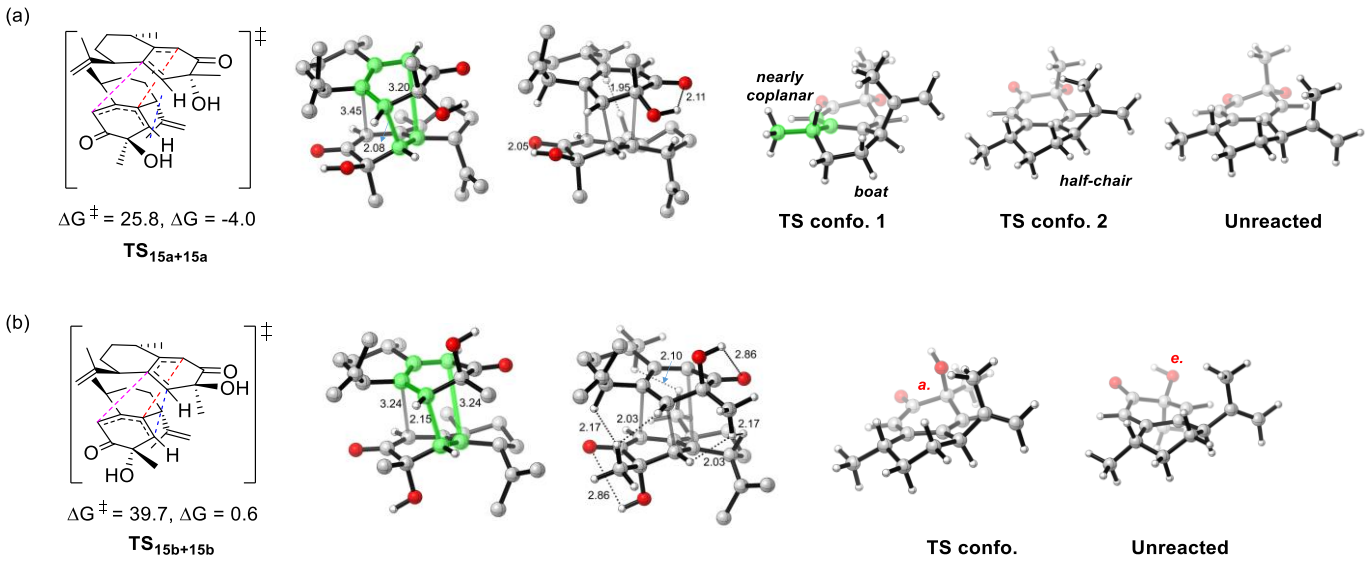


Figure S17. Trajectories of quasi-classical direct molecular dynamics simulation that are projected onto the distances of forming C-C bond. Stationary points and intrinsic reaction coordinates (IRCs) are shown in bule. Trajectories are shown in pink.

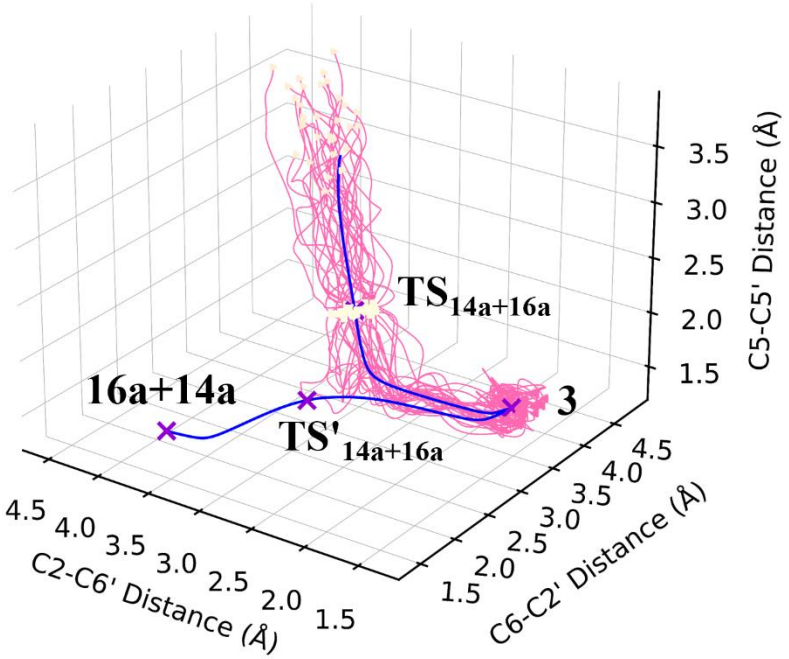


Figure S18. Energy barriers for the homo- and cross-dimerization of **14a** and **15a**

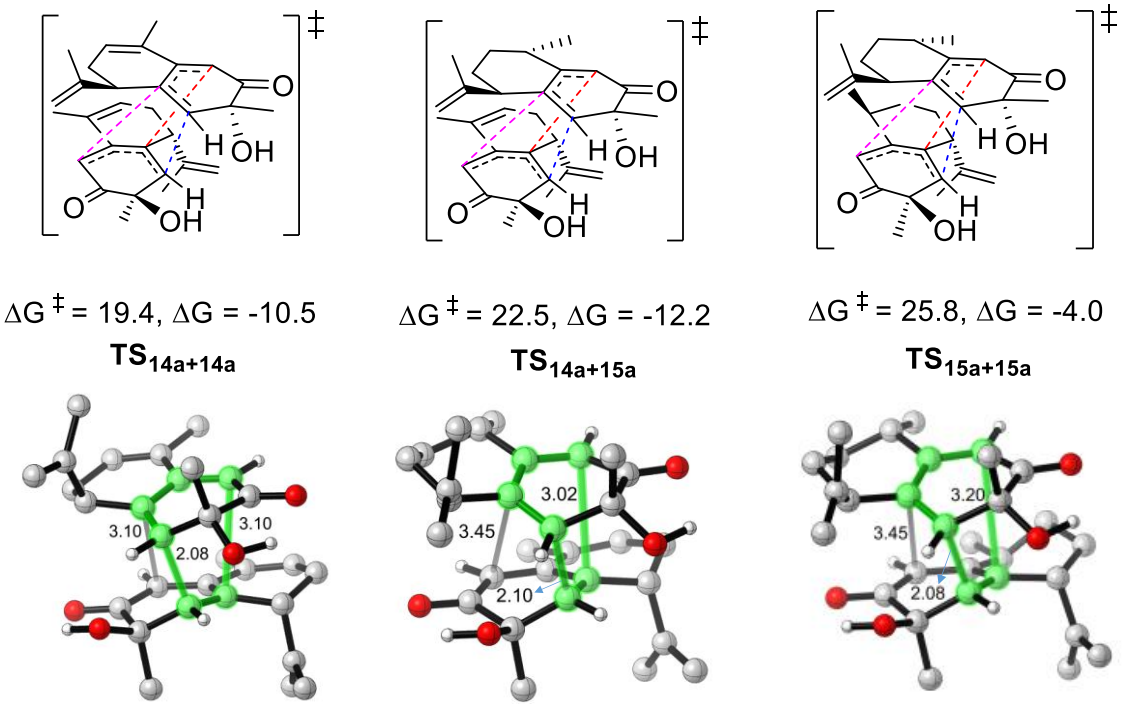
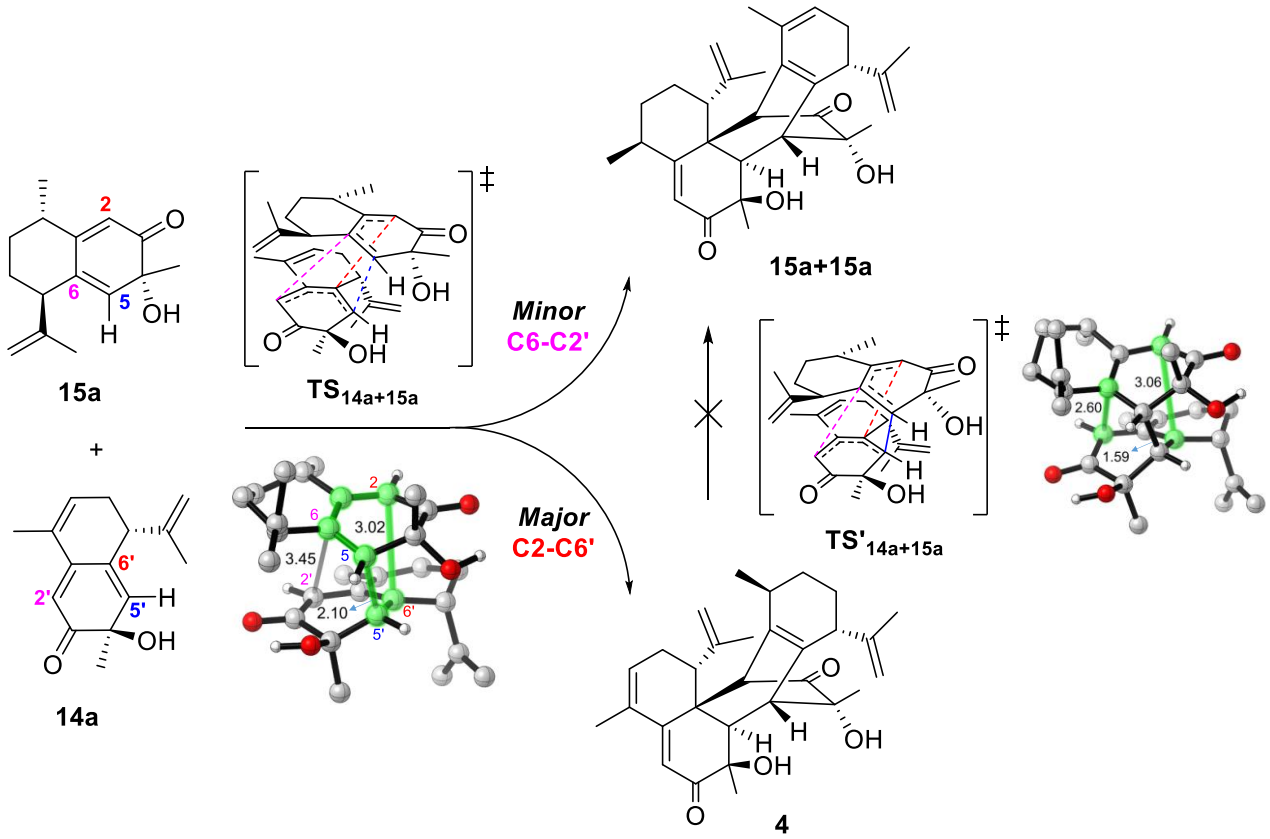


Figure S19. Reaction pathway bifurcation and the ambimodal $TS_{14a+15a}$ of the cross-dimerization reaction between **14a** and **15a**.



2.2 Cartesian Coordinates and Energies

14a

O	3.680190	0.133120	-0.558090
C	2.505770	0.120500	-0.239930
C	1.679990	1.317700	-0.115220
C	0.322440	1.237580	-0.084880
C	-0.353140	-0.081760	-0.193360
C	0.375980	-1.207000	-0.161020
C	1.850490	-1.216960	0.110230
C	2.072350	-1.424350	1.628350
H	1.602800	-0.628680	2.225540
H	3.153790	-1.437750	1.831460
H	1.646970	-2.395060	1.919190
O	2.471560	-2.241520	-0.611520
H	3.359580	-1.905670	-0.808540
H	-0.092460	-2.186880	-0.287370
C	-1.852070	-0.073570	-0.449970
C	-2.502790	-1.432410	-0.282550
C	-2.910700	-2.128010	-1.348180
H	-2.792150	-1.738140	-2.363000
H	-3.372740	-3.113630	-1.244240
C	-2.670160	-1.954570	1.120870
H	-1.739050	-1.849650	1.699840
H	-3.450020	-1.393730	1.661250
H	-2.960990	-3.013850	1.121100
C	-2.529140	1.012460	0.396800
C	-1.828700	2.328350	0.266950
C	-0.511210	2.451920	0.023310
C	0.147600	3.799950	-0.075190
H	0.880220	3.948300	0.734010
H	0.688580	3.912060	-1.027720
H	-0.596690	4.604600	-0.007650
H	-2.426200	3.235660	0.402110
H	-2.539170	0.718850	1.462110
H	-3.584010	1.109040	0.097270
H	-1.980180	0.231140	-1.504160
H	2.207610	2.271710	-0.131610

Zero-point correction= 0.297487 (Hartree/Particle)
Thermal correction to Energy= 0.313707
Thermal correction to Enthalpy= 0.314651
Thermal correction to Gibbs Free Energy= 0.254923
SCF Done: E(RwB97XD) = -732.881847535
Thermal correction to Gibbs free energy (ZPG) from GoodVibes: 0.247069

$TS_{14a+14a}$

C	2.699190	2.308630	0.720170
H	3.120950	3.264410	1.049370
C	1.915360	2.296950	-0.371230
C	1.314290	1.023420	-0.827380
C	0.436620	1.003640	-1.889800
H	0.112640	1.921580	-2.380490
C	-0.031480	-0.228300	-2.482020
O	-0.804610	-0.296480	-3.430130
C	0.522410	-1.529630	-1.915480
O	-0.424040	-2.544490	-2.103400
H	-0.911940	-2.273770	-2.898370
C	1.797910	-1.879300	-2.716320
H	2.216500	-2.819360	-2.331250
H	2.562260	-1.093910	-2.642520
H	1.523240	-2.015950	-3.772570
C	0.928600	-1.361100	-0.469260
H	1.257120	-2.281150	0.022700

C	-0.928540	-1.361150	0.469030
H	-1.257070	-2.281150	-0.023030
C	-1.602540	-0.191600	0.110840
C	-1.314310	1.023300	0.827480
C	-1.915410	2.296870	0.371470
C	-2.699270	2.308650	-0.719900
H	-3.121050	3.264460	-1.049000
C	-2.996610	1.116110	-1.570360
H	-2.377400	1.176460	-2.481640
C	-2.742860	-0.236380	-0.887900
C	-3.980060	-0.783280	-0.180810
C	-4.413430	-2.019530	-0.447450
H	-5.285200	-2.440540	0.061220
H	-3.908750	-2.654150	-1.181430
C	-4.663180	0.103450	0.824130
H	-5.063130	1.012030	0.345990
H	-5.494220	-0.418200	1.318230
H	-3.958970	0.448090	1.598580
C	-1.613080	3.553740	1.139750
H	-1.926680	3.469800	2.192510
H	-0.532360	3.770870	1.141630
H	-2.130180	4.416110	0.697840
C	-0.436700	1.003410	1.889940
H	-0.112770	1.921270	2.380790
C	0.031440	-0.228600	2.481990
O	0.804530	-0.296890	3.430130
C	-0.522340	-1.529880	1.915230
C	-1.797830	-1.879770	2.716010
H	-2.216380	-2.819780	2.330740
H	-2.562210	-1.094400	2.642370
H	-1.523150	-2.016630	3.772220
O	0.424190	-2.544690	2.102990
H	0.912010	-2.274100	2.898050
C	1.602570	-0.191580	-0.110910
C	2.742840	-0.236430	0.887890
H	2.479070	-0.968460	1.661600
C	3.980100	-0.783240	0.180850
C	4.413480	-2.019500	0.447410
H	3.908760	-2.654200	1.181300
H	5.285310	-2.440440	-0.061210
C	4.663230	0.103560	-0.824030
H	5.494720	-0.417830	-1.317640
H	5.062520	1.012470	-0.345990
H	3.959190	0.447610	-1.598900
C	2.996520	1.116000	1.570510
H	2.377270	1.176230	2.481760
H	4.037840	1.159870	1.928540
C	1.613020	3.553880	-1.139390
H	0.532300	3.771010	-1.141230
H	1.926600	3.470030	-2.192170
H	2.130130	4.416210	-0.697410
H	-4.037950	1.160000	-1.928330
H	-2.479130	-0.968320	-1.661700

Zero-point correction= 0.597942 (Hartree/Particle)
Thermal correction to Energy= 0.630102
Thermal correction to Enthalpy= 0.631046
Thermal correction to Gibbs Free Energy= 0.539378
SCF Done: E(RwB97XD) = -1465.76348056
Thermal correction to Gibbs free energy (ZPG) from GoodVibes: 0.524902

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C	-3.155040	1.253280	-1.778930
H	-3.790370	1.799790	-2.483960
C	-2.520650	1.949560	-0.817160
C	-1.641420	1.252330	0.147540
C	-1.123250	1.898730	1.214560
H	-1.293200	2.961470	1.391210
C	-0.283450	1.215980	2.193690
O	0.452980	1.796620	2.972930
C	-0.439450	-0.298430	2.310880
O	0.640250	-0.783950	3.062840
H	0.978690	-0.003210	3.532810
C	-1.732650	-0.556340	3.100770
H	-1.837730	-1.639160	3.255840
H	-2.626040	-0.190770	2.582250
H	-1.664110	-0.064820	4.082570
C	-0.480270	-0.973580	0.915880
H	-1.012560	-1.922100	1.045780
C	0.953660	-1.341970	0.441020
H	1.459820	-1.908430	1.229730
C	1.668720	-0.056440	0.119820
C	1.076930	0.674760	-0.843280
C	1.587600	1.994080	-1.262130
C	2.526390	2.570400	-0.493850
H	2.914170	3.557340	-0.765260
C	3.015300	1.952980	0.789440
H	2.412940	2.374690	1.612840
C	2.908680	0.414490	0.844760
C	4.137640	-0.306780	0.311530
C	4.719690	-1.274790	1.026910
H	5.588030	-1.821450	0.647910
H	4.346560	-1.553890	2.016410
C	4.644870	0.103010	-1.044620
H	5.432540	-0.574900	-1.402090
H	3.829290	0.121660	-1.785120
H	5.057190	1.124420	-1.017540
C	1.027090	2.636220	-2.499340
H	1.135260	1.980230	-3.378530
H	-0.050480	2.843570	-2.387560
H	1.533360	3.586670	-2.716320
C	-0.177450	0.047130	-1.394990
H	-0.616900	0.627850	-2.208810
C	0.196750	-1.324190	-1.909010
O	-0.050090	-1.734720	-3.017960
C	0.857960	-2.203220	-0.835320
C	2.205490	-2.725050	-1.316580
H	2.638830	-3.382050	-0.550000
H	2.910920	-1.911480	-1.522150
H	2.062390	-3.294090	-2.247890
O	-0.014560	-3.292740	-0.584960
H	-0.139350	-3.751880	-1.423760
C	-1.225280	-0.164770	-0.207410
C	-2.449120	-0.962140	-0.766660
H	-2.047220	-1.919050	-1.123010
C	-3.501910	-1.332760	0.267800
C	-3.553300	-2.587370	0.730320
H	-2.842360	-3.347120	0.393260
H	-4.299500	-2.892710	1.469220
C	-4.500800	-0.299210	0.720700
H	-4.013040	0.590280	1.147660
H	-5.178440	-0.717000	1.477900
H	-5.111890	0.061880	-0.121750
C	-3.055720	-0.226870	-1.970360
H	-2.451040	-0.435180	-2.871270
H	-4.051830	-0.640100	-2.198040
C	-2.702650	3.436800	-0.680830
H	-1.735880	3.963900	-0.711320
H	-3.183050	3.696300	0.276130
H	-3.333370	3.829490	-1.489500
H	4.053920	2.257670	0.992950
H	2.789780	0.115630	1.895550

Zero-point correction= 0.603638 (Hartree/Particle)
Thermal correction to Energy= 0.634937
Thermal correction to Enthalpy= 0.635881
Thermal correction to Gibbs Free Energy= 0.546831
SCF Done: E(RwB97XD) = -1465.81880309
Thermal correction to Gibbs free energy (ZPG) from GoodVibes: 0.532532

14b

O	-3.558380	0.216130	-0.870020
C	-2.450280	0.182030	-0.367430
C	-1.610740	1.358450	-0.168670
C	-0.271820	1.239760	0.040740
C	0.593900	2.435450	0.104730
C	1.915560	2.298560	-0.103940
C	2.567940	0.980220	-0.380260

H	2.545850	0.792030	-1.468850
H	3.630140	1.005970	-0.094360
C	1.863460	-0.158450	0.370140
C	0.358440	-0.100140	0.153670
C	-0.409160	-1.200630	0.141920
C	-1.906610	-1.160590	0.122110
C	-2.409560	-1.321110	1.577570
H	-2.034960	-0.521220	2.233540
H	-3.509810	-1.299150	1.575800
H	-2.075390	-2.293510	1.965220
O	-2.413800	-2.188530	-0.680900
H	-3.253620	-1.846270	-1.023620
H	0.037320	-2.194140	0.242460
C	2.465380	-1.515230	0.059990
C	2.928770	-2.294690	1.041920
H	3.362280	-3.276980	0.834740
H	2.889260	-1.978330	2.088140
C	2.522170	-1.934770	-1.385530
H	3.255960	-1.331240	-1.943990
H	1.547850	-1.796460	-1.879610
H	2.813690	-2.989150	-1.483910
H	2.022940	0.038400	1.445580
H	2.546520	3.193090	-0.105290
C	-0.038690	3.781460	0.327070
H	-0.680990	3.778330	1.221190
H	0.728050	4.557470	0.454050
H	-0.671690	4.073290	-0.526090
H	-2.088620	2.325190	-0.331770

Zero-point correction= 0.297280 (Hartree/Particle)
Thermal correction to Energy= 0.313615
Thermal correction to Enthalpy= 0.314559
Thermal correction to Gibbs Free Energy= 0.254438
SCF Done: E(RwB97XD) = -732.881265596
Thermal correction to Gibbs free energy (ZPG) from GoodVibes: 0.246560

$TS_{14b+14b}$

C	-2.710520	2.349210	-0.629310
H	-3.145450	3.309420	-0.926880
C	-1.875310	2.321330	0.422180
C	-1.266270	1.039420	0.838140
C	-0.344370	1.002700	1.855900
H	0.003150	1.915990	2.339300
C	0.106840	-0.230630	2.475870
O	0.850590	-0.257560	3.443680
C	-0.527710	-1.522130	1.950060
C	-0.957140	-1.352050	0.502380
H	-1.353460	-2.275560	0.073480
C	0.957020	-1.351690	-0.503260
H	1.353380	-2.275490	-0.075020
C	1.602880	-0.174360	-0.135090
C	1.266400	1.039980	-0.837510
C	1.875510	2.321580	-0.420680
C	2.710690	2.348710	0.630860
H	3.145660	3.308690	0.929070
C	3.055080	1.167940	1.477710
H	2.492470	1.246800	2.424710
C	2.761750	-0.203990	0.843330
C	3.986540	-0.798490	0.155680
C	4.580970	-1.880470	0.668750
H	5.465140	-2.320750	0.199610
H	4.207110	-2.361680	1.577470
C	4.465720	-0.129560	-1.101710
H	5.401520	-0.578440	-1.461830
H	3.704250	-0.235380	-1.890890
H	4.632380	0.947940	-0.943460
C	1.533310	3.568530	-1.188420
H	1.804210	3.474650	-2.252030
H	0.452260	3.779800	-1.147980
H	2.063170	4.438130	-0.776770
C	0.344570	1.003990	-1.855350
H	-0.002790	1.917620	-2.338230
C	-0.106770	-0.228890	-2.476100
O	-0.850480	-0.255130	-3.443960
C	0.527550	-1.520810	-1.951050
C	-1.602890	-0.174440	0.134970
C	-2.761770	-0.203340	-0.843460
H	-2.509810	-0.885080	-1.666900
C	-3.986600	-0.798170	-0.156150
C	-4.581060	-1.879830	-0.669840
H	-4.207230	-2.360550	-1.578830
H	-5.465260	-2.320340	-0.200950
C	-4.465750	-0.129940	1.101620
H	-4.632230	0.947680	0.944030
H	-3.704330	-0.236370	1.890780
H	-5.401630	-0.578910	1.461410
C	-3.055000	1.169030	-1.476950
H	-2.492370	1.248470	-2.423880
H	-4.116760	1.214260	-1.767570
C	-1.532990	3.567750	1.190730
H	-0.451940	3.778980	1.150380
H	-1.803850	3.473190	2.254290
H	-2.062820	4.437660	0.779670
H	4.116840	1.212910	1.768350
H	2.509710	-0.886230	1.666330
O	-1.771450	-1.648500	2.647630
H	-1.566810	-1.713690	3.587630
C	0.318020	-2.750870	2.254360
H	-0.173050	-3.647340	1.849510
H	1.336440	-2.685170	1.854700
H	0.417290	-2.857430	3.343470
C	-0.318510	-2.749160	-2.256060
H	0.172110	-3.645960	-1.851370
H	-1.337020	-2.683190	-1.856640
H	-0.417520	-2.855290	-3.345220
O	1.771270	-1.647070	-2.648670
H	1.566620	-1.711580	-3.588720

Zero-point correction= 0.597315 (Hartree/Particle)
Thermal correction to Energy= 0.630056
Thermal correction to Enthalpy= 0.631000
Thermal correction to Gibbs Free Energy= 0.538041
SCF Done: E(RwB97XD) = -1465.73784512
Thermal correction to Gibbs free energy (ZPG) from GoodVibes: 0.523342

14b+14b

C	-3.123710	1.571960	-1.568820
H	-3.744830	2.235910	-2.179300
C	-2.460240	2.096050	-0.522250
C	-1.606820	1.233470	0.322450
C	-1.070830	1.693370	1.471900
H	-1.204780	2.725130	1.800080
C	-0.282370	0.843010	2.370120
O	0.442060	1.289620	3.236770
C	-0.566480	-0.661670	2.236340
C	-0.508040	-1.097760	0.760370
H	-1.060110	-2.047230	0.758520
C	0.947800	-1.364530	0.281150
H	1.477520	-2.030570	0.972930
C	1.642990	-0.032370	0.143470
C	1.062390	0.794080	-0.744590
C	1.586820	2.139440	-1.040890
C	2.531190	2.631280	-0.223130
H	2.937200	3.631290	-0.405180
C	3.003850	1.892680	0.999360
H	2.400060	2.241680	1.856110
C	2.878550	0.354830	0.919510
C	4.111700	-0.337270	0.358010
C	4.760680	-1.251480	1.085650
H	5.644180	-1.766720	0.698770
H	4.429720	-1.519360	2.093510
C	4.546580	0.049610	-1.026850
H	5.416590	-0.538060	-1.350840
H	3.725950	-0.121890	-1.738950
H	4.809030	1.118390	-1.077400
C	1.040900	2.893340	-2.220150
H	1.142740	2.311900	-3.151010
H	-0.033570	3.108450	-2.093610

H	1.563770	3.850080	-2.354260
C	-0.181690	0.223650	-1.381450
H	-0.614070	0.893210	-2.127890
C	0.259970	-1.051860	-2.063000
O	0.189330	-1.259430	-3.250750
C	0.922500	-2.050860	-1.100630
C	-1.232120	-0.126510	-0.244470
C	-2.464220	-0.803450	-0.926030
H	-2.077870	-1.677840	-1.469770
C	-3.523450	-1.346630	0.019070
C	-3.713970	-2.667840	0.105860
H	-3.115280	-3.376150	-0.474590
H	-4.479690	-3.091180	0.761240
C	-4.378560	-0.381670	0.792750
H	-3.759240	0.233630	1.459110
H	-5.113320	-0.919520	1.407250
H	-4.922660	0.298750	0.118760
C	-3.076090	0.135470	-1.981170
H	-2.506670	0.053940	-2.924670
H	-4.091230	-0.211370	-2.234420
C	-2.585580	3.553090	-0.169760
H	-1.598840	4.041510	-0.133610
H	-3.051050	3.687540	0.819580
H	-3.204540	4.082200	-0.906640
H	4.045290	2.161680	1.235330
H	2.753480	-0.009520	1.950230
O	-1.921320	-0.851410	2.625160
H	-2.011130	-0.592040	3.547900
C	0.330760	-1.477670	3.156530
H	0.129700	-2.550120	3.020190
H	1.396600	-1.283910	2.989180
H	0.124480	-1.207300	4.202170
C	0.218750	-3.406370	-1.126560
H	0.768090	-4.103490	-0.477830
H	-0.826740	-3.366350	-0.796790
H	0.232260	-3.795420	-2.155520
O	2.258930	-2.226010	-1.519050
H	2.239440	-2.373600	-2.472250

Zero-point correction= 0.602026 (Hartree/Particle)
Thermal correction to Energy= 0.634047
Thermal correction to Enthalpy= 0.634991
Thermal correction to Gibbs Free Energy= 0.543637
SCF Done: E(RwB97XD) = -1465.80684521
Thermal correction to Gibbs free energy (ZPG) from GoodVibes: 0.529335

14a-noMe

O	-3.786860	-0.653260	0.240520
C	-2.620230	-0.433270	-0.024310
C	-2.005950	0.891090	-0.034590
C	-0.653060	1.040240	0.005730
C	0.234460	-0.149130	0.073870
C	-0.288470	-1.376870	-0.073960
C	-1.722300	-1.589670	-0.434000
O	-2.224460	-2.803550	0.011340
H	-3.158060	-2.628990	0.209530
H	0.329720	-2.273160	0.019540
C	1.693070	0.095330	0.428000
C	2.577960	-1.120080	0.233980
C	3.027650	-1.809060	1.287080
H	2.776750	-1.515150	2.310110
H	3.658550	-2.693630	1.163750
C	2.926420	-1.508390	-1.179370
H	2.032170	-1.524560	-1.822050
H	3.629770	-0.786550	-1.625440
H	3.397790	-2.499840	-1.216850
C	2.216840	1.333000	-0.312200
C	1.293610	2.499780	-0.152480
C	-0.035890	2.382650	0.018380
C	-0.920310	3.591110	0.154020
H	-1.628830	3.666040	-0.686190
H	-1.516170	3.549350	1.079110
H	-0.322650	4.512150	0.174000
H	1.731410	3.502000	-0.200640
H	2.333890	1.116720	-1.389570
H	3.221690	1.586720	0.058940
H	1.706270	0.349640	1.503100
H	-2.686470	1.741230	0.019960
H	-1.758090	-1.527880	-1.553060

Zero-point correction= 0.269560 (Hartree/Particle)
Thermal correction to Energy= 0.284338
Thermal correction to Enthalpy= 0.285283
Thermal correction to Gibbs Free Energy= 0.228427
SCF Done: E(RwB97XD) = -693.559945653
Thermal correction to Gibbs free energy (ZPG) from GoodVibes: 0.221066

$TS_{14a+14anoMe}$

C	-2.788830	2.174830	-0.436480
H	-3.251370	3.127320	-0.716800
C	-1.893280	2.168850	0.565100
C	-1.236120	0.899840	0.952030
C	-0.250890	0.889510	1.918050
H	0.117560	1.811310	2.368500
C	0.284900	-0.337790	2.457570
O	1.154770	-0.410560	3.317340
C	-0.317280	-1.628020	1.939030
O	0.567290	-2.683260	2.116130
H	1.148700	-2.390700	2.838240
C	-0.870560	-1.483210	0.549030
H	-1.251470	-2.406540	0.102320
C	0.870570	-1.483210	-0.549020
H	1.251480	-2.406540	-0.102300
C	1.585610	-0.314540	-0.264300
C	1.236120	0.899840	-0.952040
C	1.893270	2.168850	-0.565120
C	2.788820	2.174840	0.436460
H	3.251350	3.127340	0.716770
C	3.167540	0.981450	1.252140
H	2.658030	1.052850	2.228460
C	2.821290	-0.371730	0.611550
C	3.972210	-0.945620	-0.209850
C	4.477220	-2.146250	0.090710
H	5.294820	-2.582640	-0.489840
H	4.088320	-2.735780	0.925730
C	4.488020	-0.124110	-1.359590
H	4.865400	0.852080	-1.015340
H	5.300910	-0.640900	-1.887660
H	3.685980	0.090180	-2.084930
C	1.521350	3.428080	-1.298240
H	1.716150	3.340020	-2.378950
H	0.449550	3.657790	-1.181170
H	2.093420	4.285000	-0.917870
C	0.250890	0.889490	-1.918060
H	-0.117570	1.811290	-2.368520
C	-0.284900	-0.337820	-2.457570
O	-1.154770	-0.410600	-3.317340
C	0.317290	-1.628040	-1.939010
O	-0.567270	-2.683280	-2.116100
H	-1.148690	-2.390730	-2.838210
C	-1.585610	-0.314550	0.264300
C	-2.821280	-0.371750	-0.611550
H	-2.627620	-1.091610	-1.417190
C	-3.972200	-0.945630	0.209860
C	-4.477210	-2.146280	-0.090670
H	-4.088290	-2.735820	-0.925680
H	-5.294800	-2.582660	0.489890
C	-4.488040	-0.124100	1.359570
H	-5.300890	-0.640900	1.887680
H	-4.865460	0.852060	1.015290
H	-3.685990	0.090270	2.084890
C	-3.167530	0.981420	-1.252150
H	-2.658020	1.052820	-2.228470
H	-4.244060	1.013060	-1.485750
C	-1.521370	3.428090	1.298220
H	-0.449580	3.657800	1.181150
H	-1.716180	3.340030	2.378930
H	-2.093460	4.285000	0.917840

H	4.244070	1.013090	1.485730
H	2.627630	-1.091580	1.417210
H	1.228230	-1.778010	-2.567770
H	-1.228220	-1.777980	2.567790

Zero-point correction= 0.542409 (Hartree/Particle)
Thermal correction to Energy= 0.571708
Thermal correction to Enthalpy= 0.572653
Thermal correction to Gibbs Free Energy= 0.485540
SCF Done: E(RwB97XD) = -1387.11881102
Thermal correction to Gibbs free energy (ZPG) from GoodVibes: 0.472463

14b-noMe

O	3.705590	-0.677420	0.517860
C	2.593480	-0.445720	0.081750
C	1.997180	0.883550	0.001000
C	0.650260	1.043170	-0.121560
C	0.041520	2.388880	-0.061860
C	-1.265550	2.503780	0.233380
C	-2.152600	1.325980	0.489600
H	-2.101690	1.067630	1.562720
H	-3.203280	1.579750	0.284020
C	-1.740300	0.121100	-0.367280
C	-0.244150	-0.133570	-0.258870
C	0.285970	-1.363930	-0.359730
C	1.756850	-1.594430	-0.454970
O	2.162980	-2.809600	0.077370
H	3.060980	-2.647900	0.407170
H	-0.352190	-2.243540	-0.478410
C	-2.583320	-1.107000	-0.083020
C	-3.250560	-1.717150	-1.067350
H	-3.859440	-2.605680	-0.878970
H	-3.209960	-1.350360	-2.096920
C	-2.639010	-1.595860	1.340630
H	-3.206580	-0.897460	1.976760
H	-1.630070	-1.679060	1.773830
H	-3.126270	-2.578000	1.406670
H	-1.922520	0.414230	-1.416900
H	-1.701550	3.503670	0.324860
C	0.918350	3.594360	-0.260430
H	1.494810	3.519630	-1.195350
H	0.317260	4.512820	-0.296390
H	1.644610	3.702570	0.560950
H	2.663900	1.725580	0.191110
H	1.974660	-1.546620	-1.554690

Zero-point correction= 0.269474 (Hartree/Particle)
Thermal correction to Energy= 0.284343
Thermal correction to Enthalpy= 0.285288
Thermal correction to Gibbs Free Energy= 0.228071
SCF Done: E(RwB97XD) = -693.559405994
Thermal correction to Gibbs free energy (ZPG) from GoodVibes: 0.220708

$TS_{14b+14bnoMe}$

C	-2.748670	2.099130	-0.811020
H	-3.193820	3.028610	-1.181780
C	-1.915520	2.162110	0.240810
C	-1.289020	0.923370	0.751590
C	-0.367890	0.975720	1.771660
H	-0.042880	1.926790	2.194390
C	0.096170	-0.205660	2.472070
O	0.803230	-0.168140	3.468050
C	-0.455280	-1.544030	2.001350
C	-0.943660	-1.483630	0.577250
H	-1.324770	-2.439460	0.202160
C	0.944120	-1.551600	-0.356170
H	1.325420	-2.442260	0.154600
C	1.611230	-0.357880	-0.088890
C	1.289060	0.804350	-0.880310
C	1.915830	2.104320	-0.556130
C	2.747290	2.196160	0.494940
H	3.192960	3.169680	0.725550
C	3.072710	1.075340	1.427200
H	2.499630	1.226460	2.359300
C	2.771420	-0.334220	0.885660
C	3.991060	-0.980840	0.233420
C	4.635740	-1.971210	0.858130
H	5.520540	-2.439890	0.418680
H	4.304080	-2.345960	1.830800
C	4.408530	-0.470450	-1.117890
H	5.359470	-0.917960	-1.437440
H	3.640100	-0.724480	-1.866180
H	4.519130	0.625630	-1.117120
C	1.592580	3.296890	-1.413200
H	1.865060	3.123140	-2.466300
H	0.514480	3.525240	-1.392180
H	2.133130	4.186730	-1.063530
C	0.368450	0.706930	-1.897430
H	0.043570	1.585870	-2.454910
C	-0.095990	-0.564210	-2.417340
O	-0.803540	-0.672610	-3.407740
C	0.456020	-1.819380	-1.756310
C	-1.611520	-0.342010	0.138920
C	-2.773350	-0.461450	-0.826650
H	-2.516700	-1.209830	-1.590310
C	-3.991410	-1.006320	-0.084460
C	-4.638450	-2.075690	-0.558260
H	-4.309670	-2.587060	-1.467630
H	-5.522390	-2.475220	-0.053590
C	-4.404520	-0.306210	1.180430
H	-4.512240	0.778740	1.022660
H	-3.635090	-0.452810	1.955990
H	-5.355960	-0.700480	1.562520
C	-3.077170	0.853780	-1.567590
H	-2.508460	0.866930	-2.514380
H	-4.137380	0.865260	-1.865900
C	-1.589960	3.467430	0.912740
H	-0.511370	3.687940	0.858880
H	-1.863060	3.451510	1.979810
H	-2.128600	4.297030	0.435330
H	4.131620	1.130770	1.725120
H	2.513220	-0.963060	1.749990
O	-1.569730	-1.870770	2.807960
H	-1.276990	-1.830400	3.726140
O	1.570690	-2.259920	-2.506470
H	1.277950	-2.354700	-3.420630
H	-0.337570	-2.586070	-1.767530
H	0.338530	-2.300660	2.124300

Zero-point correction= 0.542205 (Hartree/Particle)
Thermal correction to Energy= 0.572218
Thermal correction to Enthalpy= 0.573162
Thermal correction to Gibbs Free Energy= 0.484287
SCF Done: E(RwB97XD) = -1387.09943352
Thermal correction to Gibbs free energy (ZPG) from GoodVibes: 0.470812

14a-noOH

O	3.832450	-0.678740	-0.034510
C	2.632470	-0.515180	-0.141680
C	2.026760	0.818100	-0.080730
C	0.684720	1.025510	-0.106290
C	-0.245920	-0.117120	-0.261990
C	0.244100	-1.362060	-0.372430
C	1.699280	-1.705110	-0.342420
C	2.018270	-2.821430	0.661080
H	1.747050	-2.512120	1.681970
H	3.094320	-3.038220	0.639110
H	1.461160	-3.738480	0.419640
H	-0.448540	-2.196670	-0.520370
C	-1.729450	0.196540	-0.392360
C	-2.626500	-1.009350	-0.192480
C	-3.274270	-1.556840	-1.225590
H	-3.178880	-1.152270	-2.237210
H	-3.922060	-2.428480	-1.096770
C	-2.761490	-1.549580	1.207420
H	-1.776480	-1.671070	1.684700
H	-3.343140	-0.861170	1.841690

H	-3.273560	-2.521450	1.213720
C	-2.114750	1.369660	0.519560
C	-1.181970	2.527050	0.342270
C	0.120290	2.384560	0.038410
C	1.034570	3.571330	-0.090880
H	1.785890	3.588350	0.714620
H	1.583610	3.550780	-1.044970
H	0.466410	4.509830	-0.039290
H	-1.582490	3.533950	0.497240
H	-2.095580	1.053670	1.578280
H	-3.151440	1.673280	0.308750
H	-1.875260	0.552070	-1.428280
H	2.734720	1.638840	0.041820
H	1.958050	-2.087300	-1.349940

Zero-point correction= 0.292770 (Hartree/Particle)
Thermal correction to Energy= 0.308170
Thermal correction to Enthalpy= 0.309114
Thermal correction to Gibbs Free Energy= 0.250181
SCF Done: E(RwB97XD) = -657.650139242
Thermal correction to Gibbs free energy (ZPG) from GoodVibes: 0.242941

$TS_{14a+14anoOH}$

C	-2.679200	2.157400	-0.730090
H	-3.100010	3.116530	-1.050550
C	-1.897360	2.132990	0.362020
C	-1.299150	0.852490	0.804890
C	-0.415150	0.812960	1.859650
H	-0.093420	1.726230	2.361330
C	0.030600	-0.424370	2.484950
O	0.752350	-0.444160	3.469900
C	-0.515750	-1.706940	1.893680
C	-1.721370	-2.172050	2.728960
H	-2.119100	-3.121610	2.342160
H	-2.531920	-1.428880	2.700280
H	-1.411970	-2.316410	3.773840
C	-0.921790	-1.524390	0.449870
H	-1.290510	-2.440370	-0.026380
C	0.921790	-1.524390	-0.449870
H	1.290510	-2.440370	0.026380
C	1.594050	-0.352310	-0.080700
C	1.299150	0.852490	-0.804890
C	1.897370	2.132990	-0.362020
C	2.679200	2.157400	0.730100
H	3.100010	3.116530	1.050560
C	2.976730	0.973330	1.593610
H	2.354110	1.037680	2.502850
C	2.727680	-0.388810	0.925940
C	3.970240	-0.944270	0.236140
C	4.442640	-2.150850	0.566110
H	5.323570	-2.572840	0.074280
H	3.969380	-2.755310	1.345250
C	4.620870	-0.093930	-0.820340
H	4.993910	0.850650	-0.393200
H	5.465310	-0.615910	-1.290780
H	3.901770	0.185590	-1.607010
C	1.594020	3.380300	-1.145000
H	1.907800	3.283960	-2.196650
H	0.512910	3.595320	-1.150110
H	2.109690	4.248520	-0.712860
C	0.415160	0.812960	-1.859650
H	0.093420	1.726230	-2.361330
C	-0.030600	-0.424370	-2.484950
O	-0.752350	-0.444150	-3.469900
C	0.515750	-1.706940	-1.893680
C	1.721360	-2.172050	-2.728960
H	2.119100	-3.121610	-2.342160
H	2.531920	-1.428880	-2.700280
H	1.411960	-2.316410	-3.773840
C	-1.594050	-0.352310	0.080700
C	-2.727680	-0.388810	-0.925940
H	-2.463220	-1.102250	-1.719900
C	-3.970240	-0.944270	-0.236140
C	-4.442640	-2.150850	-0.566110
H	-3.969380	-2.755310	-1.345250
H	-5.323560	-2.572840	-0.074280
C	-4.620870	-0.093930	0.820340
H	-5.465320	-0.615900	1.290760
H	-4.993900	0.850660	0.393200
H	-3.901780	0.185580	1.607010
C	-2.976730	0.973330	-1.593610
H	-2.354110	1.037690	-2.502850
H	-4.017400	1.021480	-1.952950
C	-1.594010	3.380300	1.145010
H	-0.512900	3.595310	1.150110
H	-1.907800	3.283960	2.196650
H	-2.109680	4.248520	0.712870
H	4.017400	1.021480	1.952950
H	2.463220	-1.102260	1.719900
H	0.271220	-2.468370	1.993620
H	-0.271230	-2.468370	-1.993620

Zero-point correction= 0.588123 (Hartree/Particle)
Thermal correction to Energy= 0.618793
Thermal correction to Enthalpy= 0.619737
Thermal correction to Gibbs Free Energy= 0.530147
SCF Done: E(RwB97XD) = -1315.29245478
Thermal correction to Gibbs free energy (ZPG) from GoodVibes: 0.516138

14b-noOH

O	-3.857880	-0.474800	-0.161940
C	-2.646790	-0.376820	-0.184200
C	-1.975130	0.923910	-0.095690
C	-0.628210	1.056530	0.017150
C	0.005060	2.390640	0.092280
C	1.335940	2.499050	-0.068590
C	2.238210	1.325390	-0.290430
H	2.333000	1.147830	-1.377020
H	3.253400	1.546510	0.073230
C	1.705680	0.067770	0.410040
C	0.237110	-0.145280	0.073060
C	-0.307950	-1.362390	-0.081670
C	-1.759770	-1.607210	-0.351000
C	-2.314240	-2.809180	0.418030
H	-2.216740	-2.652500	1.502890
H	-3.378810	-2.938850	0.185410
H	-1.772690	-3.729050	0.153280
H	0.330500	-2.248300	-0.009250
C	2.574190	-1.148520	0.155970
C	3.050710	-1.871430	1.174230
H	3.673860	-2.754230	1.005940
H	2.832920	-1.606020	2.212590
C	2.879860	-1.496430	-1.277720
H	3.577100	-0.766830	-1.720580
H	1.967840	-1.483750	-1.894900
H	3.341410	-2.490010	-1.359020
H	1.740250	0.281240	1.493560
H	1.789440	3.495370	-0.064010
C	-0.865750	3.601860	0.280900
H	-1.485580	3.511760	1.186480
H	-0.256380	4.511210	0.370050
H	-1.552690	3.738030	-0.569470
H	-2.642660	1.786460	-0.094060
H	-1.844680	-1.837820	-1.433800

Zero-point correction= 0.292688 (Hartree/Particle)
Thermal correction to Energy= 0.308087
Thermal correction to Enthalpy= 0.309031
Thermal correction to Gibbs Free Energy= 0.250304
SCF Done: E(RwB97XD) = -657.650036505
Thermal correction to Gibbs free energy (ZPG) from GoodVibes: 0.242952

$TS_{14b+14bnoOH}$

C	2.733520	2.232100	0.407390
H	3.184010	3.194460	0.673320
C	1.829170	2.199310	-0.585070
C	1.192410	0.913190	-0.952150

C	0.195710	0.867220	-1.901600
H	-0.194160	1.778940	-2.355410
C	-0.311400	-0.371940	-2.476840
O	-1.164330	-0.394980	-3.349920
C	0.346100	-1.638620	-1.970820
C	0.872370	-1.465880	-0.562230
H	1.301030	-2.381620	-0.143920
C	-0.872370	-1.465880	0.562230
H	-1.301030	-2.381620	0.143920
C	-1.566560	-0.286150	0.257780
C	-1.192410	0.913190	0.952150
C	-1.829170	2.199310	0.585070
C	-2.733510	2.232100	-0.407380
H	-3.184000	3.194460	-0.673300
C	-3.137490	1.052880	-1.232680
H	-2.633930	1.122860	-2.212690
C	-2.807380	-0.315460	-0.613560
C	-3.962550	-0.887090	0.202330
C	-4.516050	-2.055000	-0.140700
H	-5.340590	-2.486860	0.433520
H	-4.169190	-2.616260	-1.013310
C	-4.433700	-0.096550	1.392100
H	-5.252730	-0.608220	1.915750
H	-3.612490	0.069040	2.108420
H	-4.786680	0.902100	1.088960
C	-1.429120	3.442070	1.331020
H	-1.618500	3.343580	2.411820
H	-0.353550	3.651190	1.210240
H	-1.986720	4.314640	0.964700
C	-0.195700	0.867210	1.901600
H	0.194170	1.778930	2.355410
C	0.311400	-0.371950	2.476830
O	1.164330	-0.394990	3.349920
C	-0.346100	-1.638620	1.970820
C	1.566560	-0.286150	-0.257780
C	2.807380	-0.315470	0.613560
H	2.637770	-1.013880	1.444090
C	3.962550	-0.887090	-0.202340
C	4.516050	-2.055010	0.140690
H	4.169180	-2.616270	1.013300
H	5.340590	-2.486870	-0.433540
C	4.433700	-0.096550	-1.392100
H	4.786680	0.902090	-1.088960
H	3.612490	0.069050	-2.108420
H	5.252730	-0.608220	-1.915750
C	3.137490	1.052870	1.232680
H	2.633930	1.122850	2.212700
H	4.215330	1.102380	1.457180
C	1.429120	3.442070	-1.331010
H	0.353560	3.651200	-1.210220
H	1.618500	3.343590	-2.411810
H	1.986730	4.314650	-0.964680
H	-4.215330	1.102390	-1.457180
H	-2.637770	-1.013870	-1.444090
C	-0.449800	-2.899160	-2.276630
H	0.058870	-3.788550	-1.875670
H	-1.465320	-2.860770	-1.859200
H	-0.560010	-3.016030	-3.362250
C	0.449790	-2.899170	2.276630
H	-0.058900	-3.788560	1.875700
H	1.465300	-2.860800	1.859170
H	0.560030	-3.016010	3.362250
H	1.276560	-1.692480	-2.575370
H	-1.276570	-1.692480	2.575360

Zero-point correction= 0.588799 (Hartree/Particle)
Thermal correction to Energy= 0.619106
Thermal correction to Enthalpy= 0.620050
Thermal correction to Gibbs Free Energy= 0.531666
SCF Done: E(RwB97XD) = -1315.28864477
Thermal correction to Gibbs free energy (ZPG) from GoodVibes: 0.517862

$TS_{14a+14a}$-II

C	1.301570	2.850230	-1.503110
H	1.329500	3.694970	-2.199540
C	2.117810	1.807870	-1.731560
C	2.097590	0.637070	-0.825960
C	2.997820	-0.383920	-0.976180
H	3.701060	-0.416320	-1.808060
C	3.024280	-1.525830	-0.083050
O	3.683530	-2.534380	-0.267300
C	2.216900	-1.420330	1.215270
O	1.923110	-2.700680	1.684060
H	2.465630	-3.293360	1.135130
C	3.131880	-0.719630	2.243980
H	2.604750	-0.648340	3.205940
H	3.426340	0.288670	1.924420
H	4.032280	-1.335760	2.377980
C	0.979400	-0.538750	1.052500
H	0.507470	-0.342810	2.021670
C	-1.091870	0.166650	-1.428580
H	-1.218060	1.004460	-2.121620
C	-1.869980	0.078860	-0.300770
C	-1.608500	-0.958190	0.634260
C	-2.332240	-1.005700	1.913180
C	-3.099450	0.039760	2.278810
H	-3.613980	0.009030	3.244420
C	-3.233920	1.290280	1.465530
H	-2.519250	2.036820	1.863910
C	-2.971730	1.092350	-0.037260
C	-4.222770	0.698580	-0.812910
C	-4.655310	1.460080	-1.823070
H	-5.541670	1.188500	-2.402880
H	-4.139000	2.381370	-2.107740
C	-4.927220	-0.568050	-0.411770
H	-5.769400	-0.785700	-1.082570
H	-4.236810	-1.426420	-0.427340
H	-5.313930	-0.499580	0.617510
C	-2.148920	-2.205280	2.802760
H	-2.378930	-3.138630	2.265410
H	-1.108440	-2.289160	3.155890
H	-2.799630	-2.144360	3.685400
C	-0.445270	-1.739440	0.443110
H	-0.216560	-2.557920	1.125800
C	0.031150	-1.998350	-0.936690
O	0.789420	-2.896300	-1.233200
C	-0.485750	-1.066500	-2.025420
C	-1.613070	-1.839650	-2.756300
H	-2.034400	-1.198440	-3.542940
H	-2.418280	-2.141230	-2.071270
H	-1.177100	-2.738160	-3.217660
O	0.528240	-0.762320	-2.941050
H	1.129230	-1.520980	-2.932220
C	1.090840	0.602050	0.222230
C	0.486810	1.901050	0.717690
H	-0.500320	1.656960	1.136280
C	1.308720	2.438070	1.884720
C	0.830650	2.366410	3.132020
H	-0.156900	1.942920	3.339950
H	1.409790	2.722980	3.988350
C	2.659920	3.023710	1.577720
H	2.567810	3.924460	0.949830
H	3.283510	2.316280	1.008430
H	3.195200	3.299490	2.496530
C	0.301290	2.938940	-0.395240
H	-0.701650	2.820250	-0.840570
H	0.302220	3.954860	0.033250
C	3.047110	1.787380	-2.911070
H	2.806700	0.935420	-3.565720
H	4.098780	1.685120	-2.601020
H	2.954470	2.709550	-3.500200
H	-4.228610	1.740490	1.610050
H	-2.642440	2.055640	-0.453770

Zero-point correction= 0.596651 (Hartree/Particle)
Thermal correction to Energy= 0.629272
Thermal correction to Enthalpy= 0.630216
Thermal correction to Gibbs Free Energy= 0.536889
SCF Done: E(RwB97XD) = -1465.73459936

Thermal correction to Gibbs free energy (ZPG) from GoodVibes: 0.522351

17-II

C	-1.488450	-3.198330	-0.189180
H	-1.592780	-4.255370	-0.455670
C	-2.155720	-2.282880	-0.912390
C	-2.031860	-0.846290	-0.578500
C	-2.955970	0.040010	-1.005830
H	-3.775700	-0.261050	-1.659040
C	-2.849600	1.469250	-0.743060
O	-3.385850	2.321890	-1.425360
C	-2.073590	1.887240	0.502530
O	-1.782720	3.252090	0.410190
H	-2.262340	3.561110	-0.377160
C	-3.019360	1.690550	1.696440
H	-2.505320	2.004900	2.615740
H	-3.347330	0.653090	1.816720
H	-3.900890	2.330950	1.550140
C	-0.759510	1.063660	0.654530
H	-0.514160	1.082940	1.725210
C	0.503070	-0.682230	-0.710650
H	0.576270	-1.733260	-1.014340
C	1.692140	-0.242570	0.103900
C	1.681640	1.064000	0.422420
C	2.740490	1.679870	1.245420
C	3.570000	0.857620	1.909940
H	4.360570	1.275300	2.540640
C	3.406510	-0.639630	1.874860
H	2.747960	-0.928530	2.716490
C	2.789180	-1.176880	0.569050
C	3.799170	-1.443470	-0.538020
C	3.770120	-2.597640	-1.212550
H	4.465960	-2.798850	-2.031730
H	3.047710	-3.382950	-0.970700
C	4.806350	-0.367890	-0.841050
H	5.370490	-0.593270	-1.756580
H	4.323420	0.614440	-0.953940
H	5.524700	-0.261630	-0.012240
C	2.837400	3.177420	1.311200
H	2.909460	3.617820	0.303780
H	1.944670	3.615710	1.785670
H	3.716910	3.492640	1.889000
C	0.442950	1.794070	-0.035060
H	0.412760	2.855000	0.219160
C	0.224300	1.615790	-1.521690
O	-0.202140	2.458220	-2.274190
C	0.462080	0.179390	-1.996990
C	1.765290	0.121810	-2.802830
H	1.967800	-0.919530	-3.089350
H	2.631250	0.514120	-2.258660
H	1.624880	0.720790	-3.713830
O	-0.581710	-0.226430	-2.845800
H	-0.930670	0.576690	-3.257240
C	-0.791130	-0.446540	0.203640
C	-0.645040	-1.420170	1.428880
H	0.323680	-1.170430	1.882240
C	-1.665000	-1.251250	2.543470
C	-1.303030	-0.649980	3.682820
H	-0.291290	-0.259340	3.827390
H	-2.006070	-0.522630	4.510620
C	-3.047000	-1.829310	2.377270
H	-3.547800	-1.450070	1.474580
H	-3.676200	-1.597930	3.247640
H	-3.006530	-2.924760	2.268540
C	-0.579700	-2.883390	0.956000
H	0.452030	-3.139740	0.657570
H	-0.793940	-3.556350	1.802560
C	-3.042670	-2.678920	-2.058880
H	-2.744590	-2.136010	-2.968520
H	-4.099640	-2.442940	-1.857770
H	-2.973140	-3.757440	-2.254260
H	4.366870	-1.142380	2.067580
H	2.322010	-2.146900	0.796830

Zero-point correction= 0.602028 (Hartree/Particle)
Thermal correction to Energy= 0.633736
Thermal correction to Enthalpy= 0.634680
Thermal correction to Gibbs Free Energy= 0.544100
SCF Done: E(RwB97XD) = -1465.80227316
Thermal correction to Gibbs free energy (ZPG) from GoodVibes: 0.529882

$TS_{14a+14a}$-III

C	0.636000	-1.331860	-0.105360
C	1.710650	-0.429200	-0.063400
C	1.648350	0.720750	-0.885960
C	2.708690	1.751680	-0.782870
C	3.593820	1.685120	0.224830
C	3.548810	0.642700	1.300040
C	2.894820	-0.668710	0.855490
C	3.860700	-1.644370	0.173490
C	4.917770	-1.241190	-0.539070
H	5.161390	-0.185750	-0.677500
H	5.577520	-1.968050	-1.020650
C	3.545970	-3.105780	0.345800
H	2.565460	-3.360150	-0.084750
H	3.504230	-3.372890	1.414630
H	4.298490	-3.741100	-0.140710
H	2.513860	-1.181620	1.755300
H	4.560400	0.443060	1.683490
H	2.973680	1.059770	2.144290
H	4.364180	2.459030	0.305520
C	2.750980	2.855510	-1.802780
H	2.779320	2.453590	-2.827650
H	3.633750	3.492350	-1.655840
H	1.860180	3.501890	-1.737700
C	0.555560	0.905700	-1.732570
C	-0.320210	-0.179800	-2.093090
O	-1.235550	-0.126350	-2.905390
C	-0.000410	-1.532580	-1.461800
C	1.010160	-2.247280	-2.388990
H	0.553930	-2.341820	-3.385230
H	1.196730	-3.258090	-1.998860
H	1.964470	-1.709980	-2.474690
O	-1.165100	-2.302150	-1.407770
H	-1.735530	-1.931600	-2.104230
H	0.413050	1.832030	-2.289240
C	-1.364670	0.612540	0.577100
C	-2.544050	0.580800	-0.296130
C	-3.296640	-0.542280	-0.381680
C	-3.009650	-1.739070	0.415100
O	-3.757900	-2.695140	0.431500
C	-1.812340	-1.698110	1.384440
C	-1.233130	-3.089530	1.590340
H	-0.403250	-3.049320	2.311830
H	-2.019900	-3.743660	1.990730
H	-0.900860	-3.532280	0.644930
C	-0.810610	-0.574110	1.077810
H	-0.135990	-0.442630	1.927070
O	-2.374890	-1.243210	2.624150
H	-3.067200	-1.869670	2.866550
H	-4.175020	-0.608800	-1.024520
C	-2.852490	1.799030	-1.080300
C	-2.126550	2.917590	-0.902950
C	-1.037990	3.074320	0.111370
C	-1.118250	1.986300	1.177110
C	-0.119220	2.091150	2.312290
C	1.045380	2.734660	2.198360
H	1.703720	2.853420	3.063660
H	1.387800	3.168310	1.257830
C	-0.606810	1.567500	3.641160
H	0.214020	1.463550	4.364720
H	-1.127780	0.603670	3.543800
H	-1.340920	2.275150	4.063030
H	-2.097530	2.161470	1.672370
H	-1.111570	4.063580	0.591330
H	-0.056440	3.048110	-0.391560
H	-2.337880	3.782990	-1.539240

C	-3.937040	1.720570	-2.115920
H	-4.910080	1.467290	-1.666400
H	-3.691440	0.944750	-2.856870
H	-4.046480	2.678440	-2.641740
H	0.773800	-2.252600	0.465150

Zero-point correction= 0.597309 (Hartree/Particle)
Thermal correction to Energy= 0.629619
Thermal correction to Enthalpy= 0.630563
Thermal correction to Gibbs Free Energy= 0.538139
SCF Done: E(RwB97XD) = -1465.72114411
Thermal correction to Gibbs free energy (ZPG) from GoodVibes: 0.524033

17-III

C	0.694520	-1.285780	0.232050
C	1.728950	-0.190440	0.176280
C	1.333400	0.893000	-0.515550
C	2.246670	2.015580	-0.798880
C	3.358850	2.110760	-0.053270
C	3.617600	1.161490	1.084830
C	3.086380	-0.264880	0.847410
C	4.049570	-1.192960	0.109340
C	4.868270	-0.762880	-0.856400
H	4.889380	0.281380	-1.175610
H	5.543360	-1.454760	-1.367950
C	4.038810	-2.630720	0.552730
H	4.358100	-2.709310	1.605360
H	4.706590	-3.253080	-0.058740
H	3.027450	-3.062380	0.498950
H	2.920110	-0.717800	1.840460
H	4.689420	1.122200	1.327730
H	3.106360	1.569590	1.976460
H	4.069880	2.923530	-0.229310
C	1.902600	2.979740	-1.897880
H	1.702610	2.454500	-2.845520
H	2.717640	3.696880	-2.065260
H	0.993070	3.555990	-1.657740
C	-0.083720	0.807660	-1.029630
C	-0.147510	-0.422910	-1.916090
O	-0.593740	-0.452370	-3.036750
C	0.363470	-1.698160	-1.216910
C	1.544850	-2.274630	-1.992020
H	1.227720	-2.462480	-3.028510
H	1.842600	-3.230880	-1.538930
H	2.408590	-1.597600	-2.010260
O	-0.676790	-2.651050	-1.183820
H	-1.099140	-2.662110	-2.051850
H	-0.386530	1.672520	-1.624260
C	-1.120480	0.520980	0.139600
C	-2.452110	0.226480	-0.553600
C	-3.086770	-0.956160	-0.470930
C	-2.676060	-2.039000	0.429540
O	-3.288980	-3.083690	0.496050
C	-1.594920	-1.689960	1.462550
C	-0.985670	-2.955300	2.046170
H	-0.225030	-2.700480	2.799240
H	-1.774810	-3.554020	2.521460
H	-0.541590	-3.577610	1.259080
C	-0.544900	-0.681620	0.959390
H	-0.126110	-0.268820	1.886290
O	-2.302160	-0.976460	2.481960
H	-2.996860	-1.551970	2.820010
H	-4.012670	-1.144790	-1.017370
C	-3.031290	1.344260	-1.337220
C	-2.723840	2.607070	-0.997670
C	-1.807250	2.971340	0.127410
C	-1.440500	1.783540	1.022660
C	-0.462140	2.177800	2.125510
C	0.597130	2.966540	1.922350
H	1.242750	3.261310	2.754550
H	0.871370	3.350210	0.939290
C	-0.839790	1.736920	3.516640
H	-0.052890	1.972970	4.246840
H	-1.074110	0.663940	3.557550
H	-1.762130	2.257270	3.827950
H	-2.360980	1.482320	1.548690
H	-2.266250	3.760900	0.744750
H	-0.896800	3.436000	-0.291760
H	-3.158270	3.431770	-1.572230
C	-3.959650	1.025310	-2.475610
H	-4.888110	0.548010	-2.124900
H	-3.473990	0.333230	-3.180370
H	-4.238900	1.938030	-3.019110
H	1.064840	-2.154430	0.788710

Zero-point correction= 0.602261 (Hartree/Particle)
Thermal correction to Energy= 0.634146
Thermal correction to Enthalpy= 0.635090
Thermal correction to Gibbs Free Energy= 0.544456
SCF Done: E(RwB97XD) = -1465.79586759
Thermal correction to Gibbs free energy (ZPG) from GoodVibes: 0.530034

$TS_{14a+14a}$-IV=E

C	0.886260	-1.753710	-0.263590
C	1.533750	-0.578760	-0.110100
C	1.186460	0.553960	-0.952740
C	2.199590	1.585120	-1.186730
C	3.223900	1.703210	-0.316950
C	3.278470	0.948190	0.964870
C	2.676680	-0.470410	0.892140
C	3.743430	-1.511470	0.595370
C	4.007550	-2.488560	1.468440
H	3.467720	-2.567140	2.416510
H	4.771590	-3.244200	1.265810
C	4.473990	-1.380310	-0.712090
H	5.033790	-0.432390	-0.759600
H	3.764640	-1.366210	-1.554550
H	5.181650	-2.206560	-0.864900
H	2.254640	-0.711570	1.878950
H	4.306770	0.894510	1.352750
H	2.710600	1.542500	1.702700
H	4.001050	2.448350	-0.508820
C	2.104940	2.498470	-2.379070
H	3.089750	2.925660	-2.611990
H	1.737450	1.980630	-3.277950
H	1.432760	3.342350	-2.164870
C	-0.063490	0.510620	-1.630250
C	-0.608960	-0.813080	-2.034000
O	-1.537780	-0.938130	-2.804420
C	0.087510	-2.057420	-1.493690
C	1.058990	-2.521230	-2.604740
H	1.773420	-1.729280	-2.873850
H	0.482390	-2.796990	-3.500770
H	1.615910	-3.399480	-2.249410
O	-0.844030	-3.074590	-1.236950
H	-1.496210	-3.037790	-1.948630
H	-0.242710	1.254990	-2.407230
C	-1.596360	1.037560	-0.476090
C	-1.311660	2.510750	-0.197380
C	-1.308940	3.420360	-1.413550
H	-1.119940	4.454140	-1.090400
H	-2.291990	3.365770	-1.901890
H	-0.534230	3.174020	-2.145590
C	-0.050840	2.637430	0.679430
O	0.654270	3.632970	0.640200
C	0.123240	1.569890	1.648550
C	-0.701470	0.463110	1.711610
C	-0.597250	-0.513310	2.822740
C	-1.251970	-1.686060	2.733520
C	-2.174540	-2.040990	1.605280
C	-2.753290	-0.766330	0.993930
C	-3.862320	-0.938720	-0.036270
C	-4.781420	0.027370	-0.148700
H	-5.603330	-0.048940	-0.865950
H	-4.721600	0.940330	0.451540
C	-3.925850	-2.166240	-0.905240
H	-3.262230	-2.045930	-1.773760
H	-4.944870	-2.312830	-1.289410

H	-3.622880	-3.077250	-0.370110
C	-1.639940	0.214600	0.666770
H	-3.247740	-0.248500	1.839290
H	-2.989210	-2.678160	1.984640
H	-1.636290	-2.628940	0.839490
H	-1.111350	-2.428830	3.525570
C	0.274090	-0.183540	4.004210
H	1.327390	-0.037970	3.715270
H	-0.053730	0.749470	4.489340
H	0.240930	-0.987320	4.752040
H	0.863940	1.760620	2.424570
O	-2.401880	2.903320	0.642010
H	-2.264040	3.828330	0.874410
H	-2.406630	0.885970	-1.196740
H	1.144500	-2.613000	0.362630

Zero-point correction= 0.595962 (Hartree/Particle)
Thermal correction to Energy= 0.629016
Thermal correction to Enthalpy= 0.629960
Thermal correction to Gibbs Free Energy= 0.535428
SCF Done: E(RwB97XD) = -1465.71818185
Thermal correction to Gibbs free energy (ZPG) from GoodVibes: 0.520844

17-IV

C	-0.032800	-1.146580	-0.151120
C	1.310500	-0.463410	-0.072010
C	1.426750	0.635590	-0.837700
C	2.648250	1.463010	-0.840210
C	3.535820	1.264630	0.147750
C	3.287100	0.285370	1.264060
C	2.405880	-0.914670	0.867570
C	3.177860	-2.089300	0.285240
C	2.971400	-3.327790	0.745220
H	2.270200	-3.522280	1.562220
H	3.494690	-4.189730	0.321750
C	4.154940	-1.799150	-0.821120
H	5.012390	-1.219370	-0.443530
H	3.694040	-1.183710	-1.609290
H	4.538320	-2.724960	-1.272090
H	1.912240	-1.289210	1.776890
H	4.237470	-0.075030	1.687640
H	2.782760	0.836020	2.079610
H	4.443380	1.873880	0.191280
C	2.834670	2.498020	-1.911930
H	3.836760	2.944560	-1.859720
H	2.698100	2.070770	-2.918300
H	2.103520	3.315010	-1.800160
C	0.166690	0.959660	-1.606030
C	-0.222820	-0.239120	-2.437300
O	-0.584660	-0.203520	-3.587920
C	-0.264300	-1.538650	-1.624840
C	0.779050	-2.524430	-2.153600
H	1.798200	-2.122890	-2.124340
H	0.530970	-2.764680	-3.197720
H	0.744830	-3.446200	-1.556250
O	-1.538270	-2.108300	-1.777150
H	-1.822390	-1.937200	-2.684640
H	0.247480	1.826550	-2.267150
C	-1.049150	1.108480	-0.627960
C	-1.115140	2.502360	0.015120
C	-1.023840	3.644810	-0.984970
H	-1.239960	4.596620	-0.478580
H	-1.753140	3.496860	-1.794520
H	-0.019420	3.744830	-1.413090
C	-0.042820	2.623830	1.109820
O	0.651220	3.611070	1.232680
C	-0.034080	1.509980	2.062170
C	-0.570580	0.305520	1.781750
C	-0.631000	-0.745910	2.821700
C	-1.482440	-1.774420	2.668240
C	-2.433450	-1.904970	1.523430
C	-2.552210	-0.621380	0.697140
C	-3.630650	-0.727380	-0.389740
C	-4.192260	0.374020	-0.907770
H	-4.999430	0.293700	-1.641560
H	-3.893510	1.376370	-0.595530
C	-4.216270	-2.079250	-0.724150
H	-4.866540	-2.007950	-1.607480
H	-4.841620	-2.441360	0.108730
H	-3.447380	-2.834780	-0.916990
C	-1.089210	-0.080270	0.387210
H	-2.938550	0.155050	1.376080
H	-3.421630	-2.182040	1.924190
H	-2.131350	-2.751830	0.882270
H	-1.516820	-2.553420	3.437200
C	0.224920	-0.608680	4.052390
H	1.280610	-0.425870	3.796620
H	-0.105400	0.237050	4.676260
H	0.171650	-1.516710	4.668060
H	0.416710	1.726150	3.032550
O	-2.378010	2.546930	0.672060
H	-2.471400	3.404090	1.100100
H	-1.949150	1.037070	-1.252530
H	-0.043910	-2.054270	0.464530

Zero-point correction= 0.601817 (Hartree/Particle)
Thermal correction to Energy= 0.633798
Thermal correction to Enthalpy= 0.634742
Thermal correction to Gibbs Free Energy= 0.543543
SCF Done: E(RwB97XD) = -1465.79058087
Thermal correction to Gibbs free energy (ZPG) from GoodVibes: 0.529322

$TS_{14a+14a}$-V

C	2.632000	2.557530	0.333440
C	1.494320	2.506600	1.051900
C	0.816440	1.205880	1.264250
C	-0.419980	1.132020	1.849570
C	-1.001880	-0.128420	2.292280
O	-2.006500	-0.181960	2.982080
C	-0.181850	-1.392230	2.005660
C	-1.024180	-2.656570	1.998680
H	-1.847190	-2.616040	1.278350
H	-0.382270	-3.524630	1.789580
H	-1.488710	-2.784260	2.986990
C	0.722870	-1.183870	0.799090
C	-0.723030	-1.184070	-0.799000
C	-1.455550	0.002470	-0.780000
C	-0.816420	1.205560	-1.264470
C	-1.494170	2.506380	-1.052390
C	-2.631830	2.557570	-0.333920
C	-3.329100	1.354990	0.227440
C	-2.957180	0.108700	-0.572220
C	-3.683170	-1.174880	-0.221900
C	-4.154820	-1.445210	0.998210
H	-4.698470	-2.375140	1.189070
H	-3.991000	-0.782390	1.849430
C	-3.916740	-2.096510	-1.394140
H	-4.700700	-1.677780	-2.047960
H	-3.014890	-2.196440	-2.018320
H	-4.243290	-3.095160	-1.071460
H	-3.290600	0.336670	-1.606690
H	-4.419320	1.503150	0.182840
H	-3.082700	1.237150	1.296920
H	-3.084430	3.535670	-0.139620
C	-0.859390	3.747740	-1.616340
H	0.153870	3.901140	-1.212230
H	-0.763200	3.682080	-2.711720
H	-1.458400	4.637310	-1.378790
C	0.420130	1.131520	-1.849590
C	1.001910	-0.129000	-2.292210
O	2.006530	-0.182690	-2.982000
C	0.181780	-1.392700	-2.005470
C	1.023980	-2.657130	-1.998180
H	0.381800	-3.525130	-1.789630
H	1.846470	-2.616790	-1.277240
H	1.489170	-2.784710	-2.986190
O	-0.757280	-1.481730	-3.087170
H	-0.249380	-1.626070	-3.893920

H	0.956600	2.027680	-2.161840
C	1.455440	0.002640	0.779810
C	2.957120	0.108660	0.572180
C	3.683050	-1.175030	0.222150
C	4.155020	-1.445500	-0.997810
H	4.698630	-2.375500	-1.188440
H	3.991510	-0.782720	-1.849120
C	3.916260	-2.096610	1.394510
H	4.700310	-1.678050	2.048330
H	3.014350	-2.196210	2.018660
H	4.242520	-3.095380	1.071950
C	3.329270	1.354810	-0.227600
H	4.419480	1.502910	-0.182810
H	3.083090	1.236810	-1.297120
H	3.290450	0.336740	1.606660
H	-1.259320	-2.092980	-0.521490
H	1.259170	-2.092810	0.521720
O	0.757310	-1.481130	3.087300
H	0.249490	-1.625470	3.894090
H	-0.956380	2.028240	2.161780
C	0.859660	3.748140	1.615600
H	-0.153570	3.901590	1.211430
H	1.458800	4.637590	1.377900
H	0.763440	3.682690	2.710990
H	3.084670	3.535570	0.138960

Zero-point correction= 0.596913 (Hartree/Particle)
Thermal correction to Energy= 0.629399
Thermal correction to Enthalpy= 0.630343
Thermal correction to Gibbs Free Energy= 0.539189
SCF Done: E(RwB97XD) = -1465.72130478
Thermal correction to Gibbs free energy (ZPG) from GoodVibes: 0.524156

17-V

C	3.022680	2.384380	-0.035380
C	1.812790	2.639370	0.491810
C	0.966150	1.509480	0.933890
C	-0.001230	1.698040	1.852000
C	-0.763650	0.599110	2.444690
O	-1.733940	0.784410	3.151810
C	-0.154250	-0.797710	2.247860
C	-1.099660	-1.885360	2.732120
H	-2.086010	-1.808690	2.257670
H	-0.666420	-2.876930	2.533630
H	-1.262520	-1.777140	3.814160
C	0.321750	-0.993000	0.801070
C	-0.823150	-1.305730	-0.210150
C	-1.465920	-0.031960	-0.701140
C	-0.597100	0.835600	-1.254670
C	-1.024760	2.155630	-1.743990
C	-2.214430	2.611640	-1.307200
C	-3.084310	1.791150	-0.388490
C	-2.943440	0.301970	-0.709660
C	-3.811840	-0.643820	0.098230
C	-4.190560	-0.398330	1.355870
H	-4.815370	-1.112890	1.899500
H	-3.881800	0.496090	1.900030
C	-4.236370	-1.885000	-0.642290
H	-4.967960	-1.622040	-1.425250
H	-3.384790	-2.347510	-1.165790
H	-4.700310	-2.625120	0.024940
H	-3.251760	0.177090	-1.767630
H	-4.138230	2.092790	-0.475750
H	-2.786310	1.985100	0.660700
H	-2.552260	3.611870	-1.595460
C	-0.117570	2.938760	-2.649810
H	0.825530	3.200650	-2.142620
H	0.151780	2.350890	-3.541980
H	-0.595840	3.870690	-2.981040
C	0.841040	0.355090	-1.242090
C	0.752620	-0.931760	-2.047720
O	1.230730	-1.073350	-3.148270
C	-0.211170	-1.978590	-1.457130
C	0.460330	-3.327670	-1.215140
H	-0.299020	-4.036910	-0.855010
H	1.293480	-3.289210	-0.504760
H	0.862050	-3.697480	-2.170300
O	-1.256280	-2.165690	-2.391280
H	-0.846420	-2.223250	-3.263280
H	1.514380	1.040820	-1.761820
C	1.237140	0.159410	0.268780
C	2.771990	-0.084000	0.482540
C	3.301270	-1.476070	0.165920
C	3.622780	-1.872920	-1.070070
H	4.009780	-2.879670	-1.250820
H	3.504460	-1.235150	-1.947840
C	3.523700	-2.370370	1.358030
H	4.350570	-1.969820	1.969270
H	2.645590	-2.389590	2.020720
H	3.785730	-3.395630	1.060600
C	3.584520	1.010890	-0.219910
H	4.622520	0.981280	0.150410
H	3.666770	0.805700	-1.301760
H	2.907850	0.054930	1.566300
H	-1.547650	-1.993150	0.239210
H	0.935070	-1.899060	0.854220
O	1.044700	-0.822980	3.022560
H	0.808900	-0.715910	3.949870
H	-0.233650	2.690030	2.243140
C	1.303760	4.042500	0.678050
H	0.297970	4.152610	0.241970
H	1.975140	4.768920	0.200310
H	1.229140	4.308050	1.744420
H	3.649280	3.223950	-0.354520

Zero-point correction= 0.601842 (Hartree/Particle)
Thermal correction to Energy= 0.633823
Thermal correction to Enthalpy= 0.634767
Thermal correction to Gibbs Free Energy= 0.544131
SCF Done: E(RwB97XD) = -1465.80221712
Thermal correction to Gibbs free energy (ZPG) from GoodVibes: 0.529599

$TS_{14a+14a}$-VI

C	-0.493800	2.603260	2.187900
C	-1.623950	2.525700	1.459450
C	-1.981580	1.253730	0.782460
C	-3.080290	1.164500	-0.024010
C	-3.534020	-0.103780	-0.574020
O	-4.576930	-0.220790	-1.188840
C	-2.732550	-1.369460	-0.194220
C	-2.925210	-2.453790	-1.244440
H	-2.645360	-2.103520	-2.245400
H	-2.351040	-3.352830	-0.974760
H	-3.991610	-2.713200	-1.288840
C	-1.279800	-1.063980	0.220590
C	-0.232680	-1.101610	-1.344180
C	1.147840	-1.202460	-1.029270
C	1.867130	-0.011650	-0.728720
C	3.368560	-0.129460	-0.493550
C	4.026600	1.152880	-0.014490
C	4.216710	1.443240	1.275880
H	3.927380	0.761610	2.078760
H	4.687100	2.382430	1.579090
C	4.470620	2.080360	-1.115590
H	5.325190	1.637990	-1.654730
H	3.670610	2.222060	-1.859830
H	4.779240	3.062590	-0.731470
C	3.784570	-1.405290	0.235790
C	2.985630	-2.588390	-0.214100
C	1.775800	-2.508920	-0.808360
C	1.022170	-3.754830	-1.192970
H	1.625600	-4.652630	-1.004580
H	0.087840	-3.855570	-0.617470
H	0.746870	-3.746890	-2.259520
H	3.407570	-3.578290	-0.013750
H	4.856330	-1.583080	0.052890
H	3.690670	-1.305740	1.328180
H	3.720590	-0.272740	-1.534230

C	1.233540	1.198530	-0.850440
H	1.737020	2.112220	-0.524390
C	-1.119650	0.105010	1.005040
C	-0.389770	0.138450	2.333880
C	0.306740	-1.136130	2.753180
C	1.635170	-1.242940	2.797220
H	2.126010	-2.159510	3.135240
H	2.273300	-0.408850	2.507980
C	-0.599850	-2.235020	3.250000
H	-1.514290	-2.327150	2.645590
H	-0.085200	-3.205860	3.278560
H	-0.929370	-1.996850	4.275710
C	0.398810	1.436340	2.478520
H	0.802570	1.523580	3.499850
H	1.262870	1.444270	1.789150
H	-1.226980	0.239970	3.057730
C	0.194930	1.374020	-1.924810
C	-0.580490	2.677230	-1.854090
H	-1.389640	2.673850	-2.598760
H	0.116510	3.497410	-2.078340
H	-1.012100	2.845800	-0.865270
O	0.967590	1.365410	-3.140230
H	0.335290	1.439040	-3.866940
C	-0.675290	0.122380	-2.079790
O	-1.594100	0.106990	-2.868980
H	-0.665850	-1.999520	-1.779750
H	-0.838940	-1.960880	0.663340
O	-3.299380	-1.809130	1.044250
H	-4.239040	-1.959530	0.888810
H	-3.719080	2.021630	-0.237720
C	-2.524370	3.717930	1.282870
H	-2.628450	4.001920	0.223340
H	-3.538030	3.504750	1.656830
H	-2.134630	4.587420	1.828920
H	-0.215510	3.569320	2.621600

Zero-point correction= 0.596844 (Hartree/Particle)
Thermal correction to Energy= 0.629644
Thermal correction to Enthalpy= 0.630588
Thermal correction to Gibbs Free Energy= 0.537034
SCF Done: E(RwB97XD) = -1465.69479802
Thermal correction to Gibbs free energy (ZPG) from GoodVibes: 0.522440

17-VI

C	0.688760	-3.388870	0.540880
C	1.676090	-2.822440	-0.176380
C	1.912940	-1.362350	-0.063520
C	3.114540	-0.836900	-0.372600
C	3.434200	0.583530	-0.225870
O	4.415680	1.087880	-0.729850
C	2.541780	1.353460	0.758630
C	2.812880	2.847600	0.671850
H	2.663380	3.225800	-0.348190
H	2.161890	3.394460	1.369750
H	3.862270	3.046170	0.931160
C	1.051300	0.990680	0.622010
C	0.269670	1.832560	-0.415090
C	-1.208850	1.590060	-0.195250
C	-1.578290	0.300310	-0.320660
C	-3.058320	-0.026340	-0.465170
C	-3.446510	-1.495840	-0.421770
C	-4.049100	-2.073600	0.623710
H	-4.303960	-1.527230	1.533620
H	-4.335710	-3.128470	0.592520
C	-3.229700	-2.262410	-1.703700
H	-4.032230	-2.003700	-2.415330
H	-2.293010	-1.986390	-2.205030
H	-3.257880	-3.349210	-1.542050
C	-3.882430	0.895650	0.435800
C	-3.457410	2.331200	0.283370
C	-2.189490	2.671810	-0.009980
C	-1.740640	4.101700	-0.128930
H	-2.586850	4.792140	-0.011190
H	-0.991450	4.352970	0.639990
H	-1.273910	4.296520	-1.108070
H	-4.199090	3.113280	0.471810
H	-4.948400	0.779850	0.188800
H	-3.780010	0.610640	1.498300
H	-3.267320	0.292930	-1.506110
C	-0.426300	-0.618750	-0.672180
H	-0.744260	-1.659220	-0.782960
C	0.728250	-0.526230	0.418860
C	0.381880	-1.240130	1.787770
C	-0.414530	-0.487700	2.845770
C	-1.748090	-0.475140	2.869870
H	-2.296040	0.040590	3.663620
H	-2.334440	-0.984430	2.108340
C	0.390970	0.133360	3.957720
H	1.205680	0.763680	3.574580
H	-0.242340	0.721480	4.636660
H	0.877320	-0.662700	4.548000
C	-0.168060	-2.640540	1.511300
H	-0.225240	-3.204130	2.456990
H	-1.207720	-2.595940	1.140210
H	1.376910	-1.381900	2.241090
C	0.036430	-0.089150	-2.073590
C	0.996820	-0.930230	-2.907760
H	2.018280	-0.952250	-2.525010
H	1.043770	-0.492910	-3.916310
H	0.611800	-1.957290	-2.986940
O	-1.156170	0.037100	-2.843940
H	-0.927490	0.510120	-3.651570
C	0.560410	1.341870	-1.823880
O	1.072120	2.002620	-2.694140
H	0.532670	2.890100	-0.344210
H	0.616410	1.294140	1.582050
O	2.910440	0.861710	2.046980
H	3.841300	1.060830	2.193300
H	3.922040	-1.454220	-0.771130
C	2.591610	-3.646620	-1.041280
H	2.223830	-4.678210	-1.124560
H	2.680580	-3.228420	-2.055270
H	3.607800	-3.689940	-0.617950
H	0.519980	-4.466900	0.448950

Zero-point correction= 0.601899 (Hartree/Particle)
Thermal correction to Energy= 0.634091
Thermal correction to Enthalpy= 0.635035
Thermal correction to Gibbs Free Energy= 0.543179
SCF Done: E(RwB97XD) = -1465.77871095
Thermal correction to Gibbs free energy (ZPG) from GoodVibes: 0.528838

$TS_{14a+14a}$-VII

C	-1.116360	-1.149520	-0.702680
C	-1.950140	-0.037290	-0.547140
C	-1.554260	1.194540	-1.148470
C	-2.332880	2.423370	-0.853790
C	-3.155990	2.437010	0.209030
C	-3.352420	1.243480	1.097570
C	-3.210910	-0.051790	0.296370
C	-3.388090	-1.332510	1.091670
C	-2.962570	-1.472860	2.350490
H	-3.085030	-2.418540	2.884440
H	-2.474940	-0.661520	2.896880
C	-4.079880	-2.443680	0.348560
H	-4.025220	-3.398460	0.888860
H	-5.142360	-2.190550	0.195240
H	-3.641920	-2.578510	-0.653550
H	-4.030580	-0.026470	-0.449900
H	-4.342200	1.274650	1.576040
H	-2.616510	1.274320	1.922050
H	-3.698200	3.355550	0.453890
C	-2.152090	3.626680	-1.737330
H	-1.134980	4.043740	-1.661890
H	-2.310340	3.365080	-2.795000
H	-2.857430	4.423640	-1.465700
C	-0.377760	1.251420	-1.871990
C	0.296110	0.059230	-2.370550

O	1.288650	0.092320	-3.075080
C	-0.439580	-1.253690	-2.066370
C	0.416270	-2.477320	-2.324150
H	1.380210	-2.444690	-1.816450
H	0.646120	-2.525730	-3.398650
H	-0.121840	-3.385530	-2.025140
O	-1.553880	-1.293240	-2.970490
H	-1.190900	-1.397560	-3.856850
H	0.026130	2.196520	-2.237600
C	1.025890	0.325430	0.475520
C	2.351900	0.240130	-0.111860
C	2.973670	-0.968860	-0.264070
C	2.357190	-2.204620	0.175350
O	2.821990	-3.315640	-0.033140
C	1.048320	-2.126360	0.969630
C	1.457840	-2.124820	2.461400
H	2.072430	-1.253320	2.725430
H	2.027340	-3.042700	2.667280
H	0.549670	-2.121230	3.080420
O	0.291790	-3.273020	0.709670
H	0.947020	-3.935960	0.435150
C	0.278490	-0.831880	0.742760
H	-0.495780	-0.711020	1.502880
H	3.939980	-1.067540	-0.757560
C	3.000760	1.495360	-0.548440
C	2.434000	2.679700	-0.259770
C	1.147020	2.871900	0.474490
C	0.601380	1.609790	1.152220
C	0.987990	1.541100	2.628660
C	0.051610	1.421080	3.575250
H	0.313900	1.355990	4.634670
H	-1.012530	1.390100	3.325350
C	2.453210	1.604170	2.965330
H	2.894740	2.559990	2.641160
H	3.018570	0.813200	2.447130
H	2.619580	1.498730	4.046010
H	-0.498380	1.643090	1.122430
H	1.256290	3.680240	1.216600
H	0.397970	3.247450	-0.242460
H	2.928320	3.590310	-0.614690
C	4.274330	1.405710	-1.340100
H	5.074790	0.907260	-0.771090
H	4.106160	0.826950	-2.261340
H	4.631490	2.405310	-1.621530
H	-1.438430	-2.105540	-0.285760

Zero-point correction= 0.597565 (Hartree/Particle)
Thermal correction to Energy= 0.630003
Thermal correction to Enthalpy= 0.630947
Thermal correction to Gibbs Free Energy= 0.538694
SCF Done: E(RwB97XD) = -1465.72826770
Thermal correction to Gibbs free energy (ZPG) from GoodVibes: 0.524057

17-VII

C	-1.148750	-1.040830	-0.315370
C	-1.918480	0.248940	-0.157160
C	-1.259620	1.341760	-0.585550
C	-1.907350	2.664020	-0.628800
C	-3.010330	2.834780	0.122400
C	-3.540680	1.722470	0.990010
C	-3.344950	0.357700	0.321920
C	-3.767300	-0.838010	1.161090
C	-3.466880	-0.952700	2.457920
H	-3.753230	-1.840080	3.028420
H	-2.922820	-0.174000	2.999190
C	-4.504970	-1.906410	0.403300
H	-5.487010	-1.527930	0.072970
H	-3.953170	-2.174770	-0.512580
H	-4.663470	-2.811380	1.005810
H	-3.959270	0.348950	-0.600140
H	-4.605190	1.875660	1.219240
H	-3.009230	1.741960	1.961880
H	-3.521580	3.801900	0.132630
C	-1.348450	3.732380	-1.526310
H	-0.343730	4.056120	-1.210150
H	-1.249110	3.364030	-2.559970
H	-1.996460	4.619320	-1.536350
C	0.138860	1.043290	-1.074460
C	-0.047580	0.060580	-2.219810
O	0.340570	0.254760	-3.345810
C	-0.892050	-1.169190	-1.834460
C	-0.264940	-2.453940	-2.352610
H	0.771820	-2.601130	-2.042420
H	-0.257420	-2.410680	-3.452590
H	-0.859480	-3.315160	-2.023270
O	-2.170870	-1.029780	-2.442140
H	-2.031800	-0.951750	-3.392330
H	0.661890	1.916330	-1.473290
C	0.952740	0.373720	0.112160
C	2.349730	0.085810	-0.407540
C	2.824830	-1.165470	-0.595880
C	2.100760	-2.364510	-0.189560
O	2.443890	-3.487190	-0.516340
C	0.918200	-2.209060	0.764760
C	1.521970	-2.305880	2.177210
H	2.265900	-1.528100	2.379180
H	2.001620	-3.289160	2.286880
H	0.714270	-2.218930	2.917210
O	0.060110	-3.304340	0.584340
H	0.627340	-4.007820	0.230980
C	0.127050	-0.886330	0.563120
H	-0.279390	-0.653100	1.556240
H	3.798230	-1.345840	-1.054130
C	3.180480	1.263690	-0.744580
C	2.889470	2.459010	-0.200640
C	1.743670	2.723020	0.723390
C	1.042660	1.456960	1.244240
C	1.643290	1.000160	2.562140
C	0.843480	0.792660	3.614400
H	1.241530	0.476800	4.582690
H	-0.239810	0.927010	3.543050
C	3.138980	0.857970	2.682250
H	3.420840	0.493050	3.679490
H	3.642690	1.824070	2.519680
H	3.550520	0.167310	1.931170
H	0.000390	1.722620	1.466200
H	2.083470	3.336860	1.573480
H	1.013770	3.363370	0.199790
H	3.522600	3.315940	-0.454070
C	4.359960	1.081160	-1.659850
H	5.131570	0.440100	-1.204740
H	4.052940	0.607220	-2.604780
H	4.825500	2.047900	-1.893360
H	-1.706990	-1.910770	0.041330

Zero-point correction= 0.601742 (Hartree/Particle)
Thermal correction to Energy= 0.633771
Thermal correction to Enthalpy= 0.634715
Thermal correction to Gibbs Free Energy= 0.542683
SCF Done: E(RwB97XD) = -1465.79866459
Thermal correction to Gibbs free energy (ZPG) from GoodVibes: 0.528752

$TS_{14a+14a}$-VIII=A

C	-1.215820	0.988770	1.769530
C	-1.813080	0.325480	0.754900
C	-1.526830	-1.095100	0.569660
C	-2.485220	-1.925600	-0.147390
C	-3.267190	-1.334510	-1.078700
C	-3.167500	0.122120	-1.362010
C	-2.951880	0.916410	-0.062130
C	-2.932340	2.410740	-0.332010
C	-1.812970	3.109320	-0.536980
H	-1.851620	4.176020	-0.775140
H	-0.826500	2.650290	-0.460900
C	-4.293300	3.050120	-0.403910
H	-4.793890	2.998520	0.577300
H	-4.234640	4.104520	-0.706430
H	-4.946460	2.524050	-1.119080

H	-3.847610	0.719340	0.557830
H	-4.061830	0.482810	-1.889060
H	-2.306680	0.301210	-2.035320
H	-3.967910	-1.941950	-1.657430
C	-2.591810	-3.392490	0.169180
H	-1.646070	-3.918180	-0.014200
H	-3.373490	-3.863750	-0.441940
H	-2.848980	-3.537640	1.230460
C	-0.352700	-1.624890	1.140580
C	0.196980	-1.004890	2.378970
O	1.075340	-1.531980	3.026920
C	-0.501090	0.264200	2.881620
C	0.417100	1.149230	3.708760
H	-0.180400	1.946120	4.173430
H	1.208960	1.608710	3.105500
H	0.902990	0.552410	4.493680
O	-1.551750	-0.240690	3.716750
H	-1.130980	-0.680200	4.465680
C	1.215720	-1.324270	-0.028360
C	0.893490	-2.117260	-1.281000
C	2.212760	-2.300790	-2.066200
H	2.675830	-1.343480	-2.339260
H	1.995210	-2.870970	-2.980740
H	2.917710	-2.877830	-1.451100
C	-0.081230	-1.341890	-2.172710
O	-0.880220	-1.983860	-2.848910
C	0.090850	0.081280	-2.207450
C	0.951360	0.732610	-1.329980
C	1.329070	2.146700	-1.577180
C	1.996020	2.828470	-0.632750
C	2.315430	2.256080	0.711610
C	2.495410	0.732400	0.706910
C	3.911680	0.289670	0.353890
C	4.568520	-0.546650	1.164960
H	5.573440	-0.903470	0.922270
H	4.119740	-0.908620	2.094750
C	4.511990	0.794230	-0.929470
H	3.853270	0.583510	-1.786640
H	5.490900	0.333190	-1.119860
H	4.645740	1.887710	-0.904260
C	1.496330	0.048950	-0.209210
H	2.322210	0.367130	1.728750
H	3.205600	2.738920	1.143730
H	1.473620	2.516040	1.379920
H	2.272050	3.870510	-0.822560
C	0.950320	2.779770	-2.886400
H	1.363340	3.794590	-2.963810
H	1.317550	2.189900	-3.740750
H	-0.144660	2.854290	-2.987780
H	-0.399990	0.615540	-3.020860
O	0.354170	-3.378330	-1.026790
H	-0.314220	-3.480420	-1.730240
H	1.895500	-1.847930	0.654770
H	-0.237550	-2.710000	1.126320
H	-1.460820	2.038840	1.948680

Zero-point correction= 0.597243 (Hartree/Particle)
Thermal correction to Energy= 0.629744
Thermal correction to Enthalpy= 0.630688
Thermal correction to Gibbs Free Energy= 0.538013
SCF Done: E(RwB97XD) = -1465.73546166
Thermal correction to Gibbs free energy (ZPG) from GoodVibes: 0.523481

17-VIII

C	-0.114100	0.755330	1.011870
C	-1.426340	0.486730	0.302080
C	-1.793460	-0.809840	0.297660
C	-3.070970	-1.258520	-0.275640
C	-3.700860	-0.409680	-1.107560
C	-3.121310	0.941230	-1.429970
C	-2.401780	1.525680	-0.213590
C	-1.821930	2.913640	-0.400390
C	-1.448750	3.394220	-1.589700
H	-1.047520	4.406760	-1.688630
H	-1.540260	2.805350	-2.505280
C	-1.765800	3.753320	0.850040
H	-1.444420	3.163030	1.721010
H	-1.107200	4.625670	0.733810
H	-2.778540	4.118140	1.091730
H	-3.156820	1.614530	0.594500
H	-3.905450	1.635540	-1.765620
H	-2.416220	0.822260	-2.275690
H	-4.624430	-0.717770	-1.605980
C	-3.587280	-2.628480	0.058160
H	-2.887890	-3.403110	-0.291450
H	-4.566750	-2.806080	-0.406610
H	-3.693870	-2.758510	1.147330
C	-0.783210	-1.721900	0.950720
C	-0.605250	-1.235880	2.377090
O	-0.694010	-1.932120	3.358670
C	-0.373830	0.286580	2.475710
C	0.607010	0.651650	3.586160
H	0.686760	1.745550	3.657170
H	1.607170	0.219390	3.490100
H	0.195270	0.270200	4.532720
O	-1.614350	0.887070	2.839960
H	-1.899320	0.489330	3.669980
C	0.548910	-1.560120	0.174690
C	0.376540	-2.155760	-1.253500
C	1.706510	-2.680790	-1.813700
H	2.479580	-1.906960	-1.869970
H	1.536310	-3.090230	-2.820130
H	2.067770	-3.490170	-1.163720
C	-0.142380	-1.094840	-2.226290
O	-1.001340	-1.398820	-3.033080
C	0.529330	0.202010	-2.202800
C	1.155370	0.655190	-1.097310
C	1.892900	1.937680	-1.119170
C	2.629910	2.313510	-0.059290
C	2.811100	1.492790	1.176380
C	2.404650	0.027170	0.979990
C	3.538100	-0.788680	0.364530
C	3.923240	-1.923820	0.960360
H	4.741430	-2.529260	0.560930
H	3.436440	-2.292000	1.868300
C	4.270860	-0.287050	-0.853930
H	3.599090	-0.116610	-1.707770
H	5.044280	-1.004160	-1.161290
H	4.761100	0.678360	-0.652570
C	1.027860	-0.062600	0.244240
H	2.257140	-0.425990	1.964490
H	3.861870	1.546510	1.505790
H	2.232520	1.944310	1.998760
H	3.162840	3.268790	-0.103560
C	1.875080	2.763710	-2.375100
H	2.420460	3.705600	-2.229170
H	2.354880	2.222440	-3.206800
H	0.849580	3.006430	-2.685370
H	0.489730	0.779720	-3.127250
O	-0.540880	-3.212740	-1.247380
H	-1.116680	-3.039210	-2.012910
H	1.304540	-2.178590	0.677950
H	-1.076570	-2.773130	0.967100
H	0.136990	1.821780	1.002310

Zero-point correction= 0.602885 (Hartree/Particle)
Thermal correction to Energy= 0.634196
Thermal correction to Enthalpy= 0.635140
Thermal correction to Gibbs Free Energy= 0.546129
SCF Done: E(RwB97XD) = -1465.79743470
Thermal correction to Gibbs free energy (ZPG) from GoodVibes: 0.531985

17-A

C	-3.265840	1.093520	-1.443710
C	-3.101620	-0.303300	-1.972280
C	-2.146170	-1.139190	-1.541540
C	-2.106130	-2.576510	-1.964670
H	-1.115230	-2.869770	-2.336340

H	-2.854720	-2.769140	-2.745000
H	-2.340790	-3.214980	-1.097060
C	-1.140240	-0.587710	-0.502600
C	-2.090780	0.013730	0.530190
C	-2.341100	-0.582900	1.701300
C	-1.682020	-1.852400	2.158170
C	-0.260740	-1.835430	1.605400
O	0.701600	-2.019320	2.314280
C	-0.147090	-1.640810	0.104850
C	1.323770	-1.305150	-0.238440
C	1.605450	0.080400	0.287490
C	0.826000	1.030560	-0.264790
C	1.073780	2.467000	-0.033850
C	1.801520	2.798630	1.044120
C	2.276940	1.744530	2.007530
C	2.653680	0.413540	1.330680
C	4.073000	0.348490	0.772520
C	4.702420	1.408320	0.253430
H	5.720550	1.318830	-0.136400
H	4.229870	2.390840	0.192560
C	4.742530	-0.995840	0.867560
H	4.132960	-1.783870	0.399820
H	4.866240	-1.286010	1.923960
H	5.731150	-0.996700	0.387770
H	2.577400	-0.377270	2.093520
H	3.124480	2.111330	2.604520
H	1.457580	1.537290	2.722940
H	2.030590	3.848340	1.250770
C	0.563570	3.463550	-1.033320
H	-0.537250	3.469510	-1.060130
H	0.900010	4.479550	-0.784830
H	0.914790	3.221380	-2.049640
C	-0.222780	0.497570	-1.212340
C	0.513380	-0.245480	-2.310330
O	0.334510	-0.098050	-3.493920
C	1.507950	-1.289480	-1.769010
C	2.924740	-0.942360	-2.217910
H	3.277600	0.009170	-1.799380
H	2.941980	-0.865310	-3.315570
H	3.607590	-1.747160	-1.910870
O	1.153020	-2.556880	-2.285610
H	1.065610	-2.452260	-3.241440
H	-0.821130	1.286100	-1.668740
H	1.972650	-2.065350	0.211900
H	-0.375630	-2.628660	-0.318150
C	-1.697780	-1.993120	3.671480
H	-1.169300	-2.905100	3.986030
H	-1.194260	-1.141610	4.149090
H	-2.739110	-2.037030	4.021260
O	-2.377820	-2.934440	1.536020
H	-2.051900	-3.754650	1.923130
H	-3.133450	-0.185040	2.343870
C	-2.982580	1.160120	0.083000
C	-2.564850	2.539270	0.576840
C	-1.629950	2.725110	1.512440
H	-1.385840	3.728740	1.869620
H	-1.066960	1.894250	1.939780
C	-3.353480	3.691990	0.011920
H	-3.175570	3.821560	-1.067620
H	-4.436510	3.522450	0.134370
H	-3.095340	4.635520	0.511550
H	-3.958540	0.974730	0.564580
H	-3.821890	-0.658470	-2.714610
H	-4.288020	1.448300	-1.639050
H	-2.613460	1.790230	-1.996960

Zero-point correction= 0.600809 (Hartree/Particle)
Thermal correction to Energy= 0.632926
Thermal correction to Enthalpy= 0.633870
Thermal correction to Gibbs Free Energy= 0.542207
SCF Done: E(RwB97XD) = -1465.78180005
Thermal correction to Gibbs free energy (ZPG) from GoodVibes: 0.527862

$TS_{14a+14a}$-B

C	-1.172880	2.810600	-1.102080
C	-0.313180	2.119580	-2.111810
C	-0.125100	0.789000	-2.075740
C	0.659320	0.084400	-3.149230
H	0.010350	-0.606970	-3.711230
H	1.492880	-0.510810	-2.748630
H	1.072690	0.810340	-3.863070
C	-0.788300	-0.013210	-1.006810
C	-2.112010	0.499460	-0.560340
C	-3.087110	-0.341760	-0.190520
C	-2.989750	-1.836190	-0.147890
C	-1.624980	-2.363610	-0.626820
O	-1.503050	-3.552490	-0.834480
C	-0.530020	-1.413950	-0.957100
C	1.035730	-1.942810	0.300120
C	2.059440	-1.030220	-0.058300
C	1.804080	0.332140	0.173560
C	2.748590	1.412910	-0.317930
C	3.584050	1.903250	0.858400
C	3.375450	3.117160	1.378140
H	2.621550	3.793620	0.965150
H	3.951520	3.477860	2.234760
C	4.623580	0.965040	1.407310
H	5.412400	0.769360	0.663320
H	4.184010	-0.014250	1.654990
H	5.097400	1.374610	2.309770
C	3.606160	0.957920	-1.511460
C	3.948440	-0.502170	-1.505470
C	3.221770	-1.439510	-0.868670
C	3.550270	-2.903790	-0.968670
H	2.757160	-3.457770	-1.496730
H	4.488110	-3.061750	-1.517990
H	3.650660	-3.360690	0.028500
H	4.810840	-0.816330	-2.101900
H	4.523810	1.565610	-1.558390
H	3.065640	1.181380	-2.448660
H	2.123910	2.257270	-0.644210
C	0.634350	0.677650	0.840970
C	0.189430	-0.225650	1.955300
C	1.178710	-0.050350	3.133860
H	1.163760	0.997740	3.463200
H	2.205560	-0.323420	2.857060
H	0.852680	-0.696310	3.963300
O	-1.101300	0.078980	2.400300
H	-1.383930	-0.663690	2.949960
C	0.265480	-1.685400	1.525570
O	-0.290080	-2.539500	2.185330
H	0.402260	1.735170	0.987260
H	1.124620	-3.002090	0.051810
H	0.069080	-1.834820	-1.763670
C	-3.312540	-2.388250	1.243730
H	-2.633480	-1.998790	2.007970
H	-4.347220	-2.115000	1.494290
H	-3.217090	-3.484170	1.233500
O	-3.944550	-2.323450	-1.077670
H	-3.768580	-3.269520	-1.163840
H	-4.074460	0.058600	0.056580
C	-2.430580	1.974880	-0.799210
C	-3.288500	2.671050	0.247730
C	-3.159980	2.447410	1.558160
H	-3.763890	3.009080	2.277090
H	-2.467660	1.696910	1.947330
C	-4.255100	3.684060	-0.305690
H	-3.743250	4.420410	-0.947630
H	-5.013030	3.189950	-0.936560
H	-4.774910	4.231480	0.492600
H	-3.009330	1.980460	-1.741010
H	0.148350	2.707940	-2.910570
H	-1.470180	3.805660	-1.463520
H	-0.619490	2.986780	-0.163460

Zero-point correction= 0.596285 (Hartree/Particle)
Thermal correction to Energy= 0.629267
Thermal correction to Enthalpy= 0.630211
Thermal correction to Gibbs Free Energy= 0.535494

SCF Done: E(RwB97XD) = -1465.71116493
Thermal correction to Gibbs free energy (ZPG) from GoodVibes: 0.521010

17-B

C	1.009390	2.529790	1.958820
C	0.438190	1.372780	2.724640
C	0.282440	0.154480	2.189400
C	-0.189890	-1.003080	3.022750
H	0.632840	-1.720620	3.178490
H	-1.027320	-1.544930	2.557410
H	-0.514850	-0.653900	4.012750
C	0.709180	-0.045700	0.712950
C	2.087260	0.600460	0.701170
C	3.213940	-0.111610	0.621260
C	3.258050	-1.584830	0.327500
C	1.977320	-1.963720	-0.427010
O	1.988460	-2.628940	-1.434410
C	0.700170	-1.540370	0.266410
C	-0.552630	-1.880240	-0.583440
C	-1.782850	-1.240910	0.029830
C	-1.668500	0.092450	0.185550
C	-2.758760	0.931750	0.807130
C	-3.520920	1.698220	-0.263120
C	-3.381360	3.023580	-0.373950
H	-2.742830	3.588850	0.311410
H	-3.899420	3.590190	-1.152770
C	-4.399520	0.903930	-1.190540
H	-5.244540	0.454990	-0.644690
H	-3.842030	0.067570	-1.642140
H	-4.804970	1.531810	-1.996020
C	-3.648550	0.055960	1.712650
C	-3.898460	-1.331770	1.181820
C	-3.010180	-1.969390	0.400790
C	-3.210200	-3.366450	-0.112670
H	-2.454570	-4.056260	0.297270
H	-4.202080	-3.751640	0.160200
H	-3.111600	-3.401580	-1.209530
H	-4.818540	-1.841200	1.484190
H	-4.600680	0.573270	1.908340
H	-3.152210	-0.038120	2.696580
H	-2.263280	1.678870	1.445870
C	-0.334270	0.661460	-0.225730
C	-0.094870	0.324730	-1.719030
C	-0.861120	1.247100	-2.651070
H	-0.456490	2.265160	-2.560370
H	-1.931810	1.267980	-2.412360
H	-0.749650	0.896600	-3.687500
O	1.294760	0.395490	-1.998690
H	1.440460	-0.000560	-2.865490
C	-0.486580	-1.154590	-1.913770
O	-0.735770	-1.632400	-2.990070
H	-0.308310	1.748110	-0.100400
H	-0.638240	-2.957720	-0.753530
H	0.682560	-2.178170	1.159460
C	4.496360	-1.954200	-0.474630
H	4.532790	-1.388260	-1.415680
H	5.395270	-1.726270	0.116050
H	4.490440	-3.023050	-0.734830
O	3.229850	-2.282300	1.575440
H	3.438940	-3.206150	1.398130
H	4.179500	0.382470	0.768590
C	2.128420	2.099500	0.980550
C	2.246250	2.936420	-0.296210
C	1.399610	3.913290	-0.638010
H	1.567820	4.497130	-1.546620
H	0.519000	4.180660	-0.051810
C	3.446940	2.632270	-1.150270
H	3.359260	1.623200	-1.576350
H	3.542860	3.352610	-1.973890
H	4.373420	2.662470	-0.553510
H	3.085070	2.263270	1.504810
H	0.147810	1.540820	3.766100
H	1.400690	3.291360	2.648750
H	0.187190	3.028380	1.422350

Zero-point correction= 0.600626 (Hartree/Particle)
Thermal correction to Energy= 0.632955
Thermal correction to Enthalpy= 0.633899
Thermal correction to Gibbs Free Energy= 0.541293
SCF Done: E(RwB97XD) = -1465.78363232
Thermal correction to Gibbs free energy (ZPG) from GoodVibes: 0.526947

$TS_{14a+14a}$-C

C	-1.212400	-1.148010	0.155330
C	-2.167180	-0.128580	-0.047010
C	-1.885260	1.155260	0.455900
C	-2.789120	2.283180	0.116750
C	-3.777980	2.097970	-0.773430
C	-4.017880	0.819370	-1.518640
C	-3.417950	-0.429190	-0.847330
C	-4.414870	-1.147360	0.056130
C	-4.671900	-2.448130	-0.113960
H	-5.362850	-2.983120	0.543340
H	-4.198360	-3.025410	-0.913280
C	-5.057360	-0.337920	1.148910
H	-5.688600	-0.964670	1.793330
H	-5.684160	0.467170	0.732680
H	-4.296410	0.153380	1.775910
H	-3.139590	-1.145510	-1.637140
H	-5.097690	0.670030	-1.677850
H	-3.597300	0.934010	-2.534430
H	-4.427300	2.943700	-1.022210
C	-2.553410	3.617900	0.766020
H	-3.335700	4.336050	0.485700
H	-2.537030	3.533780	1.863980
H	-1.582780	4.041320	0.460670
C	-0.716940	1.368950	1.195690
C	0.028420	0.285300	1.768250
O	1.009350	0.399840	2.498710
C	-0.486520	-1.123830	1.481050
C	-1.479760	-1.507070	2.596980
H	-1.865120	-2.518960	2.408660
H	-2.323890	-0.807160	2.659330
H	-0.937220	-1.503640	3.553130
O	0.584770	-2.018880	1.496740
H	1.283770	-1.577070	2.008600
H	-0.400170	2.373780	1.476630
C	0.976030	0.270360	-0.994320
C	2.262750	0.228810	-0.280580
C	2.908490	-0.940610	-0.154060
C	2.424990	-2.220220	-0.771990
C	0.913660	-2.229750	-0.997860
O	0.353320	-3.287810	-1.185320
C	0.204500	-0.914010	-1.148070
H	-0.473000	-0.943240	-2.004650
C	3.073190	-2.357910	-2.169030
H	4.166440	-2.366540	-2.057100
H	2.753800	-3.310140	-2.617380
H	2.790160	-1.529100	-2.835790
O	2.788920	-3.306870	0.030940
H	2.077370	-3.955130	-0.065600
H	3.896390	-0.986120	0.312110
C	2.824550	1.564920	0.176510
C	4.141530	1.458290	0.926920
C	5.329420	1.663300	0.348020
H	6.254170	1.573450	0.924310
H	5.437460	1.924180	-0.706890
C	4.031180	1.107490	2.385610
H	3.464610	1.882420	2.925310
H	3.459200	0.179570	2.527950
H	5.020760	1.000670	2.850950
C	2.850910	2.514210	-1.024350
C	1.572240	2.492900	-1.798000
C	0.681790	1.477840	-1.778710
C	-0.528470	1.502950	-2.673190
H	-0.423880	0.779290	-3.498380
H	-1.443650	1.251180	-2.127280
H	-0.666070	2.498750	-3.115250

H	1.379000	3.341370	-2.462240
H	3.665630	2.234300	-1.717150
H	3.081700	3.537290	-0.687960
H	2.085500	1.966200	0.890570
H	-1.505870	-2.154750	-0.166250

Zero-point correction= 0.595782 (Hartree/Particle)
Thermal correction to Energy= 0.628829
Thermal correction to Enthalpy= 0.629773
Thermal correction to Gibbs Free Energy= 0.534828
SCF Done: E(RwB97XD) = -1465.73683223
Thermal correction to Gibbs free energy (ZPG) from GoodVibes: 0.520464

17-C

C	1.157230	1.278830	-0.053180
C	2.145440	0.166830	-0.258180
C	1.660660	-1.057020	0.019410
C	2.457910	-2.282200	-0.183110
C	3.590360	-2.176640	-0.898600
C	4.025670	-0.881690	-1.532930
C	3.538510	0.385040	-0.800290
C	4.471630	0.858670	0.305800
C	4.877010	2.131880	0.350330
H	5.524520	2.496500	1.152620
H	4.574670	2.855440	-0.412130
C	4.888360	-0.150670	1.340860
H	4.014540	-0.672580	1.762300
H	5.444150	0.323920	2.161300
H	5.529100	-0.929610	0.897550
H	3.481230	1.202520	-1.535910
H	5.121230	-0.849990	-1.638810
H	3.631030	-0.863050	-2.566880
H	4.197610	-3.067390	-1.086050
C	1.961190	-3.581230	0.383500
H	2.683530	-4.390690	0.212260
H	1.779790	-3.503970	1.467680
H	1.006120	-3.874170	-0.083110
C	0.230100	-1.051300	0.502280
C	0.172400	-0.145020	1.710910
O	-0.280470	-0.450500	2.787520
C	0.672990	1.280750	1.412610
C	1.747830	1.699430	2.406780
H	2.045550	2.737430	2.204640
H	2.635750	1.057760	2.348550
H	1.339010	1.631140	3.425490
O	-0.439050	2.147410	1.507170
H	-0.937690	1.909020	2.297480
H	-0.123530	-2.049480	0.767850
C	-0.726800	-0.390210	-0.583480
C	-2.130860	-0.206950	-0.008060
C	-2.870690	0.879290	-0.233870
C	-2.447150	2.019780	-1.109030
C	-0.936870	2.191450	-1.084130
O	-0.467670	3.295120	-1.242380
C	-0.051410	0.964200	-0.985040
H	0.372740	0.873340	-1.995200
C	-2.833980	1.700680	-2.571190
H	-3.924890	1.578350	-2.628780
H	-2.539140	2.538610	-3.220670
H	-2.360820	0.772810	-2.928480
O	-3.053860	3.210500	-0.699130
H	-2.387830	3.899480	-0.842470
H	-3.904520	0.925140	0.122500
C	-2.742210	-1.477240	0.554200
C	-3.943210	-1.249980	1.451000
C	-5.175470	-1.683030	1.166870
H	-6.000380	-1.514920	1.864250
H	-5.416090	-2.221060	0.248140
C	-3.638370	-0.526370	2.736700
H	-2.840090	-1.041730	3.293130
H	-3.266010	0.489800	2.534240
H	-4.527090	-0.447800	3.377410
C	-2.970900	-2.384380	-0.663790
C	-1.866300	-2.313590	-1.683180
C	-0.871750	-1.412970	-1.727540
C	0.116970	-1.416650	-2.863660
H	-0.005050	-0.529280	-3.506830
H	1.157080	-1.420000	-2.506860
H	-0.028770	-2.301230	-3.498500
H	-1.927720	-3.049160	-2.492580
H	-3.900550	-2.073590	-1.173590
H	-3.131820	-3.428290	-0.346820
H	-2.000610	-1.965840	1.205210
H	1.563580	2.264170	-0.316330

Zero-point correction= 0.600447 (Hartree/Particle)
Thermal correction to Energy= 0.632898
Thermal correction to Enthalpy= 0.633842
Thermal correction to Gibbs Free Energy= 0.540556
SCF Done: E(RwB97XD) = -1465.79538613
Thermal correction to Gibbs free energy (ZPG) from GoodVibes: 0.526174

$TS_{14a+14a}$-D

C	0.872220	0.328650	-1.515820
C	1.287670	-0.510500	-0.499480
C	1.794360	0.072140	0.679340
C	2.270290	-0.762220	1.788450
C	1.937680	-2.067330	1.801720
C	1.007100	-2.661490	0.798080
C	1.124930	-2.012100	-0.594330
C	2.225330	-2.677160	-1.413320
C	3.493630	-2.259590	-1.394140
H	3.798680	-1.391680	-0.804670
H	4.271590	-2.780520	-1.958570
C	1.780730	-3.873590	-2.208830
H	2.624450	-4.390690	-2.686060
H	1.072030	-3.568560	-2.997520
H	1.248100	-4.597490	-1.570020
H	0.174550	-2.197000	-1.116800
H	1.149440	-3.749670	0.722700
H	-0.017570	-2.507920	1.185790
H	2.287860	-2.701120	2.621420
C	3.089880	-0.127830	2.878590
H	3.935040	0.445170	2.465060
H	2.479170	0.570990	3.472330
H	3.490760	-0.890110	3.560590
C	1.595930	1.478970	0.823080
C	1.761580	2.338080	-0.374650
O	2.002970	3.525450	-0.325610
C	1.569230	1.644590	-1.715340
C	2.982130	1.385510	-2.291030
H	3.602770	0.787610	-1.610650
H	3.475700	2.353550	-2.466510
H	2.886440	0.851140	-3.246310
O	0.856710	2.463690	-2.599550
H	1.192650	3.359610	-2.465750
C	-0.309010	1.715480	1.016480
C	-0.448990	1.026950	2.341260
O	0.147100	1.389050	3.333850
C	-1.412240	-0.151530	2.465560
C	-1.745300	-0.765800	1.139670
C	-1.710150	-0.085500	-0.018900
C	-2.301200	-0.635530	-1.309580
C	-3.009080	-1.969390	-1.157370
C	-2.465950	-3.093220	-1.637150
H	-1.507500	-3.088170	-2.163560
H	-2.966420	-4.059940	-1.532750
C	-4.362990	-1.980440	-0.491040
H	-5.142730	-1.635710	-1.189470
H	-4.395050	-1.310240	0.381090
H	-4.637530	-2.992570	-0.163090
C	-3.205430	0.419730	-1.966960
C	-2.669630	1.813270	-1.878710
C	-1.708970	2.219720	-1.028320
C	-1.398070	3.688460	-0.899450
H	-1.865590	4.098880	0.011710
H	-1.801840	4.241020	-1.758170
H	-0.325670	3.904260	-0.837280

C	-1.098220	1.251940	-0.090980
H	-3.157680	2.561840	-2.510320
H	-4.203090	0.416430	-1.491260
H	-3.379990	0.137050	-3.017940
H	-1.453620	-0.791870	-1.993570
H	-2.186030	-1.764380	1.190740
C	-2.708850	0.412060	3.088710
H	-3.430980	-0.408330	3.206650
H	-2.486290	0.836370	4.079330
H	-3.156170	1.192390	2.454850
O	-0.853580	-1.121400	3.313510
H	-0.328800	-0.636130	3.964800
H	-0.258560	2.799800	1.152280
H	1.938120	1.963530	1.739790
H	0.416620	-0.085840	-2.419670

Zero-point correction= 0.595734 (Hartree/Particle)
Thermal correction to Energy= 0.628809
Thermal correction to Enthalpy= 0.629753
Thermal correction to Gibbs Free Energy= 0.535297
SCF Done: E(RwB97XD) = -1465.72384650
Thermal correction to Gibbs free energy (ZPG) from GoodVibes: 0.520601

17-D

C	-0.491750	-0.803350	0.857070
C	-1.319800	-0.435140	-0.349510
C	-1.828160	0.810700	-0.303680
C	-2.693400	1.356170	-1.364440
C	-2.711730	0.703210	-2.537310
C	-1.835030	-0.494140	-2.786550
C	-1.560300	-1.348110	-1.536110
C	-2.606230	-2.415800	-1.227230
C	-3.910470	-2.244440	-1.465240
H	-4.301900	-1.321400	-1.898450
H	-4.632720	-3.029600	-1.224160
C	-2.067520	-3.695590	-0.646490
H	-2.870590	-4.395100	-0.376270
H	-1.462780	-3.507310	0.254710
H	-1.402490	-4.194510	-1.371360
H	-0.616750	-1.887080	-1.720760
H	-2.254640	-1.128060	-3.581570
H	-0.863640	-0.121540	-3.163870
H	-3.325750	1.078280	-3.361530
C	-3.476360	2.608800	-1.098960
H	-4.084880	2.519090	-0.184550
H	-2.792640	3.460940	-0.960560
H	-4.147670	2.840250	-1.937140
C	-1.343310	1.616240	0.883160
C	-1.656040	0.908640	2.177340
O	-1.993790	1.448940	3.203630
C	-1.360820	-0.590920	2.122590
C	-2.676410	-1.378200	2.085080
H	-3.290360	-1.163670	1.201710
H	-3.256520	-1.132910	2.987190
H	-2.444200	-2.452480	2.108590
O	-0.653800	-0.955040	3.280540
H	-1.062510	-0.466680	4.007810
C	0.214240	1.608950	0.777660
C	0.577470	2.409150	-0.458380
O	-0.158210	3.246670	-0.930570
C	1.924590	2.157710	-1.108150
C	2.102570	0.669440	-1.237060
C	1.649030	-0.229740	-0.360240
C	2.076730	-1.693410	-0.435840
C	3.307430	-1.892520	-1.302800
C	3.216680	-2.511080	-2.484050
H	2.259970	-2.886220	-2.858920
H	4.093410	-2.661600	-3.119890
C	4.618980	-1.377110	-0.769120
H	4.531240	-0.328390	-0.446670
H	5.412950	-1.446170	-1.525020
H	4.942680	-1.951460	0.113410
C	2.295670	-2.294110	0.985630
C	2.406430	-1.259910	2.064400
C	1.705230	-0.119430	2.056480
C	1.827300	0.874690	3.176400
H	2.319420	1.807550	2.854330
H	2.427670	0.453620	3.993970
H	0.844700	1.144450	3.589810
C	0.784190	0.143910	0.847870
H	3.054440	-1.481510	2.917280
H	3.186010	-2.938570	0.981170
H	1.463620	-2.976940	1.229430
H	1.258420	-2.255590	-0.912910
H	2.738320	0.361620	-2.071330
C	3.038430	2.745890	-0.220960
H	4.004030	2.576610	-0.718220
H	2.893410	3.830800	-0.106220
H	3.070720	2.268510	0.768890
O	1.951120	2.767670	-2.364640
H	1.172160	3.344100	-2.392830
H	0.621870	2.199450	1.612340
H	-1.712550	2.644830	0.913830
H	-0.180930	-1.852240	0.836460

Zero-point correction= 0.600633 (Hartree/Particle)
Thermal correction to Energy= 0.632827
Thermal correction to Enthalpy= 0.633772
Thermal correction to Gibbs Free Energy= 0.540947
SCF Done: E(RwB97XD) = -1465.78526747
Thermal correction to Gibbs free energy (ZPG) from GoodVibes: 0.526940

17-E

C	-3.736180	0.900340	-0.478330
C	-3.040220	2.159930	-0.041950
C	-1.747870	2.283690	0.298480
C	-1.196110	3.618980	0.718900
H	-1.977720	4.389250	0.676430
H	-0.376110	3.949240	0.062420
H	-0.806940	3.603000	1.750140
C	-0.808200	1.071980	0.165620
C	-1.698330	-0.164540	0.257360
C	-1.758160	-0.948160	1.335430
C	-1.042540	-0.671440	2.620130
C	0.252580	0.082090	2.369650
O	1.166240	-0.054980	3.150820
C	0.373780	1.019150	1.184450
C	1.720900	0.711620	0.464400
C	1.535560	-0.414250	-0.524830
C	0.612010	-0.167910	-1.474700
C	0.455090	-1.039050	-2.651280
C	0.989850	-2.270710	-2.584200
C	1.671820	-2.754420	-1.333630
C	2.427510	-1.625900	-0.621060
C	3.023730	-2.049320	0.713470
C	2.283630	-2.602740	1.677170
H	2.726040	-2.876210	2.638790
H	1.207480	-2.769220	1.572010
C	4.488190	-1.757750	0.881400
H	5.082490	-2.303880	0.129500
H	4.683100	-0.685250	0.711760
H	4.853790	-2.029200	1.881310
H	3.262630	-1.311310	-1.277790
H	2.363350	-3.580360	-1.554440
H	0.907880	-3.167860	-0.646210
H	0.885380	-2.958060	-3.428900
C	-0.259080	-0.515390	-3.864990
H	-1.328770	-0.336240	-3.664530
H	0.167290	0.445390	-4.195100
H	-0.192780	-1.227560	-4.698760
C	-0.130060	1.132150	-1.262810
C	0.969160	2.181190	-1.349010
O	1.021730	3.044370	-2.192050
C	2.130980	1.946890	-0.359620
C	2.455770	3.196770	0.453270
H	3.333560	2.991220	1.081680
H	1.634060	3.540160	1.093620
H	2.698090	4.017140	-0.238820

O	3.274420	1.587740	-1.109020
H	3.364100	2.230400	-1.822520
H	-0.868250	1.360520	-2.036460
H	2.481660	0.489140	1.222400
H	0.490090	2.002730	1.659460
O	-0.753330	-1.873550	3.281400
H	0.052810	-1.704880	3.790690
C	-1.925760	0.232410	3.507360
H	-2.148990	1.190980	3.013580
H	-1.418120	0.423200	4.464990
H	-2.874280	-0.286140	3.706930
H	-2.479900	-1.769920	1.375270
C	-2.768120	-0.243720	-0.814820
C	-3.394000	-1.614880	-0.975000
C	-4.675430	-1.881900	-0.704140
H	-5.078790	-2.886950	-0.853120
H	-5.372130	-1.127160	-0.335100
C	-2.465360	-2.673100	-1.508790
H	-2.944100	-3.661520	-1.526480
H	-2.145720	-2.425090	-2.533510
H	-1.546490	-2.735290	-0.906330
H	-2.308440	-0.014680	-1.788830
H	-3.675550	3.049570	0.023120
H	-4.399140	1.112180	-1.333460
H	-4.394920	0.581870	0.349410

Zero-point correction= 0.600860 (Hartree/Particle)
Thermal correction to Energy= 0.633083
Thermal correction to Enthalpy= 0.634027
Thermal correction to Gibbs Free Energy= 0.541694
SCF Done: E(RwB97XD) = -1465.78988734
Thermal correction to Gibbs free energy (ZPG) from GoodVibes: 0.527342

$TS_{14a+14a}$-F

C	0.464990	2.886370	0.151630
C	-0.016290	2.511770	-1.205150
C	0.080020	1.235460	-1.641910
C	-0.406670	0.845020	-3.012890
H	-0.839650	1.713420	-3.528640
H	-1.175140	0.059160	-2.980660
H	0.424430	0.466320	-3.630140
C	0.770060	0.259210	-0.801350
C	1.838770	0.750740	0.063790
C	2.879110	-0.029220	0.405940
C	3.060570	-1.455830	-0.016680
C	1.890360	-1.989750	-0.865960
O	1.955590	-3.110850	-1.315610
C	0.667430	-1.143800	-1.099640
C	-0.639930	-2.038720	-0.238520
C	-1.878550	-1.332260	-0.411870
C	-2.082460	-0.181660	0.383480
C	-3.334350	0.640670	0.110660
C	-3.423530	1.924370	0.911300
C	-3.101490	3.120660	0.411060
H	-3.179370	4.025860	1.019450
H	-2.749840	3.242660	-0.615490
C	-3.939950	1.753280	2.316290
H	-5.013420	1.501240	2.292550
H	-3.433670	0.918800	2.827590
H	-3.815880	2.665740	2.916030
C	-3.575200	0.761180	-1.390540
C	-3.531480	-0.594250	-2.029730
C	-2.740400	-1.588980	-1.566710
C	-2.649250	-2.918420	-2.266860
H	-3.406430	-3.000340	-3.058350
H	-1.661390	-3.061870	-2.734930
H	-2.793450	-3.751570	-1.561720
H	-4.130080	-0.762410	-2.930230
H	-4.541330	1.252640	-1.577330
H	-2.801880	1.409380	-1.850260
H	-4.145120	-0.011920	0.491420
C	-1.183700	0.117950	1.386800
C	-0.506280	-1.002040	2.130650
C	0.693410	-0.586310	2.966450
H	1.096690	-1.466130	3.488150
H	0.361230	0.156130	3.706470
H	1.503070	-0.171630	2.358270
O	-1.527650	-1.502550	3.003510
H	-1.164220	-2.294470	3.420730
C	-0.198160	-2.172650	1.190820
O	0.283280	-3.195570	1.619280
H	-1.304910	1.041140	1.956910
H	-0.553850	-3.007690	-0.738950
H	0.299430	-1.364290	-2.106570
C	4.358300	-1.615000	-0.815410
H	4.479230	-2.664490	-1.120050
H	5.207370	-1.320720	-0.182660
H	4.351530	-0.985670	-1.718390
O	3.105550	-2.235590	1.165760
H	2.936840	-3.154760	0.922910
H	3.680440	0.381330	1.028680
C	1.796910	2.203480	0.527000
C	3.005850	2.974760	0.025670
C	3.875390	3.511160	0.888020
H	3.741520	3.413880	1.969160
H	4.752400	4.065840	0.543020
C	3.174260	3.100650	-1.463360
H	4.115090	3.606530	-1.719980
H	3.167360	2.108120	-1.941630
H	2.343130	3.670080	-1.909720
H	1.855180	2.188300	1.626640
H	-0.475850	3.272360	-1.843130
H	0.554380	3.975970	0.267250
H	-0.304550	2.552830	0.872390

Zero-point correction= 0.595408 (Hartree/Particle)
Thermal correction to Energy= 0.628563
Thermal correction to Enthalpy= 0.629507
Thermal correction to Gibbs Free Energy= 0.534430
SCF Done: E(RwB97XD) = -1465.70717817
Thermal correction to Gibbs free energy (ZPG) from GoodVibes: 0.519883

17-F

C	1.285730	2.767570	-0.199760
C	0.648310	2.229800	-1.443440
C	0.273150	0.950230	-1.571900
C	-0.312550	0.441880	-2.860150
H	-0.492940	1.277210	-3.550910
H	-1.266050	-0.085260	-2.705650
H	0.371750	-0.256480	-3.371360
C	0.509250	0.012160	-0.364730
C	1.954150	0.312690	0.036020
C	2.940700	-0.581210	-0.069060
C	2.784630	-2.001490	-0.550910
C	1.355330	-2.422410	-0.251210
O	1.145680	-3.463800	0.330470
C	0.250830	-1.496300	-0.694710
C	-1.106220	-1.972990	-0.135550
C	-2.183000	-0.936460	-0.396390
C	-1.904280	0.278820	0.120430
C	-2.973280	1.353660	0.104140
C	-2.487610	2.746770	0.460160
C	-2.164530	3.661830	-0.457940
H	-1.818530	4.656630	-0.163560
H	-2.225990	3.459340	-1.529020
C	-2.430050	3.038050	1.936560
H	-3.454160	3.133040	2.335980
H	-1.965130	2.208540	2.491510
H	-1.892520	3.972360	2.152400
C	-3.748300	1.242730	-1.209930
C	-4.208280	-0.172520	-1.446790
C	-3.467720	-1.225660	-1.054630
C	-3.873510	-2.654350	-1.279310
H	-4.884390	-2.717030	-1.704390
H	-3.183650	-3.164690	-1.971350
H	-3.856880	-3.221010	-0.334710
H	-5.148060	-0.336330	-1.982380
H	-4.603000	1.934390	-1.194040

H	-3.107440	1.558260	-2.056540
H	-3.673160	1.055100	0.911460
C	-0.536700	0.373580	0.759990
C	-0.555050	-0.621730	1.948370
C	0.760630	-0.843980	2.693740
H	0.557720	-1.501390	3.551600
H	1.130890	0.119320	3.072930
H	1.548920	-1.308210	2.092180
O	-1.509370	-0.126230	2.864130
H	-1.892830	-0.899370	3.300550
C	-1.098860	-1.949180	1.383270
O	-1.618190	-2.766780	2.100410
H	-0.343150	1.375820	1.152660
H	-1.353730	-2.978200	-0.489350
H	0.219800	-1.623520	-1.786460
C	3.064400	-2.096080	-2.061050
H	2.916930	-3.129400	-2.410030
H	4.113330	-1.819180	-2.237640
H	2.424830	-1.414790	-2.641050
O	3.659390	-2.841400	0.145080
H	3.111610	-3.562590	0.492370
H	3.966760	-0.305320	0.189680
C	2.230840	1.742170	0.491200
C	3.683370	2.139690	0.295010
C	4.484300	2.350740	1.343710
H	4.123360	2.234270	2.369520
H	5.529600	2.644470	1.214090
C	4.163870	2.297710	-1.123900
H	3.635860	3.119050	-1.634200
H	5.240340	2.513180	-1.160390
H	3.968350	1.386520	-1.710030
H	2.028680	1.773340	1.574530
H	0.478550	2.921950	-2.273370
H	1.841730	3.689160	-0.423640
H	0.495260	3.082230	0.500330

Zero-point correction= 0.600517 (Hartree/Particle)
Thermal correction to Energy= 0.632709
Thermal correction to Enthalpy= 0.633653
Thermal correction to Gibbs Free Energy= 0.541039
SCF Done: E(RwB97XD) = -1465.78794133
Thermal correction to Gibbs free energy (ZPG) from GoodVibes: 0.526817

$TS_{14a+14a}$-G

C	-0.974180	0.980510	1.189070
C	-2.048640	0.149260	0.826310
C	-1.745190	-1.211870	0.597210
C	-2.761500	-2.094440	-0.022740
C	-4.044620	-1.702380	0.006460
C	-4.474740	-0.418650	0.655480
C	-3.434420	0.705770	0.532080
C	-3.519870	1.504300	-0.771860
C	-3.957610	0.975730	-1.919610
H	-4.022370	1.583200	-2.826690
H	-4.258460	-0.070700	-2.004190
C	-3.137350	2.958500	-0.678560
H	-3.275650	3.469640	-1.641600
H	-3.762680	3.468410	0.073010
H	-2.090610	3.106350	-0.370060
H	-3.643940	1.427630	1.337970
H	-4.645980	-0.617080	1.729140
H	-5.437400	-0.079310	0.246660
H	-4.816410	-2.354280	-0.414880
C	-2.320120	-3.396240	-0.627310
H	-3.153150	-3.891100	-1.144680
H	-1.502480	-3.241860	-1.350190
H	-1.940520	-4.087030	0.142640
C	-0.464670	-1.686410	0.877510
C	0.328340	-1.039290	1.907190
O	1.140460	-1.616390	2.611370
C	-0.039900	0.409840	2.243630
C	1.200950	1.232350	2.544710
H	1.940770	1.157110	1.741410
H	1.679430	0.825660	3.446360
H	0.933930	2.283960	2.718820
O	-0.848250	0.342910	3.416450
H	-0.356490	-0.195640	4.048950
H	-0.174420	-2.706190	0.632110
C	0.840410	0.006520	-0.924030
C	2.305850	-0.034840	-0.697730
C	2.985200	1.104340	-0.488580
C	2.359650	2.470120	-0.474150
C	3.052350	3.419730	0.498340
H	2.525770	4.384830	0.513070
H	4.086340	3.574840	0.159210
H	3.071340	3.026850	1.523130
C	0.837230	2.423660	-0.240040
O	0.248440	3.461140	-0.019620
C	0.098670	1.143940	-0.494240
H	-0.793820	1.362690	-1.081380
O	2.489820	2.960870	-1.806780
H	2.132140	3.857180	-1.811710
H	4.078620	1.080150	-0.447970
C	3.058770	-1.330540	-0.968890
C	2.946730	-2.353350	0.150420
C	2.232280	-3.476740	0.049980
H	1.652440	-3.721270	-0.843700
H	2.180780	-4.180520	0.884100
C	3.760730	-2.022710	1.369950
H	3.569120	-2.725940	2.189110
H	4.836320	-2.039940	1.123160
H	3.522740	-1.013630	1.738300
C	2.657780	-1.839690	-2.356450
C	1.201580	-1.690110	-2.658290
C	0.356770	-0.846260	-2.028530
C	-1.025500	-0.634270	-2.581940
H	-1.097050	0.349680	-3.073590
H	-1.807050	-0.657080	-1.816960
H	-1.263280	-1.398700	-3.334220
H	0.824890	-2.241200	-3.526010
H	3.212160	-1.261100	-3.118150
H	2.981330	-2.884260	-2.483510
H	4.125720	-1.058480	-1.011280
H	-1.205740	2.038050	1.349980

Zero-point correction= 0.597553 (Hartree/Particle)
Thermal correction to Energy= 0.629952
Thermal correction to Enthalpy= 0.630897
Thermal correction to Gibbs Free Energy= 0.538892
SCF Done: E(RwB97XD) = -1465.70540998
Thermal correction to Gibbs free energy (ZPG) from GoodVibes: 0.524388

17-G

C	-0.885510	0.998730	1.130910
C	-1.967660	0.053630	0.676360
C	-1.506610	-1.101750	0.159310
C	-2.404540	-2.148510	-0.358120
C	-3.712090	-2.037680	-0.069510
C	-4.243730	-0.932010	0.804320
C	-3.444040	0.376720	0.719990
C	-3.806140	1.299640	-0.441530
C	-4.425290	0.867440	-1.546080
H	-4.661150	1.558110	-2.360720
H	-4.710950	-0.176830	-1.685280
C	-3.432850	2.750640	-0.274390
H	-3.775140	3.353020	-1.127130
H	-3.884360	3.162790	0.642770
H	-2.346060	2.898250	-0.174780
H	-3.624680	0.942970	1.648760
H	-4.204840	-1.286060	1.851580
H	-5.304460	-0.736550	0.586750
H	-4.413550	-2.799400	-0.423700
C	-1.827260	-3.279040	-1.160910
H	-2.619270	-3.932160	-1.551930
H	-1.234880	-2.899070	-2.008800
H	-1.153190	-3.897790	-0.545530
C	0.008010	-1.218410	0.186440
C	0.283610	-1.086920	1.673160

O	0.628240	-1.989170	2.397490
C	-0.101030	0.284860	2.248270
C	1.146630	1.012800	2.751370
H	1.924540	1.115260	1.982070
H	1.576520	0.428520	3.578360
H	0.873550	2.011010	3.118140
O	-0.988720	0.084620	3.323260
H	-0.682110	-0.706560	3.785070
H	0.359660	-2.194940	-0.150370
C	0.623100	-0.047960	-0.661550
C	2.144780	-0.062260	-0.665930
C	2.866070	1.062400	-0.633760
C	2.293600	2.447970	-0.561620
C	3.251970	3.425290	0.101540
H	2.796610	4.422690	0.177310
H	4.176980	3.486550	-0.489280
H	3.502030	3.095950	1.120680
C	0.925230	2.456000	0.123080
O	0.526810	3.438260	0.706180
C	0.007110	1.272360	-0.106220
H	-0.680370	1.670580	-0.863950
O	2.009630	2.839080	-1.909500
H	1.764850	3.771850	-1.892630
H	3.949590	1.004850	-0.779680
C	2.810470	-1.395110	-0.984880
C	3.159710	-2.229130	0.247660
C	2.920660	-3.537980	0.360960
H	2.409600	-4.123330	-0.404830
H	3.229160	-4.080520	1.257380
C	3.885720	-1.486020	1.336980
H	4.230830	-2.169740	2.123440
H	4.758830	-0.946860	0.933480
H	3.238570	-0.730530	1.805280
C	2.024560	-2.133970	-2.098330
C	0.973890	-1.293040	-2.766230
C	0.286850	-0.325070	-2.145410
C	-0.749970	0.489720	-2.860180
H	-0.420270	1.538010	-2.946560
H	-1.719250	0.477020	-2.336100
H	-0.906030	0.104280	-3.876930
H	0.745490	-1.517770	-3.812470
H	2.729490	-2.521100	-2.848390
H	1.524860	-3.027480	-1.690670
H	3.789840	-1.123080	-1.413000
H	-1.279700	1.945850	1.518260

Zero-point correction= 0.601235 (Hartree/Particle)
Thermal correction to Energy= 0.633372
Thermal correction to Enthalpy= 0.634316
Thermal correction to Gibbs Free Energy= 0.542043
SCF Done: E(RwB97XD) = -1465.78192379
Thermal correction to Gibbs free energy (ZPG) from GoodVibes: 0.527806

$TS_{14a+14a}$-H

C	-0.981500	0.977650	-1.950490
C	-1.399250	-0.157790	-1.330930
C	-1.809790	-0.137050	0.049290
C	-2.846490	-1.074770	0.492030
C	-3.423150	-1.898610	-0.412450
C	-3.069200	-1.902390	-1.864520
C	-1.634870	-1.442440	-2.126980
C	-0.584090	-2.512510	-1.904170
C	-0.794210	-3.651280	-1.237390
H	0.006210	-4.388400	-1.128270
H	-1.751000	-3.891240	-0.769120
C	0.723410	-2.203000	-2.566230
H	1.067840	-1.198150	-2.282630
H	1.509980	-2.919800	-2.299690
H	0.607800	-2.206140	-3.663460
H	-1.560820	-1.166950	-3.191090
H	-3.766790	-1.219730	-2.385170
H	-3.228320	-2.897150	-2.307770
H	-4.256440	-2.531750	-0.092280
C	-3.410000	-1.001710	1.890580
H	-4.020660	-0.092060	2.014550
H	-2.644750	-0.983370	2.675870
H	-4.065520	-1.862090	2.081390
C	-1.516880	1.045370	0.860210
C	-1.472220	2.362300	0.103240
O	-1.648780	3.408570	0.682480
C	-1.315580	2.343800	-1.422830
C	-0.376700	3.431990	-1.918890
H	0.662200	3.233600	-1.628510
H	-0.446930	3.481780	-3.014790
H	-0.667580	4.404240	-1.494250
O	-2.644820	2.601350	-1.895030
H	-2.879540	3.489410	-1.598030
C	-0.104640	1.044300	1.757880
C	-0.172950	-0.198440	2.615420
O	-0.647580	-0.175900	3.726590
C	0.459150	-1.481670	2.060270
C	1.048820	-1.254620	0.697180
C	1.645300	-0.045130	0.404030
C	2.957090	0.124900	-0.359090
C	3.611060	-1.107270	-0.944410
C	3.805840	-1.275190	-2.254850
H	4.332010	-2.153250	-2.639080
H	3.439140	-0.560340	-2.995070
C	4.180970	-2.068840	0.070890
H	3.510800	-2.211930	0.931020
H	5.122460	-1.659980	0.475150
H	4.403730	-3.048250	-0.375280
C	2.862270	1.362450	-1.245780
C	2.581280	2.537790	-0.361210
C	1.756370	2.431680	0.707360
C	1.482520	3.606940	1.608440
H	2.115680	4.460390	1.330380
H	0.433440	3.932730	1.553970
H	1.695550	3.353350	2.659030
C	1.112260	1.142560	0.957600
H	3.046810	3.500760	-0.590840
H	3.792940	1.512550	-1.810530
H	2.041220	1.239040	-1.987340
H	3.644970	0.415820	0.462410
H	1.380180	-2.157480	0.181840
C	-0.454090	-2.695700	2.146520
H	-1.269260	-2.654990	1.415640
H	0.151600	-3.589500	1.940020
H	-0.876610	-2.778990	3.159380
O	1.598410	-1.696720	2.908480
H	1.261270	-1.797950	3.807890
H	-0.255610	1.911980	2.409700
H	-2.257330	1.176790	1.658280
H	-0.701000	0.938750	-3.007830

Zero-point correction= 0.597092 (Hartree/Particle)
Thermal correction to Energy= 0.629249
Thermal correction to Enthalpy= 0.630193
Thermal correction to Gibbs Free Energy= 0.539196
SCF Done: E(RwB97XD) = -1465.69853106
Thermal correction to Gibbs free energy (ZPG) from GoodVibes: 0.524537

17-H

C	0.025190	-0.448400	-1.224750
C	1.249850	0.113620	-0.524580
C	1.797120	-0.709350	0.388360
C	3.149500	-0.494210	0.936190
C	3.945850	0.354230	0.263190
C	3.479260	1.054680	-0.984960
C	1.970530	1.371500	-0.943200
C	1.705410	2.583370	-0.053000
C	1.333560	2.491010	1.226680
H	1.209800	3.389070	1.838780
H	1.154820	1.528650	1.707920
C	1.983220	3.914620	-0.697950
H	1.805990	4.748650	-0.004750
H	3.027330	3.979450	-1.045100
H	1.346450	4.055800	-1.584750

H	1.649720	1.635870	-1.963180
H	3.670170	0.395710	-1.851360
H	4.060580	1.973630	-1.152460
H	4.973180	0.518190	0.602230
C	3.596970	-1.262440	2.146010
H	2.885210	-1.132240	2.973440
H	4.594740	-0.937580	2.471760
H	3.650060	-2.342670	1.929970
C	0.953990	-1.938190	0.651860
C	0.940090	-2.677600	-0.677260
O	1.295600	-3.820080	-0.834170
C	0.521300	-1.777690	-1.861970
C	-0.412090	-2.509290	-2.820820
H	-1.306830	-2.923440	-2.351140
H	-0.718470	-1.826150	-3.625420
H	0.145310	-3.350130	-3.260730
O	1.691470	-1.440570	-2.594820
H	2.135380	-2.264310	-2.824380
C	-0.467120	-1.449860	1.012900
C	-0.415100	-0.673460	2.316230
O	0.511280	-0.753490	3.086890
C	-1.673610	0.124330	2.656520
C	-2.054410	0.959240	1.469340
C	-1.792090	0.632610	0.200580
C	-2.405150	1.457090	-0.937520
C	-1.611100	2.698810	-1.337360
C	-1.056450	2.873950	-2.541290
H	-0.552730	3.811290	-2.790270
H	-1.082590	2.119890	-3.329650
C	-1.579000	3.791250	-0.303670
H	-2.603810	4.111530	-0.051350
H	-1.020980	4.667790	-0.659160
H	-1.104210	3.436930	0.622070
C	-2.849160	0.559120	-2.112770
C	-3.132670	-0.837100	-1.652360
C	-2.355010	-1.460710	-0.758850
C	-2.726780	-2.819960	-0.234200
H	-3.567100	-3.233500	-0.808620
H	-1.896520	-3.543420	-0.282760
H	-3.044200	-2.743130	0.818470
C	-1.136000	-0.693690	-0.184410
H	-4.007330	-1.353820	-2.057610
H	-3.732420	1.005170	-2.591800
H	-2.081740	0.521470	-2.900710
H	-3.336060	1.858210	-0.504430
H	-2.661210	1.844590	1.683780
C	-1.474920	0.972500	3.902430
H	-0.697040	1.730500	3.735630
H	-2.419190	1.476970	4.152760
H	-1.153930	0.352930	4.752340
O	-2.720570	-0.832860	2.847530
H	-2.579670	-1.252300	3.703880
H	-1.085910	-2.317250	1.276030
H	1.349830	-2.591150	1.435310
H	-0.295940	0.224910	-2.024570

Zero-point correction= 0.601062 (Hartree/Particle)
Thermal correction to Energy= 0.633167
Thermal correction to Enthalpy= 0.634112
Thermal correction to Gibbs Free Energy= 0.542521
SCF Done: E(RwB97XD) = -1465.77227878
Thermal correction to Gibbs free energy (ZPG) from GoodVibes: 0.528250

16a

O	3.704680	0.633750	-0.695070
C	2.543360	0.481320	-0.367780
C	1.546150	1.547620	-0.327790
C	0.220650	1.269220	-0.281600
C	-0.776210	2.404250	-0.154710
H	-0.360070	3.275210	-0.685360
C	-0.903360	2.791600	1.328610
H	-1.646330	3.593940	1.455690
H	-1.214360	1.937430	1.949240
H	0.060360	3.147420	1.719710
C	-2.130470	2.055260	-0.779980
C	-2.662760	0.729440	-0.253590
C	-1.728180	-0.424850	-0.639760
C	-0.262160	-0.134240	-0.312590
C	0.628560	-1.130710	-0.173700
C	2.082190	-0.897370	0.109400
O	2.862640	-1.885850	-0.497550
H	3.689780	-1.439290	-0.736270
C	2.295150	-0.916760	1.643700
H	1.697930	-0.145330	2.152300
H	3.361260	-0.747820	1.857650
H	2.011370	-1.906800	2.026870
H	0.314100	-2.177300	-0.221020
C	-2.198780	-1.753420	-0.078090
C	-2.510720	-2.769070	-0.888960
H	-2.854790	-3.729600	-0.495450
H	-2.431650	-2.675870	-1.975760
C	-2.306570	-1.867120	1.420020
H	-1.383010	-1.520610	1.910340
H	-2.495480	-2.903560	1.730900
H	-3.130050	-1.245500	1.806810
H	-1.777260	-0.501810	-1.741020
H	-2.777650	0.782990	0.840820
H	-3.664380	0.522500	-0.660200
H	-2.845290	2.868380	-0.578470
H	-2.023350	1.995370	-1.876500
H	1.909190	2.576090	-0.398650

Zero-point correction= 0.321094 (Hartree/Particle)
Thermal correction to Energy= 0.337752
Thermal correction to Enthalpy= 0.338696
Thermal correction to Gibbs Free Energy= 0.277558
SCF Done: E(RwB97XD) = -734.106727931
Thermal correction to Gibbs free energy (ZPG) from GoodVibes: 0.269758

$TS_{16a+16a}$

C	-3.271380	2.198910	-0.385170
O	-0.492170	-2.417150	-2.124720
C	-3.232420	1.084870	-1.423740
O	-0.842940	-0.121750	-3.414740
C	-2.760710	-0.268370	-0.874120
O	0.842970	-0.120740	3.414900
C	-1.631450	-0.140570	0.138940
O	0.491500	-2.416660	2.125880
C	-0.926960	-1.287390	0.511410
C	0.926580	-1.287600	-0.510680
C	1.631310	-0.140780	-0.138670
C	2.760780	-0.268470	0.874150
C	3.876780	-1.125320	0.281680
C	4.042730	-2.385060	0.698390
C	-4.042600	-2.385010	-0.698330
C	-3.876870	-1.125160	-0.281860
C	0.485180	1.107720	-1.892410
C	1.348970	1.098320	-0.824060
C	4.757840	-0.526590	-0.780620
C	3.232600	1.084840	1.423500
C	3.271700	2.198650	0.384690
C	1.912800	2.406740	-0.286370
C	1.970560	3.539070	-1.310270
C	0.476960	-1.422870	-1.944710
C	-0.045400	-0.099420	-2.486650
C	1.726890	-1.788850	-2.781530
C	-0.477330	-1.422160	1.945470
C	0.045440	-0.098620	2.486780
C	-0.484780	1.108410	1.891960
C	-1.348720	1.098750	0.823720
C	-1.912380	2.407090	0.285630
C	-1.969810	3.539740	1.309200
C	-1.727340	-1.787380	2.782510
C	-4.758310	-0.526230	0.779980
H	-0.982250	-2.139470	-2.915430
H	-2.376280	-0.846160	-1.722110
H	0.981780	-2.138700	2.916370
H	-1.243930	-2.224500	0.045680

H	1.243430	-2.224580	-0.044610
H	2.376590	-0.846200	1.722280
H	0.191350	2.036040	-2.382850
H	1.209260	2.711600	0.509780
H	-0.190640	2.036890	2.381940
H	-4.026280	1.997790	0.391210
H	-1.208960	2.711630	-0.510740
H	-3.574890	3.141150	-0.868120
H	-2.542600	1.374220	-2.232490
H	-4.219690	0.960260	-1.894800
H	4.818260	-3.029210	0.274340
H	3.400280	-2.817590	1.470190
H	-4.818260	-3.029090	-0.274410
H	-3.399830	-2.817710	-1.469760
H	5.396330	-1.289180	-1.247370
H	5.415820	0.249570	-0.357510
H	4.162680	-0.043090	-1.572040
H	2.542760	1.374420	2.232150
H	4.219830	0.960250	1.894650
H	4.026700	1.997350	-0.391550
H	3.575160	3.140990	0.867470
H	0.973920	3.849690	-1.654440
H	2.560680	3.249500	-2.193820
H	2.445960	4.423310	-0.860760
H	1.419830	-1.920310	-3.829500
H	2.145220	-2.734020	-2.408960
H	2.500430	-1.010960	-2.731550
H	-2.559460	3.250390	2.193130
H	-2.445530	4.423770	0.859630
H	-0.973040	3.850580	1.652790
H	-1.420240	-1.918640	3.830490
H	-2.146100	-2.732480	2.410270
H	-2.500550	-1.009170	2.732360
H	-4.163410	-0.043100	1.571820
H	-5.397400	-1.288610	1.246240
H	-5.415720	0.250270	0.356610

Zero-point correction= 0.646174 (Hartree/Particle)
Thermal correction to Energy= 0.678851
Thermal correction to Enthalpy= 0.679795
Thermal correction to Gibbs Free Energy= 0.587115
SCF Done: E(RwB97XD) = -1468.21196678
Thermal correction to Gibbs free energy (ZPG) from GoodVibes: 0.572465

5

C	-3.533590	1.636980	-1.151200
O	0.039050	-3.018070	-1.429220
C	-3.200160	0.321360	-1.853680
O	-0.069300	-0.900410	-3.395010
C	-2.482220	-0.712660	-0.969080
O	0.441880	0.926640	3.348510
C	-1.233740	-0.078430	-0.252090
O	0.660340	-1.581250	2.715480
C	-0.463350	-1.155650	0.600840
C	0.970410	-1.349910	0.038930
C	1.660480	-0.006840	0.038940
C	2.834650	0.270380	0.946950
C	4.064030	-0.525630	0.530310
C	4.363270	-1.668150	1.158070
C	-3.384880	-2.820110	-0.046100
C	-3.434600	-1.483050	-0.065080
C	-0.212350	0.413520	-1.377910
C	1.045760	0.921640	-0.713130
C	4.903290	-0.008530	-0.606030
C	3.039770	1.786680	1.108220
C	2.842760	2.576600	-0.184080
C	1.455530	2.370650	-0.801460
C	1.407500	2.921120	-2.228890
C	0.878360	-1.875330	-1.405600
C	0.178910	-0.778450	-2.219110
C	2.235300	-2.220520	-2.005450
C	-0.429840	-0.915960	2.133710
C	-0.303990	0.567820	2.453850
C	-1.158490	1.489080	1.707790
C	-1.617720	1.204260	0.474660
C	-2.373450	2.242260	-0.343310
C	-2.853850	3.451390	0.453970
C	-1.710950	-1.411890	2.822180
C	-4.463520	-0.747380	0.755950
H	-0.097340	-3.246960	-2.356050
H	-2.067960	-1.475500	-1.641710
H	0.987450	-0.966620	3.393460
H	-0.972090	-2.113270	0.453300
H	1.501030	-2.080750	0.657170
H	2.540160	-0.129300	1.927430
H	-0.668990	1.151600	-2.039080
H	0.722120	2.938060	-0.194190
H	-1.333280	2.454790	2.183420
H	-4.391080	1.508160	-0.476150
H	-1.635760	2.618700	-1.074620
H	-3.856260	2.377700	-1.899860
H	-2.570860	0.519670	-2.734770
H	-4.123310	-0.129590	-2.250330
H	5.220420	-2.277780	0.858060
H	3.756080	-2.032770	1.991570
H	-4.055700	-3.406390	0.588410
H	-2.659420	-3.370930	-0.651140
H	5.679190	-0.731890	-0.892240
H	5.403740	0.933650	-0.329320
H	4.289450	0.210260	-1.494490
H	2.308820	2.139110	1.854350
H	4.035680	1.987020	1.533420
H	3.601300	2.288950	-0.928810
H	2.997020	3.650560	0.007190
H	0.392610	2.907810	-2.653160
H	2.056040	2.332140	-2.896840
H	1.757440	3.964260	-2.249100
H	2.103420	-2.538820	-3.050770
H	2.692050	-3.036660	-1.428950
H	2.913730	-1.358990	-1.997430
H	-3.520800	3.148610	1.276590
H	-3.417890	4.129790	-0.202810
H	-2.021510	4.027790	0.882070
H	-1.624270	-1.247670	3.906440
H	-1.818290	-2.489280	2.635720
H	-2.609920	-0.902870	2.459920
H	-4.035160	0.116120	1.287660
H	-4.921450	-1.414780	1.499120
H	-5.272350	-0.360580	0.115450

Zero-point correction= 0.651693 (Hartree/Particle)
Thermal correction to Energy= 0.683560
Thermal correction to Enthalpy= 0.684504
Thermal correction to Gibbs Free Energy= 0.594035
SCF Done: E(RwB97XD) = -1468.26994588
Thermal correction to Gibbs free energy (ZPG) from GoodVibes: 0.579663

16b

O	3.539650	0.878050	0.760920
C	2.462240	0.618290	0.257960
C	1.433610	1.609740	-0.032680
C	0.142560	1.251820	-0.246450
C	-0.911920	2.342590	-0.335840
H	-0.490750	3.151440	-0.954610
C	-1.175490	2.929990	1.060950
H	-1.513410	2.159790	1.770460
H	-0.262340	3.378130	1.476700
H	-1.949430	3.710980	1.008890
C	-2.199430	1.845490	-0.999950
C	-2.703180	0.570830	-0.337840
C	-1.708690	-0.577590	-0.551040
C	-0.254760	-0.174990	-0.289650
C	0.692100	-1.122580	-0.166730
C	2.159040	-0.830080	-0.123600
C	2.717620	-1.014040	-1.557420
H	2.561790	-2.055730	-1.870330
H	2.231520	-0.340690	-2.279030
H	3.798070	-0.805610	-1.542600

O	2.810440	-1.693730	0.763620
H	3.574560	-1.190940	1.084980
H	0.420700	-2.182840	-0.187230
C	-2.108920	-1.828360	0.211380
C	-2.460710	-2.941840	-0.439430
H	-2.762340	-3.845860	0.096710
H	-2.460970	-2.987580	-1.532300
C	-2.100100	-1.751800	1.715080
H	-2.848180	-1.031230	2.082570
H	-1.119000	-1.416560	2.086250
H	-2.324020	-2.727710	2.166390
H	-1.759880	-0.825140	-1.626240
H	-2.865940	0.750000	0.736740
H	-3.677940	0.270890	-0.750780
H	-2.962540	2.637810	-0.953090
H	-2.013360	1.651640	-2.070340
H	1.718890	2.659850	0.072040

Zero-point correction= 0.320899 (Hartree/Particle)
Thermal correction to Energy= 0.337680
Thermal correction to Enthalpy= 0.338624
Thermal correction to Gibbs Free Energy= 0.276732
SCF Done: E(RwB97XD) = -734.105433063
Thermal correction to Gibbs free energy (ZPG) from GoodVibes: 0.269103

$TS_{16b+16b}$

C	3.297400	2.214890	0.198550
C	3.307730	1.152000	1.287360
O	0.888510	-0.091480	3.428180
C	2.781560	-0.219910	0.831700
O	-0.888520	-0.091560	-3.428180
C	1.628020	-0.119310	-0.159710
C	0.957850	-1.278540	-0.542990
C	-0.957850	-1.278520	0.543010
C	-1.628020	-0.119300	0.159710
C	-2.781570	-0.219920	-0.831690
C	-3.874940	-1.133410	-0.285030
C	-4.248300	-2.212180	-0.982770
C	4.248310	-2.212160	0.982820
C	3.874940	-1.133400	0.285050
C	-0.382820	1.106370	1.856130
C	-1.292510	1.117560	0.833100
C	-4.503960	-0.782630	1.034590
C	-3.307740	1.151970	-1.287370
C	-3.297400	2.214890	-0.198580
C	-1.887850	2.432490	0.352180
C	-1.859750	3.556380	1.386020
C	-0.479090	-1.420600	1.976740
C	0.124120	-0.105230	2.477500
C	0.479090	-1.420650	-1.976710
C	-0.124120	-0.105300	-2.477500
C	0.382820	1.106320	-1.856160
C	1.292520	1.117540	-0.833130
C	1.887860	2.432480	-0.352230
C	1.859770	3.556350	-1.386100
C	4.503950	-0.782660	-1.034580
H	2.419210	-0.715210	1.741830
H	1.341820	-2.218020	-0.138190
H	-1.341820	-2.218010	0.138240
H	-2.419210	-0.715240	-1.741820
H	-0.065280	2.028280	2.344070
H	-1.259760	2.748030	-0.500530
H	0.065290	2.028220	-2.344130
H	3.970200	1.943840	-0.631420
H	1.259750	2.748030	0.500460
H	3.674500	3.166090	0.605960
H	2.673060	1.493620	2.121750
H	4.319240	1.024750	1.701220
H	-5.033120	-2.881700	-0.619870
H	-3.793780	-2.456100	-1.947650
H	5.033120	-2.881690	0.619930
H	3.793780	-2.456070	1.947700
H	-5.202020	-1.565590	1.361420
H	-5.068090	0.161030	0.964440
H	-3.732160	-0.662520	1.810260
H	-2.673070	1.493590	-2.121780
H	-4.319250	1.024720	-1.701220
H	-3.970190	1.943850	0.631400
H	-3.674510	3.166090	-0.606000
H	-0.837230	3.860890	1.650990
H	-2.378480	3.262180	2.311630
H	-2.365550	4.445500	0.981510
H	2.378500	3.262120	-2.311700
H	2.365570	4.445470	-0.981610
H	0.837250	3.860860	-1.651090
H	3.732160	-0.662540	-1.810250
H	5.202010	-1.565630	-1.361390
H	5.068100	0.161000	-0.964440
C	0.400450	-2.627330	2.267830
H	-0.105930	-3.539760	1.921910
H	1.390010	-2.567900	1.802060
H	0.565960	-2.697550	3.352070
C	-0.400450	-2.627380	-2.267770
H	0.105950	-3.539810	-1.921870
H	-1.389990	-2.567970	-1.801950
H	-0.566000	-2.697610	-3.352000
O	-1.697910	-1.569230	2.716160
H	-1.460060	-1.625850	3.648940
O	1.697900	-1.569290	-2.716130
H	1.460050	-1.625930	-3.648910

Zero-point correction= 0.645395 (Hartree/Particle)
Thermal correction to Energy= 0.678677
Thermal correction to Enthalpy= 0.679621
Thermal correction to Gibbs Free Energy= 0.585517
SCF Done: E(RwB97XD) = -1468.18800490
Thermal correction to Gibbs free energy (ZPG) from GoodVibes: 0.570711

16b+16b

C	-3.549950	1.806220	-0.823780
C	-3.240190	0.633880	-1.750090
O	0.209360	-0.392750	-3.498320
C	-2.497040	-0.536500	-1.075930
O	0.416190	0.421660	3.466600
C	-1.238420	-0.032720	-0.278720
C	-0.485220	-1.221260	0.433460
C	0.970810	-1.322700	-0.101490
C	1.638610	0.023960	0.073840
C	2.804690	0.209730	1.013920
C	4.020810	-0.594820	0.580360
C	4.414840	-1.652970	1.297010
C	-3.551950	-2.736870	-0.682790
C	-3.444510	-1.453990	-0.317870
C	-0.214930	0.573330	-1.328450
C	1.032640	1.018660	-0.594180
C	4.742130	-0.165150	-0.665750
C	3.065160	1.708880	1.257080
C	2.874190	2.576850	0.016580
C	1.461680	2.464160	-0.563180
C	1.377230	3.143370	-1.932160
C	0.946390	-1.671210	-1.601860
C	0.258370	-0.488180	-2.295070
C	-0.545130	-1.213160	1.973460
C	-0.306730	0.200950	2.516200
C	-1.108930	1.250510	1.876170
C	-1.582370	1.150200	0.622170
C	-2.329890	2.301130	-0.033890
C	-2.722540	3.428050	0.915840
C	-4.318740	-0.896470	0.774970
H	-2.098860	-1.154770	-1.895390
H	-1.016270	-2.145900	0.173720
H	1.527340	-2.115930	0.411170
H	2.491970	-0.211720	1.982300
H	-0.666900	1.374630	-1.915170
H	0.765040	2.988300	0.121490
H	-1.249600	2.151440	2.474870
H	-4.341630	1.539880	-0.109270
H	-1.627440	2.734920	-0.768430

H	-3.947780	2.644300	-1.417780
H	-2.636910	0.992570	-2.599080
H	-4.172050	0.248930	-2.192210
H	5.274540	-2.258370	0.996600
H	3.895330	-1.948530	2.213520
H	-4.234400	-3.419440	-0.169140
H	-2.972990	-3.152110	-1.512640
H	5.512630	-0.894360	-0.951130
H	5.235570	0.809220	-0.517360
H	4.032770	-0.066350	-1.500020
H	2.359730	2.044680	2.035410
H	4.075240	1.844760	1.673450
H	3.593760	2.289610	-0.766570
H	3.085100	3.630380	0.260250
H	0.345450	3.211820	-2.307240
H	1.968490	2.592230	-2.680330
H	1.771920	4.168880	-1.873990
H	-3.370360	3.059860	1.726790
H	-3.278840	4.201610	0.366370
H	-1.846910	3.913410	1.370150
H	-3.766900	-0.207040	1.425750
H	-4.715180	-1.706220	1.401970
H	-5.177220	-0.356830	0.342660
C	0.261960	-2.993730	-1.941610
H	0.812350	-3.813840	-1.458600
H	-0.787600	-3.038900	-1.627330
H	0.293360	-3.140570	-3.031380
C	0.377540	-2.228490	2.633870
H	0.199290	-3.226360	2.207710
H	1.437860	-1.974000	2.525310
H	0.171030	-2.260690	3.713470
O	2.280300	-1.723330	-2.061530
H	2.249220	-1.622390	-3.020670
O	-1.890390	-1.539370	2.298830
H	-1.976850	-1.546670	3.257530

Zero-point correction= 0.650982 (Hartree/Particle)
Thermal correction to Energy= 0.683236
Thermal correction to Enthalpy= 0.684180
Thermal correction to Gibbs Free Energy= 0.592663
SCF Done: E(RwB97XD) = -1468.26040360
Thermal correction to Gibbs free energy (ZPG) from GoodVibes: 0.578253

15a

O	3.668910	0.393730	-0.608640
C	2.513020	0.270460	-0.251730
C	1.600710	1.388840	-0.018210
C	0.258770	1.207510	0.045650
C	-0.318430	-0.147270	-0.180800
C	0.500490	-1.211530	-0.213130
C	1.973130	-1.126260	0.051250
O	2.661590	-2.070460	-0.716830
H	3.509540	-1.650310	-0.928570
C	2.227660	-1.376820	1.557810
H	3.308850	-1.313520	1.752580
H	1.883040	-2.389410	1.809730
H	1.702970	-0.646600	2.191570
H	0.109350	-2.214060	-0.408410
C	-1.802480	-0.296700	-0.518210
C	-2.354370	-1.662500	-0.154610
C	-2.740310	-2.520270	-1.104210
H	-3.144750	-3.505130	-0.854530
H	-2.663730	-2.268070	-2.165640
C	-2.457470	-1.995960	1.310520
H	-2.719990	-3.051500	1.463720
H	-1.506660	-1.795680	1.829300
H	-3.229060	-1.382930	1.803460
C	-2.650760	0.842440	0.056920
C	-2.045740	2.192910	-0.290360
C	-0.674890	2.362050	0.369910
H	-0.849580	2.273650	1.461000
C	-0.087370	3.746580	0.109240
H	-0.834120	4.519460	0.342960
H	0.796750	3.950040	0.729140
H	0.201800	3.861590	-0.946970
H	-2.706960	3.007260	0.044020
H	-1.947490	2.295890	-1.385910
H	-3.676040	0.754780	-0.333710
H	-2.719880	0.754060	1.154630
H	-1.869460	-0.202060	-1.617170
H	2.059760	2.375550	0.042230

Zero-point correction= 0.321144 (Hartree/Particle)
Thermal correction to Energy= 0.337744
Thermal correction to Enthalpy= 0.338689
Thermal correction to Gibbs Free Energy= 0.277755
SCF Done: E(RwB97XD) = -734.106148440
Thermal correction to Gibbs free energy (ZPG) from GoodVibes: 0.269983

$TS_{15a+15a}$

C	-2.935450	1.594950	-1.526130
C	-3.389710	0.135450	-1.581220
C	-2.716390	-0.810600	-0.550500
C	-3.714330	-1.483560	0.390940
C	-3.774750	-2.817960	0.454830
H	-4.468610	-3.326420	1.130170
H	-3.123530	-3.445940	-0.159110
C	-4.592190	-0.615530	1.250980
H	-3.989180	0.045580	1.894230
H	-5.238240	-1.220250	1.901610
H	-5.240050	0.035720	0.642730
C	-1.596760	-0.184750	0.268140
C	-1.593760	1.232500	0.541010
C	-0.646190	1.778320	1.371880
C	0.190370	0.951350	2.211730
O	1.081770	1.367540	2.942150
C	-0.160490	-0.535220	2.267010
C	-1.297350	-0.701440	3.303970
H	-2.184070	-0.105570	3.052400
H	-0.923330	-0.384440	4.288430
H	-1.580160	-1.761980	3.356610
O	0.947510	-1.259880	2.715070
H	1.446110	-0.625670	3.256650
C	-0.680040	-1.014000	0.928690
C	1.065830	-1.296320	-0.158170
C	1.749780	-0.077400	-0.266630
C	1.325240	0.850340	-1.281510
C	1.943550	2.241250	-1.343170
C	0.967340	3.323480	-1.795600
H	1.456100	4.308210	-1.763500
H	0.602870	3.172600	-2.820970
H	0.098820	3.351580	-1.123590
C	2.619130	2.613410	-0.022890
C	3.624610	1.546030	0.367490
C	2.954490	0.189910	0.633350
C	3.952130	-0.959290	0.539980
C	4.076920	-1.850810	1.527720
H	4.781810	-2.684010	1.454640
H	3.465920	-1.790780	2.430430
C	4.791200	-1.046980	-0.709550
H	4.208990	-0.781190	-1.605500
H	5.643570	-0.350000	-0.666890
H	5.196920	-2.058390	-0.849870
H	2.588880	0.212220	1.667410
H	4.360600	1.458880	-0.448410
H	4.187730	1.838970	1.265540
H	1.867770	2.734580	0.773330
H	3.123170	3.585530	-0.138650
H	2.746180	2.174780	-2.103410
C	0.352740	0.484150	-2.185860
C	-0.123390	-0.873760	-2.318920
O	-0.961320	-1.249230	-3.129000
C	0.542280	-1.917970	-1.430700
C	1.756060	-2.462340	-2.221170
H	1.382830	-2.967440	-3.124000
H	2.444370	-1.662540	-2.524060
H	2.298130	-3.189800	-1.601030
O	-0.341970	-2.977260	-1.192160

H	-0.890990	-3.019930	-1.991750
H	-0.034230	1.190710	-2.920030
H	1.477870	-2.013530	0.556140
H	-0.896220	-2.085530	0.878550
H	-0.552640	2.856750	1.506020
C	-2.695550	2.062680	-0.089370
C	-2.541350	3.573920	0.034330
H	-1.651470	3.943130	-0.494880
H	-2.472360	3.896820	1.083110
H	-3.416730	4.072250	-0.406840
H	-3.603220	1.794830	0.482530
H	-2.261680	-1.634510	-1.106090
H	-4.480560	0.099310	-1.437580
H	-3.198130	-0.263050	-2.586010
H	-3.696890	2.233580	-2.000210
H	-2.008320	1.736750	-2.100610

Zero-point correction= 0.646083 (Hartree/Particle)
Thermal correction to Energy= 0.678976
Thermal correction to Enthalpy= 0.679920
Thermal correction to Gibbs Free Energy= 0.586618
SCF Done: E(RwB97XD) = -1468.20328647
Thermal correction to Gibbs free energy (ZPG) from GoodVibes: 0.572017

15a+15a

C	-3.375200	1.074040	-1.647930
C	-3.240070	-0.457390	-1.733560
C	-2.406560	-1.121320	-0.612150
C	-3.255060	-1.764080	0.484430
C	-3.010580	-3.035560	0.826690
H	-3.605910	-3.544530	1.590080
H	-2.197780	-3.602060	0.363870
C	-4.389960	-1.019720	1.139490
H	-4.032200	-0.188520	1.767160
H	-4.970610	-1.690870	1.786650
H	-5.079880	-0.589950	0.396160
C	-1.249310	-0.184350	-0.122600
C	-1.802010	1.144310	0.370900
C	-1.154010	1.845470	1.320990
C	-0.064790	1.255460	2.094350
O	0.772770	1.898970	2.703060
C	-0.097490	-0.266220	2.244050
C	-1.250790	-0.623010	3.195000
H	-2.232360	-0.374030	2.775670
H	-1.125940	-0.092710	4.150920
H	-1.216350	-1.704470	3.387490
O	1.104530	-0.664450	2.844470
H	1.469090	0.152990	3.224780
C	-0.290280	-0.945120	0.864710
C	1.079540	-1.217030	0.192010
C	1.714890	0.103810	-0.169040
C	0.948180	0.858910	-0.980710
C	1.358730	2.232630	-1.476800
C	0.208630	3.208770	-1.709730
H	0.598580	4.155570	-2.112230
H	-0.533500	2.830970	-2.428490
H	-0.307890	3.431660	-0.766270
C	2.377540	2.825620	-0.498590
C	3.518860	1.854270	-0.235670
C	3.031380	0.564620	0.435460
C	4.102410	-0.522460	0.488550
C	4.178880	-1.351520	1.535270
H	4.933450	-2.142280	1.578110
H	3.479410	-1.276510	2.371540
C	5.083740	-0.620690	-0.650790
H	4.586430	-0.583750	-1.632240
H	5.796880	0.219260	-0.629990
H	5.661790	-1.553450	-0.595440
H	2.784430	0.806770	1.482080
H	3.997440	1.620360	-1.200500
H	4.292390	2.320850	0.393990
H	1.864250	3.065260	0.448980
H	2.770330	3.772220	-0.902630
H	1.864620	2.086660	-2.451110
C	-0.346620	0.189440	-1.394190
C	0.051960	-1.119690	-2.044510
O	-0.265920	-1.465040	-3.157380
C	0.882420	-2.016150	-1.109530
C	2.194900	-2.400740	-1.780840
H	1.982240	-2.961730	-2.703420
H	2.776270	-1.513700	-2.059930
H	2.792760	-3.023220	-1.100710
O	0.132640	-3.184920	-0.826440
H	-0.049050	-3.617830	-1.668690
H	-0.905070	0.781250	-2.121510
H	1.701040	-1.798770	0.877930
H	-0.735690	-1.925270	1.064050
H	-1.432150	2.866000	1.588810
C	-3.084460	1.665070	-0.264970
C	-3.235180	3.185980	-0.275900
H	-2.457350	3.663610	-0.888100
H	-3.194000	3.619680	0.732590
H	-4.211530	3.456300	-0.704270
H	-3.874810	1.286540	0.401510
H	-1.900820	-1.980380	-1.065410
H	-4.234830	-0.926750	-1.750040
H	-2.776830	-0.717030	-2.696100
H	-4.393330	1.375370	-1.937650
H	-2.713840	1.559870	-2.383630

Zero-point correction= 0.651727 (Hartree/Particle)
Thermal correction to Energy= 0.683583
Thermal correction to Enthalpy= 0.684527
Thermal correction to Gibbs Free Energy= 0.594726
SCF Done: E(RwB97XD) = -1468.25875655
Thermal correction to Gibbs free energy (ZPG) from GoodVibes: 0.580079

15b

O	-3.508310	0.285970	-1.055000
C	-2.427990	0.256320	-0.495690
C	-1.493760	1.376210	-0.461320
C	-0.182800	1.205310	-0.154180
C	0.331250	-0.145440	0.191130
C	-0.534910	-1.164510	0.330020
C	-2.021160	-1.006250	0.260130
O	-2.606840	-2.123630	-0.344420
H	-3.395100	-1.780280	-0.792600
C	-2.558820	-0.834550	1.702730
H	-2.321330	-1.738480	2.280440
H	-2.122490	0.042330	2.203580
H	-3.652280	-0.718360	1.660250
H	-0.174820	-2.168650	0.573910
C	1.826760	-0.376320	0.410270
C	2.275910	-1.751910	-0.048560
C	2.734420	-2.648370	0.830760
H	3.069850	-3.639650	0.513600
H	2.791200	-2.421800	1.899360
C	2.193790	-2.049050	-1.522200
H	1.184410	-1.842310	-1.910860
H	2.895990	-1.420920	-2.093450
H	2.435530	-3.099640	-1.732210
C	2.671770	0.747210	-0.197790
C	2.164530	2.093670	0.289320
C	0.767980	2.393900	-0.258730
H	0.886950	2.576460	-1.343510
C	0.200170	3.668790	0.370630
H	-0.729890	4.000200	-0.109980
H	0.928480	4.488700	0.280650
H	-0.007870	3.514120	1.440770
H	2.845730	2.903950	-0.012960
H	2.141170	2.102090	1.394050
H	3.725450	0.593380	0.079710
H	2.623170	0.716220	-1.299920
H	1.994830	-0.329310	1.501060
H	-1.880650	2.333300	-0.815680

Zero-point correction= 0.320957 (Hartree/Particle)
Thermal correction to Energy= 0.337688

Thermal correction to Enthalpy= 0.338633
Thermal correction to Gibbs Free Energy= 0.276846
SCF Done: E(RwB97XD) = -734.105408565
Thermal correction to Gibbs free energy (ZPG) from GoodVibes: 0.269300

$TS_{15b+15b}$

C	-3.181660	2.156530	-0.564970
C	-3.929880	0.844340	-0.451650
C	-2.965460	-0.351930	-0.432420
C	-3.720750	-1.603720	0.000620
C	-4.114530	-2.502490	-0.909200
H	-3.870000	-2.389300	-1.969050
H	-4.713030	-3.372980	-0.626710
C	-4.086210	-1.734210	1.454420
H	-4.701570	-0.880160	1.780830
H	-3.193260	-1.739020	2.096210
H	-4.662090	-2.651900	1.637220
C	-1.695080	-0.096160	0.377770
C	-1.383940	1.202940	0.939700
C	-0.282420	1.350890	1.745640
C	0.452930	0.235120	2.305760
O	1.391050	0.366100	3.079260
C	-0.152900	-1.149910	2.034290
C	0.787150	-2.311860	2.296450
H	0.208680	-3.246180	2.262490
H	1.231310	-2.198770	3.296050
H	1.612980	-2.385270	1.584550
C	-0.837560	-1.163280	0.677060
C	0.837710	-1.163530	-0.676590
C	1.695150	-0.096220	-0.377760
C	1.383830	1.202620	-0.940110
C	2.322780	2.375950	-0.680220
C	1.674330	3.755250	-0.650790
H	1.081960	3.977820	-1.548880
H	1.025920	3.857350	0.229210
H	2.456690	4.524940	-0.578870
C	3.181580	2.156930	0.564100
C	3.929920	0.844770	0.451160
C	2.965600	-0.351580	0.432450
C	3.720960	-1.603480	-0.000180
C	4.114840	-2.501890	0.909950
H	3.870350	-2.388330	1.969770
H	4.713390	-3.372440	0.627750
C	4.086310	-1.734500	-1.453960
H	4.662730	-2.651930	-1.636360
H	3.193270	-1.740180	-2.095620
H	4.701070	-0.880220	-1.780920
H	2.669400	-0.494660	1.483690
H	4.541090	0.861670	-0.466930
H	4.627650	0.705910	1.289260
H	2.553550	2.154740	1.470820
H	3.889980	2.993910	0.664510
H	3.013040	2.358500	-1.546460
C	0.282260	1.350160	-1.746050
C	-0.452950	0.234120	-2.305800
O	-1.391020	0.364720	-3.079430
C	0.153000	-1.150750	-2.033800
C	-0.786950	-2.312900	-2.295440
H	-1.231330	-2.200160	-3.294980
H	-0.208360	-3.247130	-2.261290
H	-1.612620	-2.386160	-1.583320
O	1.232990	-1.247370	-2.973420
H	0.844360	-1.236620	-3.855560
H	-0.021640	2.331770	-2.112310
H	1.190590	-2.157720	-0.386990
H	-1.190360	-2.157620	0.387860
O	-1.232930	-1.246260	2.973890
H	-0.844360	-1.235120	3.856060
H	0.021430	2.332650	2.111530
C	-2.323060	2.376050	0.679400
C	-1.674960	3.755520	0.649770
H	-2.457530	4.524980	0.577750
H	-1.026570	3.857730	-0.230230
H	-1.082670	3.978370	1.547840
H	-3.013430	2.358650	1.545550
H	-2.669180	-0.495370	-1.483600
H	-4.541120	0.861510	0.466390
H	-4.627540	0.705110	-1.289760
H	-3.890130	2.993410	-0.665790
H	-2.553460	2.154080	-1.471580

Zero-point correction= 0.645789 (Hartree/Particle)
Thermal correction to Energy= 0.678866
Thermal correction to Enthalpy= 0.679810
Thermal correction to Gibbs Free Energy= 0.586542
SCF Done: E(RwB97XD) = -1468.18084670
Thermal correction to Gibbs free energy (ZPG) from GoodVibes: 0.571808

15b+15b

C	-3.383650	1.261490	-1.488550
C	-3.361740	-0.268990	-1.621790
C	-2.462090	-1.034010	-0.610240
C	-3.278940	-1.746870	0.461860
C	-3.339430	-3.084530	0.454360
H	-2.805040	-3.685020	-0.286710
H	-3.944970	-3.630370	1.182850
C	-4.081440	-0.961340	1.461890
H	-4.865150	-0.370980	0.959480
H	-3.436050	-0.281510	2.033580
H	-4.578230	-1.634820	2.173120
C	-1.260690	-0.161200	-0.113270
C	-1.734790	1.170640	0.455770
C	-1.014220	1.804980	1.397650
C	0.065400	1.141090	2.138300
O	0.929820	1.740900	2.744640
C	-0.105310	-0.387020	2.230480
C	1.011700	-1.029650	3.034650
H	0.852970	-2.116610	3.086520
H	1.009560	-0.620810	4.055910
H	2.003740	-0.833610	2.617650
C	-0.290990	-0.983410	0.823360
C	1.073770	-1.234680	0.111600
C	1.699800	0.103780	-0.228300
C	0.916800	0.862570	-1.020020
C	1.323340	2.210630	-1.581140
C	0.195590	3.235090	-1.685420
H	-0.645910	2.884970	-2.300910
H	-0.190420	3.487900	-0.688180
H	0.573160	4.159820	-2.146990
C	2.483180	2.785410	-0.763900
C	3.562620	1.746380	-0.502340
C	3.018500	0.593050	0.351440
C	4.085490	-0.460580	0.605520
C	4.494090	-0.715250	1.854620
H	4.068210	-0.192600	2.715750
H	5.287480	-1.440550	2.056510
C	4.728710	-1.123710	-0.580950
H	5.336410	-0.397410	-1.145010
H	5.393290	-1.940650	-0.266830
H	3.967700	-1.523570	-1.263640
H	2.764310	1.017380	1.339350
H	3.929680	1.355650	-1.466210
H	4.424470	2.198940	0.011580
H	2.088280	3.150310	0.200760
H	2.904650	3.657620	-1.288420
H	1.688320	2.018320	-2.609180
C	-0.398870	0.210350	-1.399020
C	-0.008250	-1.074920	-2.091420
O	-0.221130	-1.329390	-3.253260
C	0.834110	-2.006920	-1.205360
C	0.210290	-3.388560	-1.021100
H	-0.029790	-3.811920	-2.008130
H	0.953990	-4.035490	-0.534670
H	-0.701530	-3.388980	-0.414700
O	2.064480	-2.175990	-1.878710
H	1.852550	-2.323210	-2.809190
H	-0.967340	0.817150	-2.105510
H	1.731720	-1.841080	0.746070

H	-0.771650	-1.950800	1.022470
O	-1.340040	-0.624120	2.899420
H	-1.265460	-0.288100	3.798420
H	-1.238390	2.826190	1.710810
C	-3.025010	1.766350	-0.090440
C	-3.128570	3.288410	-0.006160
H	-4.109040	3.612760	-0.384860
H	-2.355280	3.780440	-0.612710
H	-3.043000	3.657520	1.024970
H	-3.799100	1.368120	0.585200
H	-2.014650	-1.855700	-1.183940
H	-4.383510	-0.665710	-1.528250
H	-3.035500	-0.531270	-2.638830
H	-4.385670	1.637040	-1.745770
H	-2.706260	1.727890	-2.221670

Zero-point correction= 0.651006 (Hartree/Particle)
Thermal correction to Energy= 0.683364
Thermal correction to Enthalpy= 0.684308
Thermal correction to Gibbs Free Energy= 0.592288
SCF Done: E(RwB97XD) = -1468.24939778
Thermal correction to Gibbs free energy (ZPG) from GoodVibes: 0.578076

$TS_{14a+16a}$

C	-3.133220	1.866650	-1.168060
C	-2.348120	2.225950	-0.138340
C	-1.539140	1.203340	0.560720
C	-0.700010	1.562990	1.585450
C	0.013350	0.585690	2.374510
O	0.848460	0.862040	3.226650
C	-0.361310	-0.879570	2.171410
C	-1.566750	-1.172810	3.097180
H	-2.433980	-0.539650	2.866600
H	-1.262100	-0.999980	4.139880
H	-1.855620	-2.226570	2.981180
O	0.710210	-1.687600	2.562800
H	1.182710	-1.157470	3.225480
C	-0.813420	-1.139010	0.751910
C	1.029630	-1.325350	-0.282780
C	1.679560	-0.089550	-0.192580
C	1.204690	0.968250	-1.031730
C	1.686940	2.397330	-0.843110
C	2.502400	2.858650	-2.059740
H	3.414760	2.255380	-2.184940
H	2.803880	3.910840	-1.945140
H	1.919490	2.768720	-2.987610
C	2.458960	2.575090	0.468890
C	3.501000	1.479990	0.637680
C	2.847580	0.097750	0.773600
C	3.863320	-1.026020	0.611530
C	3.965050	-2.002410	1.518140
H	4.683290	-2.818330	1.396950
H	3.322420	-2.030300	2.400200
C	4.746630	-0.989380	-0.608960
H	5.202730	-1.969720	-0.804020
H	4.182110	-0.686770	-1.504490
H	5.563520	-0.260030	-0.486610
H	2.451510	0.026090	1.796030
H	4.184650	1.497680	-0.225780
H	4.122380	1.663120	1.526730
H	2.936190	3.567380	0.479140
H	1.770780	2.544320	1.326320
H	0.778140	3.022270	-0.801560
C	0.234130	0.722790	-1.982460
C	-0.139110	-0.613270	-2.380700
O	-0.916570	-0.895110	-3.285500
C	0.531370	-1.762520	-1.636660
C	1.760530	-2.180850	-2.476920
H	2.302530	-2.985540	-1.960960
H	2.443170	-1.338380	-2.651330
H	1.403580	-2.552000	-3.448750
O	-0.354420	-2.845700	-1.559970
H	-0.875680	-2.789710	-2.376720
H	-0.214190	1.547240	-2.543110
C	-1.619530	-0.182000	0.134820
C	-2.770320	-0.619070	-0.755680
C	-3.893000	-1.151810	0.131390
C	-4.132640	-2.465920	0.188170
H	-4.918190	-2.875260	0.829530
H	-3.547190	-3.177240	-0.401300
C	-4.689140	-0.160830	0.935900
H	-4.035880	0.456650	1.573380
H	-5.230370	0.540680	0.280880
H	-5.423020	-0.666170	1.578500
C	-3.243740	0.482020	-1.714560
H	-4.282840	0.281940	-2.022250
H	-2.651110	0.425630	-2.643150
H	-2.423720	-1.469650	-1.353360
H	1.408790	-2.131990	0.349710
H	-1.060190	-2.182520	0.535690
H	-0.554930	2.605430	1.869460
C	-2.268770	3.654930	0.325150
H	-2.560910	3.753830	1.382660
H	-1.245820	4.055070	0.235210
H	-2.932170	4.295190	-0.271420
H	-3.711740	2.644520	-1.677880

Zero-point correction= 0.621618 (Hartree/Particle)
Thermal correction to Energy= 0.654249
Thermal correction to Enthalpy= 0.655193
Thermal correction to Gibbs Free Energy= 0.562358
SCF Done: E(RwB97XD) = -1466.98660655
Thermal correction to Gibbs free energy (ZPG) from GoodVibes: 0.547768

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C	-3.387280	1.271670	-1.554230
C	-2.731300	1.935070	-0.583970
C	-1.748050	1.228340	0.265980
C	-1.175090	1.837020	1.327470
C	-0.224140	1.139070	2.187320
O	0.566880	1.709130	2.919740
C	-0.325640	-0.384580	2.236180
C	-1.557260	-0.730060	3.088700
H	-2.493760	-0.376650	2.643060
H	-1.447780	-0.284250	4.088550
H	-1.611880	-1.822430	3.195200
O	0.813200	-0.871890	2.893470
H	1.165590	-0.104350	3.374540
C	-0.437370	-0.983190	0.810310
C	0.969960	-1.273640	0.220020
C	1.647720	0.048470	-0.057450
C	0.946790	0.830650	-0.895740
C	1.284730	2.259000	-1.228290
C	1.832590	2.393440	-2.653640
H	2.796970	1.873040	-2.758930
H	1.982090	3.450840	-2.920650
H	1.141460	1.953020	-3.388990
C	2.224740	2.816030	-0.151110
C	3.381790	1.860240	0.128490
C	2.899020	0.505870	0.668370
C	3.989160	-0.560240	0.686270
C	4.054370	-1.446290	1.685720
H	4.813840	-2.233340	1.699810
H	3.338930	-1.421410	2.511780
C	4.980630	-0.584230	-0.447600
H	5.704450	0.241720	-0.355470
H	5.545720	-1.526420	-0.462630
H	4.489440	-0.461290	-1.425670
H	2.587100	0.651990	1.714990
H	3.950370	1.712840	-0.802990
H	4.083450	2.306120	0.850280
H	2.611210	3.799970	-0.461120
H	1.653810	2.971890	0.778770
H	0.337630	2.827090	-1.184650
C	-0.316240	0.201370	-1.427210
C	0.064310	-1.111180	-2.069510
O	-0.237150	-1.446840	-3.190380
C	0.821180	-2.041310	-1.107460

C	2.157450	-2.458530	-1.708260
H	1.983610	-2.987800	-2.657330
H	2.685720	-3.121760	-1.009220
H	2.789740	-1.588260	-1.921960
O	0.012700	-3.184730	-0.888800
H	-0.155820	-3.580280	-1.752020
H	-0.812380	0.842610	-2.163210
C	-1.287630	-0.139660	-0.206490
C	-2.504060	-0.960610	-0.746790
C	-3.473280	-1.448930	0.320480
C	-3.436790	-2.731340	0.701110
H	-4.121320	-3.120550	1.460070
H	-2.712730	-3.430880	0.273720
C	-4.490550	-0.499450	0.899240
H	-4.020040	0.384060	1.357000
H	-5.166780	-0.114810	0.119250
H	-5.100890	-0.999990	1.663450
C	-3.214920	-0.181530	-1.861610
H	-4.196670	-0.637140	-2.069910
H	-2.647290	-0.288000	-2.803580
H	-2.080800	-1.871630	-1.187880
H	1.533520	-1.886970	0.928890
H	-0.928910	-1.955920	0.921090
H	-1.381300	2.876560	1.586100
C	-2.991640	3.393760	-0.323450
H	-3.710620	3.798160	-1.048240
H	-3.404800	3.553800	0.685270
H	-2.065990	3.987010	-0.392390
H	-4.099160	1.826610	-2.174380

Zero-point correction= 0.627164 (Hartree/Particle)
Thermal correction to Energy= 0.658866
Thermal correction to Enthalpy= 0.659810
Thermal correction to Gibbs Free Energy= 0.569866
SCF Done: E(RwB97XD) = -1467.04937960
Thermal correction to Gibbs free energy (ZPG) from GoodVibes: 0.555340

TS'$_{14a+16a}$

C	-3.247780	2.051130	-0.884570
C	-3.167200	0.755710	-1.684130
C	-2.650980	-0.446780	-0.884140
C	-3.719040	-1.175890	-0.066920
C	-3.795150	-2.509970	-0.122620
H	-4.536120	-3.063100	0.461380
H	-3.112200	-3.093720	-0.746080
C	-4.672160	-0.373590	0.776850
H	-4.145280	0.358840	1.408290
H	-5.372450	0.196640	0.145250
H	-5.265790	-1.025910	1.431840
C	-1.462690	-0.082480	-0.014940
C	-1.285310	1.233870	0.493760
C	-0.395830	1.429780	1.534660
C	0.044760	0.359790	2.405030
O	0.783100	0.515350	3.369460
C	-0.493610	-1.036390	2.112320
C	-1.829980	-1.214370	2.845040
H	-1.655790	-1.129170	3.927300
H	-2.232360	-2.213140	2.625970
H	-2.572040	-0.462460	2.550280
O	0.423710	-1.973570	2.609480
H	0.871610	-1.511650	3.337160
C	-0.658760	-1.186180	0.589430
C	0.788370	-1.360810	-0.077250
C	1.596800	-0.120340	0.003460
C	1.325040	0.893820	-0.909610
C	2.034290	2.193880	-0.827580
C	2.877100	2.410950	0.194210
C	3.102380	1.431240	1.306500
C	2.774470	-0.026500	0.945840
C	3.948610	-0.794140	0.343430
C	4.252500	-2.013540	0.800030
H	5.072850	-2.594960	0.369890
H	3.689060	-2.472330	1.617540
C	4.718890	-0.142160	-0.772170
H	5.251110	0.753390	-0.413460
H	4.049860	0.200310	-1.577190
H	5.458980	-0.831280	-1.201660
H	2.502000	-0.554680	1.868450
H	4.139630	1.497110	1.670880
H	2.471780	1.726020	2.163460
H	3.397290	3.372120	0.258380
C	1.788050	3.222660	-1.895610
H	2.427130	4.103360	-1.746590
H	0.740840	3.568110	-1.892470
H	1.988440	2.818090	-2.900610
C	0.301380	0.663850	-1.849310
C	-0.016150	-0.665780	-2.313230
O	-0.743980	-0.909150	-3.268180
C	0.597690	-1.824280	-1.531630
C	1.929880	-2.225930	-2.176910
H	2.372610	-3.053560	-1.605350
H	2.648620	-1.397340	-2.209150
H	1.737940	-2.565280	-3.205030
O	-0.287680	-2.911830	-1.594360
H	-0.748680	-2.804080	-2.441920
H	-0.069640	1.471910	-2.481810
H	1.264680	-2.161250	0.501120
H	-1.150920	-2.143310	0.382230
H	-0.105420	2.433210	1.849240
C	-1.930490	2.427320	-0.199960
C	-2.125420	3.645020	0.703230
H	-2.727990	3.390430	1.589360
H	-2.653700	4.437180	0.151950
H	-1.173850	4.071190	1.049950
H	-1.219690	2.716810	-0.994000
H	-2.303570	-1.191160	-1.611400
H	-4.150830	0.511340	-2.114260
H	-2.487440	0.892060	-2.539670
H	-4.035120	1.988330	-0.118370
H	-3.544810	2.876180	-1.551340

Zero-point correction= 0.624714 (Hartree/Particle)
Thermal correction to Energy= 0.656220
Thermal correction to Enthalpy= 0.657165
Thermal correction to Gibbs Free Energy= 0.567686
SCF Done: E(RwB97XD) = -1466.99771373
Thermal correction to Gibbs free energy (ZPG) from GoodVibes: 0.553352

16a+14a

C	-3.466490	1.427760	-1.477300
C	-3.117990	0.016890	-1.948300
C	-2.429590	-0.858080	-0.887050
C	-3.410570	-1.465310	0.107240
C	-3.375090	-2.782020	0.343410
H	-4.066910	-3.253170	1.047490
H	-2.640910	-3.428140	-0.145590
C	-4.451550	-0.601520	0.773860
H	-5.244850	-0.323520	0.061550
H	-4.928850	-1.136840	1.606350
H	-4.029250	0.336350	1.165700
C	-1.193800	-0.118480	-0.252110
C	-1.587750	1.268380	0.240920
C	-1.162240	1.753530	1.422350
C	-0.340180	0.967890	2.338490
O	0.377040	1.466640	3.188810
C	-0.462770	-0.548190	2.267050
C	-1.757560	-0.925220	3.003120
H	-1.693130	-0.580560	4.045710
H	-1.861600	-2.019030	2.998570
H	-2.648510	-0.487010	2.541530
O	0.617050	-1.100690	2.972480
H	0.932740	-0.375250	3.537390
C	-0.466640	-1.044540	0.796100
C	0.977250	-1.354620	0.320400
C	1.684350	-0.042310	0.117440
C	1.118400	0.753280	-0.810190
C	1.680760	2.073290	-1.157020
C	2.583470	2.602560	-0.314730

C	2.974320	1.922990	0.970840
C	2.892290	0.383880	0.918860
C	4.148760	-0.295590	0.395730
C	4.695020	-1.315360	1.066190
H	5.581170	-1.835650	0.691390
H	4.273090	-1.665270	2.012630
C	4.723330	0.208790	-0.900340
H	5.123510	1.228580	-0.782380
H	3.948790	0.272200	-1.681240
H	5.535390	-0.438860	-1.259380
H	2.729610	0.016240	1.941590
H	3.985390	2.230850	1.279430
H	2.295220	2.276990	1.766690
H	3.027860	3.576890	-0.540590
C	1.260370	2.743950	-2.434700
H	1.851780	3.651630	-2.616390
H	0.198890	3.040360	-2.413050
H	1.386490	2.072180	-3.299260
C	-0.133460	0.168680	-1.417610
C	0.258180	-1.156000	-2.031360
O	0.043660	-1.471360	-3.177400
C	0.912910	-2.110840	-1.022680
C	2.276470	-2.574240	-1.518840
H	2.700540	-3.292080	-0.803330
H	2.976070	-1.738010	-1.634800
H	2.161000	-3.060050	-2.499730
O	0.051670	-3.228100	-0.879030
H	-0.057730	-3.613070	-1.756420
H	-0.556820	0.793350	-2.206520
H	1.476480	-1.978830	1.068430
H	-0.990880	-2.004780	0.800160
H	-1.343450	2.785670	1.723530
C	-2.322160	2.156010	-0.753840
C	-2.811480	3.482660	-0.180760
H	-3.498810	3.323630	0.665190
H	-3.356520	4.043360	-0.954320
H	-1.983990	4.118740	0.163650
H	-1.568680	2.402480	-1.521320
H	-2.006150	-1.723790	-1.413080
H	-4.030210	-0.494440	-2.293670
H	-2.462140	0.071620	-2.830850
H	-4.340040	1.409510	-0.811020
H	-3.769230	2.036580	-2.343900

Zero-point correction= 0.627801 (Hartree/Particle)
Thermal correction to Energy= 0.659469
Thermal correction to Enthalpy= 0.660413
Thermal correction to Gibbs Free Energy= 0.570332
SCF Done: E(RwB97XD) = -1467.03798431
Thermal correction to Gibbs free energy (ZPG) from GoodVibes: 0.555994

$TS_{14a+15a}$

C	-2.688270	3.473540	-0.278130
O	0.979100	1.704690	2.798190
C	-2.540960	1.994030	-0.511870
O	0.946060	-0.932520	2.839870
C	-1.570570	1.231860	0.305450
O	-0.891270	-1.756080	-2.946310
C	-1.547980	-0.215830	0.218670
O	-0.197910	-3.167790	-0.794990
C	-0.654750	-0.939700	1.011450
C	1.143160	-1.308320	-0.012490
C	1.752300	-0.077240	-0.282490
C	2.931430	0.380600	0.573540
C	3.993650	-0.709610	0.647670
C	4.840120	-0.935930	-0.578750
C	4.164580	-1.433990	1.757590
C	3.521660	1.720980	0.113840
C	2.448910	2.678120	-0.374480
C	1.761790	2.110320	-1.617400
C	0.710680	3.067780	-2.174670
C	1.238660	0.700670	-1.374400
C	0.246080	0.179700	-2.181150
C	-0.177750	-0.302350	2.297910
C	-1.337000	-0.402290	3.319010
C	0.121610	1.181250	2.097730
C	-0.701380	1.887460	1.143570
C	-3.306260	1.349370	-1.409130
C	-3.252880	-0.120540	-1.665430
C	-2.678300	-0.933760	-0.498150
C	-3.734460	-1.339530	0.527290
C	-4.607920	-0.266000	1.116850
C	-3.848760	-2.621310	0.890720
C	0.636790	-2.111370	-1.183720
C	-0.096760	-1.223170	-2.179960
C	1.864500	-2.694480	-1.921390
H	-1.759280	4.027350	-0.485000
H	5.636960	-0.179030	-0.658160
H	4.915740	-2.227390	1.808650
H	3.547520	-1.272860	2.643730
H	1.713020	2.859470	0.424570
H	2.549870	2.000080	-2.387790
H	0.371450	2.786690	-3.181050
H	1.127390	4.083440	-2.242360
H	-0.169570	3.100070	-1.518290
H	-0.847450	-2.014400	1.079740
H	-2.244970	0.109030	2.972580
H	-1.011510	0.046890	4.268850
H	-1.568780	-1.462830	3.489060
H	-0.633530	2.975590	1.161880
H	-3.473370	3.891700	-0.922150
H	-2.957960	3.682610	0.769430
H	-5.282310	-0.676530	1.880840
H	-5.221590	0.219780	0.341350
H	-4.006410	0.533710	1.578170
H	-4.581610	-2.939350	1.637580
H	-3.207660	-3.394610	0.458120
H	-2.276230	-1.868890	-0.901070
H	-4.259360	-0.493390	-1.914000
H	-2.643730	-0.309540	-2.565320
H	-4.014120	1.934000	-2.006290
H	1.504100	-3.324220	-2.747910
H	2.450220	-3.312450	-1.226680
H	2.508010	-1.906140	-2.334000
H	1.578310	-1.901840	0.795500
H	-0.237770	0.785010	-2.948150
H	2.895860	3.652750	-0.625320
H	4.237300	1.563430	-0.709850
H	4.094030	2.155510	0.946490
H	2.556050	0.528070	1.594600
H	5.321460	-1.923360	-0.557280
H	4.240890	-0.863710	-1.499650
H	1.411840	-0.226320	3.317470
H	-0.742310	-3.346320	-1.578510

Zero-point correction= 0.622757 (Hartree/Particle)
Thermal correction to Energy= 0.654967
Thermal correction to Enthalpy= 0.655911
Thermal correction to Gibbs Free Energy= 0.564653
SCF Done: E(RwB97XD) = -1466.98519590
Thermal correction to Gibbs free energy (ZPG) from GoodVibes: 0.550054

4

C	-3.313890	3.124840	-0.370940
O	0.643290	1.996060	2.664610
C	-2.882070	1.702460	-0.604270
O	1.031920	-0.556480	2.871290
C	-1.790760	1.143510	0.223470
O	-0.234140	-1.677510	-3.100120
C	-1.239200	-0.214620	-0.175020
O	0.161610	-3.235140	-0.680870
C	-0.308200	-0.924910	0.870230
C	1.079680	-1.206740	0.240090
C	1.700020	0.105560	-0.176830
C	2.984070	0.625850	0.447120
C	4.081200	-0.429950	0.553260
C	5.067130	-0.555560	-0.579240
C	4.169600	-1.211670	1.634800

C	3.451030	1.910100	-0.249600
C	2.288520	2.831430	-0.591170
C	1.328880	2.168700	-1.584700
C	0.156010	3.094520	-1.902540
C	0.944430	0.802470	-1.048130
C	-0.328380	0.089780	-1.453800
C	-0.163430	-0.198240	2.232600
C	-1.331620	-0.541500	3.171040
C	-0.158740	1.317780	2.045560
C	-1.213010	1.873400	1.202790
C	-3.505480	0.931250	-1.514510
C	-3.212540	-0.515560	-1.748750
C	-2.410790	-1.157470	-0.609610
C	-3.304640	-1.636170	0.527140
C	-4.372740	-0.729310	1.082640
C	-3.156430	-2.882010	0.993360
C	0.911860	-2.080770	-1.017740
C	0.086210	-1.252050	-2.015690
C	2.239520	-2.493080	-1.640550
H	-2.483380	3.835280	-0.501230
H	5.772200	0.291470	-0.583650
H	4.940210	-1.983750	1.715630
H	3.463290	-1.115690	2.463260
H	1.731050	3.087600	0.326890
H	1.878250	2.003460	-2.531930
H	-0.546670	2.663240	-2.629760
H	0.531460	4.037270	-2.327630
H	-0.404830	3.338860	-0.990010
H	-0.748060	-1.903600	1.089540
H	-2.308140	-0.301430	2.735580
H	-1.218050	0.006270	4.118470
H	-1.299880	-1.619340	3.383270
H	-1.490420	2.909850	1.400490
H	-4.113280	3.408400	-1.068300
H	-3.698000	3.258370	0.653200
H	-4.917290	-1.224610	1.898310
H	-5.102170	-0.447440	0.306760
H	-3.957770	0.214300	1.468340
H	-3.783150	-3.265660	1.803390
H	-2.394530	-3.553630	0.587610
H	-1.939580	-2.067340	-0.999290
H	-4.157420	-1.063860	-1.895430
H	-2.664410	-0.635150	-2.700340
H	-4.300060	1.380410	-2.119600
H	2.049630	-3.103090	-2.536640
H	2.824300	-3.076420	-0.915740
H	2.824190	-1.618790	-1.951260
H	1.698250	-1.741650	0.965680
H	-0.891930	0.637790	-2.212950
H	2.665550	3.776110	-1.014360
H	3.974730	1.661890	-1.186930
H	4.183010	2.424800	0.392080
H	2.704610	0.887140	1.480820
H	5.654030	-1.480450	-0.493030
H	4.571250	-0.554130	-1.562250
H	1.366330	0.275160	3.247880
H	-0.012190	-3.709440	-1.502300

Zero-point correction= 0.627516 (Hartree/Particle)
Thermal correction to Energy= 0.659085
Thermal correction to Enthalpy= 0.660029
Thermal correction to Gibbs Free Energy= 0.570606
SCF Done: E(RwB97XD) = -1467.04651114
Thermal correction to Gibbs free energy (ZPG) from GoodVibes: 0.556134

TS'$_{14a+15a}$

C	3.389000	2.234890	-0.344730
C	3.238310	1.501990	0.985930
C	2.709310	0.068030	0.857440
C	3.758970	-0.980540	0.478010
C	3.805100	-2.134790	1.152620
H	4.530910	-2.912740	0.899490
H	3.108960	-2.346530	1.968600
C	4.732460	-0.697760	-0.634550
H	5.452630	0.082350	-0.339580
H	5.303740	-1.599410	-0.894650
H	4.228160	-0.339490	-1.545020
C	1.494630	0.001090	-0.052890
C	1.328930	0.937600	-1.114040
C	0.417520	0.670600	-2.117460
C	-0.055900	-0.664910	-2.403770
O	-0.821570	-0.953410	-3.315280
C	0.520540	-1.791970	-1.549110
C	1.850550	-2.246110	-2.165950
H	2.578160	-1.428780	-2.239770
H	1.660670	-2.637180	-3.175800
H	2.279690	-3.047530	-1.548340
O	-0.379130	-2.867210	-1.579000
H	-0.851750	-2.760940	-2.421560
C	0.713840	-1.277340	-0.110040
C	-0.703900	-1.214540	0.614960
C	-1.575840	-0.157520	0.046210
C	-1.336740	1.151540	0.432170
C	-2.181850	2.258210	-0.080350
C	-3.040270	2.002380	-1.080270
C	-3.154650	0.658410	-1.736810
C	-2.759030	-0.512830	-0.823010
C	-3.889110	-1.033810	0.060950
C	-4.110950	-2.349550	0.149600
H	-4.895850	-2.752780	0.795670
H	-3.512440	-3.067270	-0.418670
C	-4.709130	-0.032710	0.828070
H	-5.285650	0.612160	0.145660
H	-4.071110	0.640950	1.421160
H	-5.415110	-0.532210	1.505820
H	-2.455500	-1.353200	-1.459620
H	-4.177370	0.503130	-2.113920
H	-2.504130	0.634300	-2.628090
H	-3.683320	2.807670	-1.449360
C	-2.118180	3.597200	0.601240
H	-2.326570	3.498140	1.679110
H	-2.855850	4.289160	0.172580
H	-1.127800	4.067100	0.510140
C	-0.248170	1.373210	1.307860
C	0.113100	0.393120	2.305130
O	0.860430	0.611880	3.250420
C	-0.472610	-1.004060	2.121140
C	-1.777080	-1.125990	2.918250
H	-2.194110	-2.132440	2.773910
H	-2.528420	-0.387320	2.611600
H	-1.556500	-0.981240	3.985720
O	0.454500	-1.935850	2.615320
H	0.919720	-1.467310	3.326630
H	0.097210	2.385290	1.518660
H	-1.150170	-2.202080	0.450000
H	1.255400	-2.040700	0.460380
H	0.172820	1.435230	-2.860750
C	2.099780	2.252250	-1.178900
C	1.231430	3.473330	-0.849860
H	1.713840	4.386910	-1.227510
H	1.108930	3.593900	0.235020
H	0.232750	3.399920	-1.305370
H	2.390300	2.360440	-2.236120
H	2.379840	-0.233940	1.858910
H	4.201040	1.486520	1.519780
H	2.540280	2.047940	1.640600
H	4.194620	1.779320	-0.934170
H	3.707780	3.272890	-0.159900

Zero-point correction= 0.625118 (Hartree/Particle)
Thermal correction to Energy= 0.656398
Thermal correction to Enthalpy= 0.657343
Thermal correction to Gibbs Free Energy= 0.568700
SCF Done: E(RwB97XD) = -1466.99393807
Thermal correction to Gibbs free energy (ZPG) from GoodVibes: 0.554365

15a+14a

C	3.703830	-1.746030	-0.834410
C	3.227980	-0.581820	-1.693910
C	2.516950	0.503000	-0.867570
C	3.513640	1.292260	-0.026020
C	4.146690	0.818620	1.051720
H	4.868710	1.434190	1.595080
H	3.955880	-0.176720	1.456630
C	3.786830	2.678910	-0.543490
H	2.854070	3.265650	-0.563870
H	4.532870	3.210280	0.063340
H	4.153340	2.635920	-1.583280
C	1.271710	-0.068680	-0.111020
C	1.646270	-1.322010	0.662190
C	1.072200	-1.617590	1.843680
C	0.174540	-0.694440	2.531690
O	-0.638380	-1.033010	3.374030
C	0.379670	0.793240	2.255810
C	1.594620	1.236260	3.084170
H	2.510270	0.701460	2.815770
H	1.379010	1.070180	4.149810
H	1.758020	2.311720	2.924480
O	-0.741070	1.479200	2.751750
H	-1.134190	0.861920	3.391970
C	0.562490	1.065360	0.733420
C	-0.812770	1.407180	0.097660
C	-1.646670	0.153140	0.113280
C	-1.122090	-0.866990	-0.594440
C	-1.865350	-2.129060	-0.794030
C	-2.874700	-2.391170	0.052470
C	-3.213790	-1.465850	1.190380
C	-2.949650	0.019020	0.869070
C	-4.084740	0.718750	0.136720
C	-4.533950	1.902870	0.566060
H	-5.330450	2.436510	0.039430
H	-4.118790	2.379170	1.458830
C	-4.658630	0.042800	-1.079460
H	-5.188460	-0.882260	-0.801190
H	-3.865680	-0.259270	-1.781820
H	-5.366690	0.698020	-1.606120
H	-2.807680	0.552210	1.817750
H	-4.262120	-1.599120	1.498640
H	-2.600070	-1.741700	2.065420
H	-3.470360	-3.299550	-0.080040
C	-1.549920	-2.993950	-1.982210
H	-1.556100	-2.400080	-2.911060
H	-2.289690	-3.799420	-2.086440
H	-0.557580	-3.459780	-1.908100
C	0.215600	-0.545630	-1.216800
C	-0.054310	0.635260	-2.127220
O	0.160220	0.653640	-3.315210
C	-0.616960	1.851600	-1.366730
C	-1.897510	2.347060	-2.024700
H	-2.263630	3.236350	-1.493630
H	-2.683780	1.583920	-2.016980
H	-1.688860	2.604790	-3.074330
O	0.358930	2.880860	-1.400300
H	0.499410	3.111830	-2.325550
H	0.606730	-1.367350	-1.819000
H	-1.282340	2.217260	0.664660
H	1.179470	1.967550	0.648580
H	1.252660	-2.578050	2.335310
C	2.595020	-2.351940	0.045490
C	1.852040	-3.469090	-0.705340
H	2.520380	-4.333420	-0.833370
H	1.544320	-3.149710	-1.711180
H	0.958600	-3.802010	-0.157530
H	3.081500	-2.840230	0.904710
H	2.119380	1.235080	-1.580390
H	4.089420	-0.129070	-2.209040
H	2.554320	-0.928560	-2.493240
H	4.533220	-1.400420	-0.202420
H	4.123100	-2.539340	-1.472840

Zero-point correction= 0.626818 (Hartree/Particle)
Thermal correction to Energy= 0.658848
Thermal correction to Enthalpy= 0.659792
Thermal correction to Gibbs Free Energy= 0.568640
SCF Done: E(RwB97XD) = -1467.03124268
Thermal correction to Gibbs free energy (ZPG) from GoodVibes: 0.554196

3. Target Profiling of Natural 1−5 and Their Enantiomers 6−10

3.1 Cell culture

The HT1080 cells were obtained from ATCC and maintained in DMEM (Thermo Fisher Scientific) supplemented with 10% (vol./vol.) dialyzed fetal bovine serum (Thermo Fisher Scientific), 100 U ml^{-1} penicillin and 100 mg ml^{-1} streptomycin in a humidified atmosphere at 37 °C with 5% CO_2.

3.2 In-gel fluorescence analysis

The HT1080 cells were lysed by sonication in ice and cell lysates were collected by centrifugation (20000 *g*, 10 min) at 4 °C to remove the debris. The protein concentration was determined by using the bicinchoninic acid (BCA) protein assay kit (Pierce). Then, 100 µl of cell lysates (2 mg ml^{-1}) were incubated with compounds at 29 °C for 1 h. Then, samples were added IA-alkyne and incubated at 25 °C for an hour and then underwent click chemistry. The samples were added Rhodamine-azide (Rh-N_3), tris(2-carboxyethyl) phosphine hydrochloride (TCEP) (1 mM, 50×fresh stock in water), tris[(1-benzyl-1H-1,2,3-triazol-4-yl)methyl]amine (TBTA ligand) (100 µM, 17× stock in DMSO:*t*-butanol = 1:4), and copper(II) sulfate (1 mM, 50× stock in water) and incubated at 25 °C for an hour. The reacted samples were resolved on 10% SDS–PAGE gels and imaged by ChemiDoc XRS+ (Bio-Rad). The gels were then stained by Coomassie brilliant blue to demonstrate equal loading.

3.3 Cytotoxicity assays

The cell line HT1080 was obtained from ATCC (Manassas, VA, USA). Cells were cultured in DMEM medium (Biological Industries, Kibbutz Beit-Haemek, Israel) supplemented with 10% fetal bovine serum (Biological Industries) at 37 °C in a humidified atmosphere with 5% CO_2. The cytotoxicity assay was evaluated by the 3-(4,5-dimethylthiazol-2-yl)-5-(3-carboxymethoxyphenyl)-2-(4-sulfophenyl)-2*H*-tetrazolium, inner salt (MTS) (Promega, Madison, WI, USA) assay. Briefly, each well of a 96-well were seeded about 10^4 cells. After 12 h of incubation at 37 °C, the medium was removed and the test compound (100, 40, 10 μM) dissolved in serum-free medium was added in each well. After incubated for 24 h, cells were subjected to the MTS assay and the OD value was recorded at 490 nm. The inhibition rate was then calculated.

3.4 Competitive rdTOP-ABPP analysis of 4 and 9

The HT1080 cells were lysed in 500 μL of PBS with 0.1% Triton X-100 (Sigma-Aldrich). After sonication on ice, the cell lysates were centrifugated for 20000 *g*, 30 min at 4 °C to remove the sediment. Protein concentration was detected by using the BCA protein assay Kit and adjusted to 2 mg/mL. Then, 1000 μl of cell lysates (2 mg ml^{-1}) were incubated with compounds at 29 °C for 1 h. Samples were then added IA-alkyne and incubated at 25 °C for an hour. Then the samples reacted with 1 mM $CuSO_4$, 100 μM TBTA ligand, 100 μM acid-cleavable azide-biotin tag and 1 mM TCEP for 1 h on thermo mixer at room temperature. The products of click-labeled lysates were centrifuged for 8000 *g*, 5 min at 4 °C and washed three times with 1 mL cold methanol. The proteomes were resuspended in 1 mL PBS with 1.2% SDS. The samples were sonicated and heated at 90 °C for 10 min to dissolve the proteins, followed by centrifuging at 20000 *g*, 2 min at room temperature to remove the remaining cupric ion. The solution was diluted five times with 5 mL of PBS containing 100 μL of prewashed streptavidin Beads (Thermo Fisher Scientific) and incubated for 4 h at 29 °C on a rotator. After washing in 5 mL PBS and 5 ml distilled water for three times orderly, the resulting beads were resuspended in 500 μL PBS with 6 M urea and 10 mM DTT at 37 °C for 30 min and alkylated by addition of 20 mM iodoacetamide at 35 °C for 30 min. The beads were collected by centrifugation (1700 *g*, 3 min) and resuspended in 200 μL of 100 mM triethylammonium bicarbonate (TEAB) buffer (Sigma) and 10 ng/μL trypsin (Promega). Trypsin digestion was performed at 37 °C in a thermomixer overnight.

The beads were collected by centrifugation and washed with 1 mL PBS, 1 mL H_2O and 100 mM TEAB buffer for twice orderly, followed by suspending in 100 μL TEAB buffer. The peptides were reacted with 8 μL of 4% $D^{13}CDO$ (Sigma) for samples by adding **4** or **9** (100 μM), DCDO (Sigma) for samples by adding **4** or **9** (10 μM), or HCHO (Sigma) for samples by adding DMSO, respectively. 8 μL of 0.6 M $NaBH_3CN$ was added to the samples of DMSO and **4** or **9** (10 μM) groups and 8 μL of 0.6 M $NaBD_3CN$ was added to the samples of **4** or **9** (100 μM) group. The reaction was incubated for 1 h at room temperature and the beads were washed with 1 mL H_2O for twice. The labeled samples were combined and subjected for on-beads cleavage by using 200 μL of 2% formic acid solution (sigma) for twice. The eluant containing the peptides was collected for LC-MS/MS analysis.

3.5 LC-MS/MS and data analysis

Samples were analyzed by LC-MS/MS on Q Exactive-plus series Orbitrap mass spectrometers (Thermo Fisher Scientific) coupled with EasyNano-LC. Mobile phase A was 0.1% FA in H_2O, and mobile phase B was 0.1% FA in ACN. The flow rate was 3 μL/min for loading and 0.3 μL/min for eluting. Labeled peptide samples were loaded onto a 100 μm fused silica column packed with 15 cm × 3 μm C18 resin. Under the positive-ion mode, full-scan mass spectra were acquired over the m/z range from 350 to 1800 using the Orbitrap mass analyzer with mass resolution of 70,000. MS/MS fragmentation is performed in a data-dependent mode, of which the TOP 20 most intense ions are selected for MS2 analysis a resolution of 17,500 using collision mode of HCD. Other important parameters: isolation window, 2.0 m/z units; default charge, 2^+; normalized collision energy, 28%; maximum IT, 50 ms; and dynamic exclusion, 20.0 s. LC-MS/MS data were analyzed by ProLuCID[25] with static

modification of cysteine carbamidomethylation (+57.0215 Da). For rdTOP-ABPP data, additional modifications include N-terminus dimethyl labeling and lysine residue dimethyl labeling (+28.03130 Da (light), +32.05641 Da (medium), and +36.07567 Da (heavy)) and variable oxidation of methionine (+15.9949 Da). The ratios of rdTOP-ABPP were quantified by the CIMAGE 2.0 software as described previously.

We will take light/medium ratio as an example to explain the ratio meaning (Seeing Figure S20 below, detailed methods can can be referred to Nat. Methods, 2014, 11, 79-85; Anal. Chem., 2018, 90, 9576–9582.). The same proteome was incubated with DMSO or compound **4** (10 μM). In this 'competitive' version, cysteines of target A formed covalent bonds with **4**, but target B cannot form covalent bonds with **4**. In chemical proteomics, we cannot identify the target of **4** directly because of the lack of an alkynyl handle in **4**. Therefore, we introduced an IA-alkyne probe to the proteome. When reacted with IA-alkyne, an alkynyl handle was introduced to target B, but target A cannot carry the alkynyl handle because of the formation of a covalent bond with **4**. Therefore, target B can be enriched in the same abundance in the DMSO and compound **4** groups. However, for target A, the DMSO group was enriched much more than the compound **4** group. To show differences of target abundance in the two groups, reduction dimethylation isotope labelling was used in the two groups. The DMSO group was labelled with "light" (HCHO, $NaBH_3CN$); the compound **4** group was labelled with "medium" (DCDO, $NaBH_3CN$). Through isotope labelling, the "light" peptide B digested from target B in the DMSO group will have 4 Da less than "medium" peptide B in the compound **4** group, and the ratio of light/medium peptides B will be "1" when calculating the MS1 intensity. However, for "light" peptide A digested from target A in the DMSO group will have much more abundance than the "medium" peptide A in the compound **4** group, and the ratio of light/medium peptides A will be assigned a value of "positive infinity" (or set a number artificially, here, we set it as "15"). Therefore, we can know if the ratio of light/medium close to 15, it indicates that compound **4** binds most of target A, while IA-alkyne will form less covalent bonds with target A. If the value is closer to 1, it means that the compound **4** almost cannot bind to target A, while the IA-alkyne will bind most of target A. Hence, we can conclude that the light/medium ratio reflects the competitiveness of the given compounds with IA-alkyne. The higher the ratio value, the stronger the competition ability of the given compound against IA-alkyne.

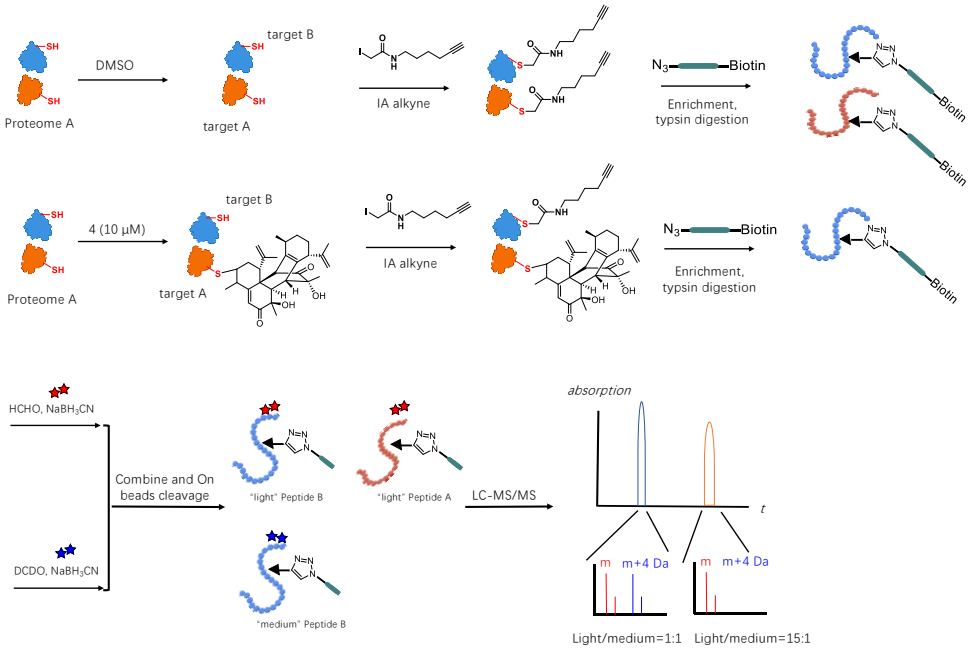
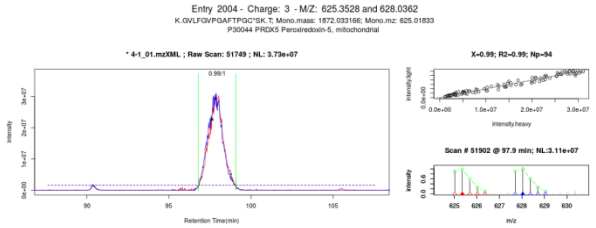


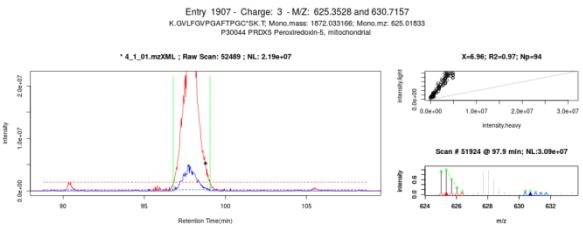
Figure S20. A simplified graph to illustrate the meaning of ratio.

3.6 Analysis of targets in the compound 4 and 9 groups

For PRDX5 C100 in the compound **4** group:

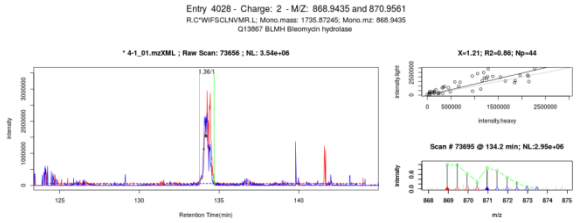


Low concentration (10 μM)

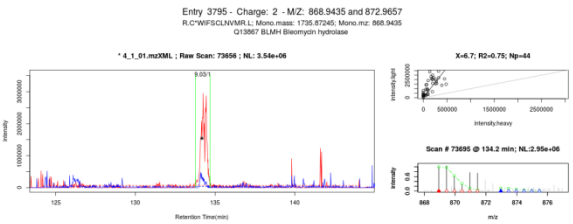


High concentration (100 μM)

For BLMH C73 in the compound **4** group:

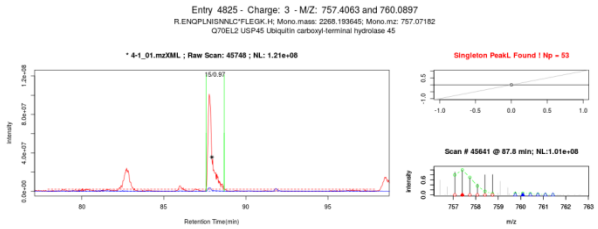


Low concentration (10 μM)

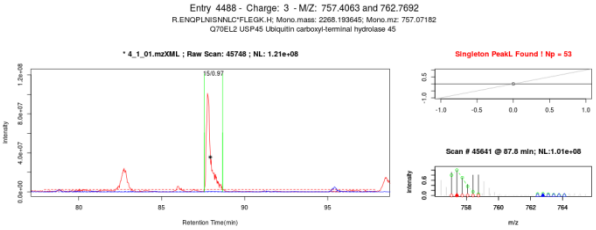


High concentration (100 μM)

For USP45 C588 in the compound **4** group:

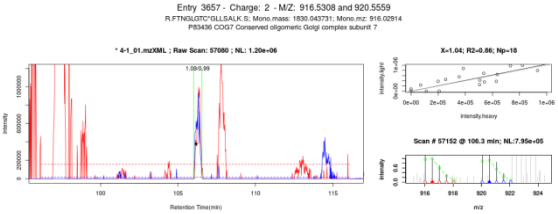


Low concentration (10 μM)

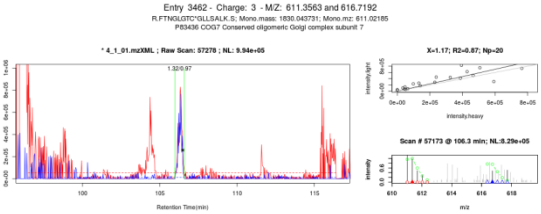


High concentration (100 μM)

For COG7 C419 in the compound **4** group:

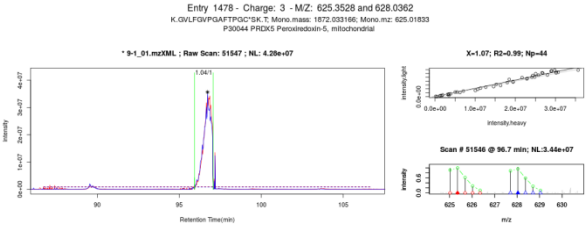


Low concentration (10 μM)

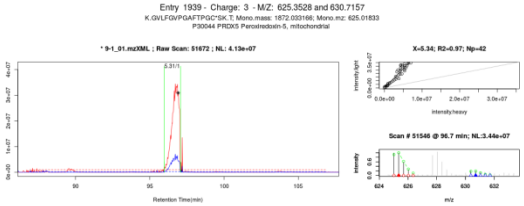


High concentration (100 μM)

For PRDX5 C100 in the compound **9** group:

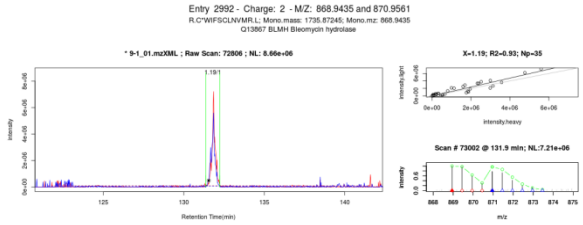


Low concentration (10 μM)

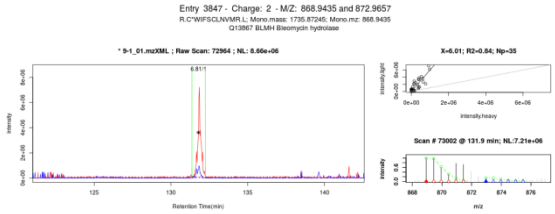


High concentration (100 μM)

For BLMH C73 in the compound **9** group:

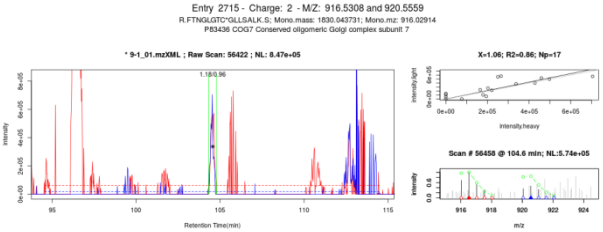


Low concentration (10 μM)

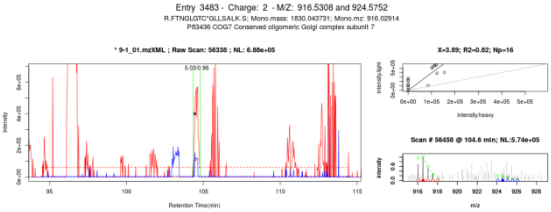


High concentration (100 μM)

For COG7 C419 in the compound **9** group:



Low concentration (10 μM)



High concentration (100 μM)

4. 1D and 2D NMR, HRESI and Optical Rotation Spectra of 1−5

Figure S21. ^{1}H NMR spectrum of natural henryinin A (**1**) at 500 MHz in pyridine-d_5

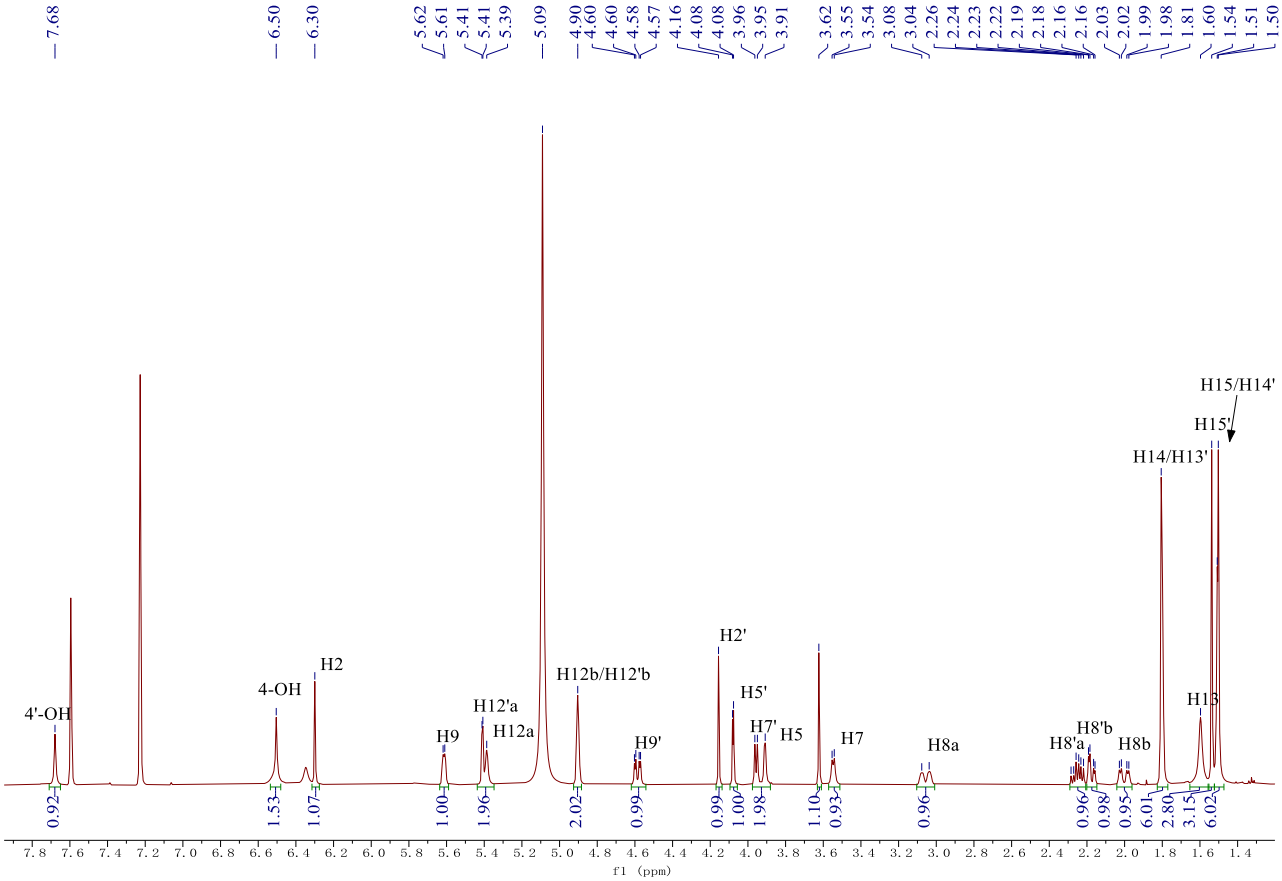


Figure S22. ^{13}C NMR spectrum of natural henryinin A (**1**) at 125 MHz in pyridine-d_5

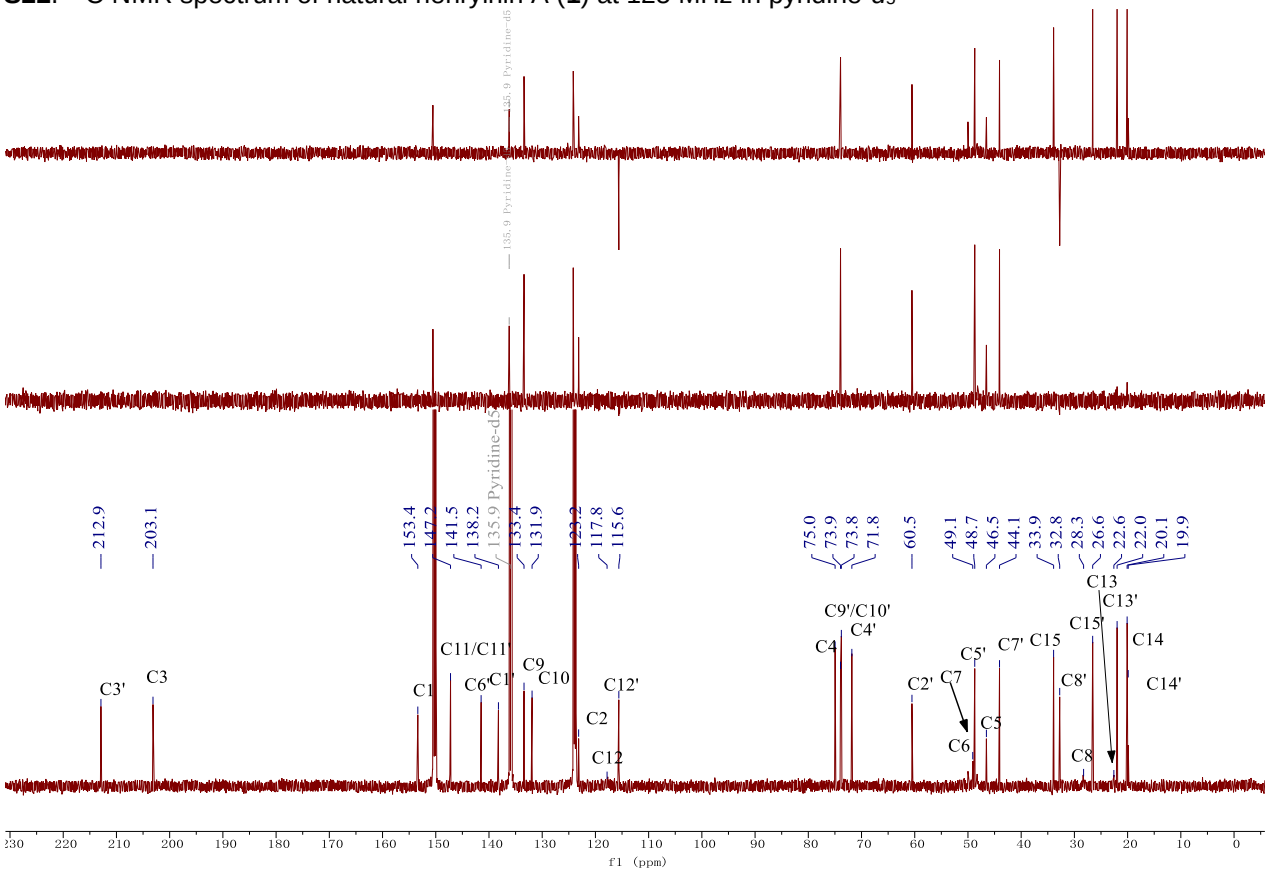


Figure S23. HSQC spectrum of natural henryinin A (**1**) in pyridine-d_5

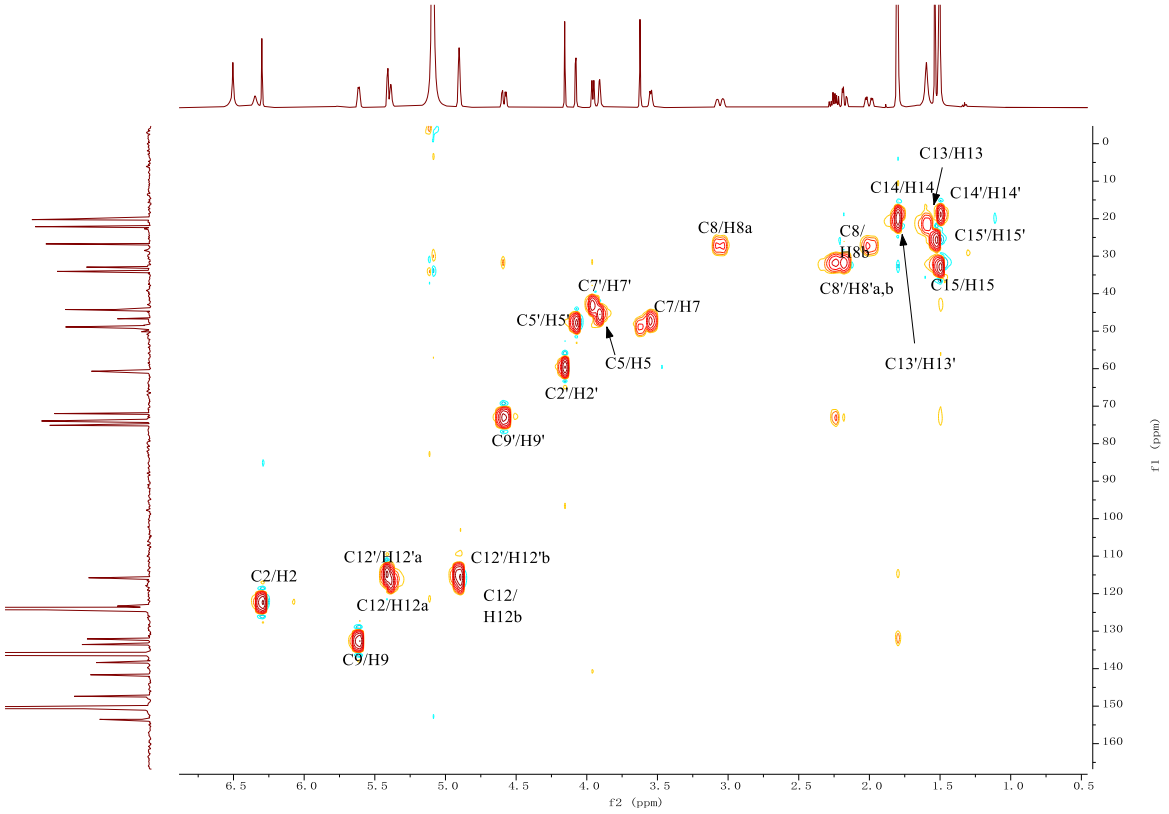


Figure S24. ^{1}H-^{1}H COSY spectrum of natural henryinin A (**1**) in pyridine-d_5

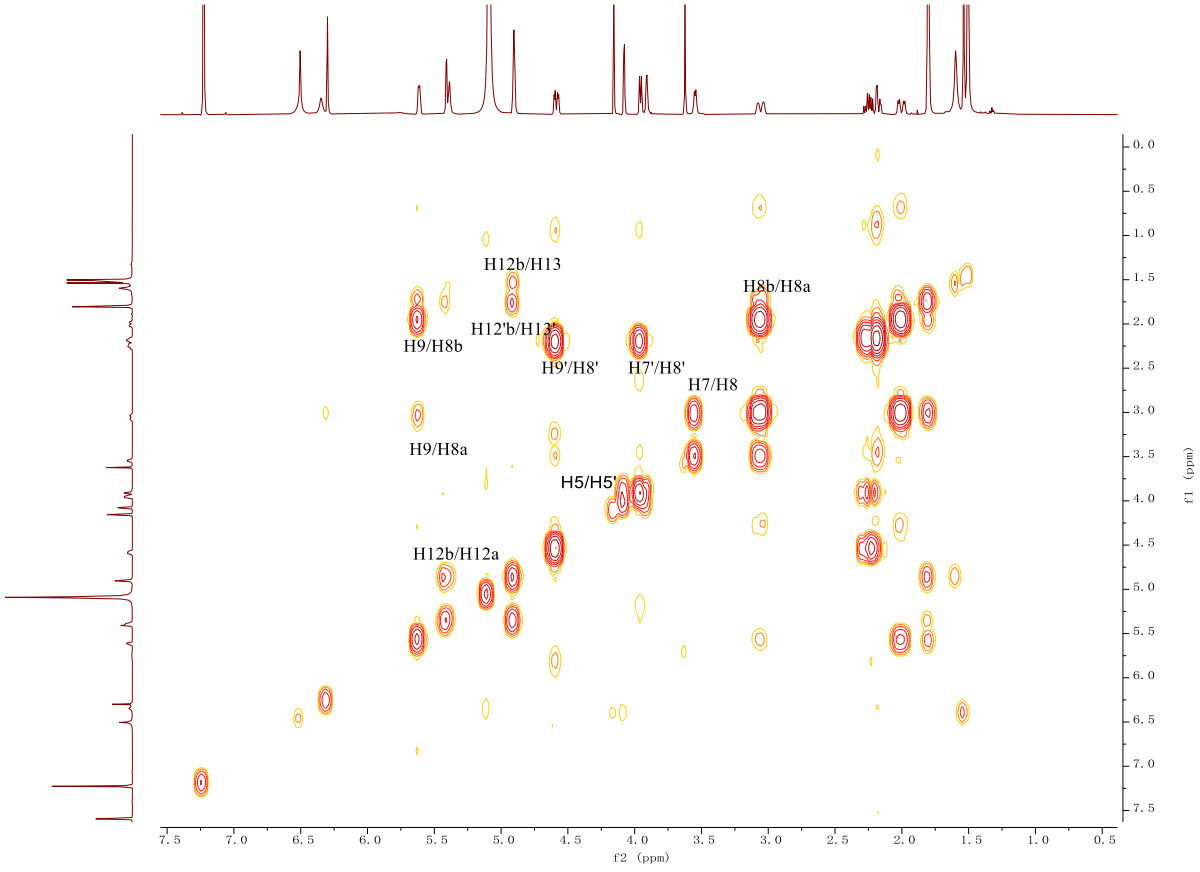


Figure S25. HMBC spectrum of natural henryinin A (**1**) in pyridine-d_5

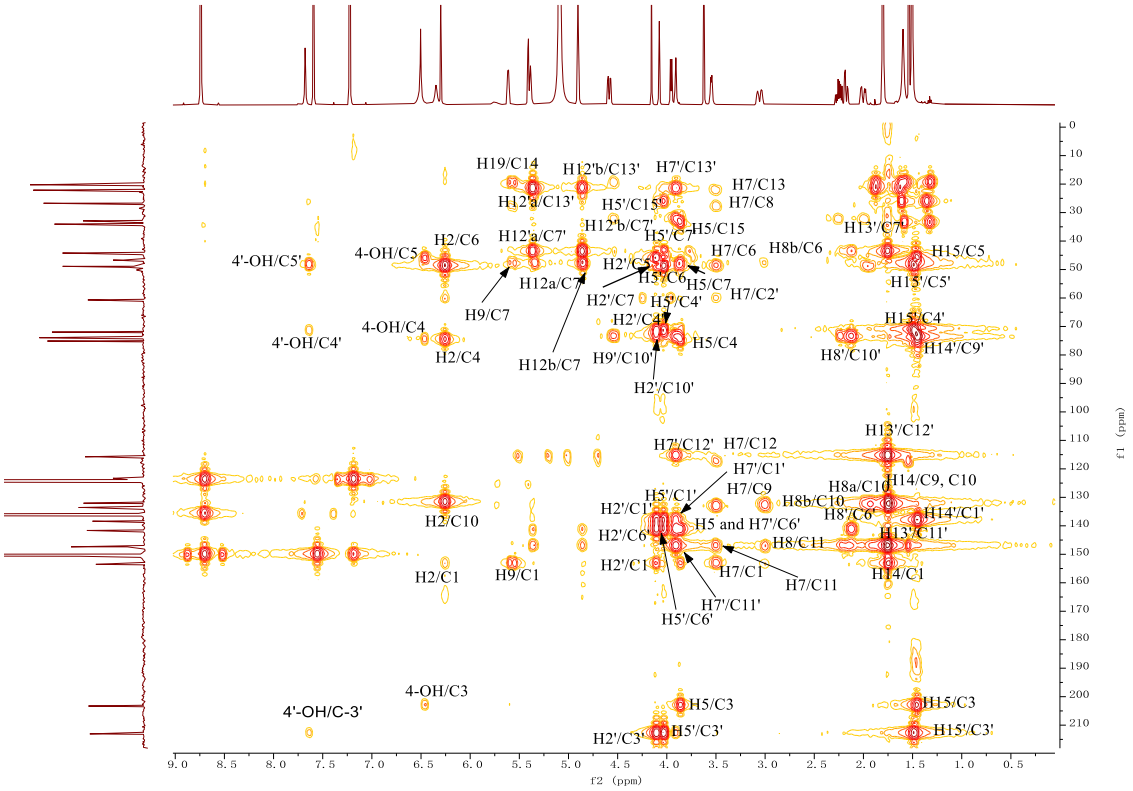


Figure S26. ROESY spectrum of natural henryinin A (**1**) in pyridine-d_5

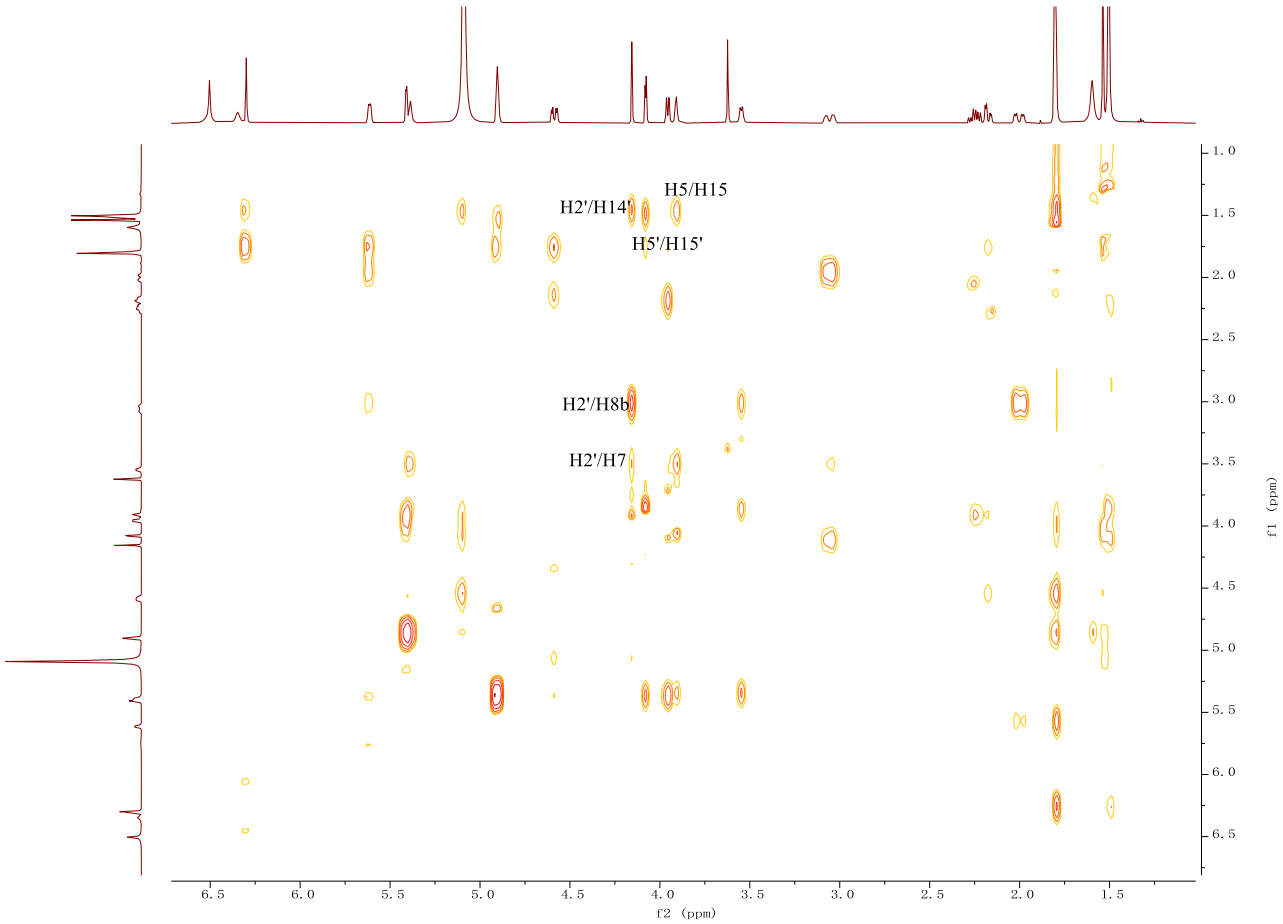


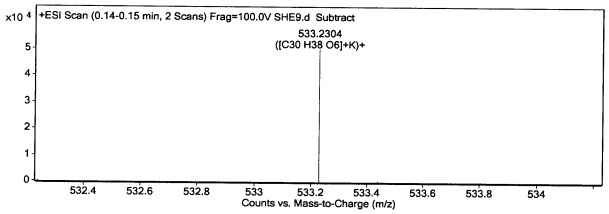
Figure S27. HRESIMS spectrum of natural henryinin A (**1**)

Data Filename	SHE9.d	**Sample Name**	SHE9
Sample Type	Sample	**Position**	P1-B3
Instrument Name	Instrument 1	**User Name**	
Acq Method	s.m	**Acquired Time**	3/27/2018 9:46:45 AM
IRM Calibration Status	[redacted]	**DA Method**	Default.m
Comment			

Sample Group	**Info.**
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125.2)

User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
100	0	ESI



Peak List

m/z	z	Abund	Formula	Ion
301.1413	1	15989.41		
517.2567	1	17959.28		
518.2597	1	6159.68		
533.2304	1	50093.55	C30 H38 O6	(M+K)+
534.2339	1	16159.08	C30 H38 O6	(M+K)+
535.2323	1	7234.27	C30 H38 O6	(M+K)+
1011.5223	1	10662.59		
1012.5247	1	6658.44		

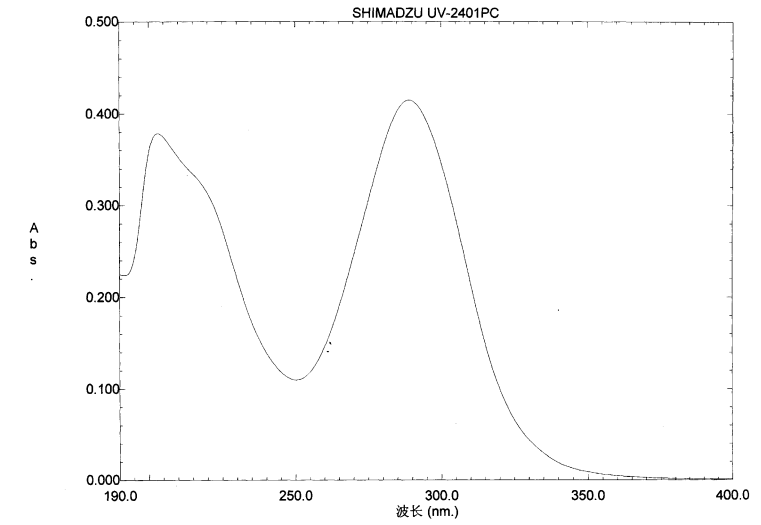
Formula Calculator Element Limits

Element	Min	Max
C	3	60
H	0	120
O	0	30

Formula Calculator Results

Formula	CalculatedMass	CalculatedMz	Mz	Diff. (mDa)	Diff. (ppm)	DBE
C30 H38 O6	494.2668	533.2300	533.2304	-0.40	-0.75	12.0000

Figure S28. UV spectrum of natural henryinin A (**1**)



文件名: SHE9

SHE9

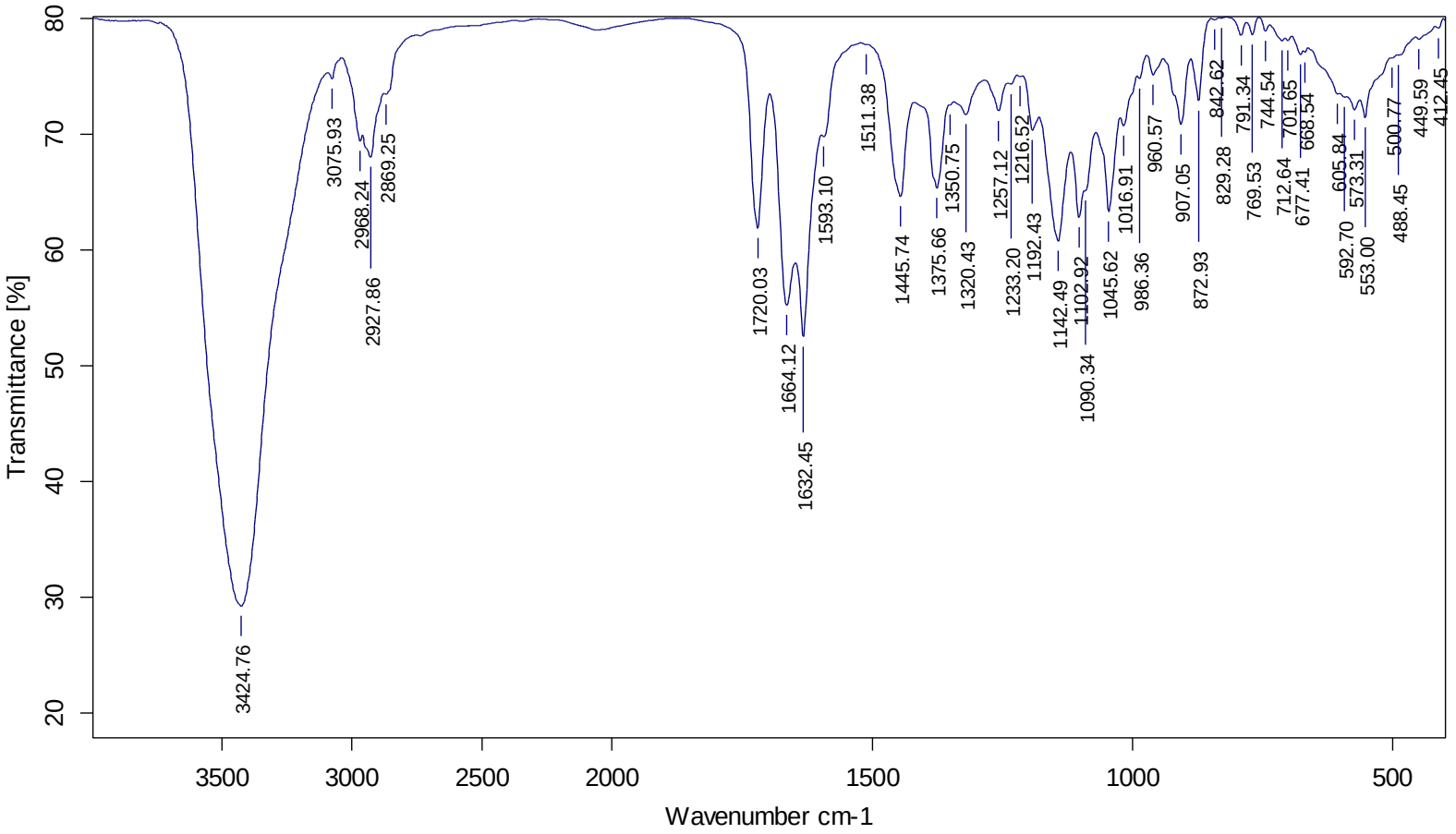
样品浓度：0.0138毫克/毫升
溶剂：甲醇

创建于: 14:36 18-02-05
数据: 原始

测量模式: Abs.
扫描速度: 中速
狭缝: 5.0
采样间隔: 0.5

否.	波长 (nm.)	Abs.
1	289.00	0.4145
2	203.00	0.3781

Figure S29. IR spectrum of natural henryinin A (**1**)



Sample : SHE9	Frequency Range : 399.246 - 3996.32	Measured on : 27/03/2018	
Technique : KBr	Resolution : 4	Instrument : Tensor27	Sample Scans : 16
Filename : 180327IR.2	Zerofilling : 2	Acquisition : Double Sided,Forv	

Figure S30. ECD spectrum of natural henryinin A (**1**) (0.1720 mg/mL in MeOH)

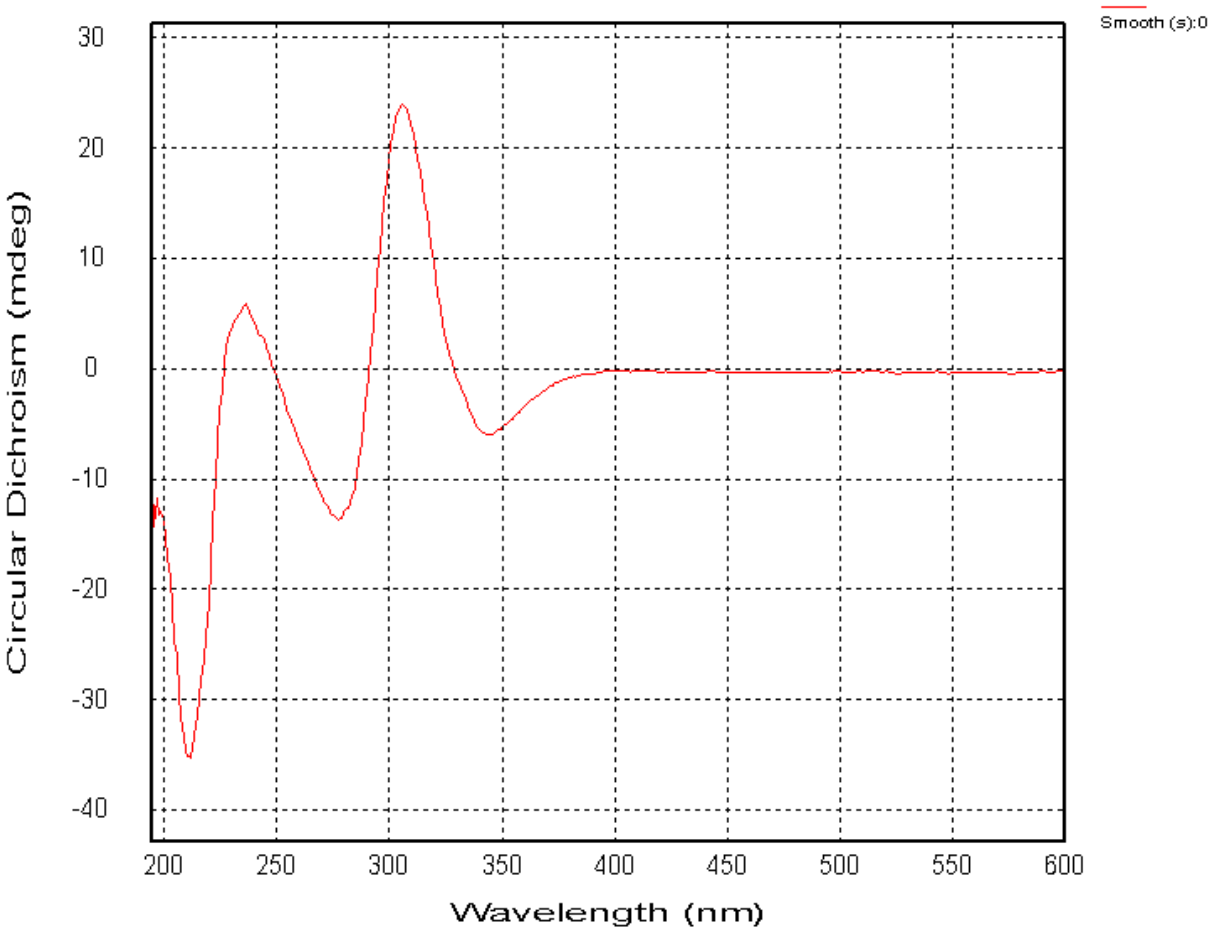


Figure S31. Specific rotation spectrum of natural henryinin A (**1**)

Optical rotation measurement

Model : P-1020 (A060460638)

No.	Sample	Mode	Data	Monitor Blank	Temp. Cell Temp Point	Date Comment Sample Name	Light Filter Operator	Cycle Time Integ Time
No.1	133 (1/3)	Sp.Rot	-68.6050	-0.0295 0.0000	19.0 50.00 Cell	Tue Jan 30 23:38:56 2018 0.00086g/mL MeOH SHE9	Na 589nm	2 sec 2 sec
No.2	133 (2/3)	Sp.Rot	-67.6740	-0.0291 0.0000	19.0 50.00 Cell	Tue Jan 30 23:39:01 2018 0.00086g/mL MeOH SHE9	Na 589nm	2 sec 2 sec
No.3	133 (3/3)	Sp.Rot	-68.6050	-0.0295 0.0000	19.0 50.00 Cell	Tue Jan 30 23:39:06 2018 0.00086g/mL MeOH SHE9	Na 589nm	2 sec 2 sec

-68.3946°

Figure S32. ^{1}H NMR spectrum of natural henryinin B (**2**) at 500 MHz in $CDCl_3$

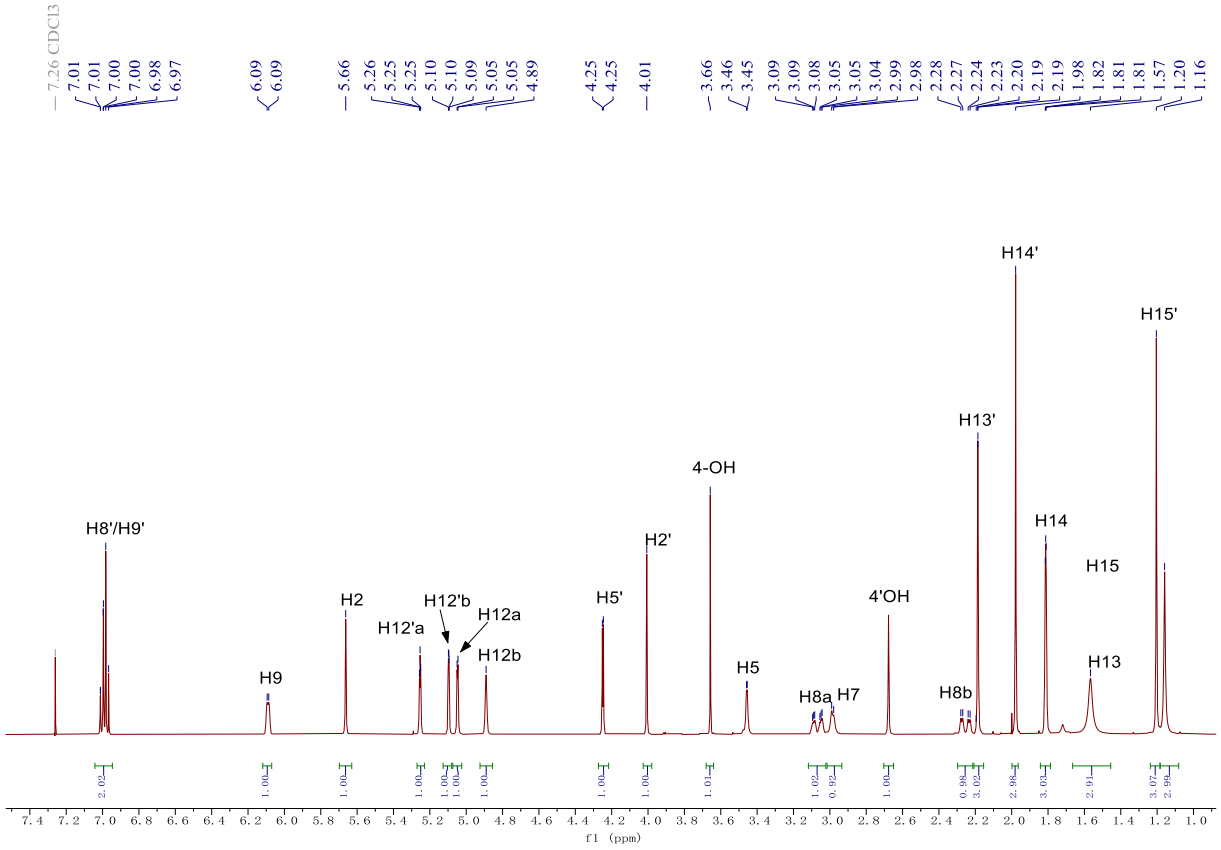


Figure S33. ^{13}C NMR spectrum of natural henryinin B (**2**) at 125 MHz in $CDCl_3$

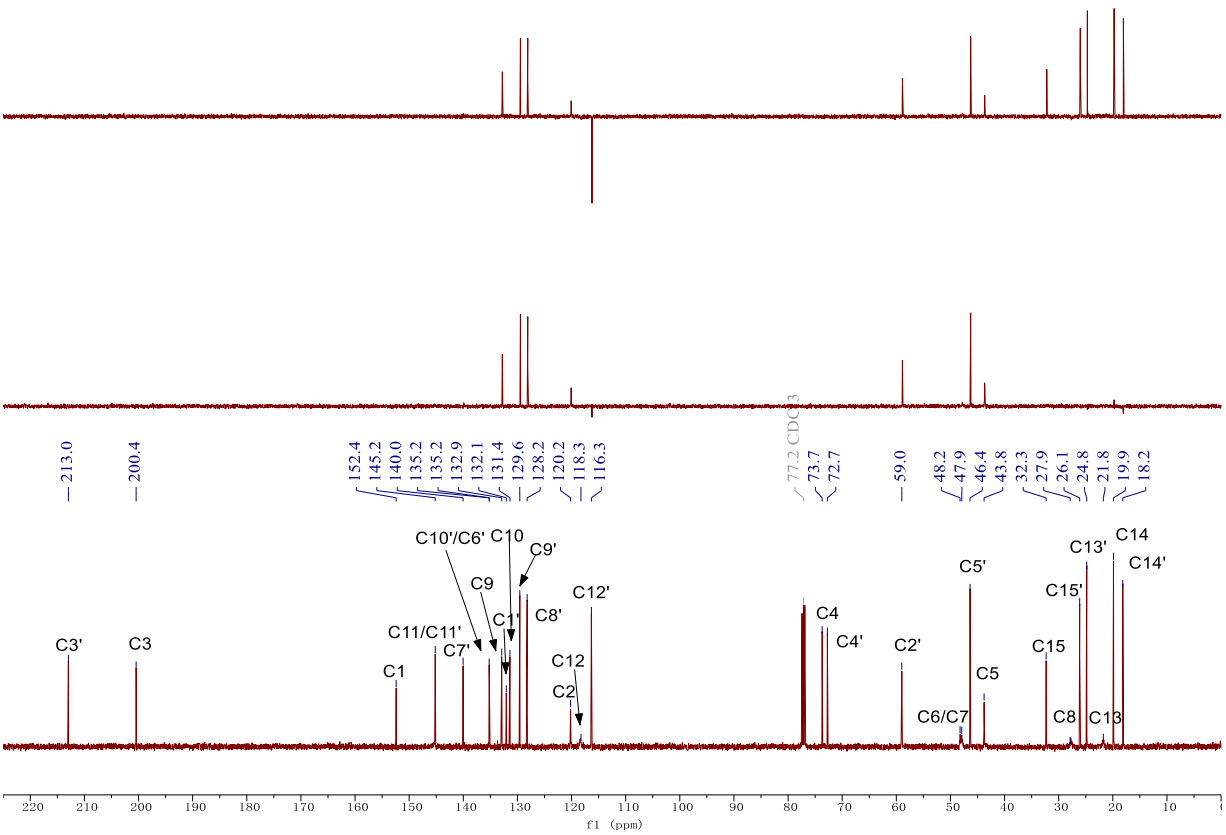


Figure S34. HSQC spectrum of natural henryinin B (**2**) in $CDCl_3$

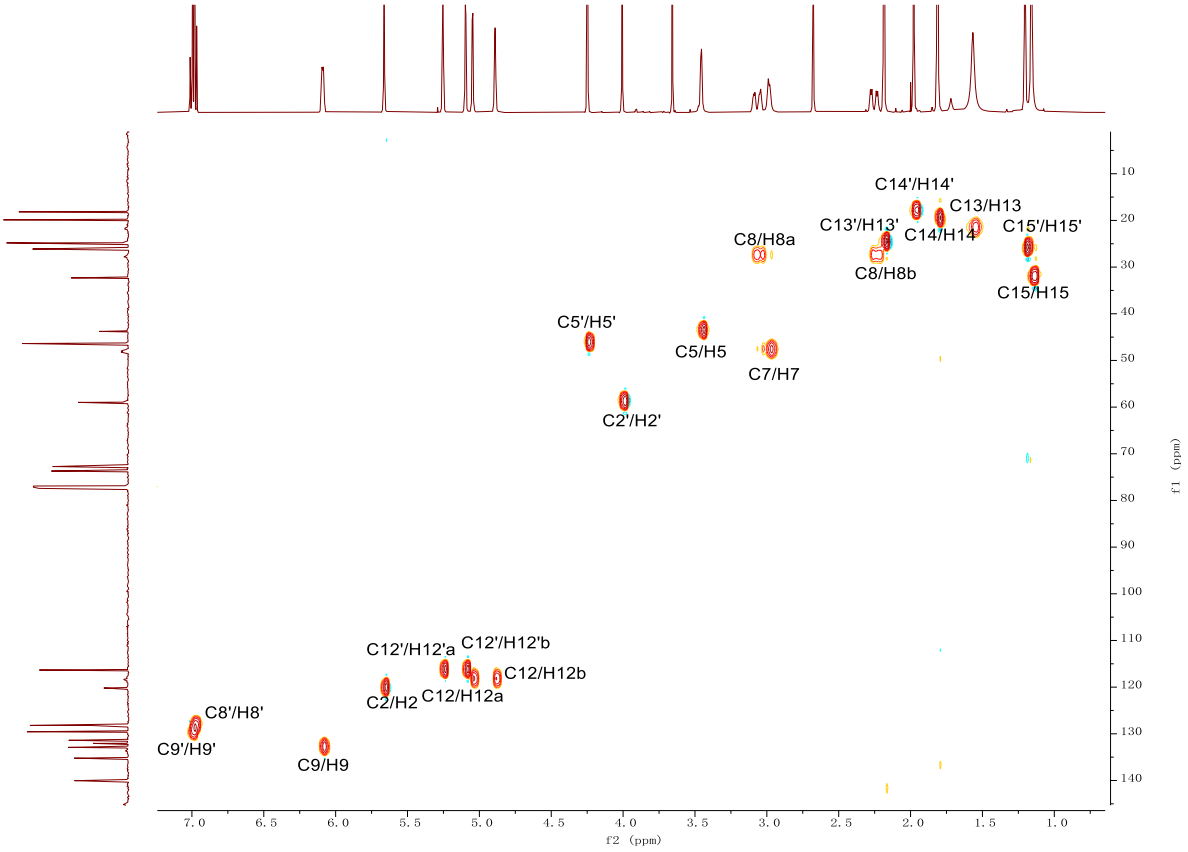


Figure S35. ^{1}H-^{1}H COSY spectrum of natural henryinin B (**2**) in $CDCl_3$

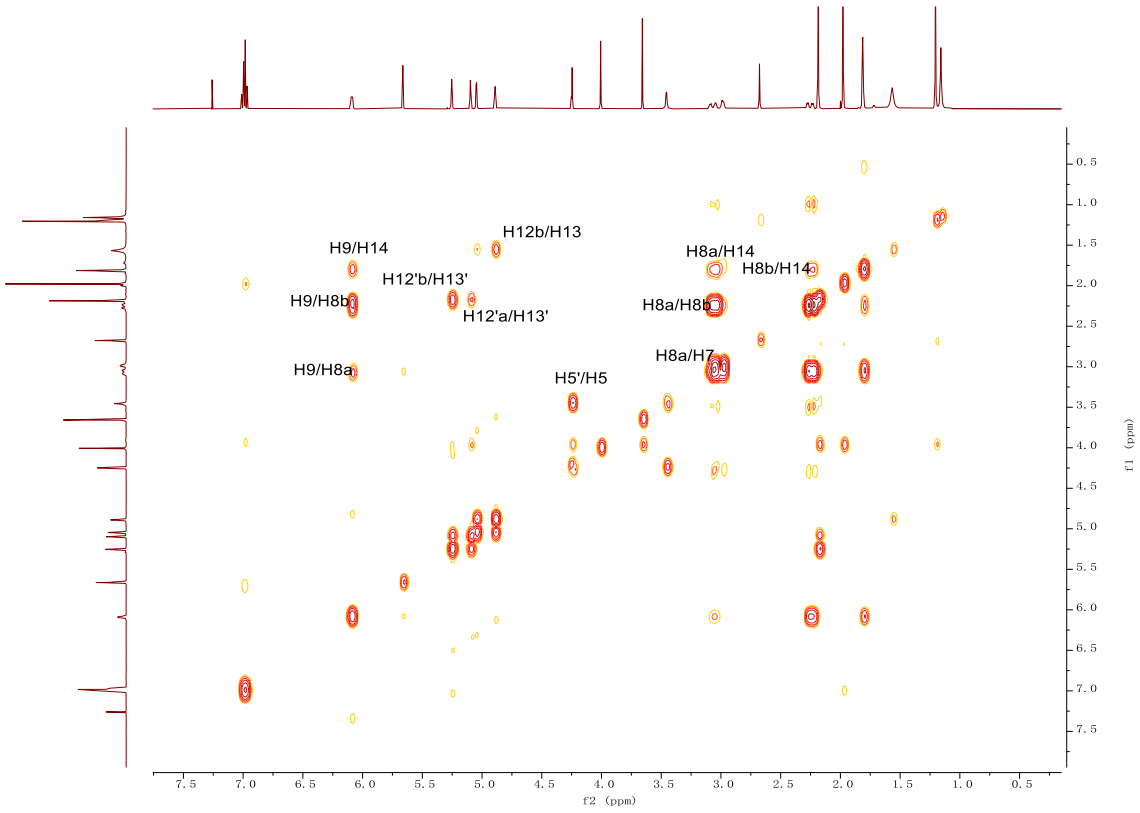


Figure S36. HMBC spectrum of natural henryinin B (**2**) in $CDCl_3$

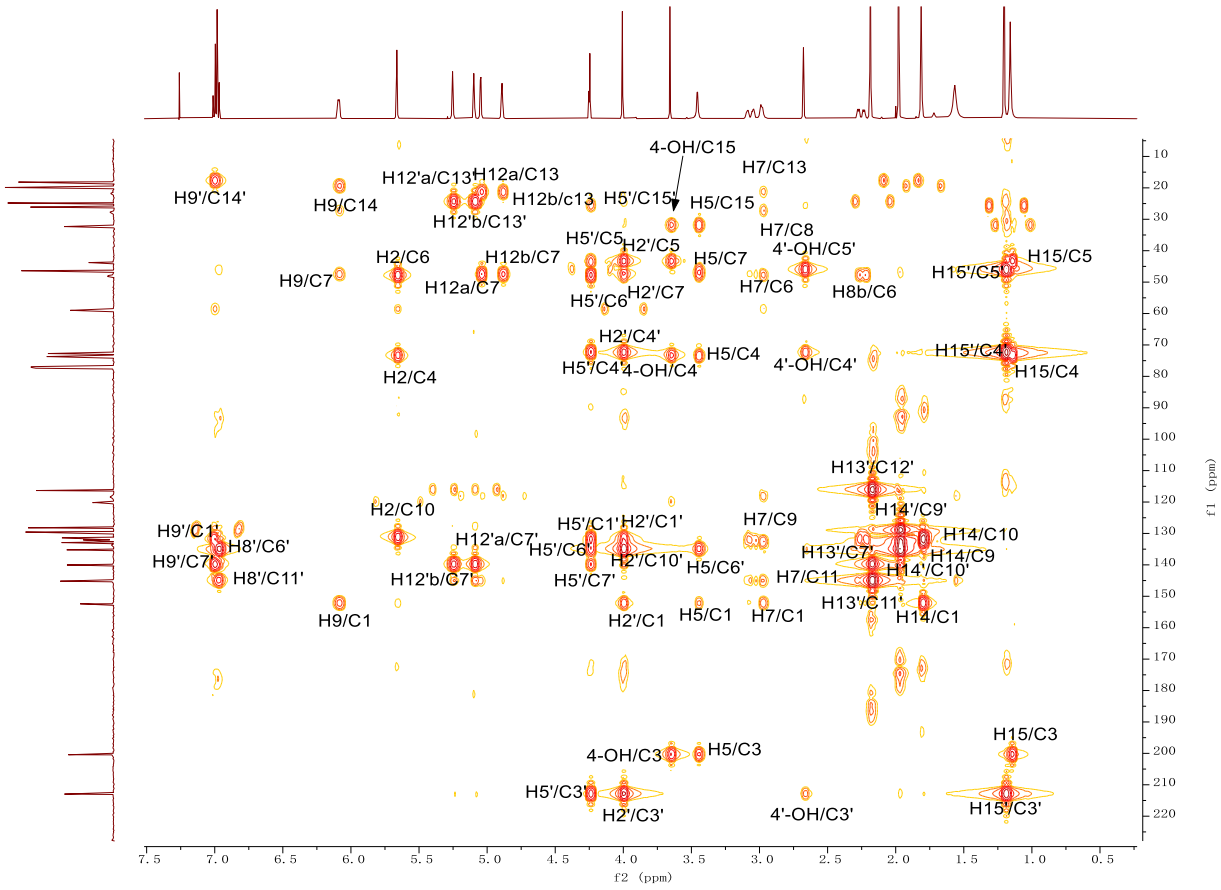


Figure S37. ROESY spectrum of natural henryinin B (**2**) in $CDCl_3$

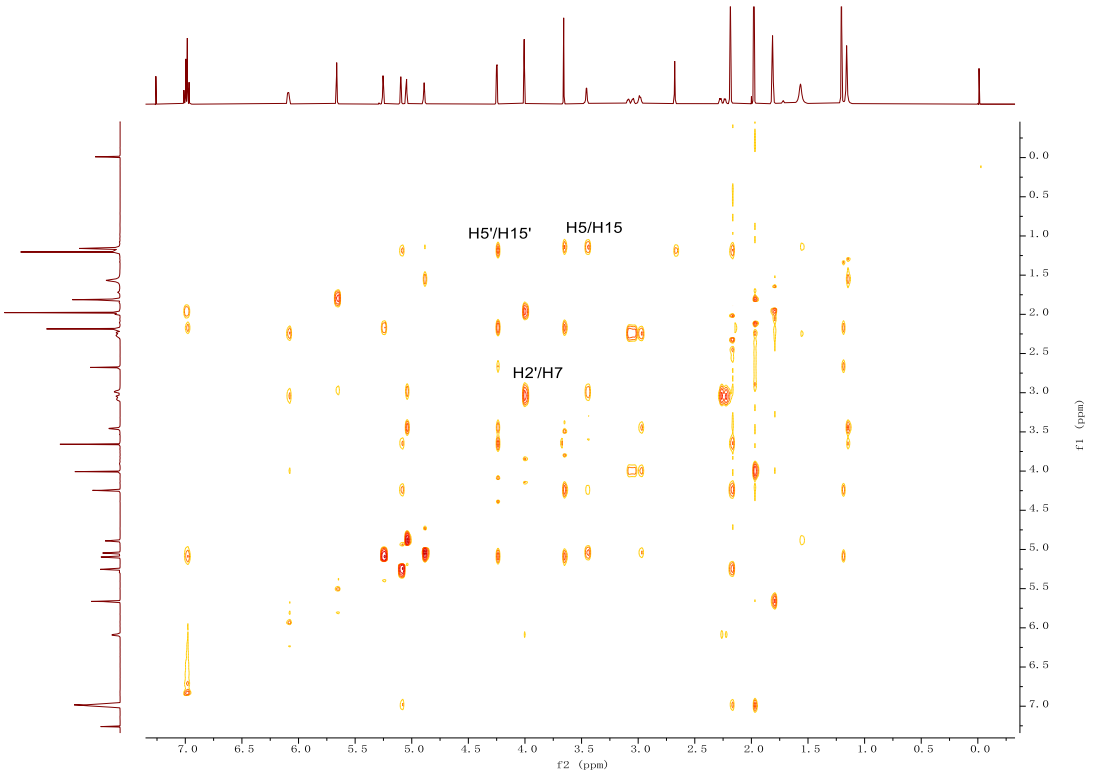
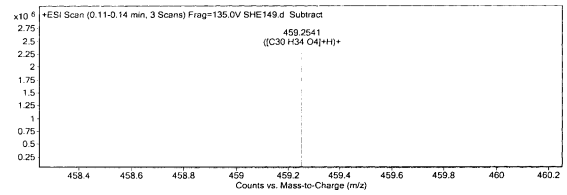


Figure S38. HRESIMS spectrum of natural henryinin B (**2**)

Data Filename	SHE149.d	**Sample Name**	SHE149
Sample Type	Sample	**Position**	P1-A3
Instrument Name	Instrument 1	**User Name**	
Acq Method	s.m	**Acquired Time**	10/19/2018 12:54:09 PM
IRM Calibration Status	Success	**DA Method**	Default.m
Comment			
Sample Group		**Info.**	
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125.2)		

User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
135	0	ESI



Peak List

m/z	z	Abund	Formula	Ion
459.2541	1	2385765.25	C30 H34 O4	(M+H)+
460.2571	1	772053.25	C30 H34 O4	(M+H)+
461.2603	1	130770.63	C30 H34 O4	(M+H)+
481.2358	1	1260642.13		
482.2394	1	382346.28		
497.21	1	218025.7		
707.3514	2	232730.42		
707.8532	2	213985.69		
939.4831	1	275049.91		
940.4862	1	182782.63		

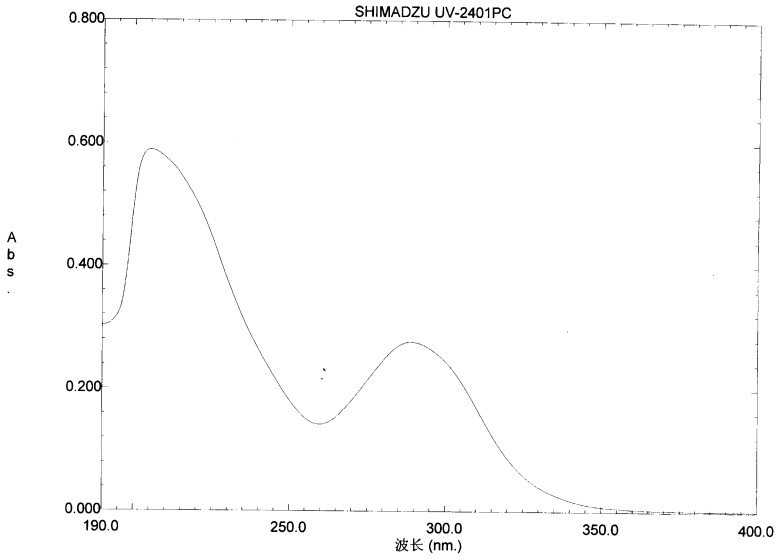
Formula Calculator Element Limits

Element	Min	Max
C	3	60
H	0	120
O	0	30

Formula Calculator Results

Formula	CalculatedMass	CalculatedMz	Mz	Diff. (mDa)	Diff. (ppm)	DBE
C30 H34 O4	458.2457	459.2530	459.2541	-1.10	-2.40	14.0000

Figure S39. UV spectrum of natural henryinin B (**2**)



文件名: SHE149

SHE149

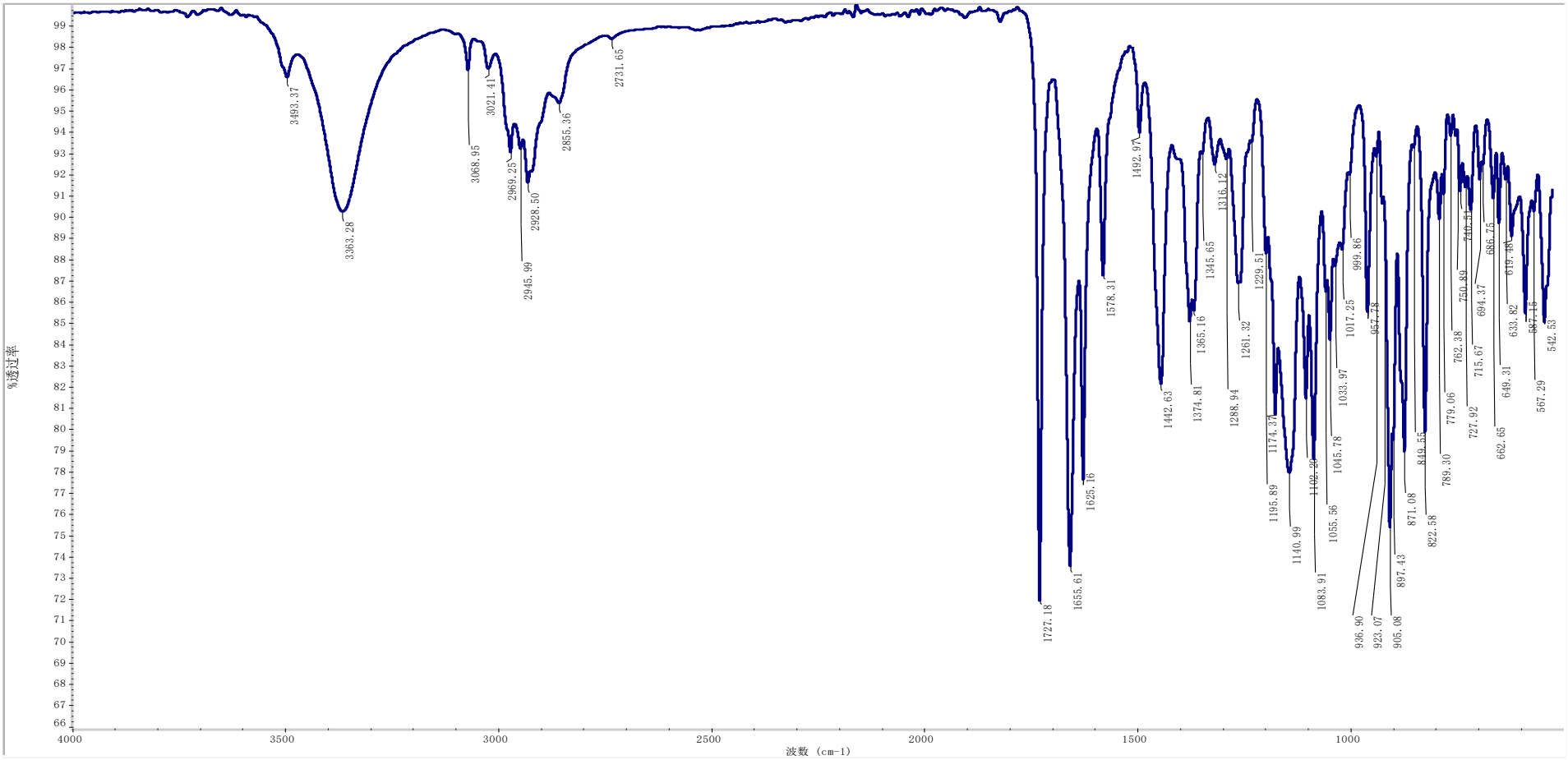
样品浓度：0.0086毫克/毫升
溶剂：甲醇

创建于: 11:07 18-10-26
数据: 原始

测量模式: Abs.
扫描速度: 中速
狭缝: 5.0
采样间隔: 0.5

否.	波长 (nm.)	Abs.
1	289.00	0.2760
2	205.50	0.5886

Figure S40. IR spectrum of natural henryinin B (**2**)



Sample Name: SHE149
ATR ITX-DIAMOND
采集时间: 星期五 11月 02 09:40:54 2018 (GMT+08:00)
仪器型号：NICOLET iS10
Software version: OMNIC 9.8.372

样品扫描次数: 16
背景扫描次数: 16
分辨率: 4.000
采样增益: 1.0
动镜速度: 0.4747
光阑: 150.00

Figure S41. ECD spectrum of natural henryinin B (**2**) (0.1209mg/mL in MeOH)

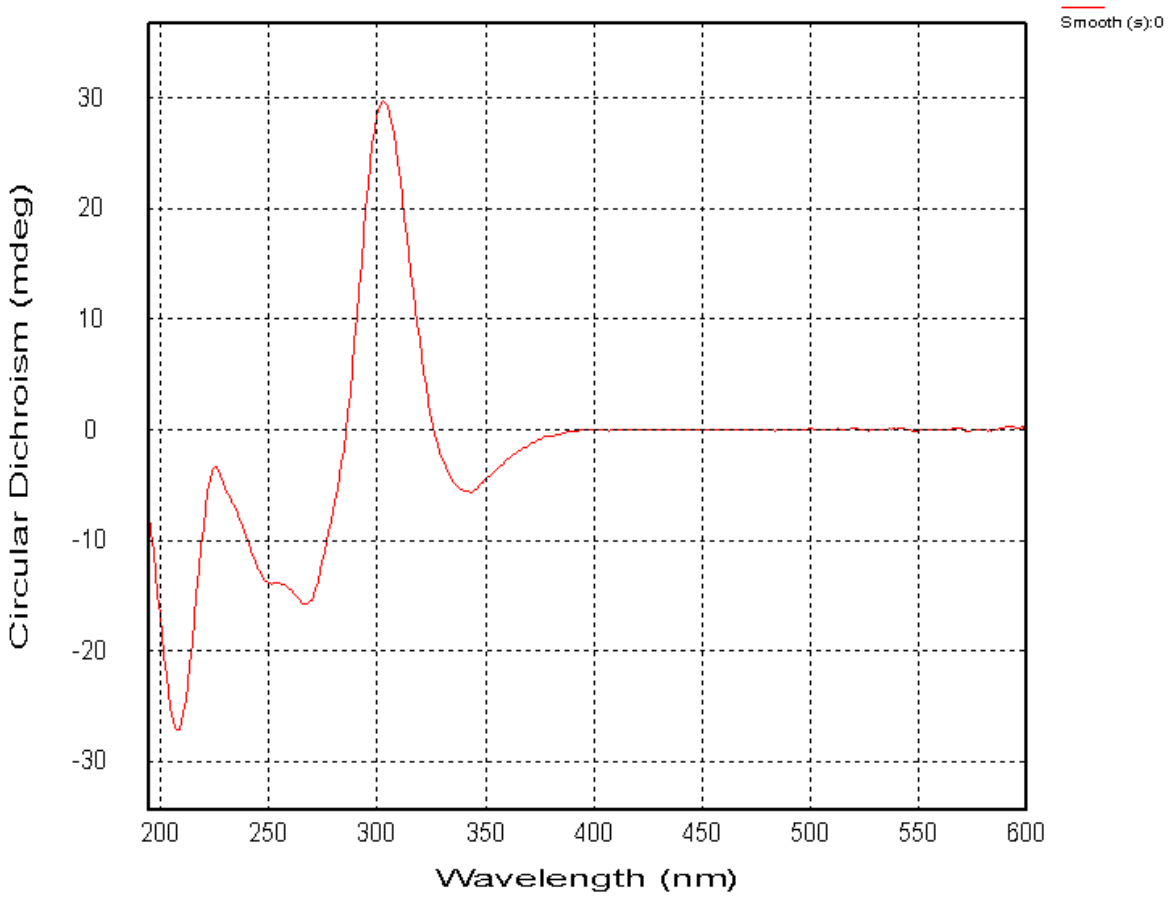


Figure S42. Specific rotation spectrum of natural henryinin B (**2**)

Optical rotation measurement

Model : P-1020 (A060460638)

No.	Sample	Mode	Data	Monitor Blank	Temp. Cell Temp Point	Date Comment Sample Name	Light Filter Operator	Cycle Time Integ Time
No.1	4 (1/3)	Sp.Rot	-6.6150	-0.0043 0.0000	24.3 50.00 Cell	Thu Oct 25 14:10:24 2018 0.00130g/mL MeOH SHE149	Na 589nm	2 sec 2 sec
No.2	4 (2/3)	Sp.Rot	-6.3080	-0.0041 0.0000	24.3 50.00 Cell	Thu Oct 25 14:10:30 2018 0.00130g/mL MeOH SHE149	Na 589nm	2 sec 2 sec
No.3	4 (3/3)	Sp.Rot	-7.5380	-0.0049 0.0000	24.3 50.00 Cell	Thu Oct 25 14:10:35 2018 0.00130g/mL MeOH SHE149	Na 589nm	2 sec 2 sec

-6.4207°

Figure S43. ^{1}H NMR spectrum of natural henryinin C (**3**) at 500 MHz in $CDCl_3$

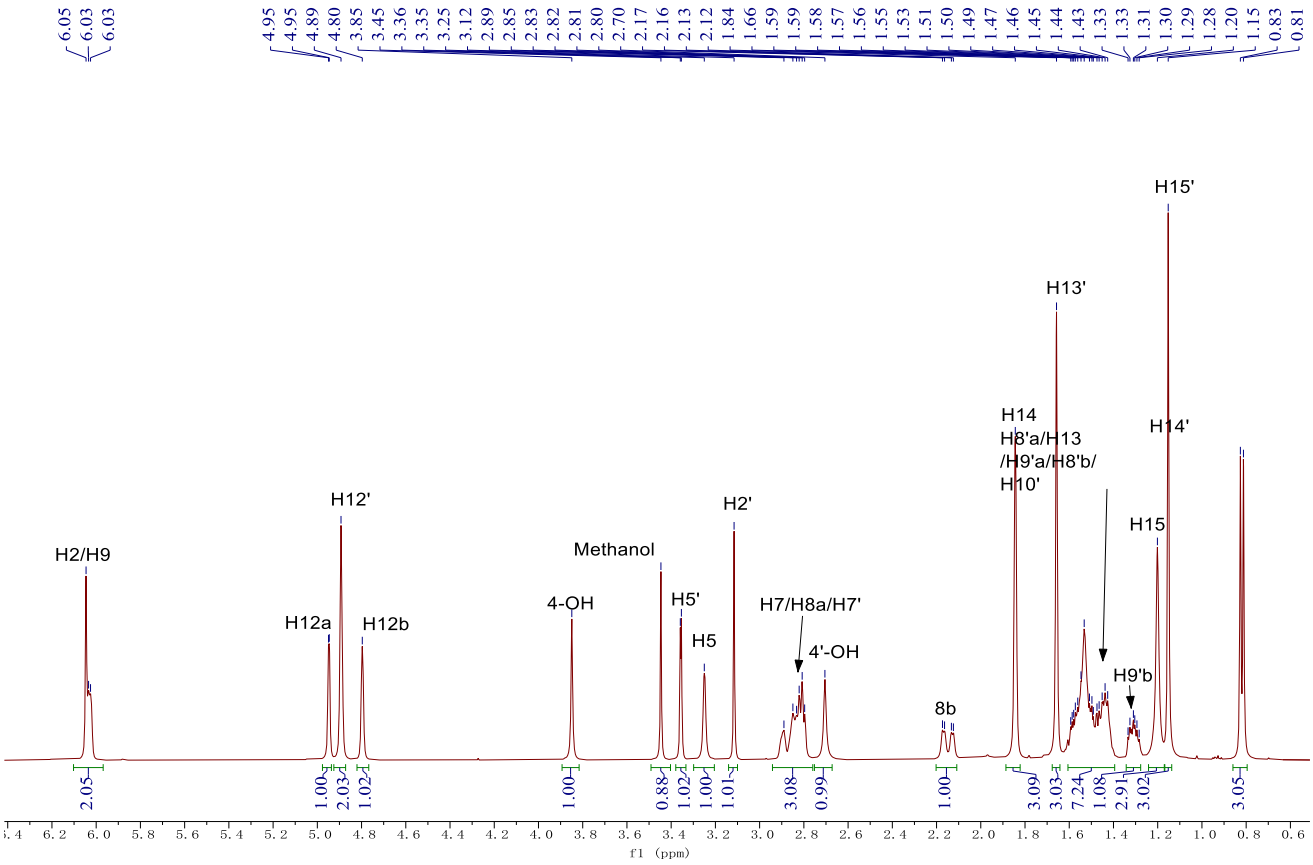


Figure S44. ^{13}C NMR spectrum of natural henryinin C (**3**) at 125 MHz in $CDCl_3$

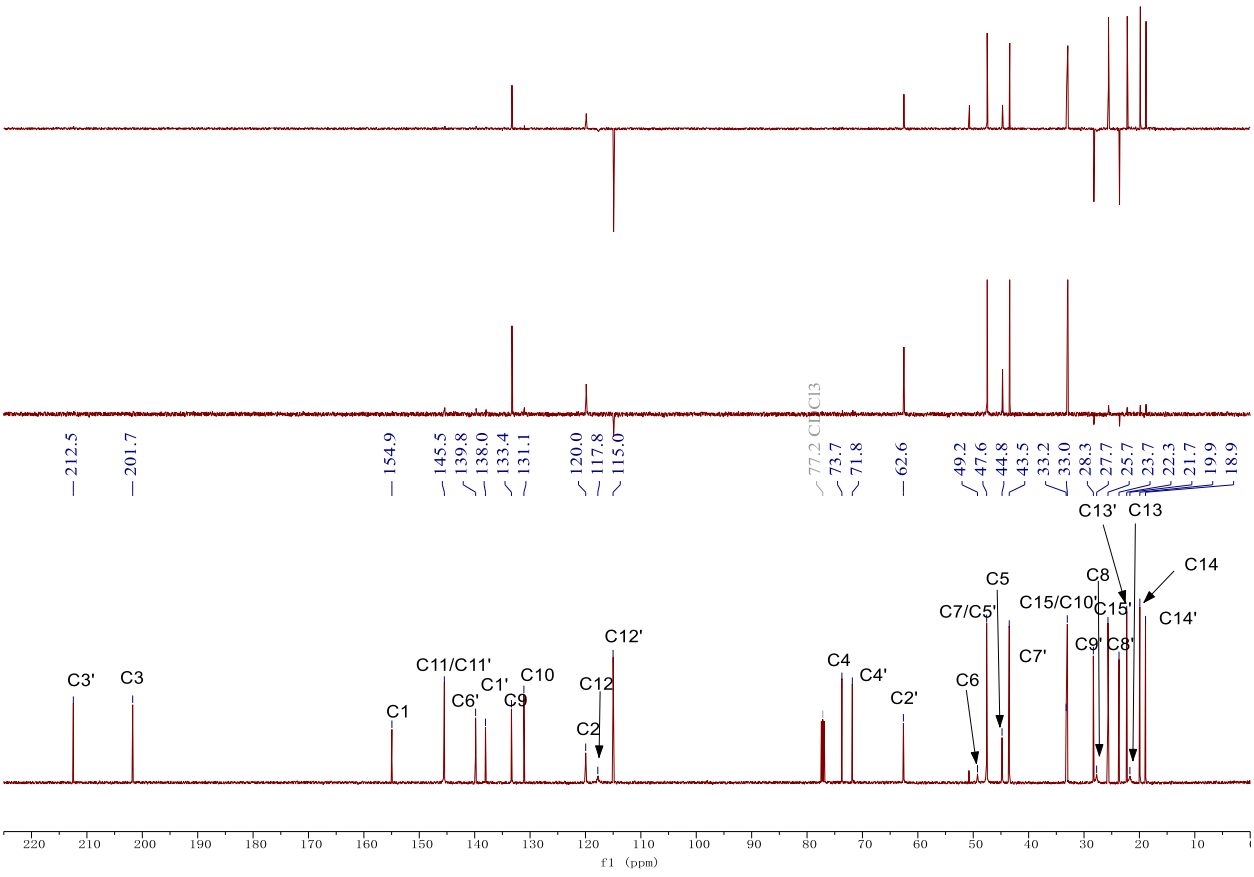


Figure S45. HSQC spectrum of natural henryinin C (**3**) in $CDCl_3$

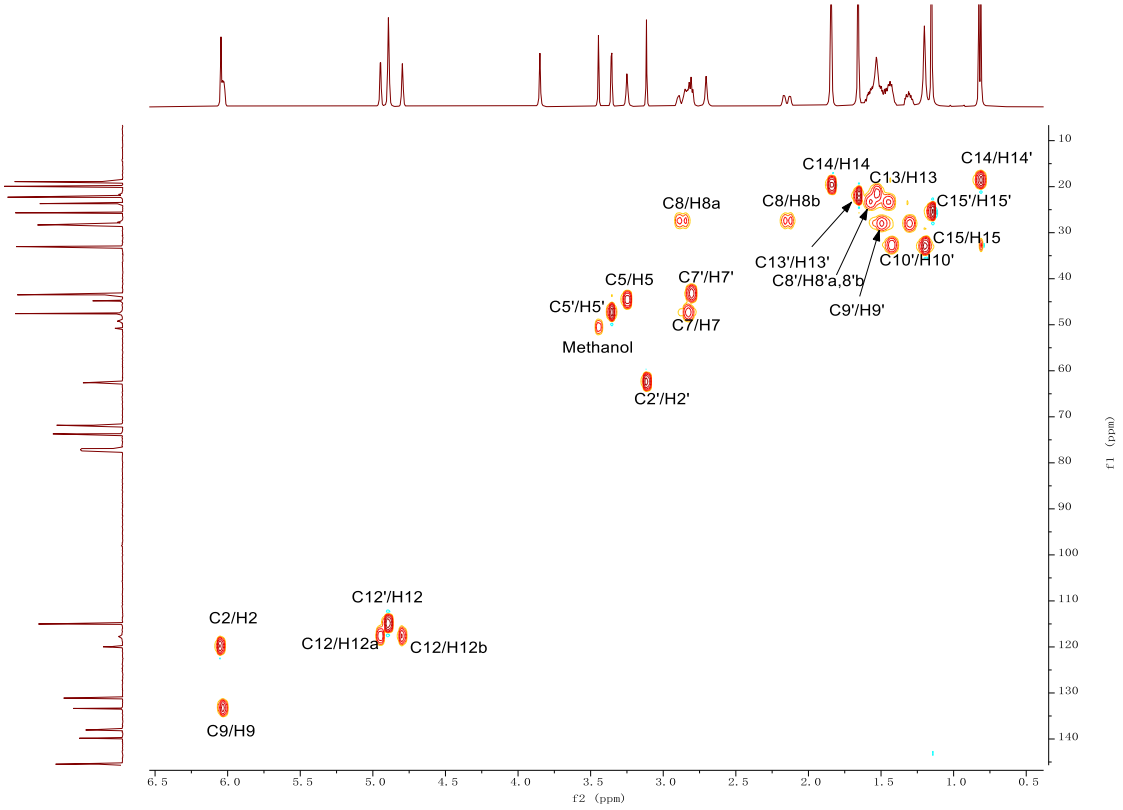


Figure S46. ^{1}H-^{1}H COSY spectrum of natural henryinin C (**3**) in $CDCl_3$

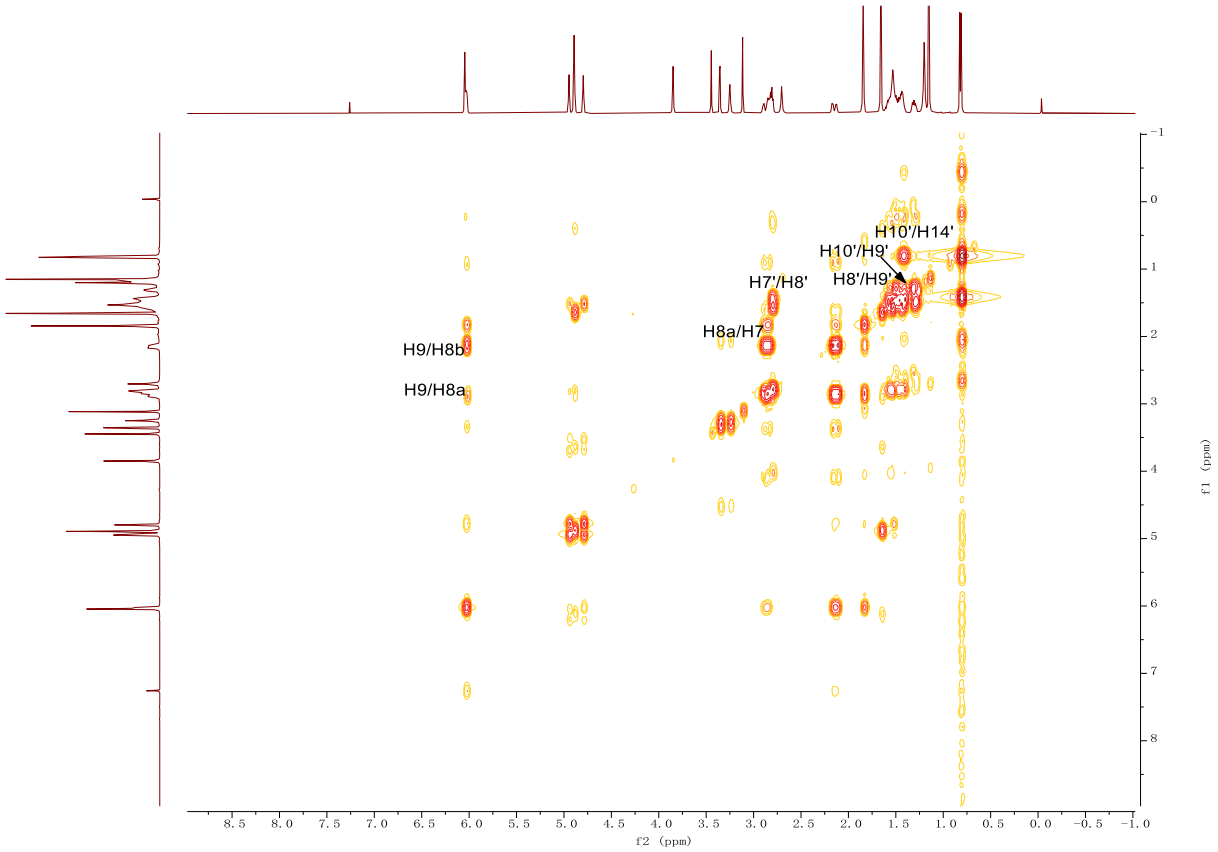


Figure S47. HMBC spectrum of natural henryinin C (**3**) in $CDCl_3$

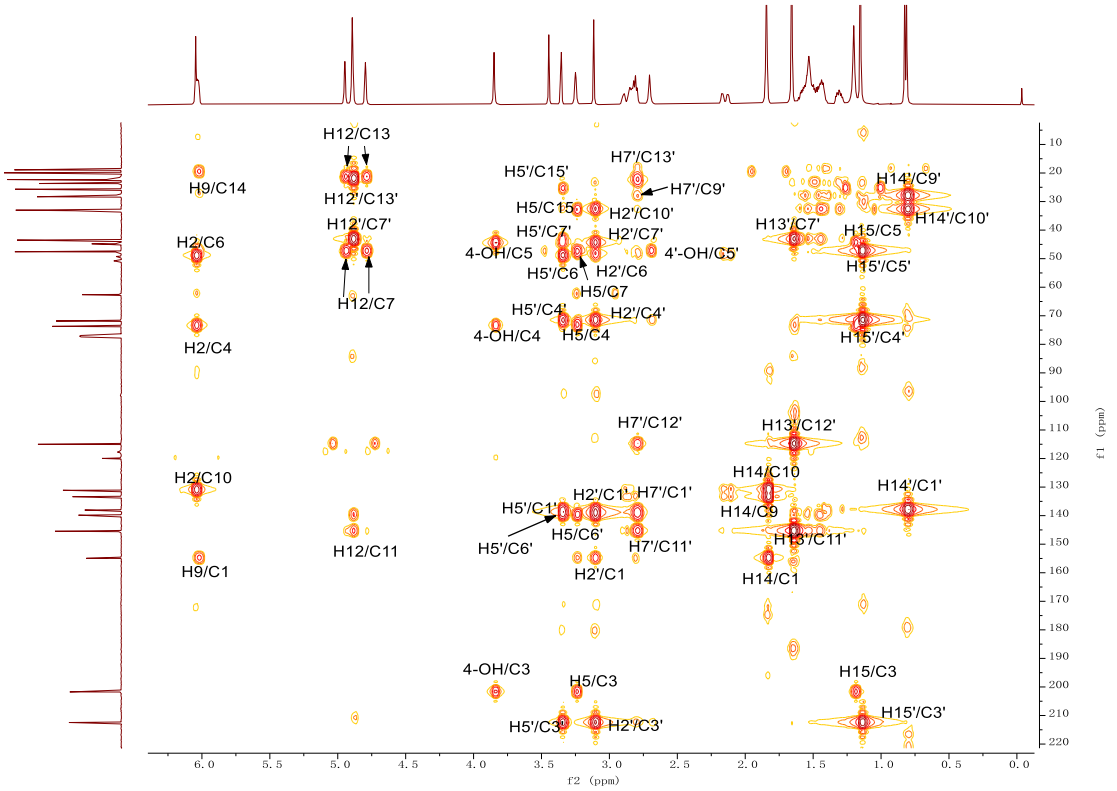


Figure S48. ROESY spectrum of natural henryinin C (**3**) in $CDCl_3$

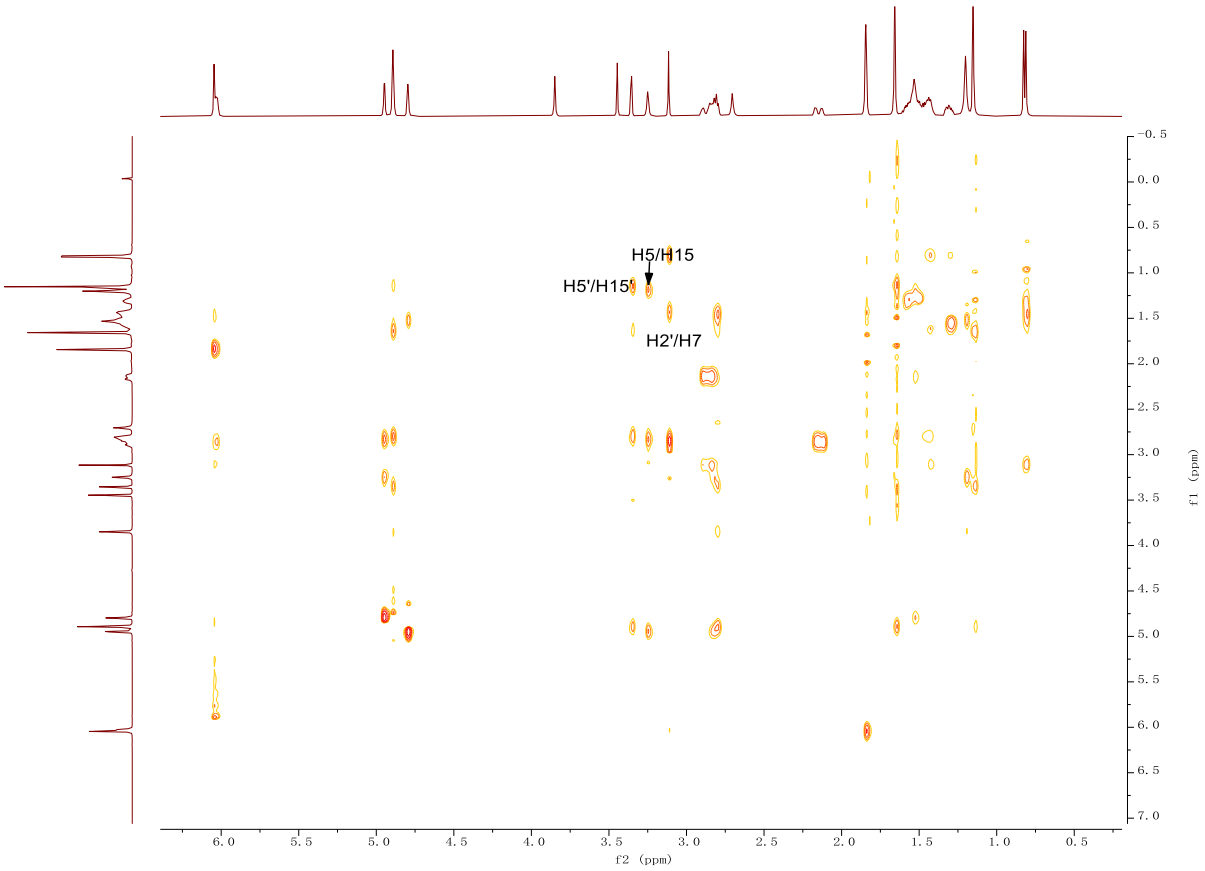


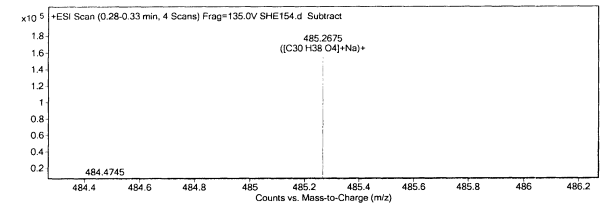
Figure S49. HRESIMS spectrum of natural henryinin C (**3**)

Data Filename	SHE154.d	**Sample Name**	SHE154
Sample Type	Sample	**Position**	P1-B2
Instrument Name	Instrument 1	**User Name**	
Acq Method	s.m	**Acquired Time**	10/16/2018 10:23:01 AM
IRM Calibration Status	Success	**DA Method**	Default.m
Comment			

Sample Group	**Info.**
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125.2)

User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
135	0	ESI



Peak List

m/z	z	Abund	Formula	Ion
102.1284	1	53237.27		
271.6335	2	20066.42		
463.2851	1	55509.54		
485.2675	1	158047.34	C30 H38 O4	(M+Na)+
486.271	1	51970.48	C30 H38 O4	(M+Na)+
501.2415	1	126009.94		
502.2445	1	40354.13		
947.5458	1	218704.47		
948.5489	1	137088.94		
949.5514	1	45704.79		

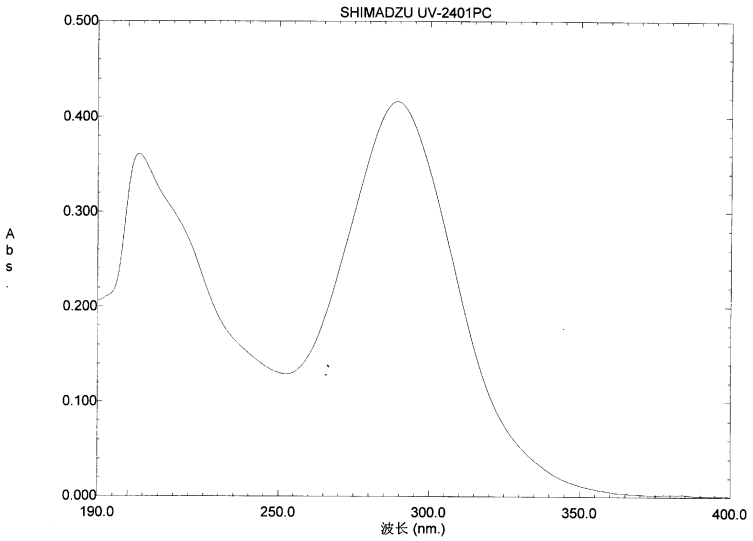
Formula Calculator Element Limits

Element	Min	Max
C	3	60
H	0	240
O	0	30

Formula Calculator Results

Formula	CalculatedMass	CalculatedMz	Mz	Diff. (mDa)	Diff. (ppm)	DBE
C30 H38 O4	462.2770	485.2662	485.2675	-1.30	-2.68	12.0000

Figure S50. UV spectrum of natural henryinin C (**3**)



文件名: SHE154

SHE154 ———

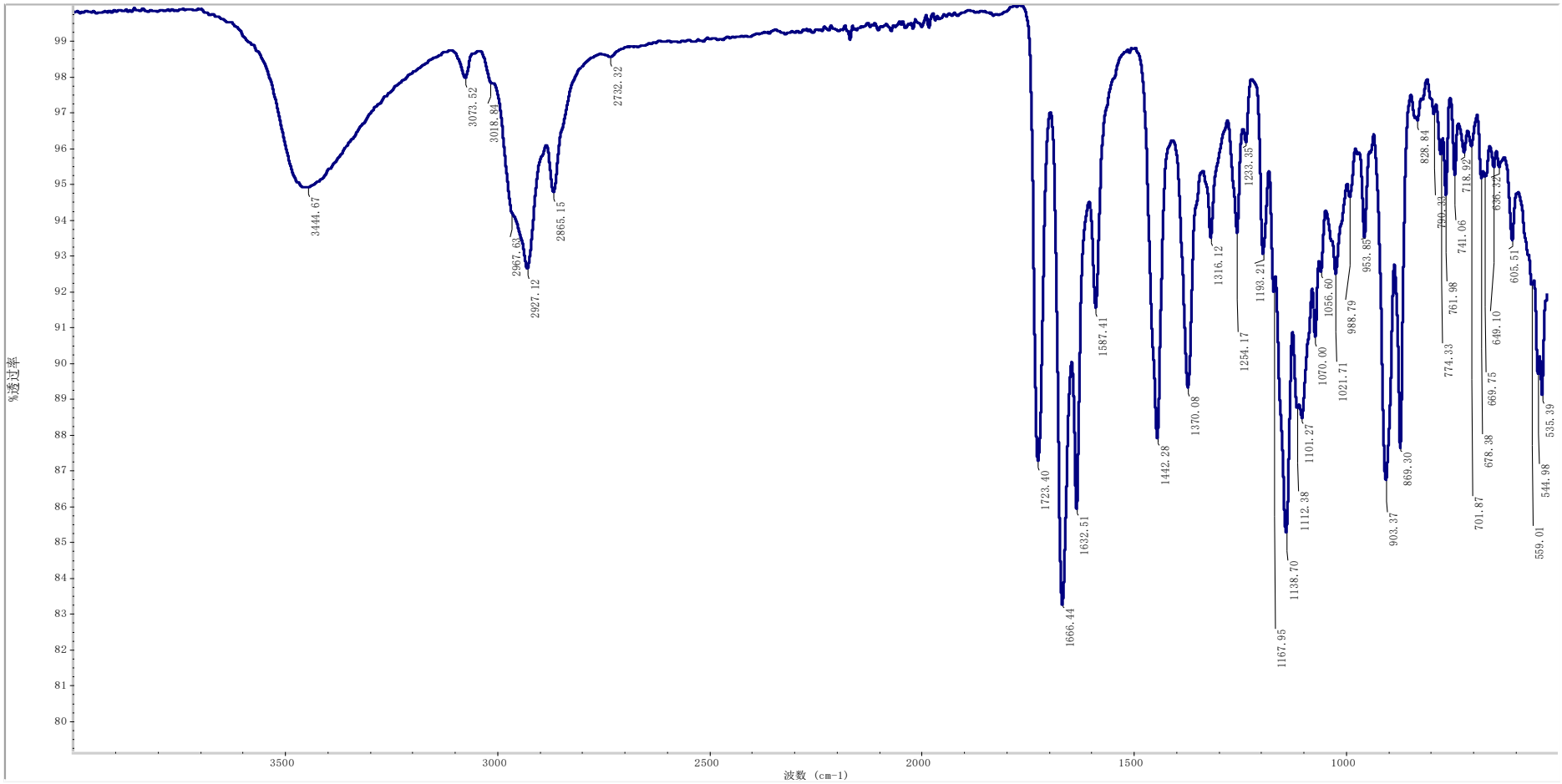
样品浓度：0.0122毫克/毫升
溶剂：甲醇

创建于: 16:15 18-10-21
数据: 原始

测量模式: Abs.
扫描速度: 中速
狭缝: 5.0
采样间隔: 0.5

否.	波长 (nm.)	Abs.
1	457.00	0.0021
2	384.00	0.0026
3	289.00	0.4158
4	203.50	0.3606

Figure S51. IR spectrum of natural henryinin C (**3**)



Sample Name: SHE154
ATR ITX-DIAMOND
采集时间: 星期五 11月 02 09:01:57 2018 (GMT+08:00)
仪器型号：NICOLET iS10
Software version: OMNIC 9.8.372

样品扫描次数: 16
背景扫描次数: 16
分辨率: 4.000
采样增益: 1.0
动镜速度: 0.4747
光阑: 150.00

Figure S52. ECD spectrum of natural henryinin C (**3**) (0.1415mg/mL in MeOH)

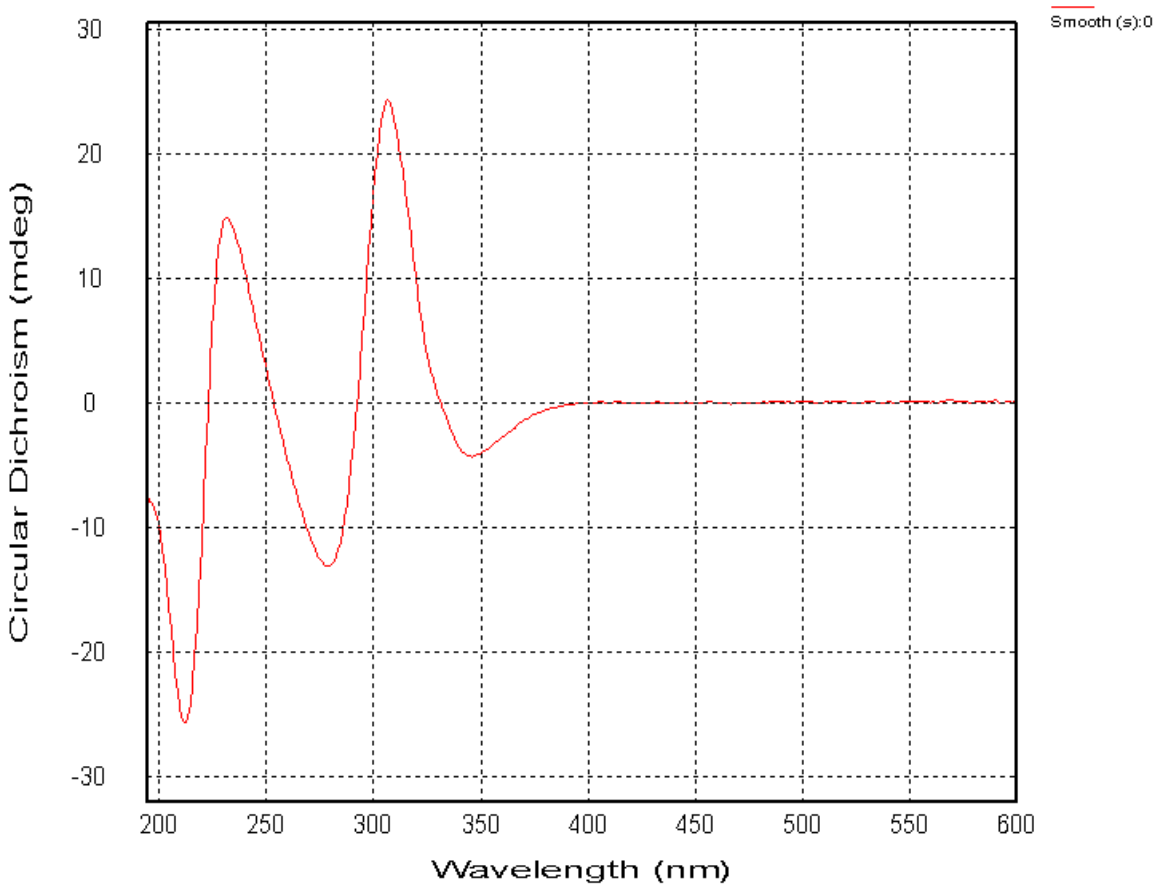


Figure S53. Specific rotation spectrum of natural henryinin C (**3**)

Optical rotation measurement

Model : P-1020 (A060460638)

No.	Sample	Mode	Data	Monitor Blank	Temp. Cell Temp Point	Date Comment Sample Name	Light Filter Operator	Cycle Time Integ Time
No.1	8 (1/3)	Sp.Rot	44.7180	0.2104 0.0000	24.3 50.00 Cell	Fri Oct 19 16:53:22 2018 0.00941g/mL MeOH SHE154	Na 589nm	2 sec 2 sec
No.2	8 (2/3)	Sp.Rot	44.6330	0.2100 0.0000	24.3 50.00 Cell	Fri Oct 19 16:53:27 2018 0.00941g/mL MeOH SHE154	Na 589nm	2 sec 2 sec
No.3	8 (3/3)	Sp.Rot	43.8040	0.2061 0.0000	24.3 50.00 Cell	Fri Oct 19 16:53:32 2018 0.00941g/mL MeOH SHE154	Na 589nm	2 sec 2 sec

Figure S54. ^{1}H NMR spectrum of natural henryinin D (**4**) at 500 MHz in $CDCl_3$

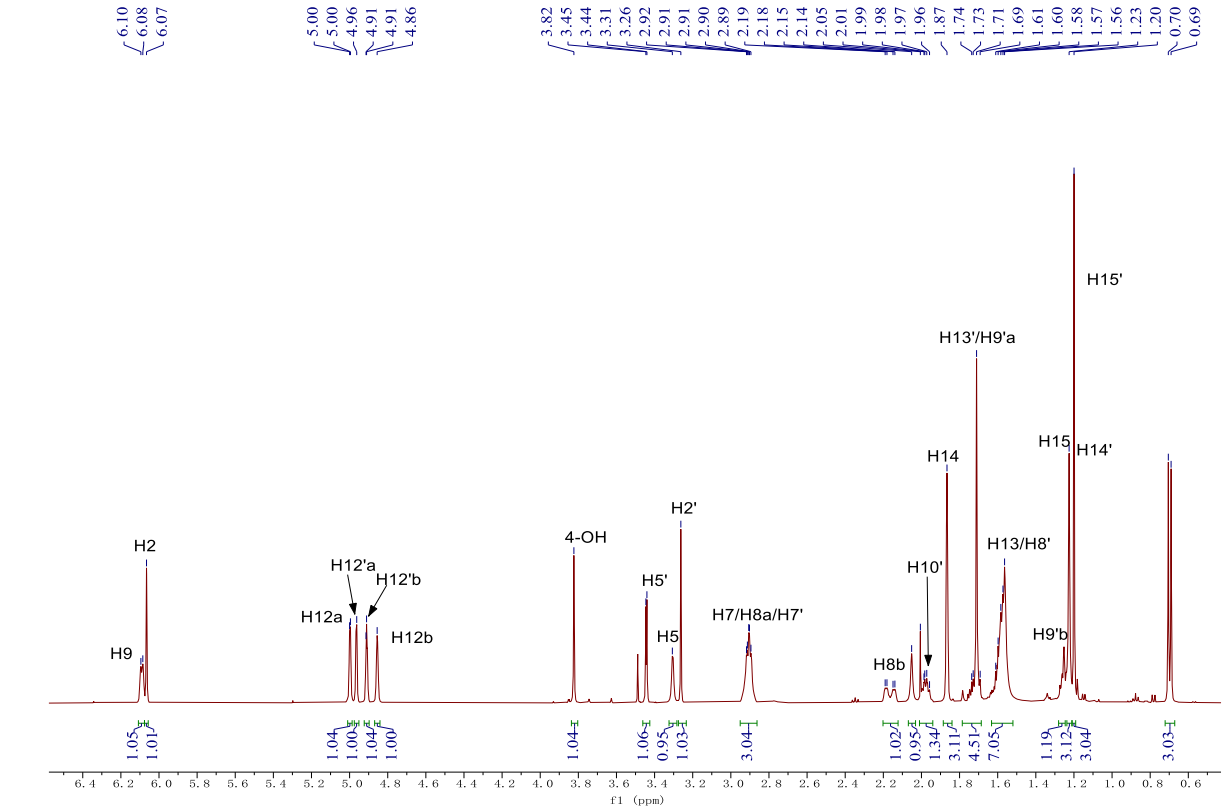


Figure S55. ^{13}C NMR spectrum of natural henryinin D (**4**) at 125 MHz in $CDCl_3$

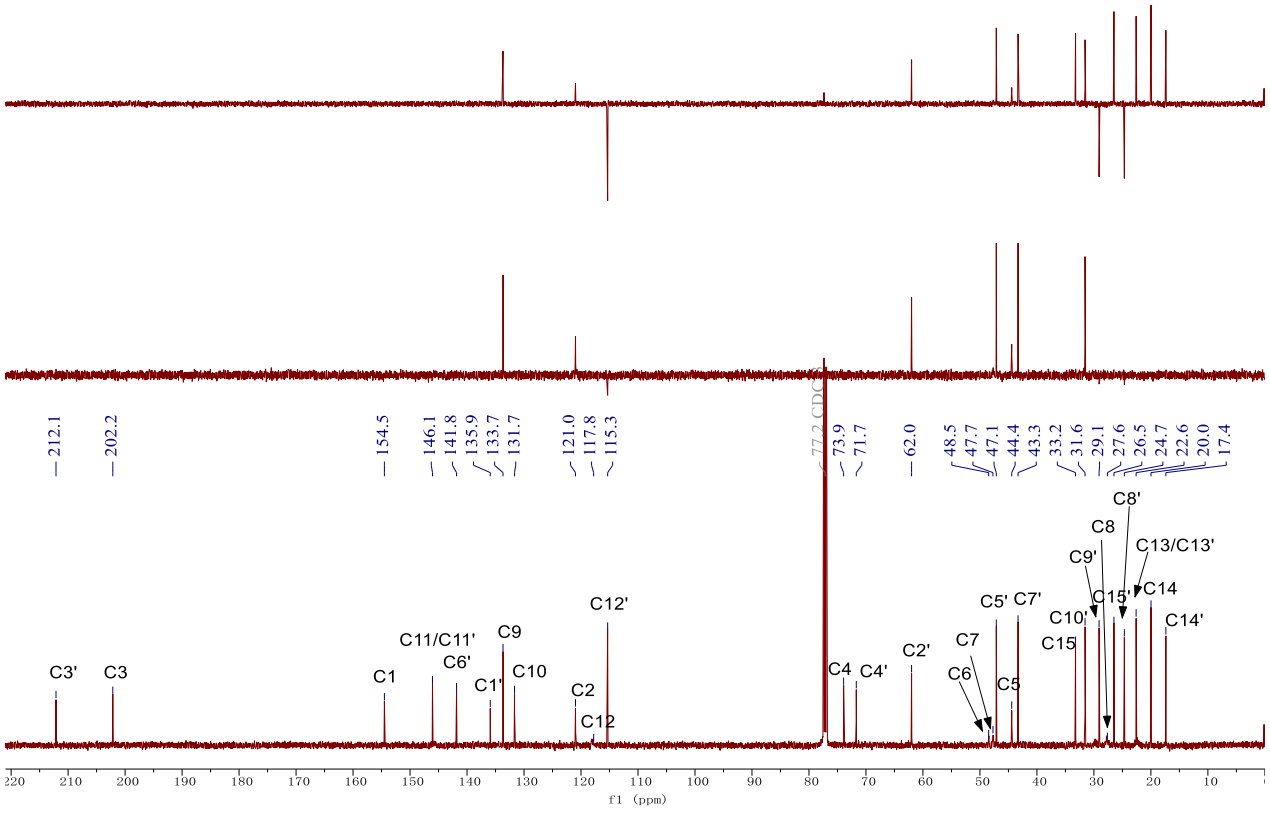


Figure S56. HSQC spectrum of natural henryinin D (**4**) in $CDCl_3$

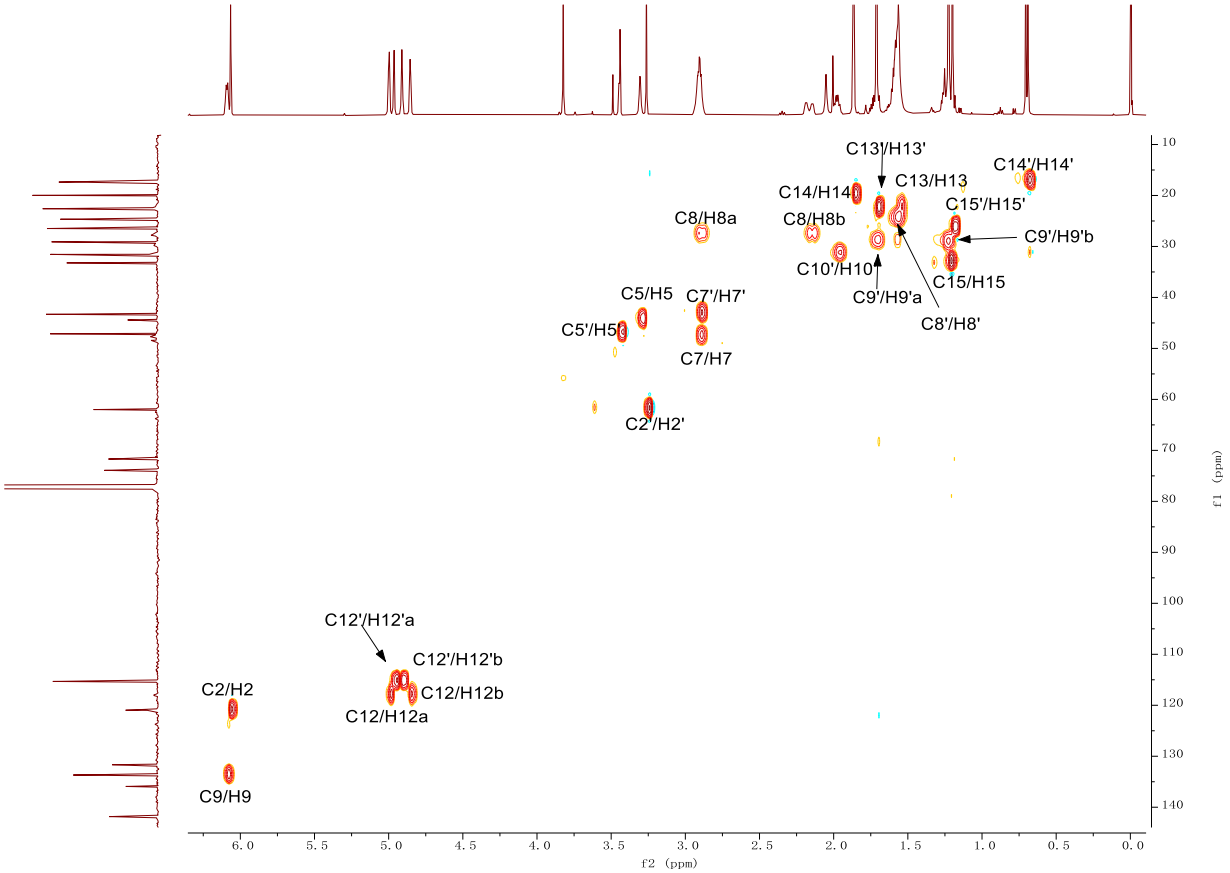


Figure S57. ^{1}H-^{1}H COSY spectrum of natural henryinin D (**4**) $CDCl_3$

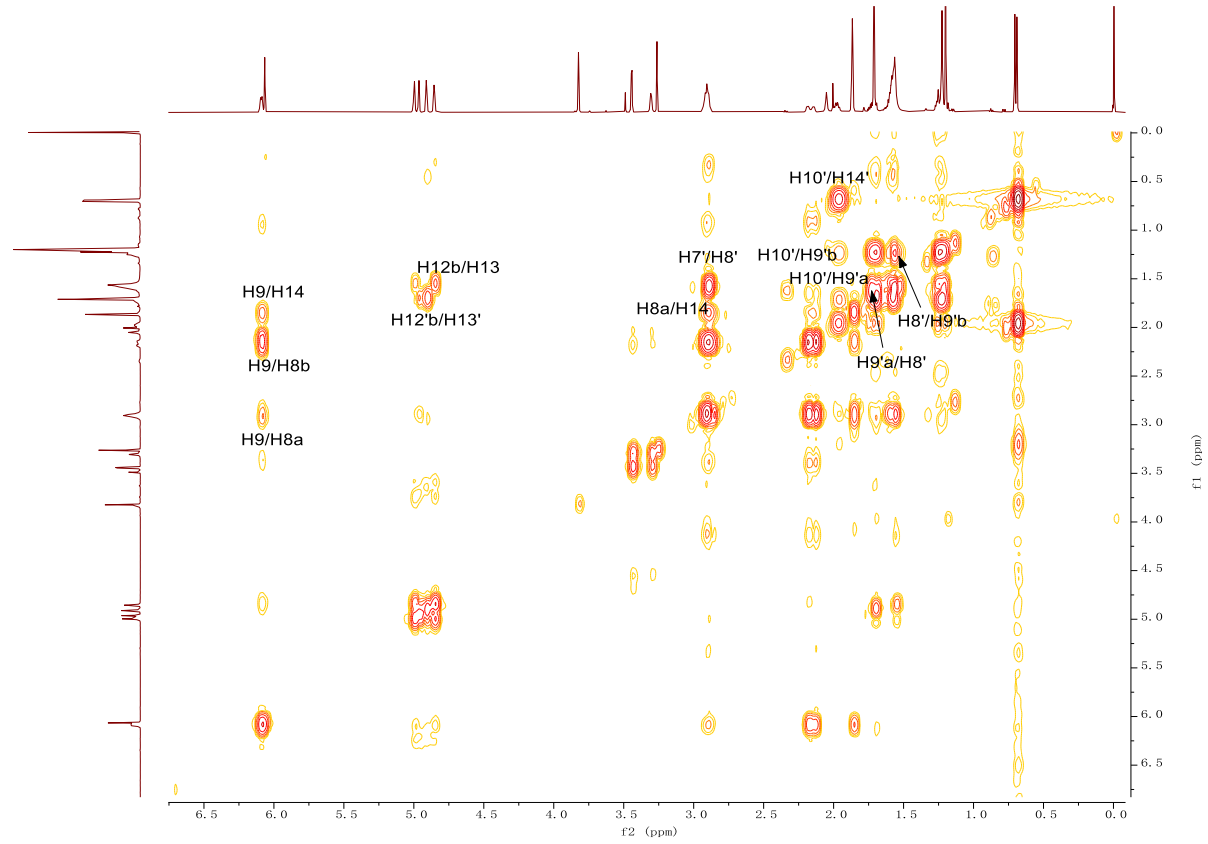


Figure S58. HMBC spectrum of natural henryinin D (**4**) $CDCl_3$

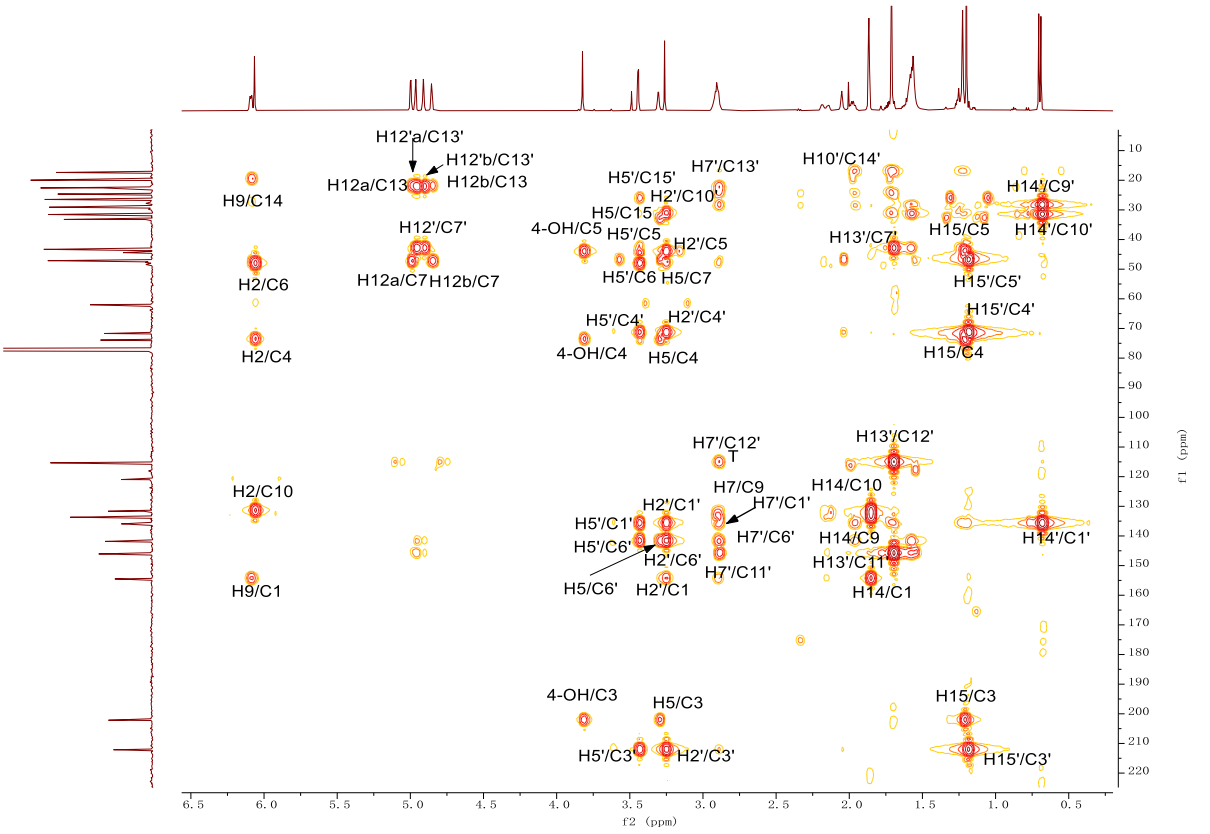


Figure S59. ROESY spectrum of natural henryinin D (**4**) $CDCl_3$

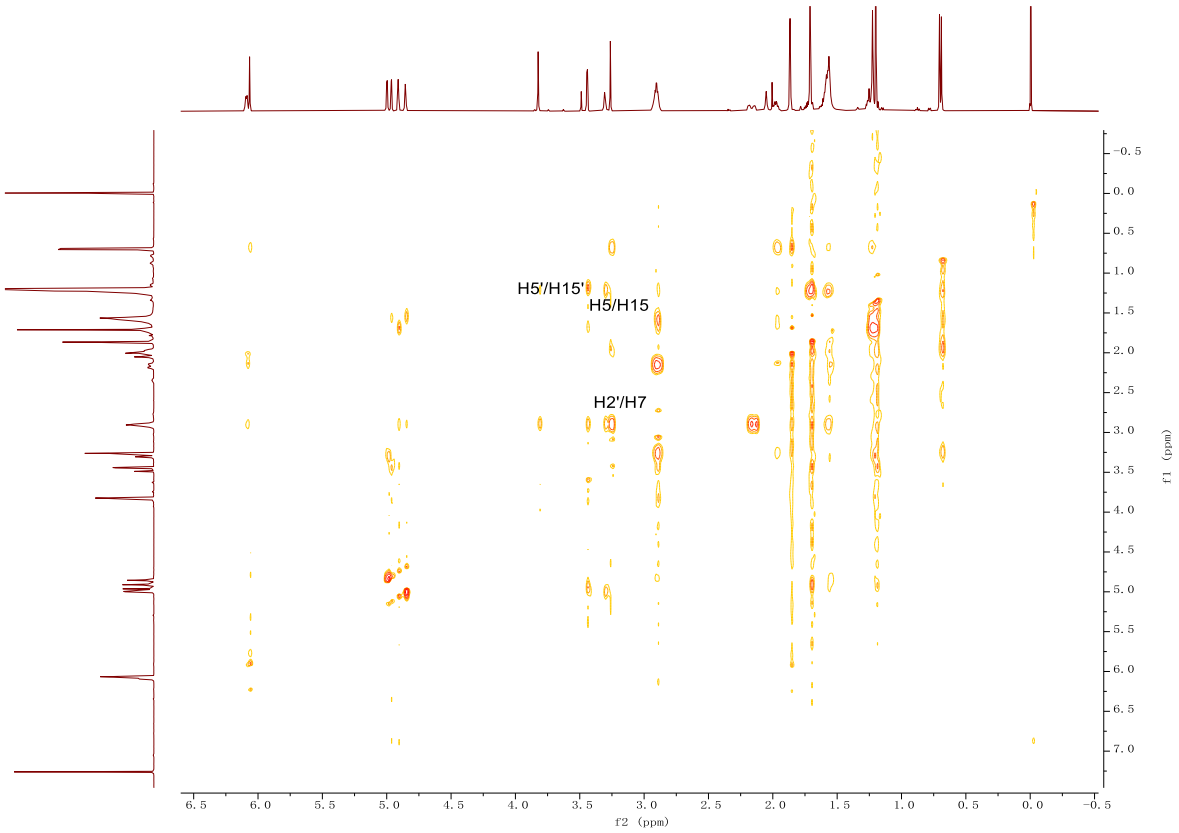


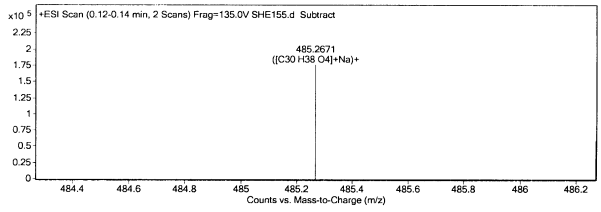
Figure S60. HRESIMS spectrum of natural henryinin D (**4**)

Data Filename	SHE155.d	**Sample Name**	SHE155
Sample Type	Sample	**Position**	P1-D4
Instrument Name	Instrument 1	**User Name**	
Acq Method	s.m	**Acquired Time**	10/15/2018 4:07:35 PM
IRM Calibration Status	Success	**DA Method**	Default.m
Comment			

Sample Group	**Info.**
Acquisition SW	6200 series TOF/6500 series
Version	Q-TOF B.05.01 (B5125.2)

User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
135	0	ESI



Peak List

m/z	z	Abund	Formula	Ion
102.1285	1	205348.59		
274.2745	1	70181.14		
318.301	1	57102.96		
463.2853	1	51536.99		
485.2671	1	175625.22	C30 H38 O4	(M+Na)+
486.2696	1	59304.95	C30 H38 O4	(M+Na)+
501.241	1	46846.72		
507.1947	1	47394.2		
947.5447	1	123877.27		
948.5477	1	80735.36		

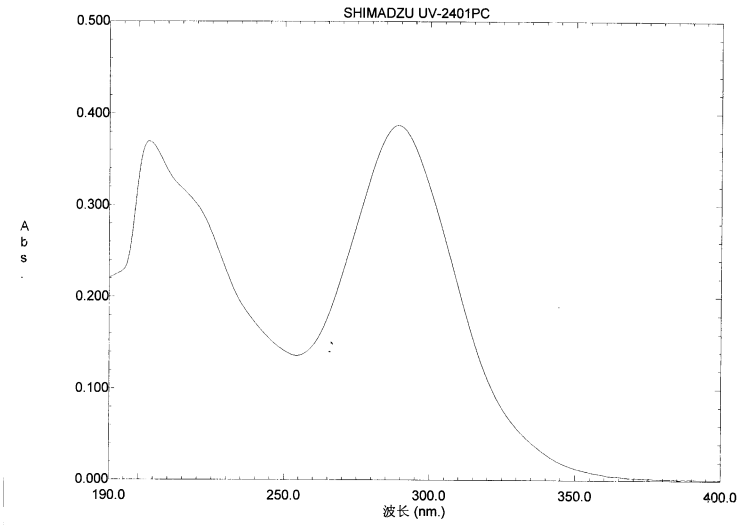
Formula Calculator Element Limits

Element	Min	Max
C	3	60
H	0	120
O	0	40
S	0	3

Formula Calculator Results

Formula	CalculatedMass	CalculatedMz	Mz	Diff. (mDa)	Diff. (ppm)	DBE
C30 H38 O4	462.2770	485.2662	485.2671	-0.90	-1.85	12.0000

Figure S61. UV spectrum of natural henryinin D (**4**)



文件名: SHE155

SHE155

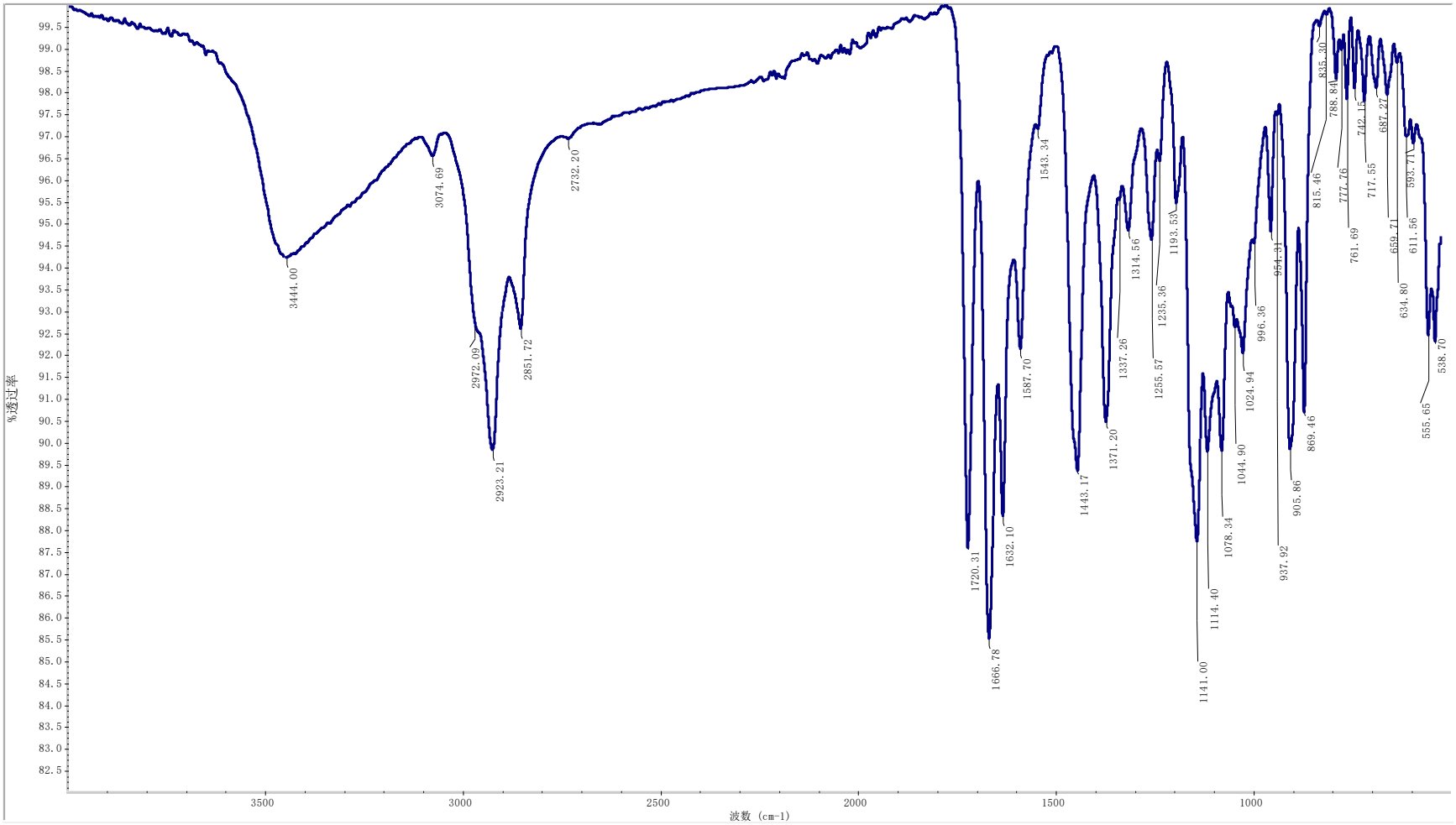
样品浓度：0.0195毫克/毫升
溶剂：甲醇

创建于: 16:20 18-10-21
数据: 原始

测量模式: Abs.
扫描速度: 中速
狭缝: 5.0
采样间隔: 0.5

否.	波长 (nm.)	Abs.
1	289.00	0.3870
2	203.50	0.3693

Figure S62. IR spectrum of natural henryinin D (**4**)



Sample Name: SHE155
ATR ITX-DIAMOND
采集时间: 星期五 11月 02 09:08:59 2018 (GMT+08:00)
仪器型号：NICOLET iS10
Software version: OMNIC 9.8.372

样品扫描次数: 16
背景扫描次数: 16
分辨率: 4.000
采样增益: 1.0
动镜速度: 0.4747
光阑: 150.00

Figure S63. ECD spectrum of natural henryinin D (**4**) (0.1950mg/mL in MeOH)

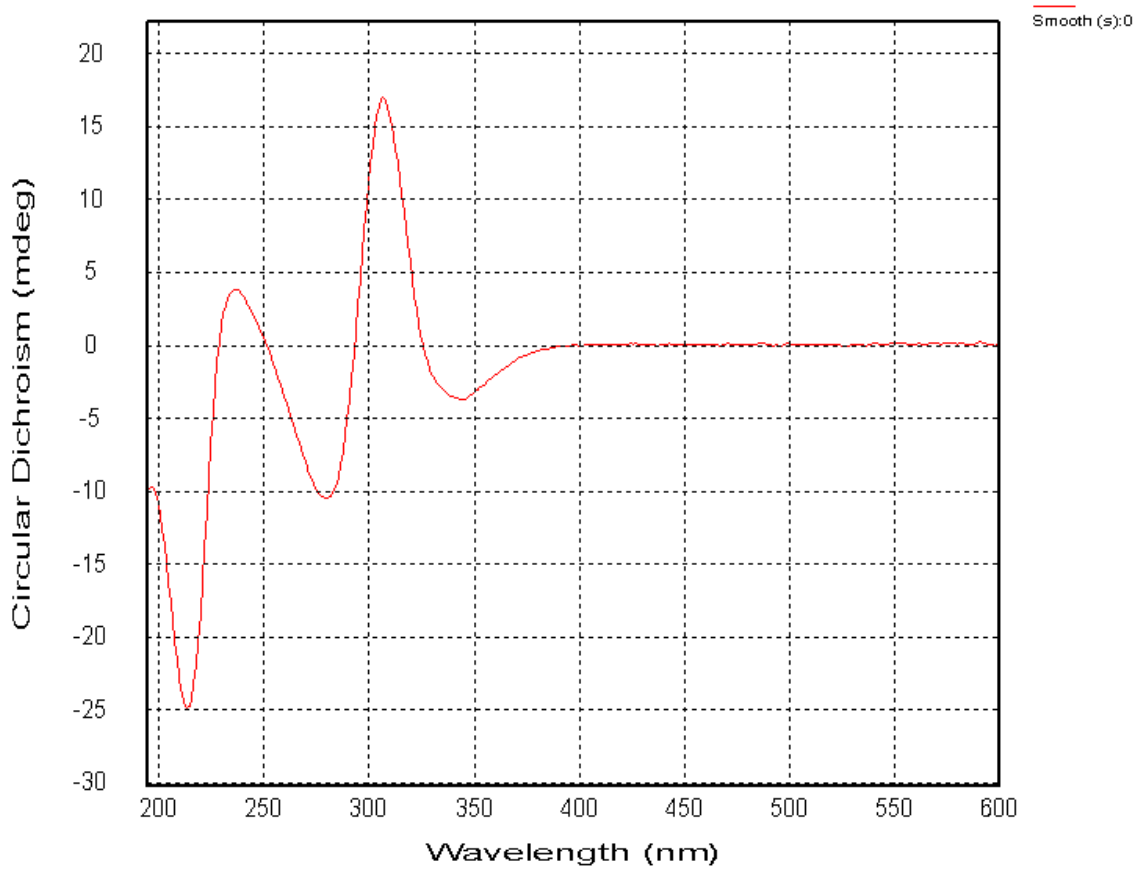


Figure S64. Specific rotation spectrum of natural henryinin D (**4**)

Optical rotation measurement

Model : P-1020 (A060460638)

No.	Sample	Mode	Data	Monitor Blank	Temp. Cell Temp Point	Date Comment Sample Name	Light Filter Operator	Cycle Time Integ Time
No.1	10 (1/3)	Sp.Rot	-54.1540	-0.0352 0.0000	24.3 50.00 Cell	Fri Oct 19 17:01:51 2018 0.00130g/mL MeOH SHE155	Na 589nm	2 sec 2 sec
No.2	10 (2/3)	Sp.Rot	-47.0770	-0.0306 0.0000	24.4 50.00 Cell	Fri Oct 19 17:01:57 2018 0.00130g/mL MeOH SHE155	Na 589nm	2 sec 2 sec
No.3	10 (3/3)	Sp.Rot	-48.1540	-0.0313 0.0000	24.3 50.00 Cell	Fri Oct 19 17:02:02 2018 0.00130g/mL MeOH SHE155	Na 589nm	2 sec 2 sec

Figure S65. ^{1}H NMR spectrum of natural henryinin E (**5**) at 500 MHz in $CDCl_3$

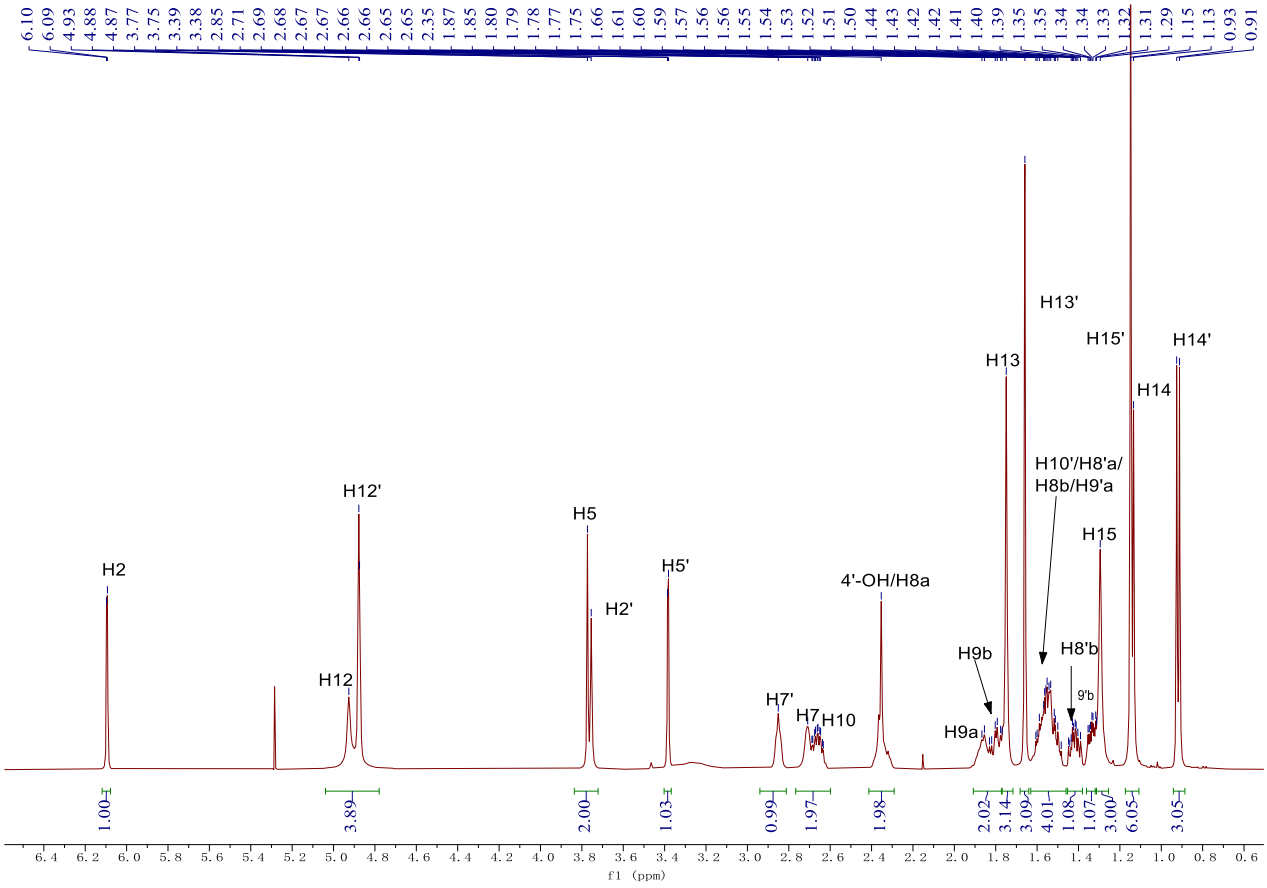


Figure S66. ^{13}C NMR spectrum of natural henryinin E (**5**) at 125 MHz in $CDCl_3$

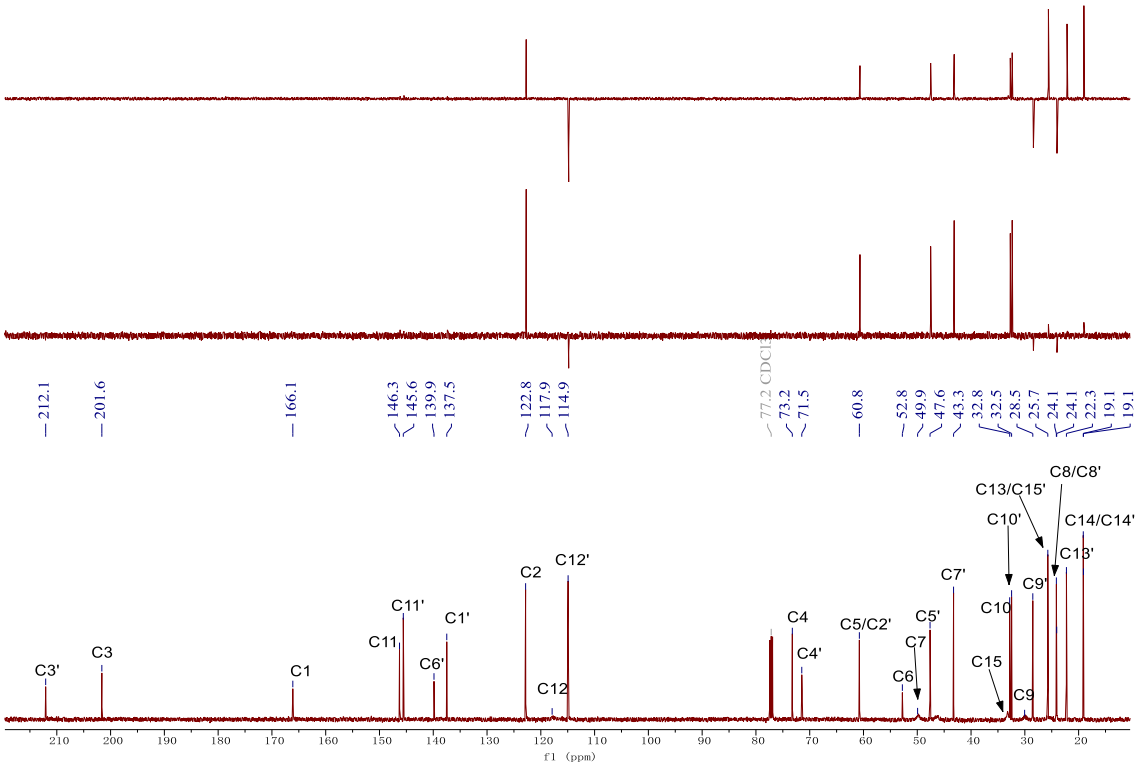


Figure S67. HSQC spectrum of natural henryinin E (**5**) in $CDCl_3$

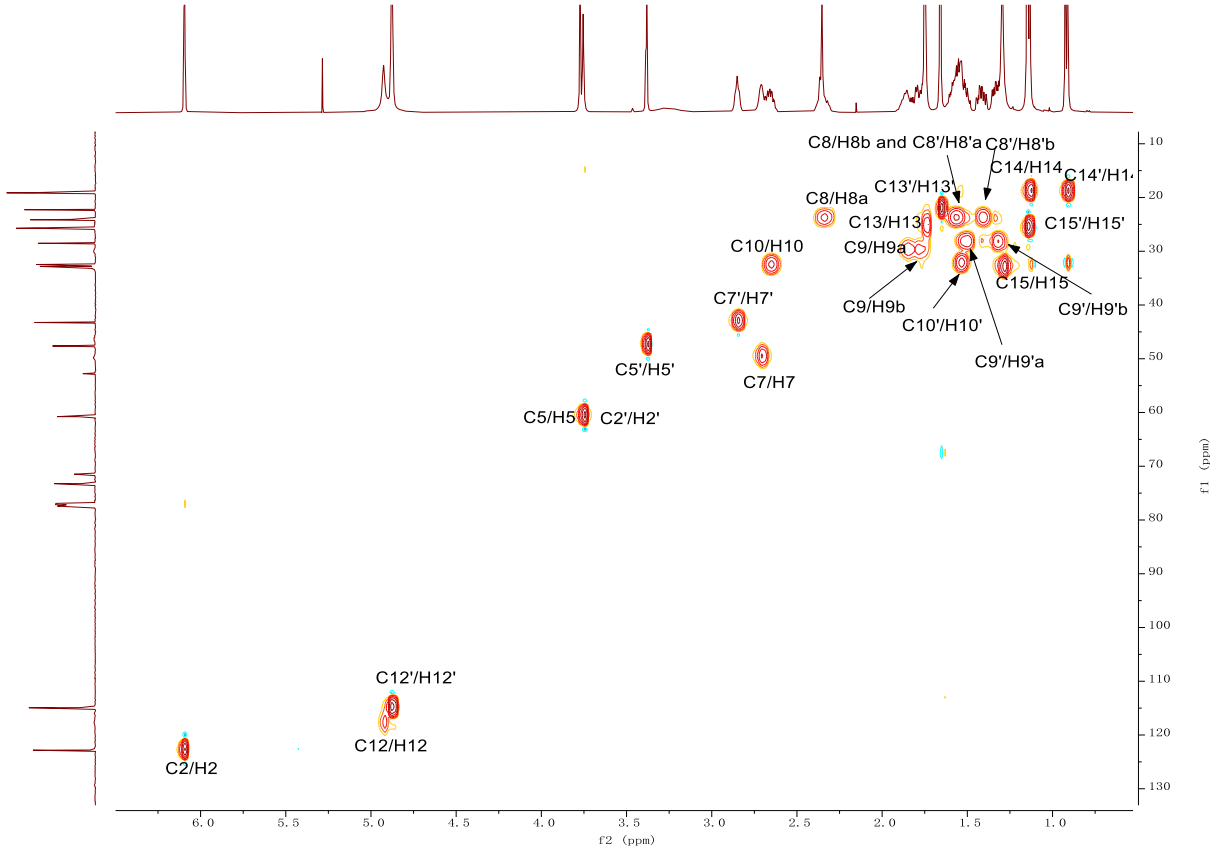


Figure S68. ^{1}H-^{1}H COSY spectrum of natural henryinin E (**5**) in $CDCl_3$

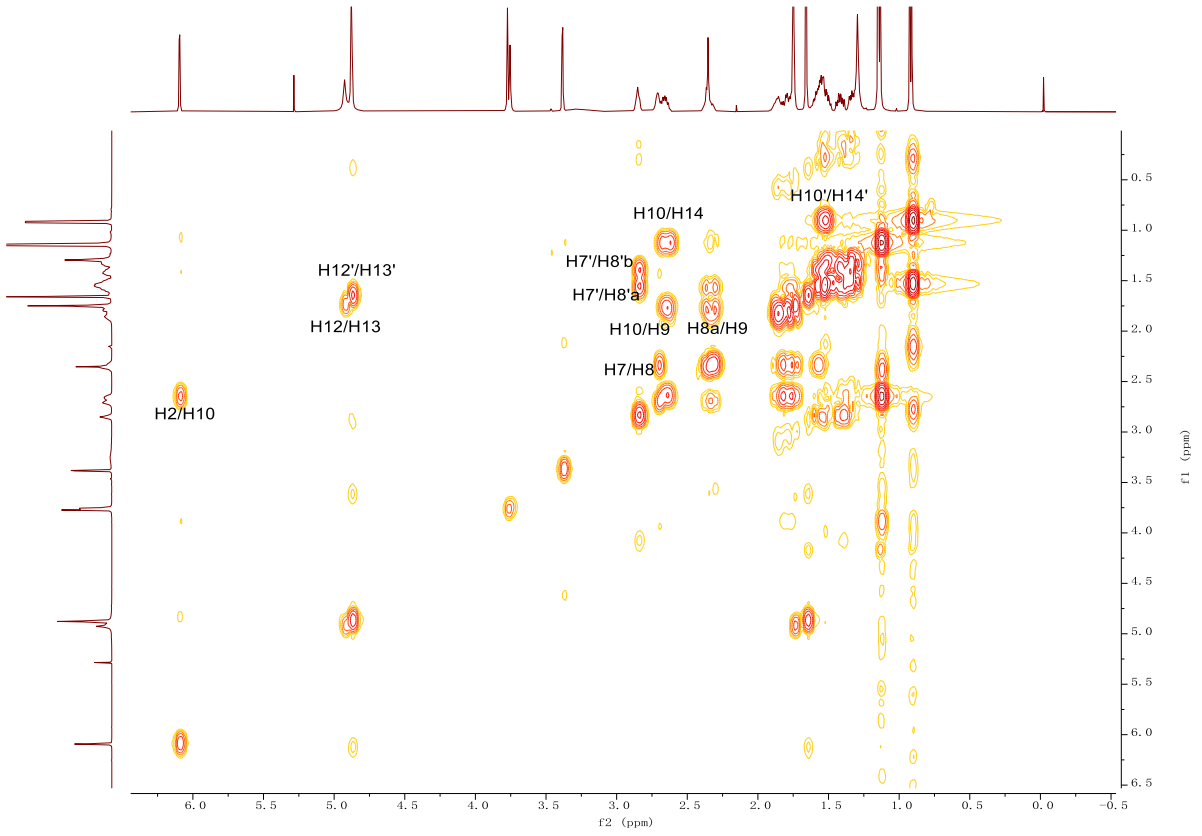


Figure S69. HMBC spectrum of natural henryinin E (**5**) in $CDCl_3$

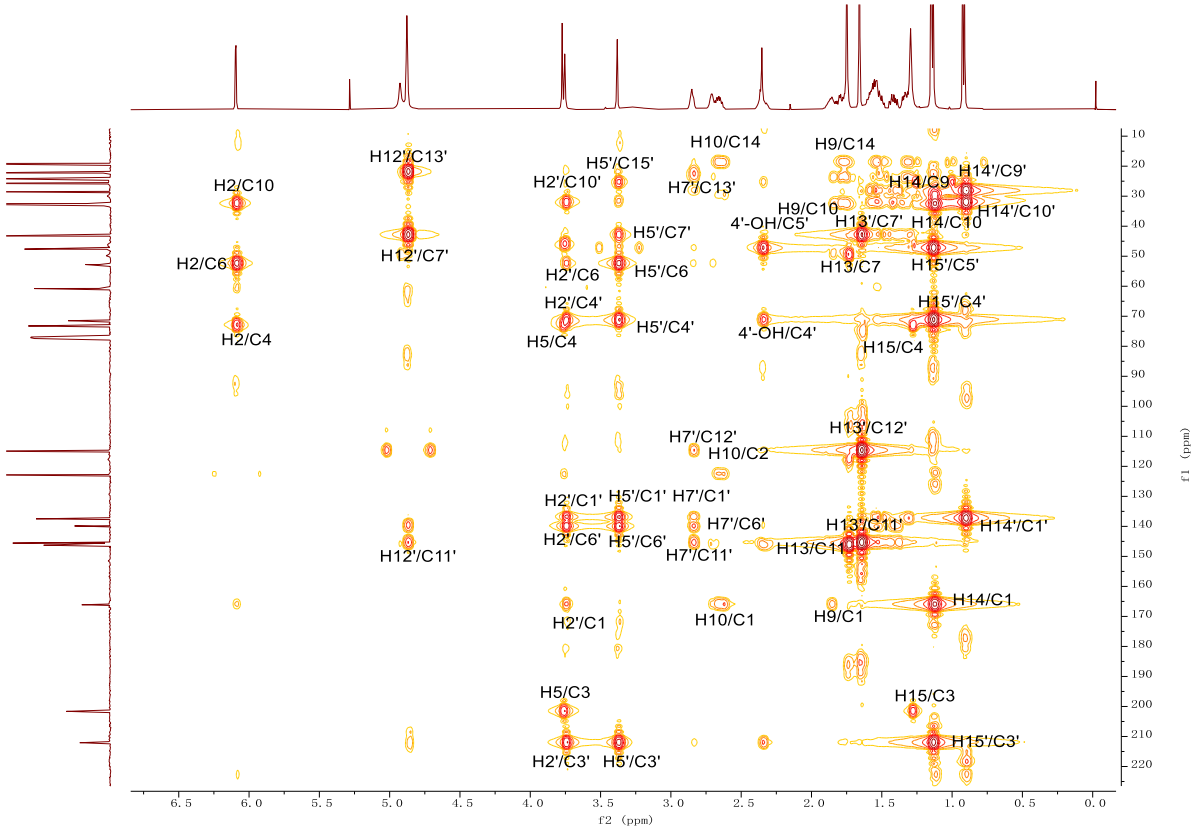


Figure S70. ROESY spectrum of natural henryinin E (**5**) in $CDCl_3$

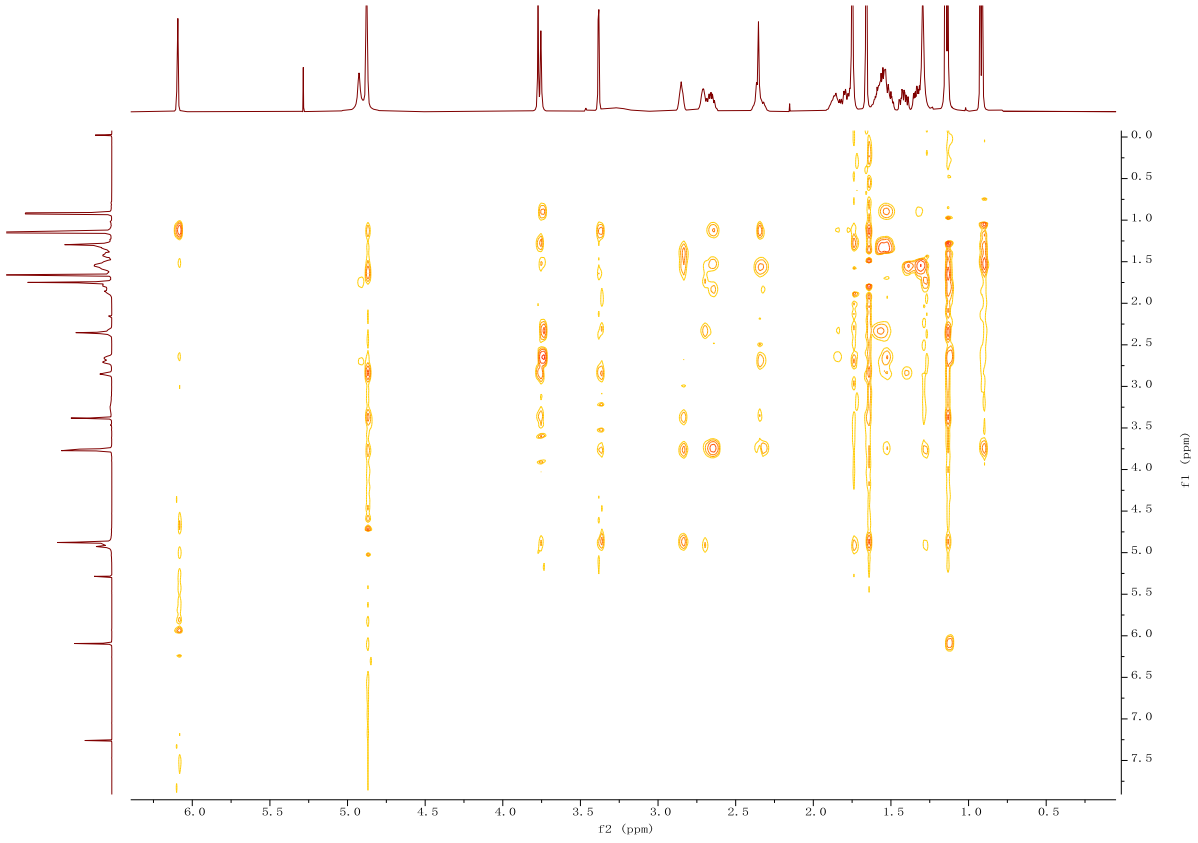


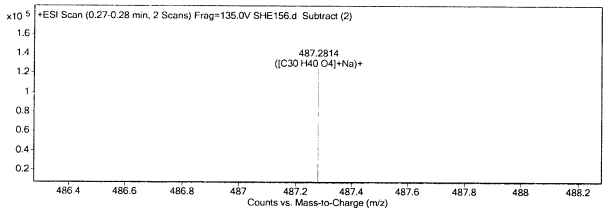
Figure S71. HRESIMS spectrum of natural henryinin E (**5**)

Data Filename	SHE156.d	**Sample Name**	SHE156
Sample Type	Sample	**Position**	P1-B2
Instrument Name	Instrument 1	**User Name**	
Acq Method	s.m	**Acquired Time**	10/26/2018 2:33:07 PM
IRM Calibration Status	Success	**DA Method**	Default.m
Comment			

Sample Group	**Info.**
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125.2)

User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
135	0	ESI



Peak List

m/z	z	Abund	Formula	Ion
252.1272	2	20944.98		
487.2814	1	123923.25	C30 H40 O4	(M+Na)+
488.2846	1	38698.34	C30 H40 O4	(M+Na)+
503.255	1	88669.36		
504.2587	1	29712.65		
765.434	1	40056.55		
766.437	1	19153.88		
951.5747	1	138155.95		
952.578	1	92881.55		
953.5813	1	29789.51		

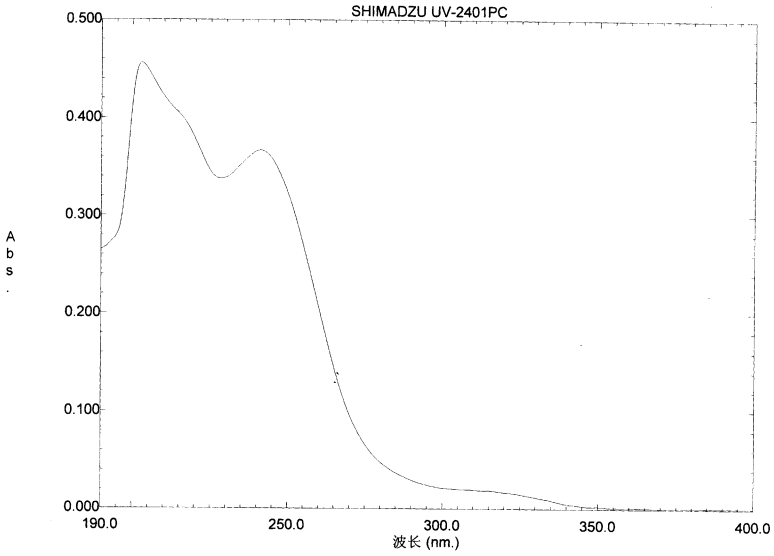
Formula Calculator Element Limits

Element	Min	Max
C	3	120
H	0	240
O	0	30

Formula Calculator Results

Formula	CalculatedMass	CalculatedMz	Mz	Diff. (mDa)	Diff. (ppm)	DBE
C30 H40 O4	464.2927	487.2819	487.2814	0.50	1.03	11.0000

Figure S72. UV spectrum of natural henryinin E (**5**)



文件名: SHE156

SHE156

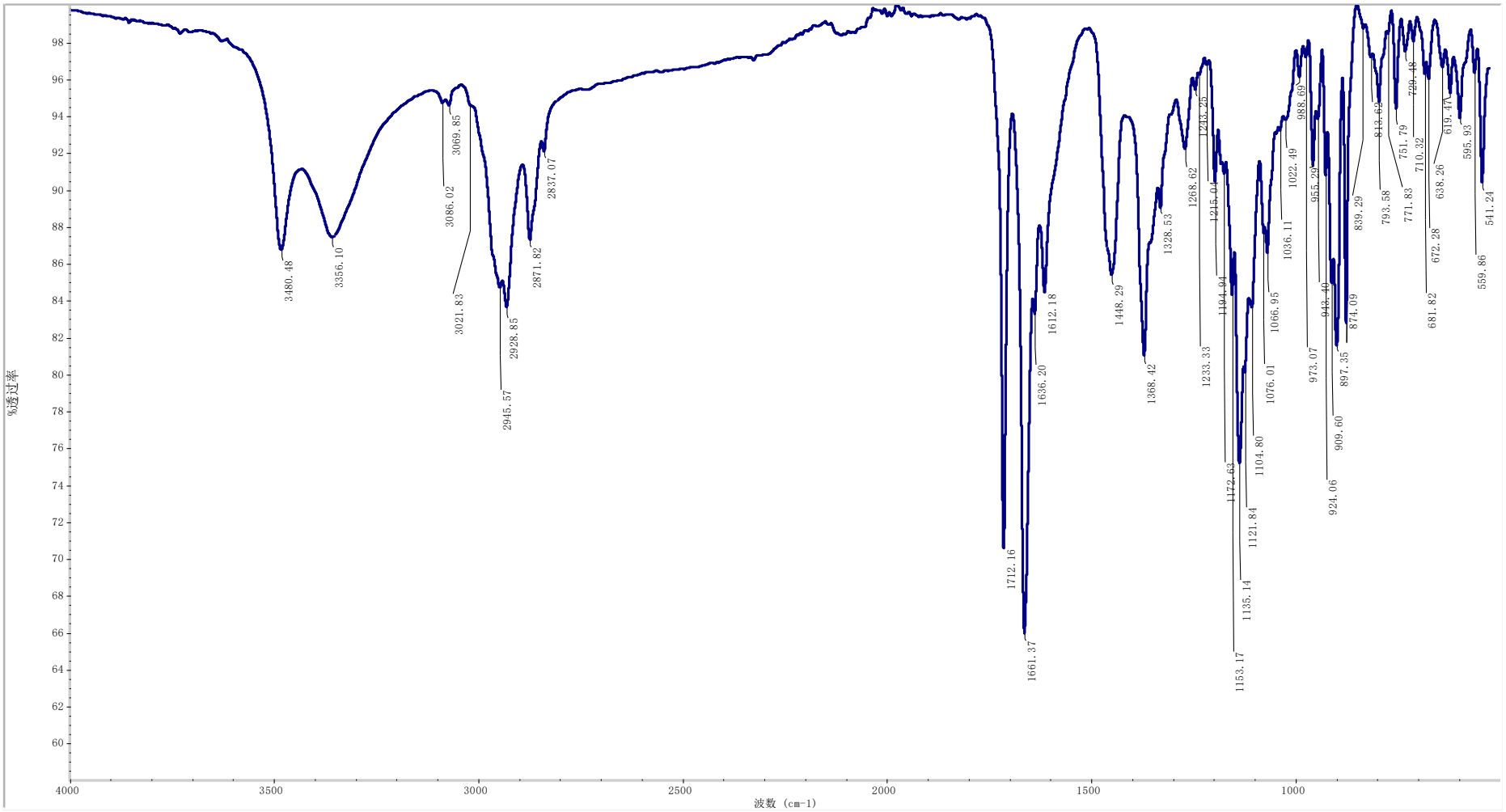
样品浓度：0.0112毫克/毫升
溶剂：甲醇

创建于: 19:23 18-10-27
数据: 原始

测量模式: Abs.
扫描速度: 中速
狭缝: 5.0
采样间隔: 0.2

否.	波长 (nm.)	Abs.
1	241.20	0.3666
2	202.80	0.4560

Figure S73. IR spectrum of natural henryinin E (**5**)



Sample Name: SHE156
ATR ITX-DIAMOND
采集时间: 星期五 11月 02 09:32:53 2018 (GMT+08:00)
仪器型号：NICOLET iS10
Software version: OMNIC 9.8.372

样品扫描次数: 16
背景扫描次数: 16
分辨率: 4.000
采样增益: 1.0
动镜速度: 0.4747
光阑: 150.00

Figure S74. ECD spectrum of natural henryinin E (**5**) (0.1344mg/mL in MeOH)

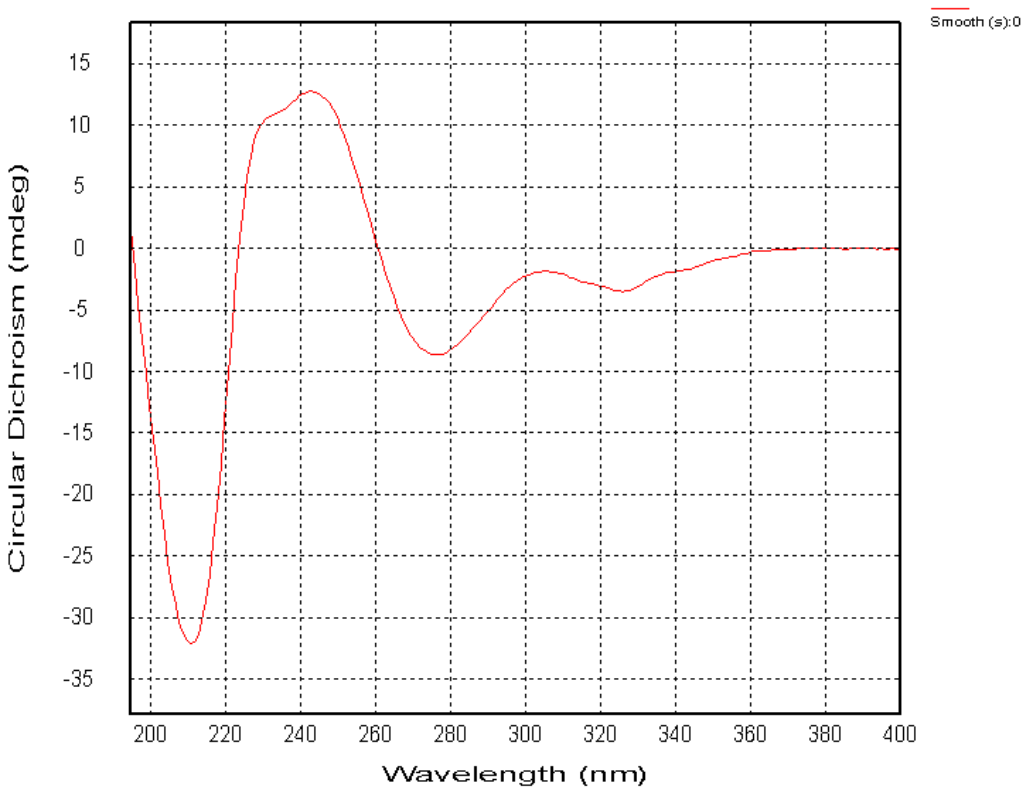


Figure S75. Specific rotation spectrum of natural henryinin E (**5**)

Optical rotation measurement

Model : P-1020 (A060460638)

No.	Sample	Mode	Data	Monitor Blank	Temp. Cell Temp Point	Date Comment Sample Name	Light Filter Operator	Cycle Time Integ Time
No.1	2 (1/3)	Sp.Rot	-78.2140	-0.0438 0.0000	22.2 50.00 Cell	Sat Oct 27 15:28:11 2018 0.00112g/mL MeOH SHE156	Na 589nm	2 sec 2 sec
No.2	2 (2/3)	Sp.Rot	-79.6430	-0.0446 0.0000	22.2 50.00 Cell	Sat Oct 27 15:28:16 2018 0.00112g/mL MeOH SHE156	Na 589nm	2 sec 2 sec
No.3	2 (3/3)	Sp.Rot	-77.3210	-0.0433 0.0000	22.2 50.00 Cell	Sat Oct 27 15:28:21 2018 0.00112g/mL MeOH SHE156	Na 589nm	2 sec 2 sec

-78.3929°

Figure S76. ^{1}H NMR spectrum of **21** at 500 MHz in $CDCl_3$

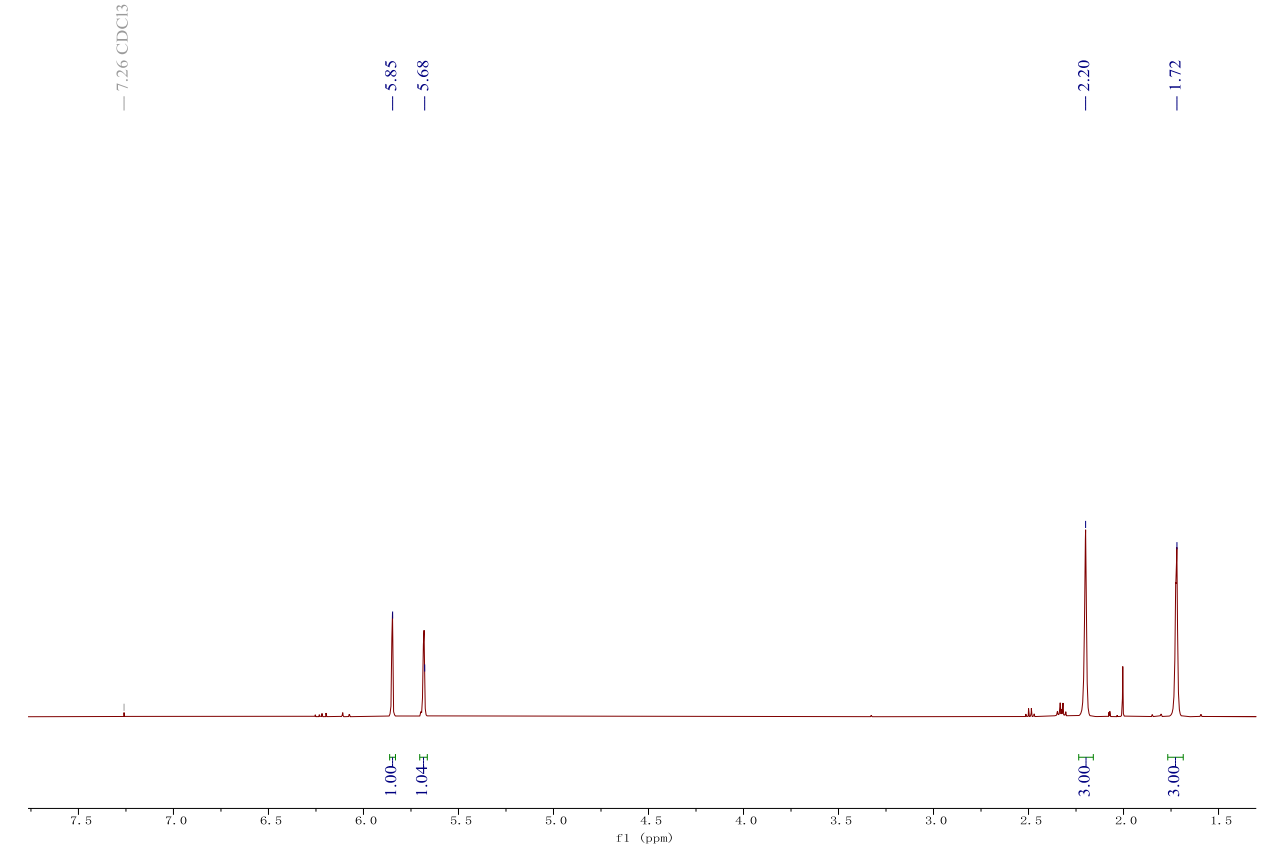


Figure S77. ^{13}C NMR spectrum of **21** at 125 MHz in $CDCl_3$

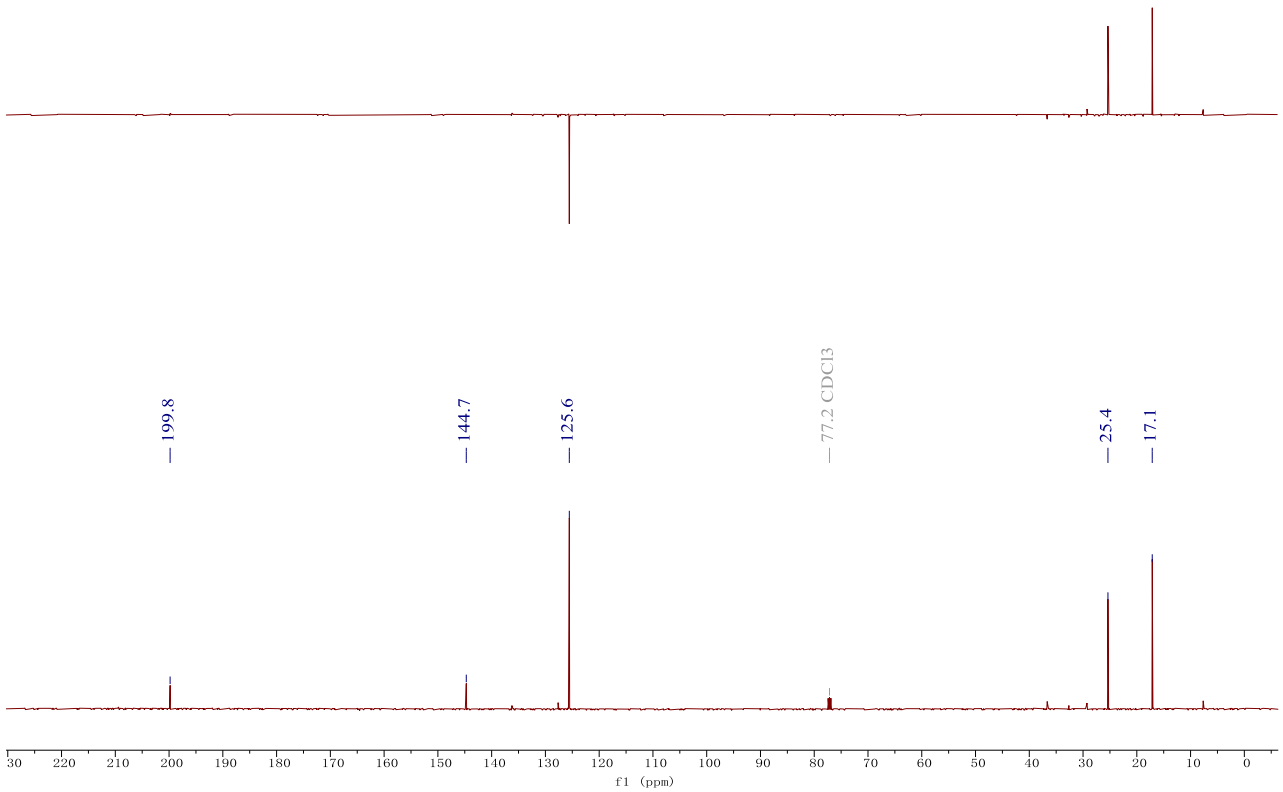


Figure S78. ^{1}H NMR spectrum of **20** at 500 MHz in $CDCl_3$

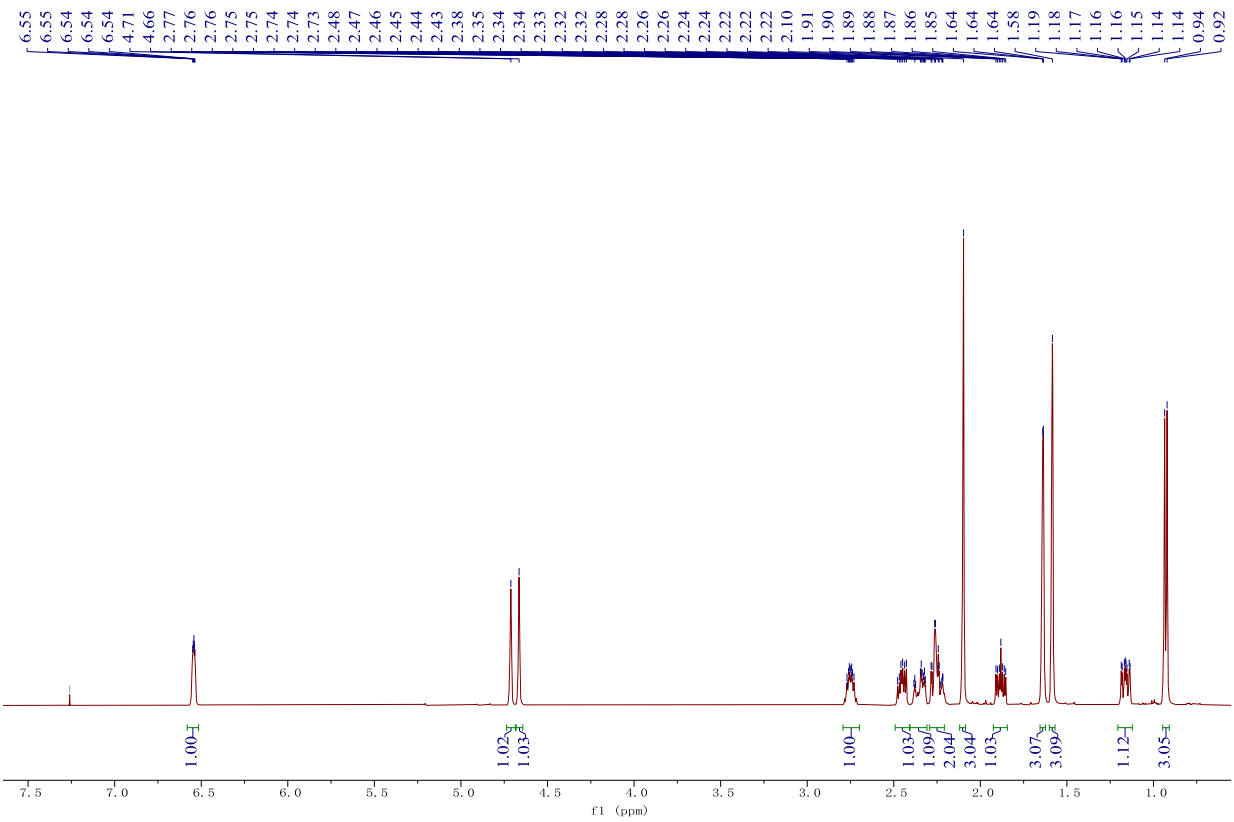


Figure S79. ^{13}C NMR spectrum of **20** at 125 MHz in $CDCl_3$

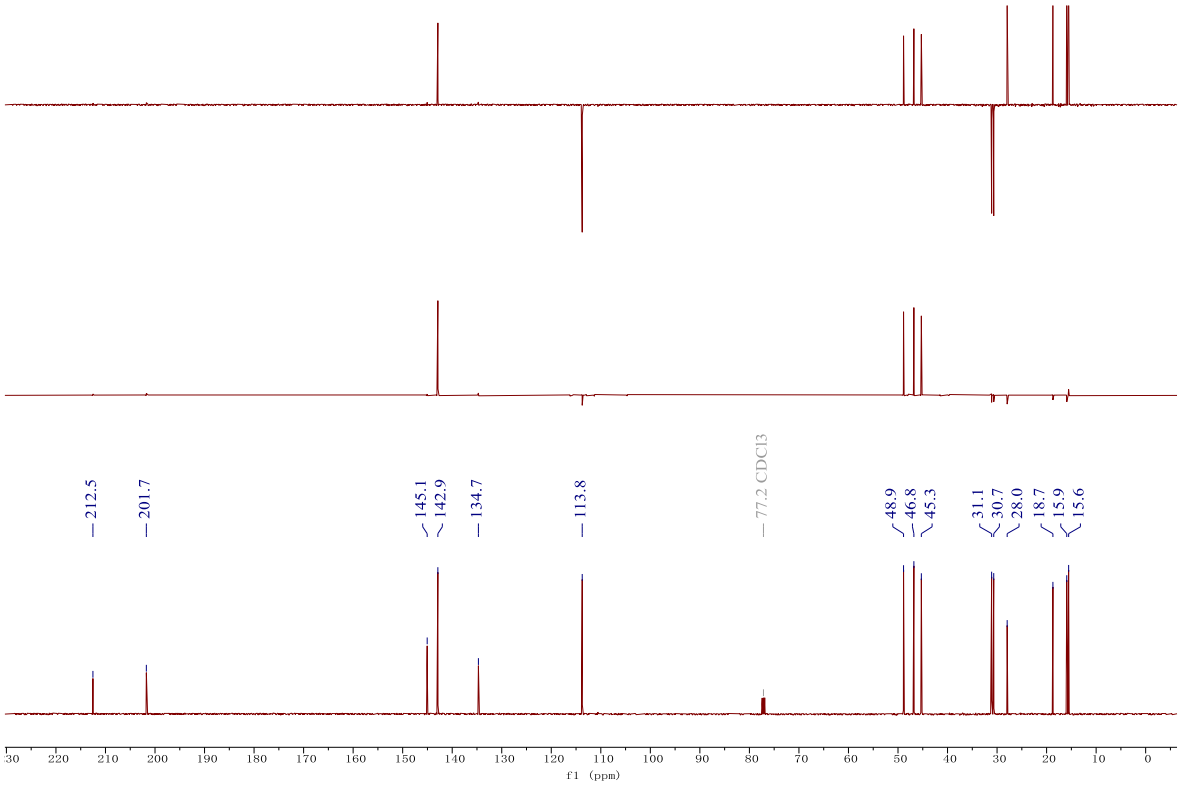


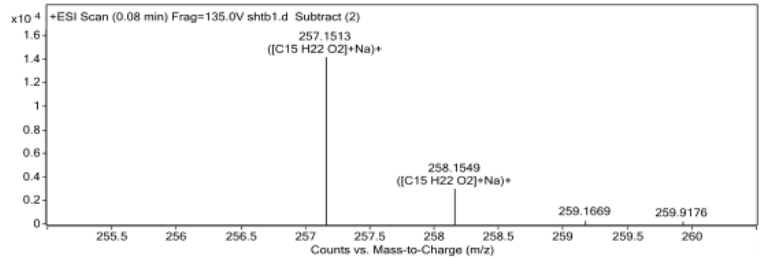
Figure S80. HRESIMS spectrum of **20**

Data Filename	shtb1.d	**Sample Name**	shtb1
Sample Type	Sample	**Position**	P1-A1
Instrument Name	Instrument 1	**User Name**	
Acq Method	s.m	**Acquired Time**	3/25/2021 10:23:07 AM
IRM Calibration Status	Success	**DA Method**	Default.m
Comment			

Sample Group	**Info.**
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125.2)

User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
135	0	ESI



Peak List

m/z	z	Abund	Formula	Ion
130.064		656.42		
235.1702	1	4954.79		
236.1721	1	804.79		
257.1513	1	14213.26	C15 H22 O2	(M+Na)+
258.1549	1	3050.26	C15 H22 O2	(M+Na)+
273.1247	1	3129.54		
280.2283		1308.65		
317.1359		856.16		
491.3145	1	2136.99		
492.3178	1	661.88		

Formula Calculator Element Limits

Element	Min	Max
C	3	60
H	0	120
O	0	10
N	0	5

Formula Calculator Results

Formula	CalculatedMass	CalculatedMz	Mz	Diff. (mDa)	Diff. (ppm)	DBE
C15 H22 O2	234.1620	257.1512	257.1513	-0.10	-0.39	5.0000

Figure S81. Specific rotation spectrum of **20**

Rudolph Research Analytical

This sample was measured on an Autopol VI, Serial #91058
Manufactured by Rudolph Research Analytical, Hackettstown, NJ, USA.

Measurement Date : Tuesday, 25-MAY-2021

Set Temperature : OFF

Time Delay : Disabled

Delay between Measurement : Disabled

n	Average	Std.Dev.	% RSD	Maximum	Minimum
5	3.17	0.71	22.39	4.29	2.55

S.No	Sample ID	Time	Result	Scale	OR °Arc	WLG.nm	Lg.mm	Conc.g/100ml	Temp.
1	SHTB1	04:23:28 PM	3.35	SR	0.0054	589	100.00	0.161	27.3
2	SHTB1	04:23:36 PM	2.61	SR	0.0042	589	100.00	0.161	27.3
3	SHTB1	04:24:05 PM	3.04	SR	0.0049	589	100.00	0.161	27.3
4	SHTB1	04:24:19 PM	4.29	SR	0.0069	589	100.00	0.161	27.3
5	SHTB1	04:24:32 PM	2.55	SR	0.0041	589	100.00	0.161	27.3

Figure S82. ^{1}H NMR spectrum of **19** at 500 MHz in $CDCl_3$

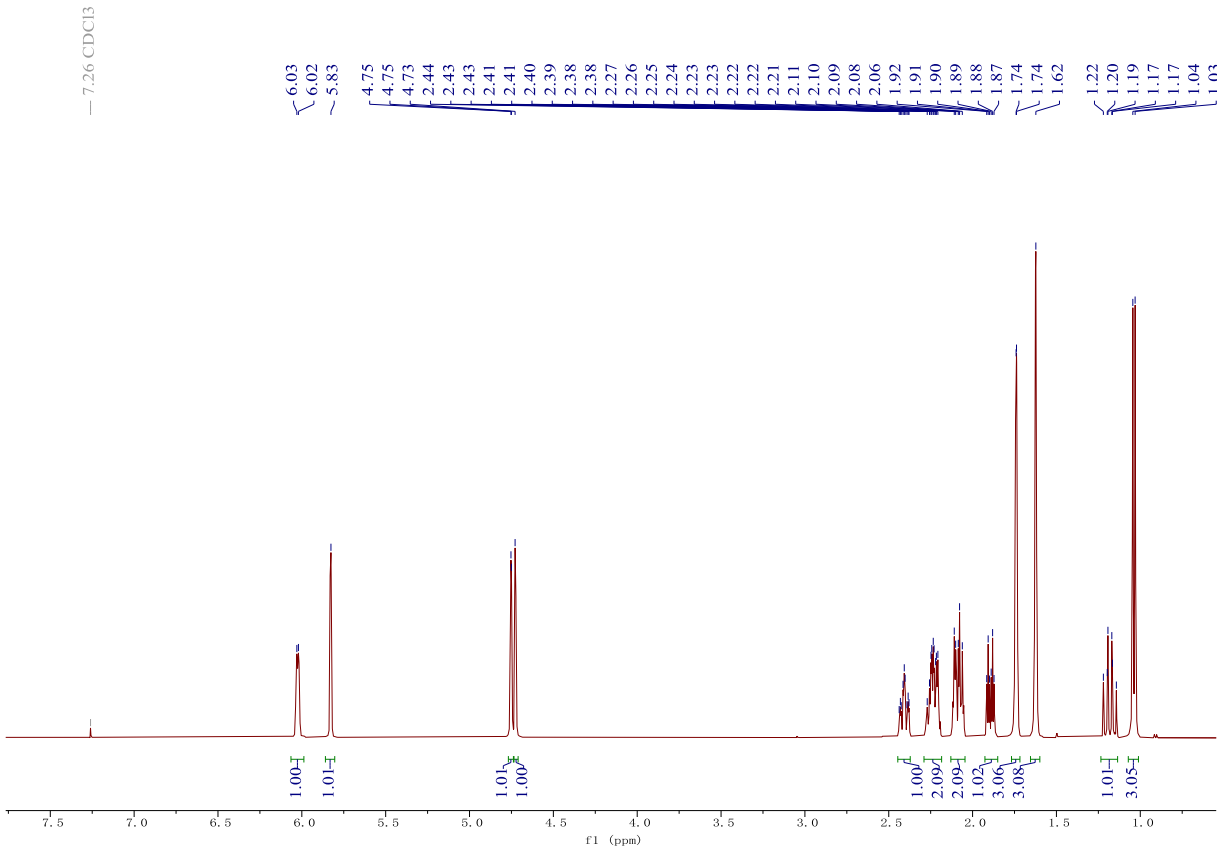


Figure S83. ^{13}C NMR spectrum of **19** at 125 MHz in $CDCl_3$

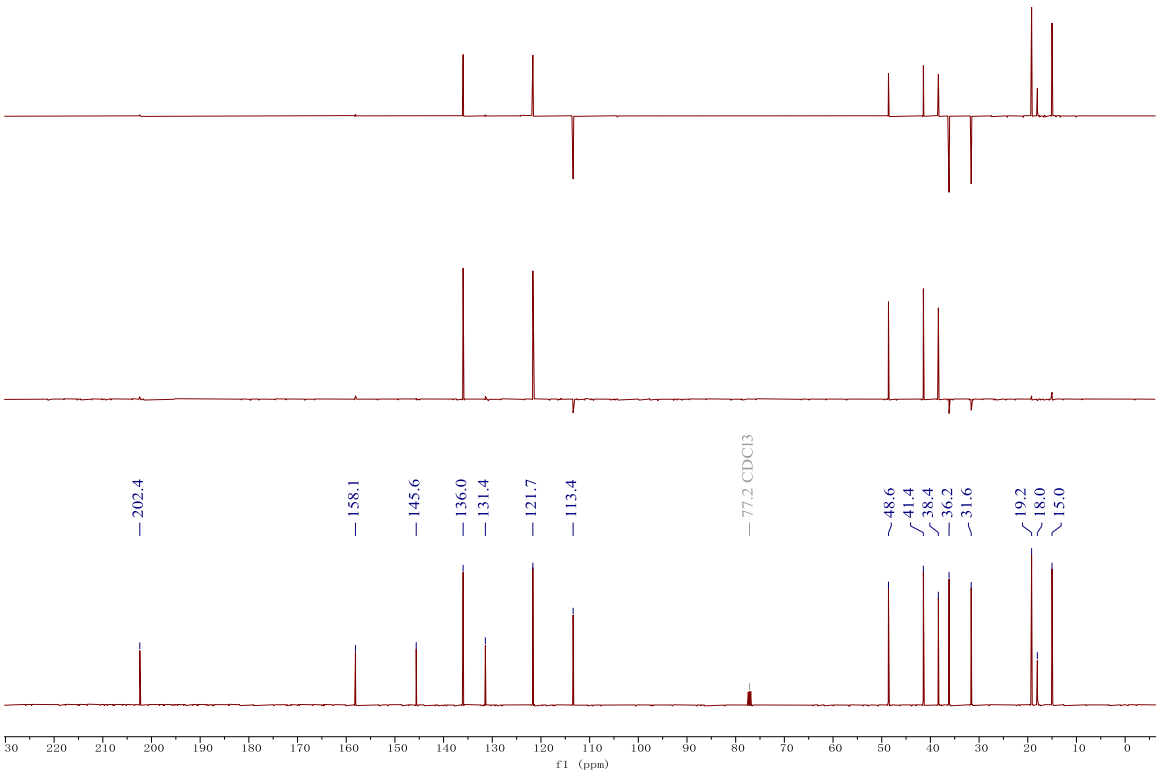


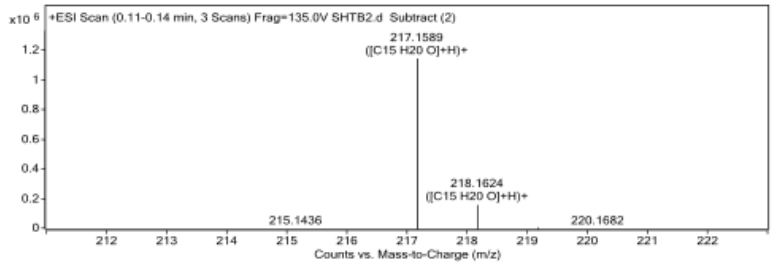
Figure S84. HRESIMS spectrum of **19**

Data Filename	SHTB2.d	**Sample Name**	SHTB2
Sample Type	Sample	**Position**	P1-A1
Instrument Name	Instrument 1	**User Name**	
Acq Method	s.m	**Acquired Time**	12/25/2020 9:36:26 AM
IRM Calibration Status	Success	**DA Method**	Default.m
Comment			

Sample Group	**Info.**
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125.2)

User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
135	0	ESI



Peak List

m/z	z	Abund	Formula	Ion
175.1119	1	26485.88		
217.1589	1	1148155.13	C15 H20 O	(M+H)+
218.1624	1	164333.36	C15 H20 O	(M+H)+
219.1657	1	14972.31	C15 H20 O	(M+H)+
239.1412	1	47203.96		
280.1674	1	14946.94		
433.3102	1	46145.74		
434.3133	1	14861.64		
452.2842	2	12069.46		
455.2921	1	25927.07		

Formula Calculator Element Limits

Element	Min	Max
C	3	120
H	0	240
O	0	30

Formula Calculator Results

Formula	CalculatedMass	CalculatedMz	Mz	Diff. (mDa)	Diff. (ppm)	DBE
C15 H20 O	216.1514	217.1587	217.1589	-0.20	-0.92	6.0000

Figure S85. Specific rotation spectrum of **20**

Rudolph Research Analytical

This sample was measured on an Autopol VI, Serial #91058
Manufactured by Rudolph Research Analytical, Hackettstown, NJ, USA.

Measurement Date : Tuesday, 25-MAY-2021

Set Temperature : OFF

Time Delay : Disabled

Delay between Measurement : Disabled

n	Average	Std.Dev.	% RSD	Maximum	Minimum
5	61.82	0.48	0.77	62.34	61.09

S.No	Sample ID	Time	Result	Scale	OR °Arc	WLG.nm	Lg.mm	Conc.g/100ml	Temp.
1	SHTB2	04:30:13 PM	61.71	SR	0.1080	589	100.00	0.175	27.3
2	SHTB2	04:30:22 PM	61.77	SR	0.1081	589	100.00	0.175	27.3
3	SHTB2	04:30:30 PM	62.17	SR	0.1088	589	100.00	0.175	27.3
4	SHTB2	04:30:38 PM	61.09	SR	0.1069	589	100.00	0.175	27.3
5	SHTB2	04:30:46 PM	62.34	SR	0.1091	589	100.00	0.175	27.3

Figure S86. ^{1}H NMR spectrum of **18a** at 500 MHz in $CDCl_3$

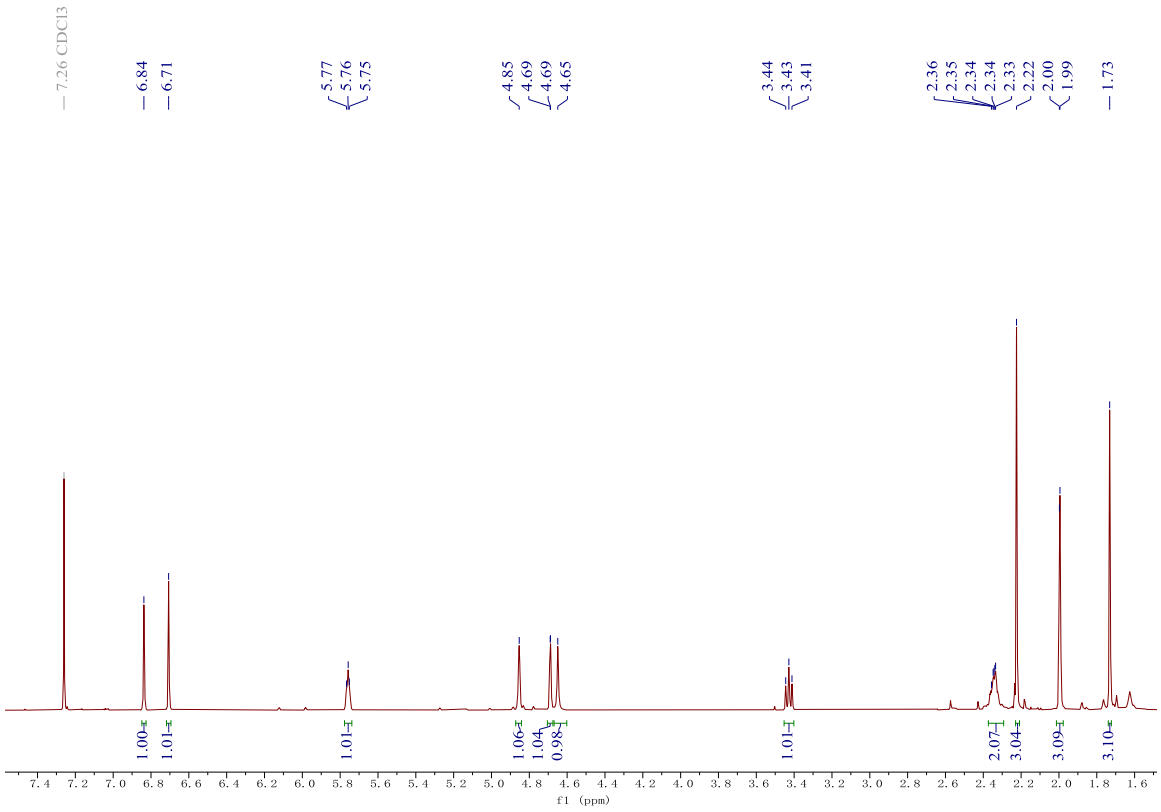


Figure S87. ^{13}C NMR spectrum of **18a** at 125 MHz in $CDCl_3$

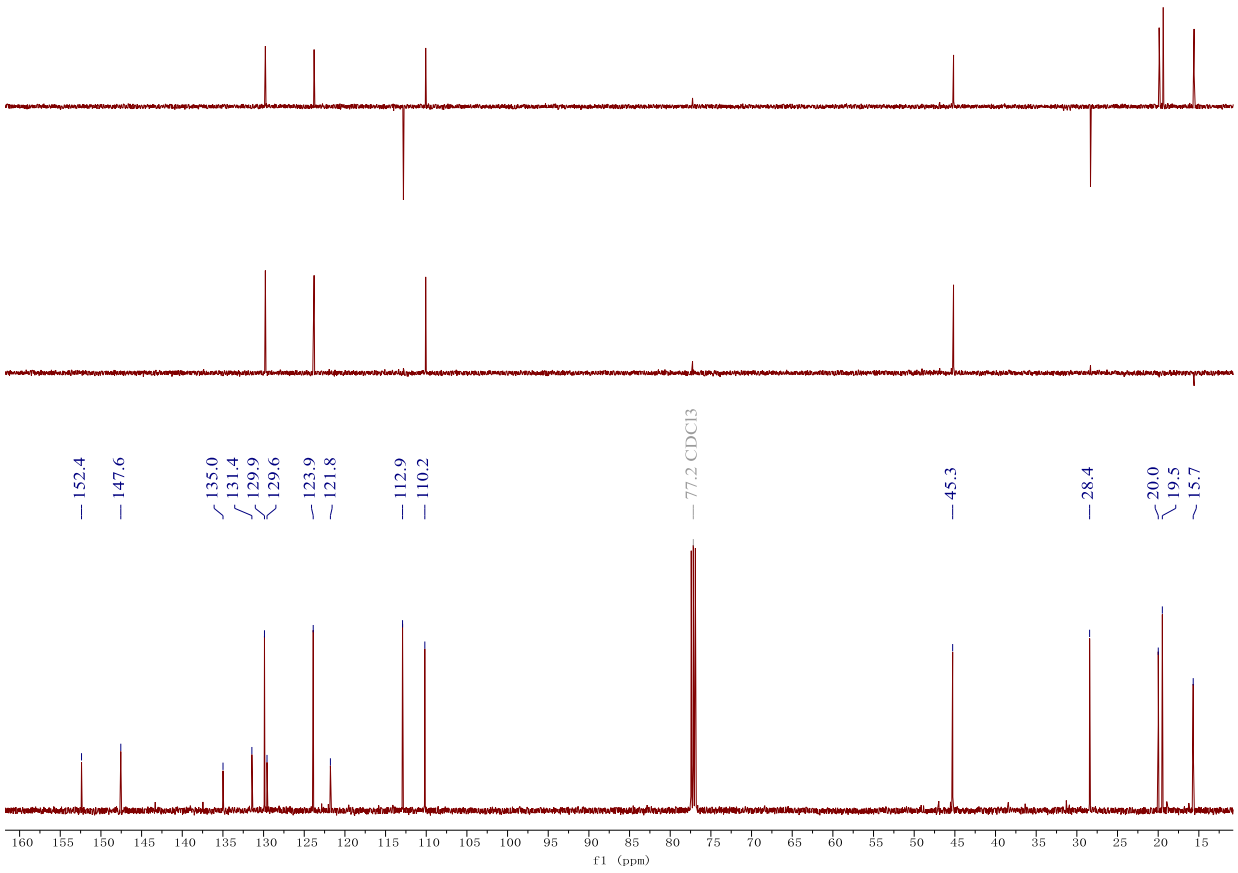


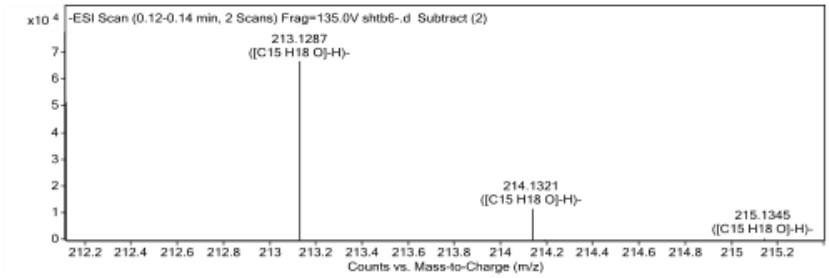
Figure S88. HRESIMS spectrum of **18a**

Data Filename	shtb6-.d	**Sample Name**	shtb6
Sample Type	Sample	**Position**	P1-D1
Instrument Name	Instrument 1	**User Name**	
Acq Method	s-.m	**Acquired Time**	1/26/2021 10:35:48 AM
IRM Calibration Status	Success	**DA Method**	Default.m
Comment			

Sample Group	**Info.**
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125.2)

User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
135	0	ESI



Peak List

m/z	z	Abund	Formula	Ion
89.0246	1	4751.79		
211.1138	1	232454.58		
212.1165	1	51775.74		
213.1287	1	66972.37	C15 H18 O	(M-H)-
214.1321	1	11864.1	C15 H18 O	(M-H)-
245.0744	1	2042.84		
245.1182	1	2858.45		
247.0894		2332.37		
423.2319	1	2725.38		
1010.0235	1	1843.96		

Formula Calculator Element Limits

Element	Min	Max
C	3	60
H	0	120
O	0	30

Formula Calculator Results

Formula	CalculatedMass	CalculatedMz	Mz	Diff. (mDa)	Diff. (ppm)	DBE
C15 H18 O	214.1358	213.1285	213.1287	-0.20	-0.94	7.0000

Figure S89. Specific rotation spectrum of **18a**

Rudolph Research Analytical

This sample was measured on an Autopol VI, Serial #91058
Manufactured by Rudolph Research Analytical, Hackettstown, NJ, USA.

Measurement Date : Thursday, 17-JUN-2021

Set Temperature : OFF

Time Delay : Disabled

Delay between Measurement : Disabled

n	Average	Std.Dev.	% RSD	Maximum	Minimum
5	-118.39	1.15	-0.97	-117.24	-119.54

S.No	Sample ID	Time	Result	Scale	OR °Arc	WLG.nm	Lg.mm	Conc.g/100ml	Temp.
1	shtb6	01:34:41 PM	-117.24	SR	-0.102	589	100.00	0.087	27.9
2	shtb6	01:34:47 PM	-118.39	SR	-0.103	589	100.00	0.087	28.0
3	shtb6	01:34:52 PM	-119.54	SR	-0.104	589	100.00	0.087	28.0
4	shtb6	01:34:58 PM	-117.24	SR	-0.102	589	100.00	0.087	28.0
5	shtb6	01:35:04 PM	-119.54	SR	-0.104	589	100.00	0.087	28.0

Figure S90. ^{1}H NMR spectrum of **18b** at 500 MHz in $CDCl_3$

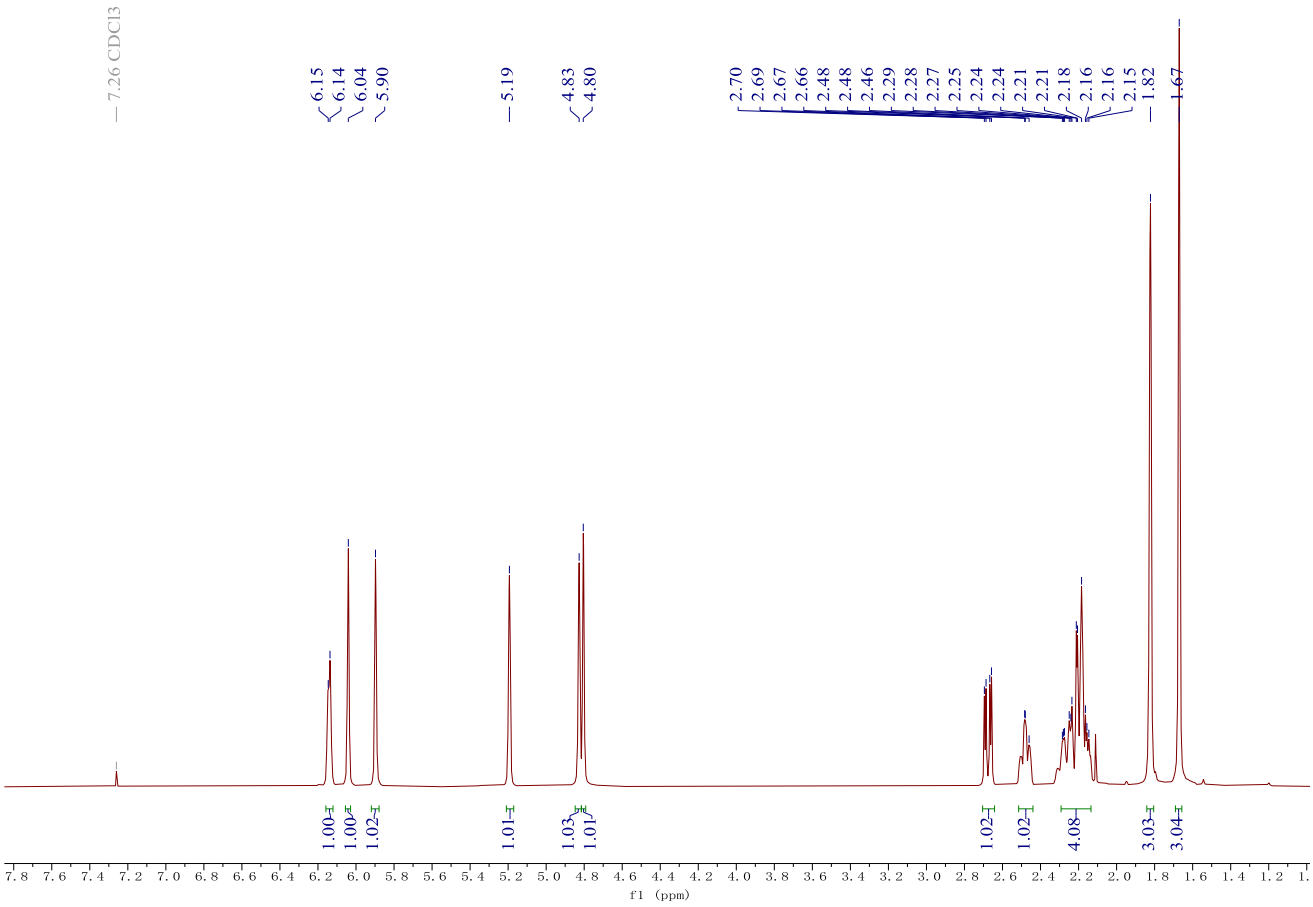


Figure S91. ^{1}C NMR spectrum of **18b** at 125 MHz in $CDCl_3$

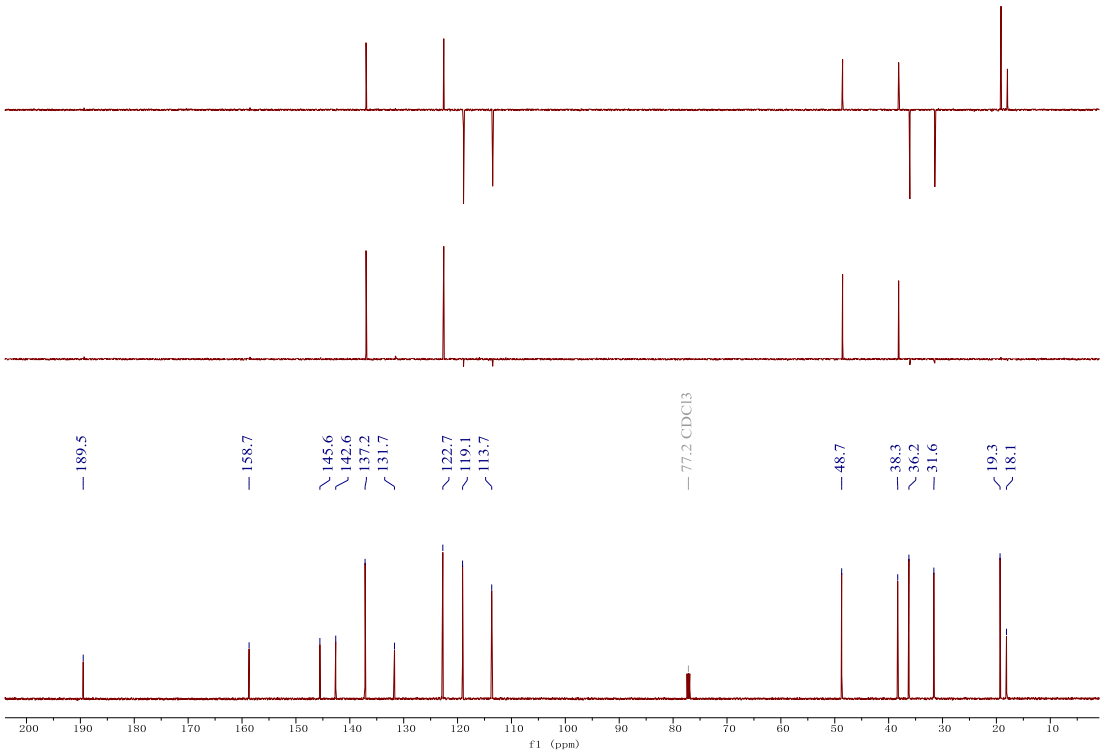


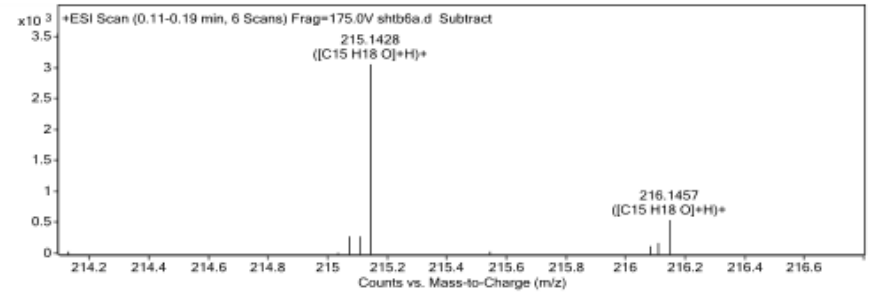
Figure S92. HRESIMS spectrum of **18b**

Data Filename	shtb6a.d	**Sample Name**	shtb6a
Sample Type	Sample	**Position**	P1-A1
Instrument Name	Instrument 1	**User Name**	
Acq Method	s.m	**Acquired Time**	12/10/2021 9:49:33 AM
IRM Calibration Status	Success	**DA Method**	PCDL.m
Comment			

Sample Group	**Info.**
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125.2)

User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
175	0	ESI



Peak List

m/z	z	Abund	Formula	Ion
102.1274	1	2994.7		
145.101	1	1444.27		
173.0958	1	1387.83		
215.1428	1	3071.17	C15 H18 O	(M+H)+
231.1373	1	1406.81		
493.2548	1	1532.54		
539.2244	1	1237.09		
555.2231	1	1199.27		
565.2294	1	1363.98		
569.2186	1	1413.79		

Formula Calculator Element Limits

Element	Min	Max
C	3	120
H	0	240
O	0	30

Formula Calculator Results

Formula	CalculatedMass	CalculatedMz	Mz	Diff. (mDa)	Diff. (ppm)	DBE
C15 H18 O	214.1358	215.1430	215.1428	0.20	0.93	7.0000

Figure S93. Specific rotation spectrum of **18b**

Rudolph Research Analytical

This sample was measured on an Autopol VI, Serial #91058
Manufactured by Rudolph Research Analytical, Hackettstown, NJ, USA.

Measurement Date : Tuesday, 25-MAY-2021

Set Temperature : OFF

Time Delay : Disabled

Delay between Measurement : Disabled

n	Average	Std.Dev.	% RSD	Maximum	Minimum
5	-12.87	0.83	-6.44	-11.78	-13.95

S.No	Sample ID	Time	Result	Scale	OR °Arc	WLG.nm	Lg.mm	Conc.g/100ml	Temp.
1	SHTB6A	05:24:05 PM	-13.95	SR	-0.0219	589	100.00	0.157	27.5
2	SHTB6A	05:24:18 PM	-12.48	SR	-0.0196	589	100.00	0.157	27.5
3	SHTB6A	05:24:27 PM	-13.38	SR	-0.0210	589	100.00	0.157	27.5
4	SHTB6A	05:24:35 PM	-12.74	SR	-0.0200	589	100.00	0.157	27.5
5	SHTB6A	05:24:43 PM	-11.78	SR	-0.0185	589	100.00	0.157	27.5

Figure S94. ^{1}H NMR spectrum of **14a** at 500 MHz in $CDCl_3$

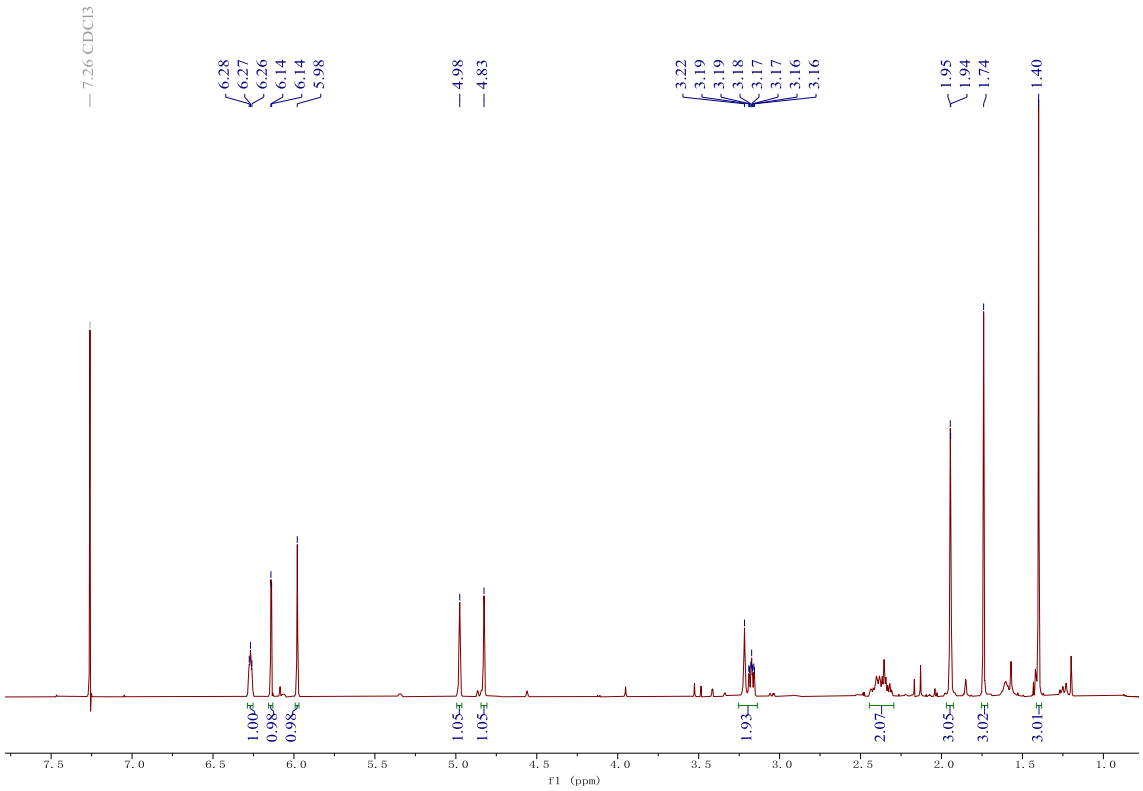


Figure S95. ^{13}C NMR spectrum of **14a** at 125 MHz in $CDCl_3$

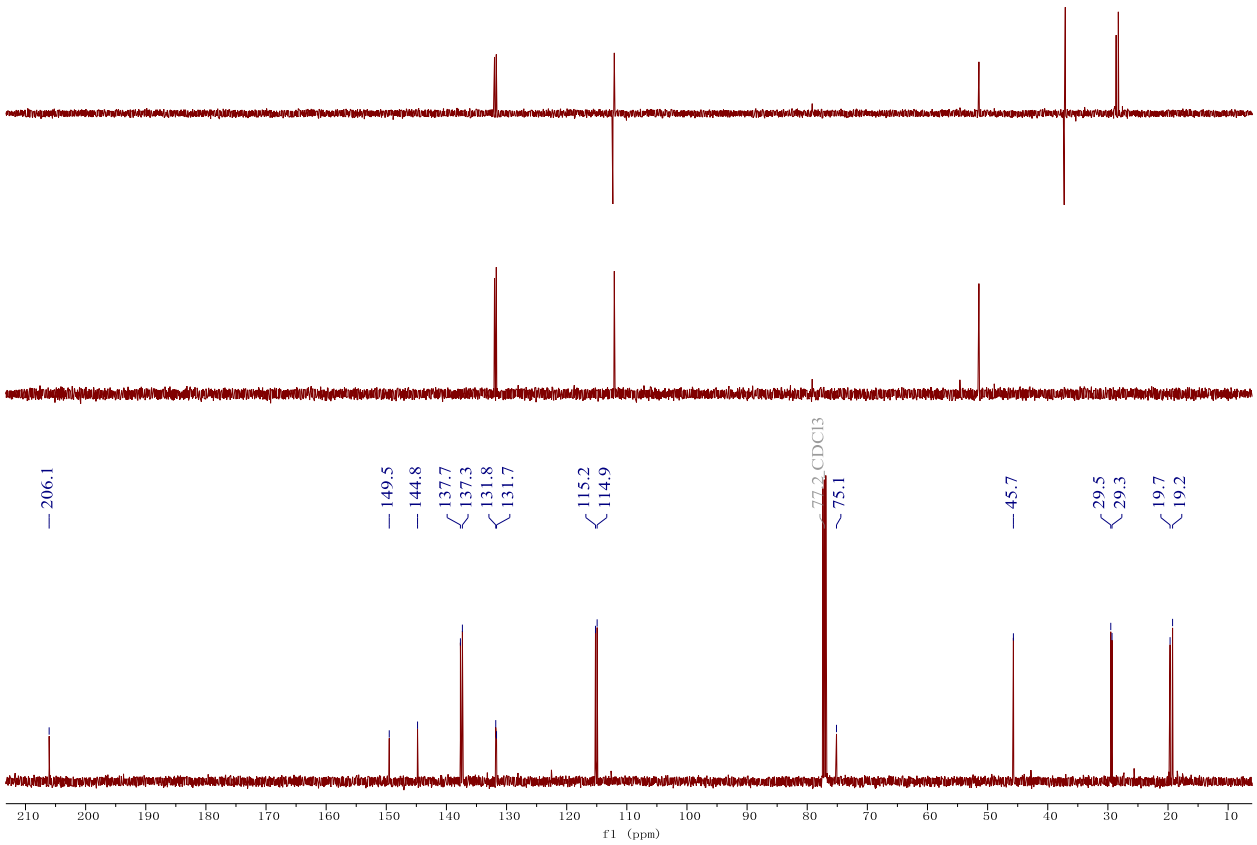


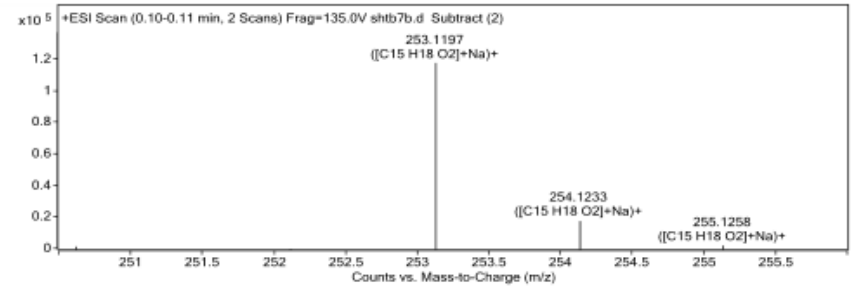
Figure S96. HRESIMS spectrum of **14a**

Data Filename	shtb7b.d	**Sample Name**	shtb7b
Sample Type	Sample	**Position**	P1-A7
Instrument Name	Instrument 1	**User Name**	
Acq Method	s.m	**Acquired Time**	5/12/2021 10:52:34 AM
IRM Calibration Status	Success	**DA Method**	Default.m
Comment			

Sample Group	**Info.**
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125.2)

User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
135	0	ESI



Peak List

m/z	z	Abund	Formula	Ion
213.127	1	27422.96		
231.1373	1	24654.32		
253.1197	1	117830.22	C15 H18 O2	(M+Na)+
254.1233	1	18362.42	C15 H18 O2	(M+Na)+
274.2736	1	20999.03		
285.1094	1	99392.77		
365.177	2	27359.05		
437.1928	1	25537.25		
483.2509	1	49048.75		
547.2307	1	18826.43		

Formula Calculator Element Limits

Element	Min	Max
C	3	60
H	0	120
O	0	30

Formula Calculator Results

Formula	CalculatedMass	CalculatedMz	Mz	Diff. (mDa)	Diff. (ppm)	DBE
C15 H18 O2	230.1307	253.1199	253.1197	0.20	0.79	7.0000

Figure S97. Specific rotation spectrum of **14a**

Rudolph Research Analytical

This sample was measured on an Autopol VI, Serial #91058
Manufactured by Rudolph Research Analytical, Hackettstown, NJ, USA.

Measurement Date : Thursday, 20-OCT-2022

Set Temperature : 20.0

Time Delay : Disabled

Delay between Measurement : Disabled

n	Average	Std.Dev.	% RSD	Maximum	Minimum
5	73.76	0.10	0.13	73.84	73.65

S.No	Sample ID	Time	Result	Scale	OR °Arc	WLG.nm	Lg.mm	Conc.g/100ml	Temp.
1	shtb7b	11:34:25 AM	73.84	SR	0.398	589	100.00	0.539	20.6
2	shtb7b	11:34:32 AM	73.65	SR	0.397	589	100.00	0.539	20.5
3	shtb7b	11:34:38 AM	73.65	SR	0.397	589	100.00	0.539	20.5
4	shtb7b	11:34:44 AM	73.84	SR	0.398	589	100.00	0.539	20.5
5	shtb7b	11:34:50 AM	73.84	SR	0.398	589	100.00	0.539	20.4

Figure S98. ^{1}H NMR spectrum of **14b** at 500 MHz in $CDCl_3$

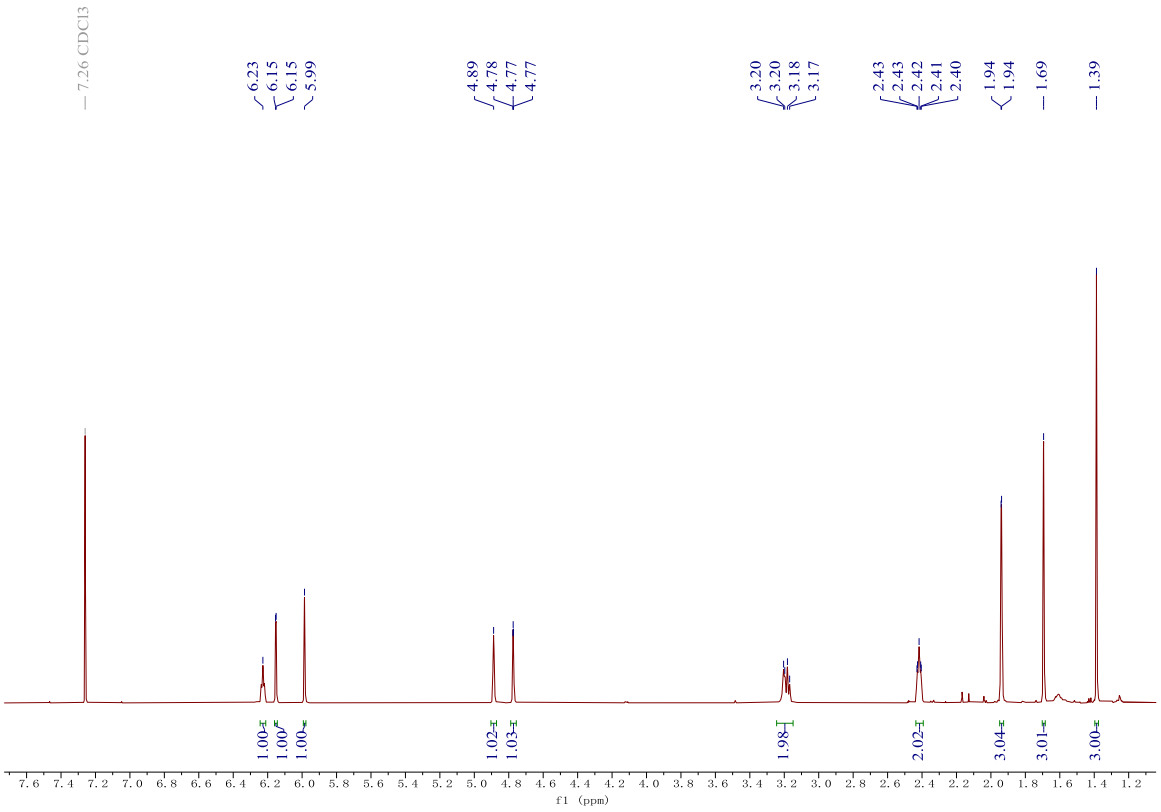


Figure S99. ^{13}C NMR spectrum of **14b** at 125 MHz in $CDCl_3$

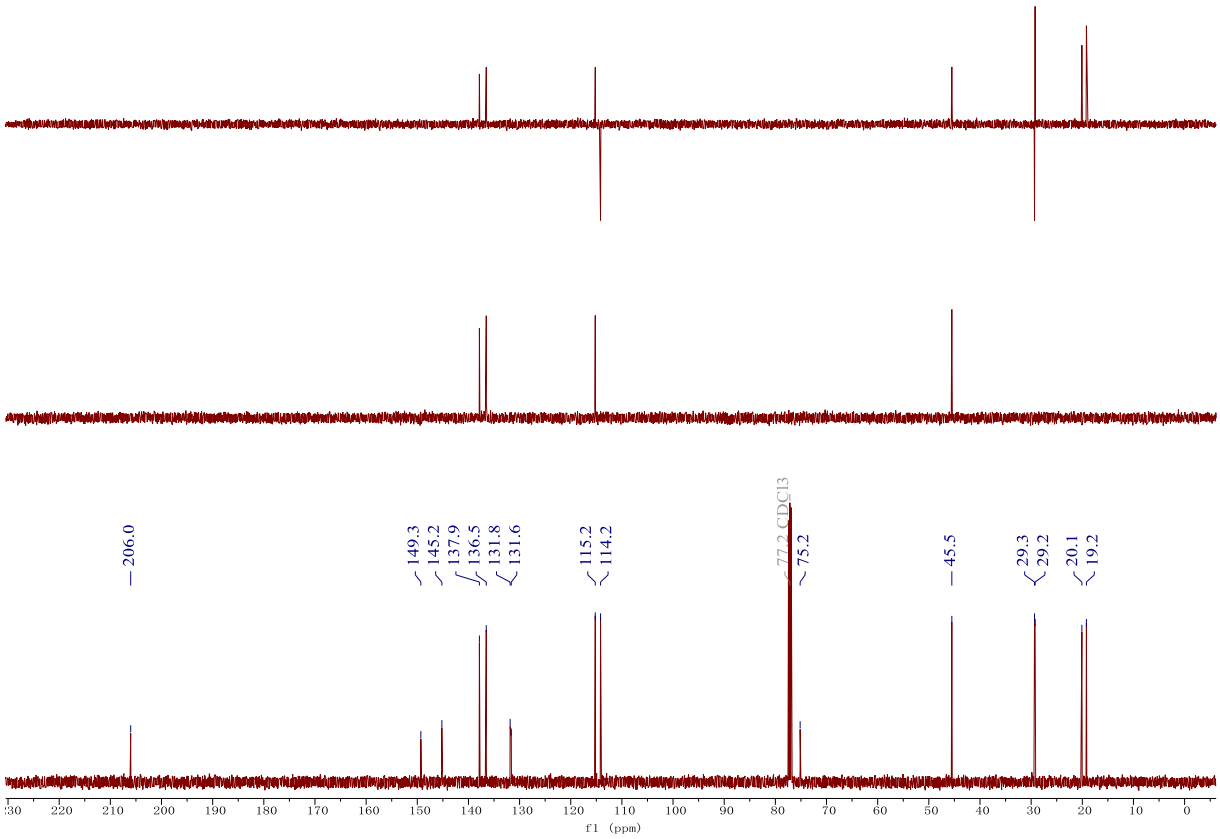


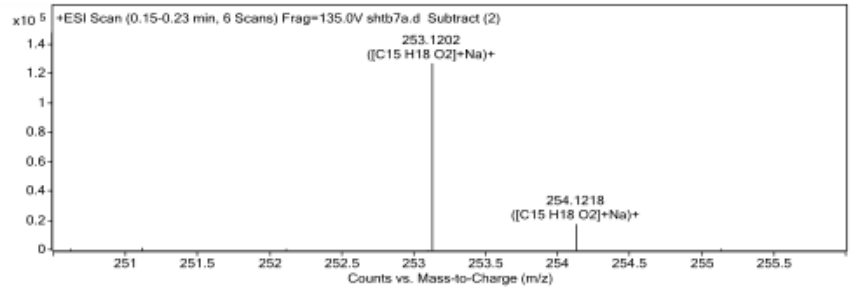
Figure S100. HRESIMS spectrum of **14b**

Data Filename	shtb7a.d	**Sample Name**	shtb7a
Sample Type	Sample	**Position**	P1-A6
Instrument Name	Instrument 1	**User Name**	
Acq Method	s.m	**Acquired Time**	5/12/2021 10:51:13 AM
IRM Calibration Status	Success	**DA Method**	Default.m
Comment			

Sample Group	**Info.**
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125.2)

User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
135	0	ESI



Peak List

m/z	z	Abund	Formula	Ion
231.1373	1	27679.39		
253.1202	1	127506.98	C15 H18 O2	(M+Na)+
269.1146	1	28896.22		
285.11	1	132182.39		
301.0842	1	32846.62		
317.1002	1	28075.12		
341.247	1	95884.38		
343.2438	1	29242.8		
483.2516	1	56621.67		
547.2308	1	37691.23		

Formula Calculator Element Limits

Element	Min	Max
C	3	60
H	0	120
O	0	30

Formula Calculator Results

Formula	CalculatedMass	CalculatedMz	Mz	Diff. (mDa)	Diff. (ppm)	DBE
C15 H18 O2	230.1307	253.1199	253.1202	-0.30	-1.19	7.0000

Figure S101. Specific rotation spectrum of **14b**

Rudolph Research Analytical

This sample was measured on an Autopol VI, Serial #91058
Manufactured by Rudolph Research Analytical, Hackettstown, NJ, USA.

Measurement Date : Thursday, 20-OCT-2022

Set Temperature : 20.0

Time Delay : Disabled

Delay between Measurement : Disabled

n	Average	Std.Dev.	% RSD	Maximum	Minimum
5	-7.20	0.73	-10.13	-6.67	-8.00

S.No	Sample ID	Time	Result	Scale	OR °Arc	WLG.nm	Lg.mm	Conc.g/100ml	Temp.
1	shtb7a	11:24:53 AM	-8.00	SR	-0.006	589	100.00	0.075	19.9
2	shtb7a	11:24:59 AM	-6.67	SR	-0.005	589	100.00	0.075	19.9
3	shtb7a	11:25:05 AM	-8.00	SR	-0.006	589	100.00	0.075	19.9
4	shtb7a	11:25:12 AM	-6.67	SR	-0.005	589	100.00	0.075	19.9
5	shtb7a	11:25:18 AM	-6.67	SR	-0.005	589	100.00	0.075	19.9

Figure S102. ^{1}H NMR spectrum of **17** at 500 MHz in $CDCl_3$

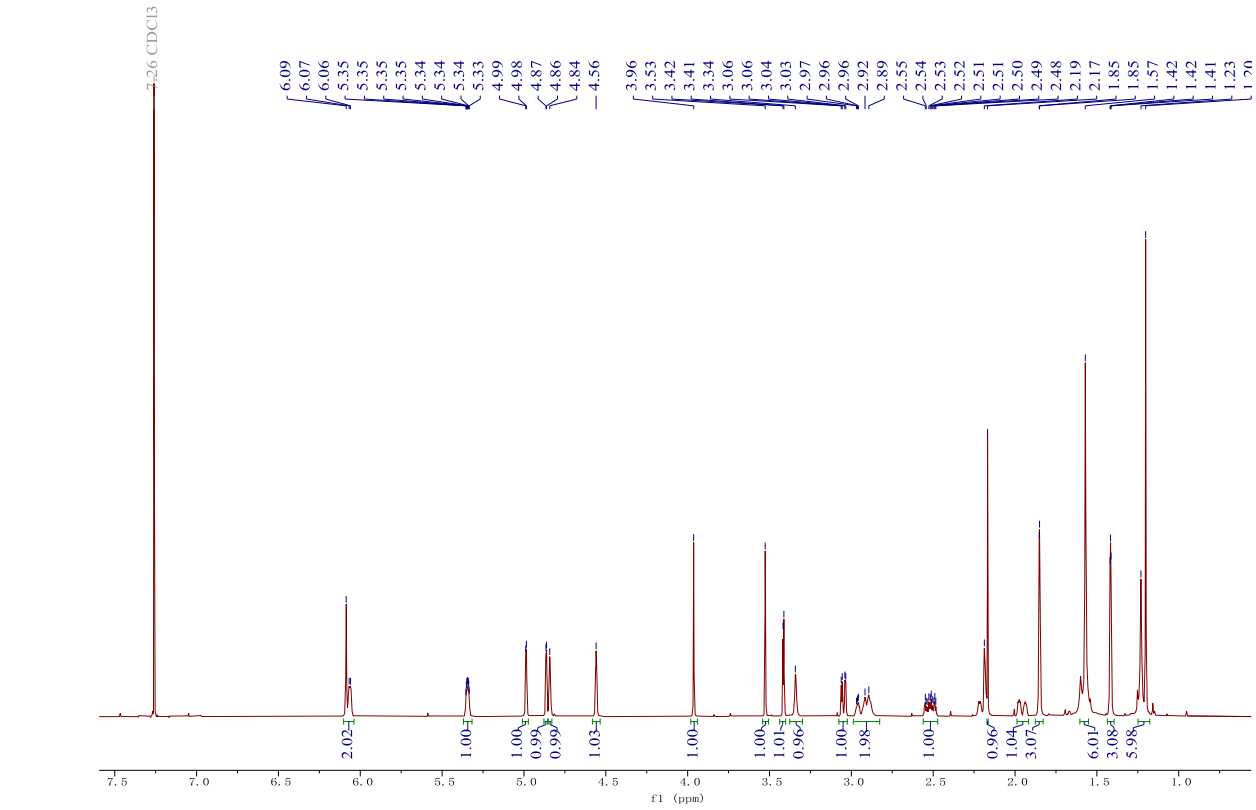


Figure S103. ^{13}C NMR spectrum of **17** at 125 MHz in $CDCl_3$

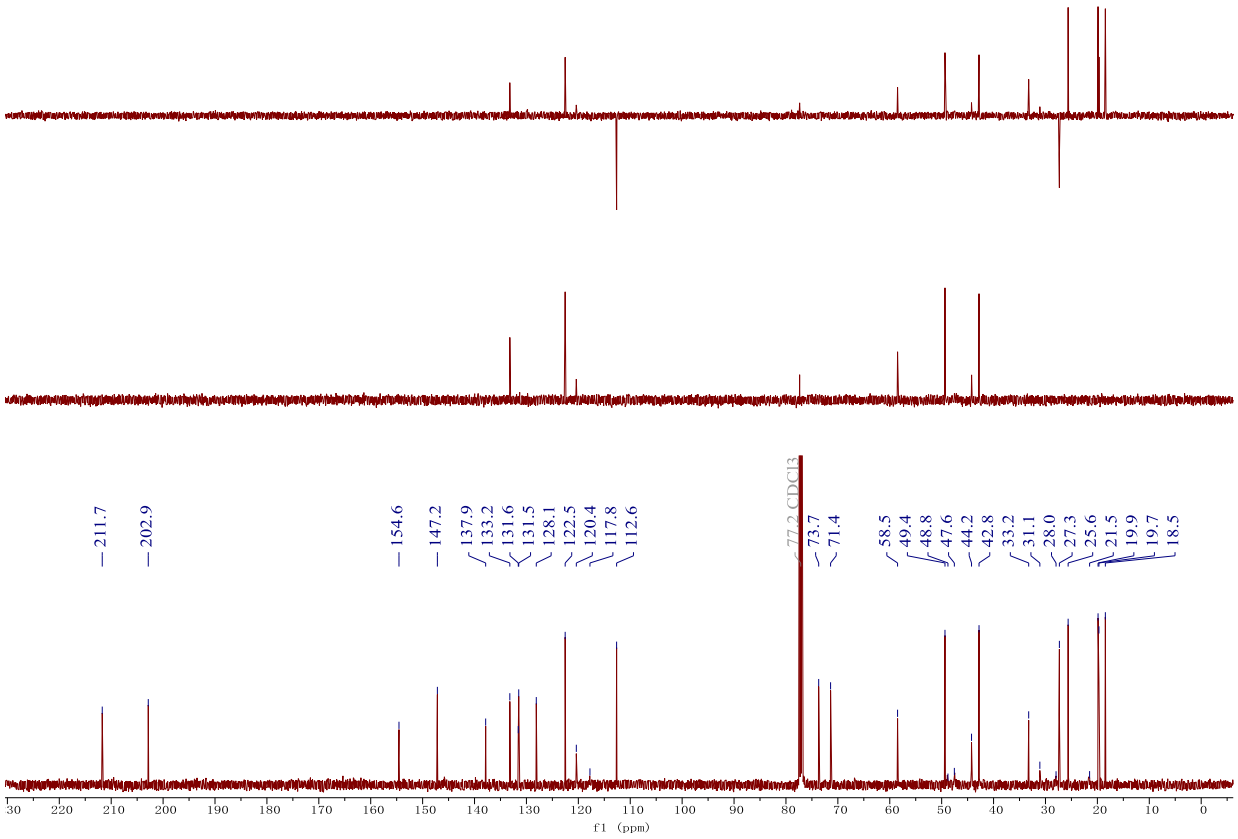


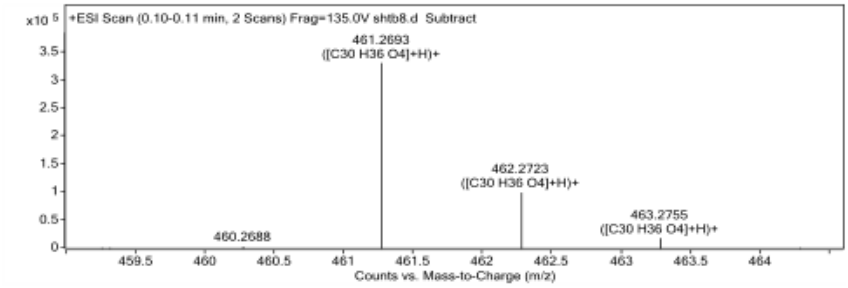
Figure S104. HRESIMS spectrum of **17**

Data Filename	shtb8.d	**Sample Name**	shtb8
Sample Type	Sample	**Position**	P1-B6
Instrument Name	Instrument 1	**User Name**	
Acq Method	s.m	**Acquired Time**	3/30/2021 2:31:59 PM
IRM Calibration Status	Success	**DA Method**	Default.m
Comment			

Sample Group	**Info.**
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125.2)

User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
135	0	ESI



Peak List

m/z	z	Abund	Formula	Ion
213.1273	1	108403		
231.1377	1	47655.39		
461.2693	1	331327.47	C30 H36 O4	(M+H)+
462.2723	1	100676.2	C30 H36 O4	(M+H)+
483.2511	1	164242.8		
484.2544	1	51716.57		
499.2246	1	47066.83		
943.5134	1	163190.94		
944.5166	1	104993.91		
945.5174	1	35662.91		

Formula Calculator Element Limits

Element	Min	Max
C	3	60
H	0	120
O	0	30

Formula Calculator Results

Formula	CalculatedMass	CalculatedMz	Mz	Diff. (mDa)	Diff. (ppm)	DBE
C30 H36 O4	460.2614	461.2686	461.2693	-0.70	-1.52	13.0000

Figure S105. Specific rotation spectrum of **17**

Rudolph Research Analytical

This sample was measured on an Autopol VI, Serial #91058
Manufactured by Rudolph Research Analytical, Hackettstown, NJ, USA.

Measurement Date : Friday, 11-JUN-2021

Set Temperature : OFF

Time Delay : Disabled

Delay between Measurement : Disabled

n	Average	Std.Dev.	% RSD	Maximum	Minimum
5	6.24	1.52	24.35	7.76	3.73

S.No	Sample ID	Time	Result	Scale	OR °Arc	WLG.nm	Lg.mm	Conc.g/100ml	Temp.
1	shtb8	04:31:45 PM	3.73	SR	0.0025	589	100.00	0.067	26.5
2	shtb8	04:31:53 PM	6.72	SR	0.0045	589	100.00	0.067	26.5
3	shtb8	04:32:02 PM	7.76	SR	0.0052	589	100.00	0.067	26.4
4	shtb8	04:32:10 PM	6.87	SR	0.0046	589	100.00	0.067	26.4
5	shtb8	04:32:18 PM	6.12	SR	0.0041	589	100.00	0.067	26.4

Figure S106. ^{1}H NMR spectrum of synthetic compound **1** at 500 MHz in pyridine-d_5

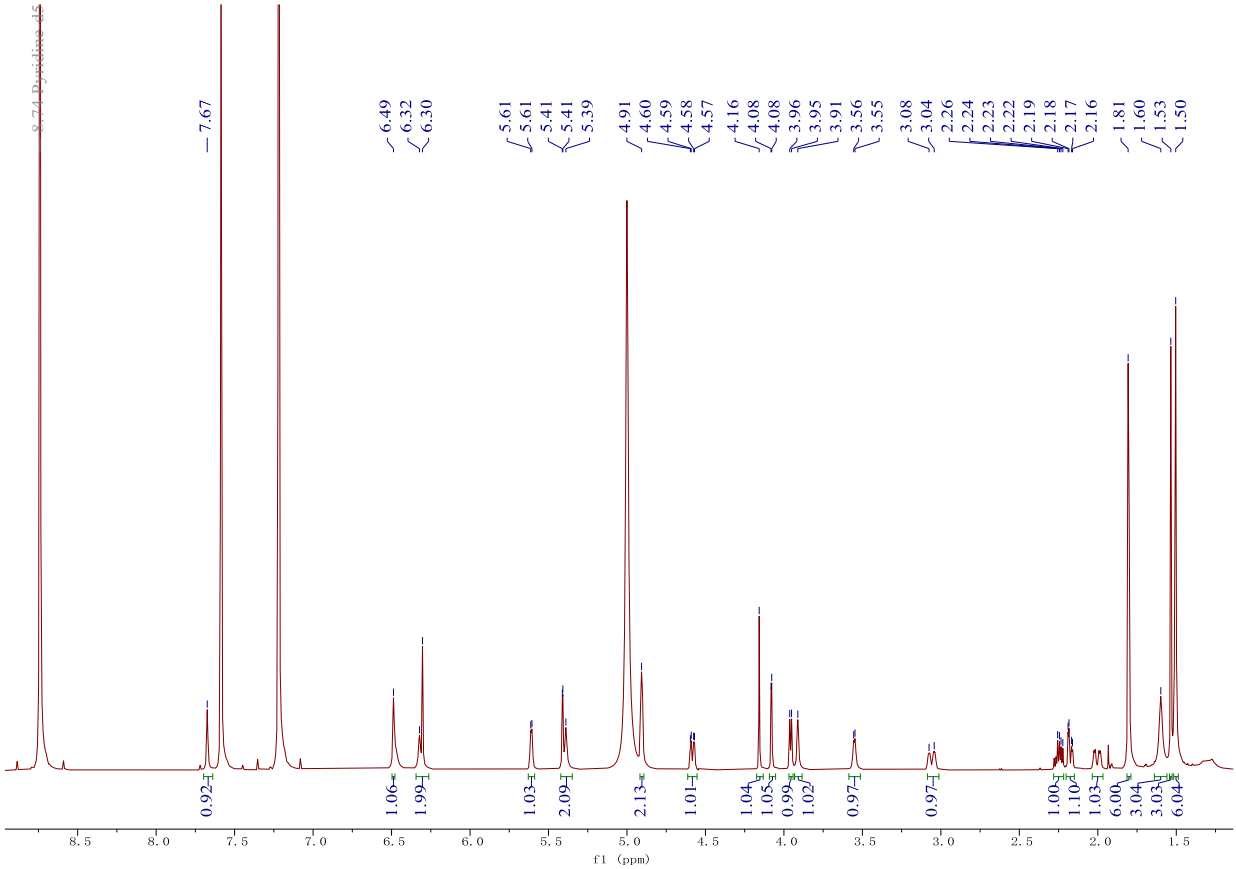


Figure S107. ^{13}C NMR spectrum of synthetic compound **1** at 125 MHz in pyridine-d_5

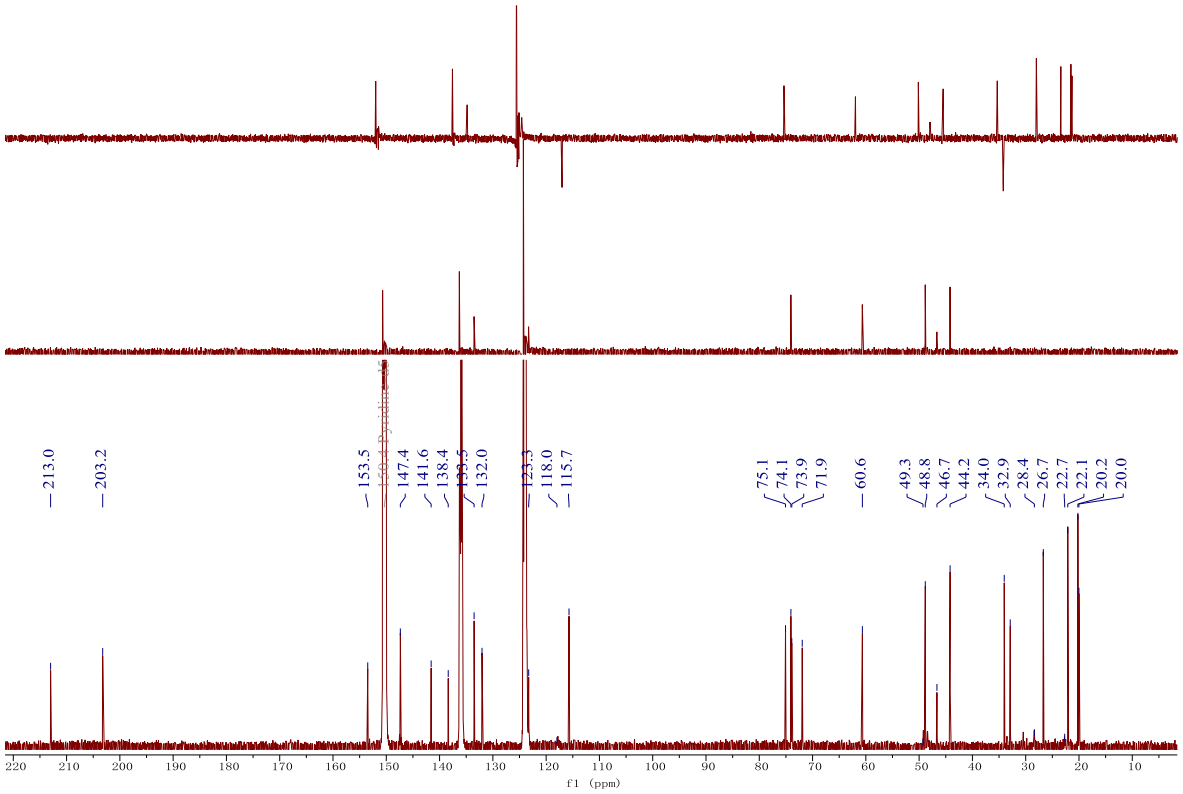


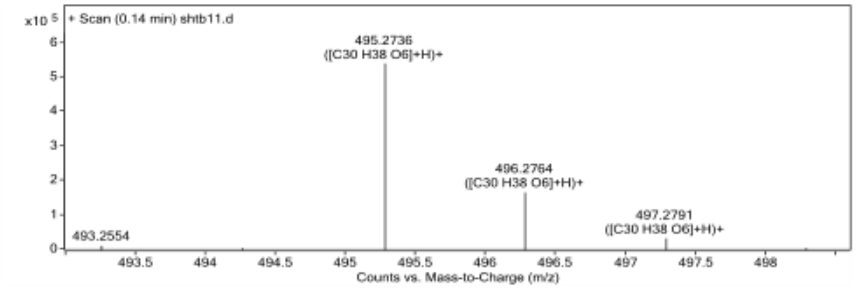
Figure S108. HRESIMS spectrum of synthetic compound **1**

Data Filename	shtb11.d	**Sample Name**	shtb11
Sample Type	Sample	**Position**	P1-D5
Instrument Name	Instrument 1	**User Name**	
Acq Method	s.m	**Acquired Time**	6/18/2021 2:27:17 PM
IRM Calibration Status	Success	**DA Method**	ZRR3.m
Comment			

Sample Group	**Info.**
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125.2)

User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
175	0	ESI



Peak List

m/z	z	Abund	Formula	Ion
327.1352	1	1699083.5		
328.1369	1	290892.66		
411.2098	1	319328.5		
459.2513	1	1014168.06		
460.2547	1	306445.19		
477.2622	1	307663.16		
495.2736	1	540047.44	C30 H38 O6	(M+H)+
675.2559	1	279267.16		
1011.5374	1	684107.56		
1012.5407	1	445229.78		

Formula Calculator Element Limits

Element	Min	Max
C	3	60
H	0	120
O	0	30

Formula Calculator Results

Formula	CalculatedMass	CalculatedMz	Mz	Diff. (mDa)	Diff. (ppm)	DBE
C30 H38 O6	494.2668	495.2741	495.2736	0.50	1.01	12.0000

Figure S109. Specific rotation spectrum of **1**

Rudolph Research Analytical

This sample was measured on an Autopol VI, Serial #91058
Manufactured by Rudolph Research Analytical, Hackettstown, NJ, USA.

Measurement Date : Thursday, 17-JUN-2021

Set Temperature : OFF

Time Delay : Disabled

Delay between Measurement : Disabled

n	Average	Std.Dev.	% RSD	Maximum	Minimum
5	-66.42	1.83	-2.75	-64.20	-69.14

S.No	Sample ID	Time	Result	Scale	OR °Arc	WLG.nm	Lg.mm	Conc.g/100ml	Temp.
1	shtb11	01:26:31 PM	-64.20	SR	-0.052	589	100.00	0.081	21.5
2	shtb11	01:26:37 PM	-65.43	SR	-0.053	589	100.00	0.081	21.5
3	shtb11	01:26:43 PM	-66.67	SR	-0.054	589	100.00	0.081	21.6
4	shtb11	01:26:48 PM	-66.67	SR	-0.054	589	100.00	0.081	21.8
5	shtb11	01:26:54 PM	-69.14	SR	-0.056	589	100.00	0.081	21.9

Figure S110. ^{1}H NMR spectrum of synthetic compound **2** at 500 MHz in $CDCl_3$

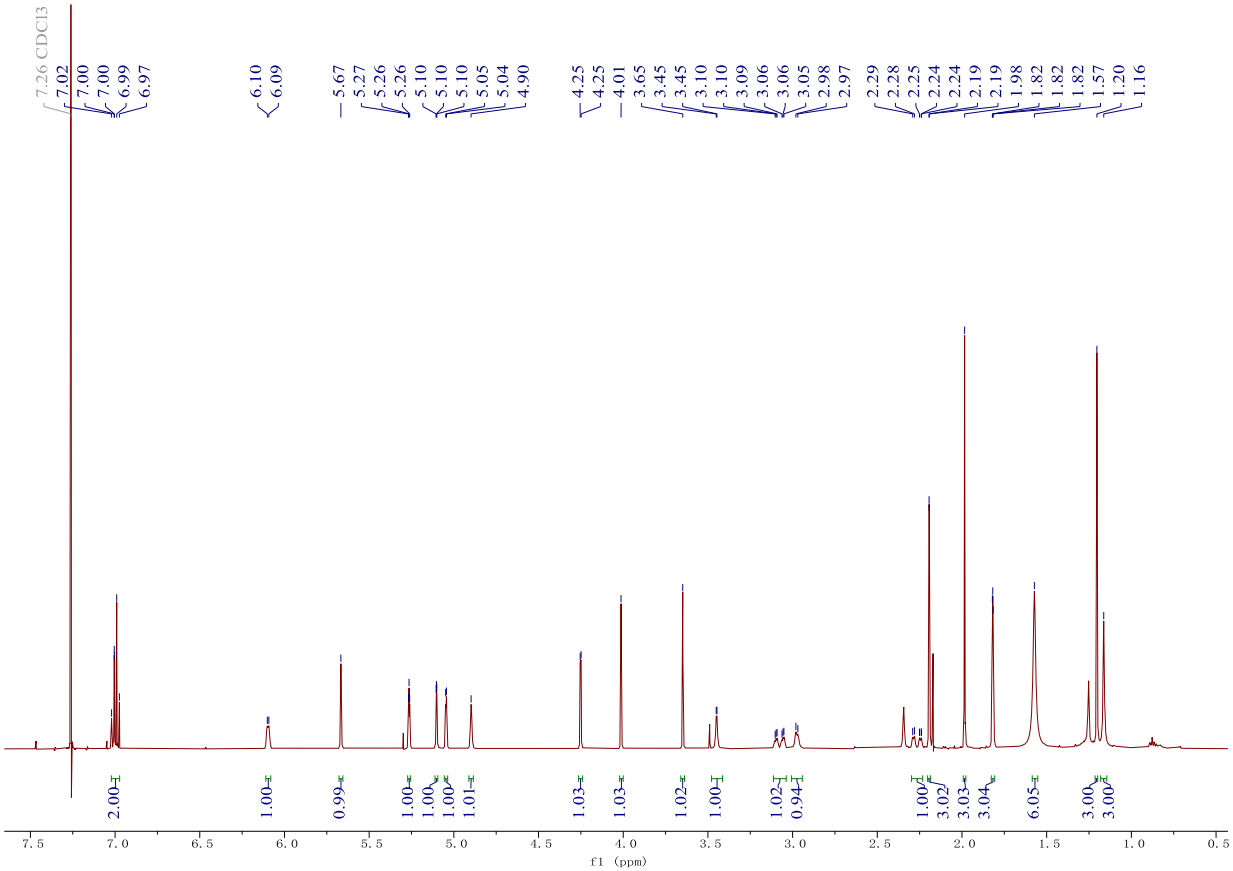


Figure S111. ^{13}C NMR spectrum of synthetic compound **2** at 500 MHz in $CDCl_3$

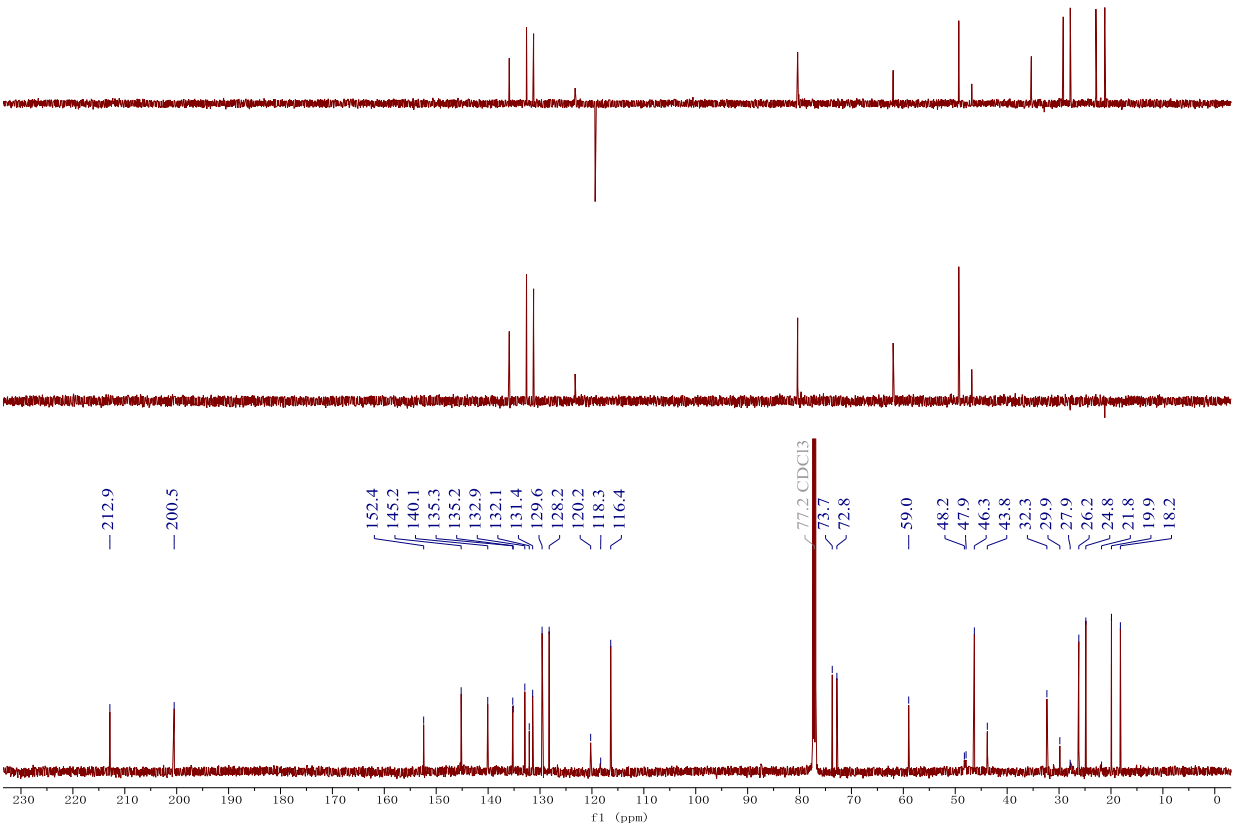


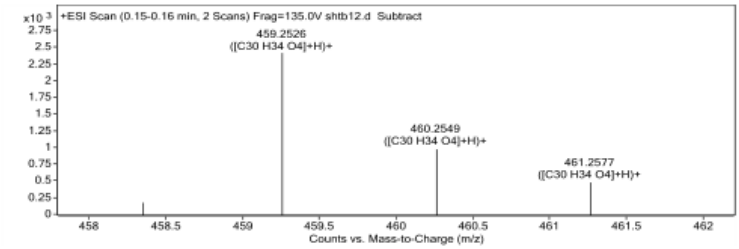
Figure S112. HRESIMS spectrum of synthetic compound **2**

Data Filename	shtb12.d	**Sample Name**	shtb12
Sample Type	Sample	**Position**	P1-C2
Instrument Name	Instrument 1	**User Name**	
Acq Method	s.m	**Acquired Time**	5/27/2021 10:16:33 AM
IRM Calibration Status	Success	**DA Method**	Default.m
Comment			

Sample Group	**Info.**
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125.2)

User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
135	0	ESI



Peak List

m/z	z	Abund	Formula	Ion
102.1274		2621.23		
118.1221	1	3342.83		
212.1177	1	3969.45		
459.2526	1	2422.29	C30 H34 O4	(M+H)+
481.2341	1	2064.52		
483.2499	1	1541.17		
497.2249	1	1509.14		
499.2403	1	1541.01		
515.2391	1	3601.7		
531.2272	1	1733.06		

Formula Calculator Element Limits

Element	Min	Max
C	3	60
H	0	120
O	0	30

Formula Calculator Results

Formula	CalculatedMass	CalculatedMz	Mz	Diff. (mDa)	Diff. (ppm)	DBE
C30 H34 O4	458.2457	459.2530	459.2526	0.40	0.87	14.0000

Figure S113. Specific rotation spectrum of **2**

Rudolph Research Analytical

This sample was measured on an Autopol VI, Serial #91058
Manufactured by Rudolph Research Analytical, Hackettstown, NJ, USA.

Measurement Date : Thursday, 20-OCT-2022

Set Temperature : 20.0

Time Delay : Disabled

Delay between Measurement : Disabled

n	Average	Std.Dev.	% RSD	Maximum	Minimum
5	-9.03	1.09	-12.07	-7.32	-9.76

S.No	Sample ID	Time	Result	Scale	OR °Arc	WLG.nm	Lg.mm	Conc.g/100ml	Temp.
1	shtb12	11:29:22 AM	-9.76	SR	-0.008	589	100.00	0.082	20.2
2	shtb12	11:29:28 AM	-9.76	SR	-0.008	589	100.00	0.082	20.2
3	shtb12	11:29:35 AM	-9.76	SR	-0.008	589	100.00	0.082	20.2
4	shtb12	11:29:41 AM	-8.54	SR	-0.007	589	100.00	0.082	20.2
5	shtb12	11:29:47 AM	-7.32	SR	-0.006	589	100.00	0.082	20.2

Figure S114. ^{1}H NMR spectrum of **25a** at 500 MHz in $CDCl_3$

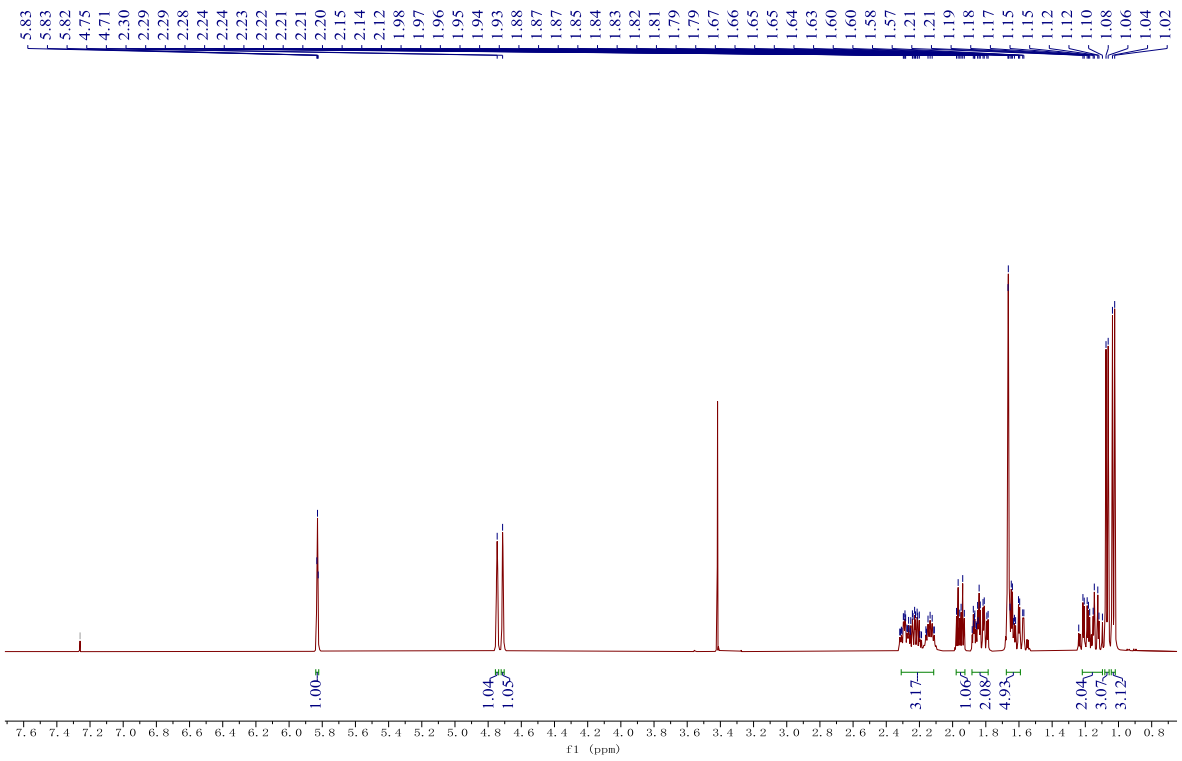


Figure S115. ^{13}C NMR spectrum of **25a** at 125 MHz in $CDCl_3$

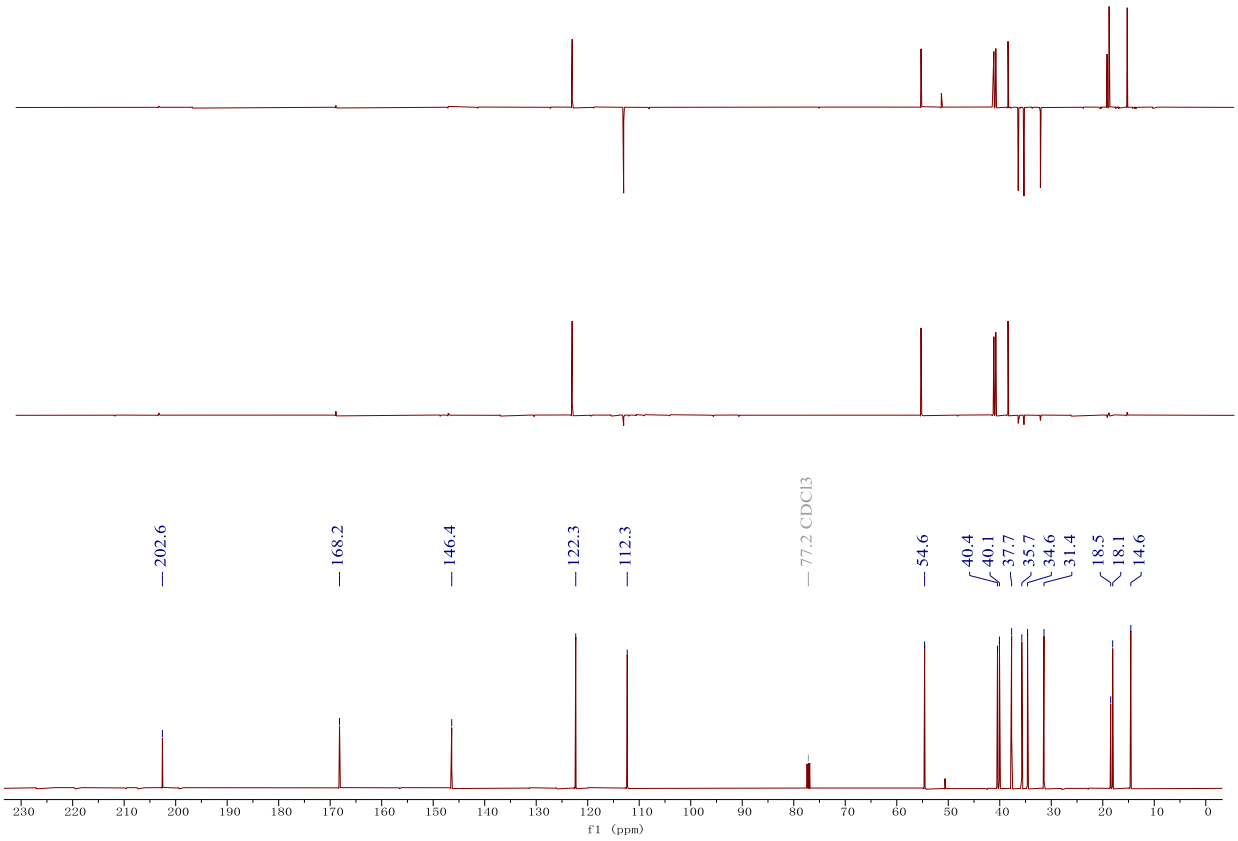


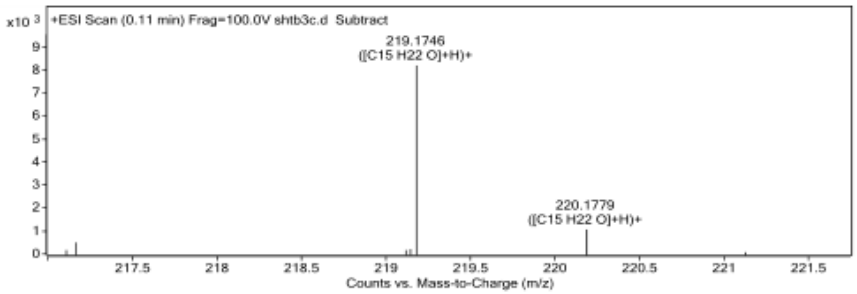
Figure S116. HRESIMS spectrum of synthetic compound **25a**

Data Filename	shtb3c.d	**Sample Name**	shtb3c
Sample Type	Sample	**Position**	P1-C7
Instrument Name	Instrument 1	**User Name**	
Acq Method	s.m	**Acquired Time**	3/5/2021 10:58:01 AM
IRM Calibration Status	Success	**DA Method**	Default.m
Comment			

Sample Group	**Info.**
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125.2)

User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
100	0	ESI



Peak List

m/z	z	Abund	Formula	Ion
105.0427		5421.56		
219.1746	1	8246.09	C15 H22 O	(M+H)+
251.1641	1	3844.96		
273.1465	1	13960.79		
473.3023	1	5605.77		
489.2972	1	14582.68		
490.3009	1	4687.91		
505.291	1	4927.05		
507.3063	1	3716.23		
521.2847	1	5351.27		

Formula Calculator Element Limits

Element	Min	Max
C	3	60
H	0	120
O	0	30

Formula Calculator Results

Formula	CalculatedMass	CalculatedMz	Mz	Diff. (mDa)	Diff. (ppm)	DBE
C15 H22 O	218.1671	219.1743	219.1746	-0.30	-1.37	5.0000

Figure S117. Specific rotation spectrum of **25a**

Rudolph Research Analytical

This sample was measured on an Autopol VI, Serial #91058
Manufactured by Rudolph Research Analytical, Hackettstown, NJ, USA.

Measurement Date : Tuesday, 25-MAY-2021

Set Temperature : OFF

Time Delay : Disabled

Delay between Measurement : Disabled

n	Average	Std.Dev.	% RSD	Maximum	Minimum
5	-2.26	3.19	-141.15	3.07	-4.47

S.No	Sample ID	Time	Result	Scale	OR °Arc	WLG.nm	Lg.mm	Conc.g/100ml	Temp.
1	SHTB3A	04:37:03 PM	-4.47	SR	-0.0051	589	100.00	0.114	27.4
2	SHTB3A	04:37:12 PM	-4.04	SR	-0.0046	589	100.00	0.114	27.4
3	SHTB3A	04:37:20 PM	-4.21	SR	-0.0048	589	100.00	0.114	27.4
4	SHTB3A	04:37:28 PM	-1.67	SR	-0.0019	589	100.00	0.114	27.4
5	SHTB3A	04:37:46 PM	3.07	SR	0.0035	589	100.00	0.114	27.4

Figure S118. ^{1}H NMR spectrum of **25b** at 500 MHz in $CDCl_3$

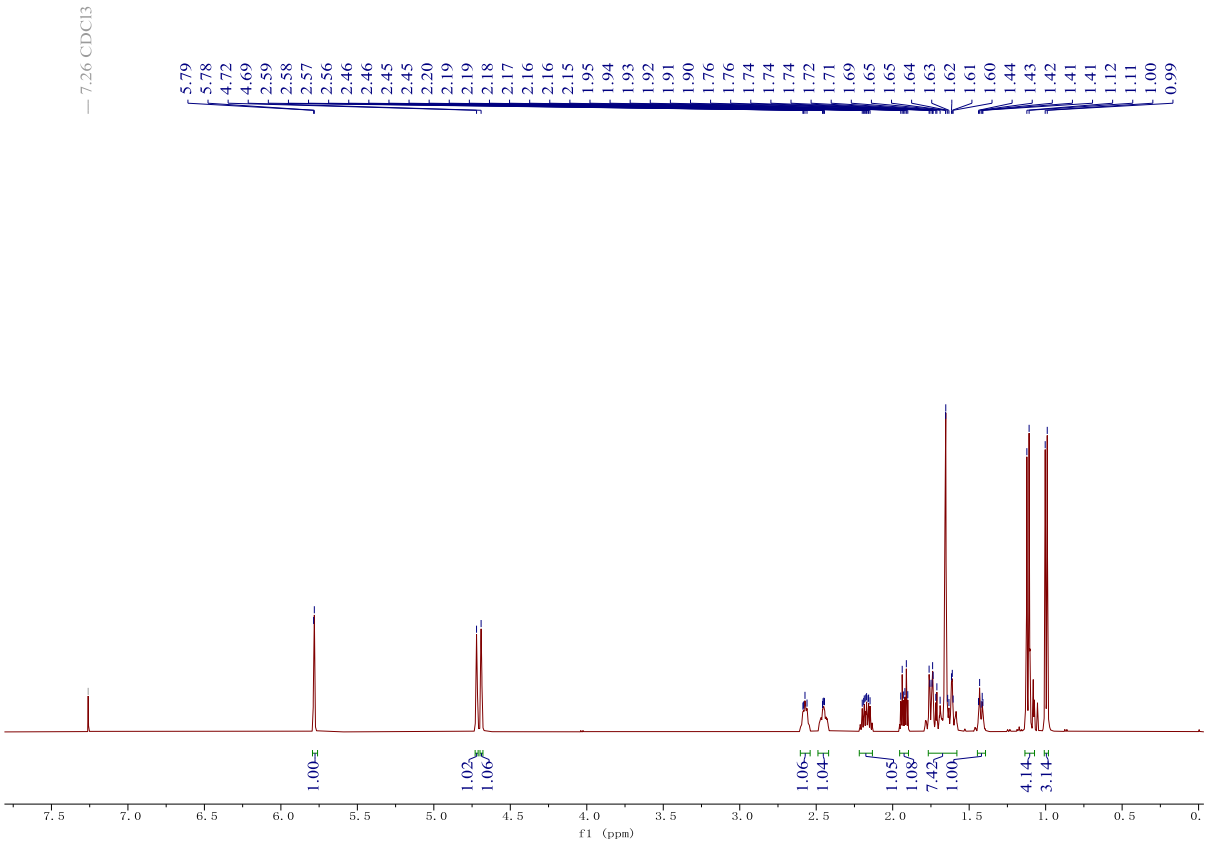


Figure S119. ^{13}C NMR spectrum of **25b** at 500 MHz in $CDCl_3$

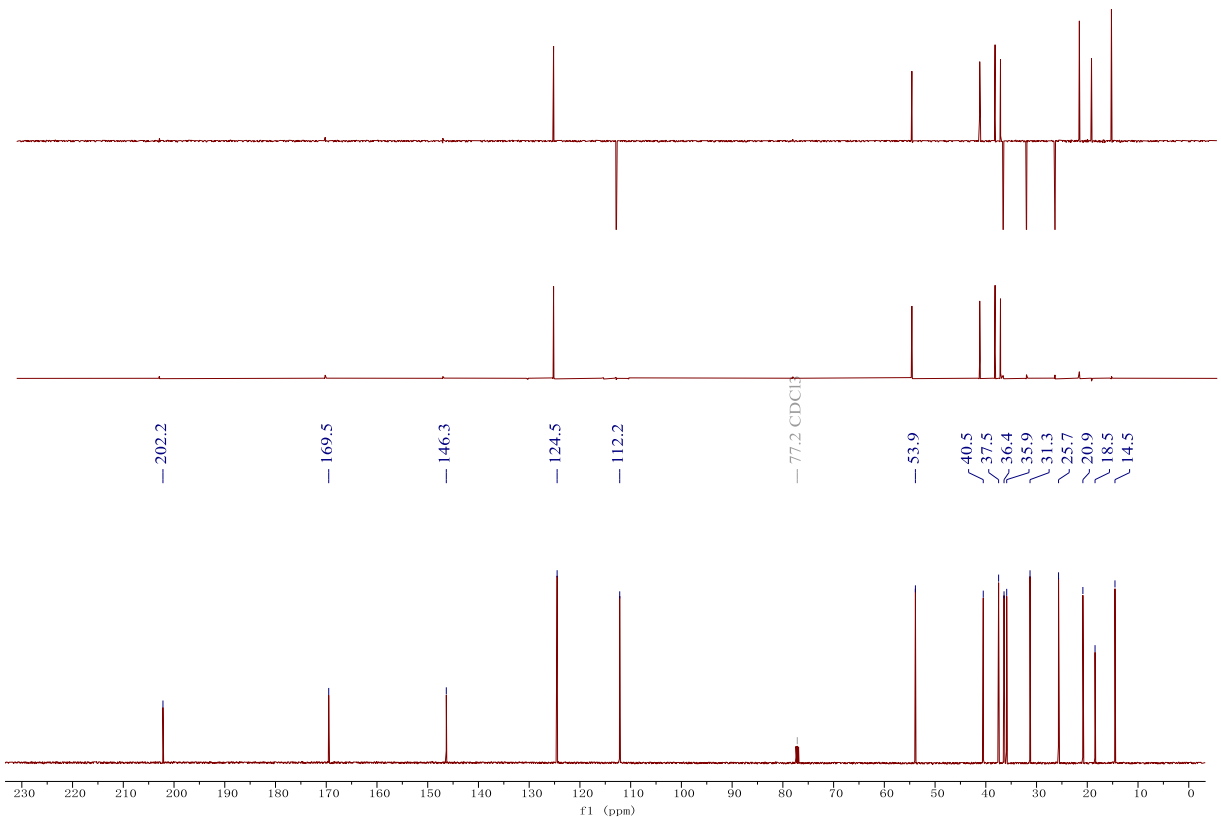


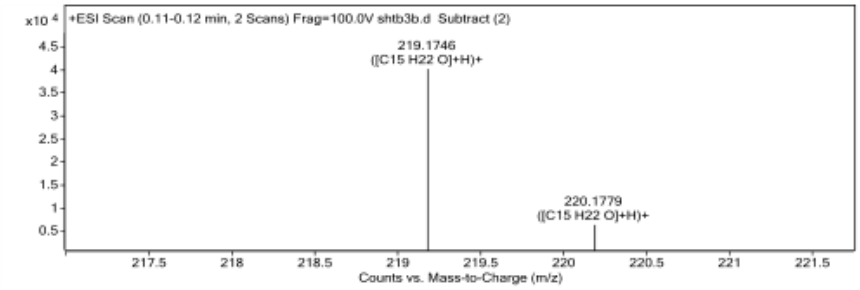
Figure S120. HRESIMS spectrum of synthetic compound **25b**

Data Filename	shtb3b.d	**Sample Name**	shtb3b
Sample Type	Sample	**Position**	P1-C6
Instrument Name	Instrument 1	**User Name**	
Acq Method	s.m	**Acquired Time**	3/5/2021 10:56:51 AM
IRM Calibration Status	Success	**DA Method**	Default.m
Comment			

Sample Group	**Info.**
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125.2)

User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
100	0	ESI



Peak List

m/z	z	Abund	Formula	Ion
219.1746	1	40434.86	C15 H22 O	(M+H)+
220.1779	1	6618.97	C15 H22 O	(M+H)+
241.1561	1	6528.09		
273.1481	1	7586.14		
282.1832		4167.29		
323.1981	1	5740.66		
327.2295	1	5734.01		
341.2662	1	3879.94		
459.3231	1	4176.1		
521.2876	1	4229.72		

Formula Calculator Element Limits

Element	Min	Max
C	3	60
H	0	120
O	0	30

Formula Calculator Results

Formula	CalculatedMass	CalculatedMz	Mz	Diff. (mDa)	Diff. (ppm)	DBE
C15 H22 O	218.1671	219.1743	219.1746	-0.30	-1.37	5.0000

Figure S121. Specific rotation spectrum of **25b**

Rudolph Research Analytical

This sample was measured on an Autopol VI, Serial #91058
Manufactured by Rudolph Research Analytical, Hackettstown, NJ, USA.

Measurement Date : Tuesday, 25-MAY-2021

Set Temperature : OFF

Time Delay : Disabled

Delay between Measurement : Disabled

n	Average	Std.Dev.	% RSD	Maximum	Minimum
5	26.35	1.25	4.74	28.27	25.20

S.No	Sample ID	Time	Result	Scale	OR °Arc	WLG.nm	Lg.mm	Conc.g/100ml	Temp.
1	SHTB3B	04:43:38 PM	25.31	SR	0.0248	589	100.00	0.098	27.4
2	SHTB3B	04:43:46 PM	25.20	SR	0.0247	589	100.00	0.098	27.4
3	SHTB3B	04:43:54 PM	26.22	SR	0.0257	589	100.00	0.098	27.4
4	SHTB3B	04:44:02 PM	26.73	SR	0.0262	589	100.00	0.098	27.4
5	SHTB3B	04:44:11 PM	28.27	SR	0.0277	589	100.00	0.098	27.4

Figure S122. ^{1}H NMR spectrum of **23** at 500 MHz in $CDCl_3$

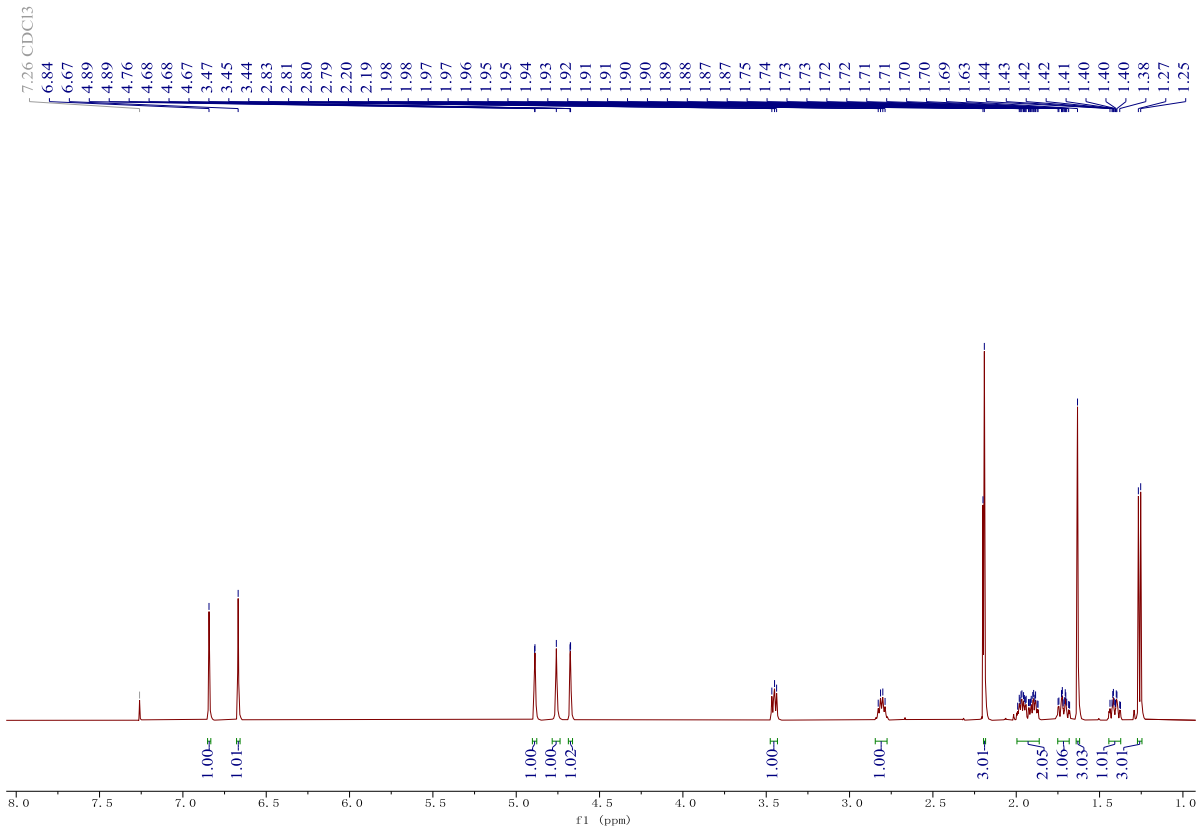


Figure S123. ^{13}C NMR spectrum of **23** at 125 MHz in $CDCl_3$

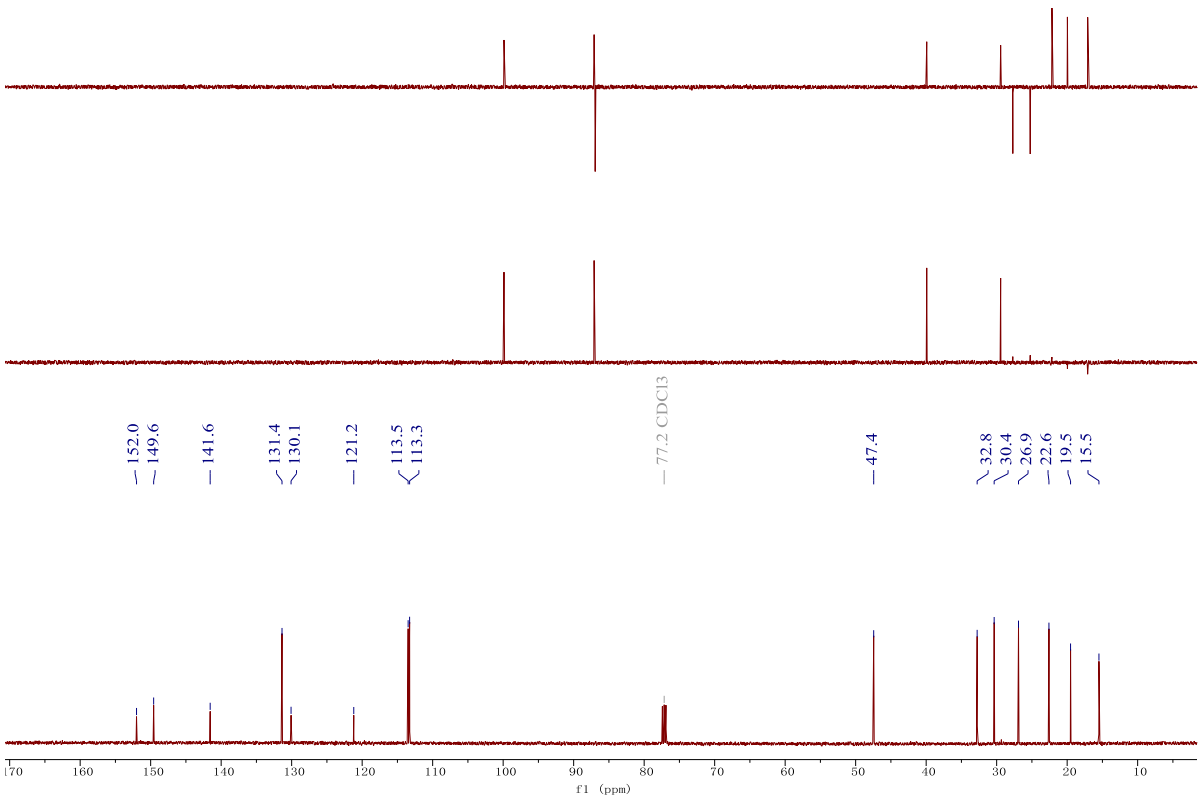


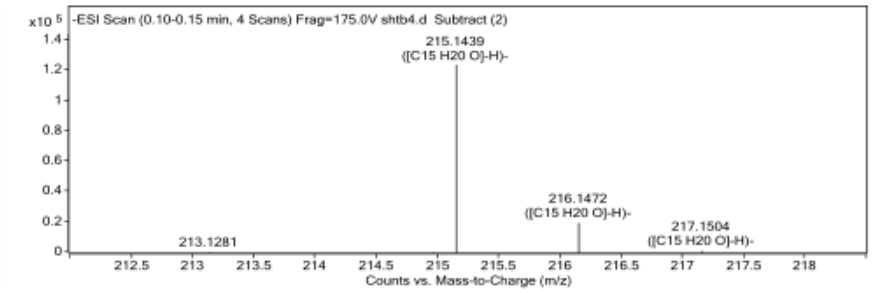
Figure S124 HRESIMS spectrum of synthetic compound **23**

Data Filename	shtb4.d	**Sample Name**	shtb4
Sample Type	Sample	**Position**	P1-A2
Instrument Name	Instrument 1	**User Name**	
Acq Method	s-.m	**Acquired Time**	3/25/2021 10:24:21 AM
IRM Calibration Status	Success	**DA Method**	Default.m
Comment			

Sample Group	**Info.**
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125.2)

User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
175	0	ESI



Peak List

m/z	z	Abund	Formula	Ion
173.0969	1	2748.09		
215.1439	1	123827.25	C15 H20 O	(M-H)-
216.1472	1	20125.21	C15 H20 O	(M-H)-
227.2016	1	3157.45		
255.2331	1	7418.11		
283.2641	1	3593.59		
485.2831	1	8593.5		
966.0006	1	6763.3		
967.004	1	2411.65		
996.011	1	9190.25		

Formula Calculator Element Limits

Element	Min	Max
C	3	60
H	0	120
O	0	10
N	0	5

Formula Calculator Results

Formula	CalculatedMass	CalculatedMz	Mz	Diff. (mDa)	Diff. (ppm)	DBE
C15 H20 O	216.1514	215.1441	215.1439	0.20	0.93	6.0000

Figure S125. Specific rotation spectrum of **23**

Rudolph Research Analytical

This sample was measured on an Autopol VI, Serial #91058
Manufactured by Rudolph Research Analytical, Hackettstown, NJ, USA.

Measurement Date : Tuesday, 25-MAY-2021

Set Temperature : OFF

Time Delay : Disabled

Delay between Measurement : Disabled

n	Average	Std.Dev.	% RSD	Maximum	Minimum
5	5.80	1.77	30.51	7.78	3.33

S.No	Sample ID	Time	Result	Scale	OR °Arc	WLG.nm	Lg.mm	Conc.g/100ml	Temp.
1	SHTB4	05:05:27 PM	5.97	SR	0.0043	589	100.00	0.072	27.4
2	SHTB4	05:05:43 PM	3.33	SR	0.0024	589	100.00	0.072	27.4
3	SHTB4	05:05:51 PM	7.78	SR	0.0056	589	100.00	0.072	27.4
4	SHTB4	05:06:03 PM	4.86	SR	0.0035	589	100.00	0.072	27.4
5	SHTB4	05:06:11 PM	7.08	SR	0.0051	589	100.00	0.072	27.4

Figure S126. ^{1}H NMR spectrum of **15a** at 600 MHz in $CDCl_3$

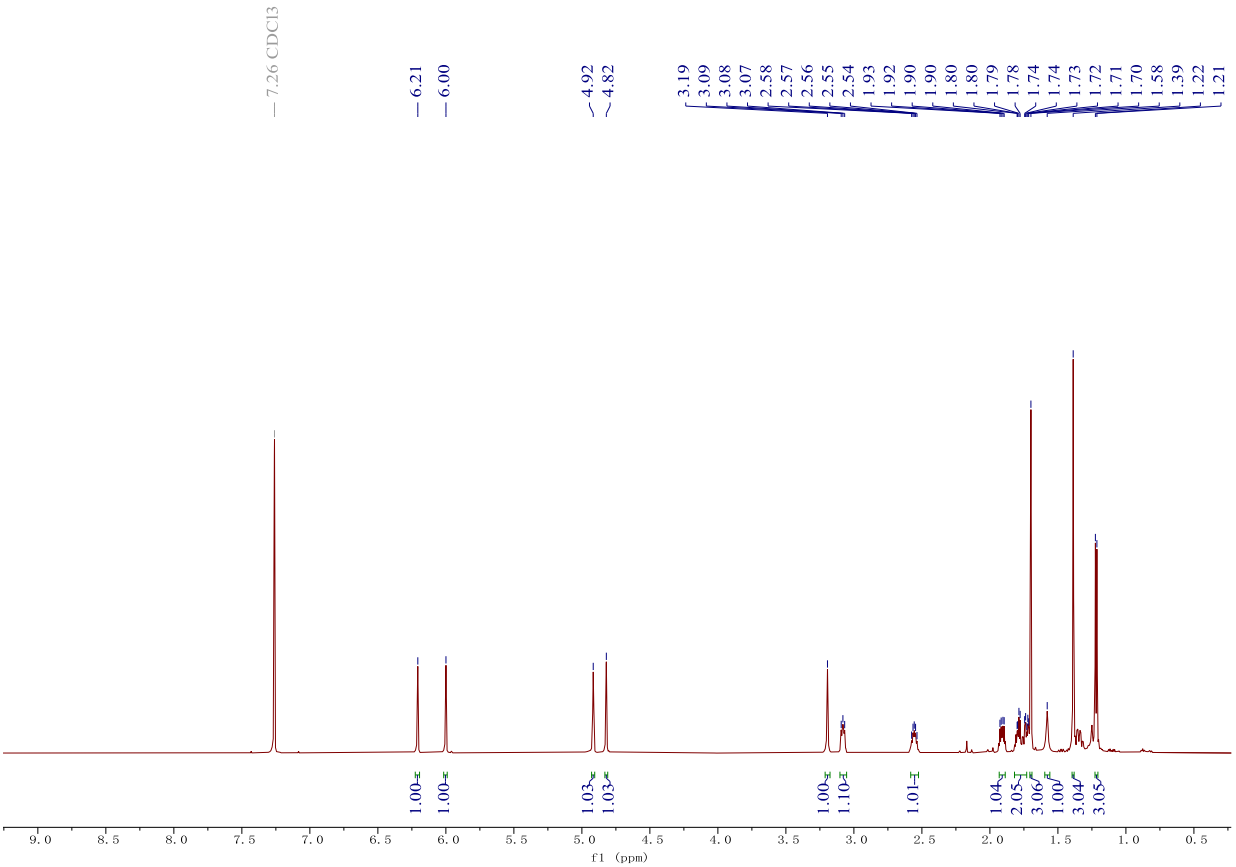


Figure S127. ^{13}C NMR spectrum of **15a** at 200 MHz in $CDCl_3$

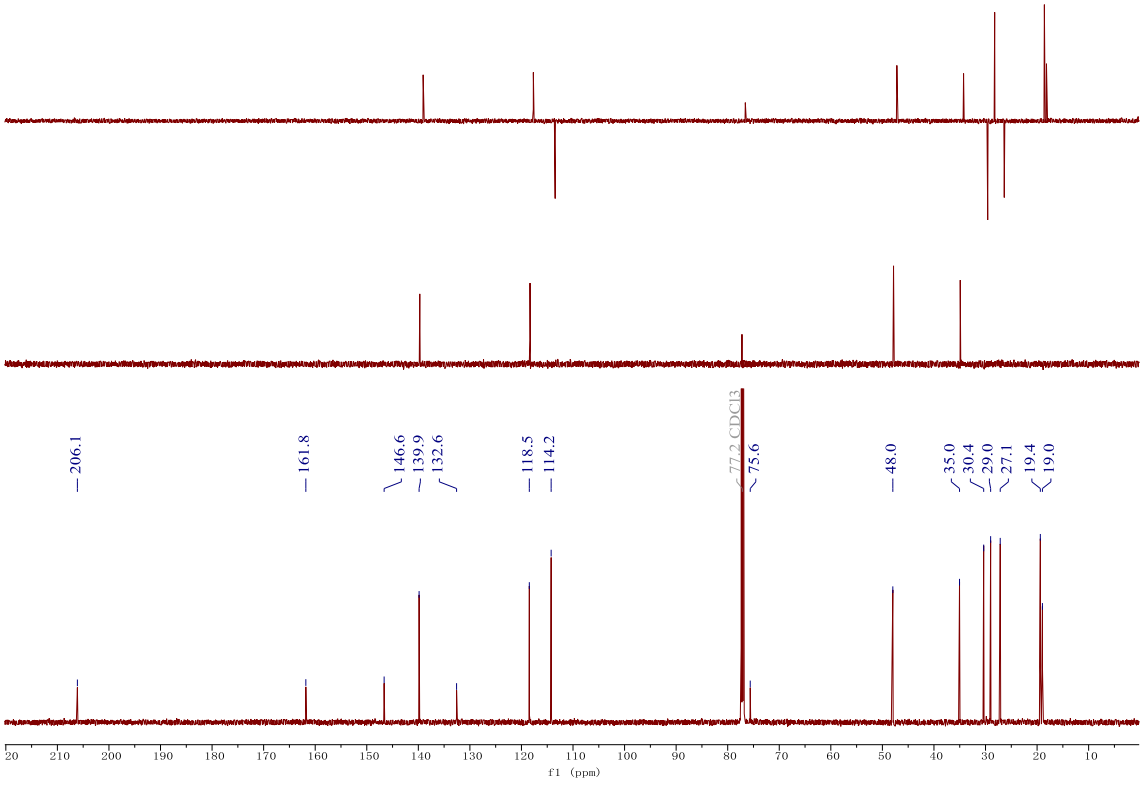


Figure S128. HRESIMS spectrum of synthetic compound **15a**

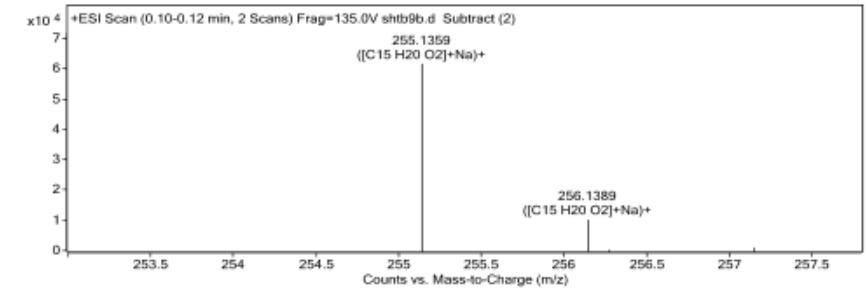
Qualitative Analysis Report

Data Filename	shtb9b.d	**Sample Name**	shtb9b
Sample Type	Sample	**Position**	P1-A9
Instrument Name	Instrument 1	**User Name**	
Acq Method	s.m	**Acquired Time**	5/12/2021 10:55:18 AM
IRM Calibration Status	Success	**DA Method**	Default.m
Comment			

Sample Group	**Info.**
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125.2)

User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
135	0	ESI



Peak List

m/z	z	Abund	Formula	Ion
233.1536	1	16380.88		
255.1359	1	61904.61	C15 H20 O2	(M+Na)+
274.2743	1	51021.09		
318.3006	1	34191.51		
340.2828	1	15702.08		
437.1939	1	45670.81		
453.168	1	19850.7		
487.2825	1	18841.72		
654.3336	1	16313.57		
659.2885	1	22187.38		

Formula Calculator Element Limits

Element	Min	Max
C	3	60
H	0	120
O	0	30

Formula Calculator Results

Formula	CalculatedMass	CalculatedMz	Mz	Diff. (mDa)	Diff. (ppm)	DBE
C15 H20 O2	232.1463	255.1356	255.1359	-0.30	-1.18	6.0000

--- End Of Report ---

Figure S129. Specific rotation spectrum of **15a**

Rudolph Research Analytical

This sample was measured on an Autopol VI, Serial #91058
Manufactured by Rudolph Research Analytical, Hackettstown, NJ, USA.

Measurement Date : Monday, 21-JUN-2021

Set Temperature : OFF

Time Delay : Disabled

Delay between Measurement : Disabled

n	Average	Std.Dev.	% RSD	Maximum	Minimum
5	-14.81	0.03	-0.20	-14.79	-14.85

S.No	Sample ID	Time	Result	Scale	OR °Arc	WLG.nm	Lg.mm	Conc.g/100ml	Temp.
1	shtb9b	10:02:11 AM	-14.79	SR	-0.244	589	100.00	1.650	25.9
2	shtb9b	10:02:16 AM	-14.85	SR	-0.245	589	100.00	1.650	25.9
3	shtb9b	10:02:22 AM	-14.85	SR	-0.245	589	100.00	1.650	25.9
4	shtb9b	10:02:28 AM	-14.79	SR	-0.244	589	100.00	1.650	25.9
5	shtb9b	10:02:33 AM	-14.79	SR	-0.244	589	100.00	1.650	25.9

Figure S130. ^{1}H NMR spectrum of **15b** at 600 MHz in $CDCl_3$

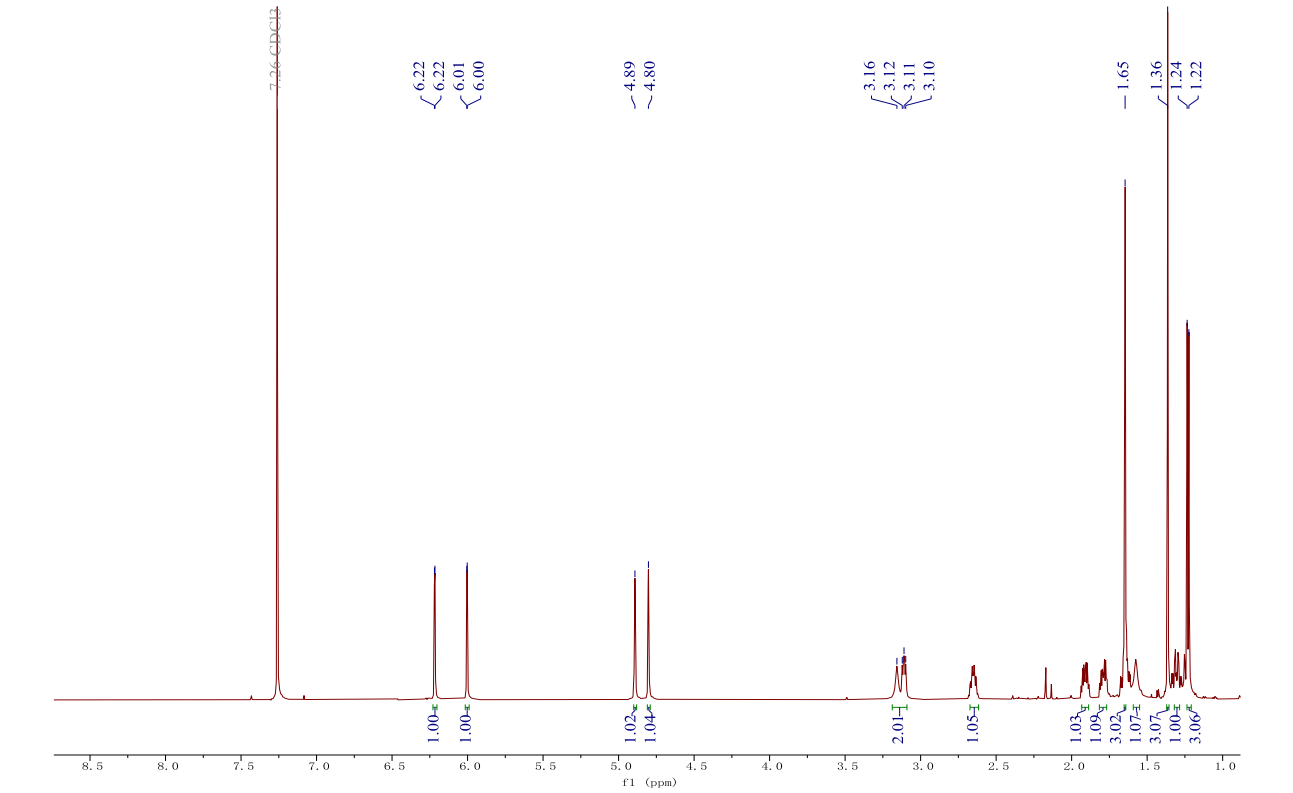


Figure S131. ^{1}C NMR spectrum of **15b** at 200 MHz in $CDCl_3$

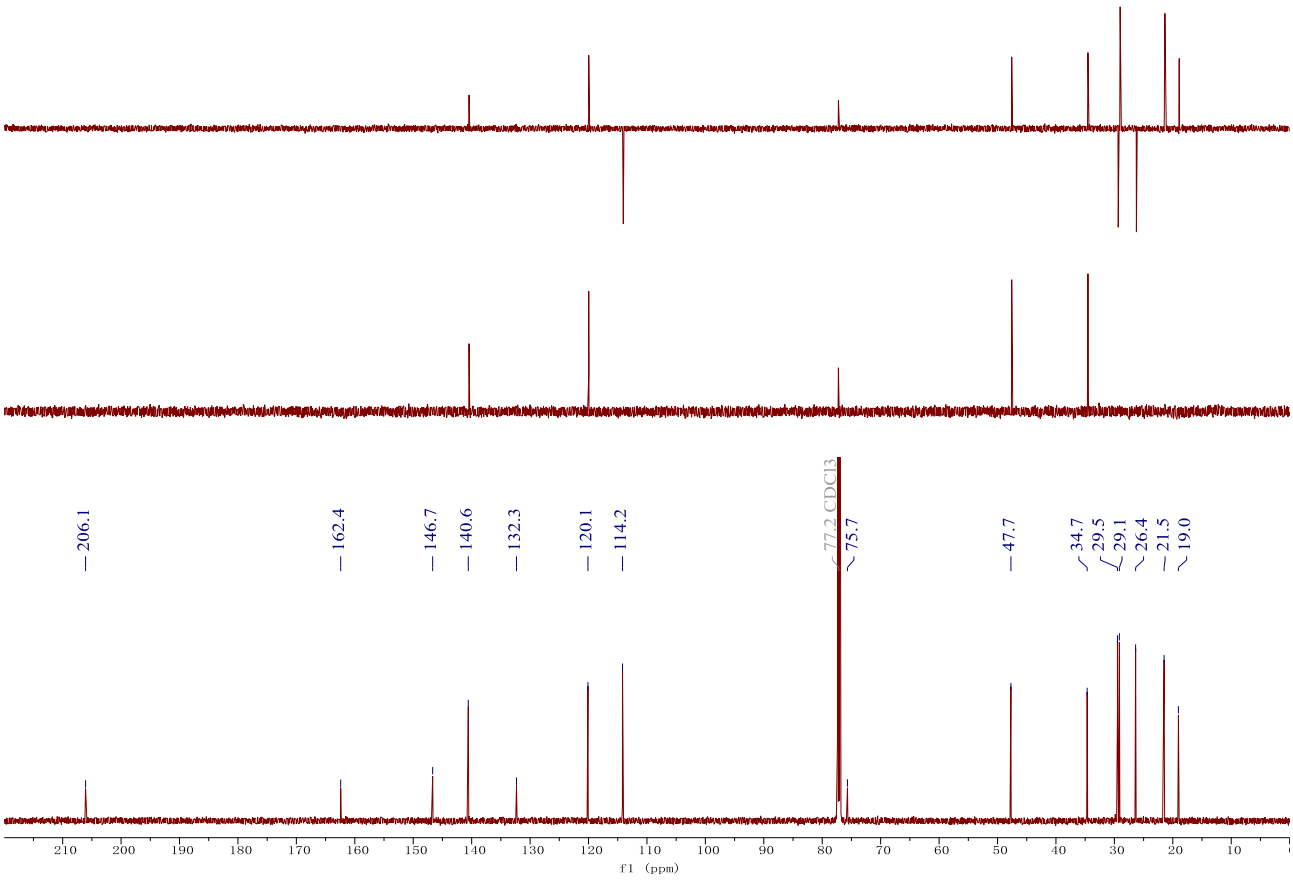


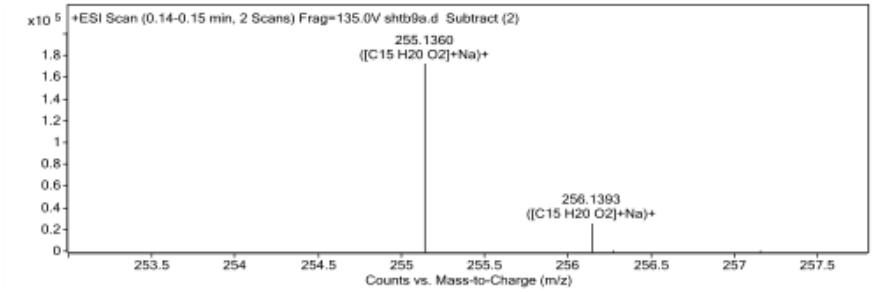
Figure S132. HRESIMS spectrum of synthetic compound **15b**

Data Filename	shtb9a.d	**Sample Name**	shtb9a
Sample Type	Sample	**Position**	P1-A8
Instrument Name	Instrument 1	**User Name**	
Acq Method	s.m	**Acquired Time**	5/12/2021 10:53:55 AM
IRM Calibration Status	Success	**DA Method**	Default.m
Comment			

Sample Group	**Info.**
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125.2)

User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
135	0	ESI



Peak List

m/z	z	Abund	Formula	Ion
102.128	1	49496.04		
233.1537	1	57223.03		
255.136	1	173165.98	C15 H20 O2	(M+Na)+
274.2745	1	81981.36		
285.1095	1	45389.63		
318.3008	1	58840.86		
319.1155	1	41147.52		
437.1944	1	59092.2		
453.1682	1	68507.31		
487.2829	1	84408.16		

Formula Calculator Element Limits

Element	Min	Max
C	3	60
H	0	120
O	0	30

Formula Calculator Results

Formula	CalculatedMass	CalculatedMz	Mz	Diff. (mDa)	Diff. (ppm)	DBE
C15 H20 O2	232.1463	255.1356	255.1360	-0.40	-1.57	6.0000

Figure S133. Specific rotation spectrum of **15b**

Rudolph Research Analytical

This sample was measured on an Autopol VI, Serial #91058
Manufactured by Rudolph Research Analytical, Hackettstown, NJ, USA.

Measurement Date : Monday, 21-JUN-2021

Set Temperature : OFF

Time Delay : Disabled

Delay between Measurement : Disabled

n	Average	Std.Dev.	% RSD	Maximum	Minimum
5	-63.96	0.92	-1.43	-62.64	-64.84

S.No	Sample ID	Time	Result	Scale	OR °Arc	WLG.nm	Lg.mm	Conc.g/100ml	Temp.
1	shtb9a	09:54:33 AM	-63.74	SR	-0.058	589	100.00	0.091	25.8
2	shtb9a	09:54:39 AM	-62.64	SR	-0.057	589	100.00	0.091	25.8
3	shtb9a	09:54:44 AM	-63.74	SR	-0.058	589	100.00	0.091	25.8
4	shtb9a	09:54:50 AM	-64.84	SR	-0.059	589	100.00	0.091	25.8
5	shtb9a	09:54:56 AM	-64.84	SR	-0.059	589	100.00	0.091	25.8

Figure S134. ^{1}H NMR spectrum of synthetic compound **4** at 500 MHz in $CDCl_3$

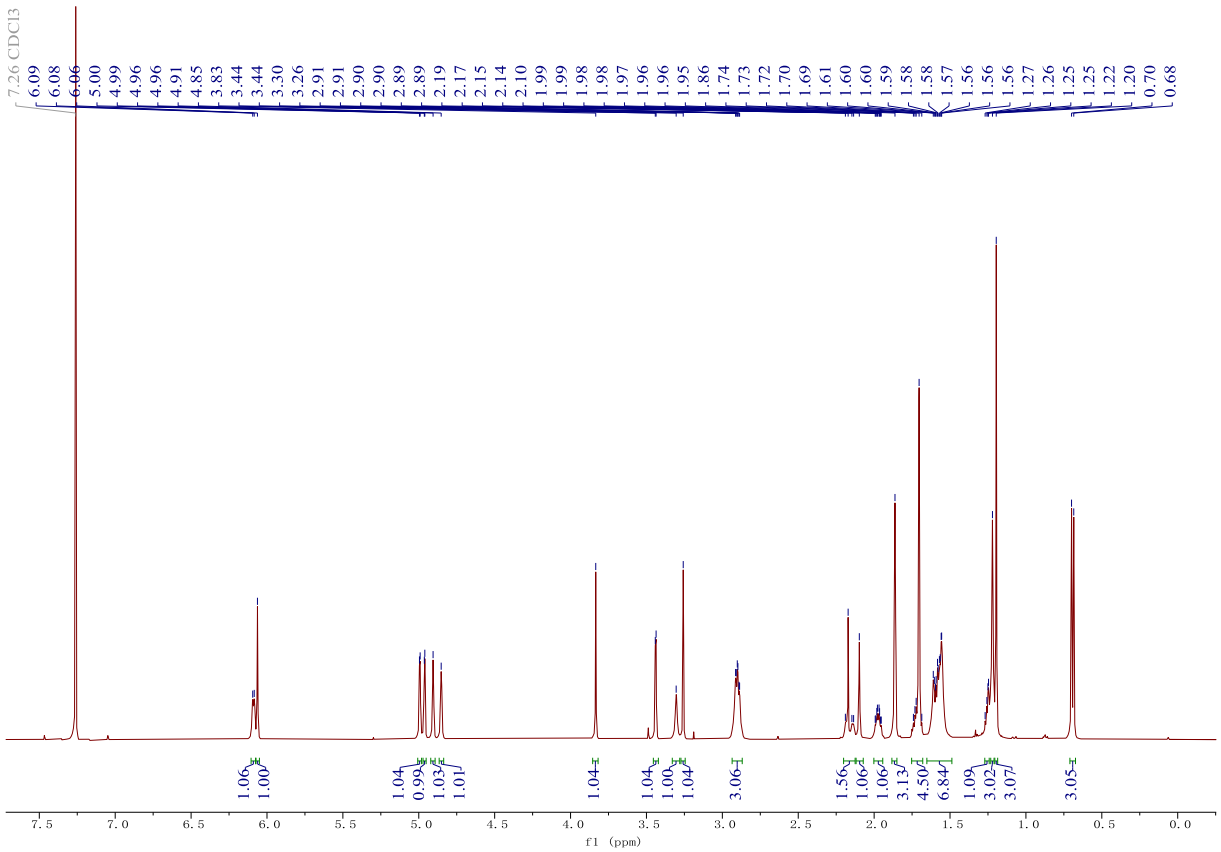


Figure S135. ^{13}C NMR spectrum of synthetic compound **4** at 125 MHz in $CDCl_3$

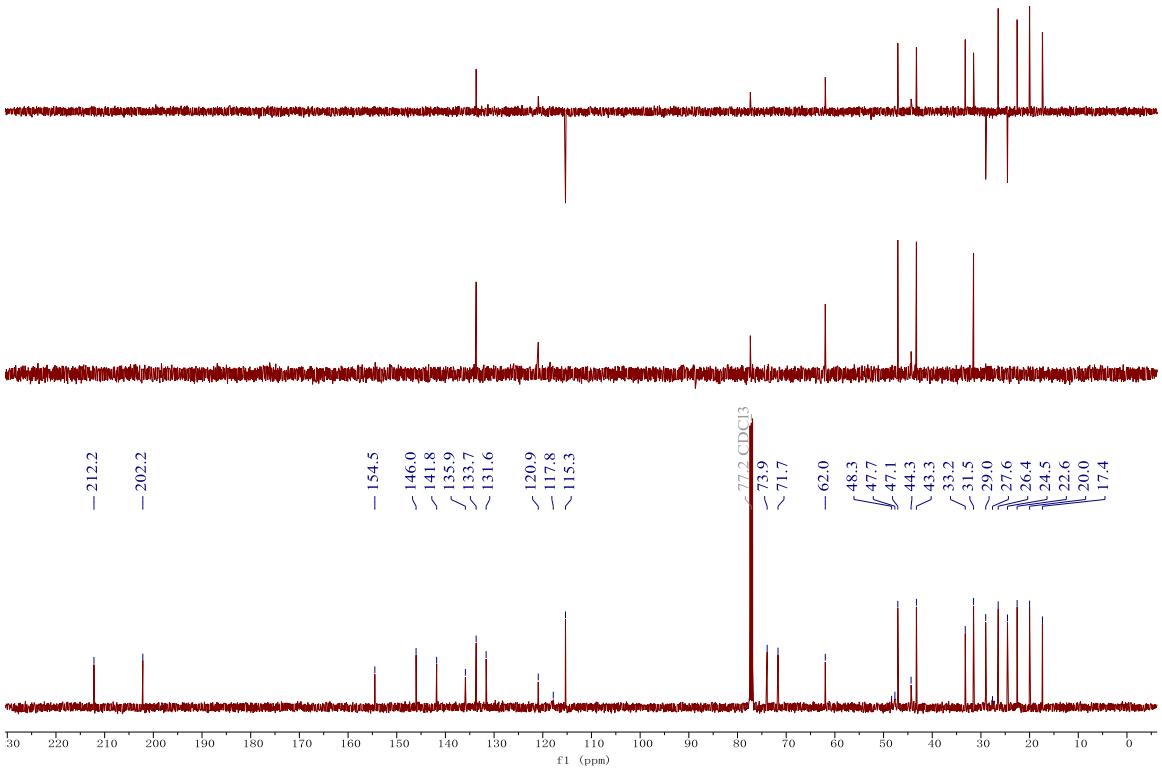


Figure S136. HRESIMS spectrum of synthetic compound **4**

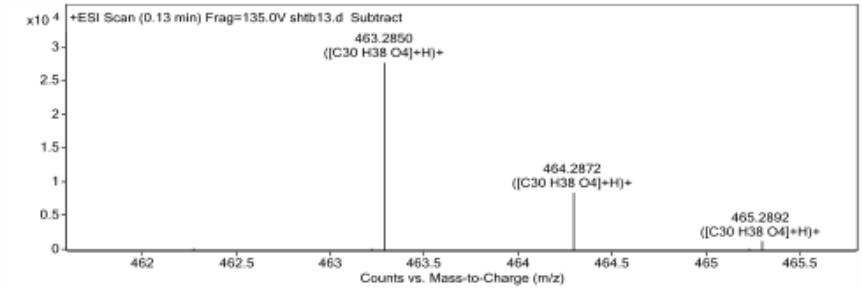
Qualitative Analysis Report

Data Filename	shtb13.d	**Sample Name**	shtb13
Sample Type	Sample	**Position**	P1-C3
Instrument Name	Instrument 1	**User Name**	
Acq Method	s.m	**Acquired Time**	5/27/2021 10:17:46 AM
IRM Calibration Status	Success	**DA Method**	Default.m
Comment			

Sample Group	**Info.**
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125.2)

User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
135	0	ESI



Peak List

m/z	z	Abund	Formula	Ion
213.1277	1	7307.28		
231.1385	1	15739.72		
463.285	1	27779.99	C30 H38 O4	(M+H)+
464.2872	1	8605.94	C30 H38 O4	(M+H)+
485.2664	1	20694.79		
486.2707	1	6948.2		
499.2456	1	11668.21		
501.2589	1	9423		
947.544	1	24102.8		
948.5488	1	14346.03		

Formula Calculator Element Limits

Element	Min	Max
C	3	60
H	0	120
O	0	30

Formula Calculator Results

Formula	CalculatedMass	CalculatedMz	Mz	Diff. (mDa)	Diff. (ppm)	DBE
C30 H38 O4	462.2770	463.2843	463.2850	-0.70	-1.51	12.0000

--- End Of Report ---

Figure S137. Specific rotation spectrum of **4**

Rudolph Research Analytical

This sample was measured on an Autopol VI, Serial #91058
Manufactured by Rudolph Research Analytical, Hackettstown, NJ, USA.

Measurement Date : Friday, 15-JAN-2021

Set Temperature : 20.0

Time Delay : Disabled

Delay between Measurement : Disabled

n	Average	Std.Dev.	% RSD	Maximum	Minimum
5	-50.24	0.33	-0.65	-50.00	-50.61

S.No	Sample ID	Time	Result	Scale	OR °Arc	WLG.nm	Lg.mm	Conc.g/100ml	Temp.
1	SHTB154-3-3	04:40:40 PM	-50.00	SR	-0.082	589	100.00	0.164	19.9
2	SHTB154-3-3	04:40:46 PM	-50.61	SR	-0.083	589	100.00	0.164	19.8
3	SHTB154-3-3	04:40:52 PM	-50.00	SR	-0.082	589	100.00	0.164	19.8
4	SHTB154-3-3	04:40:58 PM	-50.61	SR	-0.083	589	100.00	0.164	19.7
5	SHTB154-3-3	04:41:03 PM	-50.00	SR	-0.082	589	100.00	0.164	19.7

Figure S138. ^{1}H NMR spectrum of **24** at 500 MHz in $CDCl_3$

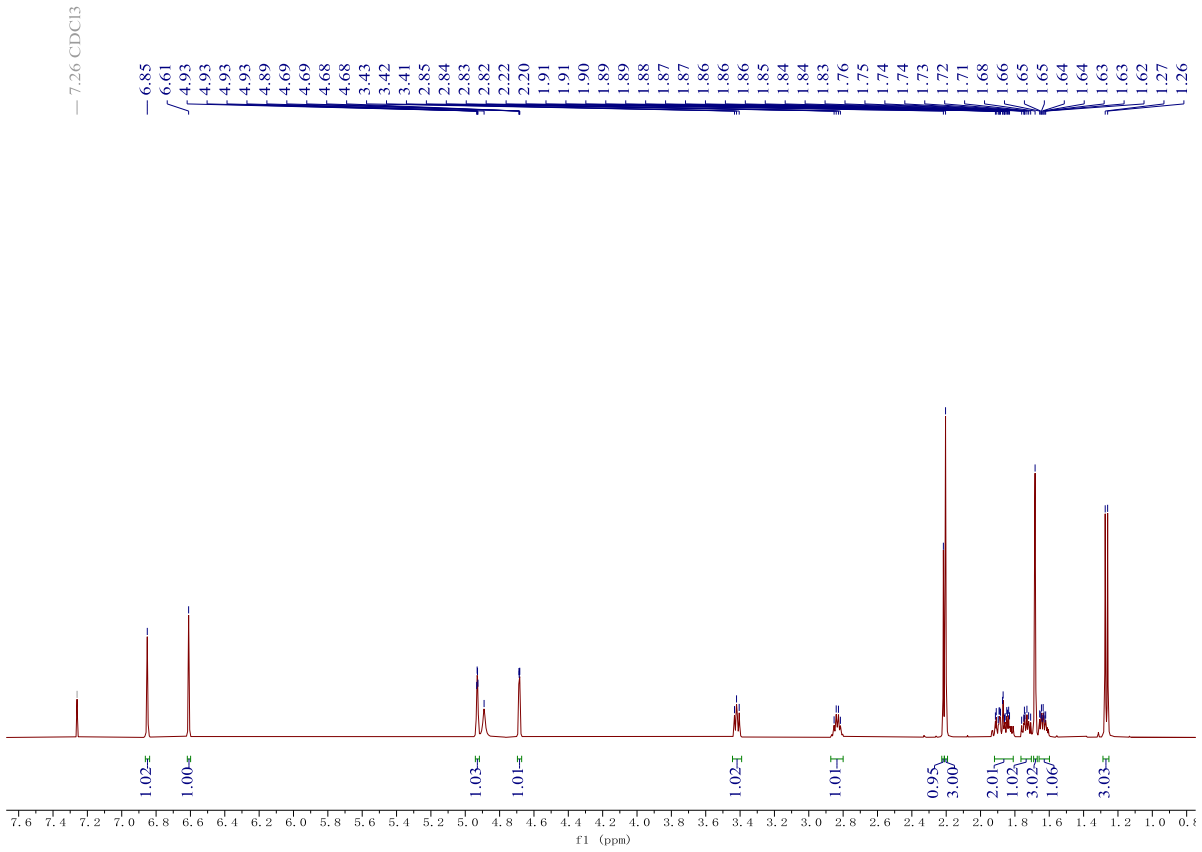


Figure S139. ^{13}C NMR spectrum of **24** at 125 MHz in $CDCl_3$

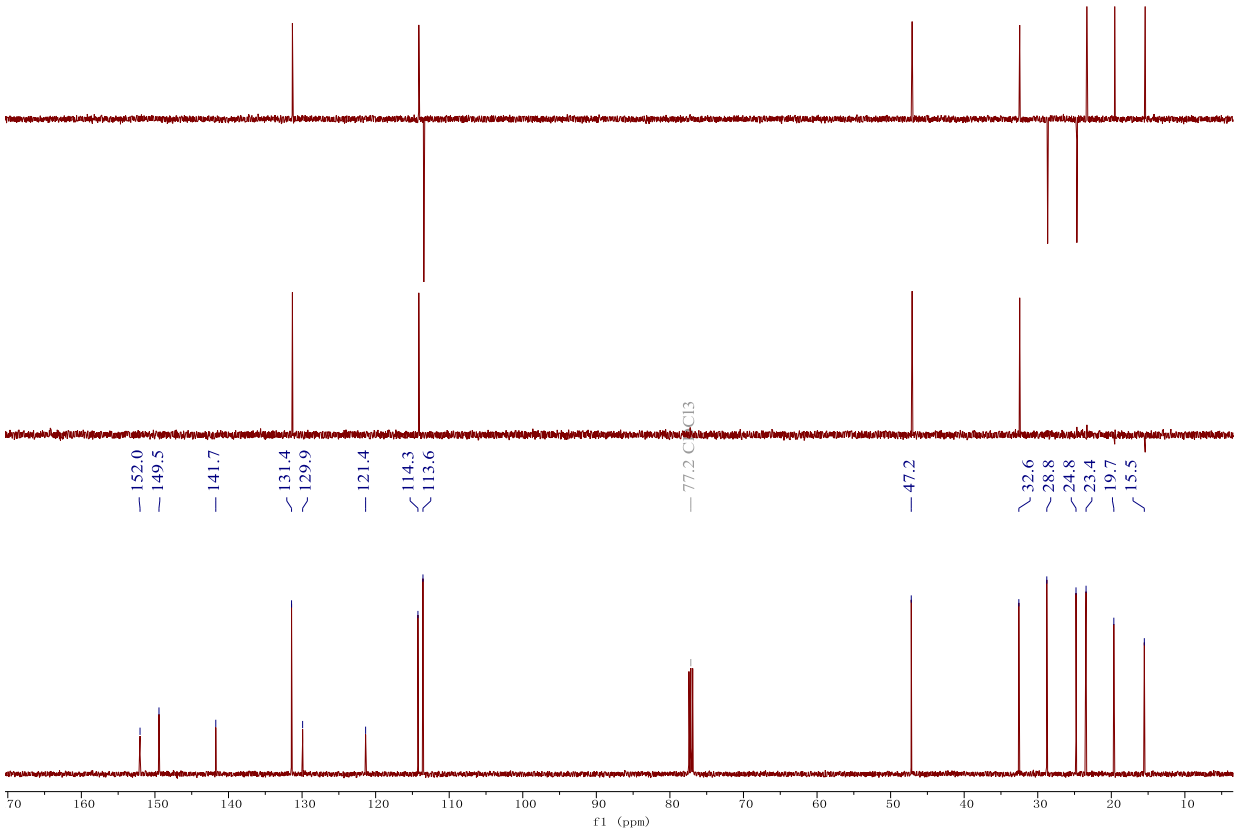


Figure S140. HRESIMS spectrum of synthetic compound **24**

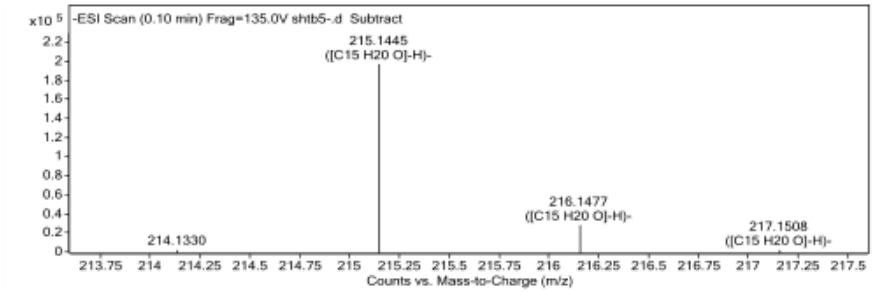
Qualitative Analysis Report

Data Filename	shtb5-.d	**Sample Name**	shtb5
Sample Type	Sample	**Position**	P1-A4
Instrument Name	Instrument 1	**User Name**	
Acq Method	s-.m	**Acquired Time**	5/10/2021 4:24:31 PM
IRM Calibration Status	Success	**DA Method**	Default.m
Comment			

Sample Group	**Info.**
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125.2)

User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
135	0	ESI



Peak List

m/z	z	Abund	Formula	Ion
119.0365	1	30283.21		
213.1289	1	16498.41		
215.1445	1	197670.78	C15 H20 O	(M-H)-
216.1477	1	28829.65	C15 H20 O	(M-H)-
247.1344	1	29362.26		
255.2334	1	29455.88		
429.2805	1	86950.37		
430.2837	1	26019.6		
1033.989	1	128687.88		
1034.9915	1	25360.93		

Formula Calculator Element Limits

Element	Min	Max
C	3	60
H	0	120
O	0	30

Formula Calculator Results

Formula	CalculatedMass	CalculatedMz	Mz	Diff. (mDa)	Diff. (ppm)	DBE
C15 H20 O	216.1514	215.1441	215.1445	-0.40	-1.86	6.0000

--- End Of Report ---

Figure S141. Specific rotation spectrum of **24**

Rudolph Research Analytical

This sample was measured on an Autopol VI, Serial #91058
Manufactured by Rudolph Research Analytical, Hackettstown, NJ, USA.

Measurement Date : Tuesday, 25-MAY-2021

Set Temperature : OFF

Time Delay : Disabled

Delay between Measurement : Disabled

n	Average	Std.Dev.	% RSD	Maximum	Minimum
5	4.02	1.63	40.54	5.65	1.63

S.No	Sample ID	Time	Result	Scale	OR °Arc	WLG.nm	Lg.mm	Conc.g/100ml	Temp.
1	SHTB5	05:11:43 PM	4.22	SR	0.0062	589	100.00	0.147	27.4
2	SHTB5	05:11:56 PM	5.31	SR	0.0078	589	100.00	0.147	27.4
3	SHTB5	05:12:04 PM	5.65	SR	0.0083	589	100.00	0.147	27.4
4	SHTB5	05:12:19 PM	1.63	SR	0.0024	589	100.00	0.147	27.4
5	SHTB5	05:12:34 PM	3.27	SR	0.0048	589	100.00	0.147	27.4

Figure S142. ^{1}H NMR spectrum of **16a** at 500 MHz in $CDCl_3$

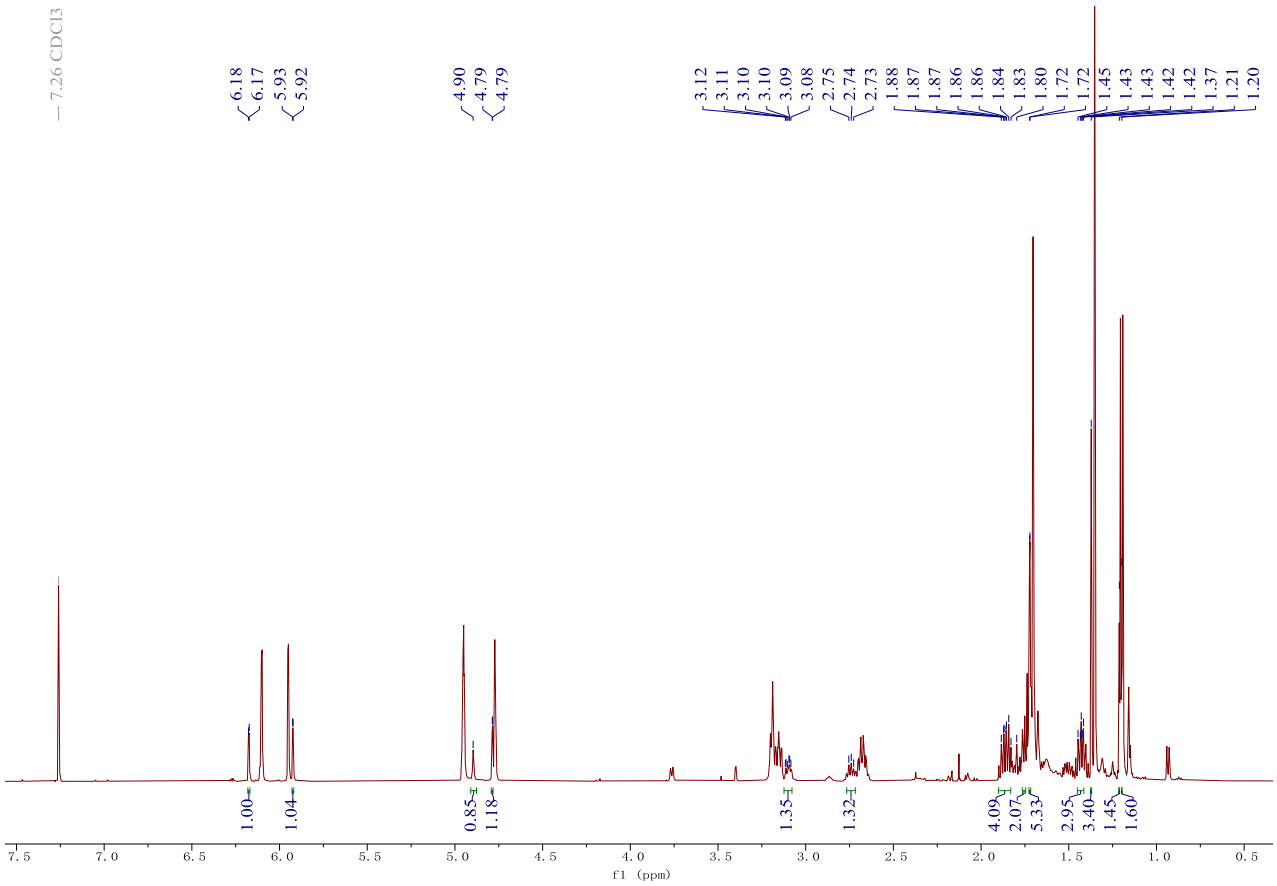


Figure S143. ^{1}C NMR spectrum of **16a** at 125 MHz in $CDCl_3$

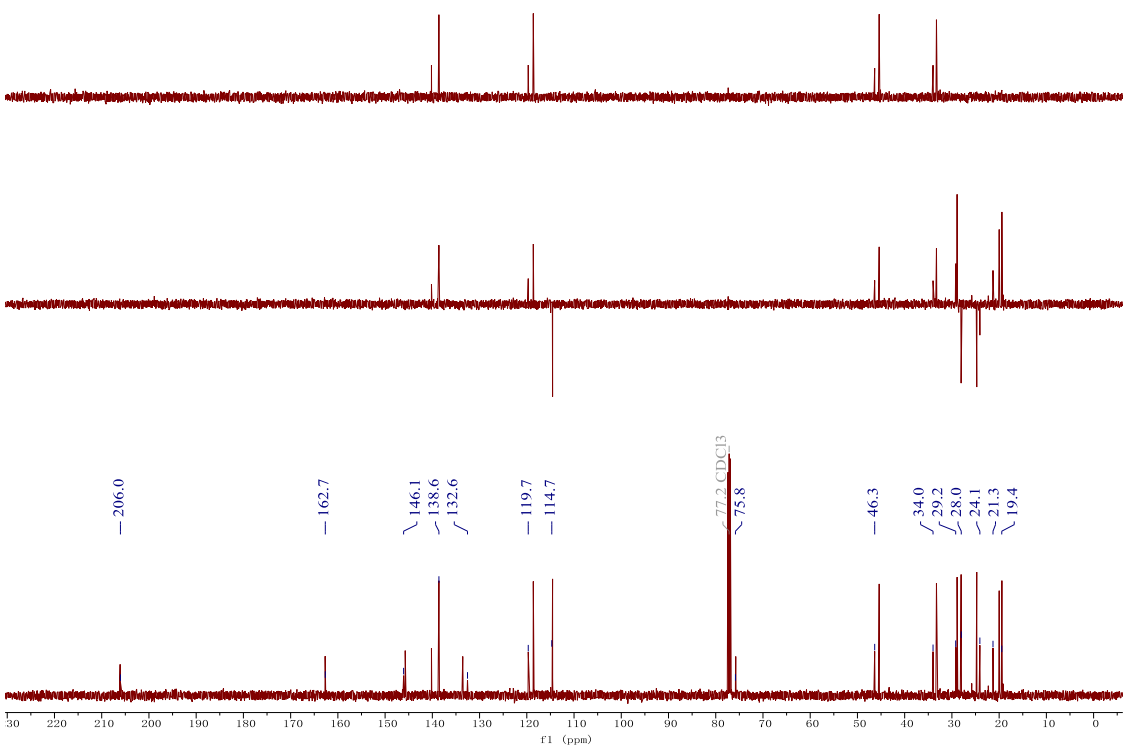


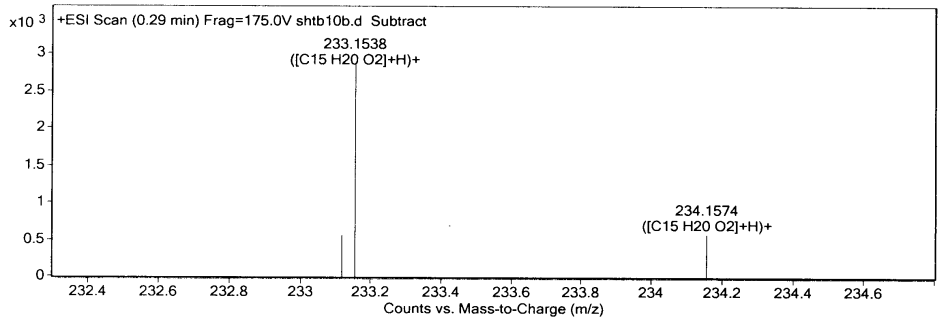
Figure S144. HRESIMS spectrum of synthetic compound **16a**

Data Filename	shtb10b.d	**Sample Name**	shtb10b
Sample Type	Sample	**Position**	P1-A7
Instrument Name	Instrument 1	**User Name**	
Acq Method	s.m	**Acquired Time**	12/14/2021 3:27:20 PM
IRM Calibration Status	Success	**DA Method**	PCDL.m
Comment			

Sample Group	**Info.**
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125.2)

User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
175	0	ESI



Peak List

m/z	z	Abund	Formula	Ion
173.0967	1	2955.46		
187.1118	1	3544.63		
215.143	1	4438.54		
231.1383	1	2780.06		
233.1538	1	2841.86	C15 H20 O2	(M+H)+
249.1516	1	1600.14		
255.1347	1	1807.27		
1240.5084	1	1538.46		
1241.0124	1	2086.55		
1242.0145	1	1449.63		

Formula Calculator Element Limits

Element	Min	Max
C	3	60
H	0	120
O	0	30

Formula Calculator Results

Formula	CalculatedMass	CalculatedMz	Mz	Diff. (mDa)	Diff. (ppm)	DBE
C15 H20 O2	232.1463	233.1536	233.1538	-0.20	-0.86	6.0000

Figure S145. ^{1}H NMR spectrum of **16b** at 800 MHz in $CDCl_3$

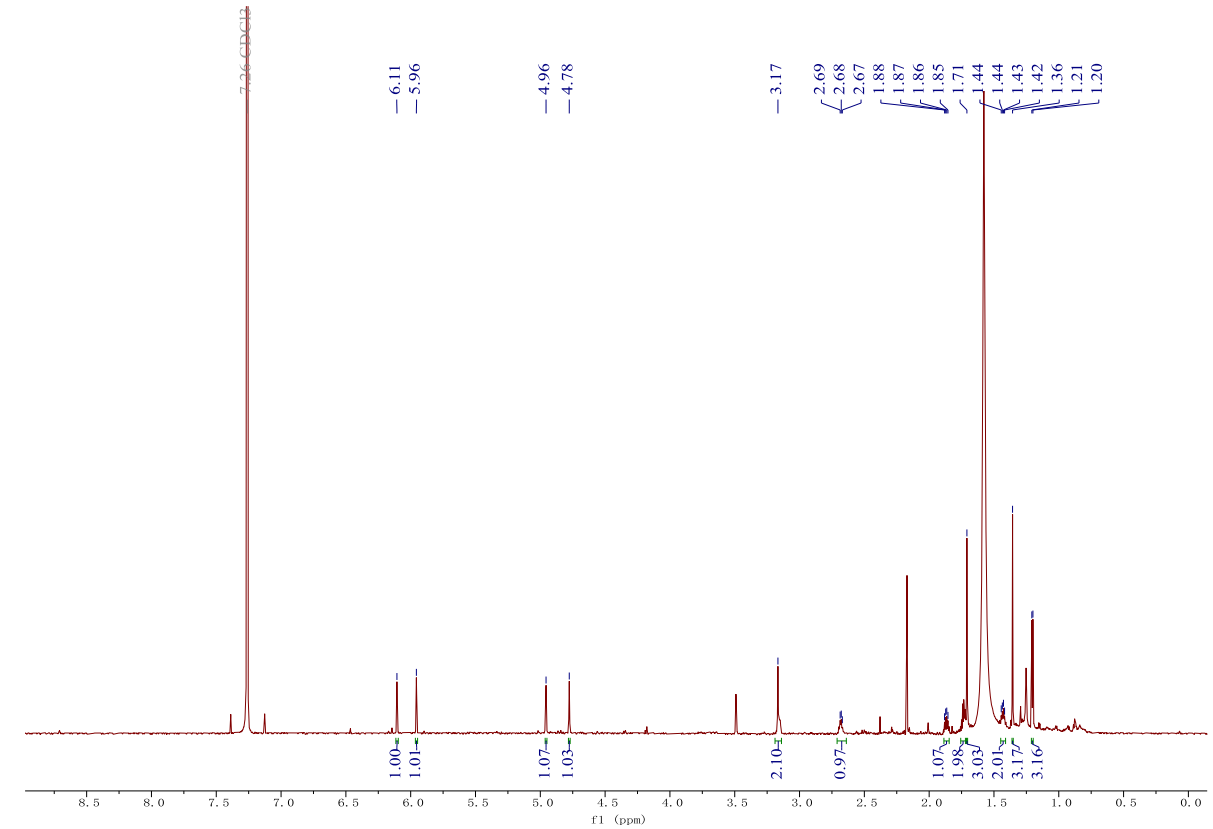


Figure S146. ^{13}C NMR spectrum of **16b** at 200 MHz in $CDCl_3$

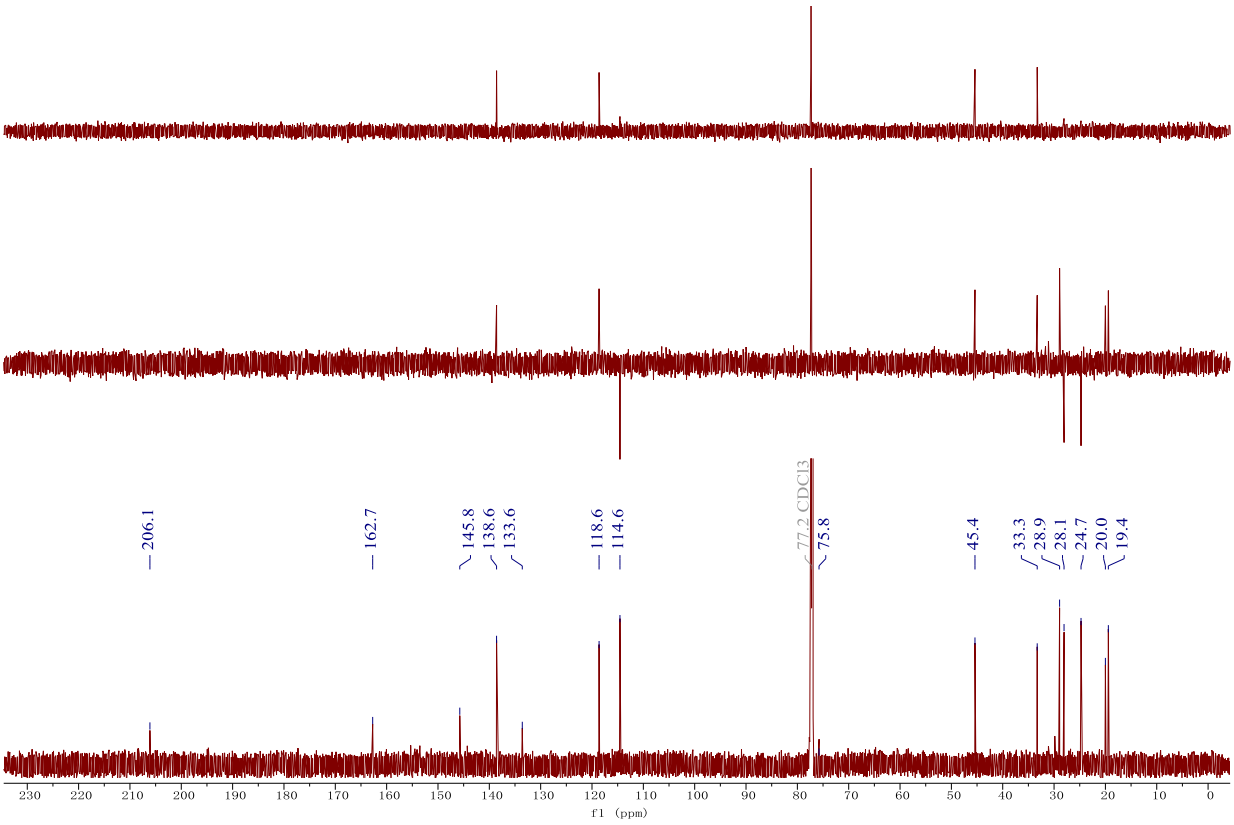


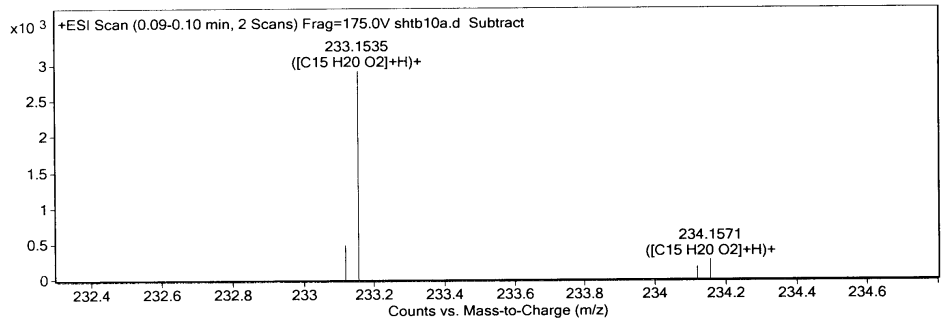
Figure S147. HRESIMS spectrum of synthetic compound **16b**

Data Filename	shtb10a.d	**Sample Name**	shtb10a
Sample Type	Sample	**Position**	P1-A6
Instrument Name	Instrument 1	**User Name**	
Acq Method	s.m	**Acquired Time**	12/14/2021 3:25:10 PM
IRM Calibration Status	Success	**DA Method**	PCDL.m
Comment			

Sample Group	**Info.**
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125.2)

User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
175	0	ESI



Peak List

m/z	z	Abund	Formula	Ion
173.0958	1	2239.06		
187.1115	1	1896.56		
191.106	1	1241.29		
215.1434	1	3974.06		
231.1378	1	3326.52		
233.1535	1	2912.84	C15 H20 O2	(M+H)+
249.1493	1	2383.2		
261.1119	1	2200.18		
485.2453	1	1301.99		
533.251	1	1892.12		

Formula Calculator Element Limits

Element	Min	Max
C	3	60
H	0	120
O	0	30

Formula Calculator Results

Formula	CalculatedMass	CalculatedMz	Mz	Diff. (mDa)	Diff. (ppm)	DBE
C15 H20 O2	232.1463	233.1536	233.1535	0.10	0.43	6.0000

Figure S148. ^{1}H NMR spectrum of synthetic compound **3** at 500 MHz in $CDCl_3$

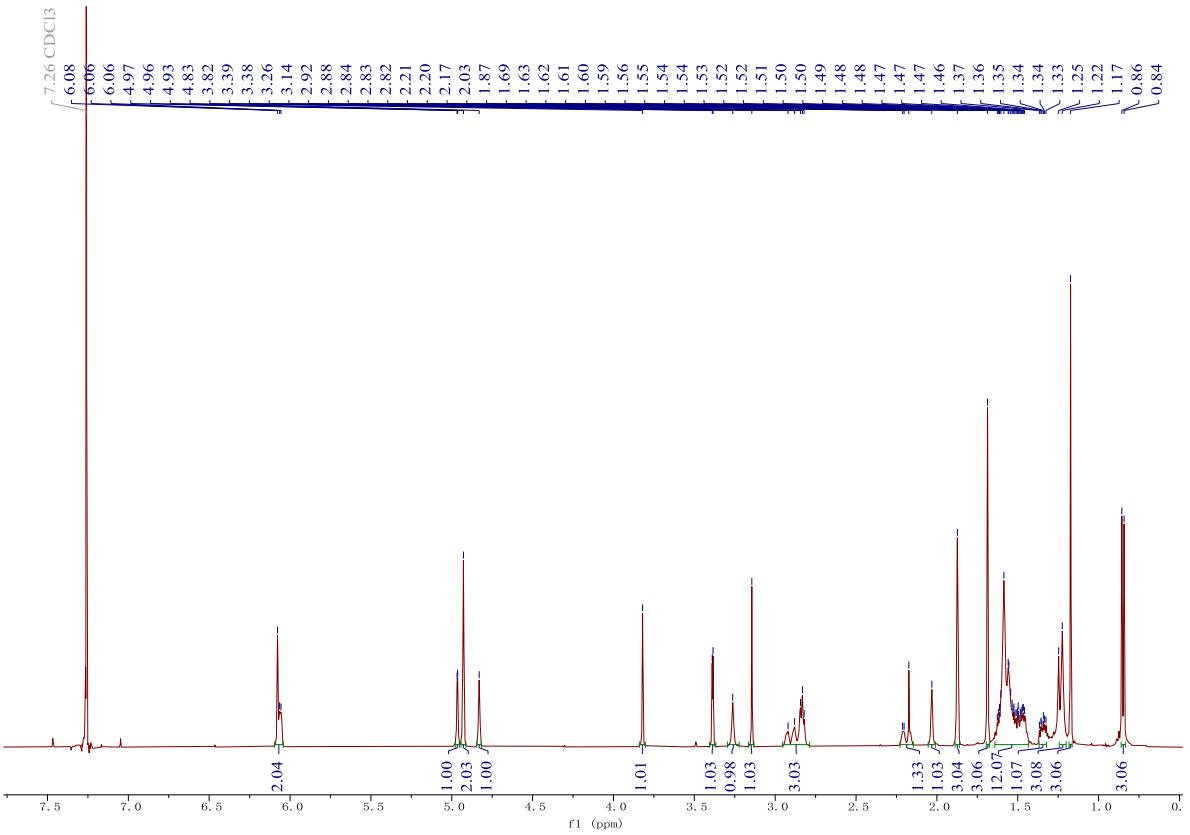


Figure S149. ^{13}C NMR spectrum of synthetic compound **3** at 125 MHz in $CDCl_3$

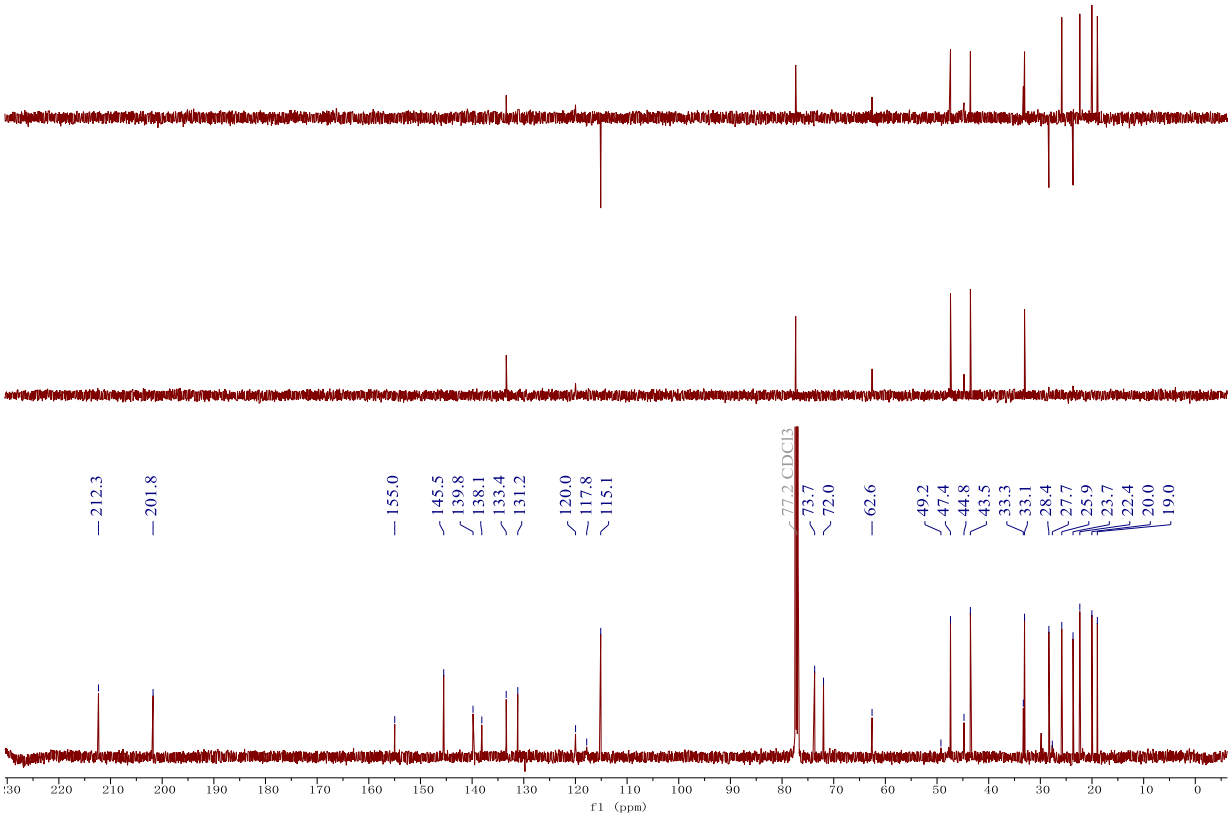


Figure S150. HRESIMS spectrum of synthetic compound **3**

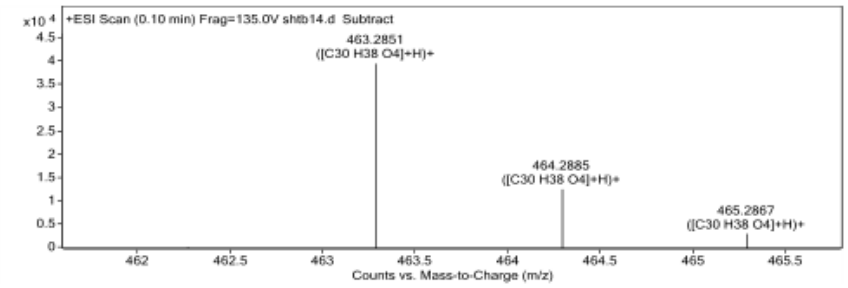
Qualitative Analysis Report

Data Filename	shtb14.d	**Sample Name**	shtb14
Sample Type	Sample	**Position**	P1-C4
Instrument Name	Instrument 1	**User Name**	
Acq Method	s.m	**Acquired Time**	5/27/2021 10:18:57 AM
IRM Calibration Status	Success	**DA Method**	Default.m
Comment			

Sample Group	**Info.**
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125.2)

User Spectra

Fragmentor Voltage	**Collision Energy**	**Ionization Mode**
135	0	ESI



Peak List

m/z	z	Abund	Formula	Ion
102.1281	1	32308.78		
231.1386	1	15034.2		
463.2851	1	39614.18	C30 H38 O4	(M+H)+
464.2885	1	12757.97	C30 H38 O4	(M+H)+
485.2664	1	18819.94		
499.2459	1	12707.11		
501.26	1	12569.34		
503.242	1	10023.2		
947.5459	1	24588.47		
948.5489	1	16004.7		

Formula Calculator Element Limits

Element	Min	Max
C	3	60
H	0	120
O	0	30

Formula Calculator Results

Formula	CalculatedMass	CalculatedMz	Mz	Diff. (mDa)	Diff. (ppm)	DBE
C30 H38 O4	462.2770	463.2843	463.2851	-0.80	-1.73	12.0000

--- End Of Report ---

Figure S151. Specific rotation spectrum of synthetic compound **3**

Rudolph Research Analytical

This sample was measured on an Autopol VI, Serial #91058
Manufactured by Rudolph Research Analytical, Hackettstown, NJ, USA.

Measurement Date : Friday, 11-JUN-2021

Set Temperature : 24.3

Time Delay : Disabled

Delay between Measurement : Disabled

n	Average	Std.Dev.	% RSD	Maximum	Minimum
5	52.57	0.14	0.26	52.78	52.38

S.No	Sample ID	Time	Result	Scale	OR °Arc	WLG.nm	Lg.mm	Conc.g/100ml	Temp.
1	shtb14	12:37:24 PM	52.58	SR	0.0794	589	100.00	0.151	24.5
2	shtb14	12:37:33 PM	52.58	SR	0.0794	589	100.00	0.151	24.5
3	shtb14	12:37:40 PM	52.38	SR	0.0791	589	100.00	0.151	24.5
4	shtb14	12:37:49 PM	52.52	SR	0.0793	589	100.00	0.151	24.4
5	shtb14	12:37:57 PM	52.78	SR	0.0797	589	100.00	0.151	24.4

Figure S152. ^{1}H NMR spectrum of synthetic compound **5** at 500 MHz in $CDCl_3$

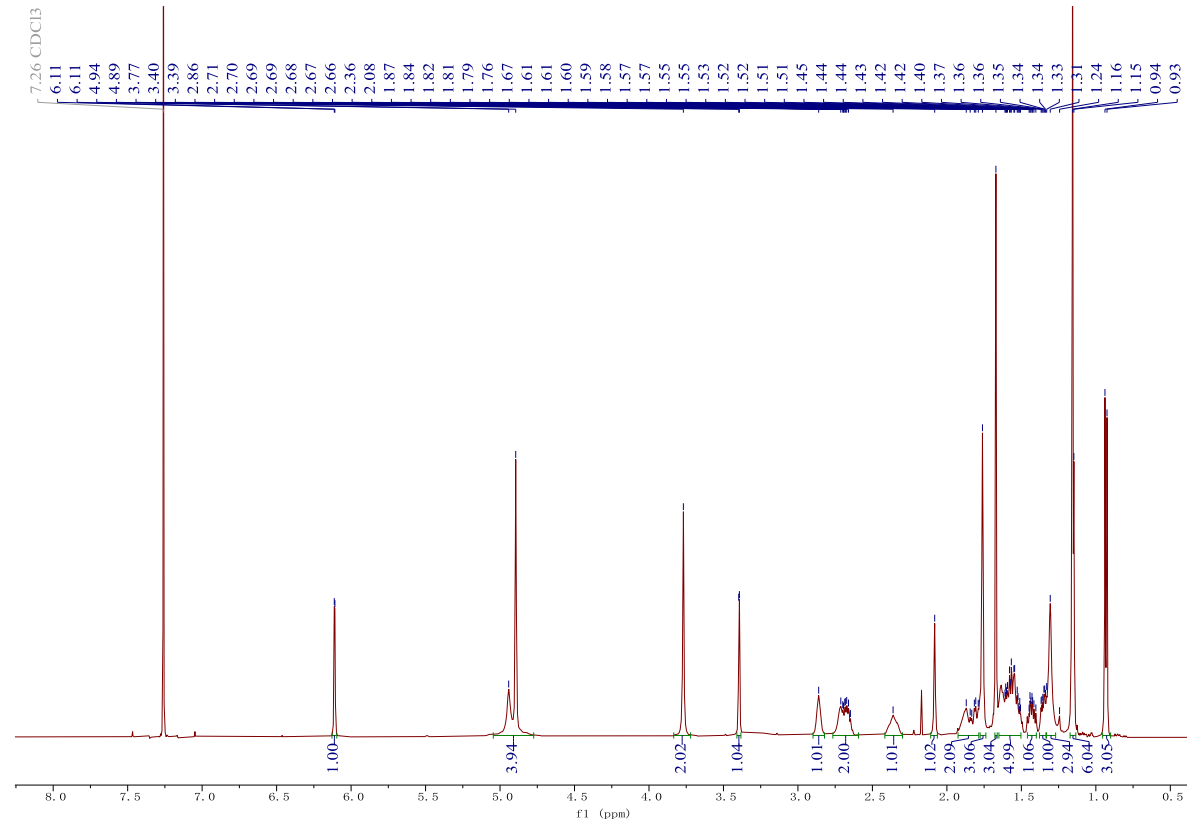


Figure S153. ^{13}C NMR spectrum of synthetic compound **5** at 125 MHz in $CDCl_3$

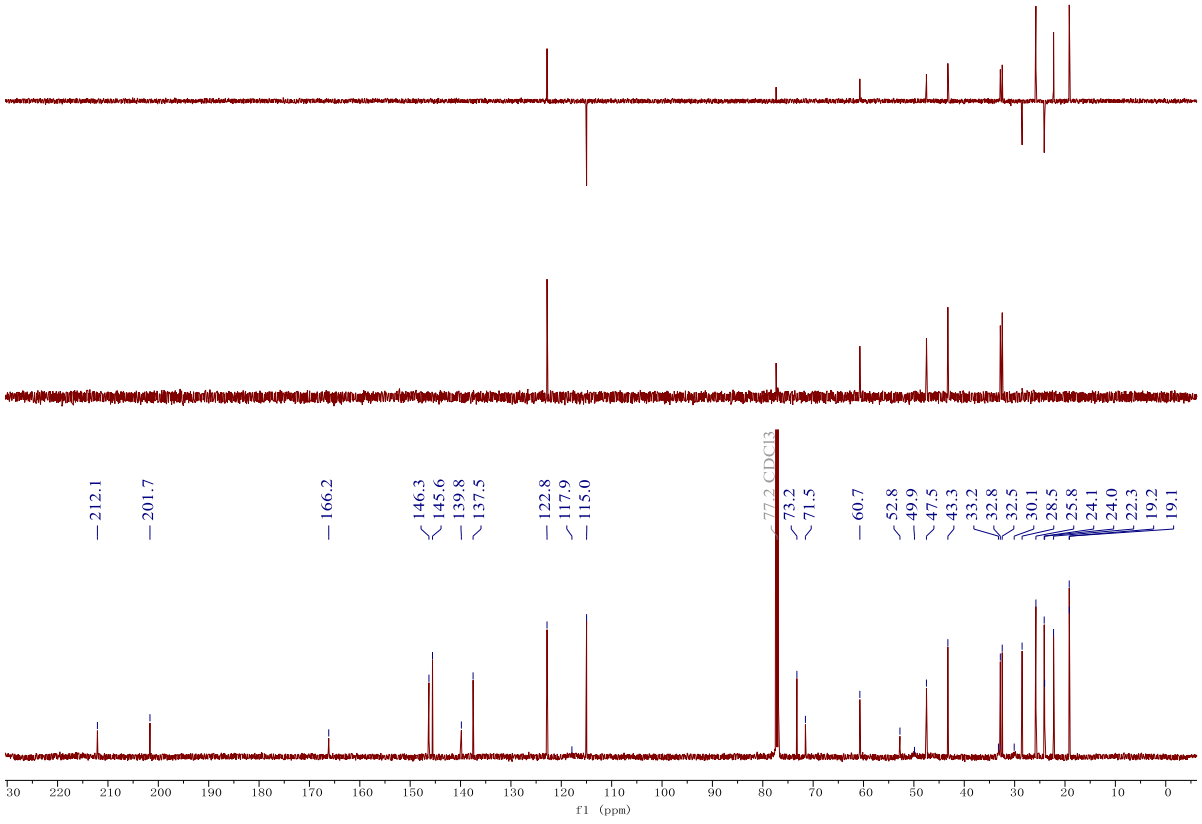


Figure S154. HRESIMS spectrum of synthetic compound **5**

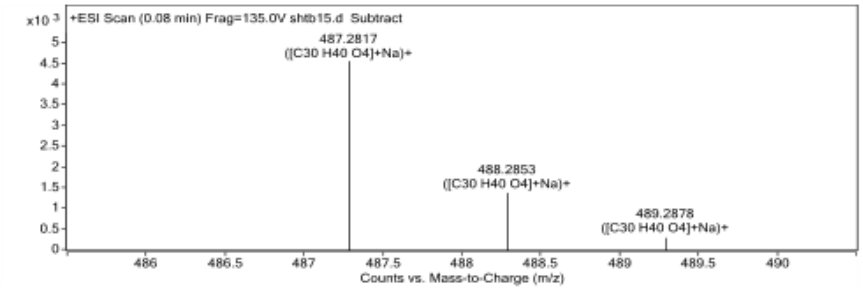
Qualitative Analysis Report

Data Filename	shtb15.d	**Sample Name**	shtb15
Sample Type	Sample	**Position**	P1-C5
Instrument Name	Instrument 1	**User Name**	
Acq Method	s.m	**Acquired Time**	5/27/2021 10:20:08 AM
IRM Calibration Status	Success	**DA Method**	Default.m
Comment			

Sample Group	**Info.**
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125.2)

User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
135	0	ESI



Peak List

m/z	z	Abund	Formula	Ion
215.1414		666.73		
233.1541	1	2142.03		
447.2909	1	858.46		
487.2817	1	4562.21	C30 H40 O4	(M+Na)+
488.2853	1	1385.87	C30 H40 O4	(M+Na)+
503.2567	1	1525.91		
504.2604	1	692.84		
951.5775	1	4427.96		
952.5792	1	2614.72		
953.5854	1	1322.34		

Formula Calculator Element Limits

Element	Min	Max
C	3	60
H	0	120
O	0	30

Formula Calculator Results

Formula	CalculatedMass	CalculatedMz	Mz	Diff. (mDa)	Diff. (ppm)	DBE
C30 H40 O4	464.2927	487.2819	487.2817	0.20	0.41	11.0000

--- End Of Report ---

Figure S155. Specific rotation spectrum of synthetic compound **5**

Rudolph Research Analytical

This sample was measured on an Autopol VI, Serial #91058
Manufactured by Rudolph Research Analytical, Hackettstown, NJ, USA.

Measurement Date : Friday, 11-JUN-2021

Set Temperature : 24.3

Time Delay : Disabled

Delay between Measurement : Disabled

n	Average	Std.Dev.	% RSD	Maximum	Minimum
5	-77.61	0.43	-0.55	-77.16	-78.28

S.No	Sample ID	Time	Result	Scale	OR °Arc	WLG.nm	Lg.mm	Conc.g/100ml	Temp.
1	shtb15	12:18:48 PM	-78.28	SR	-0.0908	589	100.00	0.116	24.9
2	shtb15	12:18:57 PM	-77.59	SR	-0.0900	589	100.00	0.116	24.8
3	shtb15	12:19:05 PM	-77.67	SR	-0.0901	589	100.00	0.116	24.7
4	shtb15	12:19:13 PM	-77.33	SR	-0.0897	589	100.00	0.116	24.6
5	shtb15	12:19:29 PM	-77.16	SR	-0.0895	589	100.00	0.116	24.4

Figure S156. ^{1}H NMR spectrum of **26** at 500 MHz in $CDCl_3$

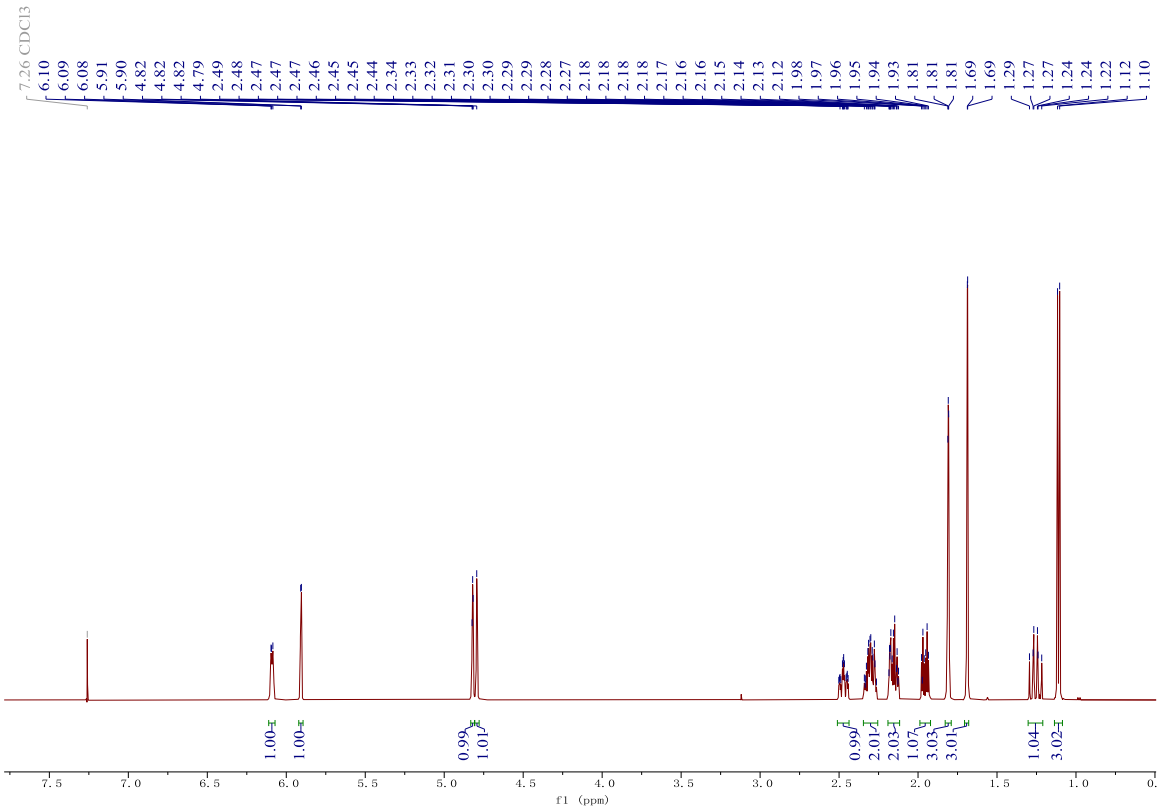


Figure S157. ^{13}C NMR spectrum of **26** at 125 MHz in $CDCl_3$

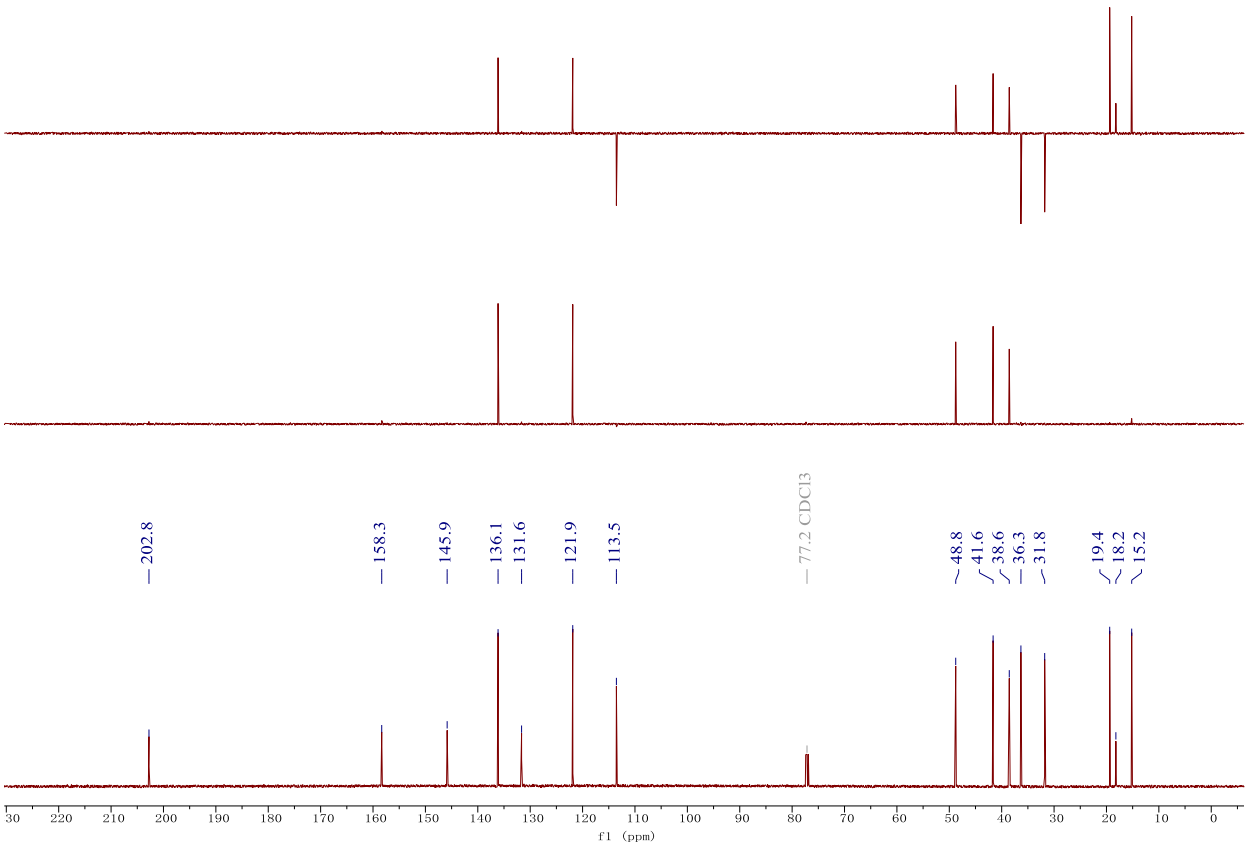


Figure S158. HRESIMS spectrum of **26**

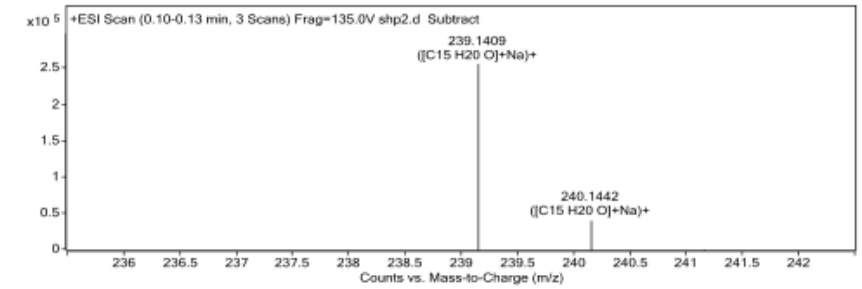
Qualitative Analysis Report

Data Filename	shp2.d	**Sample Name**	shp2
Sample Type	Sample	**Position**	P1-A5
Instrument Name	Instrument 1	**User Name**	
Acq Method	s.m	**Acquired Time**	5/12/2021 3:37:13 PM
IRM Calibration Status	Success	**DA Method**	Default.m
Comment			

Sample Group	**Info.**
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125.2)

User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
135	0	ESI



Peak List

m/z	z	Abund	Formula	Ion
217.1587	1	141091.55		
218.1621	1	21561.99		
239.1409	1	256430.16	C15 H20 O	(M+Na)+
240.1442	1	41766.03	C15 H20 O	(M+Na)+
255.1148	1	8835.31		
273.1441	1	8219.4		
303.1561		6913.2		
455.2928	1	165955.83		
456.2962	1	50895.74		
457.2997	1	9318.5		

Formula Calculator Element Limits

Element	Min	Max
C	3	60
H	0	120
O	0	30

Formula Calculator Results

Formula	CalculatedMass	CalculatedMz	Mz	Diff. (mDa)	Diff. (ppm)	DBE
C15 H20 O	216.1514	239.1406	239.1409	-0.30	-1.25	6.0000

--- End Of Report ---

Figure S159. Specific rotation spectrum of **26**

Rudolph Research Analytical

This sample was measured on an Autopol VI, Serial #91058
Manufactured by Rudolph Research Analytical, Hackettstown, NJ, USA.

Measurement Date : Tuesday, 25-MAY-2021

Set Temperature : OFF

Time Delay : Disabled

Delay between Measurement : Disabled

n	Average	Std.Dev.	% RSD	Maximum	Minimum
5	-8.03	0.53	-6.60	-7.54	-8.77

S.No	Sample ID	Time	Result	Scale	OR °Arc	WLG.nm	Lg.mm	Conc.g/100ml	Temp.
1	SHP2	03:54:08 PM	-8.77	SR	-0.0114	589	100.00	0.130	27.1
2	SHP2	03:54:17 PM	-7.85	SR	-0.0102	589	100.00	0.130	27.1
3	SHP2	03:54:25 PM	-8.38	SR	-0.0109	589	100.00	0.130	27.1
4	SHP2	03:54:34 PM	-7.54	SR	-0.0098	589	100.00	0.130	27.0
5	SHP2	03:54:41 PM	-7.62	SR	-0.0099	589	100.00	0.130	27.0

Figure S160. ^{1}H NMR spectrum of **27** at 500 MHz in $CDCl_3$

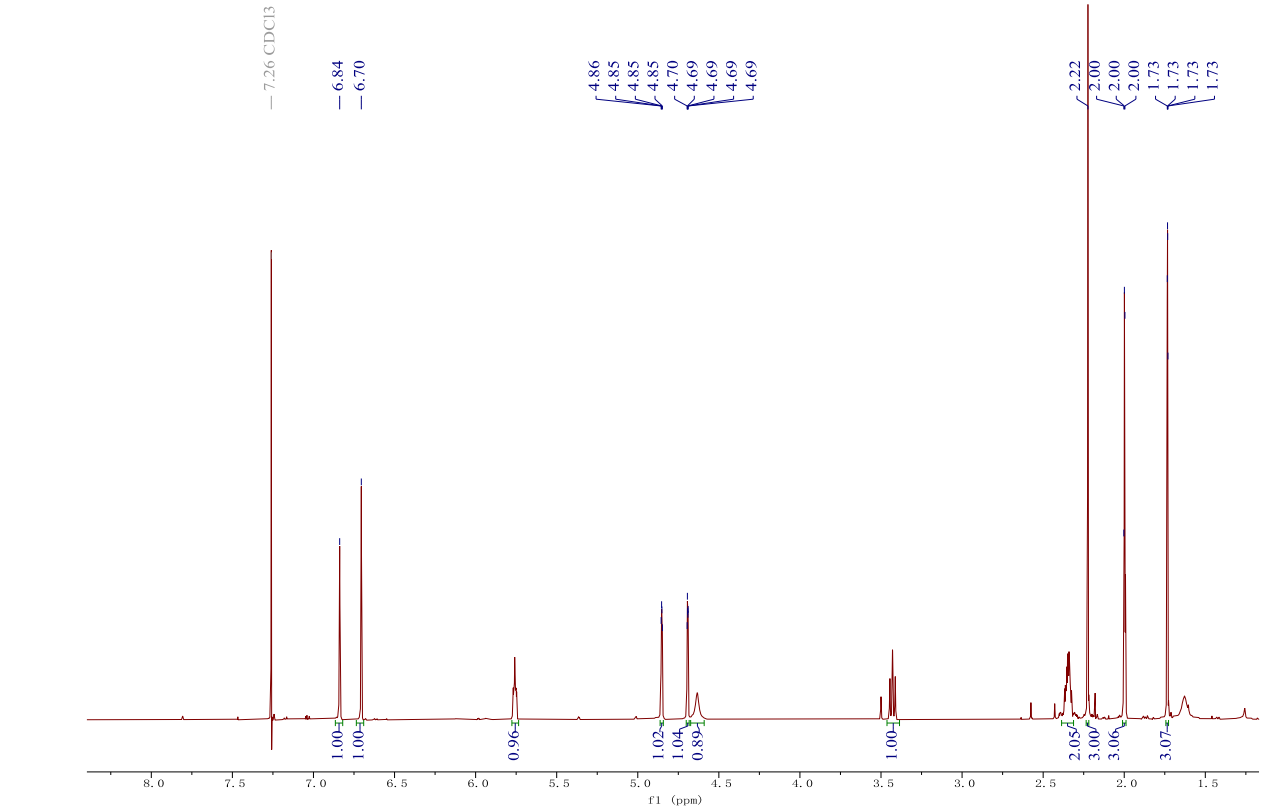


Figure S161. ^{13}C NMR spectrum of **27** at 125 MHz in $CDCl_3$

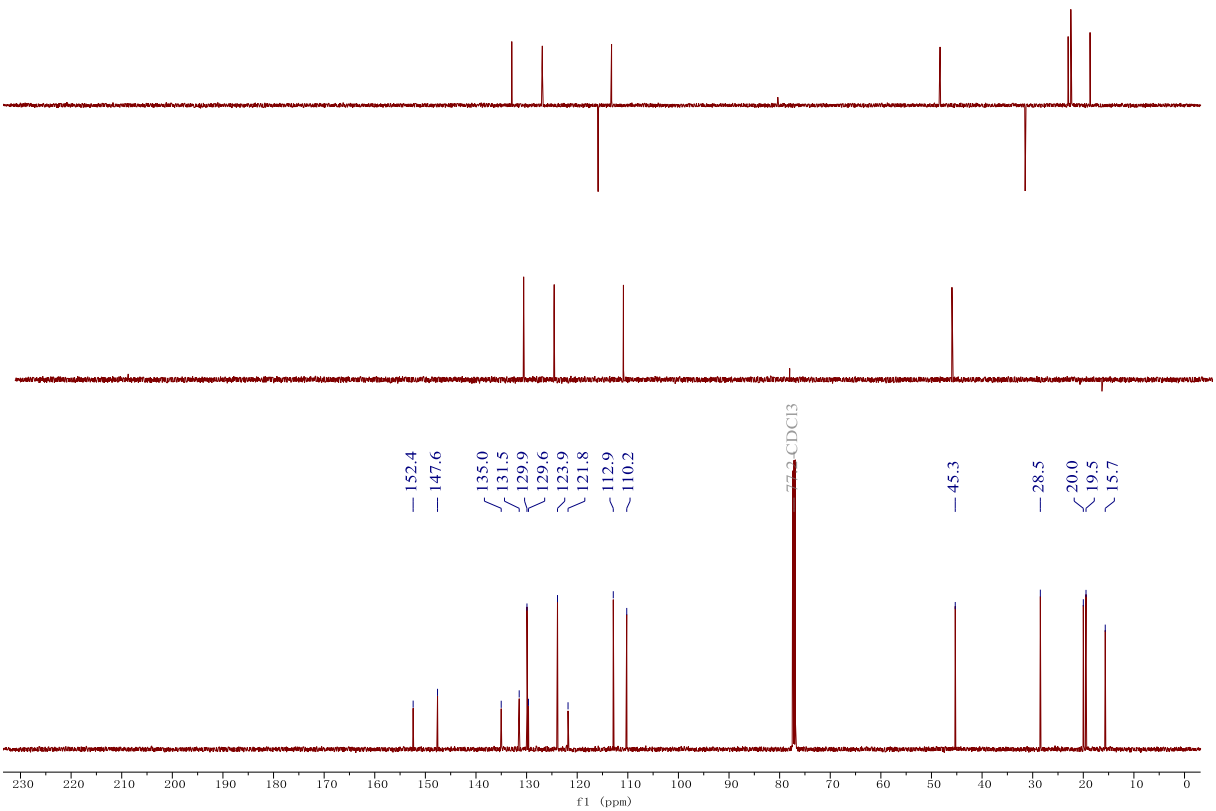


Figure S162. HRESIMS spectrum of **27**

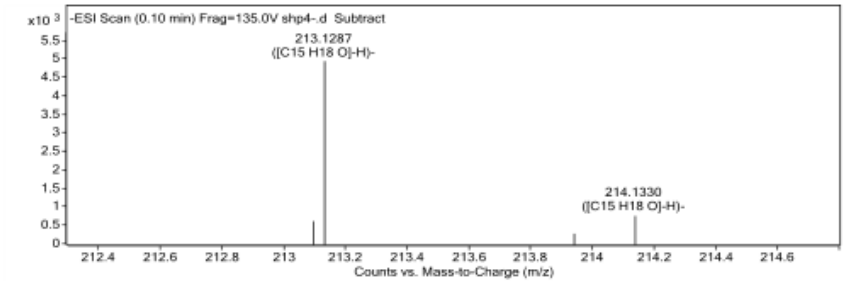
Qualitative Analysis Report

Data Filename	shp4-.d	**Sample Name**	shp4
Sample Type	Sample	**Position**	P1-A9
Instrument Name	Instrument 1	**User Name**	
Acq Method	s-.m	**Acquired Time**	5/12/2021 3:47:39 PM
IRM Calibration Status	Success	**DA Method**	Default.m
Comment			

Sample Group	**Info.**
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125.2)

User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
135	0	ESI



Peak List

m/z	z	Abund
215.1439	1	36085.23
216.1472	1	6438.84
247.1345	1	5443.9
339.2328	1	5829.52
429.2803	1	60833.18
430.2834	1	18489.7
443.2955	1	31056.43
444.2984	1	9659.97
966.0007	1	21325
1033.9882		9037.06

Formula Calculator Element Limits

Element	Min	Max
C	3	60
H	0	120
O	0	30

Formula Calculator Results

Formula	CalculatedMass	CalculatedMz	Mz	Diff. (mDa)	Diff. (ppm)	DBE
C15 H18 O	214.1358	213.1285	213.1287	-0.20	-0.94	7.0000

--- End Of Report ---

Figure S163. Specific rotation spectrum of **27**

Rudolph Research Analytical

This sample was measured on an Autopol VI, Serial #91058
Manufactured by Rudolph Research Analytical, Hackettstown, NJ, USA.

Measurement Date : Friday, 11-JUN-2021

Set Temperature : OFF

Time Delay : Disabled

Delay between Measurement : Disabled

n	Average	Std.Dev.	% RSD	Maximum	Minimum
5	125.26	0.40	0.31	125.58	124.65

S.No	Sample ID	Time	Result	Scale	OR °Arc	WLG.nm	Lg.mm	Conc.g/100ml	Temp.
1	shp6	04:41:47 PM	125.04	SR	0.1613	589	100.00	0.129	25.1
2	shp6	04:41:55 PM	125.58	SR	0.1620	589	100.00	0.129	25.0
3	shp6	04:42:03 PM	125.43	SR	0.1618	589	100.00	0.129	24.9
4	shp6	04:42:11 PM	124.65	SR	0.1608	589	100.00	0.129	24.9
5	shp6	04:42:20 PM	125.58	SR	0.1620	589	100.00	0.129	24.8

Figure S164. ^{1}H NMR spectrum of **28a** at 600 MHz in $CDCl_3$

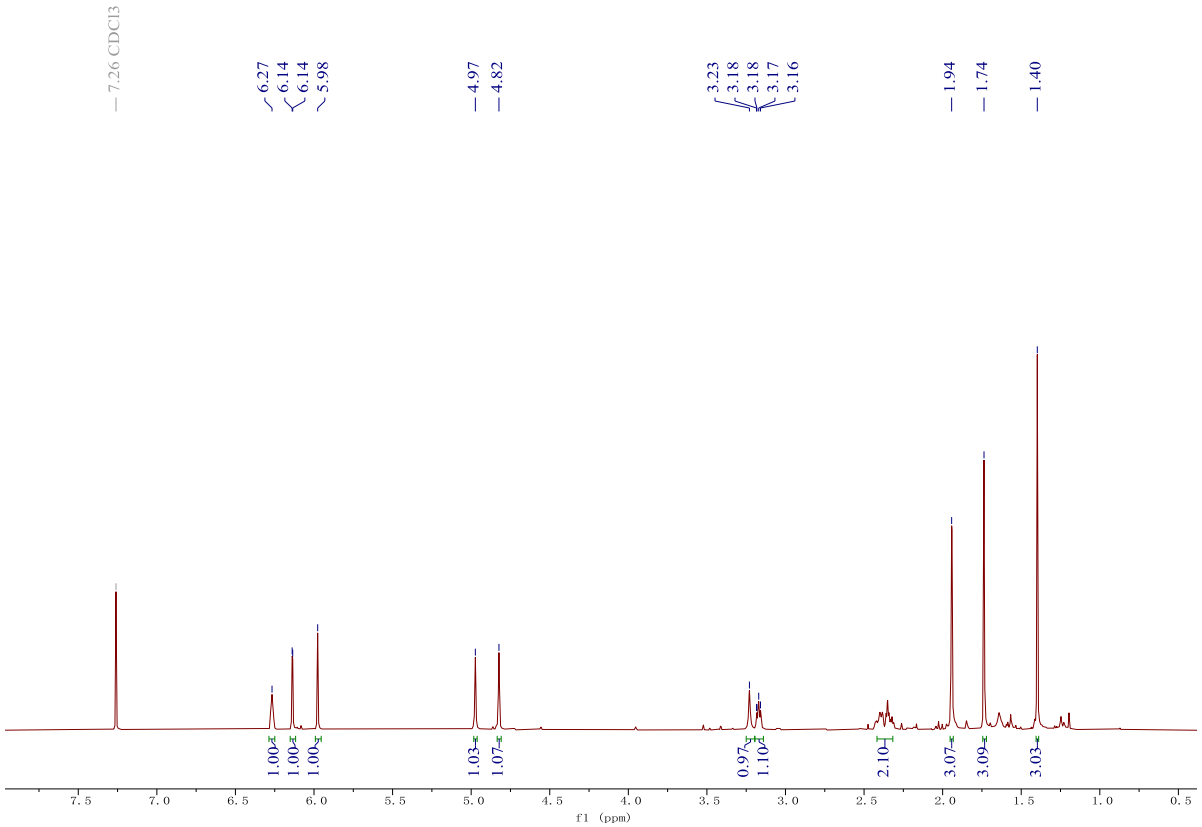


Figure S165. ^{13}C NMR spectrum of **28a** at 150 MHz in $CDCl_3$

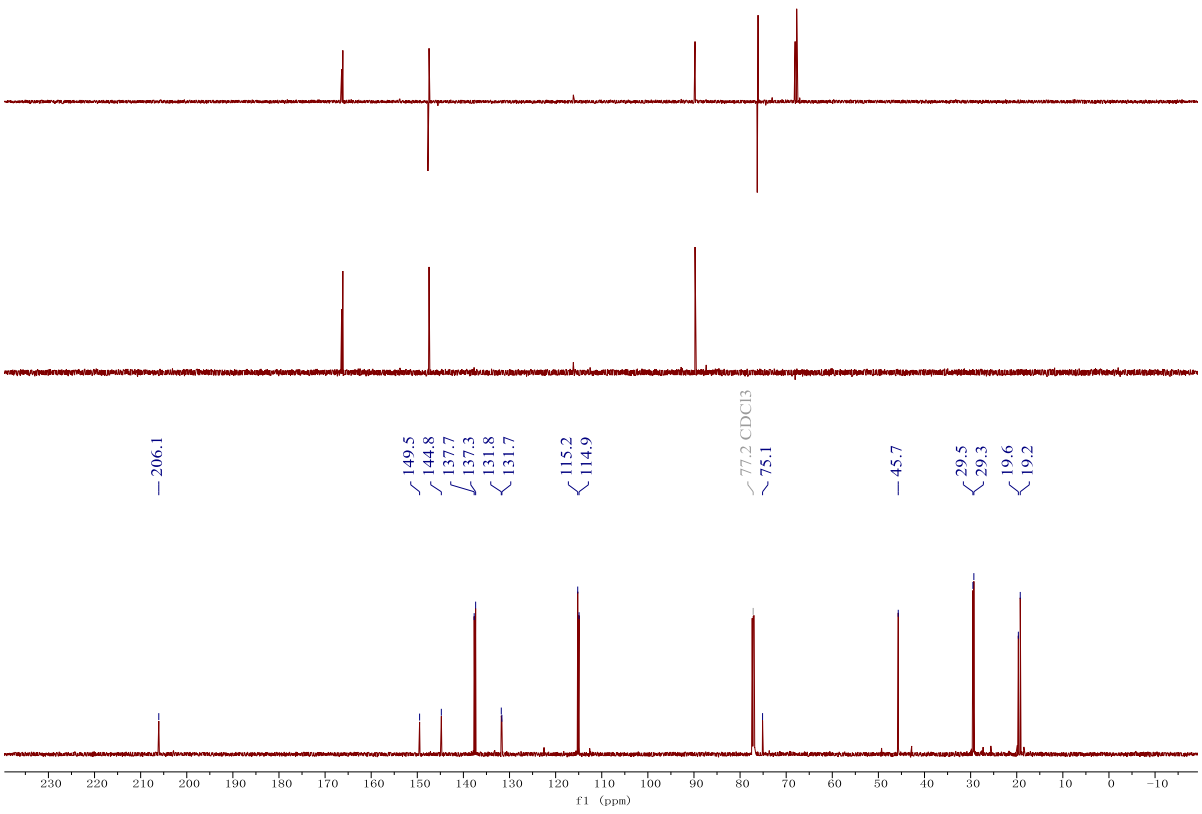


Figure S166. HRESIMS spectrum of **28a**

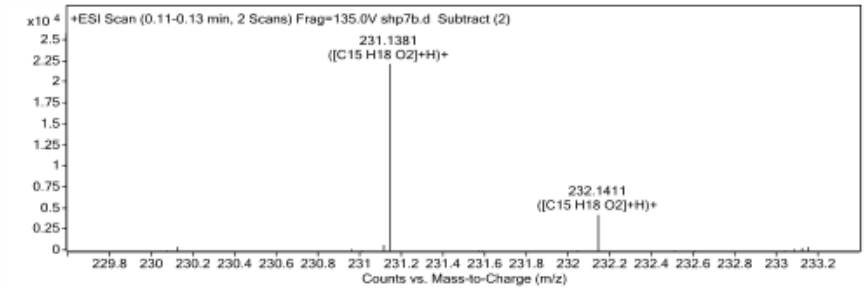
Qualitative Analysis Report

Data Filename	shp7b.d	**Sample Name**	shp7b
Sample Type	Sample	**Position**	P1-A2
Instrument Name	Instrument 1	**User Name**	
Acq Method	s.m	**Acquired Time**	6/4/2021 9:22:06 AM
IRM Calibration Status	Success	**DA Method**	Default.m
Comment			

Sample Group	**Info.**
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125.2)

User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
135	0	ESI



Peak List

m/z	z	Abund	Formula	Ion
72.0811		10404.87		
104.107	1	9783.29		
118.0864		9216.73		
144.0654		5273.05		
155.5593		4902.52		
163.0754	1	9277.79		
175.1188	1	11952.21		
231.1381	1	22220.95	C15 H18 O2	(M+H)+
253.12	1	11883.09		
269.1116	1	5762.61		

Formula Calculator Element Limits

Element	Min	Max
C	3	60
H	0	120
O	0	30

Formula Calculator Results

Formula	CalculatedMass	CalculatedMz	Mz	Diff. (mDa)	Diff. (ppm)	DBE
C15 H18 O2	230.1307	231.1380	231.1381	-0.10	-0.43	7.0000

--- End Of Report ---

Figure S167. Specific rotation spectrum of **28a**

Rudolph Research Analytical

This sample was measured on an Autopol VI, Serial #91058
Manufactured by Rudolph Research Analytical, Hackettstown, NJ, USA.

Measurement Date : Thursday, 03-JUN-2021

Set Temperature : OFF

Time Delay : Disabled

Delay between Measurement : Disabled

n	Average	Std.Dev.	% RSD	Maximum	Minimum
5	-77.01	1.73	-2.24	-75.37	-79.17

S.No	Sample ID	Time	Result	Scale	OR °Arc	WLG.nm	Lg.mm	Conc.g/100ml	Temp.
1	shp7b	11:26:42 AM	-79.17	SR	-0.0958	589	100.00	0.121	28.3
2	shp7b	11:27:00 AM	-76.61	SR	-0.0927	589	100.00	0.121	28.3
3	shp7b	11:27:08 AM	-75.45	SR	-0.0913	589	100.00	0.121	28.4
4	shp7b	11:27:16 AM	-75.37	SR	-0.0912	589	100.00	0.121	28.4
5	shp7b	11:27:25 AM	-78.43	SR	-0.0949	589	100.00	0.121	28.4

Figure S168. ^{1}H NMR spectrum of **28b** at 600 MHz in $CDCl_3$

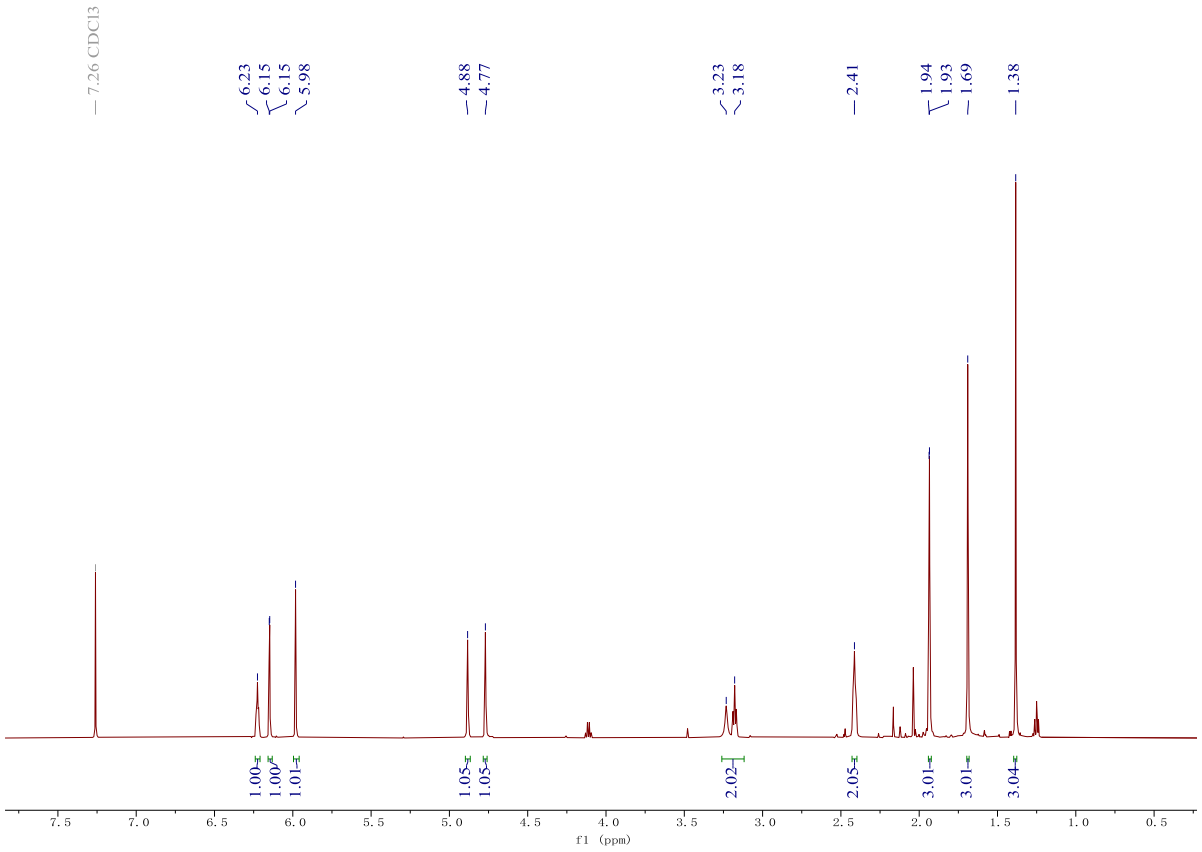


Figure S169. ^{13}C NMR spectrum of **28b** at 150 MHz in $CDCl_3$

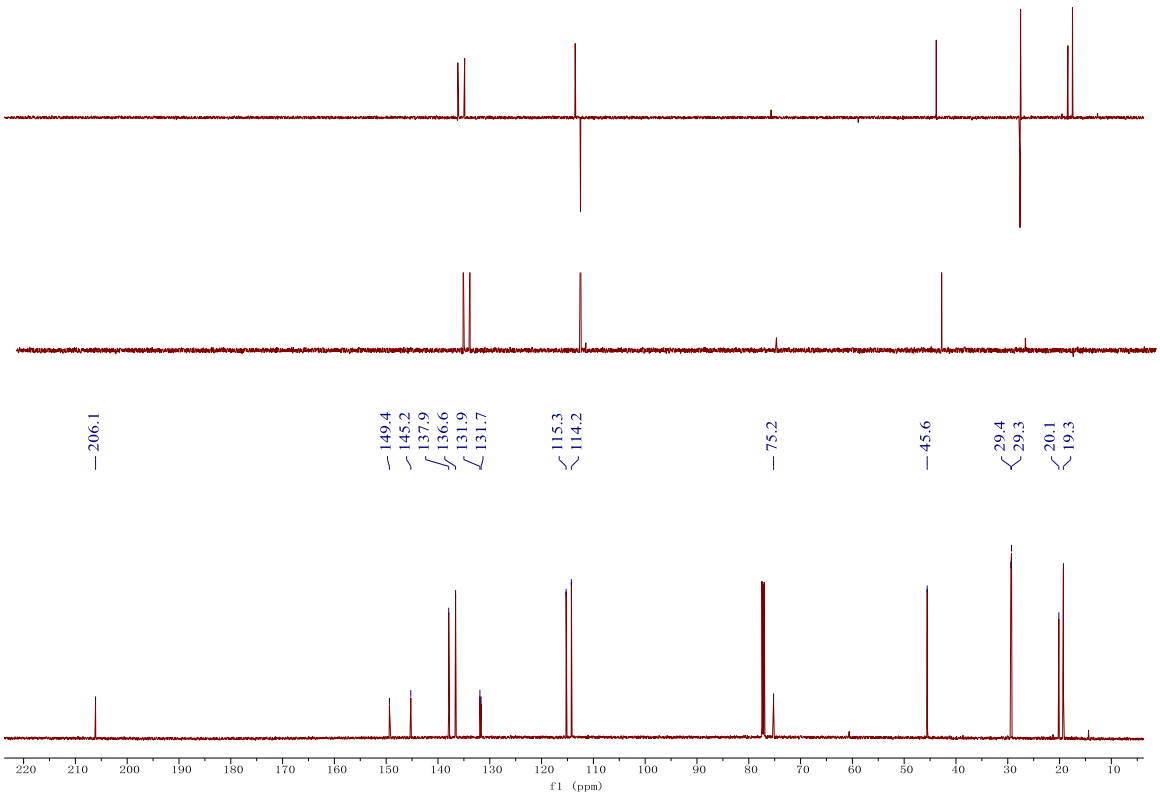


Figure S170. HRESIMS spectrum of **28b**

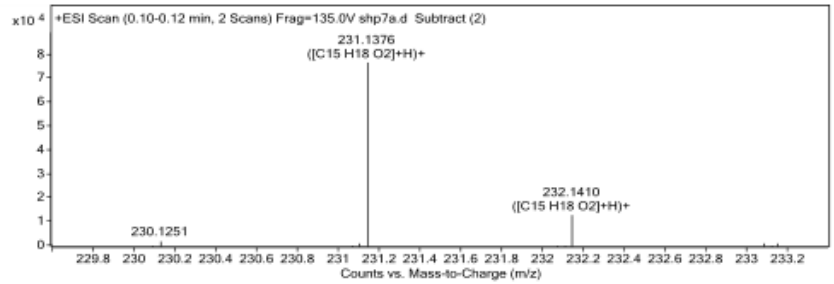
Qualitative Analysis Report

Data Filename	shp7a.d	**Sample Name**	shp7a
Sample Type	Sample	**Position**	P1-A1
Instrument Name	Instrument 1	**User Name**	
Acq Method	s.m	**Acquired Time**	6/4/2021 9:20:56 AM
IRM Calibration Status	Success	**DA Method**	Default.m
Comment			

Sample Group	**Info.**
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125.2)

User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
135	0	ESI



Peak List

m/z	z	Abund	Formula	Ion
102.1274		14148.42		
155.559	2	12716.71		
163.0752	1	45346.76		
229.1219	1	13611.36		
231.1376	1	76772.73	C15 H18 O2	(M+H)+
232.141	1	12997.43	C15 H18 O2	(M+H)+
245.1169	1	17360.4		
247.1323	1	26164.88		
253.1196	1	18992.63		
269.1145	1	22952.02		

Formula Calculator Element Limits

Element	Min	Max
C	3	60
H	0	120
O	0	30

Formula Calculator Results

Formula	CalculatedMass	CalculatedMz	Mz	Diff. (mDa)	Diff. (ppm)	DBE
C15 H18 O2	230.1307	231.1380	231.1376	0.40	1.73	7.0000

--- End Of Report ---

Figure S171. Specific rotation spectrum of **28b**

Rudolph Research Analytical

This sample was measured on an Autopol VI, Serial #91058
Manufactured by Rudolph Research Analytical, Hackettstown, NJ, USA.

Measurement Date : Thursday, 03-JUN-2021

Set Temperature : OFF

Time Delay : Disabled

Delay between Measurement : Disabled

n	Average	Std.Dev.	% RSD	Maximum	Minimum
5	15.17	2.33	15.35	17.95	12.38

S.No	Sample ID	Time	Result	Scale	OR °Arc	WLG.nm	Lg.mm	Conc.g/100ml	Temp.
1	shp7a	11:18:29 AM	13.20	SR	0.0161	589	100.00	0.122	28.3
2	shp7a	11:18:37 AM	12.38	SR	0.0151	589	100.00	0.122	28.3
3	shp7a	11:18:45 AM	15.74	SR	0.0192	589	100.00	0.122	28.3
4	shp7a	11:18:53 AM	16.56	SR	0.0202	589	100.00	0.122	28.3
5	shp7a	11:19:01 AM	17.95	SR	0.0219	589	100.00	0.122	28.3

Figure S172. ^{1}H NMR spectrum of **29** at 500 MHz in $CDCl_3$

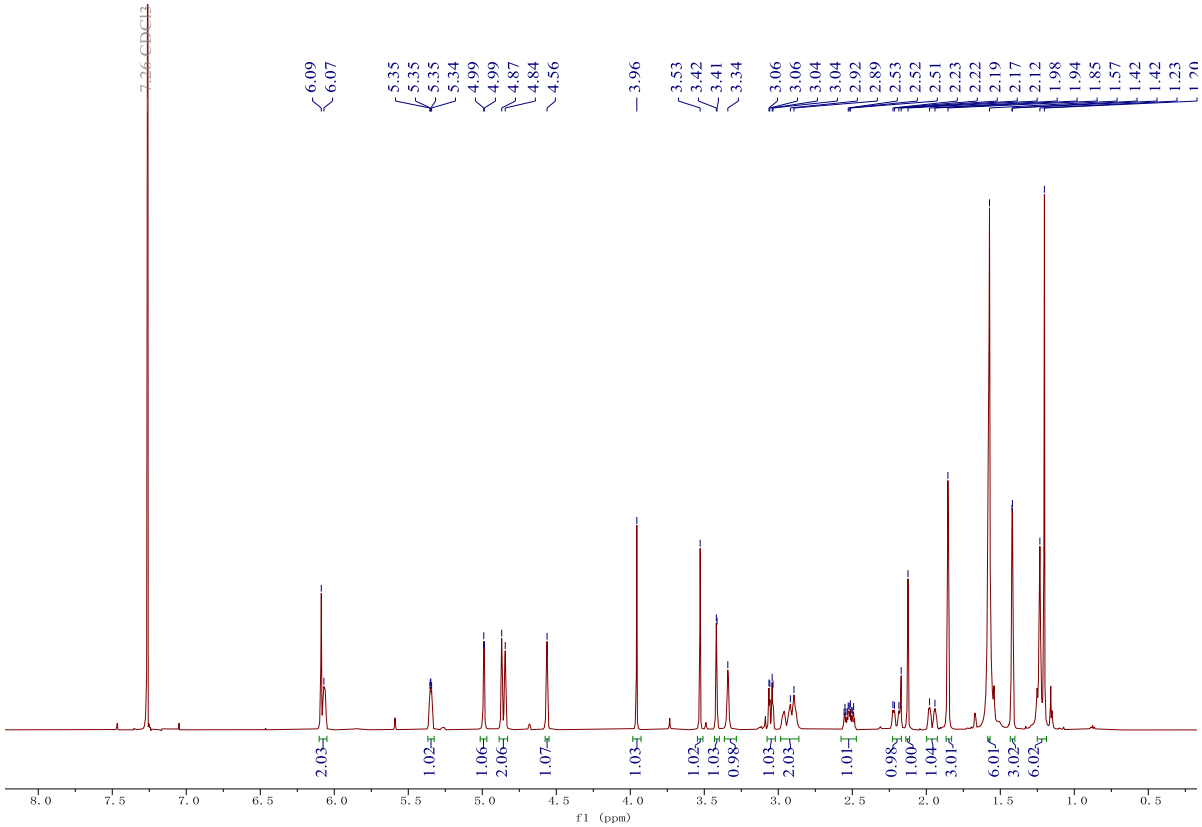


Figure S173. ^{13}C NMR spectrum of **29** at 125 MHz in $CDCl_3$

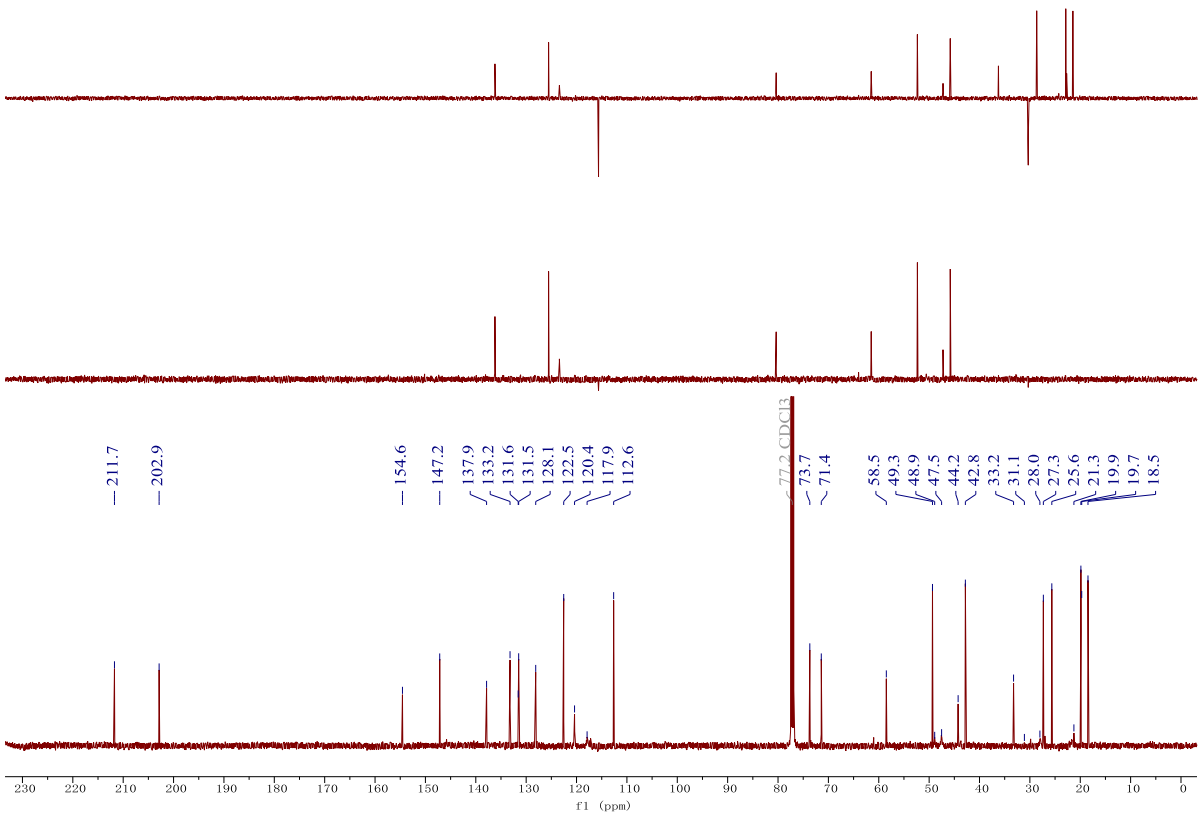


Figure S174. HRESIMS spectrum of **29**

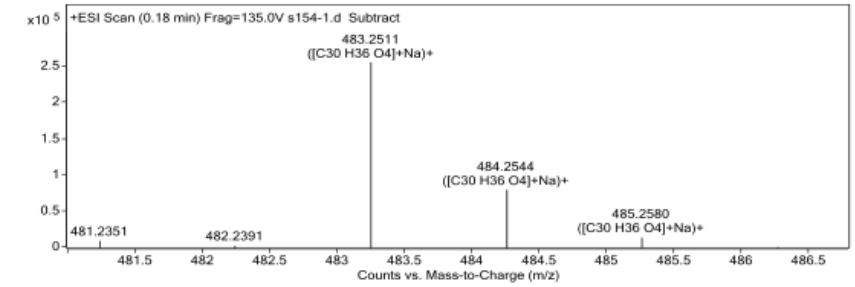
Qualitative Analysis Report

Data Filename	s154-1.d	**Sample Name**	s154-1
Sample Type	Sample	**Position**	P1-A1
Instrument Name	Instrument 1	**User Name**	
Acq Method	s.m	**Acquired Time**	11/20/2020 2:17:26 PM
IRM Calibration Status	Success	**DA Method**	Default.m
Comment			

Sample Group	**Info.**
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125.2)

User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
135	0	ESI



Peak List

m/z	z	Abund	Formula	Ion
461.2687	1	107238.28		
483.2511	1	256065.83	C30 H36 O4	(M+Na)+
484.2544	1	79954.2	C30 H36 O4	(M+Na)+
506.3266	1	73184.49		
515.2407	1	46678.7		
943.5132	1	246545.83		
944.5168	1	152572.84		
945.5197	1	54517.58		
975.5026	1	75027.11		
976.5055	1	50363.91		

Formula Calculator Element Limits

Element	Min	Max
C	3	60
H	0	120
O	0	30

Formula Calculator Results

Formula	CalculatedMass	CalculatedMz	Mz	Diff. (mDa)	Diff. (ppm)	DBE
C30 H36 O4	460.2614	483.2506	483.2511	-0.50	-1.03	13.0000

--- End Of Report ---

Figure S175. Specific rotation spectrum of **29**

Rudolph Research Analytical

This sample was measured on an Autopol VI, Serial #91058
Manufactured by Rudolph Research Analytical, Hackettstown, NJ, USA.

Measurement Date : Friday, 11-JUN-2021

Set Temperature : OFF

Time Delay : Disabled

Delay between Measurement : Disabled

n	Average	Std.Dev.	% RSD	Maximum	Minimum
5	-20.86	14.49	-69.46	5.00	-28.33

S.No	Sample ID	Time	Result	Scale	OR °Arc	WLG.nm	Lg.mm	Conc.g/100ml	Temp.
1	shp8	04:35:03 PM	-27.38	SR	-0.0115	589	100.00	0.042	26.9
2	shp8	04:35:11 PM	-27.86	SR	-0.0117	589	100.00	0.042	26.9
3	shp8	04:35:20 PM	-28.33	SR	-0.0119	589	100.00	0.042	26.9
4	shp8	04:35:27 PM	-25.71	SR	-0.0108	589	100.00	0.042	26.9
5	shp8	04:35:46 PM	5.00	SR	0.0021	589	100.00	0.042	26.8

Figure S176. ^{1}H NMR spectrum of **6** at 500 MHz in pyridine-d_5

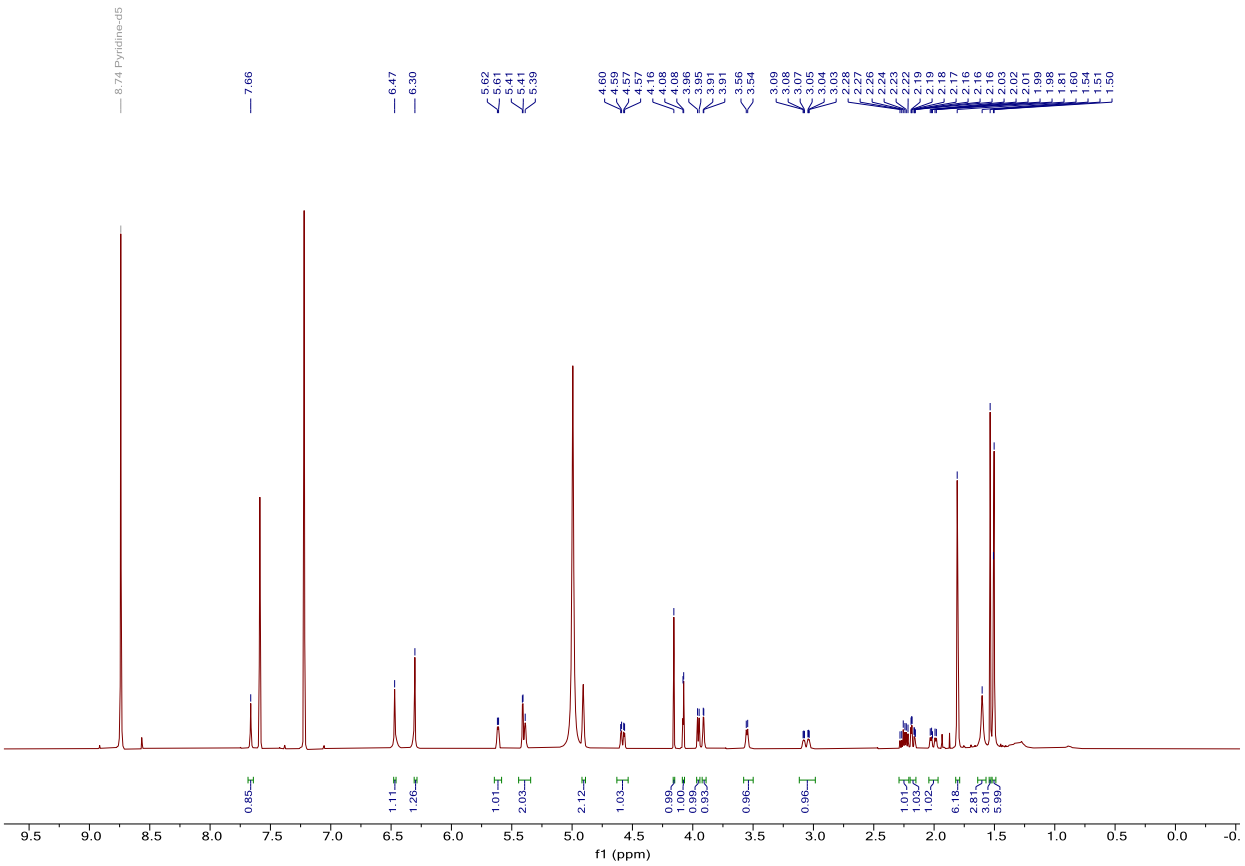


Figure S177. ^{13}C NMR spectrum of **6** at 125 MHz in pyridine-d_5

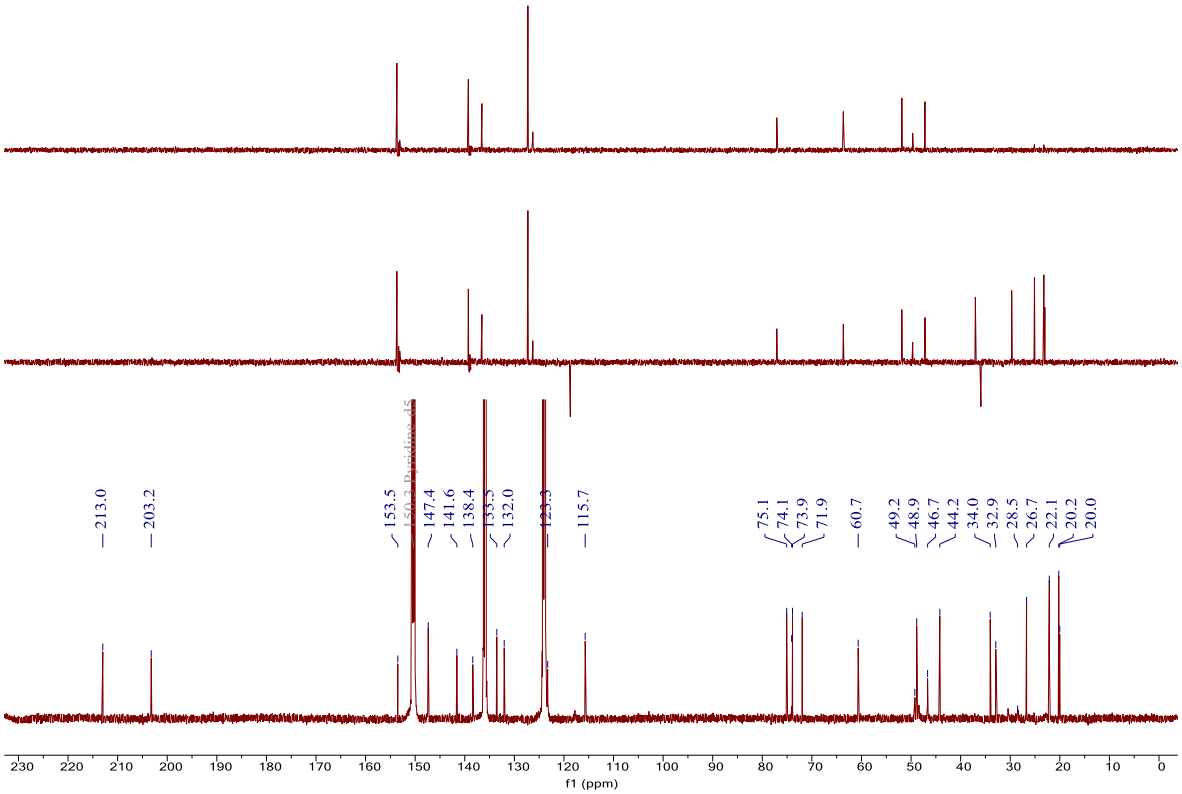


Figure S178. HRESIMS spectrum of **6**

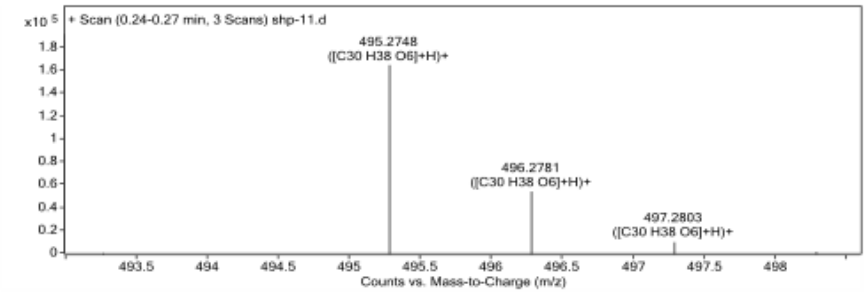
Qualitative Analysis Report

Data Filename	shp-11.d	**Sample Name**	shp-11
Sample Type	Sample	**Position**	P1-D6
Instrument Name	Instrument 1	**User Name**	
Acq Method	s.m	**Acquired Time**	6/18/2021 2:28:15 PM
IRM Calibration Status	Success	**DA Method**	ZRR3.m
Comment			

Sample Group	**Info.**
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125.2)

User Spectra

Fragmentor Voltage	**Collision Energy**	**Ionization Mode**
175	0	ESI



Peak List

m/z	z	Abund	Formula	Ion
311.1071	1	229795.67		
327.1388	1	1893224.38		
328.1408	1	335251.09		
329.1391	1	103565.76		
349.1206	1	439125.16		
350.1226	1	78041.04		
459.253	1	72792.4		
495.2748	1	164654.55	C30 H38 O6	(M+H)+
675.2549	1	364546.84		
676.2567	1	130709.02		

Formula Calculator Element Limits

Element	Min	Max
C	3	60
H	0	120
O	0	30

Formula Calculator Results

Formula	CalculatedMass	CalculatedMz	Mz	Diff. (mDa)	Diff. (ppm)	DBE
C30 H38 O6	494.2668	495.2741	495.2748	-0.70	-1.41	12.0000

--- End Of Report ---

Figure S179. Specific rotation spectrum of **6**

Rudolph Research Analytical

This sample was measured on an Autopol VI, Serial #91058
Manufactured by Rudolph Research Analytical, Hackettstown, NJ, USA.

Measurement Date : Thursday, 17-JUN-2021

Set Temperature : 19.0

Time Delay : Disabled

Delay between Measurement : Disabled

n	Average	Std.Dev.	% RSD	Maximum	Minimum
5	57.84	0.16	0.27	58.06	57.64

S.No	Sample ID	Time	Result	Scale	OR °Arc	WLG.nm	Lg.mm	Conc.g/100ml	Temp.
1	shp11	11:58:44 AM	57.78	SR	0.0416	589	100.00	0.072	19.9
2	shp11	11:58:52 AM	57.78	SR	0.0416	589	100.00	0.072	19.8
3	shp11	11:59:00 AM	57.64	SR	0.0415	589	100.00	0.072	19.7
4	shp11	11:59:08 AM	58.06	SR	0.0418	589	100.00	0.072	19.6
5	shp11	11:59:17 AM	57.92	SR	0.0417	589	100.00	0.072	19.6

Figure S180. ^{1}H NMR spectrum of **7** at 500 MHz in $CDCl_3$

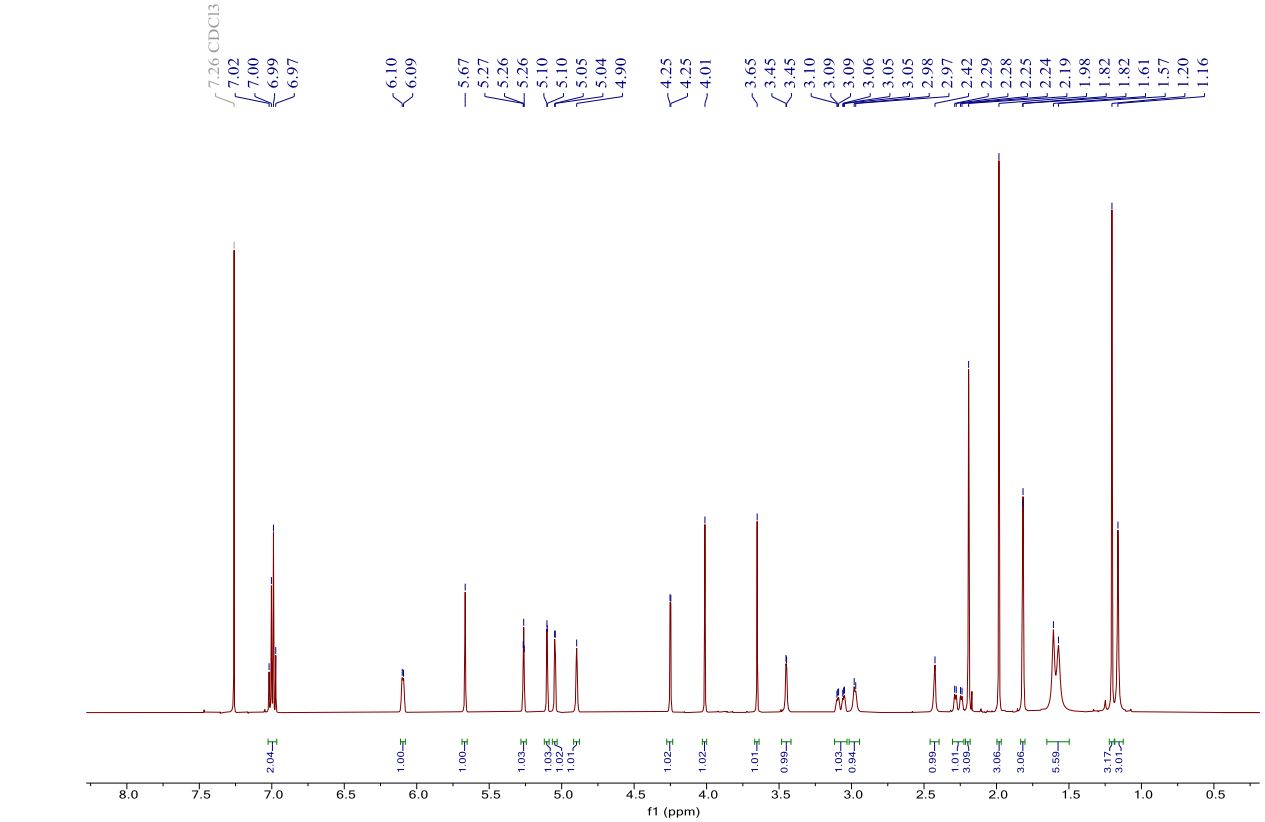


Figure S181. ^{13}C NMR spectrum of **7** at 125 MHz in $CDCl_3$

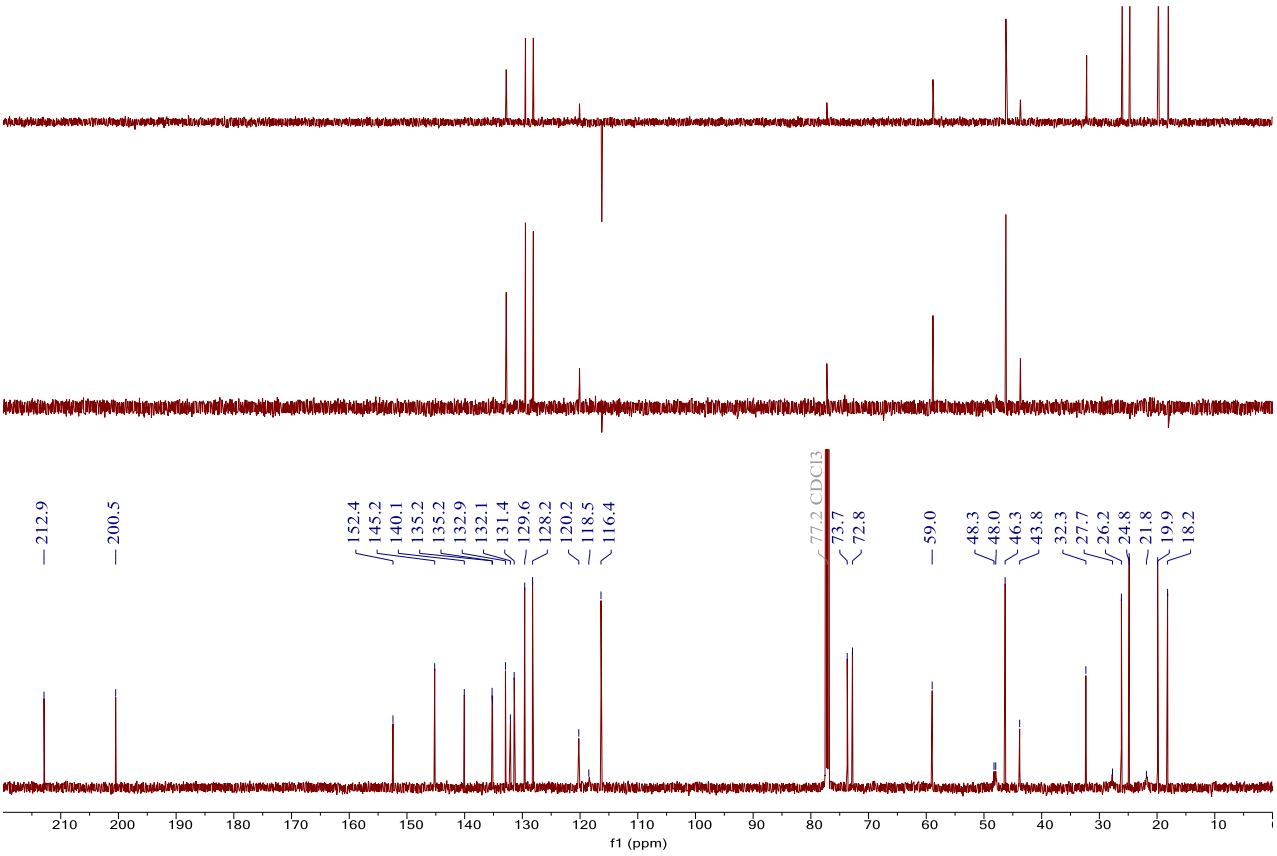


Figure S182. HRESIMS spectrum of **7**

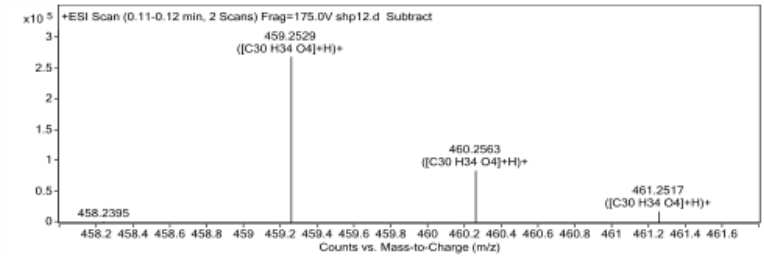
Qualitative Analysis Report

Data Filename	shp12.d	**Sample Name**	shp12
Sample Type	Sample	**Position**	P1-A5
Instrument Name	Instrument 1	**User Name**	
Acq Method	s.m	**Acquired Time**	12/10/2021 9:54:13 AM
IRM Calibration Status	Success	**DA Method**	PCDL.m
Comment			

Sample Group	**Info.**
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125.2)

User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
175	0	ESI



Peak List

m/z	z	Abund	Formula	Ion
413.2474	1	24782.79		
441.2419	1	51995.11		
459.2529	1	269466.5	C30 H34 O4	(M+H)+
460.2563	1	85216.62	C30 H34 O4	(M+H)+
475.2474	1	22732.43		
481.2343	1	99785.48		
482.2379	1	32607.86		
483.2156	1	27084.82		
497.2285	1	24259.22		
939.4802	1	25245.6		

Formula Calculator Element Limits

Element	Min	Max
C	3	120
H	0	240
O	0	30

Formula Calculator Results

Formula	CalculatedMass	CalculatedMz	Mz	Diff. (mDa)	Diff. (ppm)	DBE
C30 H34 O4	458.2457	459.2530	459.2529	0.10	0.22	14.0000

--- End Of Report ---

Figure S183. Specific rotation spectrum of **7**

Rudolph Research Analytical

This sample was measured on an Autopol VI, Serial #91058
Manufactured by Rudolph Research Analytical, Hackettstown, NJ, USA.

Measurement Date : Wednesday, 25-AUG-2021

Set Temperature : OFF

Time Delay : Disabled

Delay between Measurement : Disabled

n	Average	Std.Dev.	% RSD	Maximum	Minimum
5	4.41	0.21	4.76	4.79	4.30

S.No	Sample ID	Time	Result	Scale	OR °Arc	WLG.nm	Lg.mm	Conc.g/100ml	Temp.
1	SHP12	08:33:51 PM	4.30	SR	0.0052	589	100.00	0.121	26.8
2	SHP12	08:34:00 PM	4.30	SR	0.0052	589	100.00	0.121	26.8
3	SHP12	08:34:08 PM	4.30	SR	0.0052	589	100.00	0.121	26.7
4	SHP12	08:34:16 PM	4.38	SR	0.0053	589	100.00	0.121	26.7
5	SHP12	08:34:24 PM	4.79	SR	0.0058	589	100.00	0.121	26.7

Figure S184. ^{1}H NMR spectrum of **30a** at 500 MHz in $CDCl_3$

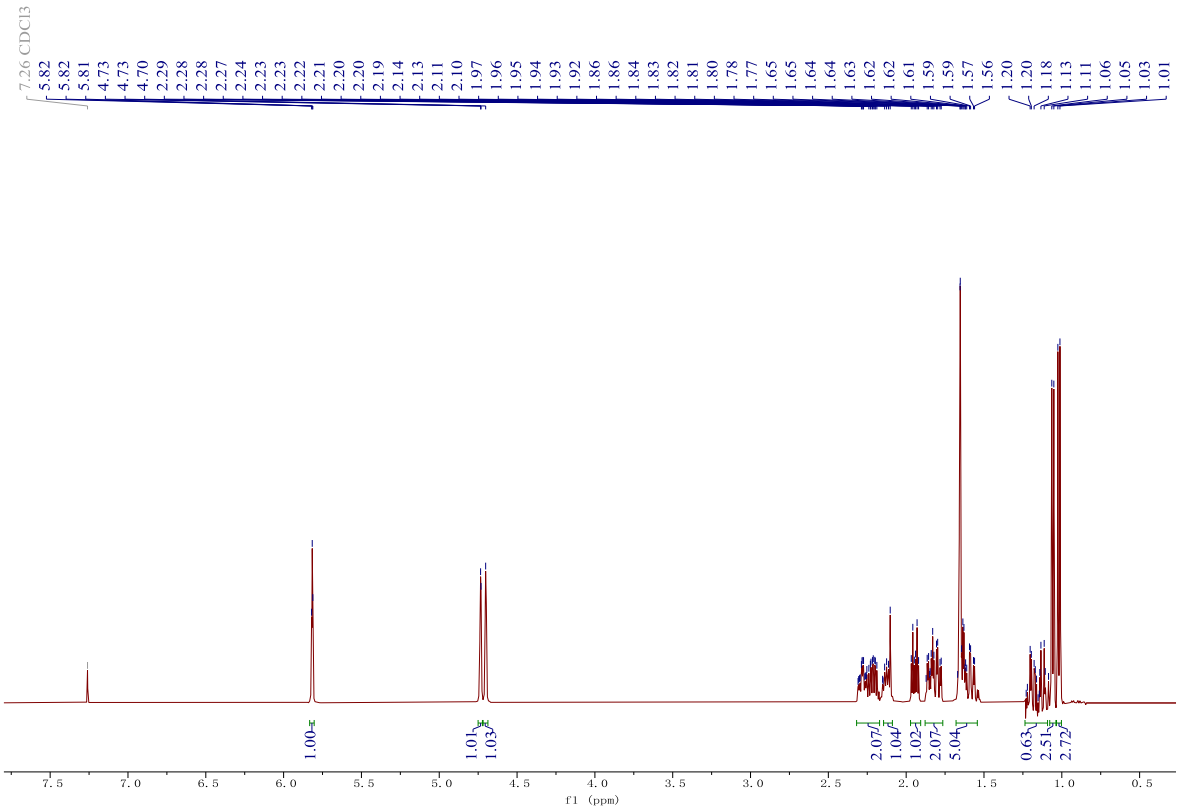


Figure S185. ^{13}C NMR spectrum of **30a** at 125 MHz in $CDCl_3$

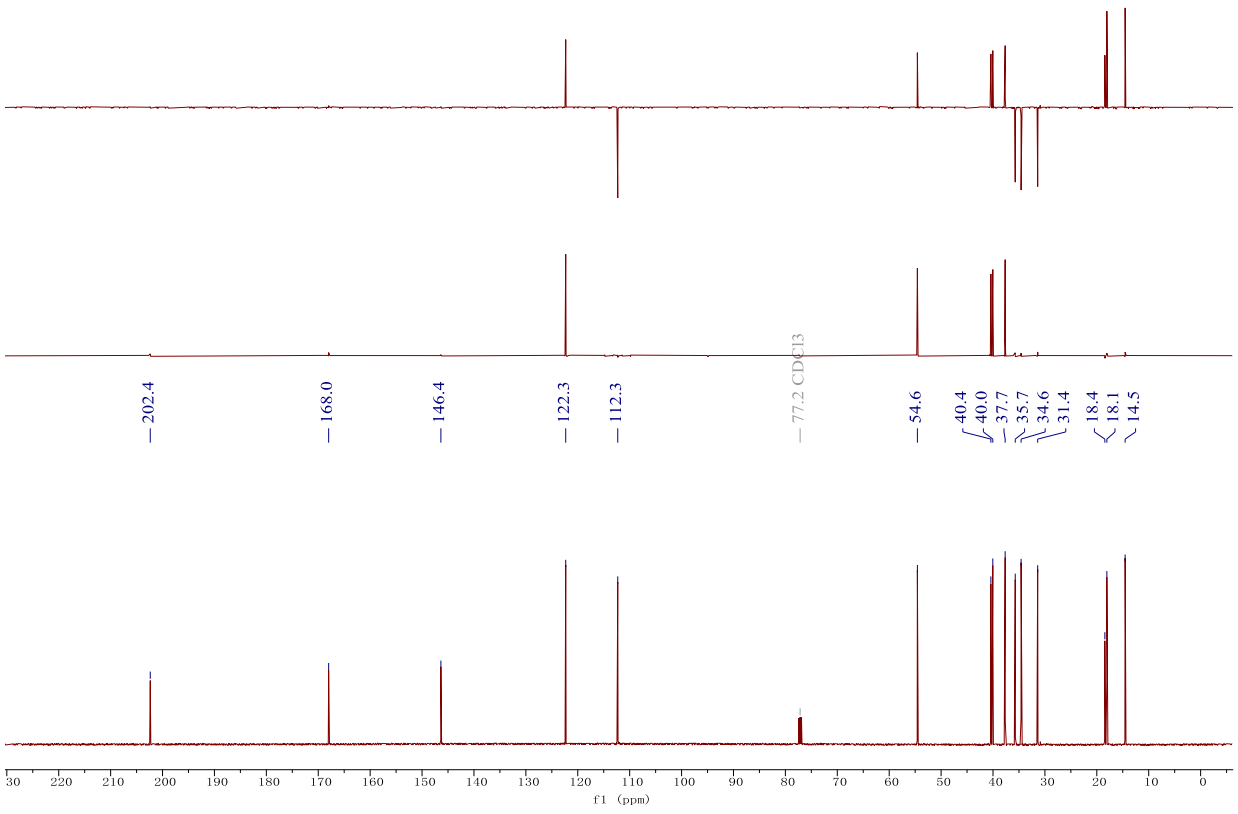


Figure S186. HRESIMS spectrum of **30a**

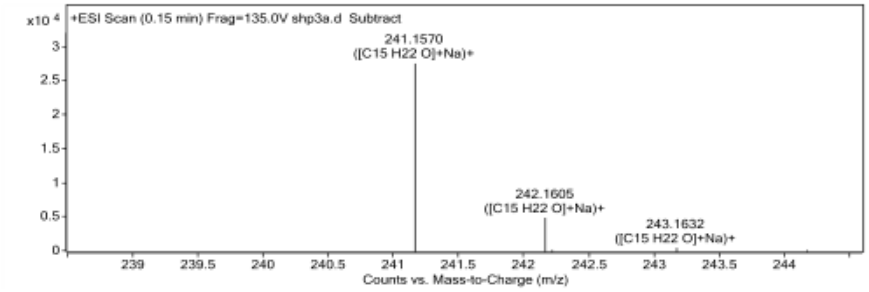
Qualitative Analysis Report

Data Filename	shp3a.d	**Sample Name**	shp3a
Sample Type	Sample	**Position**	P1-A6
Instrument Name	Instrument 1	**User Name**	
Acq Method	s.m	**Acquired Time**	5/12/2021 3:38:24 PM
IRM Calibration Status	Success	**DA Method**	Default.m
Comment			

Sample Group	**Info.**
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125.2)

User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
135	0	ESI



Peak List

m/z	z	Abund	Formula	Ion
102.1277	1	21233.87		
219.1742	1	16640.62		
235.1691		10760.63		
241.157	1	27612.54	C15 H22 O	(M+Na)+
242.1605	1	4993.65	C15 H22 O	(M+Na)+
257.1516	2	16721.5		
453.1674	1	3001.31		
457.3087	1	8417.93		
459.3235	1	8417.04		
460.3266	1	3138.87		

Formula Calculator Element Limits

Element	Min	Max
C	3	60
H	0	120
O	0	30

Formula Calculator Results

Formula	CalculatedMass	CalculatedMz	Mz	Diff. (mDa)	Diff. (ppm)	DBE
C15 H22 O	218.1671	241.1563	241.1570	-0.70	-2.90	5.0000

--- End Of Report ---

Figure S187. Specific rotation spectrum of **30a**

Rudolph Research Analytical

This sample was measured on an Autopol VI, Serial #91058
Manufactured by Rudolph Research Analytical, Hackettstown, NJ, USA.

Measurement Date : Tuesday, 25-MAY-2021

Set Temperature : OFF

Time Delay : Disabled

Delay between Measurement : Disabled

n	Average	Std.Dev.	% RSD	Maximum	Minimum
5	6.11	0.93	15.22	7.59	5.19

S.No	Sample ID	Time	Result	Scale	OR °Arc	WLG.nm	Lg.mm	Conc.g/100ml	Temp.
1	SHP3A	03:59:47 PM	7.59	SR	0.0082	589	100.00	0.108	27.1
2	SHP3A	03:59:56 PM	5.83	SR	0.0063	589	100.00	0.108	27.1
3	SHP3A	04:00:09 PM	5.56	SR	0.0060	589	100.00	0.108	27.1
4	SHP3A	04:00:18 PM	6.39	SR	0.0069	589	100.00	0.108	27.1
5	SHP3A	04:00:26 PM	5.19	SR	0.0056	589	100.00	0.108	27.1

Figure S188. ^{1}H NMR spectrum of **30b** at 500 MHz in $CDCl_3$

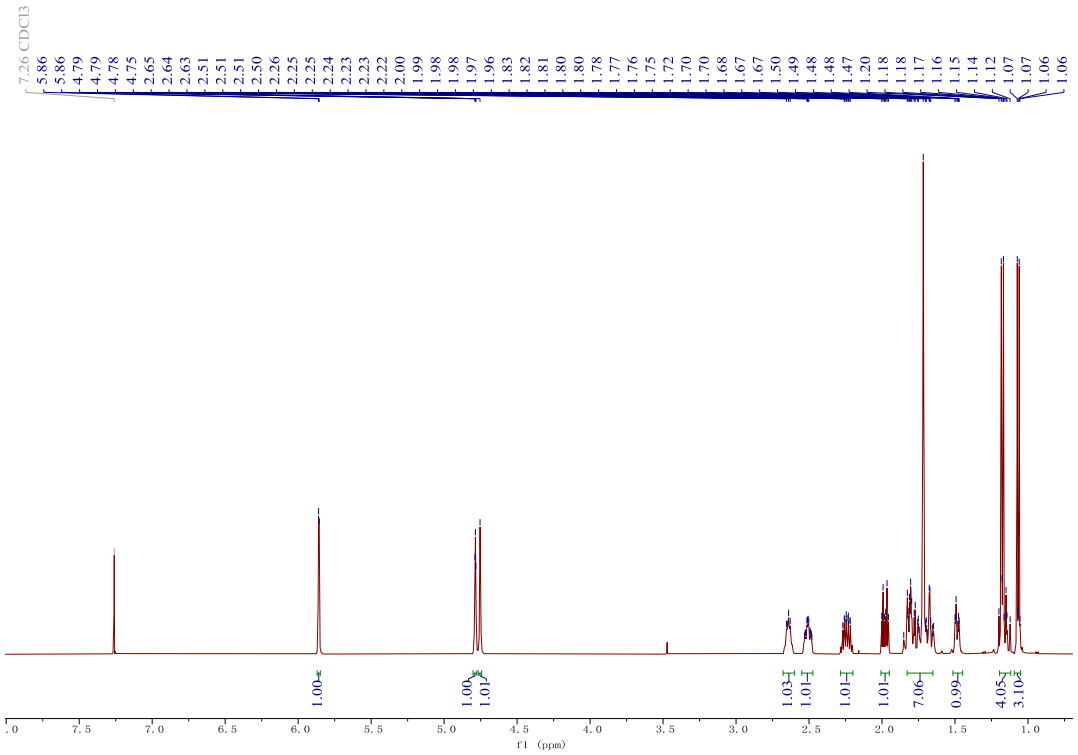


Figure S189. ^{13}C NMR spectrum of **30b** at 125 MHz in $CDCl_3$

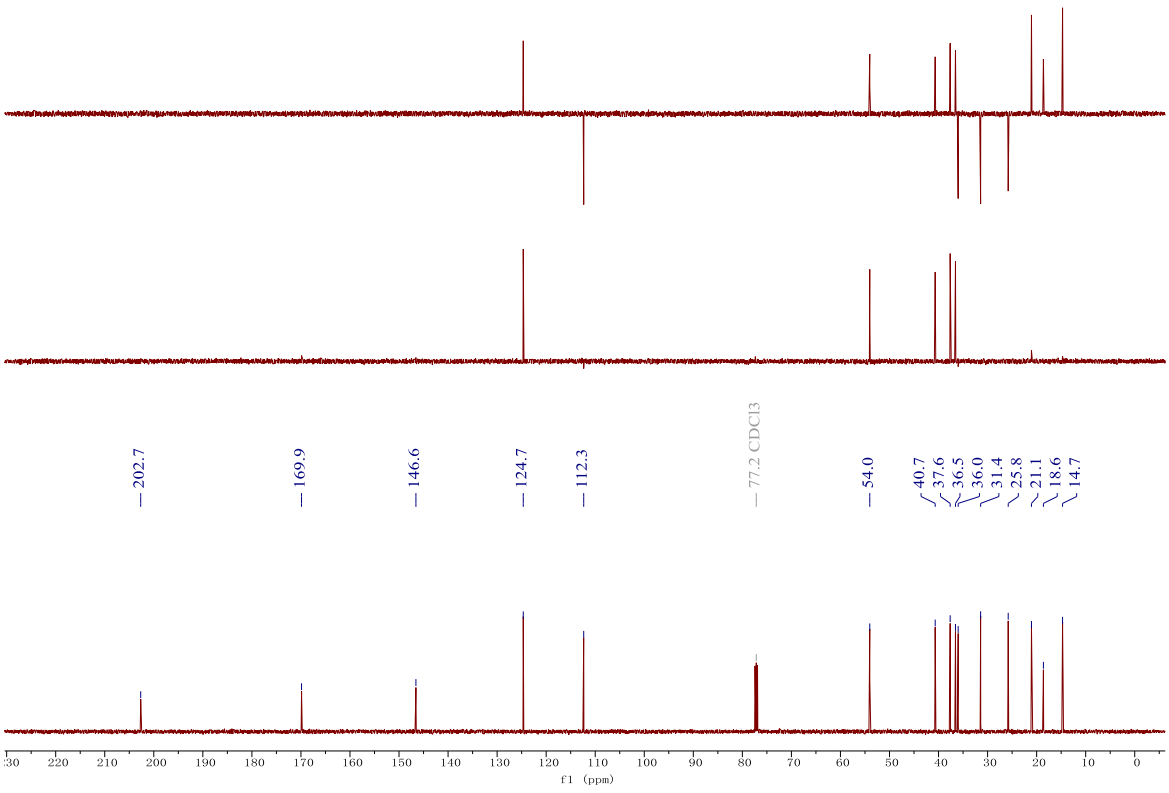


Figure S190. HRESIMS spectrum of **30b**

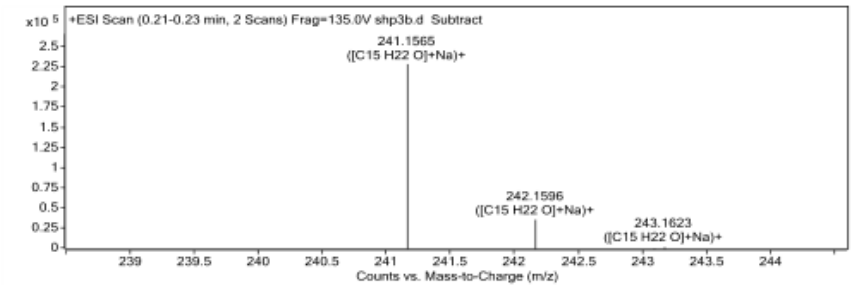
Qualitative Analysis Report

Data Filename	shp3b.d	**Sample Name**	shp3b
Sample Type	Sample	**Position**	P1-A7
Instrument Name	Instrument 1	**User Name**	
Acq Method	s.m	**Acquired Time**	5/12/2021 3:39:35 PM
IRM Calibration Status	Success	**DA Method**	Default.m
Comment			

Sample Group	**Info.**
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125.2)

User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
135	0	ESI



Peak List

m/z	z	Abund	Formula	Ion
219.174	1	101139.85		
241.1565	1	229273.97	C15 H22 O	(M+Na)+
242.1596	1	36648.56	C15 H22 O	(M+Na)+
273.1454	1	57490.64		
457.3078	2	37349.65		
459.3233	1	131135.84		
460.327	1	42421.17		
473.288	1	17914.33		
489.2971	1	52358.59		
505.2751	1	21541.46		

Formula Calculator Element Limits

Element	Min	Max
C	3	60
H	0	120
O	0	30

Formula Calculator Results

Formula	CalculatedMass	CalculatedMz	Mz	Diff. (mDa)	Diff. (ppm)	DBE
C15 H22 O	218.1671	241.1563	241.1565	-0.20	-0.83	5.0000

--- End Of Report ---

Figure S191. Specific rotation spectrum of **30b**

Rudolph Research Analytical

This sample was measured on an Autopol VI, Serial #91058
Manufactured by Rudolph Research Analytical, Hackettstown, NJ, USA.

Measurement Date : Tuesday, 25-MAY-2021

Set Temperature : OFF

Time Delay : Disabled

Delay between Measurement : Disabled

n	Average	Std.Dev.	% RSD	Maximum	Minimum
5	-9.82	0.28	-2.85	-9.41	-10.07

S.No	Sample ID	Time	Result	Scale	OR °Arc	WLG.nm	Lg.mm	Conc.g/100ml	Temp.
1	SHP3B	04:06:25 PM	-9.41	SR	-0.0127	589	100.00	0.135	27.2
2	SHP3B	04:06:34 PM	-9.70	SR	-0.0131	589	100.00	0.135	27.2
3	SHP3B	04:06:42 PM	-9.85	SR	-0.0133	589	100.00	0.135	27.2
4	SHP3B	04:06:50 PM	-10.07	SR	-0.0136	589	100.00	0.135	27.2
5	SHP3B	04:06:58 PM	-10.07	SR	-0.0136	589	100.00	0.135	27.2

Figure S192. ^{1}H NMR spectrum of **31** at 500 MHz in $CDCl_3$

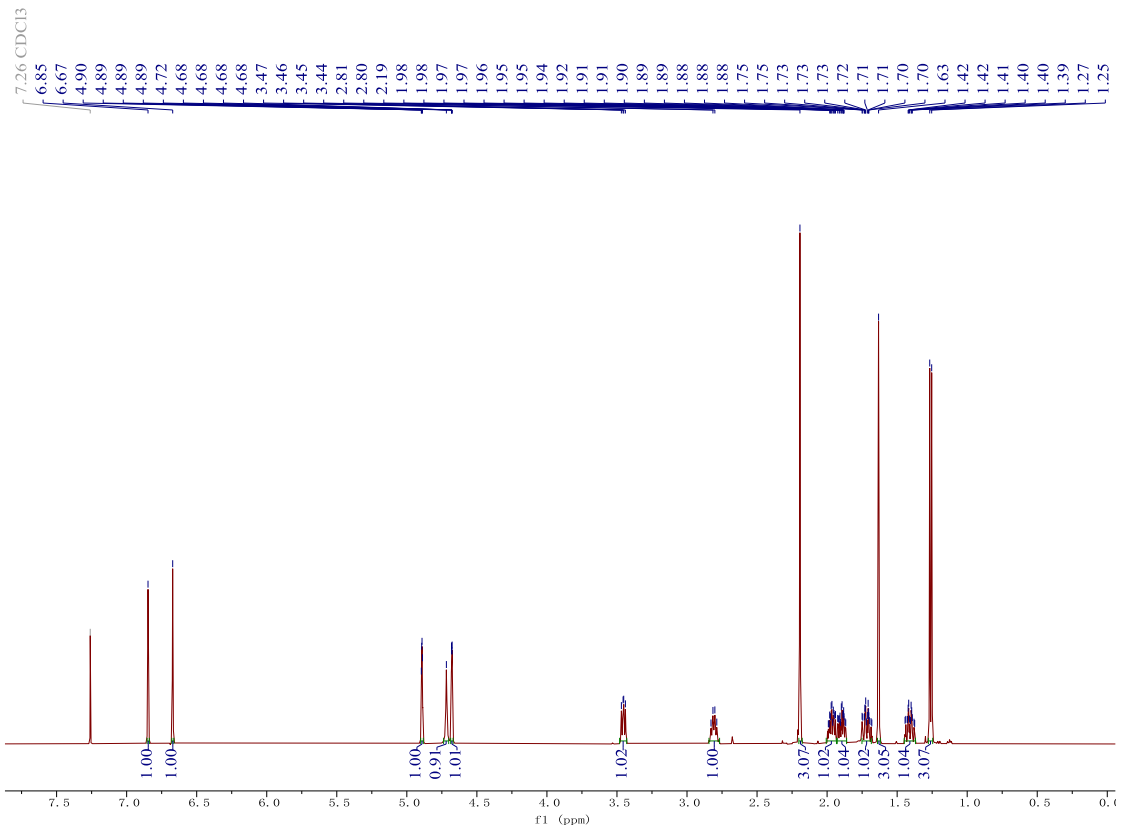


Figure S193. ^{13}C NMR spectrum of **31** at 125 MHz in $CDCl_3$

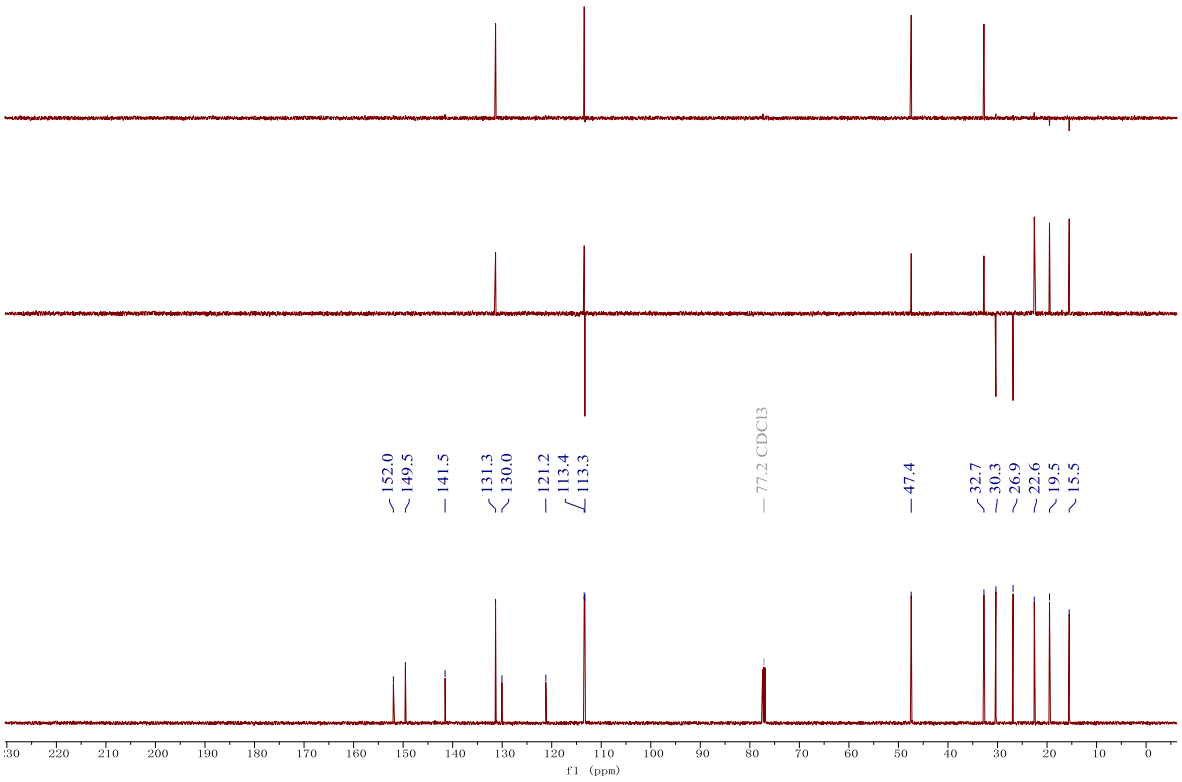


Figure S194. HRESIMS spectrum of **31**

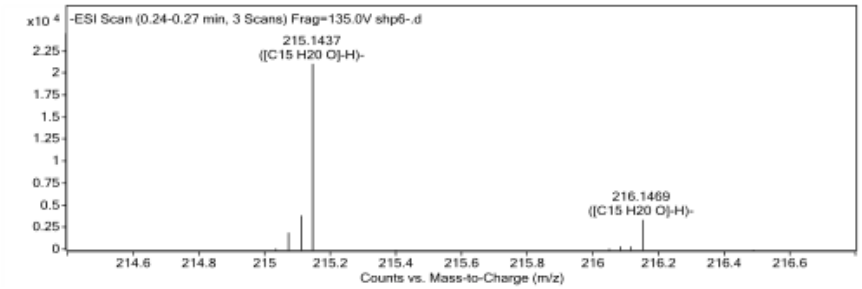
Qualitative Analysis Report

Data Filename	shp6-.d	**Sample Name**	shp6
Sample Type	Sample	**Position**	P1-A8
Instrument Name	Instrument 1	**User Name**	
Acq Method	s-.m	**Acquired Time**	5/12/2021 3:46:30 PM
IRM Calibration Status	Success	**DA Method**	Default.m
Comment			

Sample Group	**Info.**
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125.2)

User Spectra

Fragmentor Voltage	**Collision Energy**	**Ionization Mode**
135	0	ESI



Peak List

m/z	z	Abund
112.9855		90809.19
119.0361	1	55150.2
275.0927	1	56529
277.1446	1	41682.81
966.0007	1	242471.58
967.0031	1	49554.43
982.9909	1	257602
983.9931	1	49428.54
1033.9882	1	349930.16
1034.9906	1	70814.88

Formula Calculator Element Limits

Element	Min	Max
C	3	60
H	0	120
O	0	30

Formula Calculator Results

Formula	CalculatedMass	CalculatedMz	Mz	Diff. (mDa)	Diff. (ppm)	DBE
C15 H20 O	216.1514	215.1441	215.1437	0.40	1.86	6.0000

--- End Of Report ---

Figure S195. Specific rotation spectrum of **31**

Rudolph Research Analytical

This sample was measured on an Autopol VI, Serial #91058
Manufactured by Rudolph Research Analytical, Hackettstown, NJ, USA.

Measurement Date : Tuesday, 25-MAY-2021

Set Temperature : OFF

Time Delay : Disabled

Delay between Measurement : Disabled

n	Average	Std.Dev.	% RSD	Maximum	Minimum
5	26.93	4.59	17.04	31.26	20.53

S.No	Sample ID	Time	Result	Scale	OR °Arc	WLG.nm	Lg.mm	Conc.g/100ml	Temp.
1	SHP4	04:11:54 PM	20.53	SR	0.0310	589	100.00	0.151	27.2
2	SHP4	04:12:12 PM	24.44	SR	0.0369	589	100.00	0.151	27.2
3	SHP4	04:12:20 PM	27.22	SR	0.0411	589	100.00	0.151	27.2
4	SHP4	04:12:33 PM	31.26	SR	0.0472	589	100.00	0.151	27.2
5	SHP4	04:12:41 PM	31.19	SR	0.0471	589	100.00	0.151	27.2

Figure S196. ^{1}H NMR spectrum of **32a** at 800 MHz in $CDCl_3$

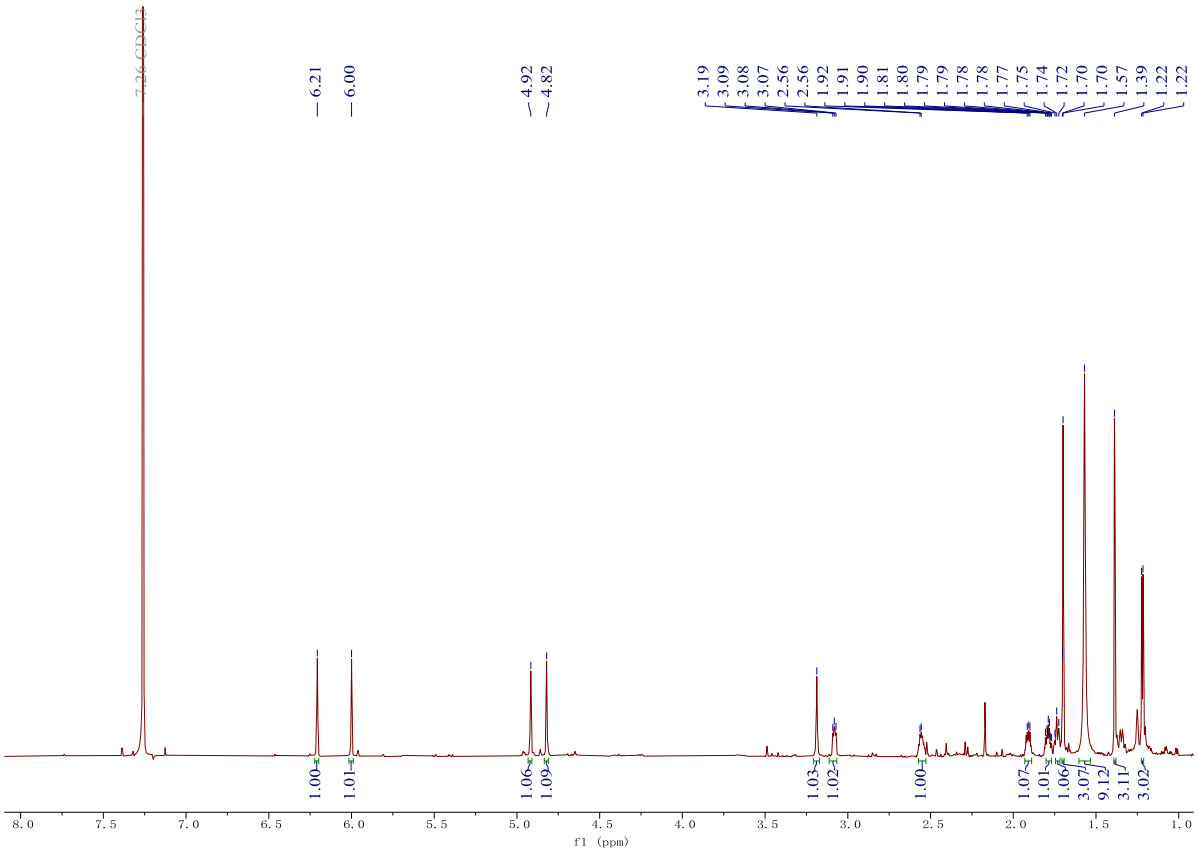


Figure S197. ^{1}C NMR spectrum of **32a** at 200 MHz in $CDCl_3$

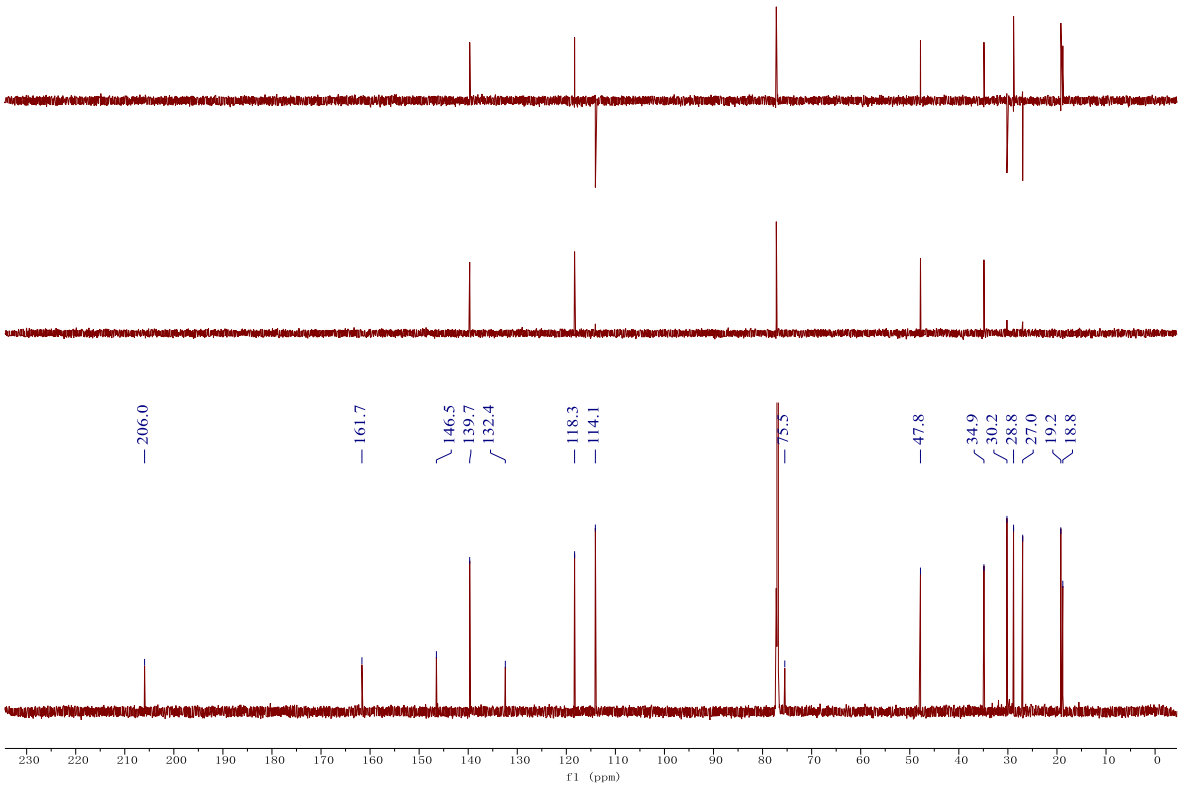


Figure S198. HRESIMS spectrum of **32a**

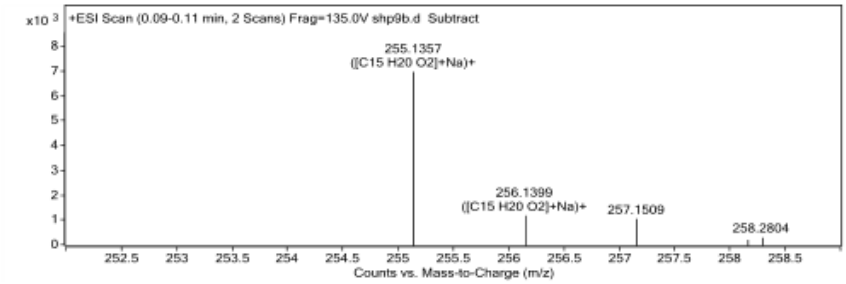
Qualitative Analysis Report

Data Filename	shp9b.d	**Sample Name**	shp9b
Sample Type	Sample	**Position**	P1-B2
Instrument Name	Instrument 1	**User Name**	
Acq Method	s.m	**Acquired Time**	5/27/2021 9:59:51 AM
IRM Calibration Status	Success	**DA Method**	Default.m
Comment			

Sample Group	**Info.**
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125.2)

User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
135	0	ESI



Peak List

m/z	z	Abund	Formula	Ion
233.1535	1	4569.12		
255.1357	1	7014.91	C15 H20 O2	(M+Na)+
274.2748	1	1959.35		
415.2129	1	3565.92		
437.1941	1	7374.59		
438.1973	1	1725.37		
453.1686	1	2254.22		
487.2837	1	1954.5		
654.3332	1	5054.54		
655.3383	1	2465.49		

Formula Calculator Element Limits

Element	Min	Max
C	3	60
H	0	120
O	0	30

Formula Calculator Results

Formula	CalculatedMass	CalculatedMz	Mz	Diff. (mDa)	Diff. (ppm)	DBE
C15 H20 O2	232.1463	255.1356	255.1357	-0.10	-0.39	6.0000

--- End Of Report ---

Figure S199. Specific rotation spectrum of **32a**

Rudolph Research Analytical

This sample was measured on an Autopol VI, Serial #91058
Manufactured by Rudolph Research Analytical, Hackettstown, NJ, USA.

Measurement Date : Thursday, 27-MAY-2021

Set Temperature : OFF

Time Delay : Disabled

Delay between Measurement : Disabled

n	Average	Std.Dev.	% RSD	Maximum	Minimum
5	9.49	0.54	5.69	10.00	8.63

S.No	Sample ID	Time	Result	Scale	OR °Arc	WLG.nm	Lg.mm	Conc.g/100ml	Temp.
1	SHP9B	03:53:40 PM	9.82	SR	0.0165	589	100.00	0.168	24.7
2	SHP9B	03:53:49 PM	10.00	SR	0.0168	589	100.00	0.168	24.7
3	SHP9B	03:53:57 PM	9.64	SR	0.0162	589	100.00	0.168	24.7
4	SHP9B	03:54:05 PM	9.35	SR	0.0157	589	100.00	0.168	24.7
5	SHP9B	03:54:13 PM	8.63	SR	0.0145	589	100.00	0.168	24.7

Figure S200. ^{1}H NMR spectrum of **32b** at 800 MHz in $CDCl_3$

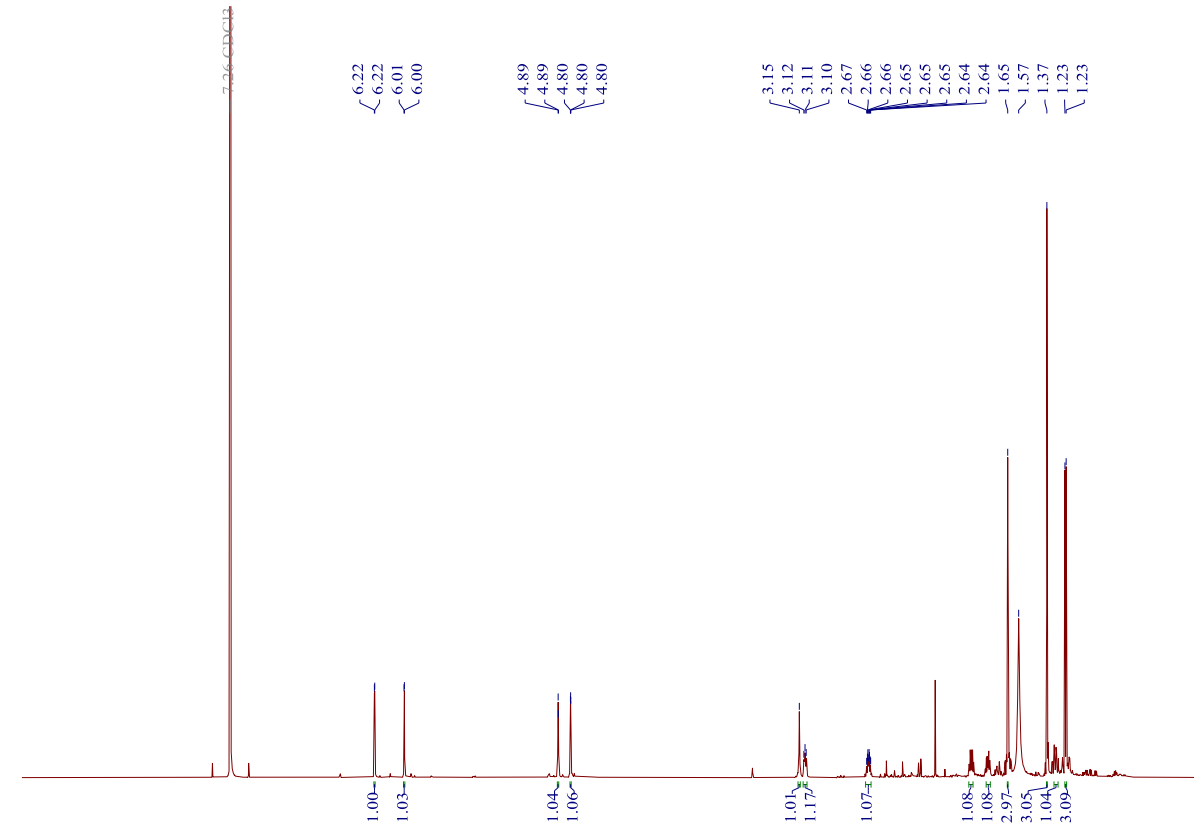


Figure S201. ^{13}C NMR spectrum of **32b** at 200 MHz in $CDCl_3$

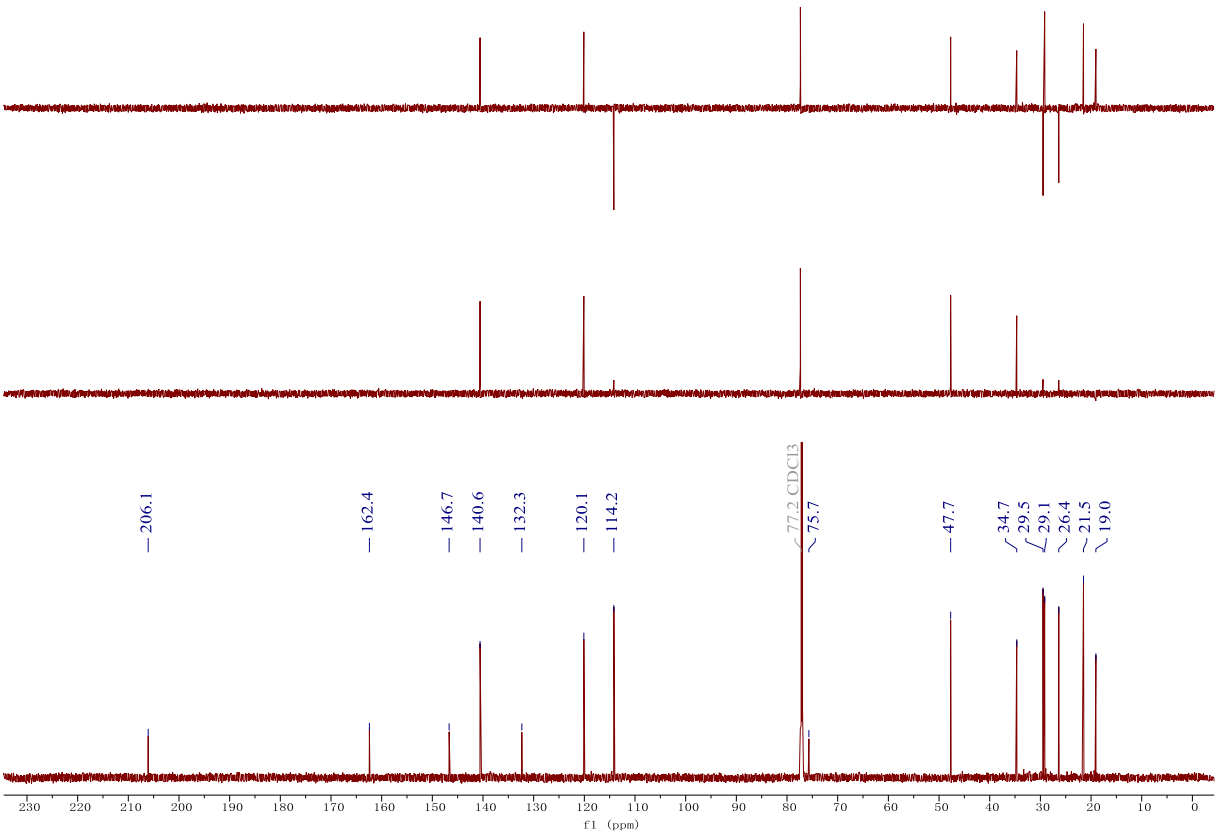


Figure S202. HRESIMS spectrum of **32b**

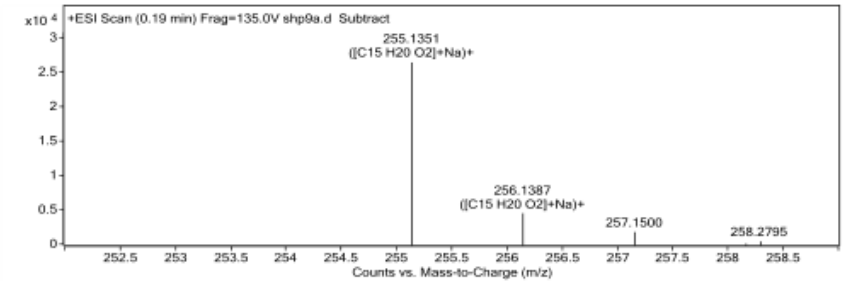
Qualitative Analysis Report

Data Filename	shp9a.d	**Sample Name**	shp9a
Sample Type	Sample	**Position**	P1-B1
Instrument Name	Instrument 1	**User Name**	
Acq Method	s.m	**Acquired Time**	5/27/2021 9:58:40 AM
IRM Calibration Status	Success	**DA Method**	Default.m
Comment			

Sample Group	**Info.**
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125.2)

User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
135	0	ESI



Peak List

m/z	z	Abund	Formula	Ion
172.0935	1	3758.13		
230.2477	1	3566.33		
233.1532	1	12660.22		
255.1351	1	26555.97	C15 H20 O2	(M+Na)+
256.1387	1	4625.34	C15 H20 O2	(M+Na)+
274.2739	1	6820.86		
437.1929	1	4774.92		
487.2804	1	10513.41		
488.2848	1	4149.43		
654.3296	1	7747.86		

Formula Calculator Element Limits

Element	Min	Max
C	3	60
H	0	120
O	0	30

Formula Calculator Results

Formula	CalculatedMass	CalculatedMz	Mz	Diff. (mDa)	Diff. (ppm)	DBE
C15 H20 O2	232.1463	255.1356	255.1351	0.50	1.96	6.0000

--- End Of Report ---

Figure S203. Specific rotation spectrum of **32b**

Rudolph Research Analytical

This sample was measured on an Autopol VI, Serial #91058
Manufactured by Rudolph Research Analytical, Hackettstown, NJ, USA.

Measurement Date : Thursday, 27-MAY-2021

Set Temperature : OFF

Time Delay : Disabled

Delay between Measurement : Disabled

n	Average	Std.Dev.	% RSD	Maximum	Minimum
5	120.51	0.89	0.73	121.76	119.62

S.No	Sample ID	Time	Result	Scale	OR °Arc	WLG.nm	Lg.mm	Conc.g/100ml	Temp.
1	SHP9A	04:03:41 PM	121.76	SR	0.2557	589	100.00	0.210	25.0
2	SHP9A	04:03:49 PM	121.10	SR	0.2543	589	100.00	0.210	25.0
3	SHP9A	04:04:02 PM	120.00	SR	0.2520	589	100.00	0.210	25.1
4	SHP9A	04:04:10 PM	119.62	SR	0.2512	589	100.00	0.210	25.1
5	SHP9A	04:04:18 PM	120.05	SR	0.2521	589	100.00	0.210	25.1

Figure S204. ^{1}H NMR spectrum of **9** at 500 MHz in $CDCl_3$

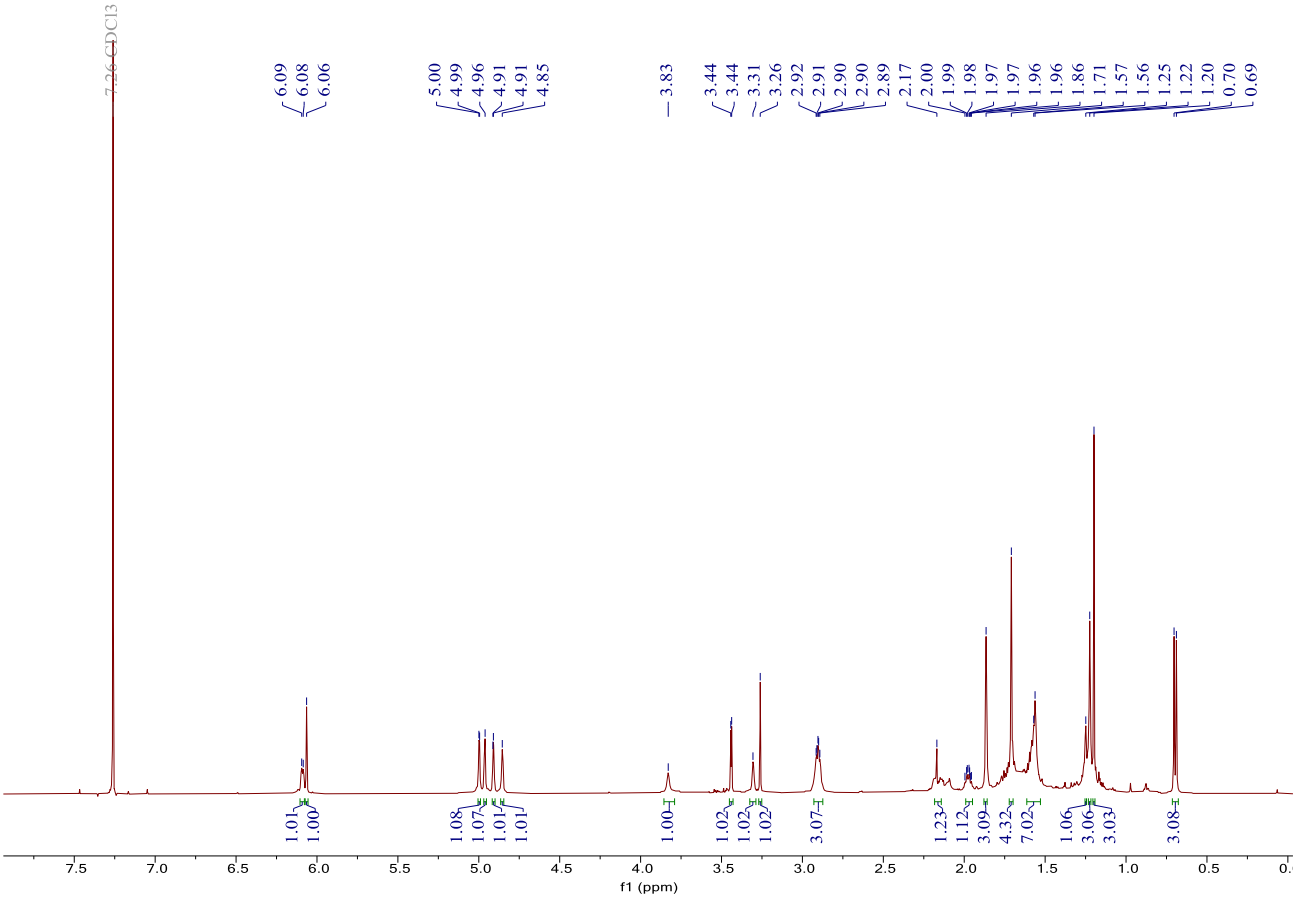


Figure S205. ^{13}C NMR spectrum of **9** at 125 MHz in $CDCl_3$

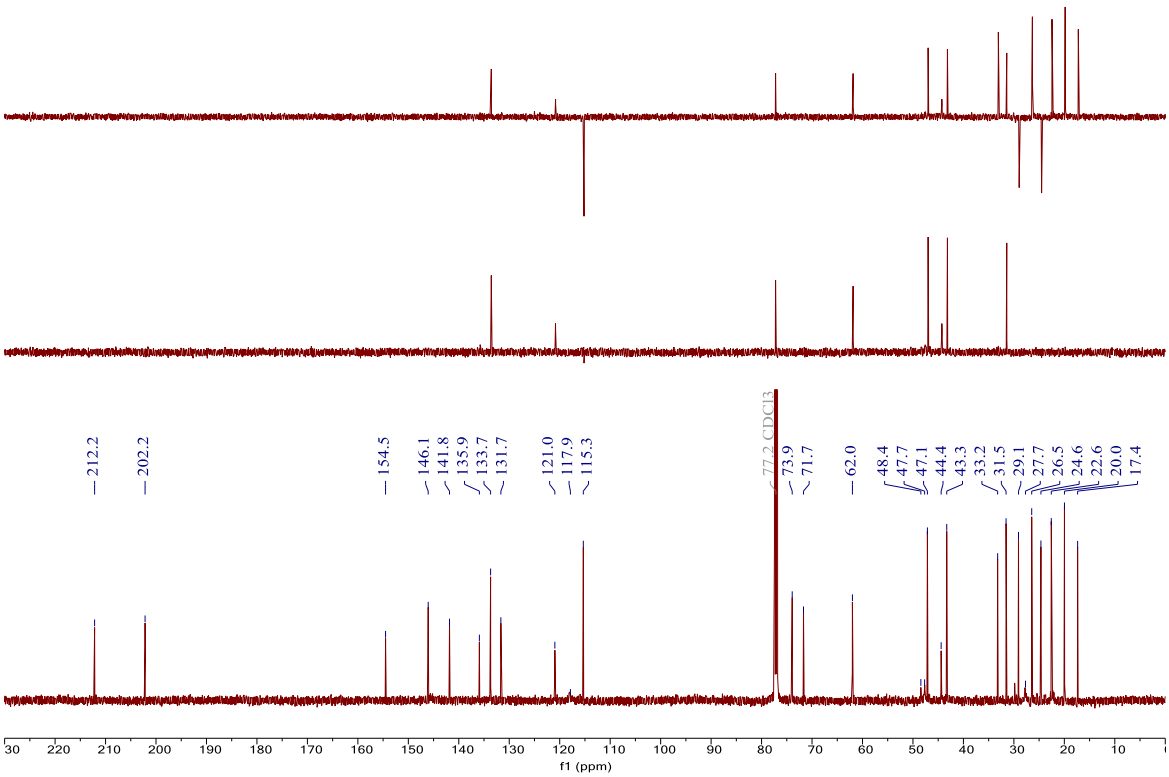


Figure S206. HRESIMS spectrum of **9**

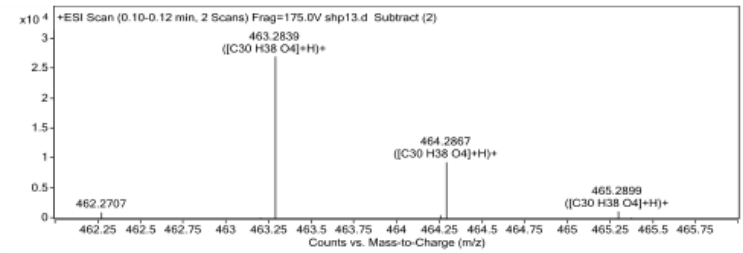
Qualitative Analysis Report

Data Filename	shp13.d	**Sample Name**	shp13
Sample Type	Sample	**Position**	P1-A6
Instrument Name	Instrument 1	**User Name**	
Acq Method	s.m	**Acquired Time**	12/10/2021 9:55:23 AM
IRM Calibration Status	Success	**DA Method**	PCDL.m
Comment			

Sample Group	**Info.**
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125.2)

User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
175	0	ESI



Peak List

m/z	z	Abund	Formula	Ion
213.1271	1	13748.36		
231.1377	1	5120.51		
461.268	1	3335.83		
463.2839	1	27083.82	C30 H38 O4	(M+H)+
464.2867	1	9508.95	C30 H38 O4	(M+H)+
479.2782	1	3355.37		
485.2667	1	9657.3		
486.2688	1	3408.15		
501.2594	1	3822.03		
517.2558	1	3612.14		

Formula Calculator Element Limits

Element	Min	Max
C	3	120
H	0	240
O	0	30

Formula Calculator Results

Formula	CalculatedMass	CalculatedMz	Mz	Diff. (mDa)	Diff. (ppm)	DBE
C30 H38 O4	462.2770	463.2843	463.2839	0.40	0.86	12.0000

--- End Of Report ---

Figure S207. Specific rotation spectrum of **9**

Rudolph Research Analytical

This sample was measured on an Autopol VI, Serial #91058
Manufactured by Rudolph Research Analytical, Hackettstown, NJ, USA.

Measurement Date : Wednesday, 25-AUG-2021

Set Temperature : OFF

Time Delay : Disabled

Delay between Measurement : Disabled

n	Average	Std.Dev.	% RSD	Maximum	Minimum
5	54.82	0.68	1.24	55.48	54.00

S.No	Sample ID	Time	Result	Scale	OR °Arc	WLG.nm	Lg.mm	Conc.g/100ml	Temp.
1	SHP13	08:39:36 PM	55.22	SR	0.0635	589	100.00	0.115	26.7
2	SHP13	08:39:44 PM	55.48	SR	0.0638	589	100.00	0.115	26.7
3	SHP13	08:39:52 PM	55.22	SR	0.0635	589	100.00	0.115	26.7
4	SHP13	08:40:00 PM	54.17	SR	0.0623	589	100.00	0.115	26.7
5	SHP13	08:40:09 PM	54.00	SR	0.0621	589	100.00	0.115	26.7

Figure S208. ^{1}H NMR spectrum of **33** at 500 MHz in $CDCl_3$

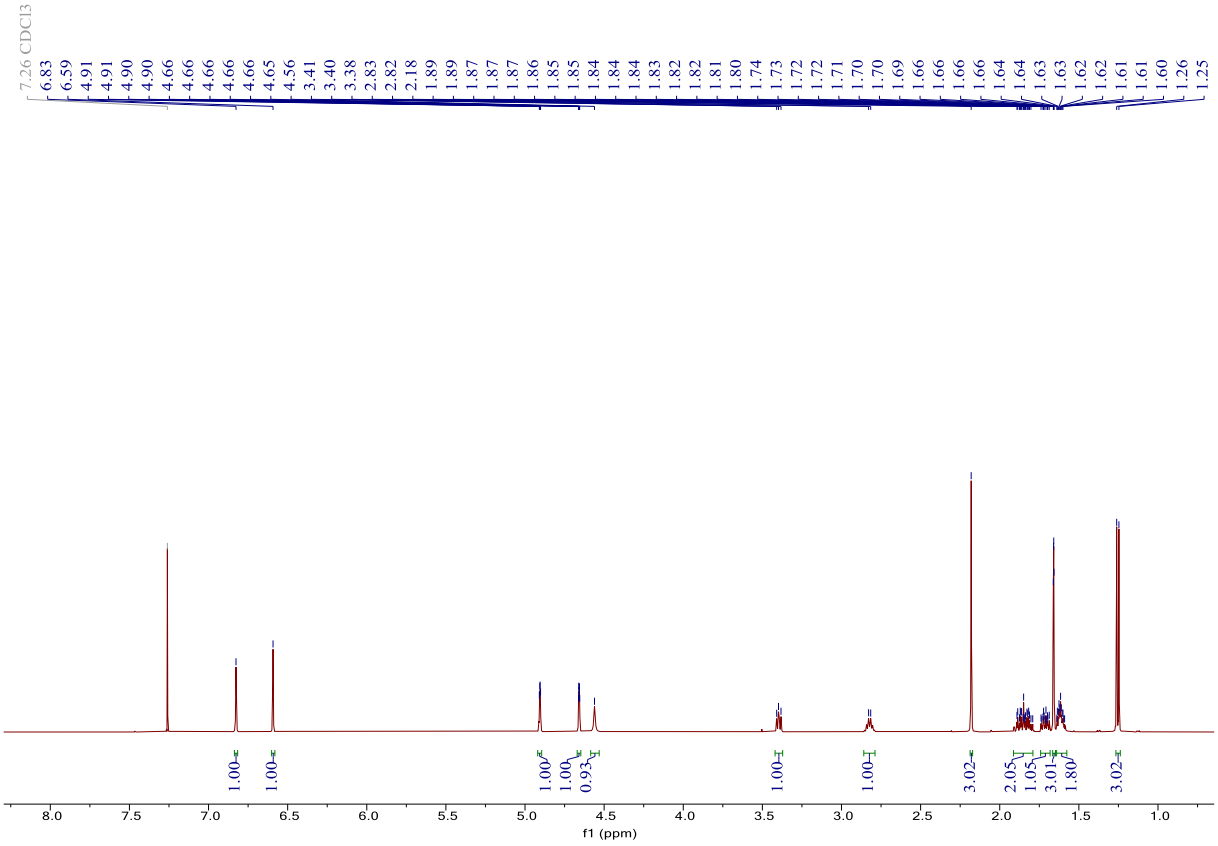


Figure S209. ^{13}C NMR spectrum of **33** at 125 MHz in $CDCl_3$

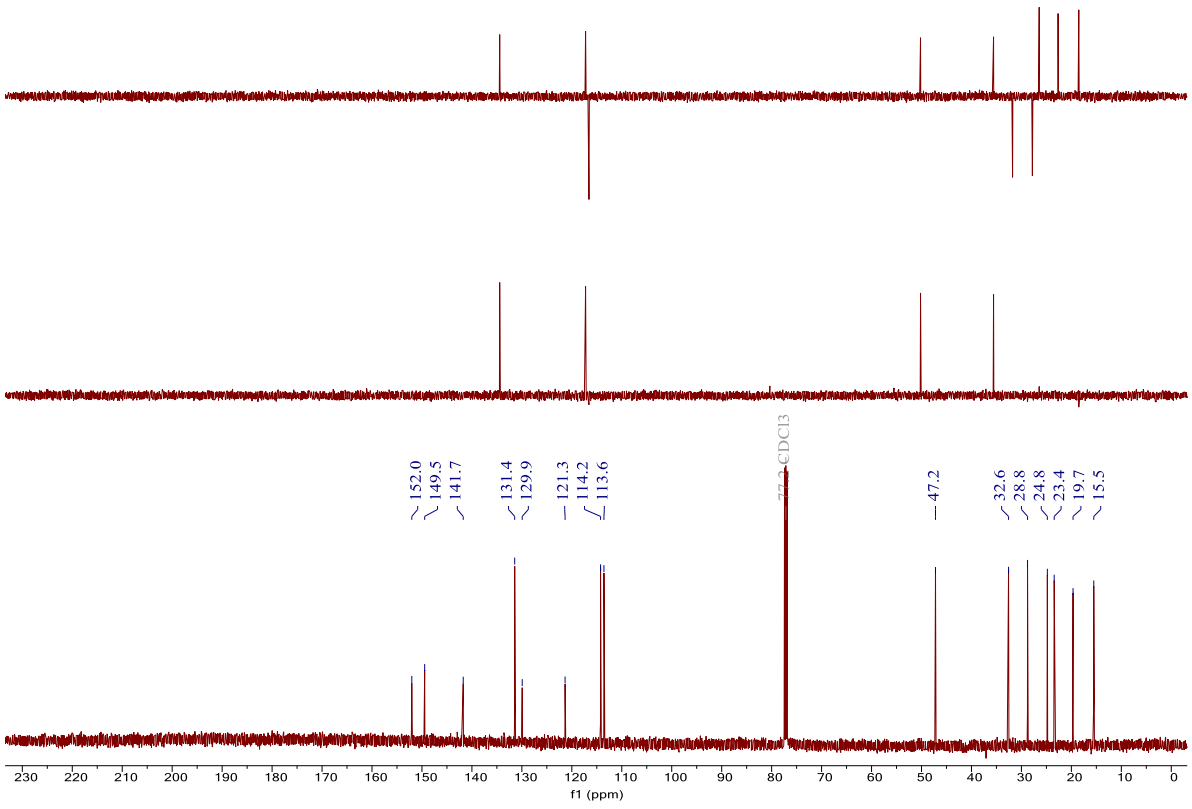


Figure S210. HRESIMS spectrum of **33**

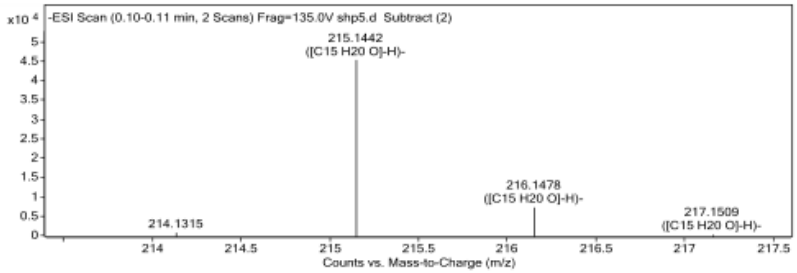
Qualitative Analysis Report

Data Filename	shp5.d	**Sample Name**	shp5
Sample Type	Sample	**Position**	P1-B1
Instrument Name	Instrument 1	**User Name**	
Acq Method	s-.m	**Acquired Time**	5/21/2021 10:03:44 AM
IRM Calibration Status	Success	**DA Method**	Default.m
Comment			

Sample Group		**Info.**	
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125.2)		

User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
135	0	ESI



Peak List

m/z	z	Abund	Formula	Ion
89.0243		1432.36		
213.1284	1	6790.01		
215.1442	1	45500.56	C15 H20 O	(M-H)-
216.1478	1	7532.74	C15 H20 O	(M-H)-
227.202	1	1655.41		
255.2331	1	8033.12		
283.2648	1	3769		
375.2754	1	2601.91		
403.3073	1	5050.66		
459.2025	1	2285.17		
485.2835	1	1928.45		
681.2957	1	3583.06		

Formula Calculator Element Limits

Element	Min	Max
C	3	60
H	0	120
O	0	30
N	0	5

Formula Calculator Results

Formula	CalculatedMass	CalculatedMz	Mz	Diff. (mDa)	Diff. (ppm)	DBE
C15 H20 O	216.1514	215.1441	215.1442	-0.10	-0.46	6.0000

--- End Of Report ---

Figure S211. Specific rotation spectrum of **33**

Rudolph Research Analytical

This sample was measured on an Autopol VI, Serial #91058
Manufactured by Rudolph Research Analytical, Hackettstown, NJ, USA.

Measurement Date : Thursday, 20-OCT-2022

Set Temperature : 20.0

Time Delay : Disabled

Delay between Measurement : Disabled

n	Average	Std.Dev.	% RSD	Maximum	Minimum
5	-4.34	0.59	-13.59	-3.95	-5.26

S.No	Sample ID	Time	Result	Scale	OR °Arc	WLG.nm	Lg.mm	Conc.g/100ml	Temp.
1	shp5	11:20:30 AM	-5.26	SR	-0.008	589	100.00	0.152	19.7
2	shp5	11:20:36 AM	-3.95	SR	-0.006	589	100.00	0.152	19.7
3	shp5	11:20:42 AM	-3.95	SR	-0.006	589	100.00	0.152	19.7
4	shp5	11:20:49 AM	-4.61	SR	-0.007	589	100.00	0.152	19.7
5	shp5	11:20:55 AM	-3.95	SR	-0.006	589	100.00	0.152	19.7

Figure S212. ^{1}H NMR spectrum of **34a** and **34b** at 800 MHz in $CDCl_3$

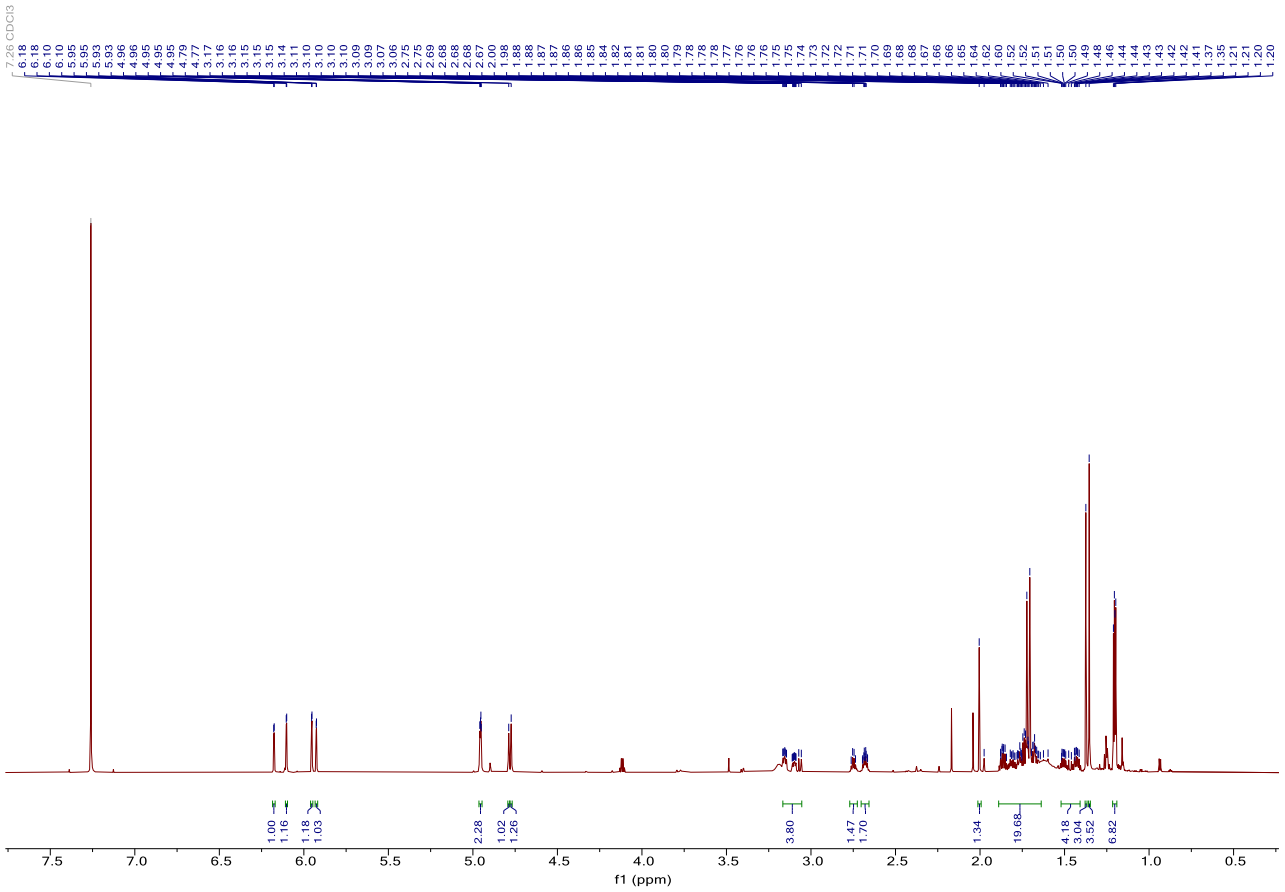


Figure S213. ^{1}C NMR spectrum of **34a** and **34b** at 200 MHz in $CDCl_3$

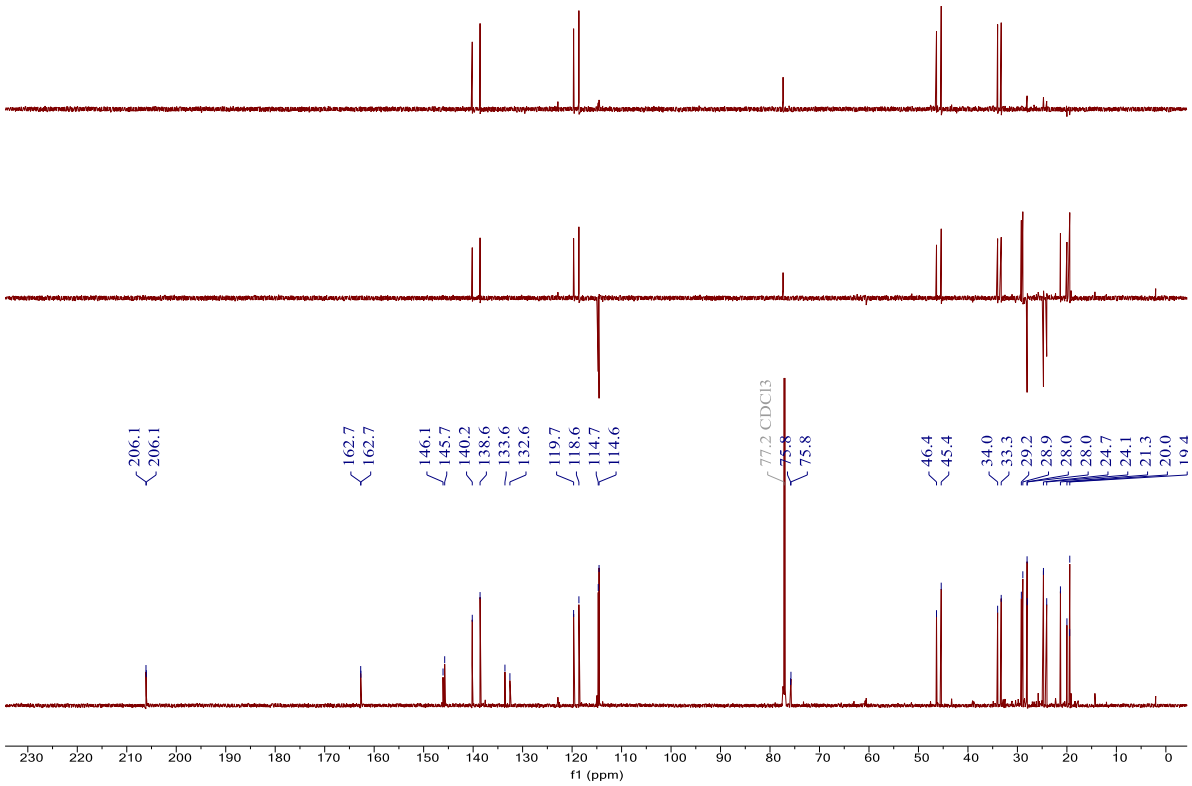


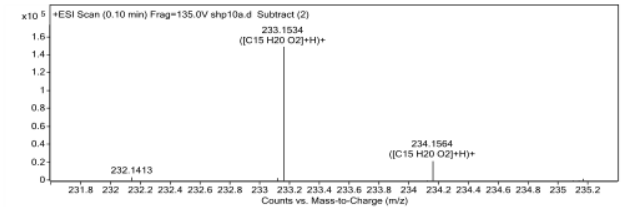
Figure S214. HRESIMS spectrum of **34a**

Data Filename	shp10a.d	**Sample Name**	shp10a
Sample Type	Sample	**Position**	P1-A6
Instrument Name	Instrument 1	**User Name**	
Acq Method	s.m	**Acquired Time**	6/4/2021 9:58:36 AM
IRM Calibration Status	Success	**DA Method**	Default.m
Comment			

Sample Group	**Info.**
Acquisition SW	6200 series TOF/6500 series
Version	Q-TOF B.05.01 (B5125.2)

User Spectra

Fragmentor Voltage	**Collision Energy**	**Ionization Mode**
135	0	ESI



Peak List

m/z	z	Abund	Formula	Ion
215.1426	1	47617.72		
231.1377	1	24217.05		
233.1534	1	149298.38	C15 H20 O2	(M+H)+
234.1564	1	22428.02	C15 H20 O2	(M+H)+
247.1324	1	27431.46		
255.1351	1	17720.22		
265.143	1	24885.11		
287.1248	1	15395.61		
303.1197		12254.04		
447.2894	1	14297.47		

Formula Calculator Element Limits

Element	Min	Max
C	3	60
H	0	120
O	0	30

Formula Calculator Results

Formula	CalculatedMass	CalculatedMz	Mz	Diff. (mDa)	Diff. (ppm)	DBE
C15 H20 O2	232.1463	233.1536	233.1534	0.20	0.86	6.0000

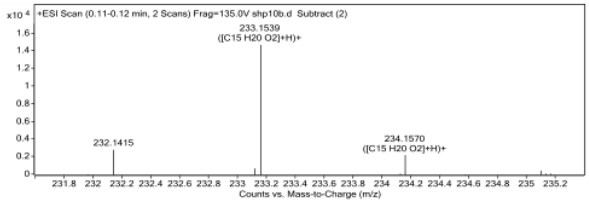
Figure S215. HRESIMS spectrum of **34b**

Data Filename	shp10b.d	**Sample Name**	shp10b
Sample Type	Sample	**Position**	P1-A7
Instrument Name	Instrument 1	**User Name**	
Acq Method	s.m	**Acquired Time**	6/4/2021 9:59:46 AM
IRM Calibration Status	Success	**DA Method**	Default.m
Comment			

Sample Group	**Info.**
Acquisition SW	6200 series TOF/6500 series
Version	Q-TOF B.05.01 (B5125.2)

User Spectra

Fragmentor Voltage	**Collision Energy**	**Ionization Mode**
135	0	ESI



Peak List

m/z	z	Abund	Formula	Ion
175.1147		5314.71		
215.1428	1	5251.69		
231.1384	1	16898.18		
233.1539	1	14720.14	C15 H20 O2	(M+H)+
249.1487	1	5607.95		
271.1302	1	10997.05		
279.1236	1	4069.97		
301.1052	1	10201.56		
319.1152	1	12178.45		
437.1939	1	4233.01		

Formula Calculator Element Limits

Element	Min	Max
C	3	60
H	0	120
O	0	30

Formula Calculator Results

Formula	CalculatedMass	CalculatedMz	Mz	Diff. (mDa)	Diff. (ppm)	DBE
C15 H20 O2	232.1463	233.1536	233.1539	-0.30	-1.29	6.0000

Figure S216. ^{1}H NMR spectrum of **8** at 500 MHz in $CDCl_3$

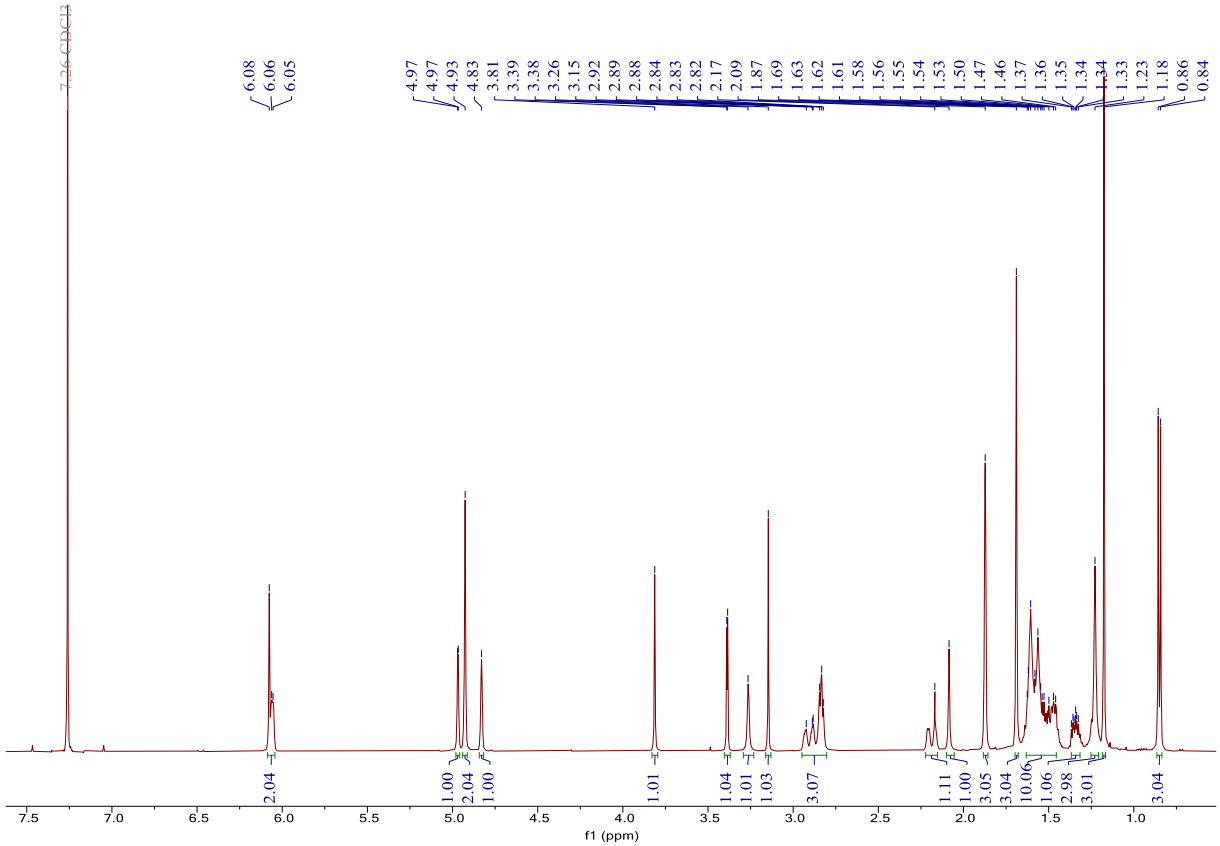


Figure S217. ^{13}C NMR spectrum of **8** at 125 MHz in $CDCl_3$

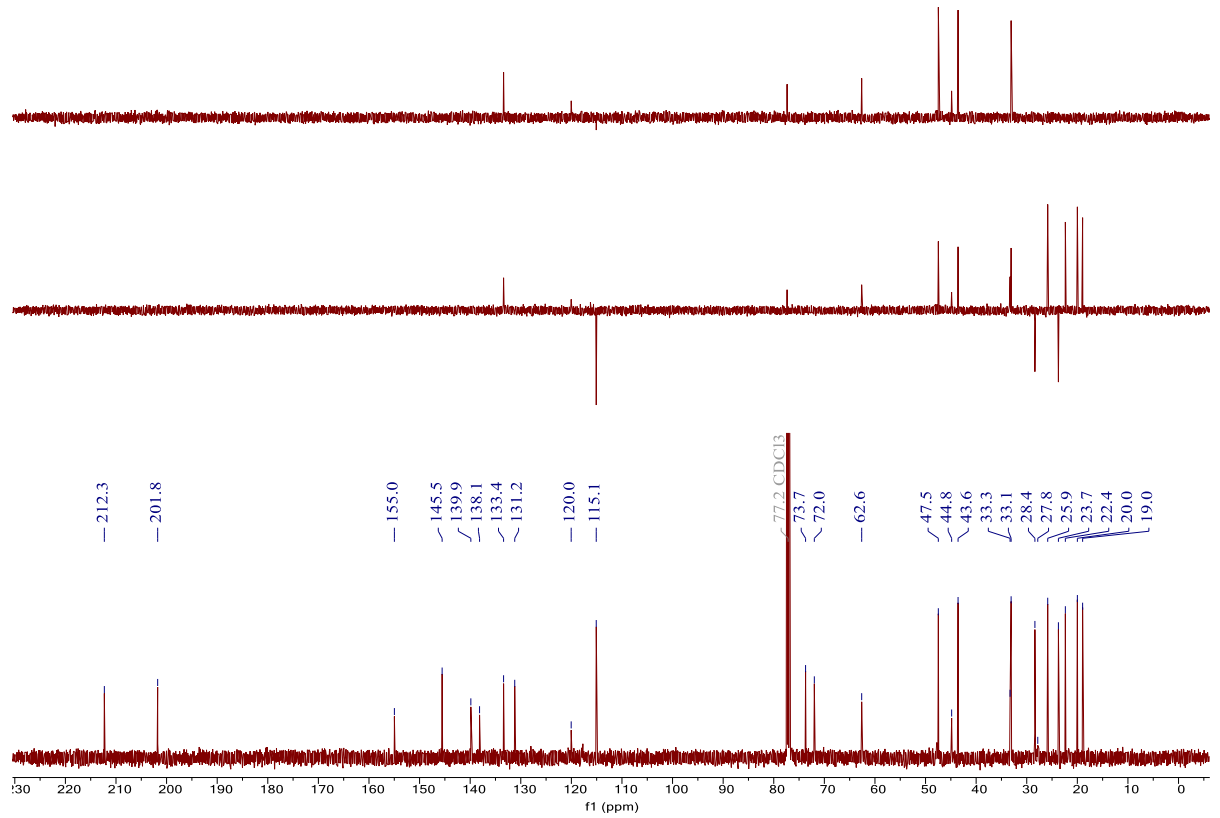


Figure S218. HRESIMS spectrum of **8**

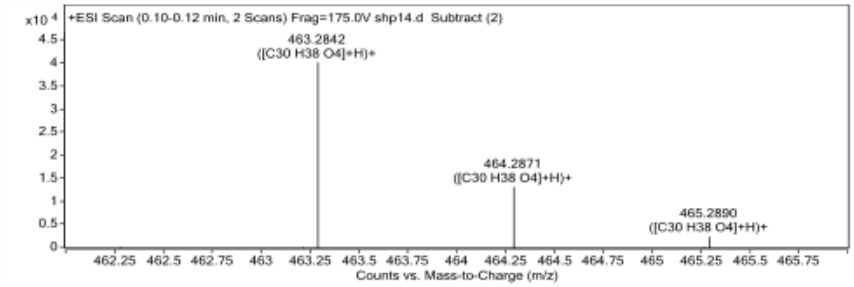
Qualitative Analysis Report

Data Filename	shp14.d	**Sample Name**	shp14
Sample Type	Sample	**Position**	P1-A7
Instrument Name	Instrument 1	**User Name**	
Acq Method	s.m	**Acquired Time**	12/10/2021 9:56:33 AM
IRM Calibration Status	Success	**DA Method**	PCDL.m
Comment			

Sample Group	**Info.**
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125.2)

User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
175	0	ESI



Peak List

m/z	z	Abund	Formula	Ion
213.1269	1	18777.09		
231.1375	1	6873.29		
463.2842	1	40247.54	C30 H38 O4	(M+H)+
464.2871	1	13233.54	C30 H38 O4	(M+H)+
479.2789	1	4586.43		
485.2656	1	16100.65		
486.2689	1	5581.3		
499.2451	1	6954.67		
501.2594	1	6127.13		
947.5423	1	5271.27		

Formula Calculator Element Limits

Element	Min	Max
C	3	120
H	0	240
O	0	30

Formula Calculator Results

Formula	CalculatedMass	CalculatedMz	Mz	Diff. (mDa)	Diff. (ppm)	DBE
C30 H38 O4	462.2770	463.2843	463.2842	0.10	0.22	12.0000

--- End Of Report ---

Figure S219. Specific rotation spectrum of **8**

Rudolph Research Analytical

This sample was measured on an Autopol VI, Serial #91058
Manufactured by Rudolph Research Analytical, Hackettstown, NJ, USA.

Measurement Date : Thursday, 26-NOV-2020

Set Temperature : OFF

Time Delay : Disabled

Delay between Measurement : Disabled

n	Average	Std.Dev.	% RSD	Maximum	Minimum
5	59.74	0.08	0.13	59.84	59.63

S.No	Sample ID	Time	Result	Scale	OR °Arc	WLG.nm	Lg.mm	Conc.g/100ml	Temp.
1	S154-3	08:48:13 PM	59.79	SR	0.1136	589	100.00	0.190	22.2
2	S154-3	08:48:21 PM	59.68	SR	0.1134	589	100.00	0.190	22.2
3	S154-3	08:48:29 PM	59.63	SR	0.1133	589	100.00	0.190	22.2
4	S154-3	08:48:38 PM	59.74	SR	0.1135	589	100.00	0.190	22.2
5	S154-3	08:48:45 PM	59.84	SR	0.1137	589	100.00	0.190	22.2

Figure S220. ^{1}H NMR spectrum of **10** at 500 MHz in $CDCl_3$

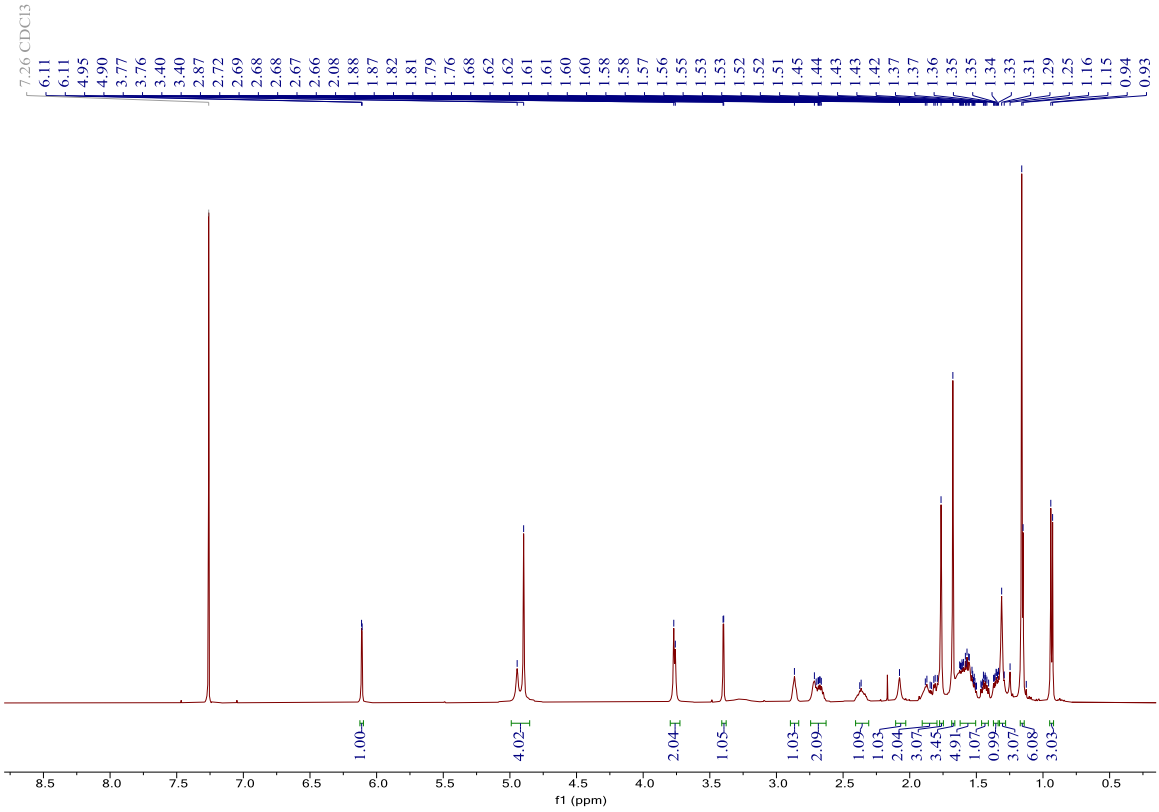


Figure S221 ^{13}C NMR spectrum of **10** at 125 MHz in $CDCl_3$

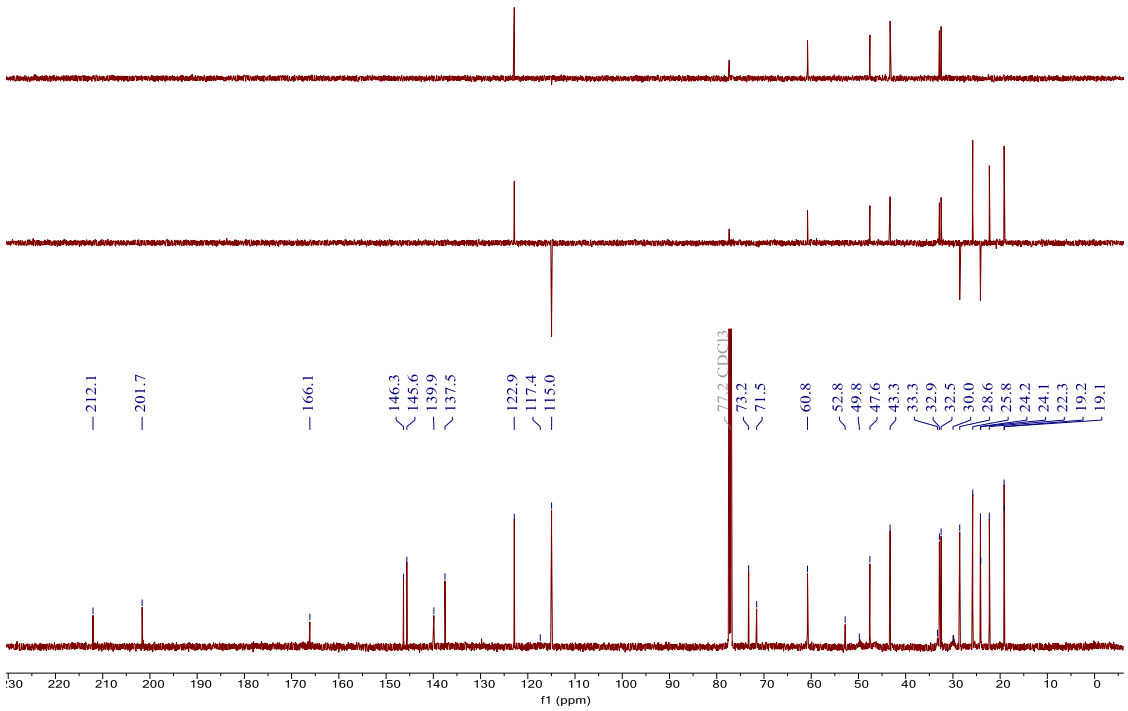


Figure S222. HRESIMS spectrum of synthetic compound **10**

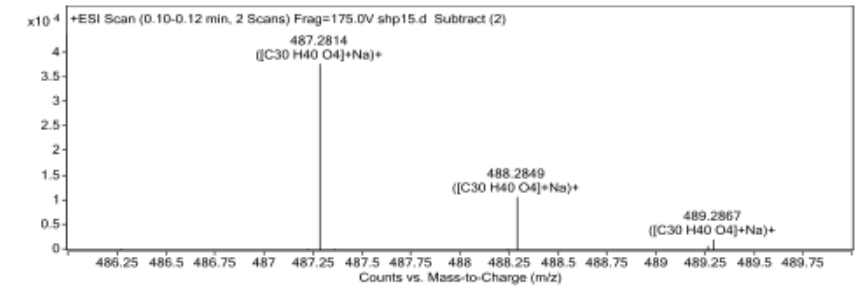
Qualitative Analysis Report

Data Filename	shp15.d	**Sample Name**	shp15
Sample Type	Sample	**Position**	P1-A8
Instrument Name	Instrument 1	**User Name**	
Acq Method	s.m	**Acquired Time**	12/10/2021 9:57:44 AM
IRM Calibration Status	Success	**DA Method**	PCDL.m
Comment			

Sample Group	**Info.**
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125.2)

User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
175	0	ESI



Peak List

m/z	z	Abund	Formula	Ion
215.1426	1	14791.27		
233.1531	1	27721.54		
234.1569	1	4890.08		
447.2888	1	13535.31		
465.2992	1	9187.26		
487.2814	1	37821.93	C30 H40 O4	(M+Na)+
488.2849	1	10759.36	C30 H40 O4	(M+Na)+
951.5741	1	23010.25		
952.5777	1	14998.05		
953.5791	1	4889.56		

Formula Calculator Element Limits

Element	Min	Max
C	3	120
H	0	240
O	0	30

Formula Calculator Results

Formula	CalculatedMass	CalculatedMz	Mz	Diff. (mDa)	Diff. (ppm)	DBE
C30 H40 O4	464.2927	487.2819	487.2814	0.50	1.03	11.0000

--- End Of Report ---

Figure S223. Specific rotation spectrum of **10**

Rudolph Research Analytical

This sample was measured on an Autopol VI, Serial #91058
Manufactured by Rudolph Research Analytical, Hackettstown, NJ, USA.

Measurement Date : Thursday, 26-NOV-2020

Set Temperature : OFF

Time Delay : Disabled

Delay between Measurement : Disabled

n	Average	Std.Dev.	% RSD	Maximum	Minimum
5	77.98	0.60	0.76	78.63	77.00

S.No	Sample ID	Time	Result	Scale	OR °Arc	WLG.nm	Lg.mm	Conc.g/100ml	Temp.
1	STPA	08:35:17 PM	77.00	SR	0.0616	589	100.00	0.080	22.1
2	STPA	08:35:26 PM	78.00	SR	0.0624	589	100.00	0.080	22.2
3	STPA	08:35:43 PM	78.63	SR	0.0629	589	100.00	0.080	22.2
4	STPA	08:35:51 PM	78.00	SR	0.0624	589	100.00	0.080	22.2
5	STPA	08:36:00 PM	78.25	SR	0.0626	589	100.00	0.080	22.3

5. References

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