Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.

Supplementary Information

Hyperforones A-C, Benzoyl-Migrated [5.3.1]-Type Polycyclic Polyprenylated Acylphloroglucinols from *Hypericum forrestii*

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I. Supplementary figures and tables

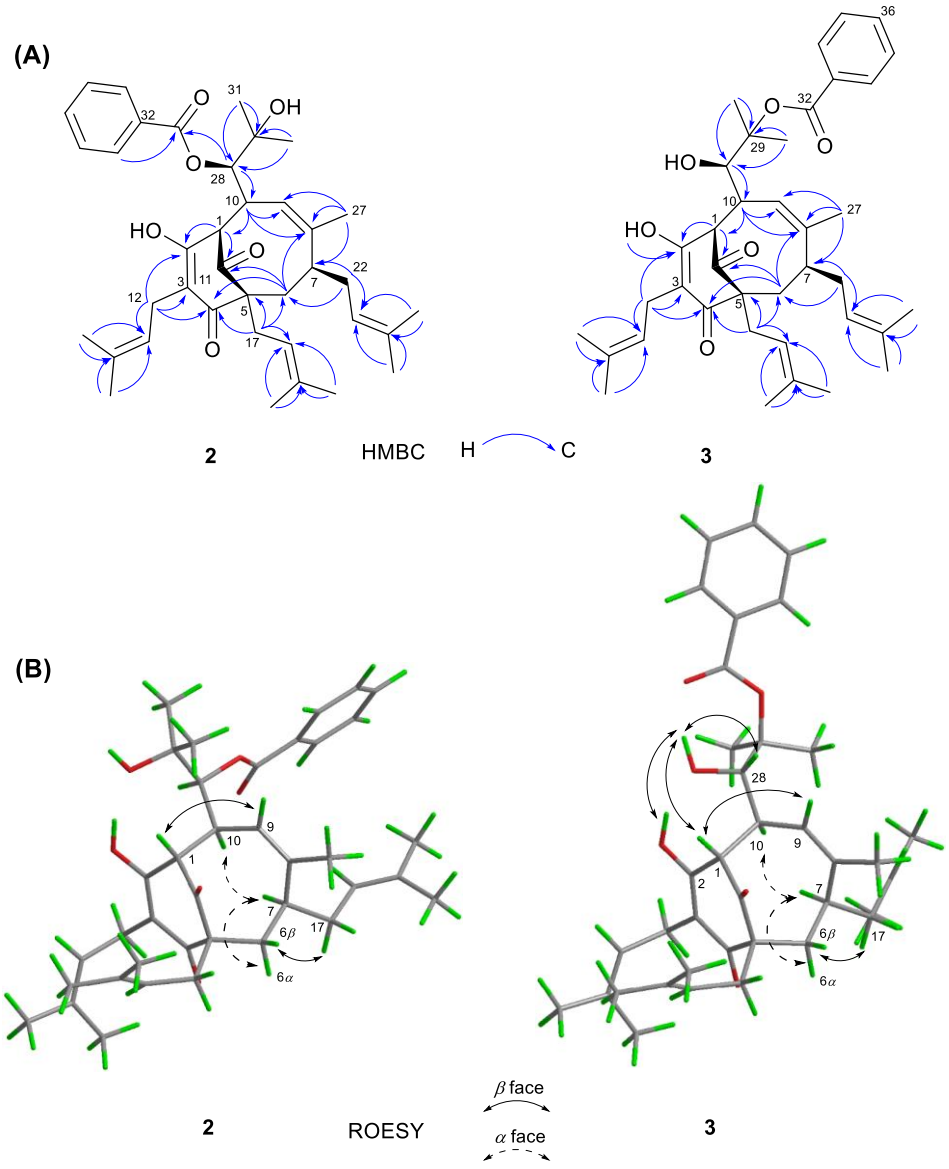


Figure S1-1. Key HMBC and ROESY correlations of compounds **2** and **3**.

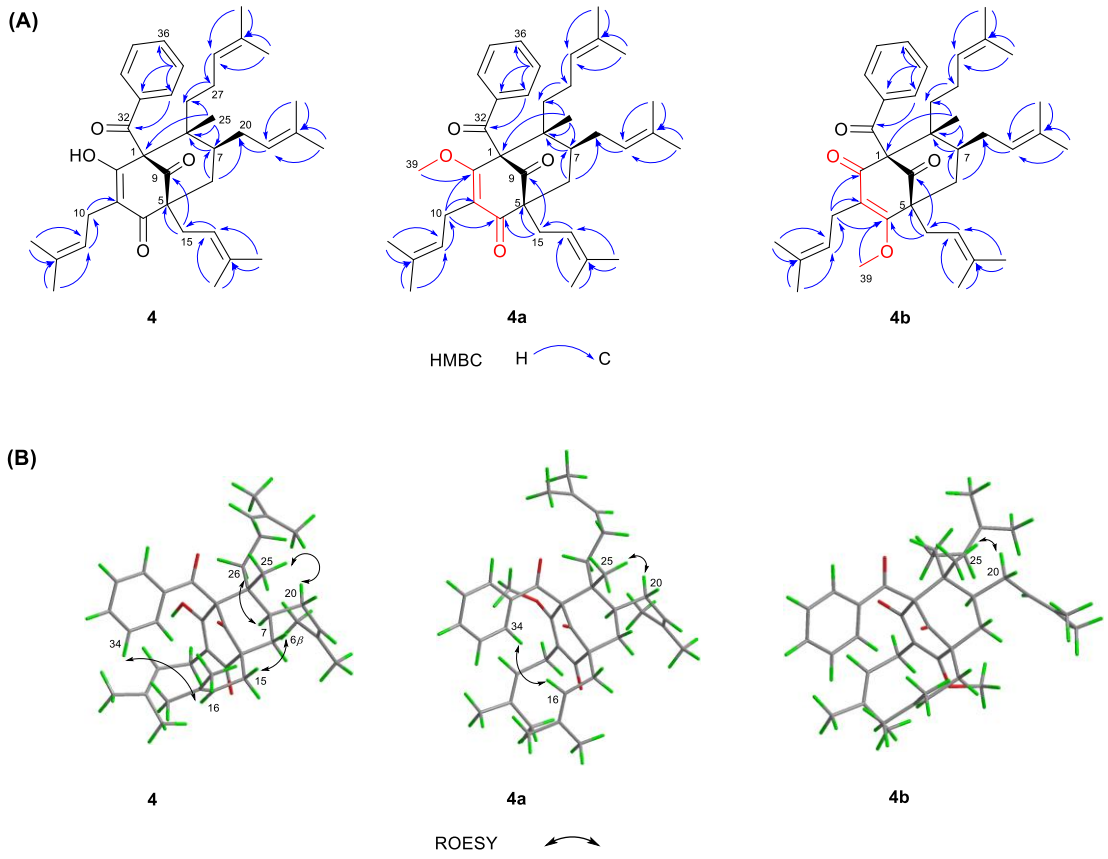


Figure S1-2. Key HMBC and ROESY correlations of compounds **4**, **4a**, and **4b**.

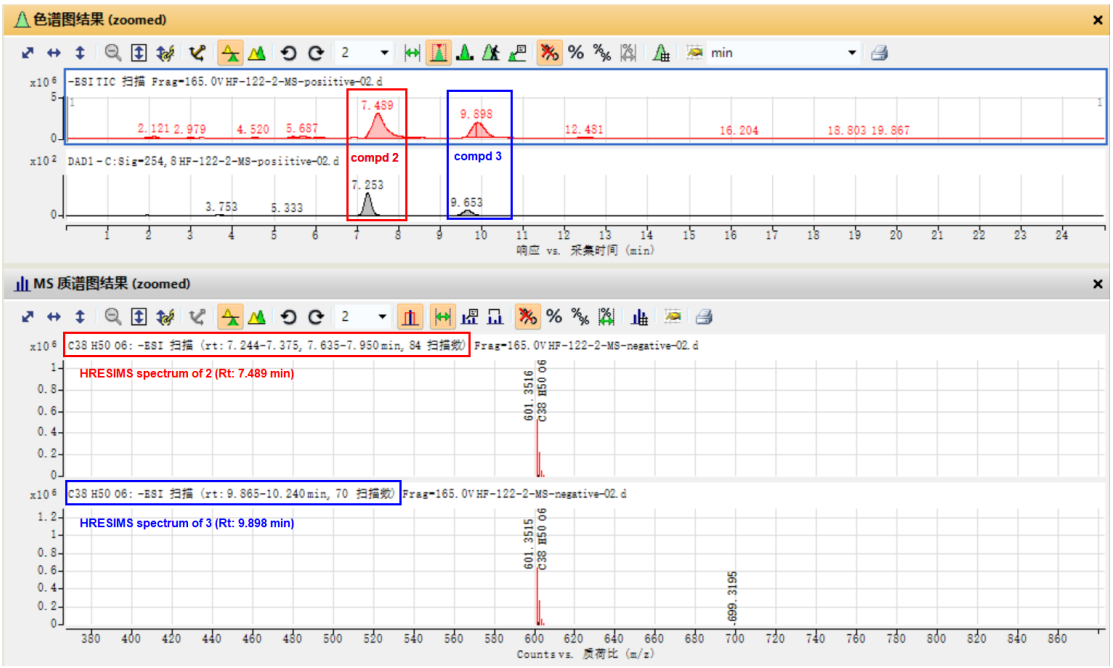


Figure S1-3. LC-MS analysis of the spontaneous interesterification from **2** to **3**.

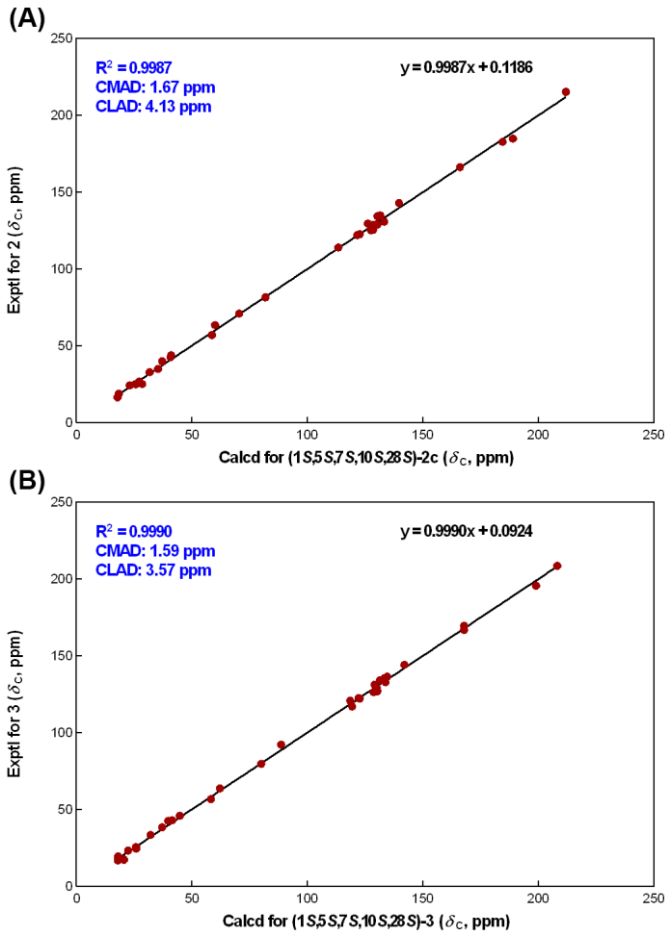


Figure S1-4. Linear correlation between the calculated and experimental ^{13}C NMR chemical shifts for **2** (A) and **3** (B).

(A) Detailed DP4+ result of 1

Functional	Solvent?	Basis Set	Type of Data
mPW1PW91	PCM	6-311+G(d,p)	Unscaled Shifts

	Isomer 1	Isomer 2	Isomer 3	Isomer 4	Isomer 5	Isomer 6
sDP4+ (H data)	0.34%	99.66%	-	-	-	-
sDP4+ (C data)	0.06%	99.94%	-	-	-	-
sDP4+ (all data)	0.00%	100.00%	-	-	-	-
uDP4+ (H data)	97.64%	2.36%	-	-	-	-
uDP4+ (C data)	0.29%	99.71%	-	-	-	-
uDP4+ (all data)	10.76%	89.24%	-	-	-	-
DP4+ (H data)	12.26%	87.74%	-	-	-	-
DP4+ (C data)	0.00%	100.00%	-	-	-	-
DP4+ (all data)	0.00%	100.00%	-	-	-	-

(B) Experimental and calculated (unscaled) NMR data of 1

Functional	Solvent?	Basis Set	Type of Data
mPW1PW91	PCM	6-311+G(d,p)	Unscaled Shifts

		DP4+	0.00%	100.00%	-	-	-
Nuclei	sp2?	Experimental	Isomer 1	Isomer 2	Isomer 3	Isomer 4	Isomer 5
C		54.00	64.89	59.08			
C	x	167.70	177.76	180.48			
C	x	120.60	130.73	127.96			
C	x	198.70	210.78	209.55			
C		61.40	69.81	69.48			
C		40.40	46.75	46.44			
C		38.10	43.68	44.46			
C	x	143.30	155.81	156.07			
C	x	121.98	131.57	131.03			
C		44.20	49.73	49.39			
C		206.60	219.81	221.35			
C		21.30	25.86	25.64			
C	x	121.94	129.53	129.49			
C	x	130.80	144.29	144.03			
C		25.60	27.98	28.11			
C		17.60	18.96	19.08			
C		36.90	42.33	41.79			
C	x	118.30	126.63	126.94			
C	x	133.70	146.69	146.64			
C		25.60	27.49	28.08			
C		17.50	19.07	19.14			
C		32.60	37.41	37.54			
C	x	122.30	130.97	130.16			
C	x	132.10	143.41	144.44			
C		25.50	27.69	28.02			
C		17.90	18.81	18.99			
C		18.00	21.06	20.86			
C		75.00	80.47	80.19			
C		88.50	93.91	96.00			
C		25.00	23.34	25.94			
C		27.00	29.00	28.76			
C	x	165.10	174.39	175.07			
C	x	128.70	134.57	134.33			
C	x	129.60	136.63	137.08			
C	x	129.10	134.24	134.70			
C	x	134.10	140.99	141.51			
C	x	129.10	134.24	134.70			
C	x	129.60	136.63	137.08			
H		3.58	3.06	3.94			
H		2.02	2.29	2.30			
H		1.21	1.47	1.51			
H		2.53	2.57	2.56			
H	x	5.24	5.91	5.78			
H		3.80	3.61	3.88			
H		3.05	3.71	3.70			
H		2.99	3.11	3.14			
H	x	4.89	5.33	5.20			
H		1.60	1.76	1.83			
H		1.65	2.01	2.05			
H		2.47	2.99	3.03			
H		2.26	2.23	2.27			
H	x	4.60	4.92	4.89			
H		1.47	1.70	1.74			
H		1.45	1.61	1.64			
H		1.99	2.34	2.37			
H		1.87	1.96	2.00			
H	x	4.91	5.09	5.20			
H		1.65	1.56	1.76			
H		1.54	1.63	1.65			
H		1.45	1.54	1.59			
H		5.40	5.91	5.59			
H		1.41	1.50	1.51			
H		1.54	1.56	1.53			
H	x	8.15	8.57	8.79			
H	x	7.62	7.95	8.05			
H	x	7.75	8.14	8.22			
H	x	7.62	7.95	8.05			
H	x	8.15	8.57	8.79			

Figure S1-5. DP4+ analyses of calculated and experimental NMR chemical shifts of **1**. Isomer 1: (1*S*,5*S*,7*S*,10*S*,28*R*)-**1**; Isomer 2: (1*S*,5*S*,7*S*,10*S*,28*S*)-**1**.

(A) Detailed DP4+ result of 2

Functional	Solvent?	Basis Set	Type of Data
mPW1PW91	PCM	6-311+G(d,p)	Unscaled Shifts

	Isomer 1	Isomer 2	Isomer 3	Isomer 4	Isomer 5	Isomer 6
sDP4+ (H data)	0.08%	0.00%	0.00%	0.00%	0.00%	99.91%
sDP4+ (C data)	0.00%	0.00%	0.00%	0.00%	0.22%	99.78%
sDP4+ (all data)	0.00%	0.00%	0.00%	0.00%	0.00%	100.00%
uDP4+ (H data)	0.00%	0.00%	99.96%	0.02%	0.02%	0.00%
uDP4+ (C data)	0.00%	0.00%	0.00%	0.00%	7.22%	92.78%
uDP4+ (all data)	0.00%	0.00%	0.00%	0.00%	90.89%	9.11%
DP4+ (H data)	0.00%	0.00%	95.90%	0.00%	0.02%	4.08%
DP4+ (C data)	0.00%	0.00%	0.00%	0.00%	0.02%	99.98%
DP4+ (all data)	0.00%	0.00%	0.00%	0.00%	0.00%	100.00%

(B) Experimental and calculated (unscaled) NMR data of 2

Functional	Solvent?	Basis Set	Type of Data
mPW1PW91	PCM	6-311+G(d,p)	Unscaled Shifts

		DP4+	0.00%	0.00%	0.00%	0.00%	0.00%	100.00%
Nuclei	sp2?	Experimental	Isomer 1	Isomer 2	Isomer 3	Isomer 4	Isomer 5	Isomer 6
C		58.70	70.92	70.10	60.33	61.88	66.32	61.75
C	x	184.50	201.56	206.91	180.71	180.76	194.94	194.21
C	x	113.40	122.97	125.03	123.04	124.96	116.81	121.66
C	x	188.90	183.92	185.55	206.62	208.08	197.03	196.52
C		60.10	64.91	64.95	66.99	68.95	67.32	68.48
C		41.05	44.28	44.81	45.31	46.37	44.51	47.82
C		37.10	43.29	42.04	41.63	41.68	41.64	43.71
C	x	139.60	155.07	153.10	152.46	154.82	150.52	152.30
C	x	128.50	131.45	135.52	133.11	131.14	135.56	137.28
C		40.10	48.06	47.12	54.00	47.76	53.69	46.49
C	x	211.90	219.94	219.11	219.18	220.69	227.95	228.44
C		23.10	26.07	26.95	25.64	25.49	27.23	27.17
C	x	127.50	127.51	128.17	129.46	129.04	135.27	133.65
C	x	126.20	153.02	152.45	142.36	142.63	138.14	138.19
C		25.60	28.19	28.23	27.41	28.44	28.13	28.04
C		17.90	19.47	19.26	18.50	19.13	19.18	19.02
C		35.30	39.33	40.28	41.85	42.91	41.45	38.32
C	x	121.60	126.31	126.17	126.53	127.82	130.02	130.36
C	x	130.40	147.57	147.36	145.31	145.18	142.64	143.24
C		25.80	28.06	27.83	27.60	27.31	28.13	27.88
C		17.80	19.04	18.83	18.67	18.60	19.21	19.52
C		31.80	36.86	36.96	36.08	36.34	36.99	36.11
C	x	122.70	130.77	131.43	130.88	130.52	132.37	130.91
C	x	131.60	143.98	143.41	143.18	143.37	142.56	143.58
C		25.50	27.72	27.44	27.47	27.38	27.89	28.28
C		17.94	18.94	19.09	18.50	18.88	18.95	18.82
C		18.40	20.96	20.81	19.99	20.22	20.61	21.32
C		81.90	92.13	83.35	80.70	80.32	84.18	87.57
C		70.50	77.13	78.74	81.95	83.05	77.10	76.47
C		28.60	27.44	28.60	29.57	31.59	32.47	28.11
C		27.30	26.96	27.16	27.55	26.79	28.77	29.72
C	x	166.10	178.76	173.80	171.85	173.71	173.65	176.86
C	x	130.30	135.38	135.26	134.31	135.04	136.99	137.43
C	x	129.70	137.61	137.49	136.49	136.91	137.48	137.49
C	x	128.60	134.76	134.52	133.52	134.86	134.06	133.96
C	x	133.20	141.47	140.75	139.69	141.29	139.80	139.45
C	x	128.60	134.76	134.52	133.52	134.86	134.06	133.96
C	x	129.70	137.61	137.49	136.49	136.91	137.48	137.49
H		3.69	3.45	4.11	4.53	4.58	4.45	4.31
H		1.79	2.08	2.08	2.25	2.33	2.29	1.88
H		0.92	1.58	1.53	1.47	1.48	1.37	1.19
H		2.49	2.63	2.89	2.42	2.41	2.64	2.61
H	x	4.98	5.96	5.73	5.89	5.96	5.97	5.45
H		3.25	3.18	4.10	3.21	3.90	3.27	3.40
H		2.94	4.03	3.78	2.97	3.03	2.93	3.56
H		2.89	3.22	3.54	3.77	3.82	3.70	2.97
H	x	5.09	5.70	5.82	5.59	5.71	5.95	5.82
H		1.55	1.98	2.01	1.77	1.78	1.84	1.74
H		1.64	2.01	2.02	1.82	1.96	1.98	2.12
H		2.27	3.18	3.21	2.86	2.95	2.84	2.78
H		2.14	2.32	2.29	2.04	2.15	2.17	2.38
H	x	4.62	5.23	5.21	4.87	4.98	5.03	5.21
H		1.47	1.67	1.57	1.65	1.61	1.73	1.93
H		1.46	1.63	1.64	1.50	1.53	1.55	1.65
H		1.89	2.50	2.61	2.44	2.36	2.56	2.14
H		1.74	2.09	1.94	1.78	1.71	1.81	2.09
H	x	4.80	5.36	5.12	5.03	4.65	5.13	5.44
H		1.56	1.75	1.52	1.65	1.07	1.71	1.74
H		1.50	1.74	1.62	1.61	1.50	1.67	1.69
H		1.37	1.72	1.59	1.48	1.44	1.54	1.65
H		4.91	5.24	5.25	5.46	5.37	5.29	5.30
H		0.96	1.04	1.18	1.19	1.36	1.04	1.07
H		1.18	1.14	1.23	1.63	1.79	1.43	1.43
H	x	8.14	8.80	8.93	8.71	8.64	8.98	9.21
H	x	7.55	8.03	7.98	7.98	7.90	8.00	8.01
H	x	7.67	8.20	8.18	8.10	8.10	8.10	8.14
H	x	7.55	8.03	7.98	7.98	7.90	8.00	8.01
H	x	8.14	8.80	8.93	8.71	8.64	8.98	9.21

Figure S1-6. DP4+ analyses of calculated and experimental NMR chemical shifts of **2**. Isomer 1: (1*S*,5*S*,7*S*,10*S*,28*R*)-**2a**; Isomer 2: (1*S*,5*S*,7*S*,10*S*,28*S*)-**2a**; Isomer 3: (1*S*,5*S*,7*S*,10*S*,28*R*)-**2b**; Isomer 4: (1*S*,5*S*,7*S*,10*S*,28*S*)-**2b**; Isomer 5: (1*S*,5*S*,7*S*,10*S*,28*R*)-**2c**; Isomer 6: (1*S*,5*S*,7*S*,10*S*,28*S*)-**2c**.

(A) Detailed DP4+ result of 3

Functional	Solvent?	Basis Set	Type of Data
mPW1PW91	PCM	6-311+G(d,p)	Unscaled Shifts

	Isomer 1	Isomer 2	Isomer 3	Isomer 4	Isomer 5	Isomer 6
sDP4+ (H data)	78.28%	21.72%	–	–	–	–
sDP4+ (C data)	0.00%	100.00%	–	–	–	–
sDP4+ (all data)	0.02%	99.98%	–	–	–	–
uDP4+ (H data)	0.01%	99.99%	–	–	–	–
uDP4+ (C data)	0.04%	99.96%	–	–	–	–
uDP4+ (all data)	0.00%	100.00%	–	–	–	–
DP4+ (H data)	0.05%	99.95%	–	–	–	–
DP4+ (C data)	0.00%	100.00%	–	–	–	–
DP4+ (all data)	0.00%	100.00%	–	–	–	–

(B) Experimental and calculated (unscaled) NMR data of 3

Functional	Solvent?	Basis Set	Type of Data
mPW1PW91	PCM	6-311+G(d,p)	Unscaled Shifts

		DP4+	0.00%	100.00%	–	–	–
Nuclei	sp2?	Experimental	Isomer 1	Isomer 2	Isomer 3	Isomer 4	Isomer 5
C		58.20	57.10	61.01			
C	x	167.90	178.26	179.42			
C	x	119.40	125.02	124.33			
C	x	199.00	204.54	206.87			
C		62.10	69.80	68.32			
C		41.40	47.62	46.51			
C		39.80	43.80	46.19			
C	x	142.00	153.83	152.69			
C	x	129.10	131.42	139.11			
C		44.80	50.47	49.71			
C		208.10	222.07	220.51			
C		22.40	25.61	25.84			
C	x	122.70	128.44	129.84			
C	x	131.40	142.22	142.27			
C		26.00	27.78	27.93			
C		18.00	18.82	19.14			
C		37.20	37.98	41.76			
C	x	118.60	128.35	128.18			
C	x	134.50	144.87	144.62			
C		25.90	27.80	27.00			
C		17.90	19.22	18.64			
C		32.20	36.12	36.44			
C	x	122.10	130.10	130.04			
C	x	133.30	143.84	143.65			
C		25.80	28.29	28.14			
C		18.07	18.76	18.66			
C		18.15	22.42	21.80			
C		80.00	83.08	85.02			
C		88.70	98.78	98.34			
C		20.60	22.84	19.73			
C		25.20	28.17	27.66			
C	x	167.80	177.47	176.73			
C	x	130.30	135.33	134.74			
C	x	130.00	136.94	137.00			
C	x	128.70	134.01	134.11			
C	x	133.80	141.00	140.91			
C	x	128.70	134.01	134.11			
C	x	130.00	136.94	137.00			
H		3.71	3.65	3.83			
H		2.18	1.88	2.35			
H		1.31	1.45	1.51			
H		2.30	2.42	2.16			
H	x	5.21	5.89	5.64			
H		2.91	3.30	2.62			
H		3.21	3.81	4.00			
H		3.05	3.04	2.90			
H	x	5.06	5.62	5.54			
H		1.65	1.76	1.78			
H		1.73	1.93	2.05			
H		2.36	2.46	2.26			
H		2.57	2.85	2.87			
H	x	4.63	5.06	4.96			
H		1.54	1.77	1.61			
H		1.52	1.59	1.47			
H		1.95	2.05	1.98			
H		1.95	1.96	2.13			
H	x	4.79	5.36	5.30			
H		1.60	1.68	1.69			
H		1.52	1.63	1.68			
H		1.53	1.82	1.78			
H		4.20	4.32	4.21			
H		1.56	1.99	1.49			
H		1.47	1.79	1.33			
H	x	7.98	8.68	8.65			
H	x	7.45	7.93	7.91			
H	x	7.60	8.13	8.13			
H	x	7.45	7.93	7.91			
H	x	7.98	8.68	8.65			

Figure S1-7. DP4+ analyses of calculated and experimental NMR chemical shifts of **3**. Isomer 1: (1*S*,5*S*,7*S*,10*S*,28*R*)-**3**; Isomer 2: (1*S*,5*S*,7*S*,10*S*,28*S*)-**3**.

Table S1-1. ^{1}H and ^{13}C NMR Spectroscopic Data for **4**, **4a**, and **4b**.

	bzhyperforin (**4**)[a]		**4a**[b]		**4b**[b]	
No.	δ_H, mult. (*J*, Hz)	δ_C	δ_H, mult. (*J*, Hz)	δ_C	δ_H, mult. (*J*, Hz)	δ_C
1		78.9		74.2		80.2
2		-[d]		170.0		194.5
3		120.5		123.0		126.9
4		-[d]		197.4		173.6
5		62.0		65.0		59.8
6a	1.42, br. dd (12.8, 4.8)	41.8	1.45, br. dd (13.0, 4.4)	42.6	1.48, br. dd (13.9, 4.0)	39.8
6b	2.04, dd (12.8, 4.8)[c]		1.96 dd (13.0, 4.4)		2.02, dd (13.9, 4.0)[c]	
7	1.97, dd (13.8, 12.8)[c]	42.7	1.81, dd (13.9, 13.0)	40.4	1.84, dd (13.9, 11.7)[c]	43.3
8		50.9		50.3		51.1
9		210.3		208.0		207.4
10a	3.15, dd (14.5, 7.5)	22.7	3.30, dd (15.7, 6.7)	23.5	3.25, dd (15.3, 6.9)	23.5
10b	3.06, dd (14.5, 7.5)		3.24, dd (15.7, 6.7)		3.17, dd (15.3, 6.9)	
11	5.13, t (7.5)	122.9	4.98, t (6.7)[c]	121.7	5.05, t (6.9)[c]	121.4
12		132.9[c]		133.1		133.2
13	1.64, br. s[c]	26.1[c]	1.68, br. s[c]	26.1	1.65, br. s[c]	26.0
14	1.66, s	18.1	1.66, br. s[c]	18.2[c]	1.63, s	18.2
15a	2.50, br.dd (14.0, 7.1)[c]	30.5	2.57, dd (14.3, 7.5)	29.6	2.58, dd (14.3, 7.2)	29.9
15b	2.50, br.dd (14.0, 7.1)[c]		2.47, dd (14.3, 7.5)		2.43, dd (14.3, 7.2)	
16	5.00, t (7.1)	121.2	5.01, t (7.5) [c]	119.8	5.01, t (7.2)[c]	119.6
17		134.8		134.7		134.5
18	1.64, br. s[c]	26.3	1.66, br. s[c]	26.2	1.67, s	26.2
19	1.64, br. s[c]	18.3	1.66, br. s[c]	18.3	1.65, br. s[c]	18.1
20a	1.80, dd (13.8, 7.2)[c]	28.8	1.70, dd (13.9, 7.1)[c]	28.3	1.83, dd (11.7, 7.2)[c]	27.4
20b	2.11, dd (13.8, 7.2)[c]		2.06, dd (13.9, 7.1)[c]		2.14, dd (11.7, 7.2)[c]	
21	5.04, t (7.2)[c]	123.9	4.93, t (7.1)	122.5	5.01, t (7.2)[c]	122.6
22		134.2		133.5		133.7
23	1.70, s	26.1[c]	1.68, s[c]	25.9	1.70, s	25.9[c]
24	1.60, br. s[c]	18.2	1.55, s	18.2[c]	1.59, s	18.0
25	1.10, s	15.7	1.20, s	15.8	1.12, s	14.2
26a	1.86, m[c]	38.0	1.90, m	37.4	2.04, m	36.7
26b	1.86, m[c]		1.74, m[c]		1.61, m[c]	
27a	1.97, m[c]	25.5	2.01, m[c]	24.3	2.17, m[c]	25.1
27b	2.04, m[c]		2.01, m[c]		1.93, m[c]	
28	5.04, t (7.2)[c]	126.1	5.02, m[c]	124.9	5.06, m[c]	124.7
29		131.7		131.2		131.3
30	1.65, s	25.9	1.66, br. s[c]	25.8	1.65, br. s[c]	25.8[c]
31	1.60, br. s[c]	17.9	1.58, s	17.8	1.61, br. s[c]	17.9
32		195.8		193.5		193.6
33		138.6		137.4		136.4
34, 38	7.57, br. d (7.7)[c]	129.7[c]	7.60, br. d. (7.8)[c]	128.5[c]	7.41, br. d (7.8)[c]	128.8[c]
35, 37	7.25, br. dd (7.7, 7.4)[c]	128.6[c]	7.30, br. dd (7.8, 7.3)[c]	128.1[c]	7.22, br.dd (7.8, 7.4)[c]	127.8[c]
36	7.41, br. t (7.4)	132.9[c]	7.43, br. t (7.3)	132.1	7.37, br. t (7.4)	132.0
39			3.39, s	61.8	4.02, s	62.6

[a] Measured in methanol-d_4. ^{1}H NMR measured in 500 MHz, ^{13}C NMR measured in 125 MHz.

[b] Measured in $CDCl_3$. ^{1}H NMR measured in 600 MHz, ^{13}C NMR measured in 150 MHz.

[c] Overlapped signals.

[d] Not observed.

II. Experimental section

2.1 General experimental procedures

Optical rotations were measured on a JASCO P-1020 polarimeter. The UV spectra were recorded on a UV-2450 UV/vis spectrophotometer. The ECD spectra were measured by a JASCO J-810 spectrometer. The IR measurements were performed on a Bruker Tensor 27 spectrometer. The 1D and 2D spectra were recorded on Bruker Avance III-500 MHz or AV-600 MHz spectrometers using standard pulse sequences in $CDCl_3$, methanol-d_4 and dimethyl sulfoxide-d_6 with TMS as an internal standard. The HRESIMS data were acquired using an Agilent 6520B UPLC-Q-TOF mass spectrometer. LC-MS analysis was performed on an Agilent 1290 series instrument with a SHIMADZU Shim-pack VP-ODS column (5 μm, 250 × 4.6 mm, i.d.) using MeOH-H_2O (94:6, v/v, 1.0 $mL \cdot min^{-1}$) as mobile phase. Column chromatography (CC) separations was carried out using silica gel (100-200 mesh and 200-300 mesh; Qingdao Haiyang Chemical Co., Ltd., Qingdao, China), Sephadex LH-20 (40-70 μm; Amersham Pharmacia Biotech AB, Uppsala, Sweden), and ODS RP-C_{18} (40-63 μm, FuJi, Japan). An Agilent 1100 series system with an Agilent ZORBAX Eclipse XDB-C18 column (5 μm, 150 × 4.6 mm, i.d.) was used for HPLC analysis. Preparative silica gel thin-layer chromatography (TLC) were performed on precoated plates GF-254 (Qingdao Haiyang Chemical Co., Ltd., Qingdao, China). Preparative HPLC was carried out using a Shimadzu LC-6AD series instrument equipped with a Shim-pack RP-C_{18} column (10 μm, 200 × 20 mm, i.d.). Recycling preparative HPLC was run on a SHIMADZU LC-20A series instrument equipped with a Shim-pack PRC-ODS (H) column (5 μm, 200 × 20 mm, i.d.).

2.2 Plant material

In October 2017, the fruits of *Hypericum forrestii* (Chittenden) N. Robson were harvested in Tengchong, Yunnan Province of China (GPS: 98°28'53" E, 25°17'39" N). The plant materials were authenticated by Professor Min-Jian Qin of China Pharmaceutical University. A voucher specimen (No. 2017GSHF) has

been stored in the Department of Natural Medicinal Chemistry, China Pharmaceutical University.

2.3 Extraction and isolation

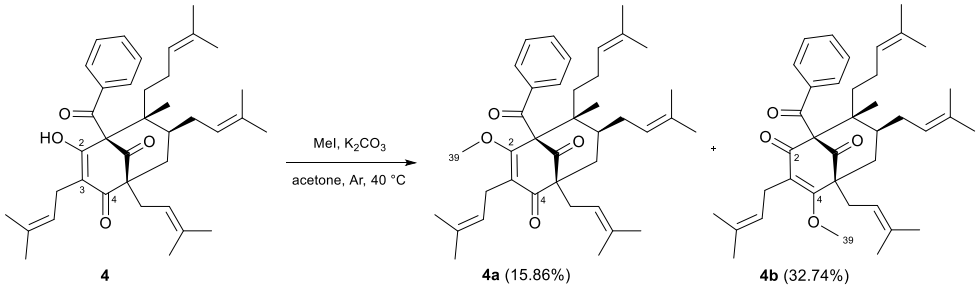
Air-dried and powdered fruits of *H. forrestii* (10.0 kg) were extracted with 95% aqueous EtOH (3 × 50.0 L, each 5.0 h) under ultrasonic agitation at 80.0 Hz and 40.0 °C. The solvent was removed under reduced pressure and yielded a dark-brown oil as crude extract (1.5 kg). The extract was then dissolved in 1.5 L of warm water and extracted with petroleum ether (3 × 3.0 L). The petroleum ether fraction (242.1 g) was subjected to a silica gel CC (100-200 mesh; 1.5 Kg; 36.0 × 9.0 cm, i.d.), and fractions Fr. 1-7 were obtained by eluting with a petroleum ether-dichloromethane gradient system (100:1, 5:2, 1:100, v/v). Further fractionation steps were guided by ^{1}H NMR analyses of the crude subfraction samples for the targeted isolations of benzoyl-PPAPs.

Fr.6 (40.5 g) was separated on an ODS CC to afford subfractions Fr. 6A-6G with a MeOH/H_2O gradient system (62:38, 72:28, 78:22, 88:12, 98:2, v/v) as mobile phase. Fr. 6F (1.1 g) was fractioned with Sephadex LH-20 CC, employing MeOH as mobile phase. Purification of compound **1** (2.5 mg) from Fr. 6F3 (40.2 mg) was carried out on preparative HPLC eluting with MeCN-H_2O (88:12, v/v, 10.0 mL·min^{-1}). Fr. 6D (1.5 g) was separated into five subfractions Fr. 6D1-6D5 by Sephadex LH-20 (MeOH) and silica gel CC with a petroleum ether-dichloromethane gradient system (5:1, 1:1, 1:5, v/v). Fr. 6D5 (20.1 mg) was then purified by recycling preparative HPLC with CH_3CN-H_2O (88:12, v/v, 10.0 mL·min^{-1}) as mobile phase to yield compound **2** (2.0 mg) and **3** (2.2 mg).

Fr. 4 (47.4 g) was loaded on an ODS CC (100.0 g; 31.0 × 2.5 cm, i.d.), and eluted with a MeOH/H_2O gradient system (65:35, 75:25, 80:20, 85:15, 95:5, v/v) to afford seven subfractions Fr. 4A-4G. Fr. 4C (8.6 g) was separated by a silica gel CC (200-300 mesh; 160.0 g; 30.0 × 4.5 cm, i.d.) to afford Fr. 4C1-4C10 with petroleum ether-acetone (50:1, 20:1, 10:1, 5:1, v/v) as mobile phase. Fr. 4C5 (760.3 mg) was separated into ten subfractions Fr. 4C5A-4C5J by Sephadex LH-

20 CC (MeOH). Fr. 4C5E (564.7 mg) was chromatographed on an ODS CC and eluted with a gradient of MeOH-H_2O (68:32, 78:22, 82:18, 88:12, 98:2, v/v) to afford six subfractions Fr. 4C5E1-4C5E6. Finally, Fr. 4C5E4 (100.2 mg) and 4C5E5 (113.1 mg) were further purified by preparative HPLC using MeCN-H_2O (90:10, v/v, 10.0 mL·min^{-1}) to give compounds **4** (50.8 mg) and **5** (3.1 mg), respectively.

2.4 Methylation of 4



To an oven-dried 25 mL round-bottom flask fitted with a magnetic stir bar was added compound **4** (48.0 mg, 84.1 μmol, dissolved in 3 mL acetone) and K_2CO_3 (232.4 mg, 1.7 mmol). Iodomethane (MeI, 62.8 μL, 1.0 mmol) was then added and allowed to stir for 24 h at 40 °C under an argon atmosphere. The mixture was quenched with H_2O (2 mL) and extracted with EtOAc (3 × 10 mL). The combined organic layer was then dried over Na_2SO_4, filtered, and concentrated in vacuo. Purifications of **4a** (7.8 mg, 15.86%) and **4b** (16.1 mg, 32.74%) were carried out on preparative TLC, eluting with petroleum ether–acetone (3:1, v/v).

2.5 Characterization data of 1-4, 4a, and 4b

*Hyperforone A (**1**)*: yellow oil; $[\alpha]^{25}_{D}$ −102 (*c* 0.1, MeOH); UV (MeOH) λ_{max} (log ε) 205 (4.50), 231 (4.34), 269 (4.10) nm; ECD (MeOH) λ_{max} ($\Delta\varepsilon$) 205 (−30.41), 212 (−13.49), 226 (+5.68), 267 (+29.41), 307 (−29.58) nm; IR (KBr) ν_{max} 3777, 3462, 2970, 2918, 1723, 1626, 1448, 1376, 1267, 1177, 1095, 1070, 1026 cm^{-1}; ^{1}H and ^{13}C NMR data see Table 1 in the manuscript; HRESIMS *m/z* 583.3424 $[M - H]^-$ (calcd for $C_{38}H_{47}O_5$, 583.3429).

*Hyperforone B (**2**)*: yellow oil; $[\alpha]^{25}_{D}$ −70 (*c* 0.1, MeOH); UV (MeOH) λ_{max} (log ε) 204 (4.22), 226 (3.97), 289 (3.80) nm; ECD (MeOH) λ_{max} ($\Delta\varepsilon$) 205

(−30.60), 213 (−13.69), 228 (−11.24), 292 (+13.59), 319 (−15.68) nm; IR (KBr) ν_{max} 3908, 3778, 3447, 2952, 2853, 1716, 1595, 1448, 1384, 1285, 1114, 1069 cm^{-1}; ^{1}H and ^{13}C NMR data see Table 1 in the manuscript; HRESIMS *m/z* 601.3531 $[M - H]^-$ (calcd for $C_{38}H_{49}O_6$, 601.3535).

*Hyperforone C (**3**)*: yellow oil; $[\alpha]^{25}_D$ −115 (*c* 0.1, MeOH); UV (MeOH) λ_{max} (log ε) 204 (4.46), 229 (4.30), 274 (4.08) nm; ECD (MeOH) λ_{max} ($\Delta\varepsilon$) 206 (−56.62), 217 (−25.21), 230 (−21.61), 272 (+43.77), 316 (−31.05) nm; IR (KBr) ν_{max} 3777, 3449, 2970, 2922, 1716, 1600, 1447, 1382, 1284, 1114, 1070 cm^{-1}; ^{1}H and ^{13}C NMR data see Table 1 in the manuscript; HRESIMS *m/z* 601.3540 $[M - H]^-$ (calcd for $C_{38}H_{49}O_6$, 601.3535).

*Bzhyperforin (**4**)*: light-yellow oil; $[\alpha]^{25}_D$ −66 (*c* 0.2, MeOH); UV (MeOH) λ_{max} (log ε) 203 (4.56), 245 (4.21), 281 (4.09) nm; ECD (MeOH) λ_{max} ($\Delta\varepsilon$) 206 (+3.62), 223(−9.87), 247 (+39.32), 270 (−38.78), 302 (+4.24) nm; IR (KBr) ν_{max} 3449, 2967, 2917, 1722, 1601, 1447, 1378, 1222, 1022 cm^{-1}; ^{1}H and ^{13}C NMR data see Table S1-1; HRESIMS *m/z* 569.3639 $[M - H]^-$ (calcd for $C_{38}H_{49}O_4$, 569.3636).

*Compound **4a***: light-yellow oil; UV (MeOH) λ_{max} (log ε) 207 (4.52), 245 (4.28), 270 (4.11) nm; ECD (MeOH) λ_{max} ($\Delta\varepsilon$) 204 (+3.19), 220(−24.68), 246 (+14.89), 268 (−11.40), 300 (−4.47) nm; ^{1}H and ^{13}C NMR data see Table S1-1; HRESIMS *m/z* 585.3944 $[M + H]^-$ (calcd for $C_{39}H_{53}O_4$, 585.3938).

*Compound **4b***: light-yellow oil; UV (MeOH) λ_{max} (log ε) 207 (4.39), 247 (4.24), 275 (4.04) nm; ECD (MeOH) λ_{max} ($\Delta\varepsilon$) 202 (+5.92), 210 (+12.51), 229(−10.94), 247 (+20.16), 269 (−38.32), 304 (+4.75) nm; ^{1}H and ^{13}C NMR data see Table S1-1; HRESIMS *m/z* 585.3941 $[M + H]^-$ (calcd for $C_{39}H_{53}O_4$, 585.3938).

2.6 Biological assays

Cell culture

The human cancer cell lines MDA-MB-231, A549 and HOS were purchased from the Chinese Academic of Sciences. MDA-MB-231 cells were cultured in L-12 medium. A549 cells were cultured in F12K medium. HOS cells were cultured in DMEM medium.

All the cells were supplemented with FBS (10%), penicillin (100 U/mL), and streptomycin (100 U/mL) at 37 °C in a humidified atmosphere with 5% CO_2.

Cytotoxicity bioassay

The cells were seeded onto 96-well culture plates (5.0×10^3 cells per well), and were treated with different concentrations of each compound for 48 h. MTT (5 mg/ml) was dissolved in PBS and sterile filtered, then 20 μL of the prepared solution was added to each well and cells were incubated for 4 h. The formed formazan crystals were dissolved in DMSO (150 μL/well) by constant shaking for 10 min. The absorbance was measured on a microplate reader (SpectraMax Plus384, Molecular Devices) at a test wavelength of 570 nm and a reference wavelength of 630 nm. In each experiment, three replicates of wells were prepared for each sample. The ratio of the living cells was determined by the difference of the absorbance between those of samples and controls. These differences were expressed in percentage, and cytotoxic activity was indicated as an IC_{50} value.

Statistical analysis

All experiments were performed at least three times. The results were analyzed using one-way ANOVA with Tukey's multiple comparison test. The data are given as the mean ± SD.

III. Computational details

3.1 Conformational analyses

Conformational analyses was performed in Yinfo Cloud Platform (http://cloud.yinfotek.com) using Gentor with systematic search algorithm that all rotatable bonds among atoms C-10, C-28, C-29, C-30, C-31, and C-32 were rotated by every 60 degrees.[1] The output conformers were then optimized at MMFF94 force field and filtered by RMSD threshold of 0.5 Å and energy window of 5 kcal/mol.

3.2 NMR calculations

The theoretical calculations were carried out using Gaussian 09.[2] At first, conformers were optimized at PM6 and HF/6-31G(d) theory levels, consecutively. Room-temperature equilibrium populations were calculated according to Boltzmann distribution law (1), based on which dominative conformers were saved with the values over 1%. The chosen conformers were finally optimized at B3LYP/6-31G(d) in gas phase (Table S3-1). Vibrational frequency analysis confirmed the stable structures. NMR calculations were carried out following Tantillo and co-workers' recommendations, using the Gauge-Including Atomic Orbitals (GIAO) method at mPW1PW91/6-311+G(2d,p) level in DMSO (for **1**-**2**) or chloroform (for **3**) simulated by the IEFPCM model.[3] Finally, the TMS-corrected NMR chemical shift values were averaged according to Boltzmann distribution and fitted to the experimental values by linear regression. DP4+ statistical analyses were performed using the Excel spreadsheed from sarotti-nmr.weebly.com.[4]

$$\frac{N_i}{N} = \frac{g_i e^{-\frac{E_i}{k_B T}}}{\sum g_i e^{-\frac{E_i}{k_B T}}} \qquad \textbf{(1)}$$

In eq. 1, N_i is the number of conformer i with energy E_i and degeneracy g_i at temperature T, and k_B is Boltzmann constant.

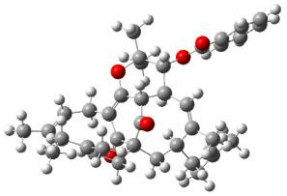
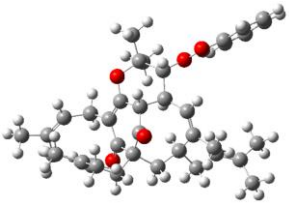
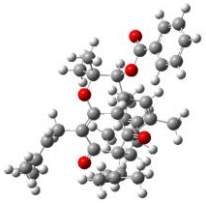
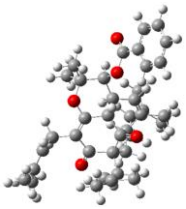
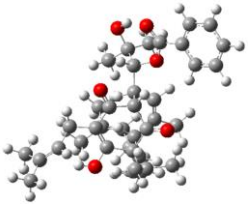
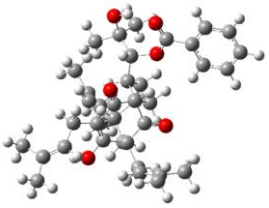
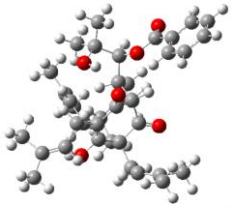
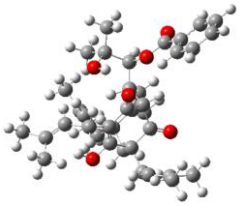
3.3 ECD calculations

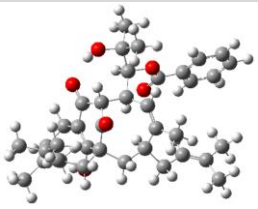
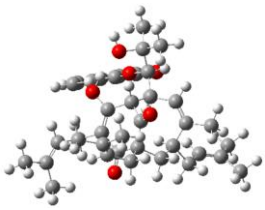
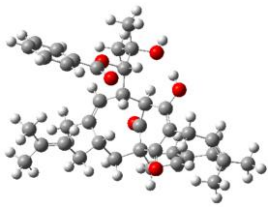
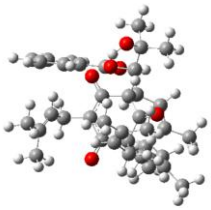
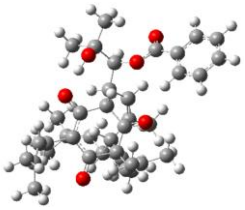
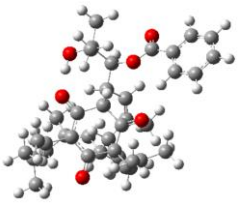
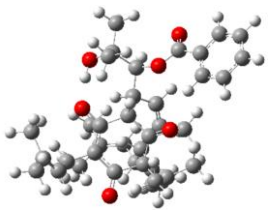
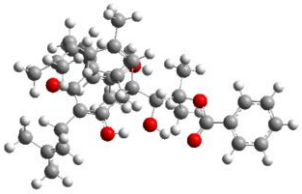
In order to confirm the absolute configurations, (1*S*,5*S*,7*S*,10*S*,28*S*) for **1**-**3** and (1*S*,5*R*,7*S*,8*R*)-**4a**, ECD calculations were conducted. Structures were obtained directly from the above-mentioned optimizations. The calculations were executed in methanol with IEFPCM model using Time-dependent Density functional theory (TD-DFT). Rotatory strengths for 50 excited states were calculated. The ECD spectra were simulated in Yinfo Cloud Platform (http://cloud.yinfotek.com) by overlapping Gaussian functions for each transition according to (2). The σ values were set 0.3 eV for all compounds and UV-shift values were 4 nm for (1*S*,5*S*,7*S*,10*S*,28*S*)-**1**, 11 nm for (1*S*,5*S*,7*S*,10*S*,28*S*)-**2a/b**, −10 nm for (1*S*,5*S*,7*S*,10*S*,28*S*)-**2c**, 7 nm for (1*S*,5*S*,7*S*,10*S*,28*S*)-**3**, and −2 nm for (1*S*,5*R*,7*S*,8*R*)-**4a**.

$$\Delta\varepsilon(E) = \frac{1}{2.297\times10^{-39}} \times \frac{1}{\sqrt{2\pi\sigma}} \sum_i^A \Delta E_i R_i e^{-\left(\frac{E-E_i}{2\sigma}\right)^2} \qquad \textbf{(2)}$$

In eq. 2, σ represents the width of the band at $1/e$ height, and ΔE_i and R_i are the excitation energies and rotatory strengths for transition i, respectively.

Table S3-1 Energies of Compounds at B3LYP/6-31G(d) in gas phase.

Configurations	Conformers	Structures	E (Hartree)	E (kcal/mol)	Populations (%)
(1*S*,5*S*,7*S*,10*S*,28*R*)-**1**	1		−1853.11871142	−1162849.54	34.99
(1*S*,5*S*,7*S*,10*S*,28*R*)-**1**	2		−1853.11929645	−1162849.91	65.01
(1*S*,5*S*,7*S*,10*S*,28*S*)-**1**	1		−1853.12011948	−1162850.42	34.35
(1*S*,5*S*,7*S*,10*S*,28*S*)-**1**	2		−1853.12073104	−1162850.81	65.65
(1*S*,5*S*,7*S*,10*S*,28*R*)-**2a**	1		−1929.57787058	−1210828.38	35.89
(1*S*,5*S*,7*S*,10*S*,28*R*)-**2a**	2		−1929.57841820	−1210828.73	64.11
(1*S*,5*S*,7*S*,10*S*,28*S*)-**2a**	1		−1929.57456989	−1210826.31	31.17
(1*S*,5*S*,7*S*,10*S*,28*S*)-**2a**	5		−1929.57464974	−1210826.36	33.92

Configurations	Conformers	Structures	E (Hartree)	E (kcal/mol)	Populations (%)
(1*S*,5*S*,7*S*,10*S*,28*S*)-**2a**	7		−1929.57467673	−1210826.38	34.91
(1*S*,5*S*,7*S*,10*S*,28*R*)-**2b**	1		−1929.57716935	−1210827.94	100.00
(1*S*,5*S*,7*S*,10*S*,28*S*)-**2b**	1		−1929.57451895	−1210826.28	100.00
(1*S*,5*S*,7*S*,10*S*,28*R*)-**2c**	1		−1929.11215690	−1210536.15	100.00
(1*S*,5*S*,7*S*,10*S*,28*S*)-**2c**	1		−1929.11514635	−1210538.02	96.47
(1*S*,5*S*,7*S*,10*S*,28*S*)-**2c**	6		−1929.11123285	−1210535.56	1.53
(1*S*,5*S*,7*S*,10*S*,28*S*)-**2c**	8		−1929.11148786	−1210535.72	2
(1*S*,5*S*,7*S*,10*S*,28*R*)-**3**	4		−1929.56528806	−1210820.49	98.04

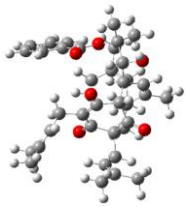
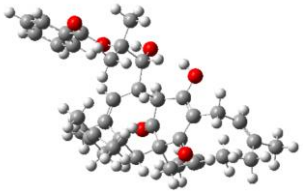
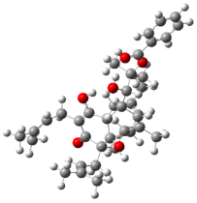
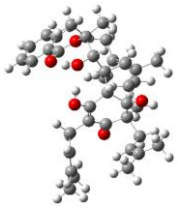
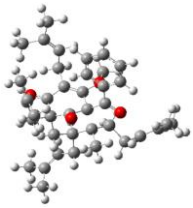
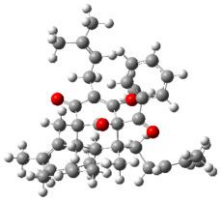
Configurations	Conformers	Structures	E (Hartree)	E (kcal/mol)	Populations (%)
(1*S*,5*S*,7*S*,10*S*,28*R*)-**3**	6		−1929.56035195	−1210817.39	0.53
(1*S*,5*S*,7*S*,10*S*,28*R*)-**3**	11		−1929.56129911	−1210817.99	1.43
(1*S*,5*S*,7*S*,10*S*,28*S*)-**3**	1		−1929.57192763	−1210824.66	95.25
(1*S*,5*S*,7*S*,10*S*,28*S*)-**3**	2		−1929.56909702	−1210822.88	4.75
(1*S*,5*R*,7*S*,8*R*)-**4a**	1		−1818.75693847	−1141287.20	74.49
(1*S*,5*R*,7*S*,8*R*)-**4a**	7		−1818.75592676	−1141286.57	25.51

Table S3-2. Experimental and Computed ^{1}H and ^{13}C NMR Chemical Shifts of **1**.

No.	Experimental (^{1}H)	Calculated (^{1}H)		Experimental (^{13}C)	Calculated (^{13}C)	
		(28*R*)-**1**	(28*S*)-**1**		(28*R*)-**1**	(28*S*)-**1**
1	3.58	2.87	3.64	54.00	59.81	54.33
2				167.70	166.79	169.16
3				120.60	122.22	119.48
4				198.70	198.08	196.65
5				61.40	64.48	64.17
6a	2.02	2.14	2.08	40.40	42.63	42.38
6b	1.21	1.36	1.34			
7	2.53	2.41	2.34	38.10	39.72	40.51
8				143.30	145.98	146.08
9	5.24	5.58	5.39	121.98	123.01	122.39
10	3.80	3.39	3.59	44.20	45.45	45.17
11				206.60	206.64	207.82
12a	3.05	3.49	3.41	21.30	22.83	22.71
12b	2.99	2.92	2.88			
13	4.89	5.03	4.84	121.94	121.08	120.93
14				130.80	135.06	134.68
15	1.60	1.64	1.64	25.60	24.84	25.05
16	1.65	1.87	1.85	17.60	16.28	16.51
17a	2.47	2.81	2.78	36.90	38.43	37.98
17b	2.26	2.08	2.06			
18	4.60	4.64	4.55	118.30	118.33	118.52
19				133.70	137.34	137.15
20	1.47	1.58	1.55	25.60	24.37	25.02
21	1.45	1.49	1.46	17.50	16.39	16.56
22a	1.99	2.18	2.16	32.60	33.77	33.96
22b	1.87	1.82	1.81			
23	4.91	4.80	4.84	122.30	122.44	121.56
24				132.10	134.23	135.08
25	1.65	1.45	1.57	25.50	24.56	24.96
26	1.54	1.51	1.47	17.90	16.15	16.42
27	1.45	1.42	1.41	18.00	18.27	18.19
28	5.40	5.58	5.21	75.00	74.58	74.31
29				88.50	87.32	89.26
30	1.41	1.39	1.34	25.00	20.44	23.00
31	1.54	1.44	1.36	27.00	25.80	25.66
32				165.10	163.59	164.04
33				128.70	125.86	125.51
34	8.15	8.11	8.24	129.60	127.81	128.11
35	7.62	7.52	7.54	129.10	125.54	125.86
36	7.75	7.70	7.71	134.10	131.94	132.30
37	7.62	7.52	7.54	129.10	125.54	125.86
38	8.15	8.11	8.24	129.60	127.81	128.11

Table S3-3. Experimental and Computed ^{1}H NMR Chemical Shifts of **2**.

No.	Experimental (^{1}H)	Calculated (^{1}H)					
		(28*R*)-**2a**	(28*S*)-**2a**	(28*R*)-**2b**	(28*S*)-**2b**	(28*R*)-**2c**	(28*S*)-**2c**
1	3.69	3.07	3.65	4.15	4.19	4.01	3.87
6a	1.79	1.77	1.74	1.99	2.05	2.00	1.63
6b	0.92	1.30	1.21	1.26	1.25	1.14	0.99
7	2.49	2.29	2.49	2.15	2.14	2.33	2.30
9	4.98	5.44	5.17	5.43	5.49	5.43	4.93
10	3.25	2.81	3.63	2.90	3.55	2.91	3.04
12a	2.94	3.61	3.34	2.67	2.72	2.59	3.18
12b	2.89	2.85	3.11	3.43	3.47	3.31	2.63
13	5.09	5.19	5.26	5.15	5.26	5.41	5.27
15	1.55	1.68	1.67	1.53	1.53	1.59	1.50
16	1.64	1.71	1.68	1.59	1.70	1.71	1.85
17a	2.27	2.82	2.80	2.57	2.64	2.52	2.46
17b	2.14	2.00	1.93	1.79	1.89	1.89	2.09
18	4.62	4.75	4.68	4.47	4.57	4.55	4.70
20	1.47	1.39	1.25	1.42	1.37	1.48	1.67
21	1.46	1.35	1.32	1.28	1.30	1.31	1.41
22a	1.89	2.17	2.24	2.17	2.08	2.25	1.87
22b	1.74	1.79	1.60	1.55	1.47	1.56	1.82
23	4.80	4.87	4.60	4.62	4.25	4.64	4.92
25	1.56	1.47	1.20	1.42	0.86	1.46	1.50
26	1.50	1.45	1.30	1.39	1.27	1.42	1.46
27	1.37	1.43	1.27	1.26	1.21	1.30	1.42
28	4.91	4.75	4.72	5.03	4.93	4.79	4.79
30	0.96	0.79	0.88	0.99	1.14	0.84	0.88
31	1.18	0.89	0.93	1.40	1.55	1.20	1.21
34	8.14	8.11	8.19	8.10	8.04	8.23	8.39
35	7.55	7.39	7.29	7.41	7.33	7.32	7.29
36	7.67	7.54	7.48	7.52	7.53	7.41	7.41
37	7.55	7.39	7.29	7.41	7.33	7.32	7.29
38	8.14	8.11	8.19	8.10	8.04	8.23	8.39

Table S3-4. Experimental and Computed ^{13}C NMR Chemical Shifts of **2**.

No.	Experimental (^{13}C)	Calculated (^{13}C)					
		(28*R*)-**2a**	(28*S*)-**2a**	(28*R*)-**2b**	(28*S*)-**2b**	(28*R*)-**2c**	(28*S*)-**2c**
1	58.70	65.68	65.03	56.19	57.40	61.23	57.08
2	184.50	189.56	194.56	171.59	170.74	183.96	182.58
3	113.40	115.03	117.04	116.30	117.55	109.41	113.85
4	188.90	172.83	174.33	196.43	196.79	185.95	184.77
5	60.10	59.99	60.16	62.57	64.15	62.19	63.45
6	41.05	40.43	41.09	41.78	42.62	40.42	43.88
7	37.10	39.49	38.47	38.26	38.15	37.68	39.98
8	139.60	145.47	143.61	144.51	146.01	141.57	142.87
9	128.50	123.08	126.97	125.96	123.44	127.30	128.64
10	40.10	44.01	43.28	50.12	43.95	49.18	42.62
11	211.90	206.98	206.11	208.47	208.81	215.46	215.02
12	23.10	23.17	24.18	22.92	22.72	23.93	24.32
13	127.50	119.34	120.01	122.45	121.44	127.02	125.20
14	126.20	143.53	143.00	134.82	134.39	129.76	129.51
15	25.60	25.17	25.39	24.62	25.52	24.78	25.14
16	17.90	16.91	16.90	16.08	16.65	16.25	16.60
17	35.30	35.73	36.80	38.46	39.33	37.50	34.88
18	121.60	118.21	118.12	119.65	120.27	122.01	122.08
19	130.40	138.36	138.18	137.65	136.82	134.06	134.28
20	25.80	25.05	25.01	24.81	24.45	24.79	24.99
21	17.80	16.49	16.49	16.25	16.15	16.27	17.07
22	31.80	33.39	33.65	32.94	33.06	33.25	32.79
23	122.60	122.43	123.10	123.82	122.85	124.26	122.60
24	131.60	134.95	134.44	135.61	135.10	133.98	134.61
25	25.50	24.73	24.64	24.68	24.52	24.56	25.36
26	17.94	16.41	16.73	16.08	16.41	16.03	16.40
27	18.40	18.32	18.37	17.51	17.69	17.61	18.77
28	81.90	85.80	77.58	75.71	74.99	78.28	81.55
29	70.50	71.57	73.21	76.91	77.59	71.51	71.03
30	28.60	24.47	25.75	26.70	28.53	28.93	25.21
31	27.30	24.01	24.38	24.76	23.95	25.40	26.73
32	166.10	167.93	163.21	163.10	164.02	163.65	166.15
33	130.30	126.80	126.72	127.11	127.16	128.66	128.78
34	129.70	128.92	128.84	129.20	128.94	129.13	128.84
35	128.60	126.22	126.02	126.35	126.99	125.87	125.50
36	133.20	132.57	131.92	132.27	133.11	131.34	130.70
37	128.60	126.22	126.02	126.35	126.99	125.87	125.50
38	129.70	128.92	128.84	129.20	128.94	129.13	128.84

Table S3-5. Experimental and Computed ^{1}H and ^{13}C NMR Chemical Shifts of **3**.

No.	Experimental (^{1}H)	Calculated (^{1}H)		Experimental (^{13}C)	Calculated (^{13}C)	
		(28*R*)-**3**	(28*S*)-**3**		(28*R*)-**3**	(28*S*)-**3**
1	3.71	3.37	3.60	58.20	53.23	56.75
2				167.90	168.76	169.43
3				119.40	118.00	117.01
4				199.00	193.83	195.55
5				62.10	65.34	63.70
6a	2.18	1.74	2.25	41.40		
6b	1.31	1.34	1.48		44.19	42.95
7	2.30	2.24	2.07	39.80	40.55	42.65
8				142.00	145.46	143.99
9	5.21	5.44	5.27	129.10	124.09	131.07
10	2.91	3.06	2.49	44.80	46.90	45.99
11				208.10	210.54	208.53
12a	3.21	3.52	3.76	22.40	23.20	23.28
12b	3.05	2.81	2.75			
13	5.06	5.20	5.17	122.70	121.25	122.25
14				131.40	134.39	134.08
15	1.65	1.63	1.72	26.00	25.27	25.27
16	1.73	1.79	1.97	18.00	16.72	16.90
17a	2.36	2.28	2.17	37.20	35.00	38.42
17b	2.57	2.63	2.72			
18	4.63	4.68	4.64	118.60	121.16	120.67
19				134.50	136.92	136.32
20	1.54	1.64	1.57	25.90	25.28	24.38
21	1.52	1.48	1.44	17.90	17.11	16.42
22a	1.95	1.90	1.91	32.20	33.22	33.37
22b	1.95	1.81	2.04			
23	4.79	4.95	4.95	122.10	122.83	122.44
24				133.30	135.94	135.39
25	1.60	1.56	1.64	25.80	25.75	25.46
26	1.52	1.51	1.63	18.07	16.67	16.45
27	1.53	1.69	1.72	18.15	20.16	19.43
28	4.20	3.99	3.95	80.00	78.00	79.60
29				88.70	92.97	92.27
30	1.56	1.84	1.46	20.60	20.55	17.47
31	1.47	1.66	1.31	25.20	25.64	25.01
32				167.80	168.01	166.87
33				130.30	127.82	126.91
34	7.98	8.02	8.02	130.00	129.36	129.06
35	7.45	7.32	7.34	128.70	126.57	126.31
36	7.60	7.51	7.54	133.80	133.24	132.78
37	7.45	7.32	7.34	128.70	126.57	126.31
38	7.98	8.02	8.02	130.00	129.36	129.06

Table S3-6. Statistics of Ordinary Least Squares Linear Regression (OLS-LR) of Experimental and Computed ^{1}H and ^{13}C NMR Chemical Shifts.

Type	Compound	CMAD[a]	CLAD[b]	R^2	RMSE	F	p value
^{1}H NMR	(28*R*)-**1**	0.16	0.71	0.9910	0.23	3089.98	< 0.01
	(28*S*)-**1**	0.12	0.36	0.9961	0.15	7181.44	< 0.01
	(28*R*)-**2a**	0.20	0.67	0.9870	0.27	2125.63	< 0.01
	(28*S*)-**2a**	0.19	0.53	0.9905	0.24	2913.01	< 0.01
	(28*R*)-**2b**	0.20	0.54	0.9891	0.25	2539.12	< 0.01
	(28*S*)-**2b**	0.26	0.70	0.9825	0.32	1572.64	< 0.01
	(28*R*)-**2c**	0.19	0.45	0.9906	0.23	2950.85	< 0.01
	(28*S*)-**2c**	0.14	0.26	0.9949	0.17	5504.55	< 0.01
	(28*R*)-**3**	0.13	0.44	0.9941	0.18	4717.10	< 0.01
	(28*S*)-**3**	0.14	0.55	0.9930	0.19	3982.23	< 0.01
^{13}C NMR	(28*R*)-**1**	1.84	6.56	0.9983	2.41	20967.66	< 0.01
	(28*S*)-**1**	1.56	3.88	0.9989	1.90	33626.00	< 0.01
	(28*R*)-**2a**	3.30	17.33	0.9921	5.20	4511.57	< 0.01
	(28*S*)-**2a**	3.31	16.80	0.9924	5.11	4687.40	< 0.01
	(28*R*)-**2b**	3.20	12.91	0.9944	4.39	6359.94	< 0.01
	(28*S*)-**2b**	3.10	13.76	0.9944	4.39	6358.18	< 0.01
	(28*R*)-**2c**	1.92	8.41	0.9982	2.50	19690.84	< 0.01
	(28*S*)-**2c**	1.67	4.13	0.9987	2.14	26781.18	< 0.01
	(28*R*)-**3**	1.88	5.17	0.9983	2.39	21419.70	< 0.01
	(28*S*)-**3**	1.59	3.57	0.9990	1.88	34617.56	< 0.01

[a] CMAD = corrected mean absolute deviation, computed as $(1/n)\sum_i^n |\delta_{\text{calc}} - \delta_{\text{exp}}|$, where δ_{calc} and δ_{exp} refer to the calculated and experimental chemical shifts.

[b] CLAD = corrected largest absolute deviation, computed as $max(|\delta_{\text{calc}} - \delta_{\text{exp}}|)$.

Table S3-7. DFT Coordinates for the Conformers of **1.**

(1*S*,5*S*,7*S*,10*S*,28*R*)-**1** (conformer 1)					
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-2.835688	-1.637134	-0.138535
2	8	0	0.714068	-2.509215	-0.874050
3	8	0	2.987490	1.592125	-1.238457
4	8	0	1.597168	-0.088696	2.950929
5	8	0	-3.571892	-2.331411	1.895990
6	6	0	-7.771261	-1.053072	-0.582476
7	1	0	-8.784393	-0.844424	-0.915796
8	6	0	-6.688256	-0.746480	-1.409957
9	1	0	-6.857730	-0.298077	-2.384907
10	6	0	-5.387319	-1.013335	-0.987250
11	1	0	-4.542961	-0.771471	-1.622545
12	6	0	-5.166450	-1.589177	0.272001
13	6	0	-3.803137	-1.895632	0.785907
14	6	0	-1.463843	-1.858232	0.250341
15	1	0	-1.469203	-2.509680	1.127430
16	6	0	-0.763688	-2.587539	-0.954305
17	6	0	1.264852	-1.369582	-0.365380
18	6	0	2.140118	-0.596883	-1.053875
19	6	0	2.668238	-0.953336	-2.428338
20	1	0	2.018054	-1.720917	-2.862902
21	1	0	2.612821	-0.067763	-3.065095
22	6	0	4.081810	-1.491995	-2.370877
23	1	0	4.169421	-2.460133	-1.875528
24	6	0	5.202977	-0.932083	-2.851817
25	6	0	6.527319	-1.650963	-2.736285
26	1	0	7.253303	-1.054726	-2.165771
27	1	0	6.974322	-1.815689	-3.727232
28	1	0	6.425099	-2.624791	-2.246572
29	6	0	-1.151807	-1.977357	-2.306812
30	1	0	-0.896971	-0.914209	-2.361533
31	1	0	-2.223780	-2.082860	-2.488401
32	1	0	-0.607366	-2.498080	-3.099798
33	6	0	5.268752	0.405837	-3.548484
34	1	0	6.101521	0.999858	-3.149124
35	1	0	4.359883	0.995962	-3.422898
36	1	0	5.465877	0.278536	-4.622886
37	6	0	2.481412	0.740298	-0.513034
38	6	0	2.213703	1.113948	0.968048
39	6	0	1.354308	2.420686	1.075077
40	1	0	1.447184	2.783435	2.105933
41	1	0	1.854396	3.147629	0.426187
42	6	0	-0.151676	2.371974	0.680011
43	1	0	-0.217883	1.829420	-0.269321
44	6	0	-0.640112	3.812658	0.356652
45	1	0	-0.603866	4.420600	1.272818
46	1	0	0.083419	4.262665	-0.329379
47	6	0	-2.025756	3.852079	-0.232813
48	1	0	-2.794242	3.362408	0.366488
49	6	0	-2.419678	4.396507	-1.395284
50	6	0	-3.868097	4.331158	-1.821739
51	1	0	-4.287617	5.338607	-1.954174
52	1	0	-4.486836	3.800019	-1.091592
53	1	0	-3.972629	3.823430	-2.791248
54	6	0	-1.520079	5.116210	-2.370912
55	1	0	-0.470194	5.129884	-2.070302
56	1	0	-1.844535	6.158591	-2.498123
57	1	0	-1.578565	4.651708	-3.365043
58	6	0	-1.039256	1.668611	1.720114
59	6	0	-1.502122	2.483421	2.906825
60	1	0	-0.650356	2.941035	3.427713
61	1	0	-2.031065	1.854376	3.628546
62	1	0	-2.171934	3.302404	2.618388
63	6	0	-1.360562	0.363310	1.643546
64	1	0	-1.956769	-0.094508	2.430386

65	6	0	-0.771430	-0.534217	0.593250
66	1	0	-0.705683	0.037880	-0.335919
67	6	0	0.688130	-0.990580	0.956135
68	1	0	0.619213	-1.876363	1.598041
69	6	0	1.518132	0.007709	1.740743
70	6	0	3.604636	1.417771	1.622653
71	1	0	3.990060	2.314860	1.122421
72	1	0	3.424185	1.670176	2.669158
73	6	0	4.616871	0.309990	1.485871
74	1	0	4.958258	0.130450	0.465849
75	6	0	5.153162	-0.447877	2.456091
76	6	0	6.194024	-1.490882	2.121143
77	1	0	7.133433	-1.297842	2.658776
78	1	0	6.415624	-1.519704	1.049681
79	1	0	5.862254	-2.492558	2.429171
80	6	0	4.815954	-0.350401	3.923949
81	1	0	4.561799	-1.342312	4.321246
82	1	0	3.970782	0.307359	4.130464
83	1	0	5.685150	0.000757	4.498625
84	6	0	-1.068335	-4.082324	-0.915303
85	1	0	-0.705517	-4.525462	0.017232
86	1	0	-0.580857	-4.590752	-1.752633
87	1	0	-2.147676	-4.249784	-0.986581
88	6	0	-6.255845	-1.891376	1.101516
89	1	0	-6.062925	-2.332667	2.073691
90	6	0	-7.553706	-1.625519	0.673726
91	1	0	-8.395558	-1.862592	1.318120

(1*S*,5*S*,7*S*,10*S*,28*R*)-**1** (conformer 2)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-2.661279	-1.849576	0.195343
2	8	0	0.953066	-2.688434	-0.169725
3	8	0	2.993101	1.230582	-1.778822
4	8	0	1.568683	0.863605	2.710396
5	8	0	-3.441779	-1.951863	2.327119
6	6	0	-7.597675	-1.735124	-0.518749
7	1	0	-8.605772	-1.698934	-0.923088
8	6	0	-6.499027	-1.621274	-1.374083
9	1	0	-6.651407	-1.494738	-2.442310
10	6	0	-5.204485	-1.668414	-0.860074
11	1	0	-4.348594	-1.574229	-1.518641
12	6	0	-5.005553	-1.828671	0.518588
13	6	0	-3.650207	-1.881539	1.132576
14	6	0	-1.295549	-1.854575	0.661277
15	1	0	-1.301197	-2.195115	1.699296
16	6	0	-0.514719	-2.883265	-0.236948
17	6	0	1.421310	-1.414349	-0.037020
18	6	0	2.271812	-0.841793	-0.923687
19	6	0	2.863436	-1.576074	-2.109314
20	1	0	2.251029	-2.461503	-2.314098
21	1	0	2.813190	-0.923775	-2.983603
22	6	0	4.286124	-2.022874	-1.847370
23	1	0	4.376051	-2.802174	-1.089179
24	6	0	5.412639	-1.584816	-2.431212
25	6	0	6.749167	-2.188796	-2.067008
26	1	0	7.432270	-1.426532	-1.666365
27	1	0	7.244575	-2.611670	-2.952762
28	1	0	6.651768	-2.985457	-1.322378
29	6	0	-0.893147	-2.762768	-1.718502
30	1	0	-0.702197	-1.756568	-2.104814
31	1	0	-1.949368	-2.995176	-1.871468
32	1	0	-0.289831	-3.468344	-2.296836
33	6	0	5.473989	-0.503783	-3.484072
34	1	0	6.282692	0.202503	-3.254007
35	1	0	4.550400	0.072497	-3.557127
36	1	0	5.706758	-0.930404	-4.470613
37	6	0	2.517378	0.616407	-0.827506
38	6	0	2.183854	1.415607	0.458118
39	6	0	1.250602	2.633405	0.142072

40	1	0	1.290381	3.302003	1.010541
41	1	0	1.728400	3.154299	-0.694668
42	6	0	-0.238319	2.375771	-0.235671
43	1	0	-0.245850	1.561919	-0.970972
44	6	0	-0.782242	3.616476	-0.995711
45	1	0	-0.722788	4.504767	-0.357455
46	1	0	-0.090818	3.801212	-1.831807
47	6	0	-2.172022	3.418815	-1.544650
48	1	0	-2.345801	2.433333	-1.981660
49	6	0	-3.189447	4.293405	-1.586837
50	6	0	-4.511209	3.910587	-2.210243
51	1	0	-5.332119	4.003227	-1.485205
52	1	0	-4.504202	2.881751	-2.583747
53	1	0	-4.761728	4.575628	-3.048936
54	6	0	-3.134582	5.706794	-1.058798
55	1	0	-3.950165	5.888499	-0.345301
56	1	0	-3.273220	6.428462	-1.876158
57	1	0	-2.191668	5.948074	-0.562473
58	6	0	-1.123832	1.974568	0.954699
59	6	0	-1.690547	3.089315	1.801741
60	1	0	-0.895862	3.757238	2.160457
61	1	0	-2.208171	2.689912	2.678740
62	1	0	-2.399898	3.704654	1.236814
63	6	0	-1.364548	0.691867	1.285608
64	1	0	-1.967963	0.463947	2.162028
65	6	0	-0.687587	-0.449380	0.581606
66	1	0	-0.618732	-0.195025	-0.479639
67	6	0	0.781805	-0.678548	1.090919
68	1	0	0.741204	-1.321578	1.977743
69	6	0	1.527176	0.566596	1.531409
70	6	0	3.536197	1.992938	0.999919
71	1	0	3.887684	2.709333	0.247075
72	1	0	3.311561	2.549117	1.911763
73	6	0	4.609042	0.960581	1.231975
74	1	0	4.987980	0.486144	0.326197
75	6	0	5.156829	0.582761	2.398392
76	6	0	6.260829	-0.448683	2.423427
77	1	0	7.173922	-0.038401	2.878164
78	1	0	6.511823	-0.805054	1.419449
79	1	0	5.975689	-1.317434	3.033565
80	6	0	4.773559	1.122000	3.754964
81	1	0	4.570633	0.295016	4.448609
82	1	0	3.883655	1.752351	3.732989
83	1	0	5.602628	1.697199	4.191897
84	6	0	-0.733693	-4.304114	0.275185
85	1	0	-0.374057	-4.402914	1.304043
86	1	0	-0.192749	-5.020425	-0.350569
87	1	0	-1.798898	-4.554936	0.250815
88	6	0	-6.110859	-1.938440	1.374320
89	1	0	-5.935351	-2.057690	2.438300
90	6	0	-7.402172	-1.893716	0.855872
91	1	0	-8.256181	-1.980925	1.521633

(1*S*,5*S*,7*S*,10*S*,28*S*)-**1** (conformer 1)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	2.985118	-0.314956	0.775956
2	8	0	0.107680	-1.054957	2.239654
3	8	0	-3.758253	0.292661	-0.072064
4	8	0	0.157870	-0.974864	-2.388393
5	8	0	4.627191	0.769225	1.907322
6	6	0	7.085720	-2.404532	-1.145630
7	1	0	7.808456	-2.994275	-1.703269
8	6	0	5.725362	-2.502112	-1.447785
9	1	0	5.389194	-3.163873	-2.240942
10	6	0	4.793672	-1.749227	-0.735322
11	1	0	3.738256	-1.817687	-0.973725
12	6	0	5.226433	-0.890547	0.286063
13	6	0	4.286793	-0.053100	1.079351
14	6	0	1.966927	0.505904	1.388852

15	1	0	2.461766	1.396761	1.781265
16	6	0	1.272757	-0.209159	2.603191
17	6	0	-0.593589	-0.780235	1.106929
18	6	0	-1.943906	-0.642559	1.101523
19	6	0	-2.803820	-0.855026	2.331035
20	1	0	-2.173110	-0.748943	3.221217
21	1	0	-3.563402	-0.071500	2.364010
22	6	0	-3.439076	-2.228937	2.350984
23	1	0	-2.729200	-3.045852	2.489608
24	6	0	-4.737697	-2.543683	2.224459
25	6	0	-5.188568	-3.983235	2.313424
26	1	0	-5.694907	-4.298087	1.390001
27	1	0	-5.916964	-4.118721	3.125853
28	1	0	-4.351558	-4.665623	2.493341
29	6	0	0.727283	0.862525	3.558824
30	1	0	0.028026	1.538542	3.055665
31	1	0	1.546831	1.459336	3.973017
32	1	0	0.196009	0.380248	4.383920
33	6	0	-5.849414	-1.544347	2.009044
34	1	0	-6.527028	-1.896137	1.219662
35	1	0	-5.484475	-0.560813	1.709015
36	1	0	-6.461170	-1.436345	2.916573
37	6	0	-2.601497	-0.121000	-0.114357
38	6	0	-1.865267	-0.059669	-1.478786
39	6	0	-1.853352	1.404872	-2.036765
40	1	0	-1.584390	1.345298	-3.098172
41	1	0	-2.892914	1.744681	-1.980509
42	6	0	-0.953687	2.463785	-1.331736
43	1	0	-1.084251	2.328537	-0.252444
44	6	0	-1.501492	3.888495	-1.630253
45	1	0	-1.408834	4.092316	-2.707265
46	1	0	-2.574612	3.882316	-1.418126
47	6	0	-0.809490	4.969193	-0.841379
48	1	0	0.271769	5.016466	-0.976661
49	6	0	-1.351882	5.858253	0.006249
50	6	0	-0.483004	6.871734	0.714594
51	1	0	-0.791231	7.897906	0.469041
52	1	0	0.573320	6.762914	0.449216
53	1	0	-0.571985	6.775430	1.806035
54	6	0	-2.820822	5.963781	0.337813
55	1	0	-3.436152	5.206625	-0.152991
56	1	0	-3.211139	6.950102	0.050087
57	1	0	-2.979070	5.874108	1.421436
58	6	0	0.538388	2.322603	-1.674528
59	6	0	1.015188	2.937454	-2.970837
60	1	0	0.424829	2.572229	-3.821765
61	1	0	2.062183	2.684561	-3.161604
62	1	0	0.926072	4.030447	-2.972755
63	6	0	1.401230	1.633781	-0.904360
64	1	0	2.435350	1.520797	-1.223870
65	6	0	0.949095	0.860860	0.300683
66	1	0	0.184870	1.457463	0.807215
67	6	0	0.275721	-0.510929	-0.071250
68	1	0	1.066505	-1.263731	-0.134209
69	6	0	-0.433511	-0.559330	-1.408420
70	6	0	-2.681998	-0.939508	-2.483847
71	1	0	-3.656606	-0.449737	-2.599319
72	1	0	-2.171054	-0.899136	-3.447637
73	6	0	-2.899365	-2.360042	-2.030419
74	1	0	-3.544436	-2.463478	-1.157266
75	6	0	-2.418877	-3.488398	-2.577163
76	6	0	-2.784239	-4.834255	-1.995237
77	1	0	-3.289314	-5.463386	-2.742206
78	1	0	-3.444923	-4.740211	-1.127699
79	1	0	-1.886404	-5.386393	-1.683213
80	6	0	-1.517690	-3.553733	-3.786155
81	1	0	-0.639364	-4.177527	-3.571651
82	1	0	-1.151915	-2.576710	-4.104526
83	1	0	-2.036607	-4.028789	-4.631250

84	6	0	2.216203	-1.159039	3.334425
85	1	0	2.541216	-1.967330	2.674990
86	1	0	1.697248	-1.598428	4.191429
87	1	0	3.097401	-0.619093	3.692374
88	6	0	6.593463	-0.791459	0.583174
89	1	0	6.907078	-0.117552	1.373530
90	6	0	7.519115	-1.548125	-0.129659
91	1	0	8.577147	-1.470938	0.104427

(1*S*,5*S*,7*S*,10*S*,28*S*)-**1** (conformer 2)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-2.737982	-1.132612	-0.717570
2	8	0	0.257150	-1.606499	-2.066281
3	8	0	3.720456	1.013209	-0.266804
4	8	0	0.125395	-0.466151	2.415918
5	8	0	-4.541061	-0.722635	-2.033848
6	6	0	-6.366412	-3.443960	1.801689
7	1	0	-6.965368	-4.004904	2.514219
8	6	0	-5.024880	-3.172193	2.080632
9	1	0	-4.580318	-3.517492	3.009690
10	6	0	-4.251602	-2.454563	1.169902
11	1	0	-3.212534	-2.235035	1.387975
12	6	0	-4.825391	-2.003097	-0.027931
13	6	0	-4.058948	-1.222744	-1.036401
14	6	0	-1.895148	-0.297573	-1.541342
15	1	0	-2.552057	0.359465	-2.115353
16	6	0	-1.054080	-1.129400	-2.575155
17	6	0	0.868575	-0.937205	-1.052688
18	6	0	2.159934	-0.525756	-1.126551
19	6	0	3.063553	-0.838783	-2.301967
20	1	0	2.438104	-1.071338	-3.171597
21	1	0	3.648712	0.052143	-2.538312
22	6	0	3.964779	-2.022775	-2.024026
23	1	0	3.436604	-2.973518	-1.936923
24	6	0	5.298863	-2.033203	-1.877421
25	6	0	6.032592	-3.332253	-1.636537
26	1	0	6.582382	-3.305677	-0.685036
27	1	0	6.781843	-3.513628	-2.420522
28	1	0	5.353031	-4.190327	-1.614060
29	6	0	-0.730774	-0.234720	-3.781052
30	1	0	-0.200345	0.675788	-3.482777
31	1	0	-1.650548	0.056650	-4.299151
32	1	0	-0.094881	-0.782624	-4.481780
33	6	0	6.184440	-0.812040	-1.949829
34	1	0	6.898847	-0.812786	-1.115807
35	1	0	5.625523	0.123605	-1.898400
36	1	0	6.784698	-0.817534	-2.871324
37	6	0	2.675515	0.390853	-0.088886
38	6	0	1.923280	0.615132	1.249369
39	6	0	1.597856	2.133685	1.457296
40	1	0	1.330255	2.264778	2.512697
41	1	0	2.544877	2.658683	1.291688
42	6	0	0.509866	2.800341	0.564058
43	1	0	0.685391	2.456241	-0.462617
44	6	0	0.751821	4.334070	0.529620
45	1	0	0.673009	4.749519	1.539959
46	1	0	1.798836	4.481188	0.224479
47	6	0	-0.146009	5.057613	-0.440852
48	1	0	-0.265709	4.552177	-1.401495
49	6	0	-0.776673	6.232533	-0.286732
50	6	0	-1.616832	6.809992	-1.401634
51	1	0	-2.655982	6.960812	-1.076683
52	1	0	-1.628427	6.161831	-2.283491
53	1	0	-1.242386	7.796452	-1.709731
54	6	0	-0.711076	7.091285	0.953301
55	1	0	-1.719959	7.312738	1.328054
56	1	0	-0.247160	8.061146	0.725085
57	1	0	-0.140757	6.636247	1.766498
58	6	0	-0.927472	2.438578	0.968068

59	6	0	-1.554918	3.237601	2.085732
60	1	0	-0.920334	3.233507	2.982136
61	1	0	-2.526484	2.820546	2.366525
62	1	0	-1.703211	4.284950	1.799540
63	6	0	-1.611113	1.425224	0.404624
64	1	0	-2.608193	1.183823	0.767409
65	6	0	-0.987260	0.500161	-0.599346
66	1	0	-0.350094	1.102439	-1.253676
67	6	0	-0.055732	-0.582191	0.059143
68	1	0	-0.677555	-1.442945	0.320796
69	6	0	0.629134	-0.173457	1.346735
70	6	0	2.892261	0.182249	2.400500
71	1	0	3.738113	0.879886	2.368572
72	1	0	2.369072	0.334463	3.346324
73	6	0	3.415719	-1.225347	2.276679
74	1	0	4.081195	-1.388432	1.428289
75	6	0	3.180549	-2.271558	3.084886
76	6	0	3.835245	-3.606597	2.815800
77	1	0	4.450011	-3.924274	3.670208
78	1	0	4.475728	-3.577946	1.928729
79	1	0	3.081937	-4.393415	2.668159
80	6	0	2.295046	-2.244092	4.306918
81	1	0	1.576006	-3.073823	4.273624
82	1	0	1.721324	-1.321365	4.402487
83	1	0	2.890134	-2.385877	5.220659
84	6	0	-1.770669	-2.400320	-3.020050
85	1	0	-1.933012	-3.070117	-2.172334
86	1	0	-1.158170	-2.921620	-3.761616
87	1	0	-2.737948	-2.155275	-3.467676
88	6	0	-6.173976	-2.273172	-0.302130
89	1	0	-6.599532	-1.910422	-1.231943
90	6	0	-6.940429	-2.993584	0.609560
91	1	0	-7.984131	-3.203597	0.393288

Table S3-8. DFT Coordinates for the Conformers of **2.**

(1*S*,5*S*,7*S*,10*S*,28*R*)-**2a** (conformer 1)					
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	3.049413	0.767354	0.608345
2	8	0	2.546233	2.942541	2.887245
3	1	0	3.279027	2.297259	2.942289
4	8	0	-3.626919	-1.131261	-0.415775
5	1	0	-4.132707	-1.280241	0.413276
6	8	0	0.823840	-1.587741	-1.925636
7	8	0	4.278168	0.803373	2.514206
8	6	0	6.950570	-2.059449	-0.650267
9	1	0	7.679980	-2.692249	-1.149133
10	6	0	5.700075	-1.843297	-1.234051
11	1	0	5.453097	-2.310846	-2.183016
12	6	0	4.760789	-1.030504	-0.601341
13	1	0	3.784966	-0.875244	-1.048932
14	6	0	5.075268	-0.433397	0.629253
15	6	0	4.110385	0.431589	1.361916
16	6	0	1.836123	1.331608	1.204981
17	1	0	1.653332	0.799250	2.142986
18	6	0	1.981101	2.847120	1.580884
19	6	0	-0.389998	-0.957278	1.399969
20	8	0	0.082940	-1.046546	2.531489
21	6	0	-1.833548	-1.037248	1.146836
22	6	0	-2.734666	-1.030489	2.374668
23	1	0	-2.083861	-1.281662	3.221445
24	1	0	-3.091358	-0.010417	2.565649
25	6	0	-3.886684	-2.005920	2.326815
26	1	0	-3.593899	-3.031505	2.094736
27	6	0	-5.192922	-1.778140	2.570948
28	6	0	-6.191148	-2.911541	2.526661
29	1	0	-6.997742	-2.703516	1.810493
30	1	0	-6.672024	-3.043188	3.505709
31	1	0	-5.722693	-3.860611	2.249125
32	6	0	0.600284	3.504563	1.720573
33	1	0	-0.039434	2.926706	2.396831
34	1	0	0.095830	3.625628	0.757007
35	1	0	0.741800	4.493353	2.167280
36	6	0	-5.783052	-0.438199	2.940734
37	1	0	-6.622358	-0.186615	2.278710
38	1	0	-5.062590	0.381863	2.902808
39	1	0	-6.192680	-0.473852	3.959424
40	6	0	-2.305676	-1.085362	-0.131329
41	6	0	-1.478005	-1.174442	-1.401179
42	6	0	-1.829008	0.012909	-2.361485
43	1	0	-1.346103	-0.194285	-3.323250
44	1	0	-2.910189	-0.034628	-2.528410
45	6	0	-1.451579	1.437404	-1.871648
46	1	0	-1.640942	1.473969	-0.792728
47	6	0	-2.395732	2.499931	-2.497750
48	1	0	-2.266643	2.502419	-3.590017
49	1	0	-3.426182	2.177488	-2.317802
50	6	0	-2.166076	3.887443	-1.957932
51	1	0	-1.190031	4.314935	-2.190262
52	6	0	-2.997040	4.643313	-1.221633
53	6	0	-2.579891	6.021515	-0.763321
54	1	0	-2.603180	6.098437	0.332730
55	1	0	-3.268454	6.789710	-1.142932
56	1	0	-1.569732	6.275410	-1.099111
57	6	0	-4.385081	4.239690	-0.786508
58	1	0	-4.470644	4.275614	0.308468
59	1	0	-4.670077	3.236392	-1.111392
60	1	0	-5.132908	4.943976	-1.176985
61	6	0	0.029533	1.710161	-2.122552
62	6	0	0.431177	2.145460	-3.514025
63	1	0	0.043872	1.457754	-4.277906
64	1	0	1.519852	2.174857	-3.616193

65	1	0	0.043072	3.140639	-3.764118
66	6	0	0.973228	1.474723	-1.196963
67	1	0	2.016004	1.588200	-1.480847
68	6	0	0.725900	0.954306	0.199937
69	1	0	-0.199179	1.387554	0.586622
70	6	0	0.525322	-0.629046	0.227912
71	1	0	1.500731	-1.087292	0.402792
72	6	0	0.031321	-1.171065	-1.100074
73	6	0	-1.831614	-2.505198	-2.156940
74	1	0	-2.850885	-2.392655	-2.544744
75	1	0	-1.158364	-2.565101	-3.013437
76	6	0	-1.764840	-3.751358	-1.313900
77	1	0	-2.547588	-3.830742	-0.558680
78	6	0	-0.893139	-4.769159	-1.400905
79	6	0	-1.015889	-5.962062	-0.481813
80	1	0	-1.134731	-6.891500	-1.056510
81	1	0	-1.869227	-5.872708	0.198028
82	1	0	-0.108112	-6.087002	0.124686
83	6	0	0.247450	-4.854651	-2.385479
84	1	0	0.080793	-5.675206	-3.098031
85	1	0	1.184408	-5.084950	-1.860941
86	1	0	0.405409	-3.931486	-2.944265
87	6	0	2.847886	3.638604	0.586868
88	1	0	3.857061	3.220983	0.519970
89	1	0	2.934798	4.667474	0.949781
90	1	0	2.415289	3.657605	-0.418580
91	6	0	6.327970	-0.660541	1.217357
92	1	0	6.547065	-0.197324	2.173712
93	6	0	7.263550	-1.467968	0.576734
94	1	0	8.234671	-1.638568	1.032971

(1*S*,5*S*,7*S*,10*S*,28*R*)-**2a** (conformer 2)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	3.020112	0.325468	0.759614
2	8	0	2.764898	2.002223	3.470130
3	1	0	3.445923	1.309174	3.358636
4	8	0	-3.806969	-0.824371	-0.329702
5	1	0	-4.300262	-1.105166	0.472148
6	8	0	0.550858	-1.262912	-2.094659
7	8	0	4.313799	-0.123285	2.567391
8	6	0	6.621686	-2.469343	-1.243641
9	1	0	7.276812	-3.039972	-1.896743
10	6	0	5.375924	-2.040542	-1.707655
11	1	0	5.058032	-2.281011	-2.718229
12	6	0	4.531763	-1.305662	-0.876562
13	1	0	3.558651	-0.986385	-1.234189
14	6	0	4.937178	-1.002201	0.432416
15	6	0	4.075029	-0.236414	1.373868
16	6	0	1.881059	0.845314	1.519146
17	1	0	1.682614	0.144377	2.335167
18	6	0	2.171405	2.231567	2.193495
19	6	0	-0.517627	-1.264493	1.339891
20	8	0	-0.021285	-1.623242	2.406181
21	6	0	-1.969666	-1.185771	1.140153
22	6	0	-2.832247	-1.366068	2.382494
23	1	0	-2.179927	-1.833246	3.130796
24	1	0	-3.098689	-0.383285	2.791624
25	6	0	-4.060508	-2.223264	2.190400
26	1	0	-3.858295	-3.199900	1.746961
27	6	0	-5.336910	-1.953250	2.530559
28	6	0	-6.424808	-2.977184	2.304838
29	1	0	-7.231910	-2.568914	1.681494
30	1	0	-6.886447	-3.268961	3.258179
31	1	0	-6.043162	-3.882125	1.822566
32	6	0	0.859552	2.962241	2.512904
33	1	0	0.179001	2.315241	3.077302
34	1	0	0.358712	3.320292	1.608198
35	1	0	1.096289	3.822784	3.145795
36	6	0	-5.806167	-0.675271	3.184031

37	1	0	-6.635726	-0.230860	2.618114
38	1	0	-5.021438	0.077660	3.284170
39	1	0	-6.195284	-0.885912	4.189503
40	6	0	-2.478987	-0.933386	-0.099118
41	6	0	-1.695740	-0.812752	-1.394351
42	6	0	-1.978459	0.570126	-2.073445
43	1	0	-1.533873	0.534177	-3.074539
44	1	0	-3.063714	0.633457	-2.205619
45	6	0	-1.484912	1.837091	-1.322906
46	1	0	-1.647380	1.666413	-0.250982
47	6	0	-2.364389	3.058154	-1.698192
48	1	0	-2.301082	3.251406	-2.774348
49	1	0	-3.409061	2.768664	-1.505419
50	6	0	-2.040401	4.289124	-0.892108
51	1	0	-1.922357	4.103087	0.177602
52	6	0	-1.908163	5.558740	-1.307894
53	6	0	-1.599264	6.663525	-0.324733
54	1	0	-2.388713	7.428383	-0.327790
55	1	0	-0.666420	7.180251	-0.590701
56	1	0	-1.497055	6.285087	0.697101
57	6	0	-2.063760	6.021534	-2.736575
58	1	0	-2.895160	6.735367	-2.820616
59	1	0	-2.255734	5.207211	-3.439142
60	1	0	-1.164309	6.555323	-3.073259
61	6	0	0.006174	2.056345	-1.564922
62	6	0	0.403435	2.772601	-2.834563
63	1	0	-0.069574	2.323240	-3.718230
64	1	0	1.486565	2.735821	-2.983449
65	1	0	0.100113	3.825815	-2.809442
66	6	0	0.953525	1.560973	-0.752349
67	1	0	1.993308	1.666106	-1.049742
68	6	0	0.710312	0.772002	0.513520
69	1	0	-0.165384	1.176835	1.026665
70	6	0	0.387357	-0.763704	0.222242
71	1	0	1.327916	-1.316559	0.256434
72	6	0	-0.183423	-0.977407	-1.165960
73	6	0	-2.172843	-1.926963	-2.393370
74	1	0	-3.200159	-1.677381	-2.683801
75	1	0	-1.548521	-1.836470	-3.283580
76	6	0	-2.147065	-3.327447	-1.841029
77	1	0	-2.890824	-3.525255	-1.068282
78	6	0	-1.353241	-4.349258	-2.200821
79	6	0	-1.509994	-5.703581	-1.549647
80	1	0	-1.732252	-6.477587	-2.297887
81	1	0	-2.312711	-5.711665	-0.805348
82	1	0	-0.580039	-6.011748	-1.052018
83	6	0	-0.274663	-4.283571	-3.254240
84	1	0	-0.531442	-4.925012	-4.109437
85	1	0	0.671848	-4.668064	-2.851290
86	1	0	-0.086440	-3.272598	-3.617579
87	6	0	3.089888	3.135935	1.354327
88	1	0	4.057763	2.659402	1.171529
89	1	0	3.272018	4.057072	1.916679
90	1	0	2.646433	3.398189	0.388605
91	6	0	6.184468	-1.442625	0.898230
92	1	0	6.474161	-1.205610	1.916582
93	6	0	7.025059	-2.170393	0.060693
94	1	0	7.992410	-2.506517	0.423419

(1*S*,5*S*,7*S*,10*S*,28*S*)-**2a** (conformer 1)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-2.659419	-1.326236	0.709983
2	8	0	-0.670482	-0.714984	2.915011
3	1	0	-1.368247	-0.076401	2.680116
4	8	0	2.876489	2.195176	0.164338
5	1	0	2.912309	2.659319	1.030482
6	8	0	-0.362963	0.509052	-2.840522
7	8	0	-3.569437	-3.230386	-0.132657
8	6	0	-7.314809	0.153593	-0.203935

9	1	0	-8.245861	0.704837	-0.308265
10	6	0	-7.264331	-1.200743	-0.546177
11	1	0	-8.153537	-1.703553	-0.916445
12	6	0	-6.071720	-1.906323	-0.413187
13	1	0	-6.007019	-2.957562	-0.674332
14	6	0	-4.923474	-1.260020	0.065552
15	6	0	-3.675127	-2.062727	0.188690
16	6	0	-1.367623	-1.945589	0.889877
17	1	0	-1.456433	-2.971912	0.526794
18	6	0	-1.049092	-2.001419	2.412682
19	6	0	-0.683446	1.245425	0.610768
20	8	0	-1.667845	1.493293	1.312889
21	6	0	0.632951	1.826801	0.889063
22	6	0	0.802481	2.445274	2.270820
23	1	0	-0.203098	2.760565	2.576760
24	1	0	1.086443	1.656251	2.977719
25	6	0	1.727277	3.634682	2.355637
26	1	0	1.462292	4.459015	1.690366
27	6	0	2.781837	3.821762	3.175068
28	6	0	3.546941	5.124486	3.158667
29	1	0	4.612805	4.956858	2.952505
30	1	0	3.494578	5.616592	4.139608
31	1	0	3.158026	5.820700	2.409418
32	6	0	0.162094	-2.911317	2.651899
33	1	0	1.035968	-2.589546	2.077058
34	1	0	-0.066807	-3.947033	2.380662
35	1	0	0.427678	-2.879015	3.713155
36	6	0	3.279553	2.814269	4.183218
37	1	0	4.351634	2.622103	4.042766
38	1	0	2.753705	1.858451	4.138274
39	1	0	3.167139	3.210689	5.201598
40	6	0	1.623362	1.736771	-0.045717
41	6	0	1.458829	1.246445	-1.473306
42	6	0	2.559035	0.197665	-1.843866
43	1	0	2.460691	-0.003921	-2.916840
44	1	0	3.523813	0.694194	-1.696859
45	6	0	2.559348	-1.139677	-1.057457
46	1	0	2.351730	-0.899669	-0.006614
47	6	0	3.978935	-1.763344	-1.075141
48	1	0	4.286710	-1.971526	-2.105513
49	1	0	4.669441	-0.989361	-0.705645
50	6	0	4.101574	-2.984774	-0.201060
51	1	0	3.614652	-2.888247	0.771857
52	6	0	4.741066	-4.138285	-0.450770
53	6	0	4.766159	-5.244450	0.577935
54	1	0	5.797051	-5.493769	0.866924
55	1	0	4.325100	-6.167780	0.176681
56	1	0	4.216083	-4.972771	1.484326
57	6	0	5.493341	-4.451567	-1.721719
58	1	0	6.557813	-4.621116	-1.506722
59	1	0	5.430209	-3.658183	-2.470121
60	1	0	5.119231	-5.378761	-2.177325
61	6	0	1.469117	-2.078160	-1.572556
62	6	0	1.808298	-2.958217	-2.752887
63	1	0	2.211622	-2.370771	-3.589130
64	1	0	0.921044	-3.484509	-3.116607
65	1	0	2.565477	-3.706086	-2.490548
66	6	0	0.222269	-2.078344	-1.073984
67	1	0	-0.523579	-2.719659	-1.543281
68	6	0	-0.284268	-1.197665	0.044538
69	1	0	0.537736	-0.976029	0.727386
70	6	0	-0.766617	0.214042	-0.509827
71	1	0	-1.797713	0.133949	-0.852485
72	6	0	0.064369	0.642079	-1.709920
73	6	0	1.640994	2.466027	-2.451730
74	1	0	2.693265	2.768957	-2.390828
75	1	0	1.466670	2.083540	-3.458774
76	6	0	0.770244	3.658445	-2.157582
77	1	0	1.033260	4.202341	-1.249734

78	6	0	-0.253567	4.138091	-2.882646
79	6	0	-0.986445	5.383368	-2.441167
80	1	0	-0.944422	6.160776	-3.217188
81	1	0	-0.571109	5.802134	-1.518882
82	1	0	-2.051530	5.173355	-2.270829
83	6	0	-0.763562	3.536613	-4.169348
84	1	0	-0.573628	4.214813	-5.013631
85	1	0	-1.852077	3.401010	-4.118948
86	1	0	-0.325537	2.563650	-4.394402
87	6	0	-2.259442	-2.528333	3.200456
88	1	0	-3.096770	-1.826477	3.143592
89	1	0	-1.982929	-2.644513	4.253026
90	1	0	-2.600692	-3.496784	2.817366
91	6	0	-4.972919	0.100086	0.408239
92	1	0	-4.079452	0.599024	0.770384
93	6	0	-6.170929	0.800165	0.270165
94	1	0	-6.210704	1.853695	0.533037

(1*S*,5*S*,7*S*,10*S*,28*S*)-**2a** (conformer 5)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-2.552214	-1.477490	0.654029
2	8	0	-0.538675	-0.831842	2.841220
3	1	0	-1.288111	-0.234430	2.663456
4	8	0	2.658291	2.469768	0.296972
5	1	0	2.758655	2.562911	1.268669
6	8	0	-0.511273	0.817762	-2.811035
7	8	0	-3.304550	-3.379521	-0.335725
8	6	0	-7.336002	-0.351970	-0.094322
9	1	0	-8.313909	0.119973	-0.145298
10	6	0	-6.246717	0.354833	0.420632
11	1	0	-6.375943	1.376141	0.768226
12	6	0	-4.988907	-0.243110	0.490552
13	1	0	-4.137679	0.304635	0.882418
14	6	0	-4.824264	-1.561494	0.038142
15	6	0	-3.507929	-2.256440	0.083018
16	6	0	-1.206777	-1.989403	0.762316
17	1	0	-1.216981	-2.995686	0.337510
18	6	0	-0.836746	-2.110630	2.269517
19	6	0	-0.817797	1.256563	0.685318
20	8	0	-1.801984	1.367279	1.422168
21	6	0	0.444952	1.935751	0.968451
22	6	0	0.605258	2.612793	2.321129
23	1	0	0.699862	3.697220	2.184544
24	1	0	-0.333747	2.451740	2.862655
25	6	0	1.756526	2.058054	3.128806
26	1	0	1.722932	0.974153	3.243064
27	6	0	2.768052	2.726256	3.717249
28	6	0	3.817547	1.982399	4.510518
29	1	0	3.823571	2.316561	5.557254
30	1	0	4.825197	2.176053	4.117537
31	1	0	3.647274	0.901727	4.500927
32	6	0	0.446176	-2.937514	2.418107
33	1	0	1.274489	-2.514607	1.841181
34	1	0	0.287746	-3.969249	2.087732
35	1	0	0.742539	-2.949907	3.471565
36	6	0	2.944852	4.227037	3.699982
37	1	0	2.221774	4.745151	3.065733
38	1	0	3.953250	4.498411	3.359750
39	1	0	2.842734	4.631112	4.716483
40	6	0	1.438959	1.950265	0.033437
41	6	0	1.295102	1.558867	-1.422714
42	6	0	2.457550	0.626725	-1.895755
43	1	0	2.348840	0.506140	-2.979915
44	1	0	3.387353	1.179367	-1.725151
45	6	0	2.577714	-0.767796	-1.225631
46	1	0	2.391803	-0.632627	-0.152300
47	6	0	4.036497	-1.281068	-1.337576
48	1	0	4.322418	-1.380590	-2.390215
49	1	0	4.682678	-0.490846	-0.924564

50	6	0	4.277051	-2.558626	-0.575027
51	1	0	3.802519	-2.589376	0.408266
52	6	0	5.007448	-3.625969	-0.934591
53	6	0	5.149080	-4.811829	-0.009440
54	1	0	6.203105	-4.992428	0.245187
55	1	0	4.783948	-5.731891	-0.487170
56	1	0	4.594370	-4.671245	0.923525
57	6	0	5.756822	-3.758519	-2.238603
58	1	0	6.836523	-3.849748	-2.054192
59	1	0	5.607353	-2.911902	-2.912779
60	1	0	5.456446	-4.672312	-2.769634
61	6	0	1.538191	-1.737670	-1.785764
62	6	0	1.899932	-2.500186	-3.038807
63	1	0	2.234956	-1.823811	-3.837151
64	1	0	1.039894	-3.059199	-3.418721
65	1	0	2.714919	-3.209839	-2.855309
66	6	0	0.309270	-1.859188	-1.258369
67	1	0	-0.406739	-2.514125	-1.754692
68	6	0	-0.219686	-1.100230	-0.063921
69	1	0	0.608240	-0.856745	0.603836
70	6	0	-0.832903	0.298830	-0.504032
71	1	0	-1.859698	0.153948	-0.838317
72	6	0	-0.064141	0.883086	-1.682573
73	6	0	1.377517	2.864700	-2.300391
74	1	0	2.408970	3.230988	-2.226384
75	1	0	1.213795	2.552708	-3.333322
76	6	0	0.435876	3.969585	-1.902576
77	1	0	0.671685	4.450762	-0.952771
78	6	0	-0.620290	4.444326	-2.583195
79	6	0	-1.425097	5.599850	-2.035675
80	1	0	-1.428273	6.445265	-2.738278
81	1	0	-1.034735	5.956795	-1.077337
82	1	0	-2.476038	5.313489	-1.890898
83	6	0	-1.100225	3.924469	-3.916133
84	1	0	-0.968104	4.687081	-4.697014
85	1	0	-2.175680	3.707002	-3.873299
86	1	0	-0.596224	3.009748	-4.230175
87	6	0	-1.978555	-2.775709	3.055053
88	1	0	-2.869316	-2.140750	3.060950
89	1	0	-1.662720	-2.931235	4.091349
90	1	0	-2.253869	-3.744283	2.622413
91	6	0	-5.918093	-2.267943	-0.481548
92	1	0	-5.764039	-3.284650	-0.828003
93	6	0	-7.170791	-1.664343	-0.546242
94	1	0	-8.017528	-2.213739	-0.948449

(1*S*,5*S*,7*S*,10*S*,28*S*)-**2a** (conformer 7)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-2.560775	1.840997	0.574286
2	8	0	0.229964	4.227302	0.420883
3	1	0	0.709924	3.732074	1.118145
4	8	0	2.873532	-2.159499	0.465630
5	1	0	3.179051	-2.234492	1.396784
6	8	0	1.949511	1.256423	-2.656079
7	8	0	-2.194264	0.149093	2.037369
8	6	0	-7.160711	0.002979	1.181914
9	1	0	-8.226103	-0.209798	1.152461
10	6	0	-6.629810	1.018449	0.383175
11	1	0	-7.280513	1.594940	-0.268527
12	6	0	-5.264161	1.295819	0.418922
13	1	0	-4.846288	2.080883	-0.200707
14	6	0	-4.421618	0.553214	1.257551
15	6	0	-2.953716	0.803186	1.344718
16	6	0	-1.156336	2.220590	0.606610
17	1	0	-0.815639	2.090794	1.638103
18	6	0	-1.114304	3.752007	0.314251
19	6	0	1.819536	1.364544	0.915333
20	8	0	1.788993	2.264746	1.765200
21	6	0	2.340940	0.033973	1.221615

22	6	0	2.639610	-0.254722	2.687819
23	1	0	2.754503	0.724662	3.168033
24	1	0	1.757924	-0.710593	3.155392
25	6	0	3.879589	-1.077791	2.943257
26	1	0	4.783618	-0.682266	2.476475
27	6	0	4.010728	-2.188450	3.696384
28	6	0	5.362991	-2.838051	3.876286
29	1	0	5.343522	-3.889902	3.560377
30	1	0	5.655378	-2.837619	4.935368
31	1	0	6.144514	-2.323828	3.308803
32	6	0	-1.974101	4.477834	1.367716
33	1	0	-1.650578	4.211185	2.381256
34	1	0	-3.037951	4.240869	1.273091
35	1	0	-1.838553	5.556675	1.244667
36	6	0	2.886918	-2.863545	4.445733
37	1	0	2.833530	-3.929580	4.187540
38	1	0	1.907237	-2.419197	4.257766
39	1	0	3.072649	-2.816314	5.527421
40	6	0	2.463105	-0.896756	0.227661
41	6	0	2.275493	-0.659245	-1.259824
42	6	0	1.256757	-1.675364	-1.881475
43	1	0	1.318222	-1.556734	-2.969610
44	1	0	1.635416	-2.675695	-1.645931
45	6	0	-0.225762	-1.585769	-1.430766
46	1	0	-0.229827	-1.425199	-0.345957
47	6	0	-0.922564	-2.954155	-1.645751
48	1	0	-0.896851	-3.230593	-2.705669
49	1	0	-0.310562	-3.706924	-1.124624
50	6	0	-2.326858	-2.992155	-1.096486
51	1	0	-2.455613	-2.455306	-0.154553
52	6	0	-3.403336	-3.611898	-1.605630
53	6	0	-4.735278	-3.556950	-0.895236
54	1	0	-5.078065	-4.564308	-0.617843
55	1	0	-5.512763	-3.133988	-1.547000
56	1	0	-4.691142	-2.948794	0.013179
57	6	0	-3.408063	-4.419740	-2.881314
58	1	0	-3.653351	-5.470467	-2.670906
59	1	0	-2.450778	-4.403692	-3.407742
60	1	0	-4.181653	-4.055071	-3.571163
61	6	0	-0.954731	-0.421057	-2.104832
62	6	0	-1.546153	-0.674476	-3.472230
63	1	0	-0.796184	-1.080326	-4.165049
64	1	0	-1.932062	0.251049	-3.909587
65	1	0	-2.367436	-1.398976	-3.426658
66	6	0	-1.017858	0.808488	-1.565569
67	1	0	-1.509890	1.593918	-2.131805
68	6	0	-0.369614	1.190620	-0.257716
69	1	0	-0.372636	0.298063	0.371781
70	6	0	1.158476	1.579673	-0.437402
71	1	0	1.230741	2.630013	-0.718700
72	6	0	1.809855	0.775738	-1.547601
73	6	0	3.651247	-0.893839	-1.987171
74	1	0	3.855031	-1.970362	-1.944595
75	1	0	3.494873	-0.629261	-3.034094
76	6	0	4.822823	-0.151579	-1.400879
77	1	0	5.154445	-0.518886	-0.428987
78	6	0	5.513030	0.867879	-1.937660
79	6	0	6.696592	1.458350	-1.207368
80	1	0	7.607864	1.396507	-1.818987
81	1	0	6.891223	0.949894	-0.257504
82	1	0	6.536747	2.524963	-0.997104
83	6	0	5.219769	1.507608	-3.272695
84	1	0	6.034843	1.308046	-3.983103
85	1	0	5.161965	2.598890	-3.165340
86	1	0	4.279282	1.174568	-3.712996
87	6	0	-1.577156	4.130021	-1.096142
88	1	0	-0.903097	3.720491	-1.853262
89	1	0	-1.564176	5.220197	-1.197401
90	1	0	-2.594099	3.775114	-1.289620

91	6	0	-4.958157	-0.465770	2.057398
92	1	0	-4.289295	-1.025761	2.702652
93	6	0	-6.323383	-0.738878	2.019715
94	1	0	-6.735805	-1.527052	2.643540

(1*S*,5*S*,7*S*,10*S*,28*R*)-**2b** (conformer 1)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-2.157492	-1.621537	1.136914
2	8	0	-0.543353	-1.781177	3.345887
3	1	0	-0.453037	-2.219761	4.198350
4	8	0	2.063573	0.626491	-2.439334
5	8	0	1.873559	1.972633	2.086203
6	8	0	-4.236929	-0.957649	0.537248
7	6	0	-3.517672	-5.275485	-1.953643
8	1	0	-3.578415	-6.164381	-2.571683
9	6	0	-2.328853	-4.966533	-1.294257
10	1	0	-1.464456	-5.611526	-1.401813
11	6	0	-2.244196	-3.826707	-0.500373
12	1	0	-1.320333	-3.575366	0.003896
13	6	0	-3.358616	-2.989619	-0.367517
14	6	0	-3.330491	-1.752823	0.460121
15	6	0	-1.959094	-0.427759	1.934950
16	1	0	-2.904762	0.116552	1.942196
17	6	0	-1.696832	-0.898490	3.387891
18	6	0	0.998389	-1.052073	0.508073
19	8	0	0.767368	-2.288414	0.985707
20	1	0	0.286279	-2.235280	1.836028
21	6	0	1.517169	-0.899201	-0.737319
22	6	0	1.775388	-2.082202	-1.650504
23	1	0	1.031657	-2.856518	-1.440471
24	1	0	1.623705	-1.747930	-2.675972
25	6	0	3.152452	-2.678581	-1.473251
26	1	0	3.306272	-3.178857	-0.518846
27	6	0	4.168899	-2.667390	-2.344079
28	6	0	5.470775	-3.358461	-2.016349
29	1	0	6.306135	-2.647923	-2.021851
30	1	0	5.707764	-4.121638	-2.767730
31	1	0	5.439707	-3.843236	-1.038341
32	6	0	-2.899983	-1.700799	3.899209
33	1	0	-3.056419	-2.589007	3.287537
34	1	0	-3.811434	-1.099097	3.885102
35	1	0	-2.724483	-2.017958	4.932247
36	6	0	4.131097	-2.003116	-3.698535
37	1	0	5.042905	-1.415844	-3.854416
38	1	0	3.284325	-1.329077	-3.817270
39	1	0	4.103621	-2.752820	-4.499284
40	6	0	1.817520	0.435284	-1.254138
41	6	0	1.932294	1.639568	-0.287200
42	6	0	1.098921	2.832197	-0.845503
43	1	0	1.386536	3.733890	-0.296650
44	1	0	1.431337	2.954905	-1.878957
45	6	0	-0.444265	2.681587	-0.837954
46	1	0	-0.672656	1.652704	-1.134500
47	6	0	-1.073432	3.580012	-1.931688
48	1	0	-0.810402	4.626403	-1.756946
49	1	0	-0.592465	3.302574	-2.878694
50	6	0	-2.561942	3.395245	-2.065448
51	1	0	-2.894468	2.359902	-1.997087
52	6	0	-3.503361	4.322522	-2.278335
53	6	0	-4.955682	3.933442	-2.409439
54	1	0	-5.354766	4.229470	-3.387097
55	1	0	-5.567660	4.442712	-1.655392
56	1	0	-5.099348	2.857771	-2.293523
57	6	0	-3.237659	5.799748	-2.426522
58	1	0	-3.528917	6.141155	-3.427029
59	1	0	-2.191834	6.068426	-2.278869
60	1	0	-3.841671	6.375378	-1.715367
61	6	0	-1.015788	2.928254	0.553970
62	6	0	-1.273686	4.360703	0.951735

63	1	0	-0.383034	4.980526	0.801752
64	1	0	-1.553709	4.430430	2.004142
65	1	0	-2.077604	4.798271	0.353870
66	6	0	-1.213664	1.944729	1.441338
67	1	0	-1.558385	2.220937	2.432218
68	6	0	-0.936512	0.478928	1.189904
69	1	0	-1.150775	0.285327	0.137805
70	6	0	0.594552	0.106599	1.383921
71	1	0	0.766795	-0.156571	2.425836
72	6	0	1.505503	1.311004	1.140783
73	6	0	3.434255	2.088293	-0.276526
74	1	0	3.661674	2.400911	-1.300427
75	1	0	3.507480	2.967166	0.363337
76	6	0	4.414811	1.024706	0.137031
77	1	0	4.500060	0.186103	-0.550861
78	6	0	5.202711	1.009868	1.219729
79	6	0	6.171313	-0.125622	1.445957
80	1	0	7.202040	0.245038	1.504771
81	1	0	6.120166	-0.868248	0.647745
82	1	0	5.968053	-0.630435	2.398052
83	6	0	5.231905	2.078537	2.283179
84	1	0	6.179719	2.630147	2.250033
85	1	0	5.170896	1.622266	3.277491
86	1	0	4.409763	2.786533	2.199890
87	6	0	-1.397748	0.273215	4.330880
88	1	0	-0.515155	0.834530	4.024059
89	1	0	-1.219110	-0.111026	5.339497
90	1	0	-2.247744	0.957723	4.386713
91	6	0	-4.549097	-3.299480	-1.035084
92	1	0	-5.396104	-2.634087	-0.923817
93	6	0	-4.627787	-4.440811	-1.823670
94	1	0	-5.551123	-4.679668	-2.338714

(1*S*,5*S*,7*S*,10*S*,28*S*)-**2b** (conformer 1)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	2.648870	-1.964821	-0.135140
2	8	0	-0.290791	-3.926490	-0.838540
3	1	0	-0.460331	-4.724100	-1.363980
4	8	0	-2.596250	2.020390	1.538310
5	8	0	-1.747330	0.089790	-2.701350
6	8	0	2.478030	-1.268561	2.014450
7	6	0	7.360600	-0.676321	0.898360
8	1	0	8.427970	-0.472692	0.881970
9	6	0	6.711030	-1.086541	-0.268330
10	1	0	7.271200	-1.199241	-1.192390
11	6	0	5.342620	-1.350211	-0.251410
12	1	0	4.832160	-1.661621	-1.155520
13	6	0	4.616890	-1.201481	0.938660
14	6	0	3.154060	-1.464621	1.024130
15	6	0	1.228390	-2.239261	-0.172240
16	1	0	0.929160	-2.573250	0.825320
17	6	0	1.063769	-3.470881	-1.108610
18	6	0	-1.811950	-1.309320	0.539830
19	8	0	-1.858270	-2.580890	0.988670
20	1	0	-1.379181	-3.172030	0.366540
21	6	0	-2.346000	-0.309550	1.291580
22	6	0	-2.962030	-0.570460	2.654040
23	1	0	-2.447620	-1.422120	3.115030
24	1	0	-2.777210	0.305300	3.278820
25	6	0	-4.440380	-0.883020	2.577080
26	1	0	-4.670580	-1.841820	2.110370
27	6	0	-5.467850	-0.136020	3.011230
28	6	0	-6.888560	-0.635739	2.882380
29	1	0	-7.498050	0.049761	2.276340
30	1	0	-7.376900	-0.694119	3.865900
31	1	0	-6.934290	-1.628909	2.423540
32	6	0	2.025149	-4.587401	-0.676470
33	1	0	1.913359	-4.802281	0.391210
34	1	0	3.066049	-4.321241	-0.872480

35	1	0	1.798829	-5.504341	-1.235490
36	6	0	-5.332530	1.217990	3.667260
37	1	0	-6.047940	1.925900	3.227330
38	1	0	-4.336300	1.649160	3.554480
39	1	0	-5.573920	1.160540	4.738850
40	6	0	-2.323450	1.070810	0.803590
41	6	0	-2.054720	1.371440	-0.692140
42	6	0	-0.980650	2.495500	-0.816440
43	1	0	-0.990380	2.860940	-1.850440
44	1	0	-1.337260	3.308190	-0.175100
45	6	0	0.471430	2.138020	-0.400310
46	1	0	0.407340	1.540310	0.517270
47	6	0	1.240410	3.425749	-0.007450
48	1	0	1.258380	4.125179	-0.850460
49	1	0	0.647930	3.917150	0.779040
50	6	0	2.627240	3.152169	0.516630
51	1	0	2.694720	2.286139	1.178220
52	6	0	3.757120	3.842009	0.293500
53	6	0	5.059080	3.419469	0.932700
54	1	0	5.461200	4.215049	1.576380
55	1	0	5.826850	3.218869	0.171890
56	1	0	4.943390	2.516199	1.539290
57	6	0	3.856911	5.079829	-0.565660
58	1	0	4.172041	5.942609	0.038130
59	1	0	2.916741	5.346469	-1.054280
60	1	0	4.621241	4.953989	-1.345300
61	6	0	1.176120	1.316439	-1.478150
62	6	0	1.818120	2.076139	-2.615690
63	1	0	1.108730	2.773419	-3.080970
64	1	0	2.171680	1.394559	-3.395350
65	1	0	2.671510	2.669019	-2.267170
66	6	0	1.177950	-0.027101	-1.490490
67	1	0	1.656670	-0.526191	-2.328060
68	6	0	0.492260	-0.895810	-0.459790
69	1	0	0.551270	-0.376800	0.499860
70	6	0	-1.060590	-1.066170	-0.744670
71	1	0	-1.212940	-1.905710	-1.424170
72	6	0	-1.634270	0.140920	-1.490320
73	6	0	-3.389580	1.931750	-1.296580
74	1	0	-3.593930	2.868410	-0.763490
75	1	0	-3.197750	2.177610	-2.342930
76	6	0	-4.578130	1.017900	-1.151970
77	1	0	-4.908910	0.860480	-0.124960
78	6	0	-5.274180	0.404880	-2.123130
79	6	0	-6.474850	-0.446529	-1.780470
80	1	0	-7.383260	-0.062639	-2.266910
81	1	0	-6.656380	-0.482799	-0.701790
82	1	0	-6.345260	-1.477260	-2.140320
83	6	0	-4.974510	0.497550	-3.599790
84	1	0	-5.784920	1.020100	-4.128510
85	1	0	-4.915600	-0.507520	-4.039440
86	1	0	-4.032460	1.002530	-3.818110
87	6	0	1.210869	-3.175061	-2.604280
88	1	0	0.473320	-2.447330	-2.951940
89	1	0	1.077669	-4.099001	-3.181650
90	1	0	2.212340	-2.792771	-2.825180
91	6	0	5.271450	-0.785391	2.107070
92	1	0	4.691270	-0.675031	3.017290
93	6	0	6.639480	-0.525931	2.086080
94	1	0	7.143980	-0.206881	2.993720

(1*S*,5*S*,7*S*,10*S*,28*R*)-**2c** (conformer 1)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-2.042665	-1.706910	1.109390
2	8	0	-0.382883	-1.785658	3.450042
3	1	0	-0.036876	-2.029875	2.547167
4	8	0	2.066005	0.786861	-2.443507
5	8	0	1.786343	2.131617	2.085139
6	8	0	-4.210265	-1.291873	0.561800

7	6	0	-2.965173	-5.508304	-1.925644
8	1	0	-2.916754	-6.404990	-2.539458
9	6	0	-1.817955	-5.042084	-1.279314
10	1	0	-0.875436	-5.571219	-1.392126
11	6	0	-1.869015	-3.892568	-0.489962
12	1	0	-0.977513	-3.518856	0.007454
13	6	0	-3.084856	-3.205208	-0.353360
14	6	0	-3.198120	-1.965643	0.475160
15	6	0	-1.915827	-0.522739	1.942584
16	1	0	-2.901364	-0.049423	1.974520
17	6	0	-1.580853	-1.027917	3.376786
18	6	0	1.012668	-1.005618	0.550788
19	8	0	0.815433	-2.161170	1.034428
20	6	0	1.482458	-0.761337	-0.753591
21	6	0	1.706562	-1.937673	-1.687740
22	1	0	0.931995	-2.692312	-1.497717
23	1	0	1.591244	-1.589097	-2.716583
24	6	0	3.051885	-2.596361	-1.487133
25	1	0	3.135876	-3.153580	-0.552850
26	6	0	4.124328	-2.555666	-2.294019
27	6	0	5.389905	-3.302548	-1.937889
28	1	0	6.249301	-2.620586	-1.846918
29	1	0	5.659720	-4.031020	-2.718995
30	1	0	5.288640	-3.846255	-0.992187
31	6	0	-2.736487	-1.926002	3.869175
32	1	0	-2.811533	-2.821729	3.246895
33	1	0	-3.703306	-1.407043	3.858996
34	1	0	-2.520141	-2.247086	4.893730
35	6	0	4.178282	-1.791407	-3.598424
36	1	0	5.139329	-1.265049	-3.691511
37	1	0	3.387570	-1.041018	-3.669763
38	1	0	4.112571	-2.466866	-4.466471
39	6	0	1.766428	0.544324	-1.252485
40	6	0	1.826395	1.761345	-0.284491
41	6	0	0.938608	2.915844	-0.839286
42	1	0	1.183388	3.837256	-0.294324
43	1	0	1.259490	3.044754	-1.878786
44	6	0	-0.597166	2.694900	-0.823481
45	1	0	-0.770193	1.656120	-1.128949
46	6	0	-1.269252	3.569897	-1.913466
47	1	0	-1.059125	4.630511	-1.732201
48	1	0	-0.772909	3.321712	-2.863807
49	6	0	-2.747536	3.313814	-2.054464
50	1	0	-3.024685	2.259713	-1.992430
51	6	0	-3.741296	4.192733	-2.258879
52	6	0	-5.172511	3.726176	-2.391232
53	1	0	-5.596305	4.010077	-3.366228
54	1	0	-5.814223	4.190259	-1.627843
55	1	0	-5.257652	2.640085	-2.287131
56	6	0	-3.557309	5.685813	-2.391517
57	1	0	-3.882684	6.030931	-3.384097
58	1	0	-2.521256	6.004549	-2.254670
59	1	0	-4.177097	6.223876	-1.659669
60	6	0	-1.187124	2.903342	0.569732
61	6	0	-1.518547	4.320782	0.978205
62	1	0	-0.655387	4.987461	0.843099
63	1	0	-1.809209	4.366369	2.032650
64	1	0	-2.340620	4.734312	0.380874
65	6	0	-1.337099	1.901610	1.451897
66	1	0	-1.704463	2.150034	2.445828
67	6	0	-0.958137	0.458580	1.201254
68	1	0	-1.144943	0.251732	0.143224
69	6	0	0.588711	0.189812	1.415146
70	1	0	0.761030	-0.060828	2.462196
71	6	0	1.428651	1.426474	1.151435
72	6	0	3.301715	2.285217	-0.291135
73	1	0	3.500098	2.613656	-1.318759
74	1	0	3.354526	3.160210	0.361195
75	6	0	4.332567	1.253999	0.083876

76	1	0	4.422744	0.431210	-0.624821
77	6	0	5.136772	1.234072	1.158454
78	6	0	6.139558	0.118599	1.344210
79	1	0	7.166634	0.510344	1.409981
80	1	0	6.101850	-0.603172	0.522064
81	1	0	5.956009	-0.426667	2.281571
82	6	0	5.138685	2.269165	2.258139
83	1	0	6.069440	2.857813	2.247487
84	1	0	5.092589	1.778595	3.240487
85	1	0	4.288164	2.949832	2.199111
86	6	0	-1.425577	0.162478	4.342175
87	1	0	-0.608752	0.823681	4.041162
88	1	0	-1.184458	-0.230721	5.335696
89	1	0	-2.348957	0.750438	4.420101
90	6	0	-4.233756	-3.670794	-1.005684
91	1	0	-5.158505	-3.115084	-0.885918
92	6	0	-4.174842	-4.821171	-1.788560
93	1	0	-5.068056	-5.181623	-2.293183

(1*S*,5*S*,7*S*,10*S*,28*S*)-**2c** (conformer 1)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	2.916811	0.493359	1.012210
2	8	0	1.285271	0.095499	3.435200
3	1	0	0.315671	0.089180	3.194810
4	8	0	-3.632230	-1.020639	-1.278030
5	8	0	1.041410	-1.287851	-1.242320
6	6	0	1.964971	1.485449	1.493460
7	1	0	2.407401	2.468469	1.307440
8	6	0	1.807241	1.347239	3.041130
9	6	0	-1.263129	-0.108120	1.335750
10	8	0	-1.219549	0.199150	2.567580
11	6	0	-2.469140	-0.413450	0.683570
12	6	0	-3.754440	-0.376449	1.493970
13	1	0	-3.687489	0.458121	2.203900
14	1	0	-4.587749	-0.183369	0.814220
15	6	0	-3.989130	-1.638529	2.291490
16	1	0	-3.318720	-1.752969	3.144390
17	6	0	-4.887630	-2.608849	2.062760
18	6	0	-4.992751	-3.798919	2.989120
19	1	0	-4.803121	-4.742769	2.455140
20	1	0	-6.003891	-3.887678	3.417280
21	1	0	-4.281091	-3.731499	3.819140
22	6	0	0.912771	2.496329	3.556310
23	1	0	-0.116209	2.374260	3.208210
24	1	0	1.285702	3.480519	3.244190
25	1	0	0.897711	2.466019	4.651340
26	6	0	-5.851770	-2.617928	0.897500
27	1	0	-5.907461	-3.624688	0.458200
28	1	0	-5.544620	-1.933039	0.103850
29	1	0	-6.875890	-2.365358	1.216240
30	6	0	-2.557700	-0.765120	-0.690390
31	6	0	-1.279780	-0.805250	-1.575990
32	6	0	-1.369329	0.427330	-2.531840
33	1	0	-0.646409	0.293330	-3.347080
34	1	0	-2.372129	0.375710	-2.970890
35	6	0	-1.160579	1.812420	-1.860160
36	1	0	-1.522069	1.739430	-0.828270
37	6	0	-2.046099	2.892250	-2.540690
38	1	0	-1.750008	2.995910	-3.595420
39	1	0	-3.072869	2.513551	-2.551890
40	6	0	-1.977598	4.237850	-1.868750
41	1	0	-1.025838	4.760100	-1.979610
42	6	0	-2.918648	4.847011	-1.129920
43	6	0	-2.655757	6.199881	-0.509670
44	1	0	-2.745457	6.157441	0.585390
45	1	0	-3.389747	6.944971	-0.851600
46	1	0	-1.655307	6.573120	-0.752100
47	6	0	-4.285848	4.281861	-0.829350
48	1	0	-4.429308	4.180241	0.255400

49	1	0	-4.457228	3.299591	-1.274240
50	1	0	-5.075648	4.959921	-1.185210
51	6	0	0.322191	2.151970	-1.839250
52	6	0	0.929271	2.699109	-3.113490
53	1	0	0.693251	2.064999	-3.979200
54	1	0	2.019081	2.761789	-3.034150
55	1	0	0.553452	3.703400	-3.352620
56	6	0	1.112341	1.891749	-0.788140
57	1	0	2.174371	2.099169	-0.910440
58	6	0	0.716191	1.355179	0.581410
59	1	0	-0.044709	2.022980	1.001010
60	6	0	0.077611	-0.108480	0.586770
61	1	0	0.762290	-0.732281	1.170550
62	6	0	0.030830	-0.768560	-0.785800
63	6	0	-1.317740	-2.086920	-2.461410
64	1	0	-2.203600	-1.988570	-3.099350
65	1	0	-0.433310	-2.089050	-3.102050
66	6	0	-1.446300	-3.370420	-1.685090
67	1	0	-2.383110	-3.459020	-1.135530
68	6	0	-0.580651	-4.392930	-1.604720
69	6	0	-0.917431	-5.620020	-0.788640
70	1	0	-0.902621	-6.530140	-1.408250
71	1	0	-1.906161	-5.541040	-0.325370
72	1	0	-0.179801	-5.779330	0.011770
73	6	0	0.765589	-4.445111	-2.286270
74	1	0	0.786189	-5.226871	-3.061500
75	1	0	1.548959	-4.707571	-1.560700
76	1	0	1.047719	-3.492971	-2.737260
77	6	0	3.192691	1.442559	3.699490
78	1	0	3.796891	0.571989	3.429420
79	1	0	3.066871	1.437759	4.787320
80	1	0	3.729271	2.349719	3.402760
81	8	0	4.577781	2.018008	0.711350
82	6	0	6.472200	-2.318342	-1.022640
83	1	0	7.073900	-3.123353	-1.438770
84	6	0	5.084670	-2.454122	-0.939610
85	1	0	4.602220	-3.358802	-1.300460
86	6	0	4.304880	-1.430142	-0.400350
87	1	0	3.223250	-1.516331	-0.365050
88	6	0	4.925161	-0.256322	0.049920
89	6	0	4.140591	0.882648	0.618210
90	6	0	6.315221	-0.112162	-0.052580
91	1	0	6.767841	0.814408	0.286520
92	6	0	7.088020	-1.144013	-0.579620
93	1	0	8.167630	-1.033683	-0.648410

(1*S*,5*S*,7*S*,10*S*,28*S*)-**2c** (conformer 6)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	2.900680	0.547401	1.016690
2	8	0	0.559119	2.144800	3.372870
3	1	0	-0.203040	1.566790	3.101690
4	8	0	-3.611309	-1.243792	-1.291200
5	8	0	1.041591	-1.276180	-1.183490
6	6	0	1.925210	1.533771	1.465920
7	1	0	2.349969	2.521591	1.269850
8	6	0	1.736570	1.436721	3.023870
9	6	0	-1.350820	0.007149	1.281050
10	8	0	-1.353300	0.449659	2.469600
11	6	0	-2.520719	-0.440381	0.642340
12	6	0	-3.820979	-0.415472	1.429040
13	1	0	-3.821580	0.484348	2.057580
14	1	0	-4.652369	-0.343272	0.724100
15	6	0	-3.988699	-1.609852	2.340180
16	1	0	-3.347809	-1.587822	3.222770
17	6	0	-4.798568	-2.667422	2.177410
18	6	0	-4.852948	-3.769112	3.211040
19	1	0	-4.567748	-4.740762	2.779080
20	1	0	-5.872658	-3.898443	3.607230
21	1	0	-4.187218	-3.567692	4.057520

22	6	0	2.891879	2.193241	3.698460
23	1	0	2.896479	3.240901	3.379770
24	1	0	3.865420	1.756632	3.454570
25	1	0	2.752219	2.166281	4.784490
26	6	0	-5.706558	-2.864693	0.984000
27	1	0	-5.663868	-3.909543	0.643000
28	1	0	-5.419189	-2.233612	0.139790
29	1	0	-6.760358	-2.668283	1.239020
30	6	0	-2.566069	-0.877421	-0.709350
31	6	0	-1.280689	-0.848481	-1.589250
32	6	0	-1.417870	0.388199	-2.538490
33	1	0	-0.719910	0.261150	-3.376470
34	1	0	-2.432020	0.322159	-2.949550
35	6	0	-1.204020	1.780429	-1.884800
36	1	0	-1.555600	1.720409	-0.849250
37	6	0	-2.099851	2.849599	-2.569940
38	1	0	-1.815941	2.939639	-3.629250
39	1	0	-3.126171	2.469269	-2.564890
40	6	0	-2.026221	4.203599	-1.915600
41	1	0	-1.079882	4.729699	-2.050780
42	6	0	-2.955062	4.814149	-1.162750
43	6	0	-2.686562	6.173079	-0.558700
44	1	0	-2.748612	6.136719	0.538300
45	1	0	-3.433843	6.910748	-0.887740
46	1	0	-1.694702	6.551029	-0.827440
47	6	0	-4.311511	4.243168	-0.826840
48	1	0	-4.424591	4.138538	0.261110
49	1	0	-4.491301	3.261248	-1.269330
50	1	0	-5.113072	4.918978	-1.159860
51	6	0	0.277909	2.131280	-1.883960
52	6	0	0.870069	2.655060	-3.174920
53	1	0	0.635920	1.999110	-4.024730
54	1	0	1.959639	2.731931	-3.104450
55	1	0	0.481529	3.649390	-3.434260
56	6	0	1.076190	1.909230	-0.830030
57	1	0	2.135299	2.129131	-0.959500
58	6	0	0.684690	1.398560	0.549070
59	1	0	-0.049110	2.090300	0.975610
60	6	0	0.011060	-0.039810	0.570100
61	1	0	0.657731	-0.673970	1.184890
62	6	0	0.010171	-0.755140	-0.778320
63	6	0	-1.245719	-2.119341	-2.489000
64	1	0	-2.120819	-2.050901	-3.145470
65	1	0	-0.349139	-2.074590	-3.111140
66	6	0	-1.336108	-3.420761	-1.737470
67	1	0	-2.281528	-3.558531	-1.214080
68	6	0	-0.430708	-4.408370	-1.658300
69	6	0	-0.735637	-5.666760	-0.878020
70	1	0	-0.669677	-6.560910	-1.517260
71	1	0	-1.737307	-5.638651	-0.437200
72	1	0	-0.010627	-5.815780	-0.064000
73	6	0	0.931412	-4.390460	-2.309830
74	1	0	0.995143	-5.137640	-3.116250
75	1	0	1.706422	-4.659129	-1.577330
76	1	0	1.192362	-3.411190	-2.713010
77	6	0	1.688420	-0.004749	3.569540
78	1	0	0.764501	-0.505320	3.273920
79	1	0	1.700160	0.038761	4.664790
80	1	0	2.545941	-0.597319	3.235350
81	8	0	4.582290	2.060532	0.781290
82	6	0	6.484801	-2.274927	-0.950780
83	1	0	7.090132	-3.080957	-1.359510
84	6	0	5.094881	-2.401728	-0.899590
85	1	0	4.614342	-3.300258	-1.277970
86	6	0	4.310231	-1.375848	-0.370810
87	1	0	3.227311	-1.455529	-0.359260
88	6	0	4.928460	-0.209578	0.101950
89	6	0	4.138970	0.931282	0.660590
90	6	0	6.321460	-0.074527	0.031630

91	1	0	6.772600	0.846633	0.387080
92	6	0	7.098581	-1.108017	-0.485710
93	1	0	8.180121	-1.004647	-0.530110

(1*S*,5*S*,7*S*,10*S*,28*S*)-**2c** (conformer 8)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-2.712330	-0.719181	1.126800
2	8	0	-0.093549	-1.823640	3.474970
3	1	0	0.584290	-1.193640	3.112730
4	8	0	3.436819	1.559641	-1.694440
5	8	0	-1.180200	1.097950	-1.326420
6	6	0	-1.606150	-1.542320	1.601980
7	1	0	-1.919089	-2.585970	1.515440
8	6	0	-1.359040	-1.282920	3.132560
9	6	0	1.460520	0.317481	1.097310
10	8	0	1.559840	-0.011419	2.319930
11	6	0	2.537460	0.824541	0.350670
12	6	0	3.877460	1.019651	1.041100
13	1	0	3.907490	0.383071	1.927930
14	1	0	4.666550	0.688922	0.352770
15	6	0	4.160259	2.461392	1.396850
16	1	0	4.419719	3.085592	0.540800
17	6	0	4.106659	3.040692	2.606080
18	6	0	4.443509	4.504232	2.778880
19	1	0	5.271008	4.645272	3.492240
20	1	0	3.590138	5.068531	3.185330
21	1	0	4.735178	4.969262	1.830730
22	6	0	-2.388109	-2.097361	3.932320
23	1	0	-2.283749	-3.164261	3.708560
24	1	0	-3.415459	-1.798511	3.702470
25	1	0	-2.206409	-1.952601	5.002650
26	6	0	3.712019	2.322921	3.876900
27	1	0	4.581319	2.153352	4.532200
28	1	0	3.223330	1.366181	3.679150
29	1	0	3.007349	2.937181	4.456510
30	6	0	2.464490	1.133881	-1.035150
31	6	0	1.151850	0.885141	-1.833880
32	6	0	1.385680	-0.410699	-2.678930
33	1	0	0.642740	-0.437930	-3.487030
34	1	0	2.367510	-0.273309	-3.147070
35	6	0	1.357961	-1.752859	-1.899310
36	1	0	1.754670	-1.565489	-0.895490
37	6	0	2.323391	-2.781579	-2.549810
38	1	0	1.991131	-2.992099	-3.578000
39	1	0	3.302871	-2.302449	-2.642120
40	6	0	2.425411	-4.071989	-1.781470
41	1	0	1.500141	-4.648059	-1.730150
42	6	0	3.486091	-4.573399	-1.128860
43	6	0	3.381502	-5.882849	-0.381530
44	1	0	3.600632	-5.746239	0.687160
45	1	0	4.110712	-6.616558	-0.756770
46	1	0	2.382412	-6.322629	-0.466200
47	6	0	4.845481	-3.921598	-1.050040
48	1	0	4.901951	-2.970638	-1.583600
49	1	0	5.621211	-4.586458	-1.457970
50	1	0	5.119201	-3.729958	-0.003240
51	6	0	-0.075639	-2.252580	-1.779440
52	6	0	-0.676659	-2.941030	-2.986560
53	1	0	-0.575679	-2.329360	-3.893870
54	1	0	-1.742699	-3.137490	-2.835260
55	1	0	-0.187709	-3.900390	-3.203760
56	6	0	-0.837389	-2.023590	-0.700270
57	1	0	-1.871339	-2.363220	-0.747940
58	6	0	-0.435800	-1.352530	0.605420
59	1	0	0.392511	-1.919900	1.042340
60	6	0	0.070050	0.147020	0.463240
61	1	0	-0.614560	0.761610	1.056580
62	6	0	-0.077680	0.729200	-0.941550
63	6	0	0.932149	2.056331	-2.836860

64	1	0	1.775609	2.018411	-3.535820
65	1	0	0.015909	1.859600	-3.397990
66	6	0	0.918439	3.424881	-2.208850
67	1	0	1.870649	3.710361	-1.763280
68	6	0	-0.085621	4.313780	-2.155210
69	6	0	0.119878	5.664370	-1.507820
70	1	0	-0.081822	6.483340	-2.215670
71	1	0	1.141488	5.784451	-1.133150
72	1	0	-0.570352	5.809890	-0.663550
73	6	0	-1.471451	4.090520	-2.711320
74	1	0	-1.665332	4.752200	-3.569870
75	1	0	-2.229421	4.336659	-1.953580
76	1	0	-1.640441	3.056860	-3.014960
77	6	0	-1.450720	0.198860	3.546860
78	1	0	-2.380990	0.661819	3.202780
79	1	0	-0.599700	0.765690	3.164460
80	1	0	-1.416200	0.256960	4.641010
81	8	0	-4.213399	-2.427941	1.126250
82	6	0	-6.685891	1.473658	-0.893720
83	1	0	-7.398811	2.161748	-1.342570
84	6	0	-7.137880	0.296978	-0.288820
85	1	0	-8.200770	0.068728	-0.264640
86	6	0	-6.223440	-0.586352	0.279690
87	1	0	-6.547710	-1.512862	0.743160
88	6	0	-4.854220	-0.288951	0.261100
89	6	0	-3.911870	-1.273101	0.877770
90	6	0	-4.398110	0.887109	-0.350930
91	1	0	-3.332480	1.089109	-0.404370
92	6	0	-5.319591	1.760758	-0.930030
93	1	0	-4.964431	2.665809	-1.415990

Table S3-9. DFT coordinates for the conformers of **3.**

(1*S*,5*S*,7*S*,10*S*,28*R*)-**3** (conformer 4)					
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	2.009320	0.041730	1.656731
2	1	0	2.873680	-0.331830	1.954601
3	8	0	4.376140	-0.385110	-0.316579
4	8	0	-4.547530	-0.061190	-0.051219
5	8	0	-0.542280	-1.101240	-2.264469
6	6	0	2.123310	0.433660	0.289521
7	1	0	2.730030	1.349360	0.222881
8	6	0	2.916860	-0.637950	-0.548539
9	6	0	-1.214210	-0.295230	1.210401
10	8	0	-0.558380	-0.329630	2.381931
11	1	0	0.420190	-0.281320	2.230111
12	6	0	-2.574440	-0.238110	1.214821
13	6	0	-3.360580	-0.230600	2.514371
14	1	0	-2.792960	0.334510	3.263441
15	1	0	-4.299590	0.296800	2.339201
16	6	0	-3.609260	-1.623950	3.049701
17	1	0	-2.716180	-2.123420	3.427171
18	6	0	-4.771580	-2.291690	3.107221
19	6	0	-4.831210	-3.676340	3.709611
20	1	0	-5.188720	-4.413450	2.976281
21	1	0	-5.537980	-3.711630	4.551371
22	1	0	-3.853870	-4.007210	4.075871
23	6	0	2.829800	-0.439870	-2.062349
24	1	0	3.198060	0.546110	-2.358039
25	1	0	1.801730	-0.570950	-2.407239
26	1	0	3.459850	-1.190110	-2.551049
27	6	0	-6.096030	-1.760490	2.612001
28	1	0	-6.612010	-2.525760	2.016161
29	1	0	-5.990880	-0.874750	1.983261
30	1	0	-6.763870	-1.522440	3.452951
31	6	0	-3.321080	-0.176940	-0.034969
32	6	0	-2.591870	-0.196310	-1.402189
33	6	0	-2.678350	1.259950	-1.973249
34	1	0	-2.417250	1.222550	-3.037409
35	1	0	-3.736250	1.536570	-1.907309
36	6	0	-1.808310	2.324860	-1.246239
37	1	0	-1.715190	2.030320	-0.194779
38	6	0	-2.527800	3.702350	-1.226209
39	1	0	-2.669520	4.052210	-2.259209
40	1	0	-3.531990	3.540350	-0.823069
41	6	0	-1.792730	4.748870	-0.430839
42	1	0	-0.827680	5.047420	-0.842809
43	6	0	-2.167140	5.334300	0.718191
44	6	0	-1.281470	6.364480	1.379781
45	1	0	-1.008190	6.054990	2.398441
46	1	0	-1.800950	7.328250	1.478301
47	1	0	-0.357800	6.533320	0.817171
48	6	0	-3.453480	5.057110	1.457841
49	1	0	-3.242520	4.716310	2.480831
50	1	0	-4.079950	4.301370	0.979171
51	1	0	-4.049300	5.975480	1.555211
52	6	0	-0.414560	2.378250	-1.860529
53	6	0	-0.251560	3.173410	-3.137519
54	1	0	-0.973610	2.855790	-3.901599
55	1	0	0.751210	3.048810	-3.557079
56	1	0	-0.418420	4.245850	-2.979029
57	6	0	0.634820	1.705730	-1.363699
58	1	0	1.573760	1.802420	-1.898489
59	6	0	0.677430	0.854730	-0.107499
60	1	0	0.404120	1.515380	0.725271
61	6	0	-0.347070	-0.365760	-0.023339
62	1	0	0.252080	-1.273010	0.095861
63	6	0	-1.125640	-0.602320	-1.315939
64	6	0	-3.350700	-1.148840	-2.374119

65	1	0	-4.351700	-0.721700	-2.503409
66	1	0	-2.845260	-1.115310	-3.341169
67	6	0	-3.493460	-2.561090	-1.868179
68	1	0	-4.120540	-2.656680	-0.981829
69	6	0	-2.976180	-3.687350	-2.384409
70	6	0	-3.274670	-5.026260	-1.750299
71	1	0	-3.764819	-5.702080	-2.465899
72	1	0	-3.925660	-4.929280	-0.875839
73	1	0	-2.350039	-5.530220	-1.434279
74	6	0	-2.096410	-3.758210	-3.608909
75	1	0	-2.611740	-4.280300	-4.428099
76	1	0	-1.189780	-4.340130	-3.393309
77	1	0	-1.777370	-2.778030	-3.965509
78	6	0	2.614520	-2.103460	-0.210109
79	1	0	2.513570	-2.284370	0.859981
80	1	0	3.423490	-2.730890	-0.597569
81	1	0	1.695720	-2.412910	-0.715969
82	8	0	4.483550	-0.885780	1.901191
83	6	0	9.286180	-0.413790	0.504341
84	1	0	10.369450	-0.362090	0.435241
85	6	0	8.506100	-0.247740	-0.642849
86	1	0	8.980980	-0.067700	-1.603109
87	6	0	7.117100	-0.314100	-0.559189
88	1	0	6.505620	-0.187550	-1.445149
89	6	0	6.502120	-0.547010	0.679861
90	6	0	5.023600	-0.630200	0.827151
91	6	0	7.288700	-0.712740	1.829411
92	1	0	6.795800	-0.892580	2.778801
93	6	0	8.676370	-0.646530	1.739981
94	1	0	9.282860	-0.775640	2.631831

(1*S*,5*S*,7*S*,10*S*,28*R*)-**3** (conformer 6)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	0.959010	-2.067791	3.660400
2	1	0	0.757450	-1.706141	4.534800
3	8	0	2.920750	0.412399	1.673080
4	8	0	-1.510000	0.727879	-2.153610
5	8	0	-2.392580	-2.929201	0.732490
6	6	0	1.149440	-0.969621	2.758500
7	1	0	0.636290	-0.087671	3.143140
8	6	0	2.668130	-0.608331	2.708510
9	6	0	-1.370250	0.363809	1.383220
10	8	0	-1.344910	0.994049	2.580260
11	1	0	-1.292350	1.956679	2.448940
12	6	0	-1.521640	0.995059	0.188490
13	6	0	-1.608530	2.505879	0.052180
14	1	0	-0.938740	2.987589	0.784140
15	1	0	-1.204200	2.762979	-0.928270
16	6	0	-3.010460	3.051019	0.219890
17	1	0	-3.418470	2.971529	1.229410
18	6	0	-3.792660	3.603649	-0.720750
19	6	0	-5.165080	4.127319	-0.367040
20	1	0	-5.945690	3.610159	-0.942170
21	1	0	-5.254180	5.194459	-0.615520
22	1	0	-5.390260	4.008129	0.697720
23	6	0	3.550430	-1.775661	2.267940
24	1	0	3.383960	-2.629931	2.928680
25	1	0	4.605480	-1.487071	2.320300
26	1	0	3.320350	-2.078541	1.244000
27	6	0	-3.405730	3.771909	-2.171270
28	1	0	-4.235390	3.463419	-2.820860
29	1	0	-2.533190	3.179799	-2.453370
30	1	0	-3.207050	4.828169	-2.403760
31	6	0	-1.592830	0.199529	-1.045160
32	6	0	-1.899580	-1.314561	-0.974300
33	6	0	-0.936300	-2.099191	-1.917000
34	1	0	-1.321980	-3.121091	-2.013960
35	1	0	-1.029520	-1.617151	-2.895740
36	6	0	0.565570	-2.139911	-1.525800

37	1	0	0.850010	-1.129811	-1.209550
38	6	0	1.429970	-2.436561	-2.782770
39	1	0	1.188350	-3.440931	-3.160070
40	1	0	1.122240	-1.738511	-3.566970
41	6	0	2.911400	-2.334431	-2.531200
42	1	0	3.314460	-3.075821	-1.839830
43	6	0	3.780490	-1.444411	-3.037460
44	6	0	5.243070	-1.499071	-2.660370
45	1	0	5.572370	-0.554451	-2.203280
46	1	0	5.875700	-1.648311	-3.546990
47	1	0	5.454530	-2.307671	-1.953540
48	6	0	3.429350	-0.337231	-4.001740
49	1	0	3.660060	0.643709	-3.563210
50	1	0	2.376220	-0.328001	-4.290270
51	1	0	4.029460	-0.417781	-4.918920
52	6	0	0.814360	-3.111371	-0.372000
53	6	0	0.966670	-4.577351	-0.712830
54	1	0	0.113610	-4.937901	-1.303500
55	1	0	1.019250	-5.185351	0.194980
56	1	0	1.866470	-4.779691	-1.306890
57	6	0	0.798490	-2.729461	0.916550
58	1	0	0.898580	-3.484961	1.691660
59	6	0	0.503000	-1.331711	1.401210
60	1	0	0.869550	-0.608151	0.670220
61	6	0	-1.070790	-1.101951	1.508060
62	1	0	-1.402180	-1.481731	2.478560
63	6	0	-1.842530	-1.883691	0.445780
64	6	0	-3.353930	-1.514271	-1.534810
65	1	0	-3.323010	-1.190591	-2.582550
66	1	0	-3.558490	-2.586511	-1.523080
67	6	0	-4.427180	-0.741661	-0.814300
68	1	0	-4.366670	0.340979	-0.929440
69	6	0	-5.443300	-1.225451	-0.081300
70	6	0	-6.455990	-0.286791	0.532660
71	1	0	-7.470890	-0.511381	0.174200
72	1	0	-6.237750	0.760449	0.300610
73	1	0	-6.483950	-0.396401	1.626080
74	6	0	-5.698950	-2.687351	0.194210
75	1	0	-6.626950	-3.017691	-0.294610
76	1	0	-5.839960	-2.851131	1.271010
77	1	0	-4.883240	-3.336141	-0.127590
78	6	0	3.129750	-0.073711	4.070290
79	1	0	2.519280	0.770139	4.399890
80	1	0	4.173630	0.251239	4.011100
81	1	0	3.069750	-0.873971	4.814600
82	8	0	1.543430	2.025219	2.506800
83	6	0	3.855940	4.214909	-1.398510
84	1	0	4.224950	4.877759	-2.176650
85	6	0	4.292860	2.888979	-1.346200
86	1	0	5.003680	2.521309	-2.081200
87	6	0	3.822530	2.034159	-0.350540
88	1	0	4.153830	1.002959	-0.307810
89	6	0	2.908600	2.507159	0.602010
90	6	0	2.375220	1.643529	1.698410
91	6	0	2.474280	3.838949	0.546460
92	1	0	1.772710	4.189639	1.296090
93	6	0	2.946120	4.689279	-0.450290
94	1	0	2.606650	5.720589	-0.488200

(1*S*,5*S*,7*S*,10*S*,28*R*)-**3** (conformer 11)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	1.244240	-1.925780	2.153810
2	1	0	1.961270	-2.310040	1.621180
3	8	0	3.515660	-0.749750	1.295450
4	8	0	-3.494621	1.771629	-0.125450
5	8	0	-0.912920	-1.740710	-1.980040
6	6	0	1.256050	-0.508850	1.927680
7	1	0	0.620419	-0.117310	2.727680
8	6	0	2.675049	0.054710	2.203920

9	6	0	-1.713200	-0.936111	1.329870
10	8	0	-1.581590	-1.654171	2.469460
11	1	0	-0.717760	-2.116290	2.451620
12	6	0	-2.708531	-0.020841	1.194110
13	6	0	-3.688111	0.291009	2.309890
14	1	0	-3.197371	0.095439	3.271340
15	1	0	-3.916241	1.358009	2.266060
16	6	0	-4.952340	-0.537471	2.238820
17	1	0	-4.805720	-1.596981	2.452820
18	6	0	-6.197731	-0.121111	1.959320
19	6	0	-7.355220	-1.092711	1.981980
20	1	0	-7.853480	-1.140301	1.003350
21	1	0	-8.121940	-0.774981	2.703230
22	1	0	-7.036770	-2.104711	2.252730
23	6	0	3.072730	-0.242800	3.655990
24	1	0	2.973920	-1.308870	3.874610
25	1	0	2.411309	0.307230	4.334580
26	1	0	4.099639	0.075260	3.840430
27	6	0	-6.574871	1.302489	1.623270
28	1	0	-7.235251	1.321989	0.745940
29	1	0	-5.711471	1.929879	1.394900
30	1	0	-7.140291	1.763929	2.446040
31	6	0	-2.817381	0.747059	-0.057120
32	6	0	-2.168221	0.210929	-1.358450
33	6	0	-1.433691	1.349030	-2.134690
34	1	0	-1.232261	0.979660	-3.147430
35	1	0	-2.163271	2.161119	-2.219490
36	6	0	-0.127181	1.930700	-1.528200
37	1	0	-0.323521	2.134100	-0.469950
38	6	0	0.164079	3.323280	-2.156350
39	1	0	0.355609	3.206350	-3.232730
40	1	0	-0.752551	3.915510	-2.078680
41	6	0	1.318819	4.047120	-1.513600
42	1	0	2.301129	3.610430	-1.698470
43	6	0	1.282159	5.145200	-0.740820
44	6	0	2.555999	5.733300	-0.179530
45	1	0	2.525669	5.769660	0.918600
46	1	0	2.695579	6.769510	-0.518920
47	1	0	3.438889	5.158030	-0.475600
48	6	0	0.030909	5.898890	-0.359740
49	1	0	-0.068601	5.951410	0.733300
50	1	0	-0.885181	5.454370	-0.754590
51	1	0	0.082189	6.937850	-0.714420
52	6	0	1.049509	0.956440	-1.641580
53	6	0	1.807369	0.925950	-2.949790
54	1	0	1.127759	0.743940	-3.792980
55	1	0	2.555289	0.127610	-2.950520
56	1	0	2.322939	1.870580	-3.159790
57	6	0	1.369379	0.078950	-0.672020
58	1	0	2.181970	-0.619160	-0.853510
59	6	0	0.553709	-0.100630	0.584720
60	1	0	0.080489	0.856910	0.812650
61	6	0	-0.632930	-1.107780	0.297410
62	1	0	-0.234930	-2.124780	0.328190
63	6	0	-1.214560	-0.949240	-1.106670
64	6	0	-3.341120	-0.281701	-2.281530
65	1	0	-3.936151	0.610139	-2.515080
66	1	0	-2.892940	-0.634401	-3.212640
67	6	0	-4.241440	-1.326061	-1.675540
68	1	0	-4.844300	-0.980191	-0.835880
69	6	0	-4.402180	-2.601541	-2.064430
70	6	0	-5.398630	-3.494151	-1.361860
71	1	0	-6.154030	-3.872871	-2.065460
72	1	0	-5.919270	-2.971281	-0.553560
73	1	0	-4.904390	-4.378491	-0.935020
74	6	0	-3.662170	-3.264101	-3.201300
75	1	0	-4.347550	-3.493191	-4.030150
76	1	0	-3.242390	-4.224101	-2.871870
77	1	0	-2.836240	-2.663851	-3.585340

78	6	0	2.762789	1.550930	1.894470
79	1	0	2.601299	1.750730	0.833180
80	1	0	3.736469	1.944600	2.187750
81	1	0	1.988609	2.078490	2.464280
82	8	0	5.474449	0.269310	1.842330
83	6	0	6.821460	-3.186909	-1.558440
84	1	0	7.335760	-3.842879	-2.255610
85	6	0	5.437670	-3.287360	-1.398170
86	1	0	4.873900	-4.019400	-1.969480
87	6	0	4.774950	-2.447390	-0.504820
88	1	0	3.700490	-2.527440	-0.384150
89	6	0	5.495180	-1.497980	0.234530
90	6	0	4.856070	-0.562080	1.207850
91	6	0	6.884450	-1.402339	0.069060
92	1	0	7.425560	-0.662029	0.648630
93	6	0	7.543810	-2.243399	-0.823190
94	1	0	8.620200	-2.163979	-0.946600

(1*S*,5*S*,7*S*,10*S*,28*S*)-**3** (conformer 1)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-1.709788	-1.921868	-0.075101
2	1	0	-2.583146	-2.338602	-0.278218
3	8	0	-4.370939	-0.258942	-0.191459
4	8	0	4.081603	1.020579	-0.841310
5	8	0	1.606492	-0.671311	2.809943
6	6	0	-1.958618	-0.594278	0.382317
7	1	0	-2.421382	-0.652800	1.377822
8	6	0	-2.978158	0.148681	-0.543942
9	6	0	1.223080	-1.114572	-0.717751
10	8	0	0.506633	-1.921038	-1.518801
11	1	0	-0.360751	-2.111888	-1.078132
12	6	0	2.366049	-0.548478	-1.197366
13	6	0	2.849519	-0.817100	-2.611518
14	1	0	1.978144	-0.956796	-3.262571
15	1	0	3.388052	0.066759	-2.958085
16	6	0	3.718010	-2.053439	-2.699544
17	1	0	3.178815	-2.990057	-2.552799
18	6	0	5.038974	-2.119598	-2.927928
19	6	0	5.736682	-3.457355	-3.015194
20	1	0	6.525808	-3.544586	-2.254542
21	1	0	6.232922	-3.581540	-3.988740
22	1	0	5.041169	-4.292318	-2.881977
23	6	0	-2.738134	-0.120508	-2.031525
24	1	0	-2.855494	-1.174837	-2.283742
25	1	0	-1.720620	0.176695	-2.304516
26	1	0	-3.439770	0.466041	-2.632463
27	6	0	5.937449	-0.922178	-3.132384
28	1	0	6.860459	-1.036676	-2.548082
29	1	0	5.470952	0.015438	-2.824813
30	1	0	6.247044	-0.836758	-4.184484
31	6	0	3.152477	0.359672	-0.371871
32	6	0	2.871173	0.500561	1.142197
33	6	0	2.598643	2.005238	1.450538
34	1	0	2.673633	2.153818	2.533976
35	1	0	3.425525	2.551646	0.985264
36	6	0	1.252033	2.578355	0.926499
37	1	0	1.058695	2.123739	-0.052908
38	6	0	1.372453	4.104289	0.665172
39	1	0	1.595273	4.617162	1.612024
40	1	0	2.246042	4.260710	0.025571
41	6	0	0.138191	4.706078	0.045556
42	1	0	-0.737742	4.733462	0.695533
43	6	0	-0.013203	5.197275	-1.195678
44	6	0	-1.339103	5.770761	-1.640017
45	1	0	-1.723458	5.244145	-2.525041
46	1	0	-1.234994	6.825753	-1.930601
47	1	0	-2.096595	5.710670	-0.851868
48	6	0	1.068890	5.250962	-2.246915
49	1	0	0.749187	4.723227	-3.156077

50	1	0	2.014823	4.811331	-1.923856
51	1	0	1.264797	6.290005	-2.546796
52	6	0	0.116913	2.209898	1.875896
53	6	0	-0.037770	3.037745	3.131740
54	1	0	0.908749	3.110830	3.682693
55	1	0	-0.780063	2.598504	3.804734
56	1	0	-0.350847	4.065948	2.910996
57	6	0	-0.665480	1.135996	1.687863
58	1	0	-1.382885	0.885816	2.468882
59	6	0	-0.597163	0.163314	0.528015
60	1	0	-0.420375	0.725443	-0.394817
61	6	0	0.640767	-0.838654	0.649250
62	1	0	0.270601	-1.774307	1.077495
63	6	0	1.707641	-0.357687	1.638654
64	6	0	4.172361	0.081957	1.905230
65	1	0	4.947007	0.796266	1.601132
66	1	0	3.989311	0.218925	2.972658
67	6	0	4.646870	-1.314268	1.597017
68	1	0	4.969885	-1.465585	0.566565
69	6	0	4.733599	-2.364818	2.428702
70	6	0	5.272651	-3.687212	1.934303
71	1	0	6.161476	-3.990899	2.506066
72	1	0	5.546835	-3.647398	0.875420
73	1	0	4.532546	-4.489428	2.065299
74	6	0	4.340126	-2.356017	3.885693
75	1	0	5.220994	-2.508144	4.526222
76	1	0	3.653959	-3.186764	4.099254
77	1	0	3.841059	-1.435738	4.192118
78	6	0	-3.052325	1.652632	-0.264449
79	1	0	-3.244019	1.850545	0.793428
80	1	0	-3.872460	2.079767	-0.849403
81	1	0	-2.127670	2.160398	-0.546267
82	8	0	-4.236349	-2.498856	-0.583674
83	6	0	-9.119988	-1.682870	0.251449
84	1	0	-10.194860	-1.746596	0.397950
85	6	0	-8.481514	-0.441329	0.307087
86	1	0	-9.058016	0.459727	0.496085
87	6	0	-7.103842	-0.354968	0.119749
88	1	0	-6.602128	0.604819	0.161787
89	6	0	-6.357424	-1.517338	-0.124250
90	6	0	-4.884170	-1.485499	-0.329854
91	6	0	-7.002163	-2.762060	-0.179124
92	1	0	-6.409513	-3.650606	-0.368295
93	6	0	-8.379266	-2.842526	0.007803
94	1	0	-8.875576	-3.807750	-0.035179

(1*S*,5*S*,7*S*,10*S*,28*S*)-**3** (conformer 2)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	0.591527	0.651709	3.419726
2	1	0	1.106762	1.377027	2.987758
3	8	0	3.214633	0.139786	1.667938
4	8	0	-1.964186	0.525108	-2.313024
5	8	0	-2.531740	-2.524995	1.266443
6	6	0	1.082463	-0.567341	2.859117
7	1	0	0.801322	-1.339667	3.586377
8	6	0	2.650612	-0.563090	2.847915
9	6	0	-1.506772	0.831298	1.207290
10	8	0	-1.469698	1.751740	2.186527
11	1	0	-0.933065	1.370336	2.922246
12	6	0	-1.801712	1.215182	-0.065153
13	6	0	-1.974440	2.675892	-0.439882
14	1	0	-1.328161	3.280378	0.207919
15	1	0	-1.627662	2.800209	-1.467677
16	6	0	-3.398594	3.163542	-0.285839
17	1	0	-3.735196	3.241902	0.748578
18	6	0	-4.262859	3.505244	-1.254855
19	6	0	-5.641965	4.017530	-0.908315
20	1	0	-6.424284	3.374848	-1.336722
21	1	0	-5.806150	5.021961	-1.324891

22	1	0	-5.799559	4.071664	0.173845
23	6	0	3.247157	-1.966025	2.689371
24	1	0	2.981081	-2.406737	1.728283
25	1	0	2.892265	-2.623216	3.489423
26	1	0	4.337717	-1.904242	2.756540
27	6	0	-3.967024	3.438333	-2.735043
28	1	0	-4.807164	2.973409	-3.268378
29	1	0	-3.072922	2.855700	-2.964329
30	1	0	-3.851841	4.446478	-3.159803
31	6	0	-1.947358	0.215170	-1.120911
32	6	0	-2.200278	-1.264605	-0.751203
33	6	0	-1.285989	-2.177162	-1.619630
34	1	0	-1.656176	-3.206411	-1.543878
35	1	0	-1.444071	-1.845535	-2.650842
36	6	0	0.236900	-2.145156	-1.316223
37	1	0	0.523049	-1.099151	-1.154041
38	6	0	1.027269	-2.621326	-2.564678
39	1	0	0.737855	-3.657545	-2.796044
40	1	0	0.689573	-2.021358	-3.414589
41	6	0	2.523344	-2.541752	-2.416951
42	1	0	2.940872	-3.152844	-1.615165
43	6	0	3.394019	-1.825595	-3.146168
44	6	0	4.876000	-1.896794	-2.860521
45	1	0	5.279083	-0.902055	-2.624461
46	1	0	5.431161	-2.256221	-3.738745
47	1	0	5.100473	-2.565306	-2.022828
48	6	0	3.028912	-0.911034	-4.290128
49	1	0	3.394699	0.107061	-4.097963
50	1	0	1.954315	-0.848181	-4.473718
51	1	0	3.510369	-1.242898	-5.220806
52	6	0	0.534467	-2.945800	-0.053397
53	6	0	0.633661	-4.449149	-0.187926
54	1	0	-0.246835	-4.862657	-0.696491
55	1	0	0.704547	-4.929241	0.792639
56	1	0	1.507259	-4.754846	-0.776762
57	6	0	0.584881	-2.386588	1.166707
58	1	0	0.671347	-3.055234	2.022911
59	6	0	0.384492	-0.925846	1.509289
60	1	0	0.802742	-0.293333	0.720117
61	6	0	-1.175045	-0.594196	1.591009
62	1	0	-1.504353	-0.777051	2.619820
63	6	0	-2.016140	-1.557341	0.739657
64	6	0	-3.685737	-1.590248	-1.144348
65	1	0	-3.745343	-1.463426	-2.232586
66	1	0	-3.856863	-2.645289	-0.921694
67	6	0	-4.720655	-0.712744	-0.491566
68	1	0	-4.684361	0.335078	-0.790265
69	6	0	-5.675720	-1.069712	0.382459
70	6	0	-6.656581	-0.043897	0.901465
71	1	0	-7.690235	-0.322782	0.650395
72	1	0	-6.463298	0.951898	0.490681
73	1	0	-6.612952	0.024278	1.997774
74	6	0	-5.889642	-2.464405	0.918290
75	1	0	-6.856071	-2.865888	0.580470
76	1	0	-5.927369	-2.447390	2.015905
77	1	0	-5.102453	-3.163165	0.631797
78	6	0	3.208922	0.078654	4.126619
79	1	0	2.908524	1.118705	4.246062
80	1	0	4.301989	0.023396	4.113182
81	1	0	2.846931	-0.476049	4.998280
82	8	0	2.266181	2.176864	2.021456
83	6	0	5.721826	3.045881	-1.513674
84	1	0	6.394352	3.465091	-2.257219
85	6	0	5.869926	1.715993	-1.111050
86	1	0	6.659353	1.102925	-1.536491
87	6	0	5.009283	1.173192	-0.158970
88	1	0	5.116521	0.141654	0.155671
89	6	0	3.997958	1.967738	0.400510
90	6	0	3.072842	1.452952	1.443840

91	6	0	3.853673	3.303132	-0.004416
92	1	0	3.067468	3.903115	0.441036
93	6	0	4.712093	3.837996	-0.960908
94	1	0	4.595869	4.871364	-1.274538

Table S3-10. DFT coordinates for the conformers of **4a.**

(1*S*,5*R*,7*S*,8*R*)-**4a** (conformer 1)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.155904	0.113765	-2.199483
2	6	0	1.807040	0.076651	-0.692339
3	6	0	0.297798	-0.517206	-0.501868
4	6	0	0.141561	-1.968077	-1.086270
5	6	0	-1.196774	-2.656558	-1.080674
6	6	0	-2.391627	-2.094684	-0.604840
7	6	0	-3.578006	-2.826902	-0.633212
8	6	0	-3.592077	-4.126931	-1.140182
9	6	0	-2.409482	-4.695508	-1.620288
10	6	0	-1.225198	-3.966703	-1.589146
11	8	0	1.108808	-2.555685	-1.540210
12	6	0	-0.115252	-0.547776	0.971062
13	8	0	0.260527	-1.740966	1.495659
14	6	0	0.581823	-1.948978	2.872438
15	6	0	-0.794486	0.449946	1.604807
16	6	0	-1.108001	1.686776	0.854927
17	6	0	-0.746161	1.803241	-0.637734
18	6	0	0.688930	2.426126	-0.706723
19	6	0	1.803461	1.540914	-0.117573
20	6	0	3.167858	2.268953	-0.249959
21	6	0	3.244626	3.507604	0.606358
22	6	0	3.497921	4.774015	0.239964
23	6	0	3.549909	5.877618	1.270714
24	6	0	3.761315	5.231945	-1.174097
25	6	0	-1.758445	2.707031	-1.384719
26	6	0	-3.197304	2.271479	-1.266401
27	6	0	-4.017520	1.829467	-2.232991
28	6	0	-5.448426	1.465439	-1.909595
29	6	0	-3.644713	1.654837	-3.683922
30	6	0	-0.600286	0.442137	-1.283849
31	8	0	-1.025102	0.162956	-2.388497
32	8	0	-1.634638	2.649165	1.406191
33	6	0	-1.390578	0.402761	3.008401
34	6	0	-2.648644	-0.436664	3.058495
35	6	0	-3.910790	-0.016379	3.240027
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38	6	0	2.815195	-0.806680	0.128872
39	6	0	4.164483	-1.173465	-0.531304
40	6	0	5.038691	-1.961191	0.412708
41	6	0	5.223438	-3.290395	0.443742
42	6	0	4.558981	-4.267566	-0.497155
43	6	0	6.150719	-3.920496	1.456225
44	1	0	1.464947	0.739526	-2.769234
45	1	0	2.136157	-0.881776	-2.638643
46	1	0	3.158821	0.524493	-2.340283
47	1	0	-2.420589	-1.086484	-0.211192
48	1	0	-4.493236	-2.374796	-0.261436
49	1	0	-4.519517	-4.693274	-1.163103
50	1	0	-2.411986	-5.706423	-2.018991
51	1	0	-0.298885	-4.393211	-1.957726
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60	1	0	3.075511	3.323720	1.669895
61	1	0	2.813771	6.662591	1.047524
62	1	0	3.351739	5.504666	2.280430
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68	1	0	-1.442970	2.764678	-2.429216
69	1	0	-3.606595	2.358575	-0.260857
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71	1	0	-5.651990	0.413364	-2.155441
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73	1	0	-3.830678	0.620343	-4.002315
74	1	0	-2.596119	1.871763	-3.888794
75	1	0	-4.268081	2.297447	-4.322088
76	1	0	-0.671138	0.026836	3.740680
77	1	0	-1.601184	1.434309	3.290011
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79	1	0	-3.526835	2.134055	3.196222
80	1	0	-5.173042	1.659852	2.767905
81	1	0	-4.670520	1.602721	4.451783
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87	1	0	3.971235	-1.741385	-1.444487
88	1	0	4.709134	-0.270565	-0.836617
89	1	0	5.562777	-1.364574	1.162282
90	1	0	3.796965	-3.808696	-1.130838
91	1	0	4.074684	-5.073848	0.070765
92	1	0	5.301709	-4.752715	-1.146811
93	1	0	5.617399	-4.644192	2.089186
94	1	0	6.613604	-3.173272	2.108973
95	1	0	6.955850	-4.480961	0.959699

(1*S*,5*R*,7*S*,8*R*)-**4a** (conformer 7)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.787164	0.522780	-2.204482
2	6	0	1.470293	0.206087	-0.722322
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4	6	0	0.050987	-1.945298	-1.401220
5	6	0	-1.163373	-2.834814	-1.425530
6	6	0	-1.001963	-4.089319	-2.039401
7	6	0	-2.058237	-4.991528	-2.110507
8	6	0	-3.301511	-4.655601	-1.568782
9	6	0	-3.476257	-3.412869	-0.958668
10	6	0	-2.417702	-2.508144	-0.887954
11	8	0	1.062351	-2.315547	-1.973255
12	6	0	-0.391731	-0.802664	0.804280
13	8	0	0.150908	-1.972587	1.220512
14	6	0	0.458254	-2.276743	2.582783
15	6	0	-1.229191	0.013012	1.506733
16	6	0	-1.701308	1.268439	0.878346
17	6	0	-1.230854	1.644885	-0.550054
18	6	0	0.128366	2.399684	-0.397469
19	6	0	1.314630	1.545955	0.084577
20	6	0	2.608074	2.409785	0.112703
21	6	0	2.518844	3.597820	1.040453
22	6	0	3.019203	3.716235	2.280920
23	6	0	2.833509	4.990426	3.070752
24	6	0	3.795044	2.642471	3.004869
25	6	0	-2.303776	2.542954	-1.225939
26	6	0	-1.908787	3.134824	-2.553754
27	6	0	-1.741476	4.432461	-2.859962
28	6	0	-1.893721	5.583221	-1.894556
29	6	0	-1.384569	4.847437	-4.268644
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36	6	0	-5.260123	-2.244464	2.833365
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39	6	0	3.952138	-0.776816	-0.750700
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41	6	0	5.240790	-2.895631	-0.114994
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45	1	0	1.023194	1.156318	-2.663283
46	1	0	1.860961	-0.386903	-2.797377
47	1	0	-0.031841	-4.334592	-2.456982
48	1	0	-1.913641	-5.956354	-2.589184
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56	1	0	-0.036764	3.226639	0.301818
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59	1	0	3.453898	1.777270	0.393441
60	1	0	1.978640	4.457732	0.643567
61	1	0	2.265141	5.739390	2.510510
62	1	0	2.304010	4.798189	4.014582
63	1	0	3.802606	5.432035	3.343322
64	1	0	3.288290	2.364565	3.939704
65	1	0	3.930440	1.732014	2.416178
66	1	0	4.790415	3.009282	3.291980
67	1	0	-2.574647	3.311704	-0.500858
68	1	0	-3.200221	1.925325	-1.370739
69	1	0	-1.776033	2.407506	-3.352494
70	1	0	-2.661614	6.285216	-2.248781
71	1	0	-0.959404	6.158562	-1.827328
72	1	0	-2.167789	5.271012	-0.884499
73	1	0	-2.153181	5.509510	-4.692448
74	1	0	-1.276578	3.984777	-4.933470
75	1	0	-0.443123	5.414894	-4.289892
76	1	0	-1.111236	-0.622598	3.589432
77	1	0	-2.232743	0.671104	3.246943
78	1	0	-2.652436	-2.307159	2.509723
79	1	0	-4.756463	-3.188994	2.603880
80	1	0	-5.822488	-2.377264	3.768477
81	1	0	-6.007355	-2.054498	2.049914
82	1	0	-4.241430	1.081280	3.138133
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88	1	0	4.383121	0.221697	-0.897737
89	1	0	5.402058	-1.075181	0.884066
90	1	0	5.437151	-4.103662	-1.896282
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94	1	0	7.086708	-3.978806	0.207409
95	1	0	6.651193	-2.888054	1.537668

3.4 References

(1) Tian Lu, molclus program, Version 1.8.9, http://www.keinsci.com/research/molclus.html (accessed Oct 1st, 2019).

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(4) N. Grimblat, M. M. Zanardi and A. M. Sarotti, Beyond DP4: an improved probability for the stereochemical assignment of isomeric compounds using quantum chemical calculations of NMR shifts, *J. Org. Chem.,* 2015, **80**, 12526-12534.

IV. Original spectra of compounds 1-4, 4a, and 4b

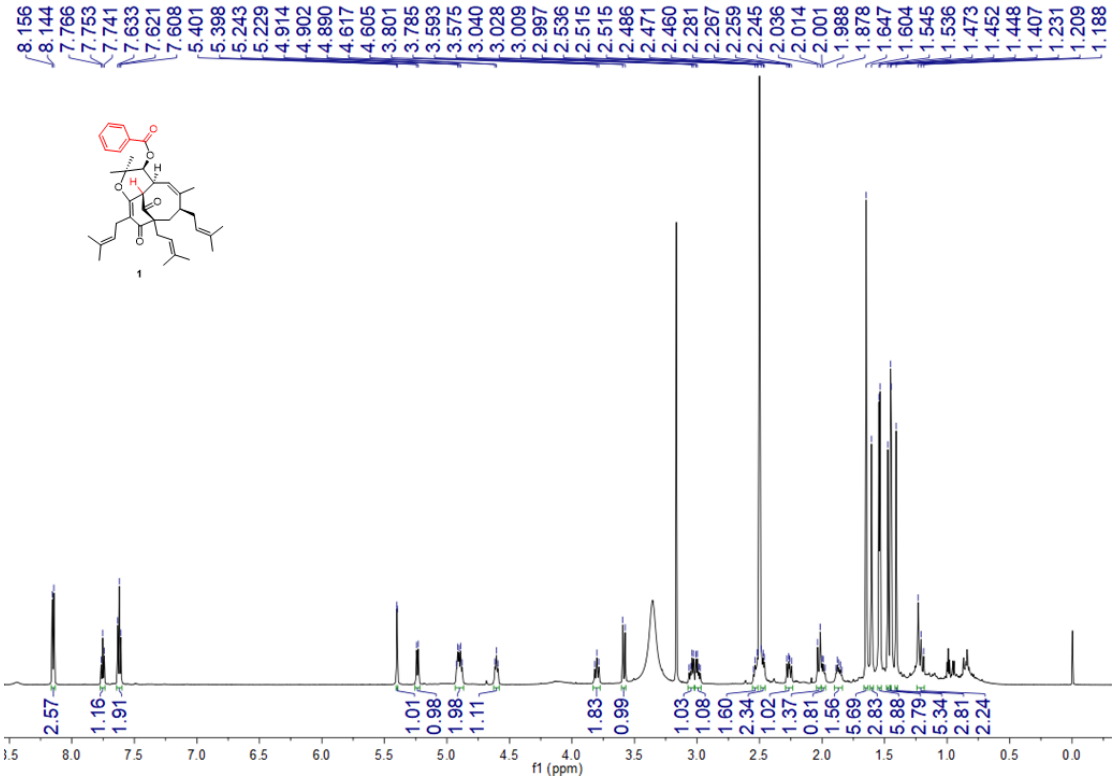


Figure S4-1. ^{1}H NMR spectrum of **1** (dimethyl sulfoxide-d_6)

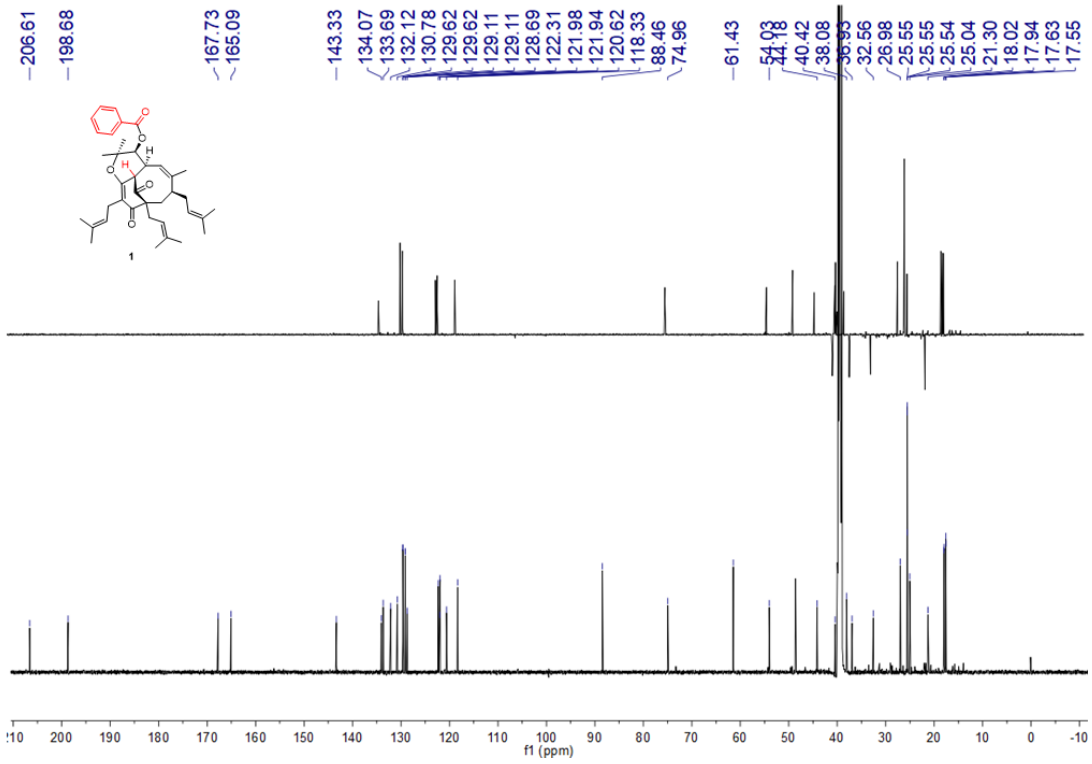


Figure S4-2. ^{13}C NMR and DEPT spectra of **1** (dimethyl sulfoxide-d_6)

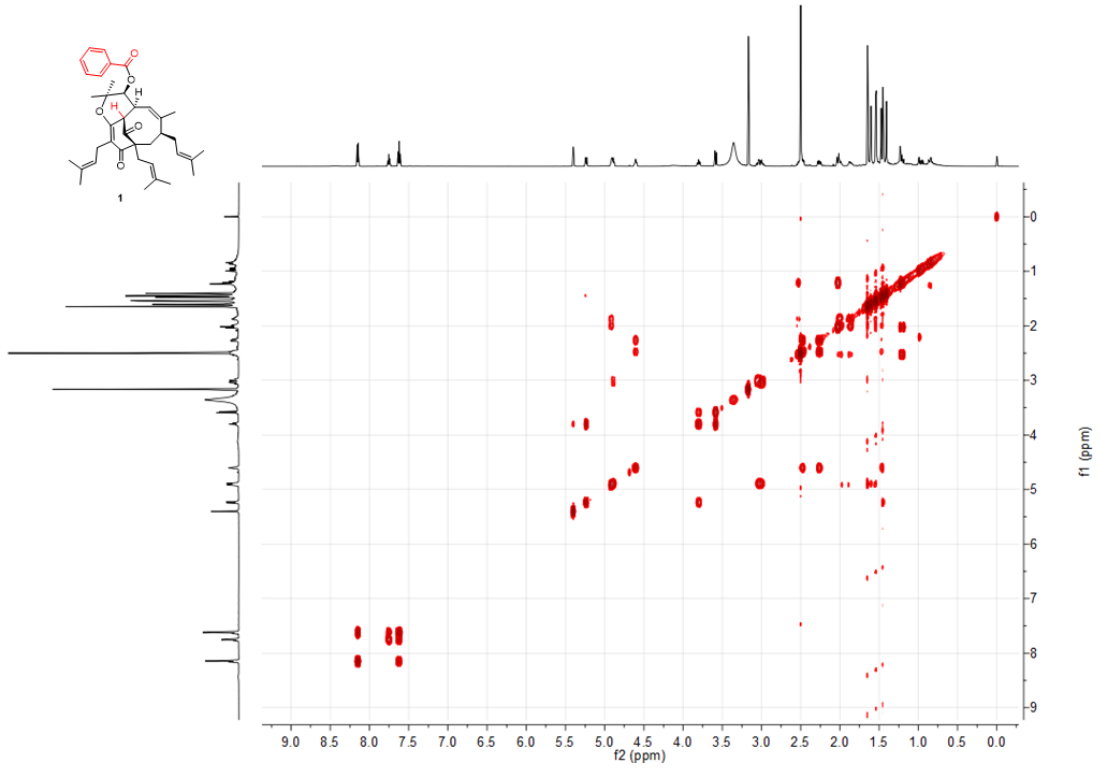


Figure S4-3. ^{1}H-^{1}H COSY spectrum of **1** (dimethyl sulfoxide-d_6)

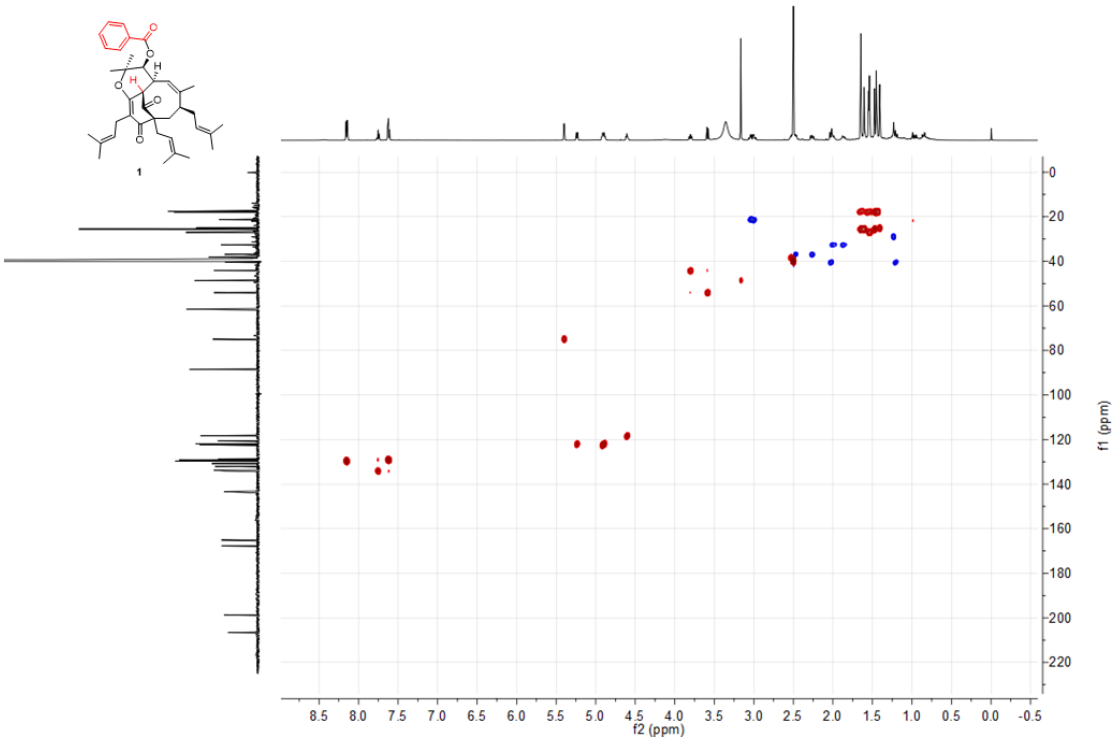


Figure S4-4. HSQC spectrum of **1** (dimethyl sulfoxide-d_6)

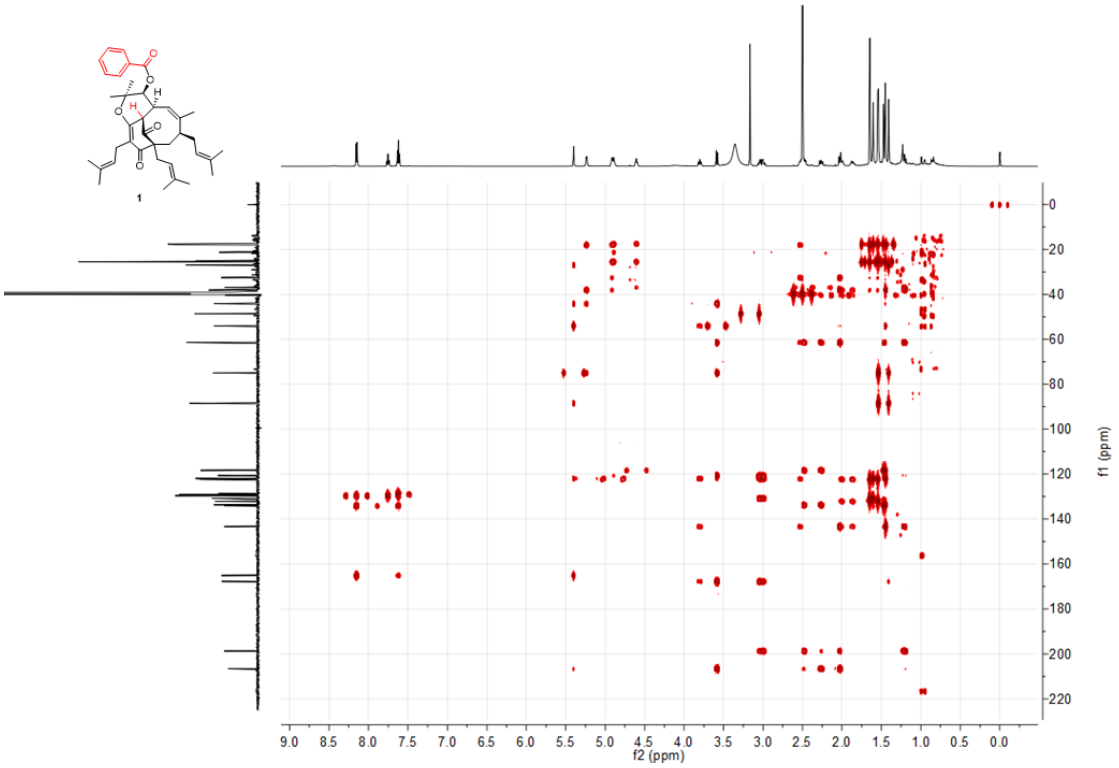


Figure S4-5. HMBC spectrum of **1** (dimethyl sulfoxide-d_6)

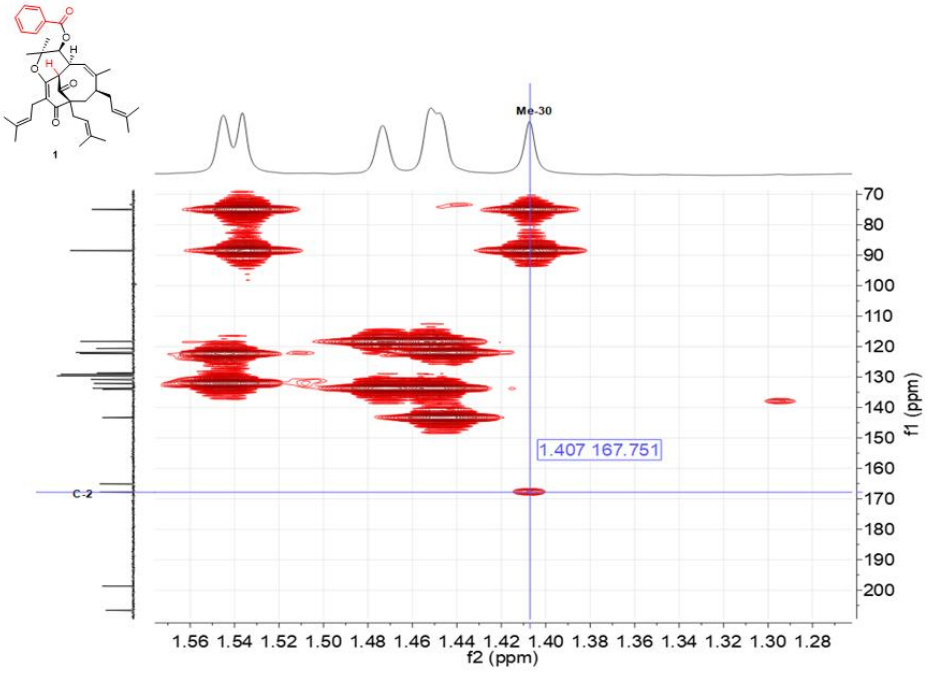


Figure S4-6. Partially expending HMBC spectrum of **1** (dimethyl sulfoxide-d_6)

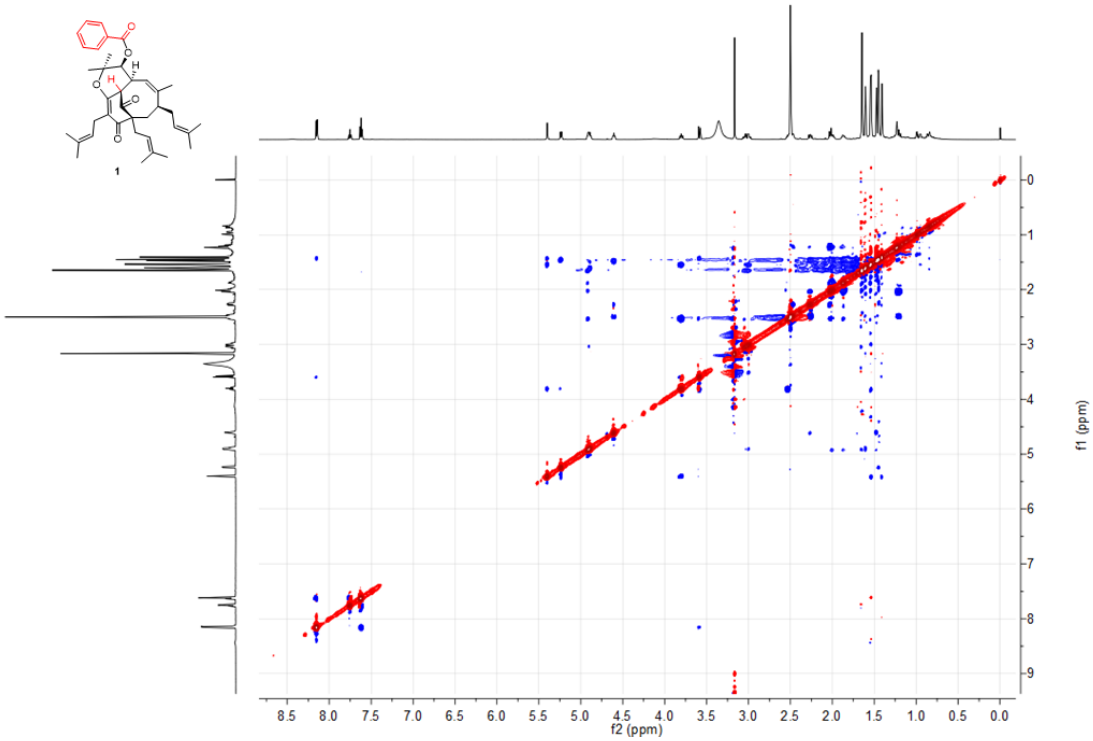
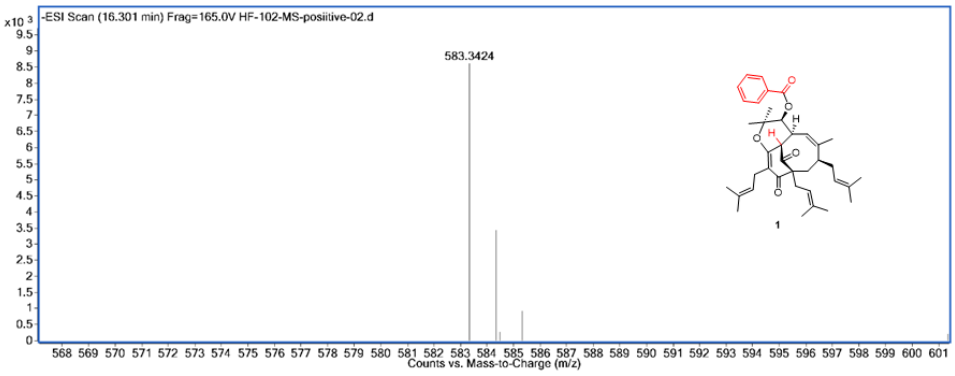


Figure S4-7. ROESY spectrum of **1** (dimethyl sulfoxide-d_6)



Elemental Composition Calculator

Target m/z:	583.3424	**Result type:**	Negative ions	**Species:**	$[M-H]^-$
Elements:		C (0-80); H (0-120); O (0-30)			
Ion Formula		**Calculated m/z**		**PPM Error**	
$C_{38}H_{47}O_5$		583.3429		0.9	

Figure S4-8. HRESIMS of **1**

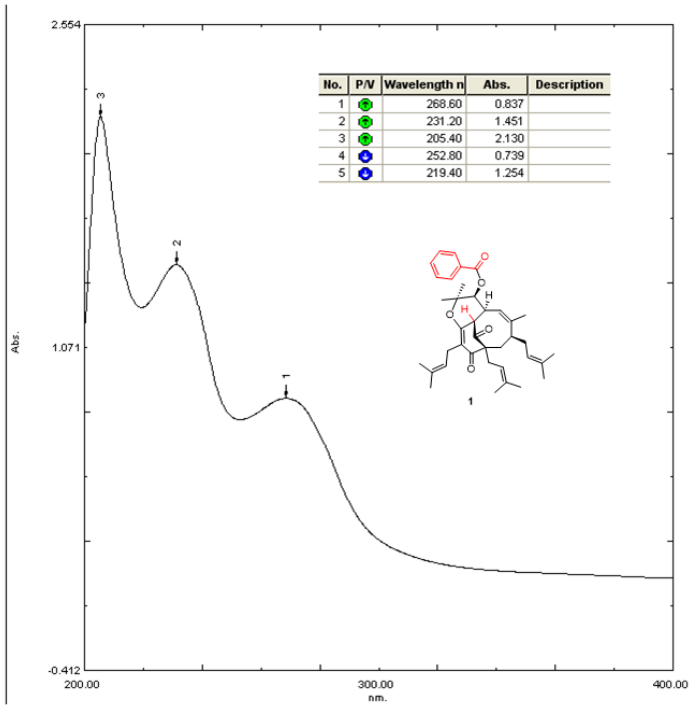


Figure S4-9. UV spectrum of **1** (MeOH)

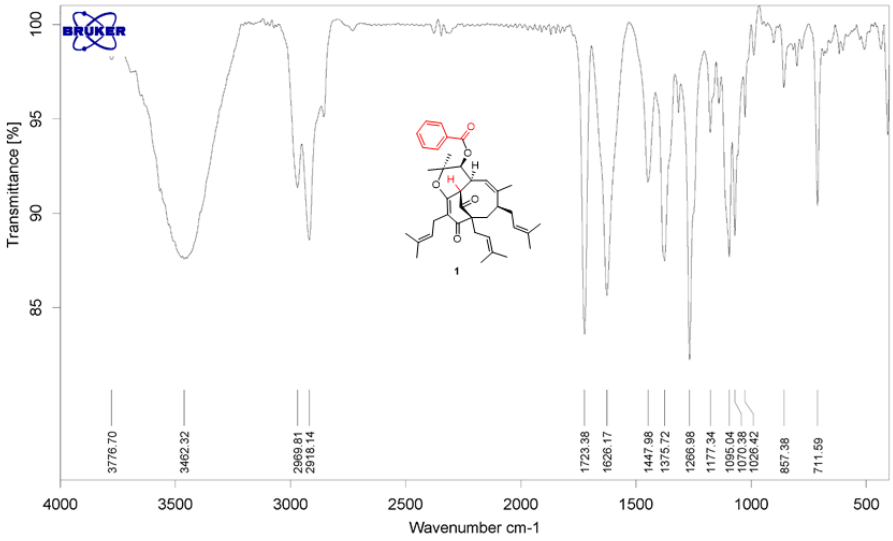


Figure S4-10. IR spectrum of **1**

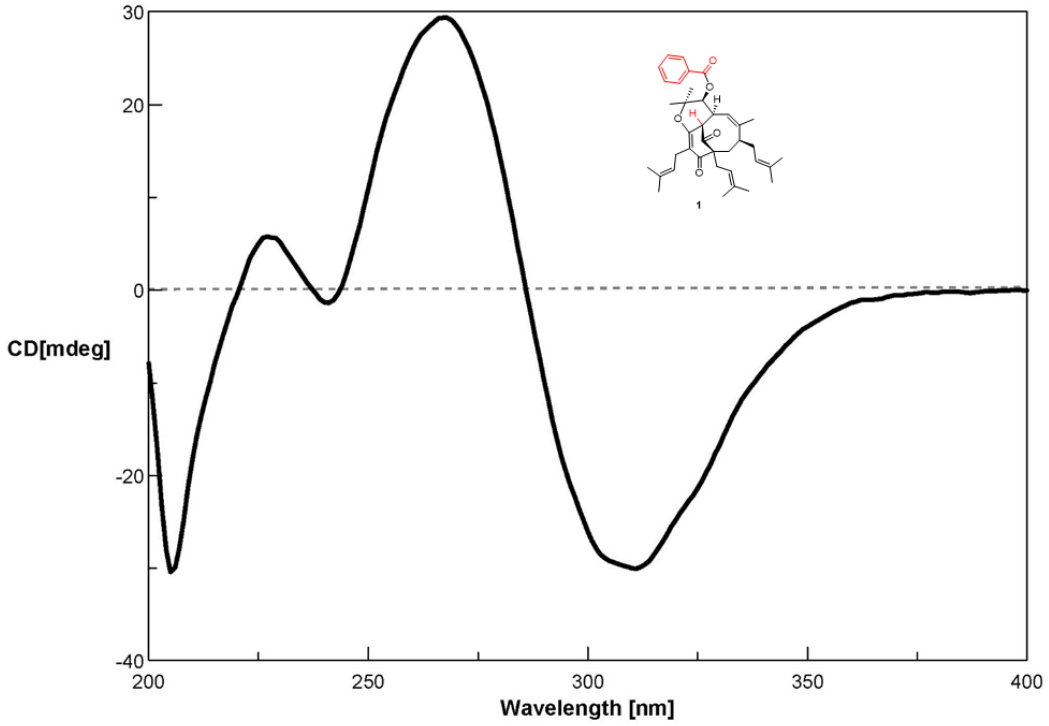


Figure S4-11. ECD spectrum of **1**

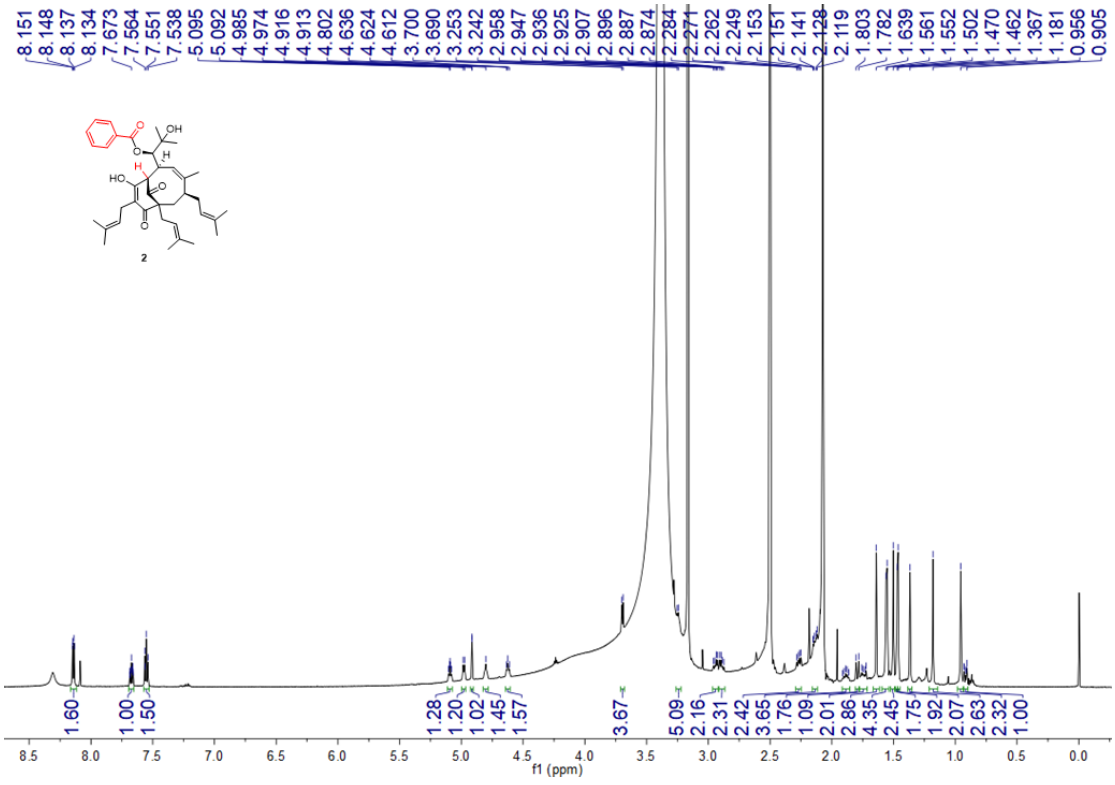


Figure S4-12. ^{1}H NMR spectrum of **2** (dimethyl sulfoxide-d_6)

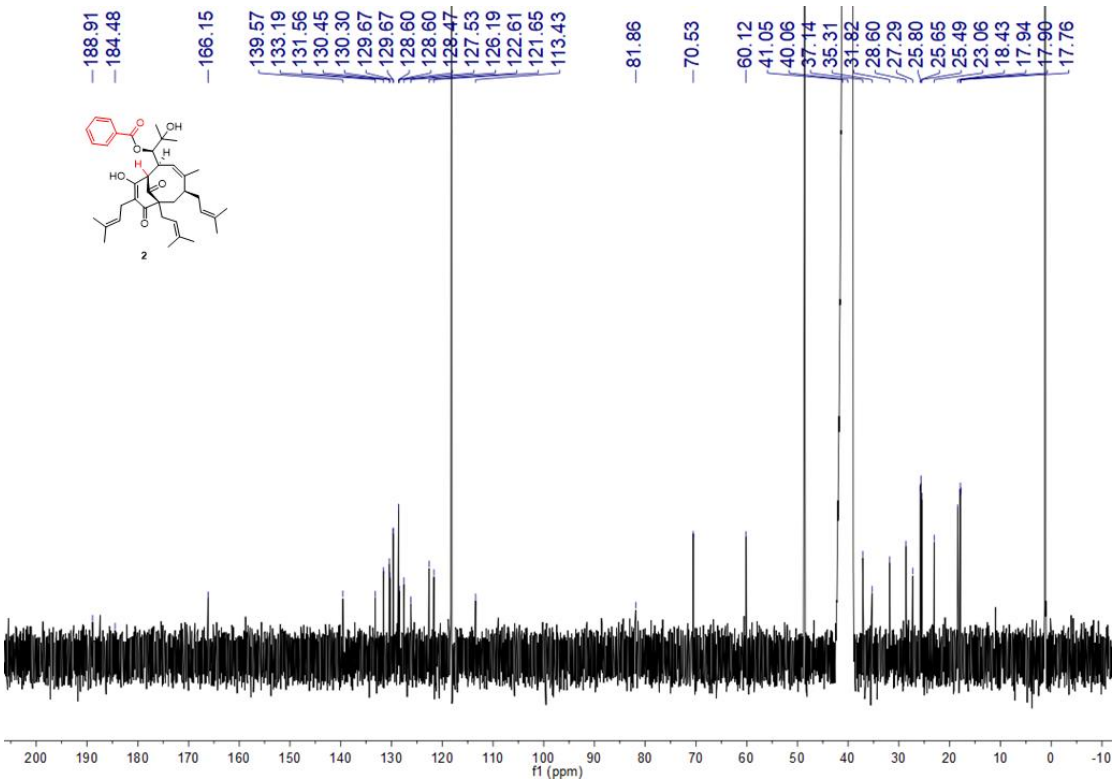


Figure S4-13. ^{13}C NMR spectrum of **2** (dimethyl sulfoxide-d_6)

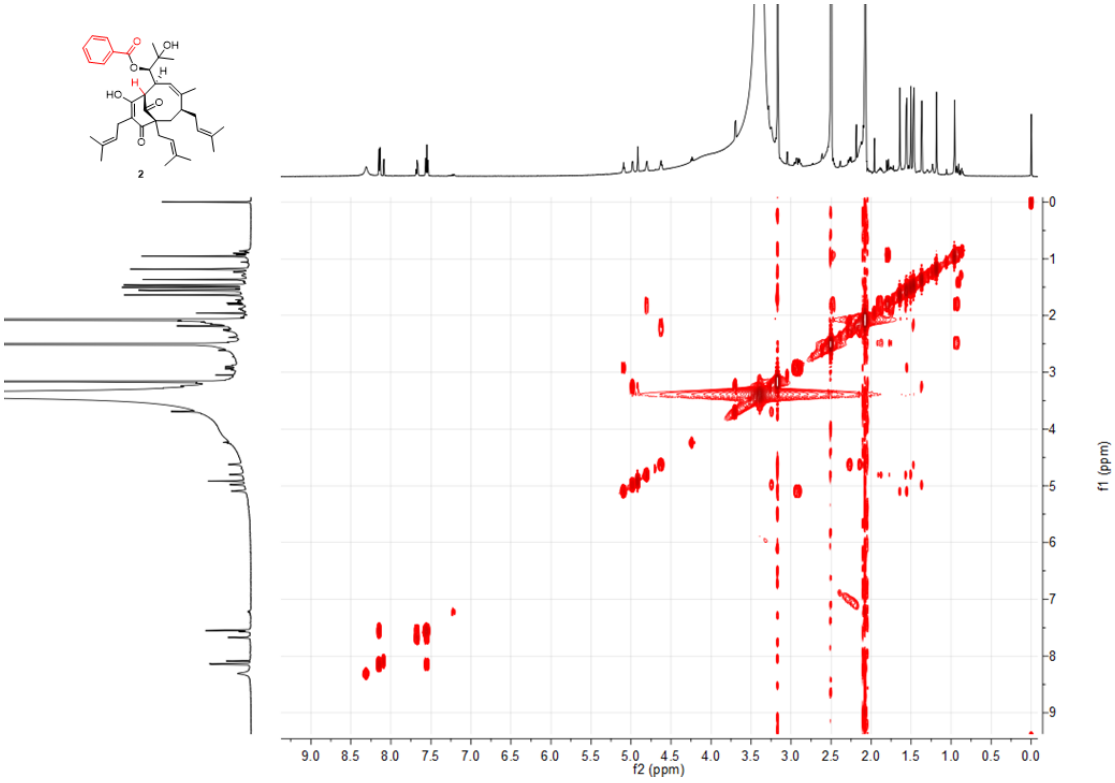


Figure S4-14. ^{1}H-^{1}H COSY spectrum of **2** (dimethyl sulfoxide-d_6)

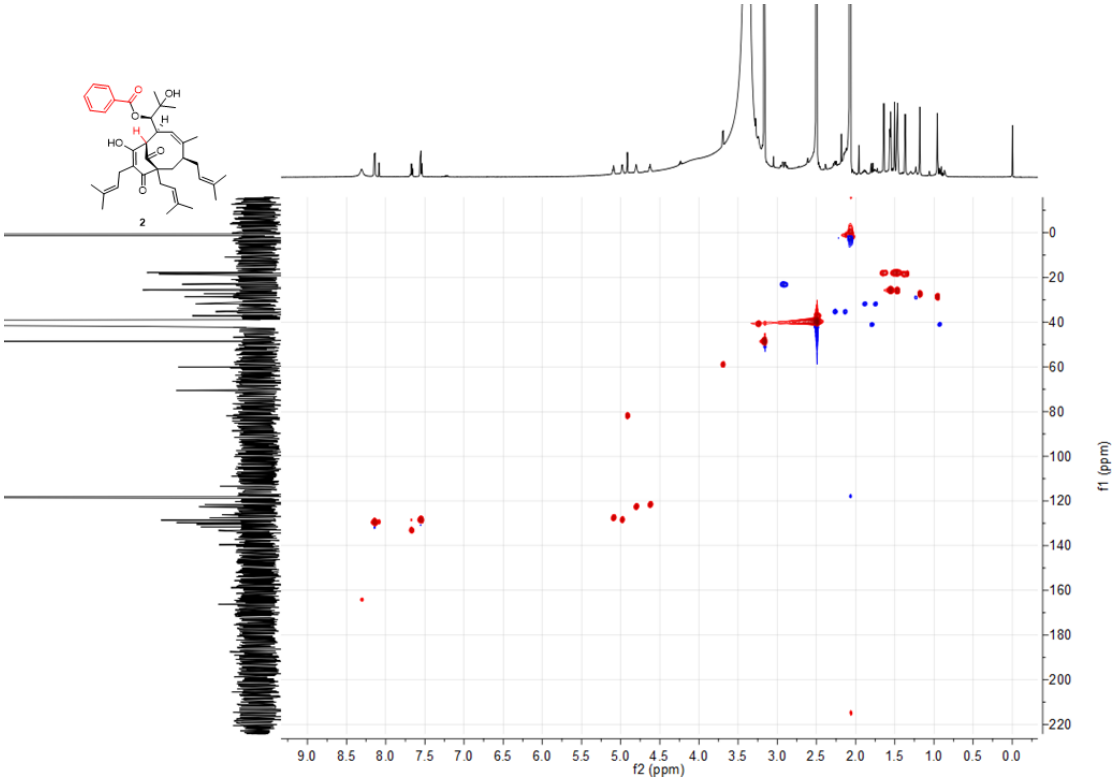


Figure S4-15. HSQC spectrum of **2** (dimethyl sulfoxide-d_6)

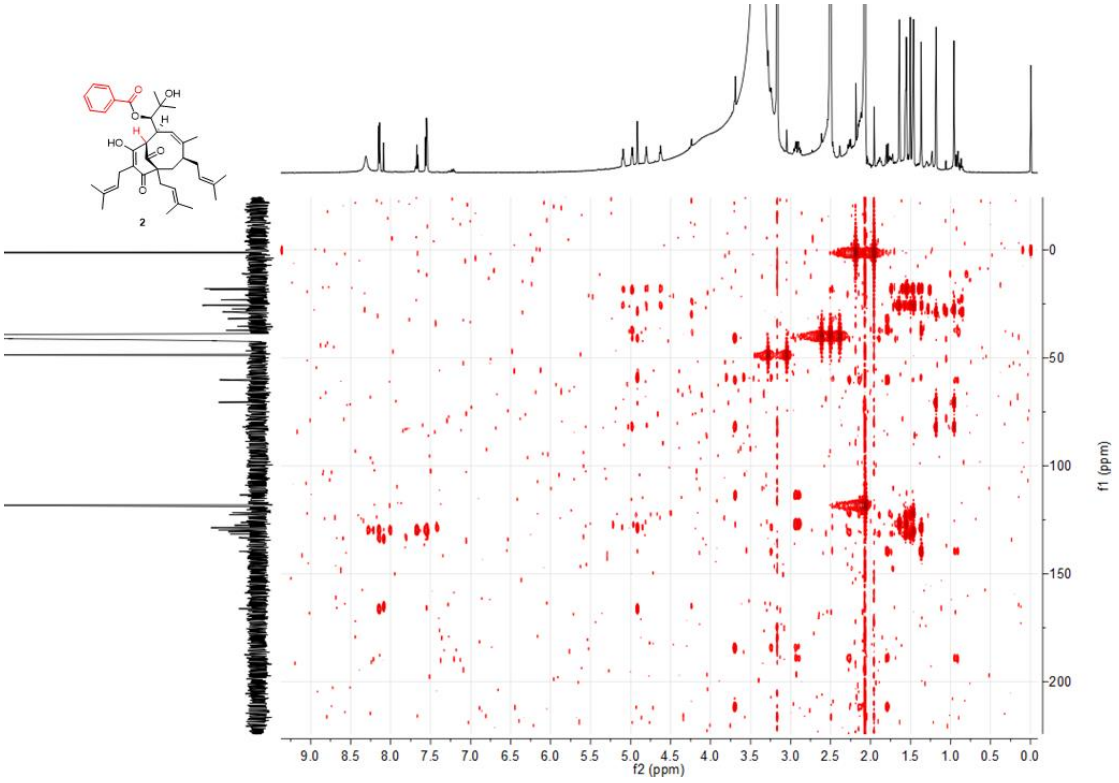


Figure S4-16. HMBC spectrum of **2** (dimethyl sulfoxide-d_6)

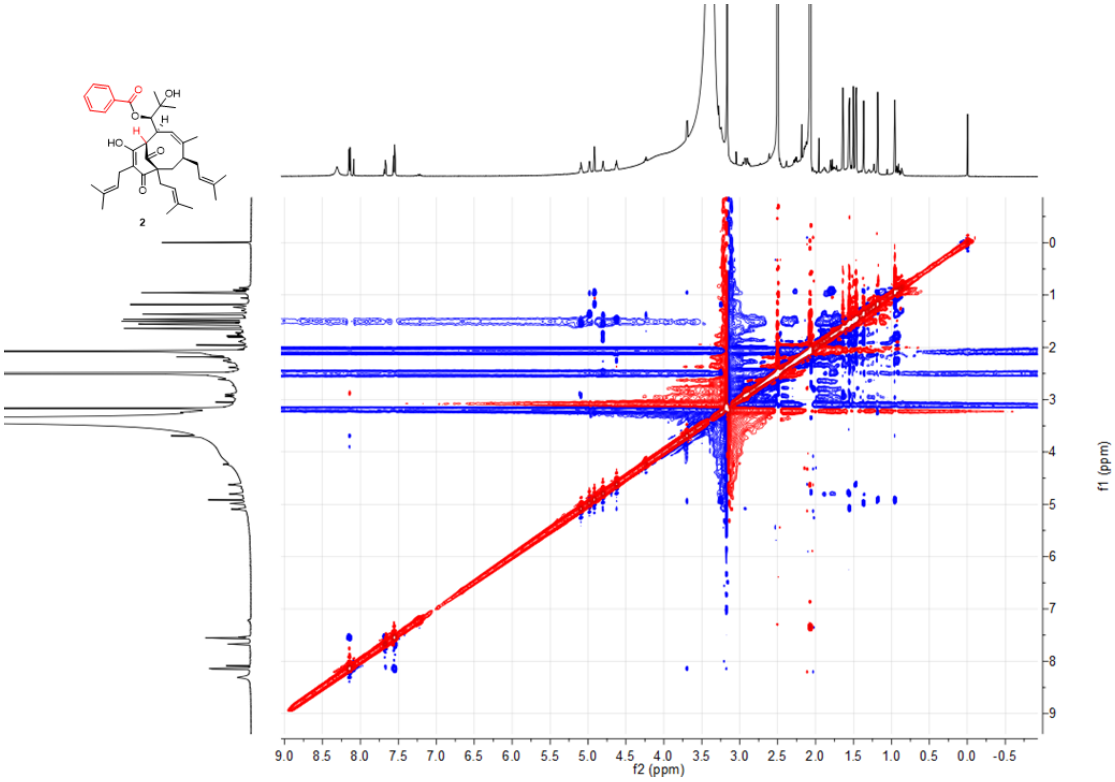


Figure S4-17. ROESY spectrum of **2** (dimethyl sulfoxide-d_6)

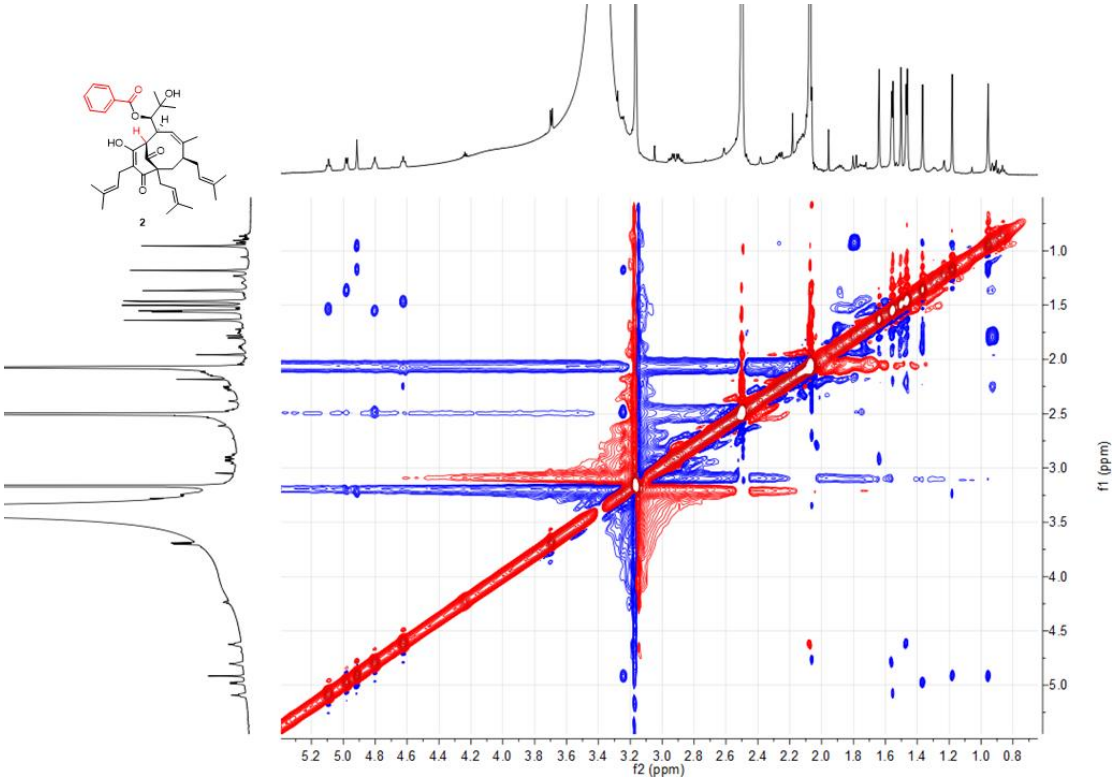
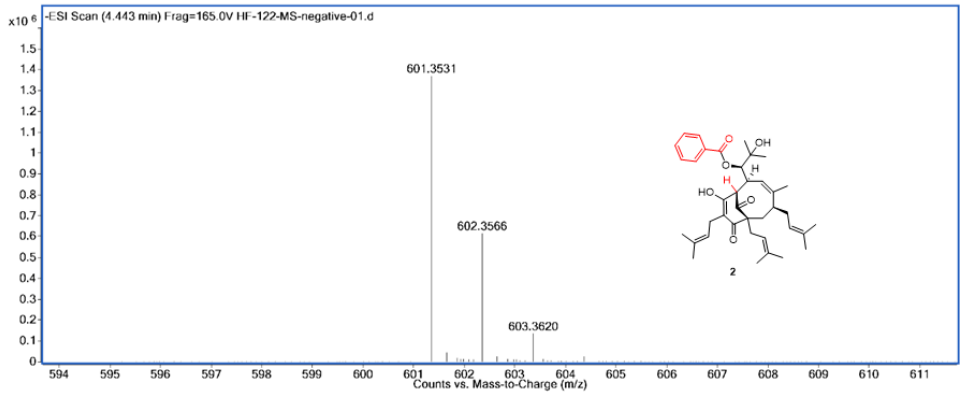


Figure S4-18. Partially expending ROESY spectrum of **2** (dimethyl sulfoxide-d_6)



Elemental Composition Calculator

Target m/z:	601.3531	**Result type:**	Negative ions	**Species:**	$[M-H]^-$
Elements:		C (0-80); H (0-120); O (0-30)			
Ion Formula		**Calcalated m/z**		**PPM Error**	
C38H49O6		601.3535		0.61	

Figure S4-19. HRESIMS of **2**

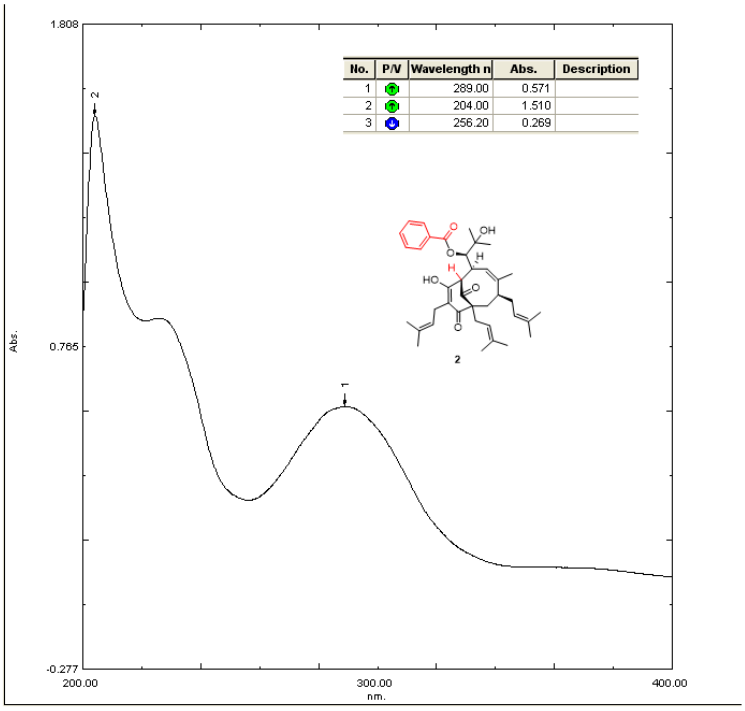


Figure S4-20. UV spectrum of **2** (MeOH)

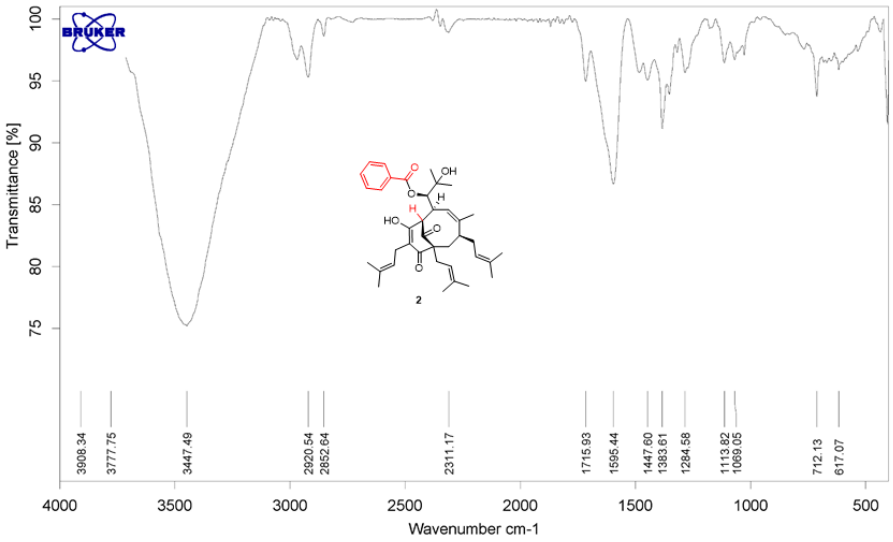


Figure S4-21. IR spectrum of **2**

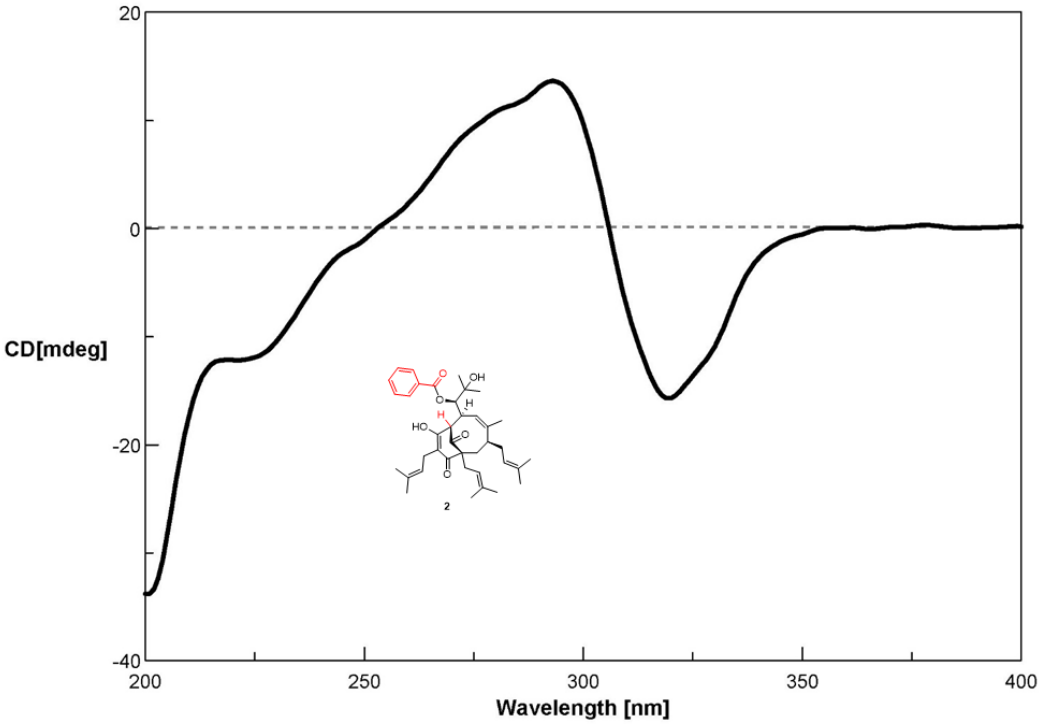


Figure S4-22. ECD spectrum of **2** (MeOH)

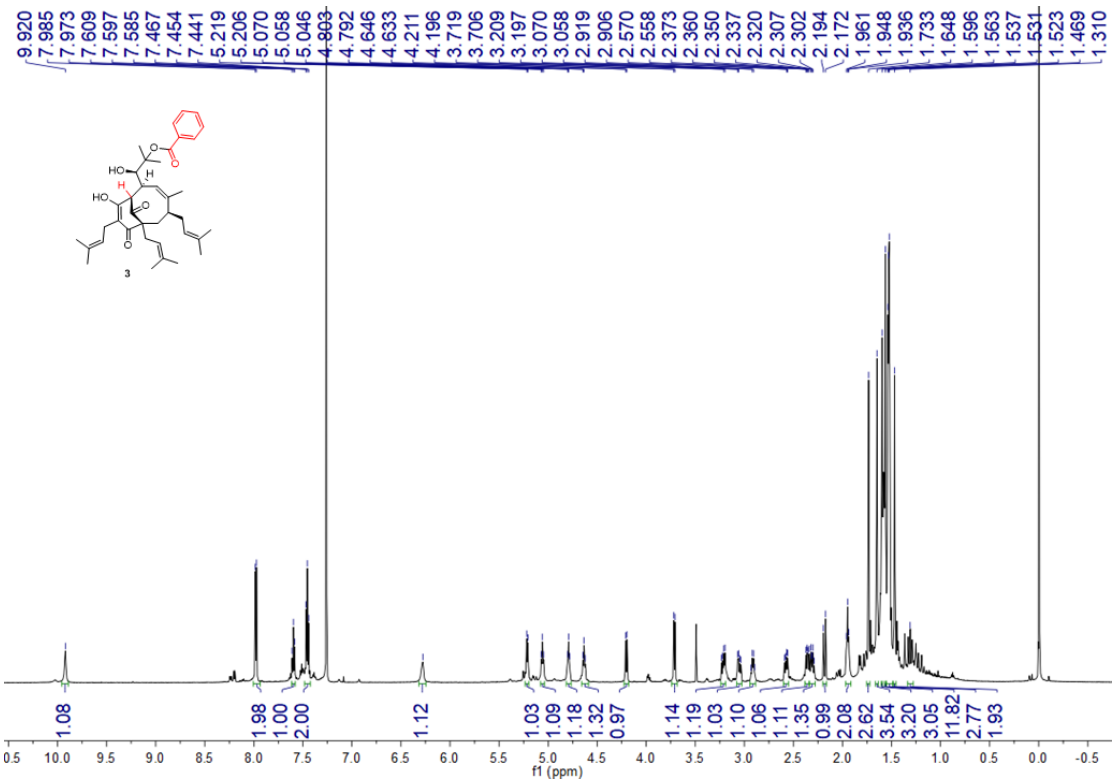


Figure S4-23. ^{1}H NMR spectrum of **3** ($CDCl_3$)

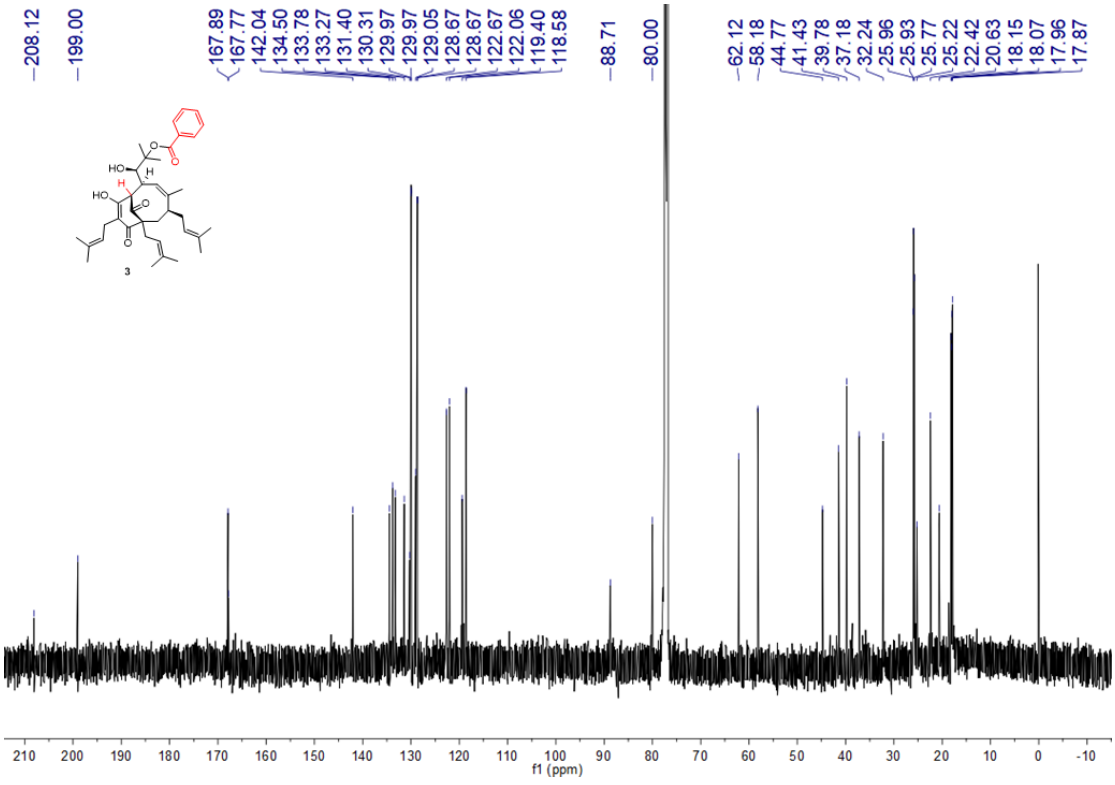


Figure S4-24. ^{13}C NMR spectrum of **3** ($CDCl_3$)

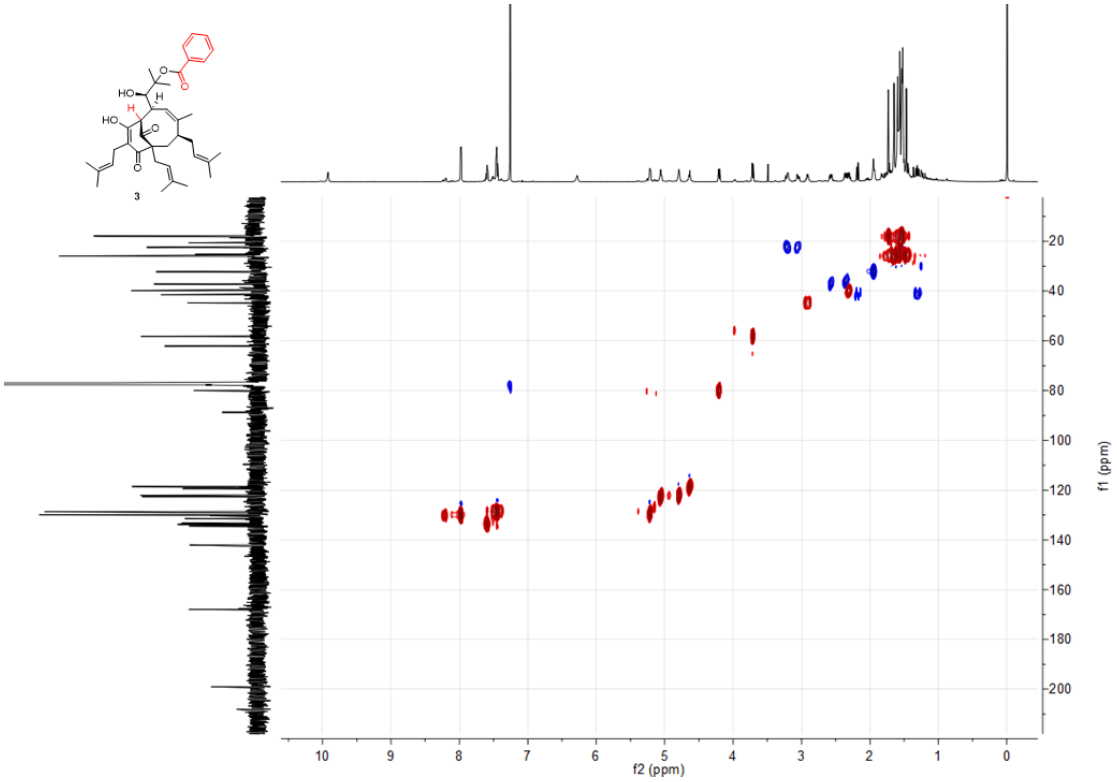


Figure S4-25. HSQC spectrum of **3** ($CDCl_3$)

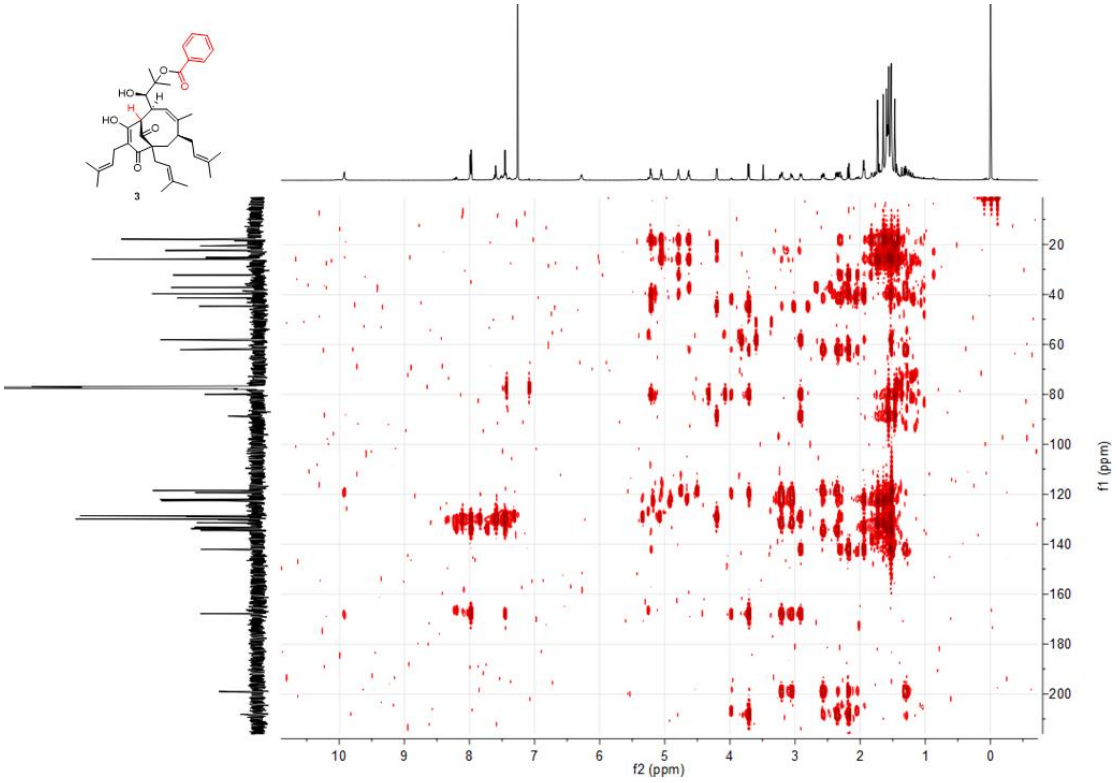


Figure S4-26. HMBC spectrum of **3** ($CDCl_3$)

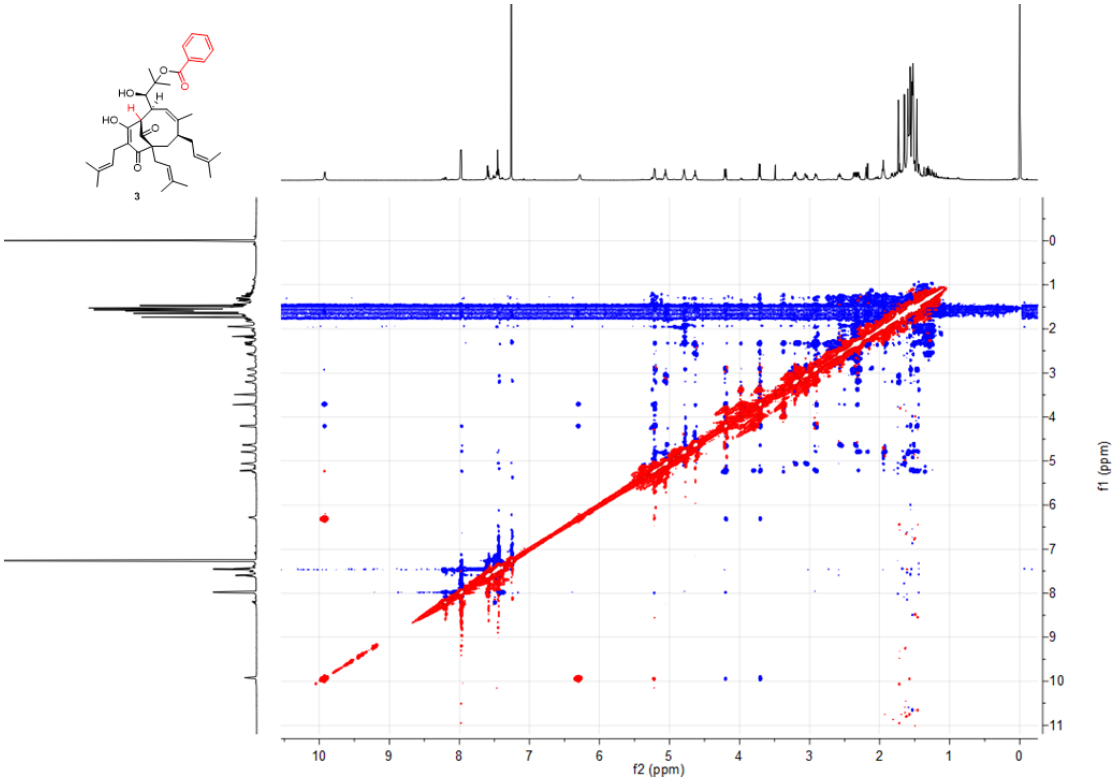


Figure S4-27. ROESY spectrum of **3** ($CDCl_3$)

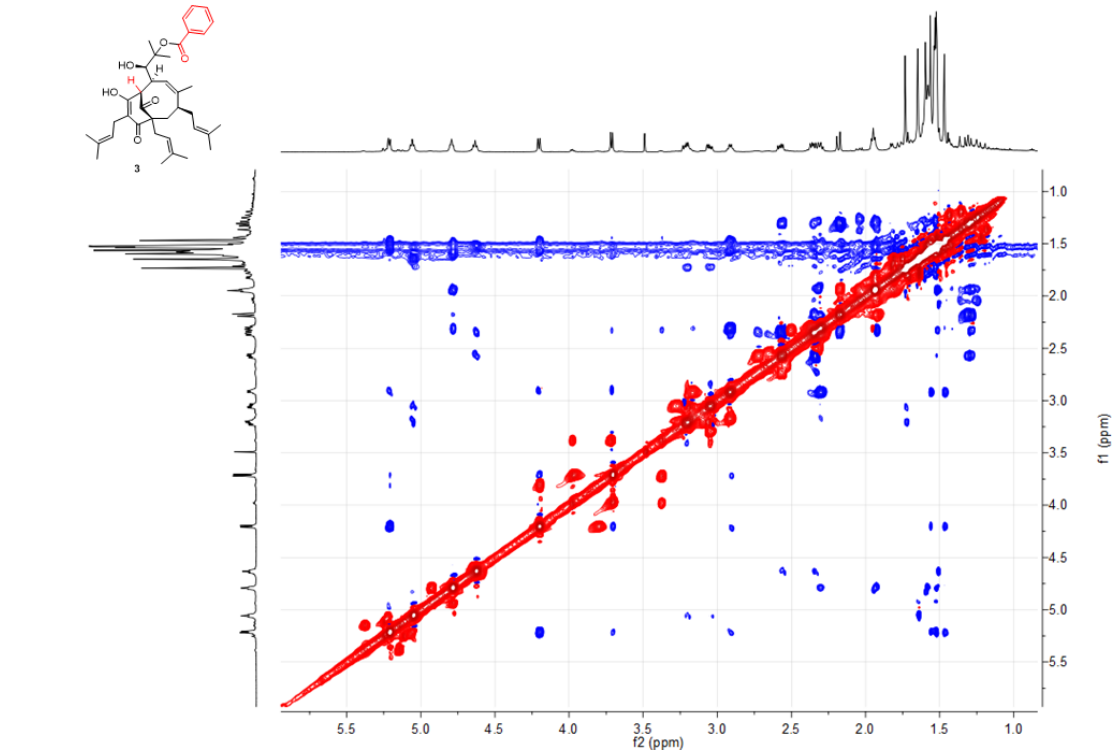
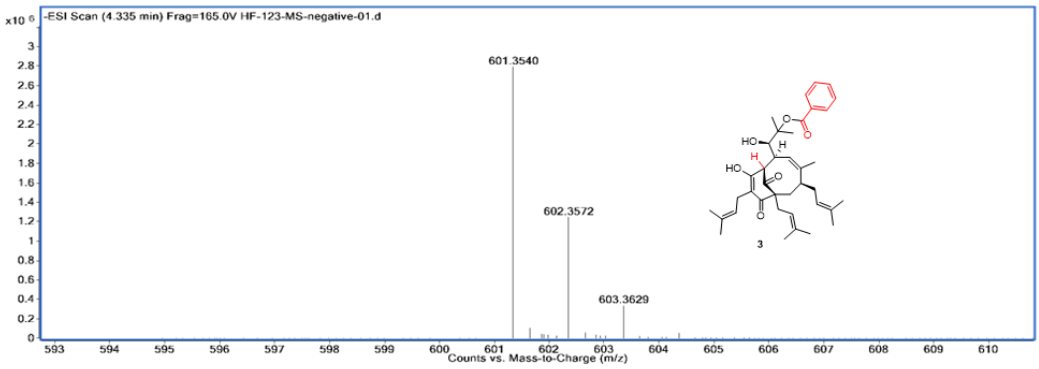


Figure S4-28. Partially expending ROESY spectrum of **3** ($CDCl_3$)



Elemental Composition Calculator

Target m/z:	601.3540	**Result type:**	Negative ions	**Species:**	$[M-H]^-$
Elements:		C (0-80); H (0-120); O (0-30)			
Ion Formula		**Calcalated m/z**		**PPM Error**	
C38H49O6		601.3535		-0.87	

Figure S4-29. HRESIMS of **3**

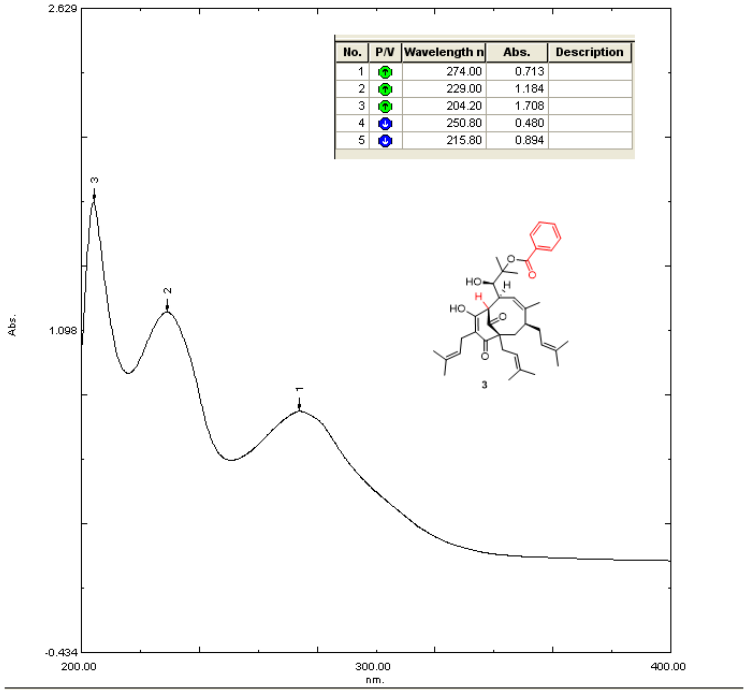


Figure S4-30. UV spectrum of **3** (MeOH)

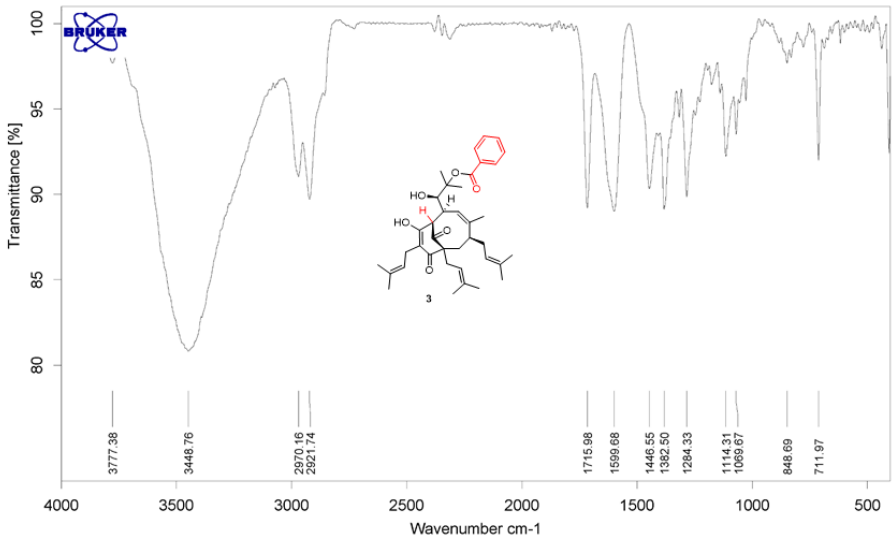


Figure S4-31. IR spectrum of **3**

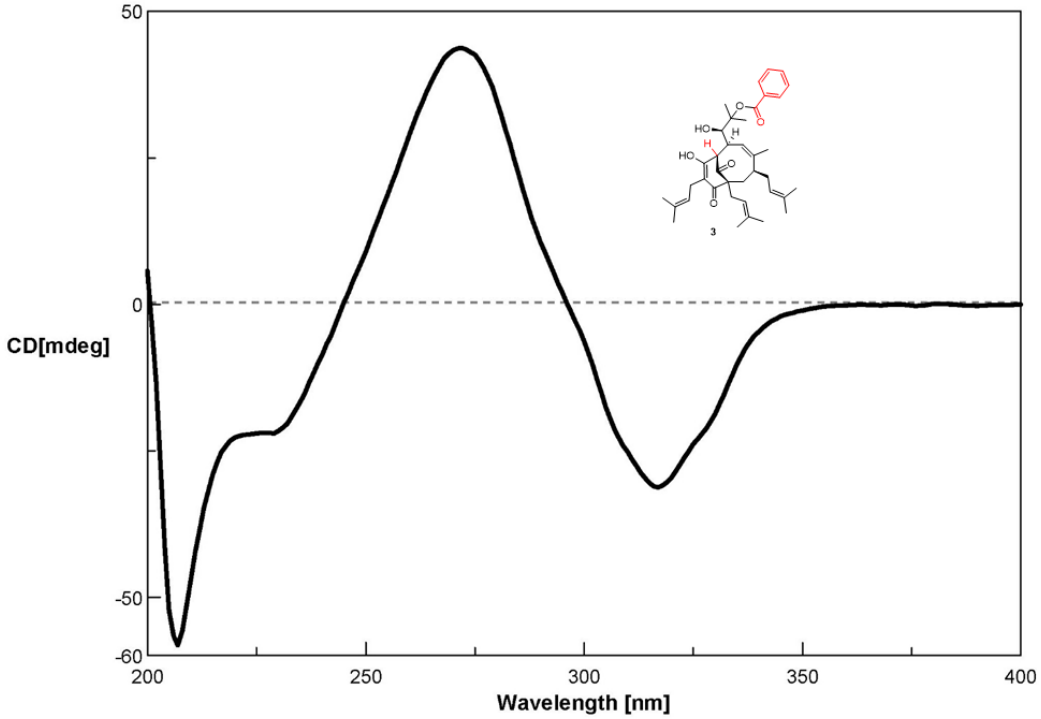


Figure S4-32. ECD spectrum of **3** (MeOH)

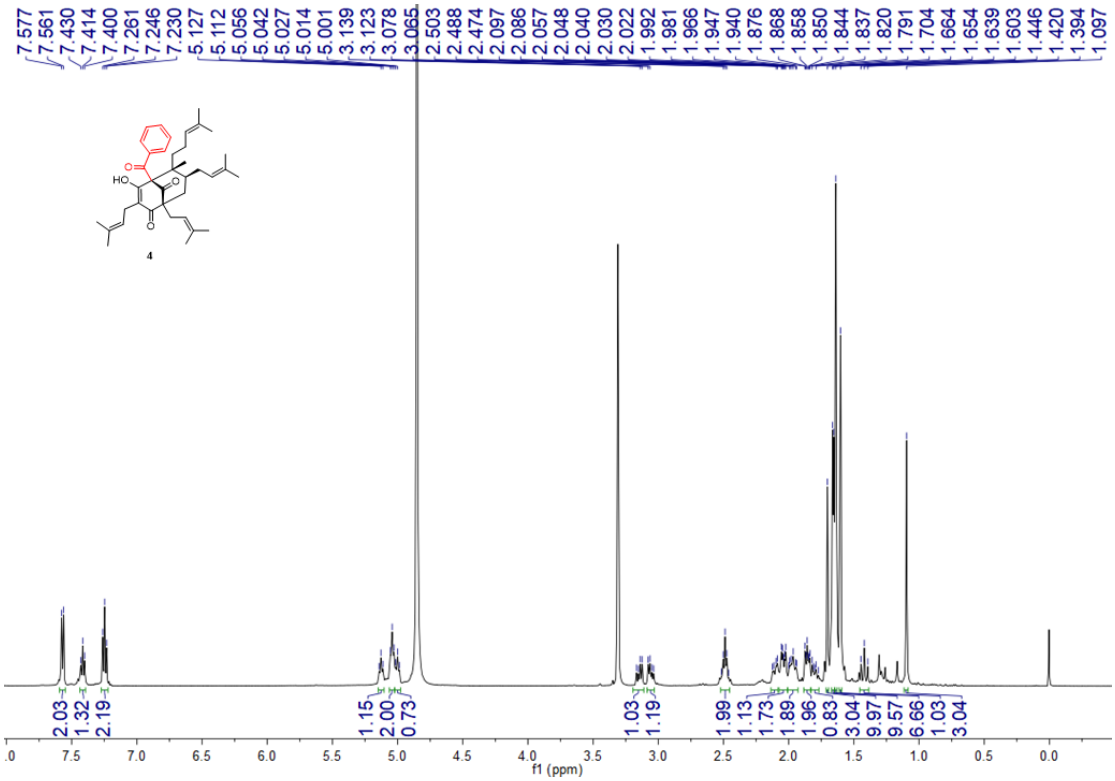


Figure S4-33. ^{1}H NMR spectrum of **4** (methanol-d_4)

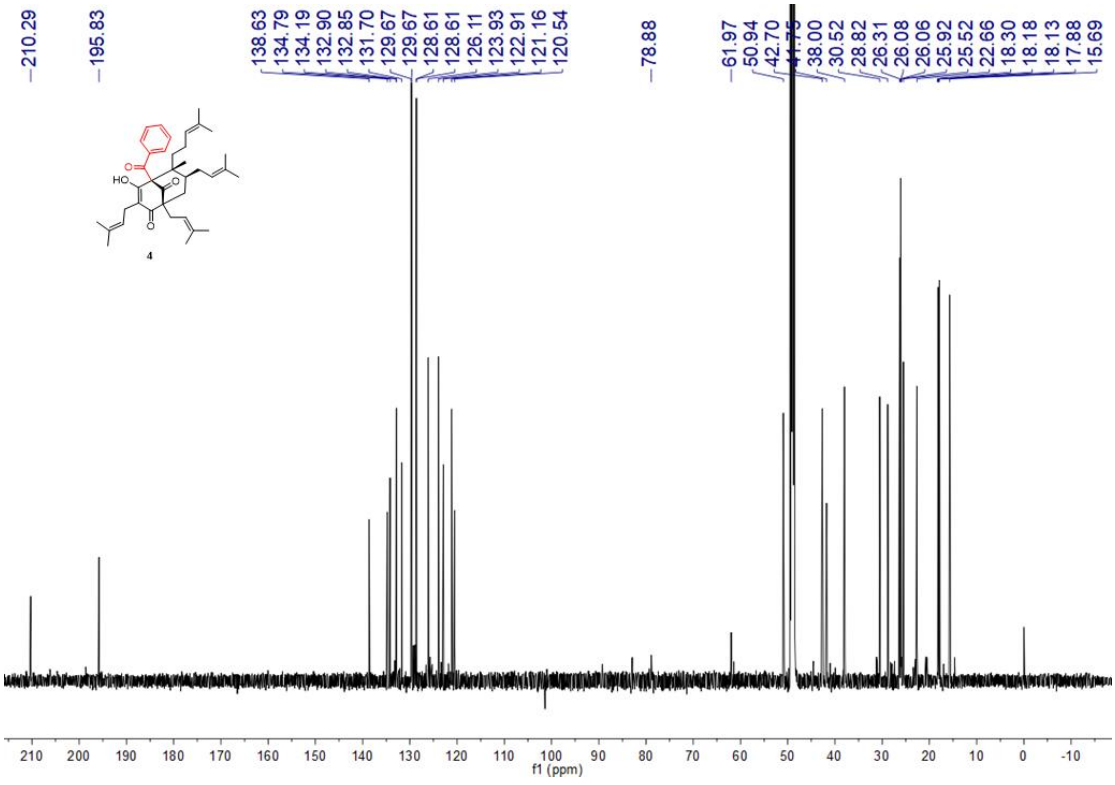


Figure S4-34. ^{13}C NMR spectrum of **4** (methanol-d_4)

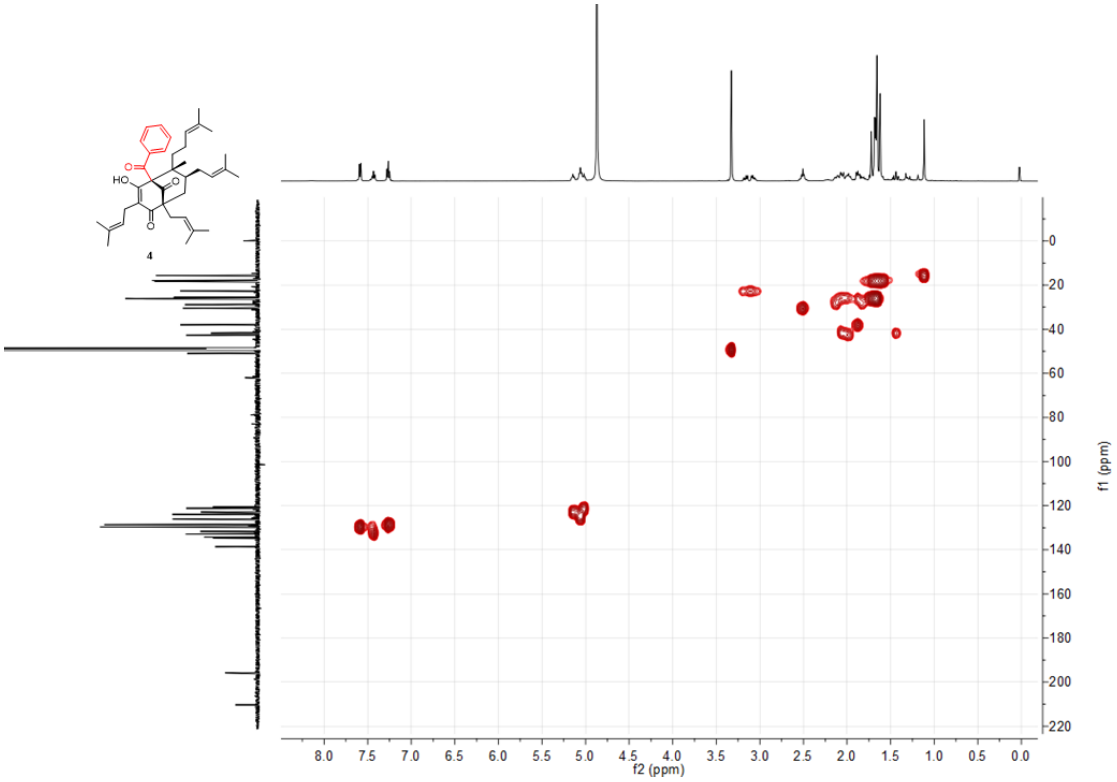


Figure S4-35. HSQC spectrum of **4** (methanol-d_4)

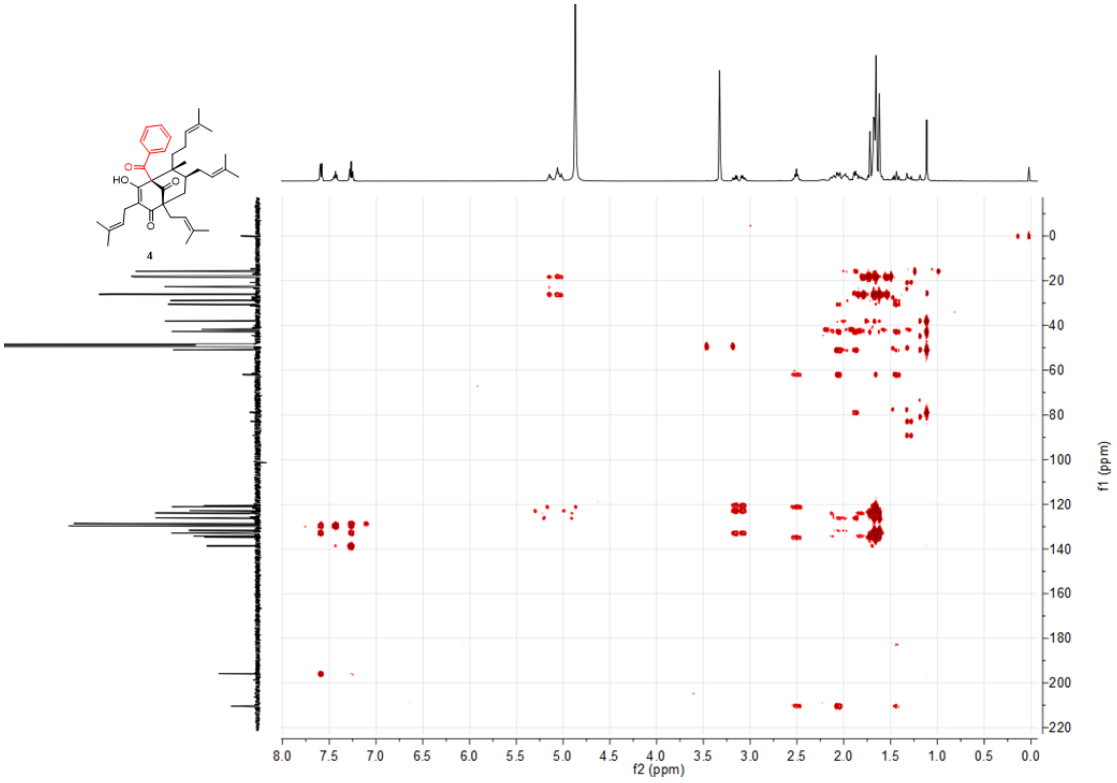


Figure S4-36. HMBC spectrum of **4** (methanol-d_4)

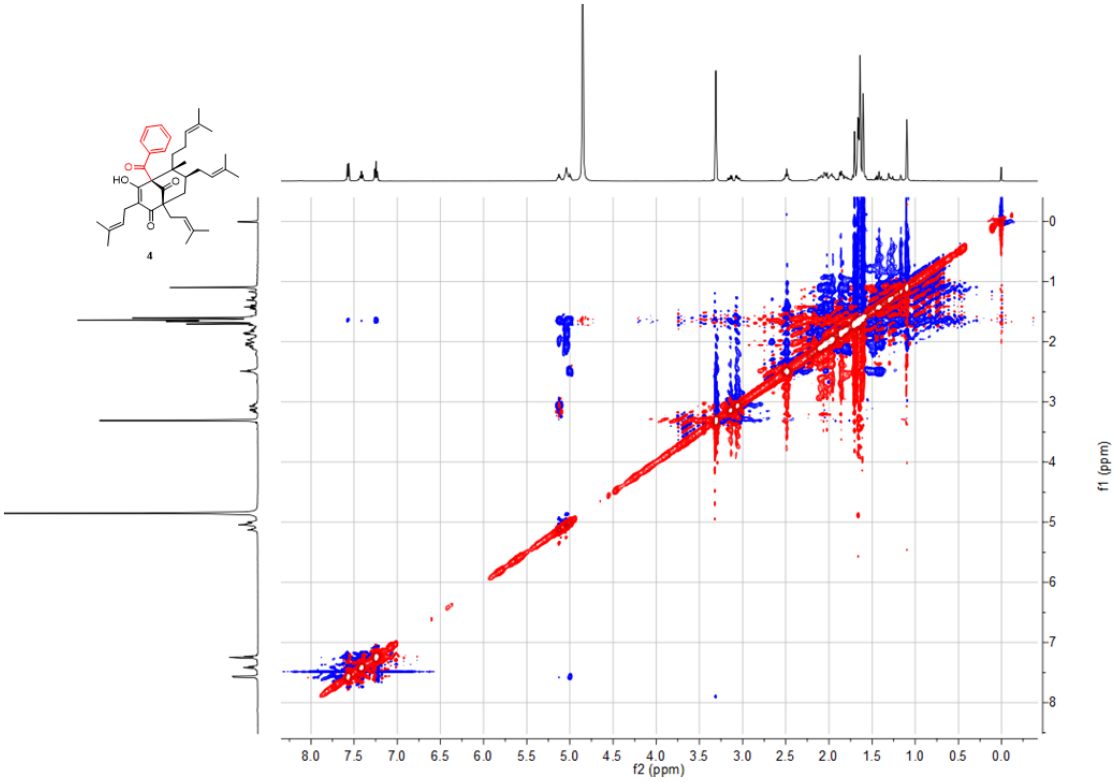


Figure S4-37. ROESY spectrum of **4** (methanol-d_4)

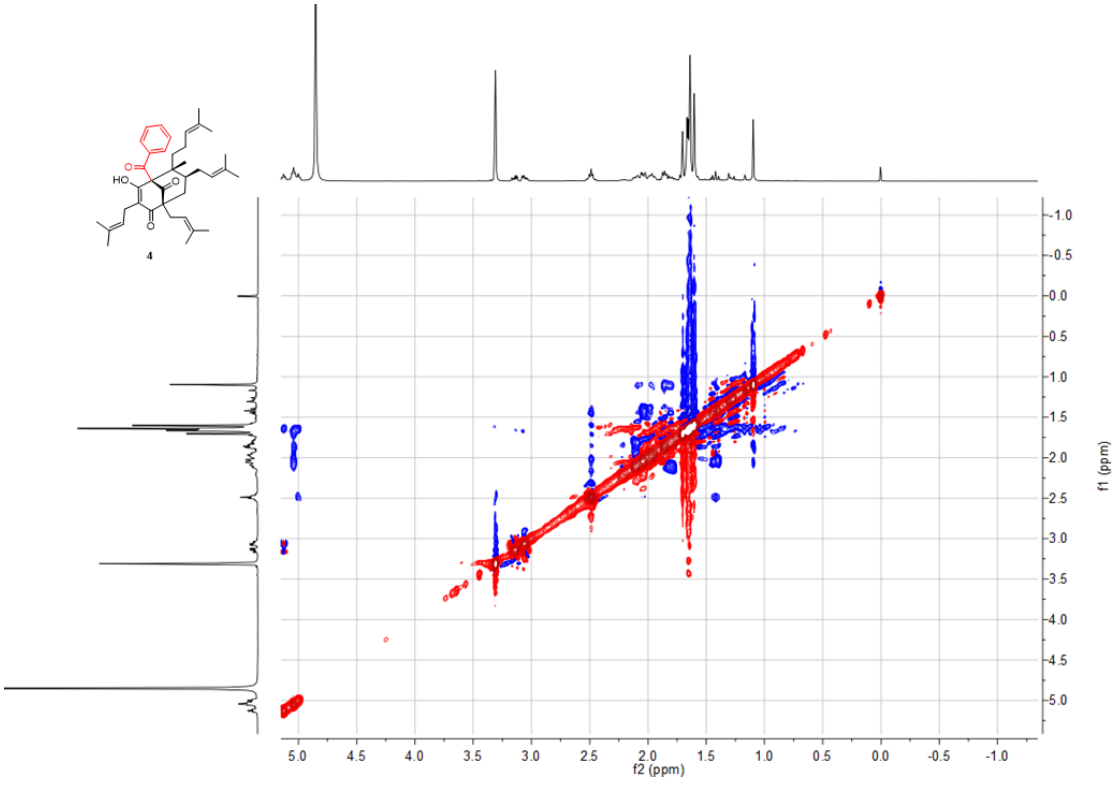
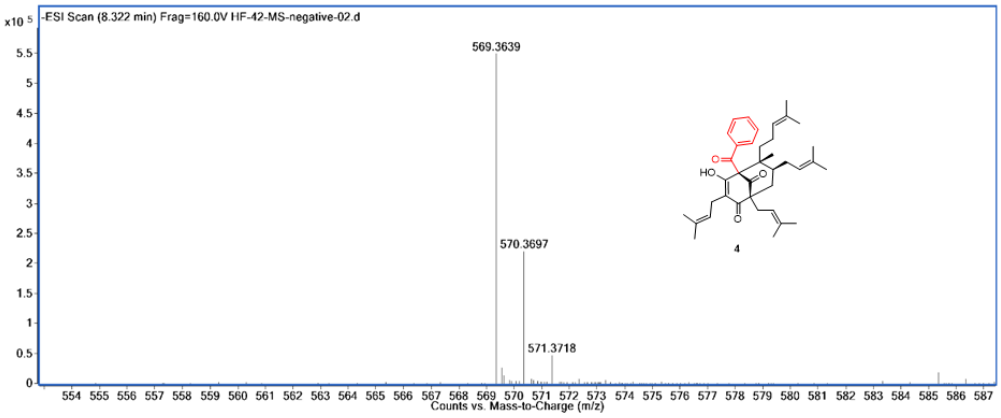


Figure S4-38. Partially expending ROESY spectrum of **4** (methanol-d_4)



Elemental Composition Calculator

Target m/z:	569.3639	**Result type:**	Negative ions	**Species:**	$[M-H]^-$
Elements:		C (0-80); H (0-120); O (0-30)			
Ion Formula		**Calcalated m/z**		**PPM Error**	
C38H49O4		569.3636		-0.40	

Figure S4-39. HRESIMS of **4**

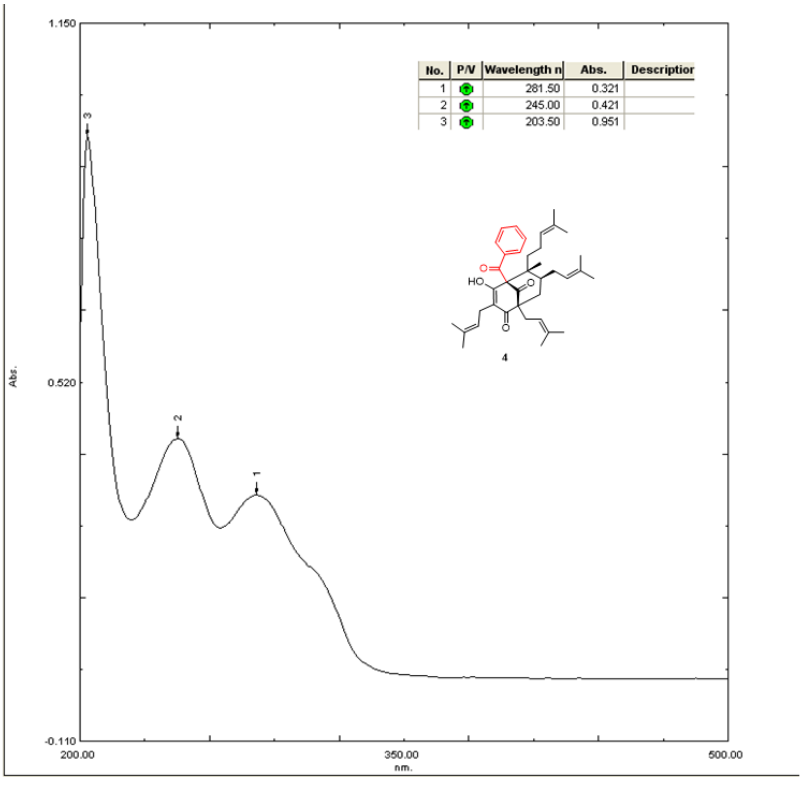


Figure S4-40. UV spectrum of **4** (MeOH)

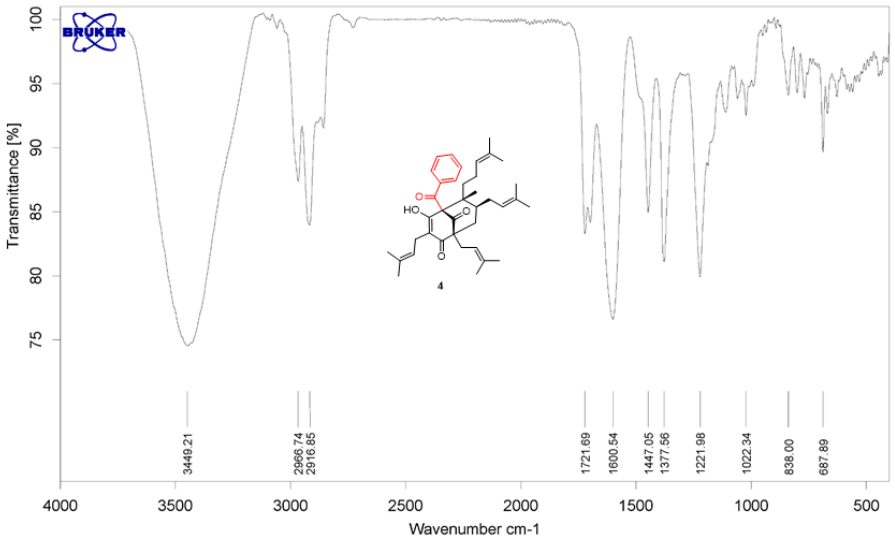


Figure S4-41. IR spectrum of **4**

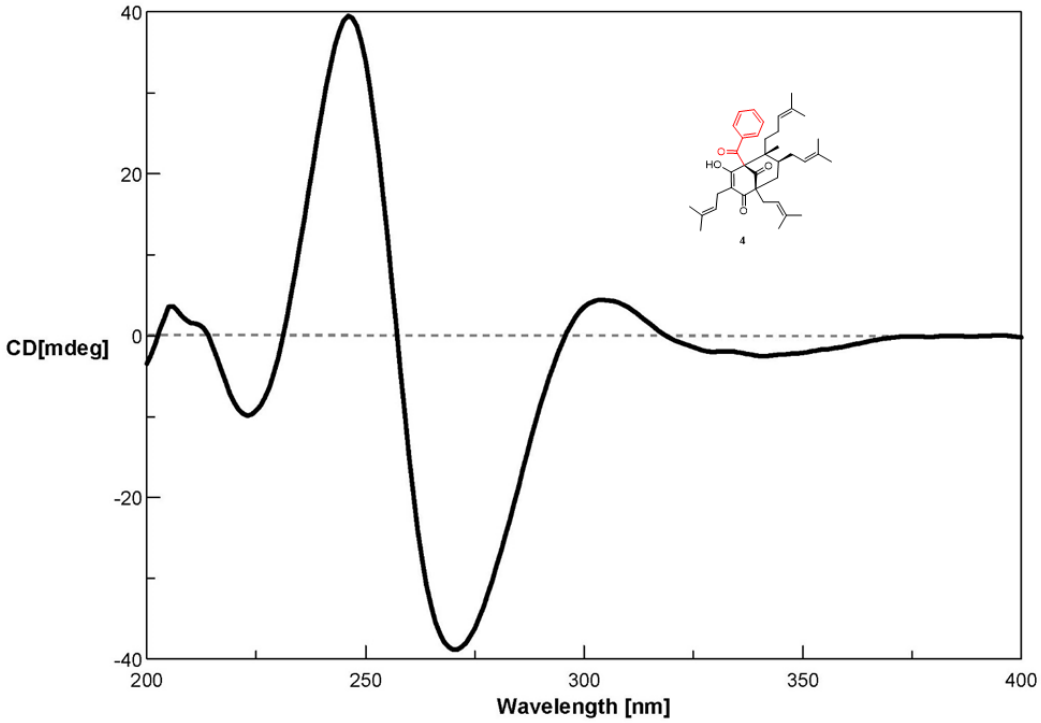


Figure S4-42. ECD spectrum of **4** (MeOH)

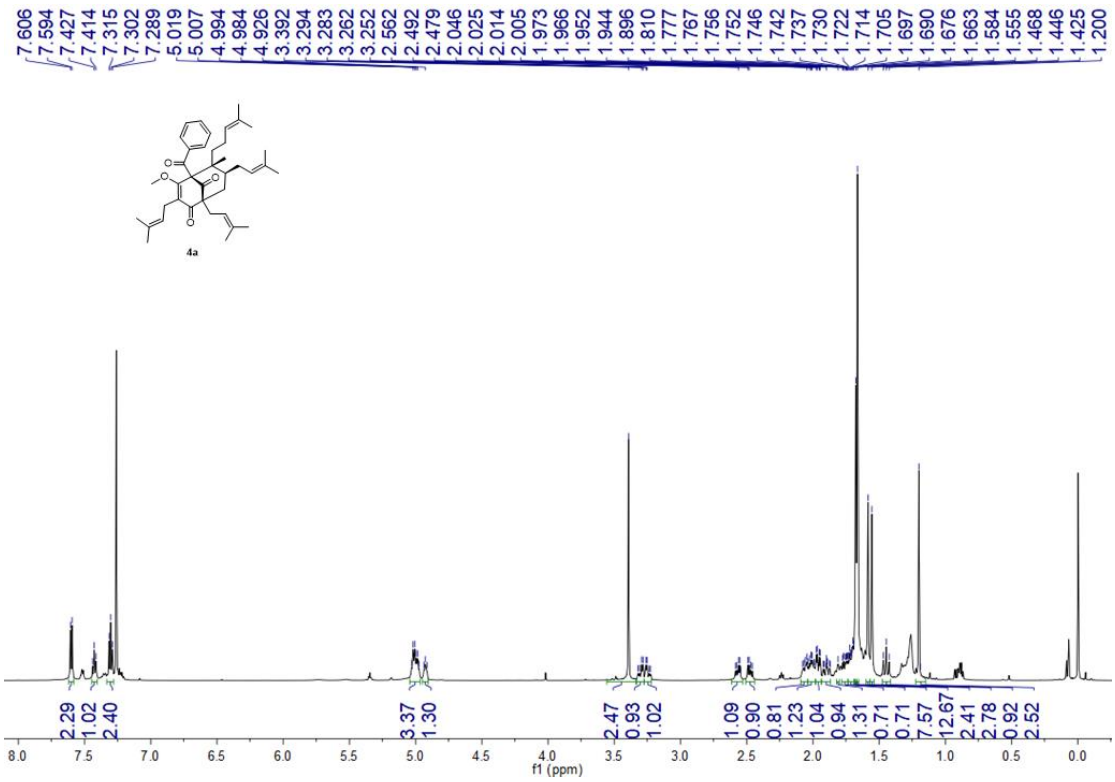


Figure S4-43. ^{1}H NMR spectrum of **4a** ($CDCl_3$)

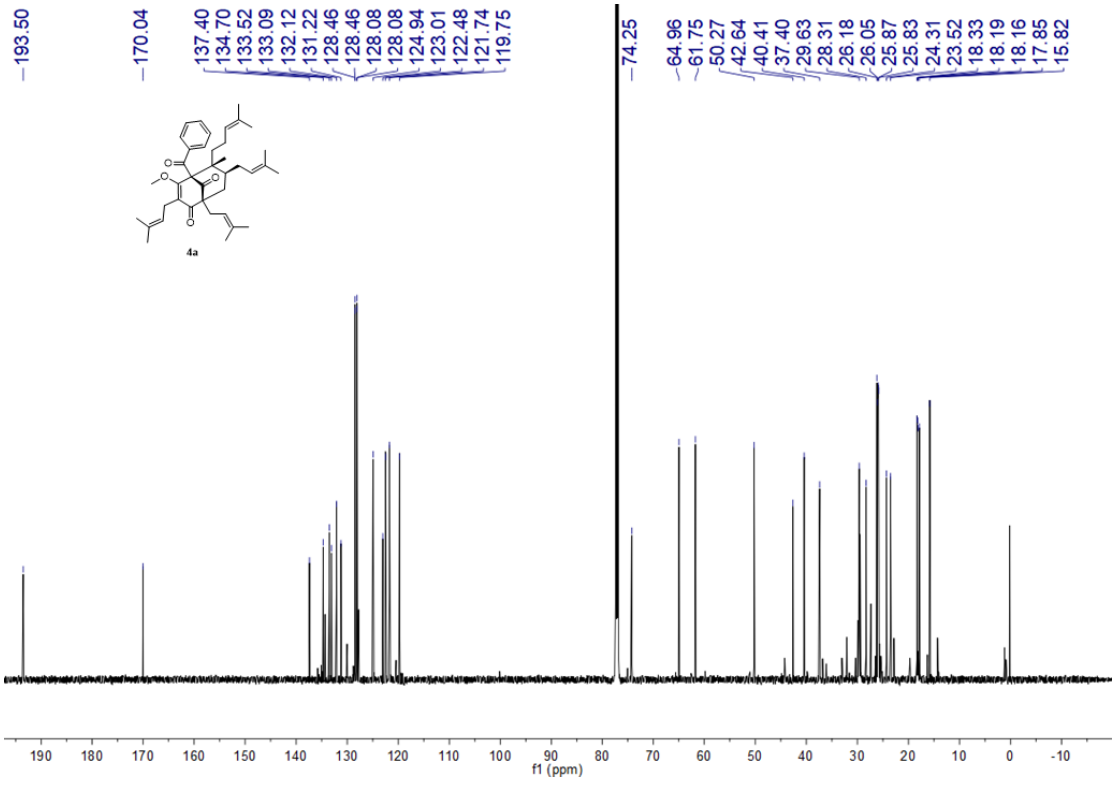


Figure S4-44. ^{13}C NMR spectrum of **4a** ($CDCl_3$)

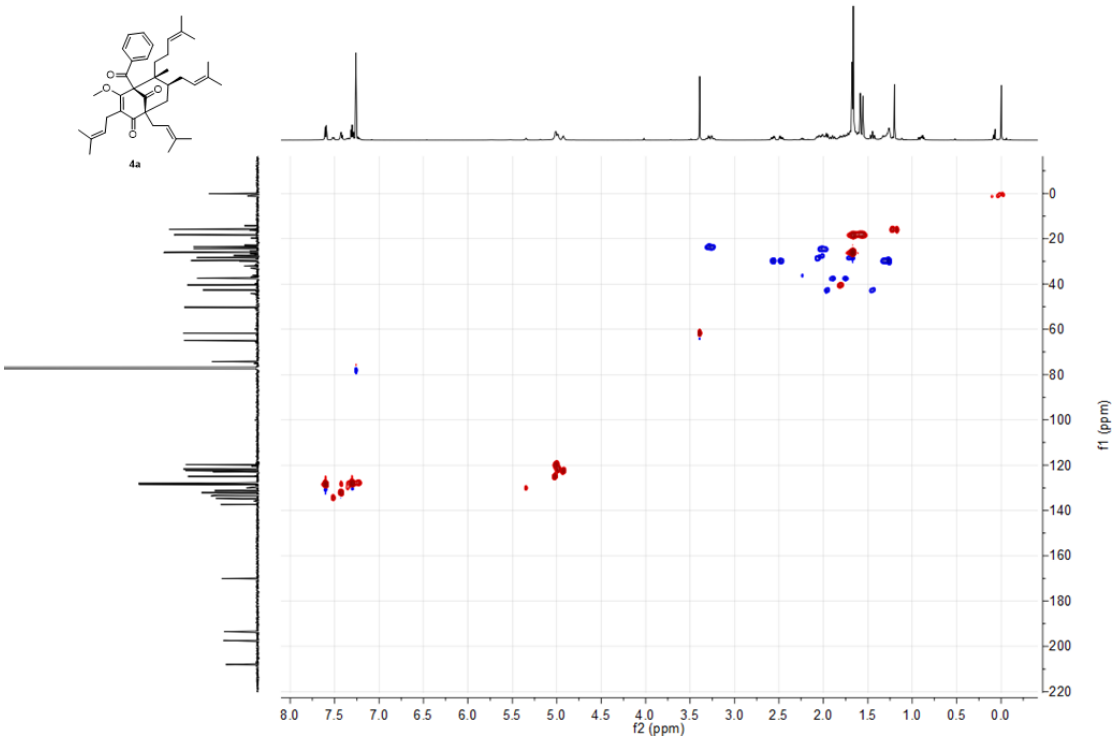


Figure S4-45. HSQC spectrum of **4a** ($CDCl_3$)

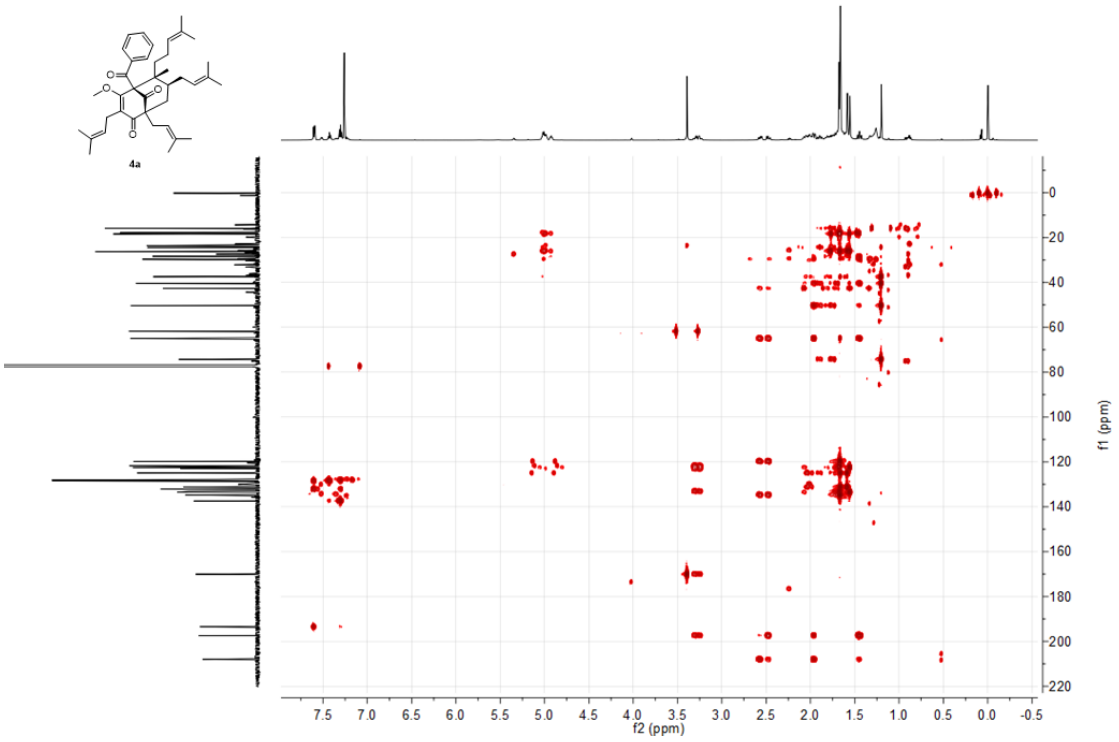


Figure S4-46. HMBC spectrum of **4a** ($CDCl_3$)

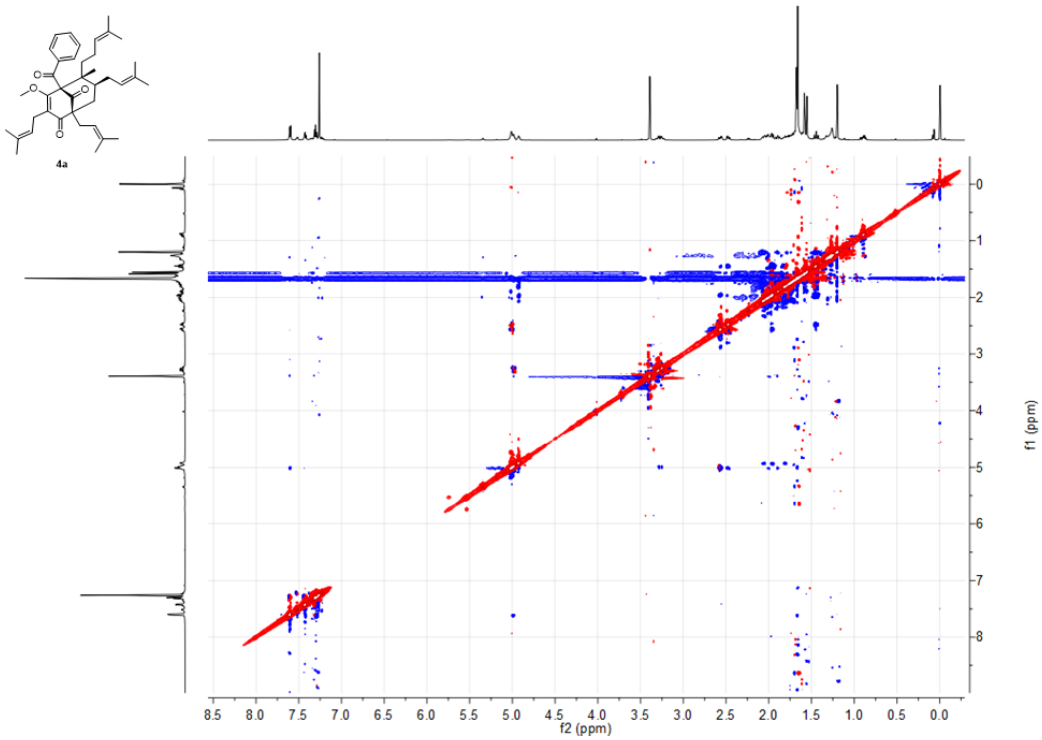
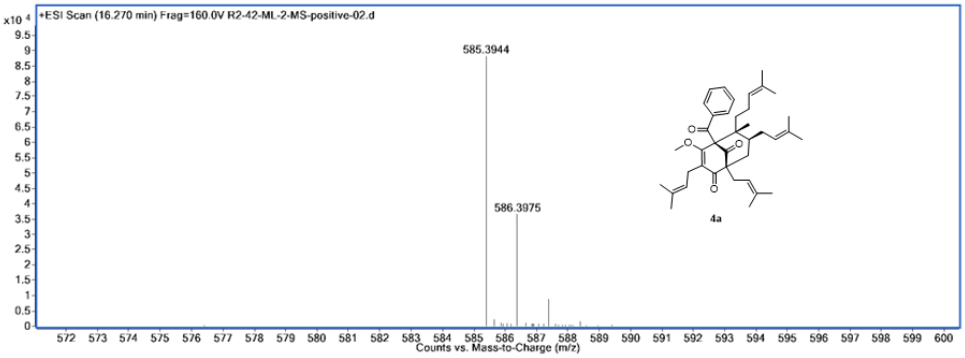


Figure S4-47. ROESY spectrum of **4a** ($CDCl_3$)



Elemental Composition Calculator

Target m/z:	585.3944	**Result type:**	Positive ions	**Species:**	$[M+H]^+$
Elements:		C (0-80); H (0-120); O (0-30)			
Ion Formula		**Calcalated m/z**		**PPM Error**	
C39H53O4		585.3938		-1.04	

Figure S4-48. HRESIMS of **4a**

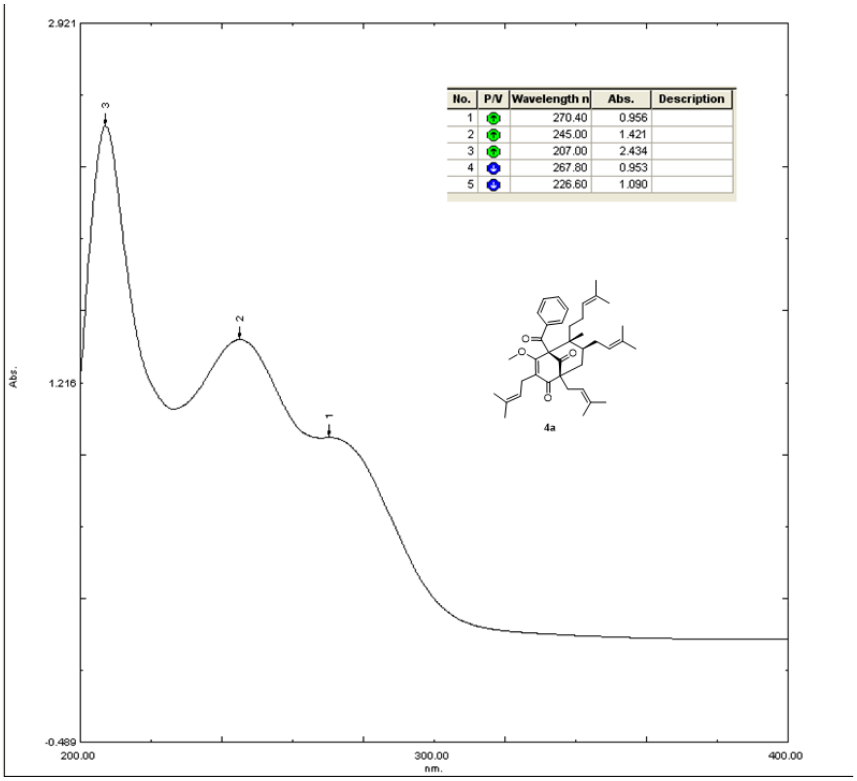


Figure S4-49. UV spectrum of **4a** (MeOH)

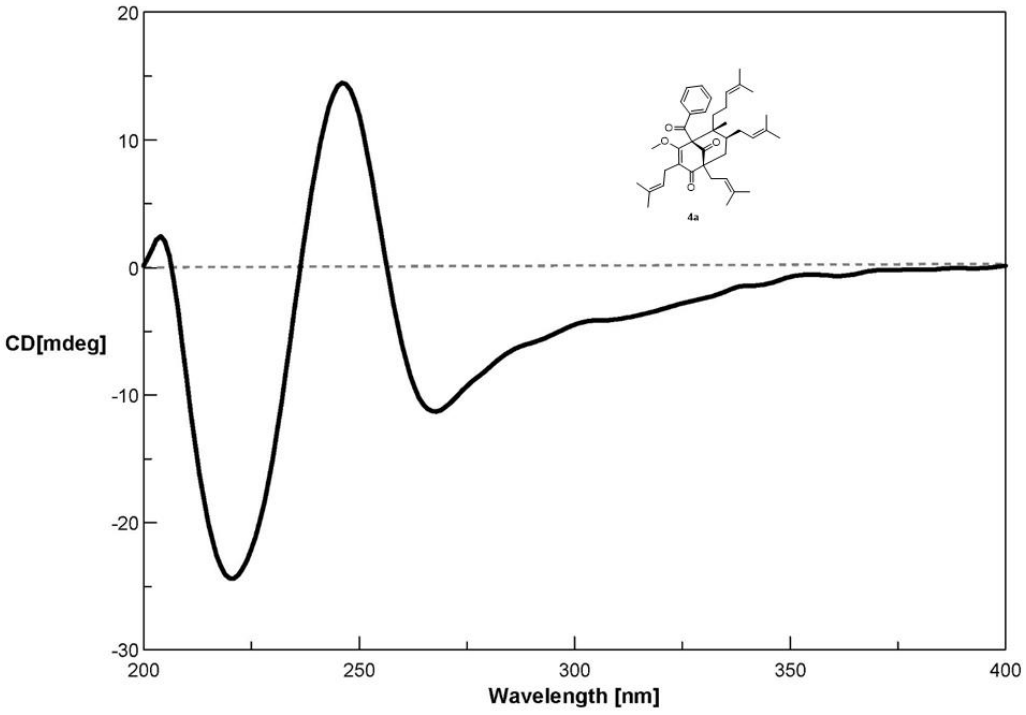


Figure S4-50. ECD spectrum of **4a** (MeOH)

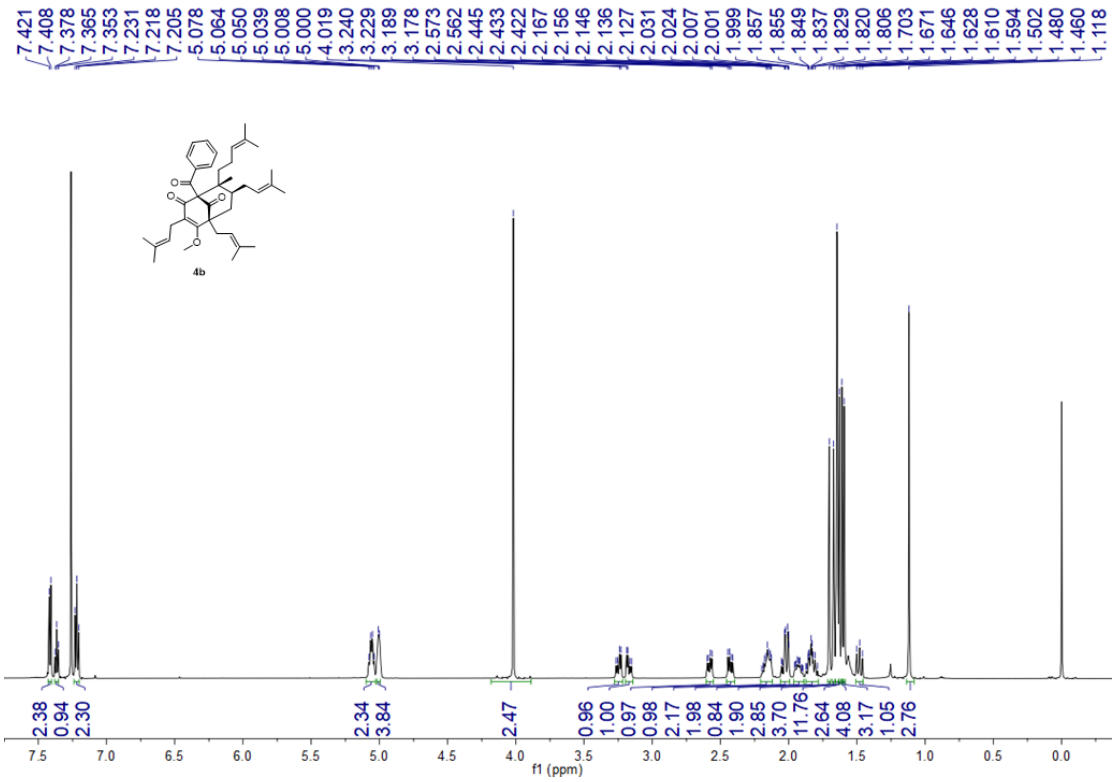


Figure S4-51. ^{1}H NMR spectrum of **4b** ($CDCl_3$)

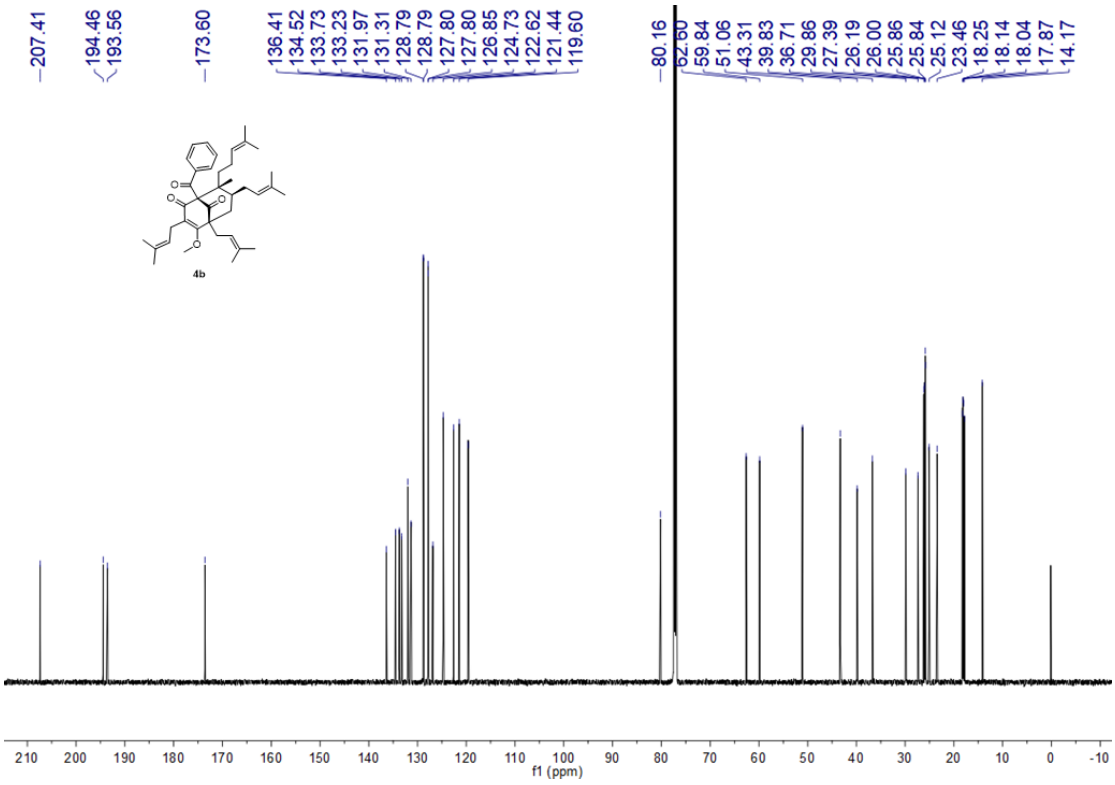


Figure S4-52. ^{13}C NMR spectrum of **4b** ($CDCl_3$)

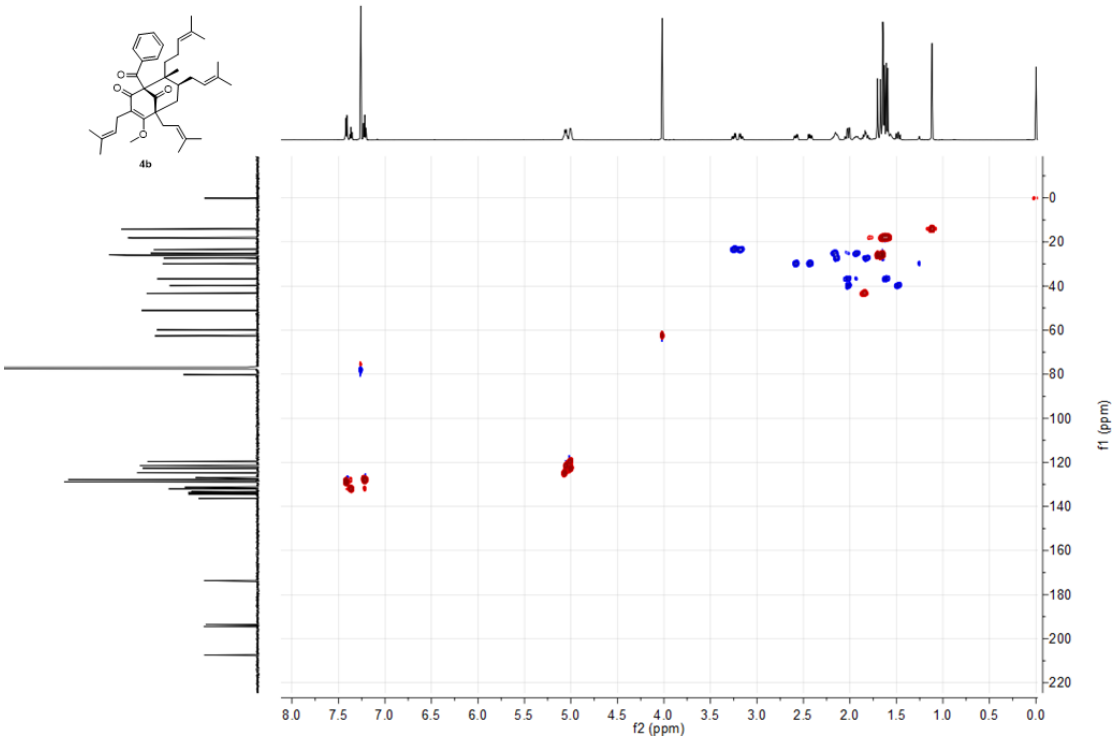


Figure S4-53. HSQC spectrum of **4b** ($CDCl_3$)

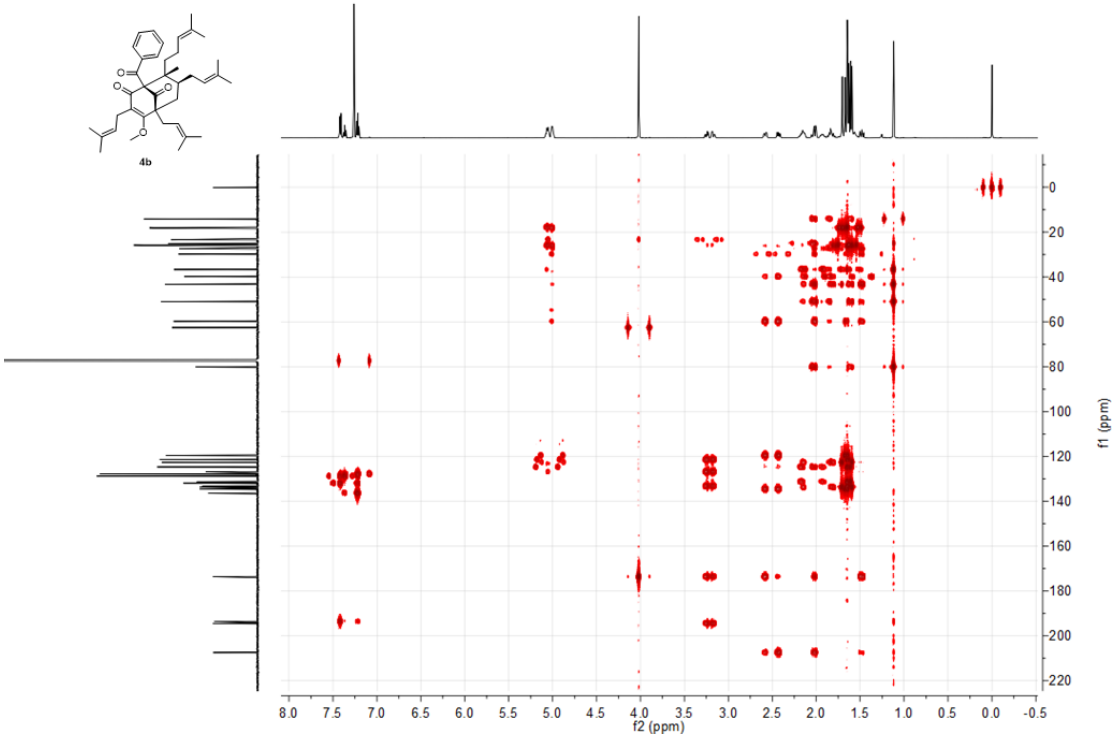


Figure S4-54. HMBC spectrum of **4b** ($CDCl_3$)

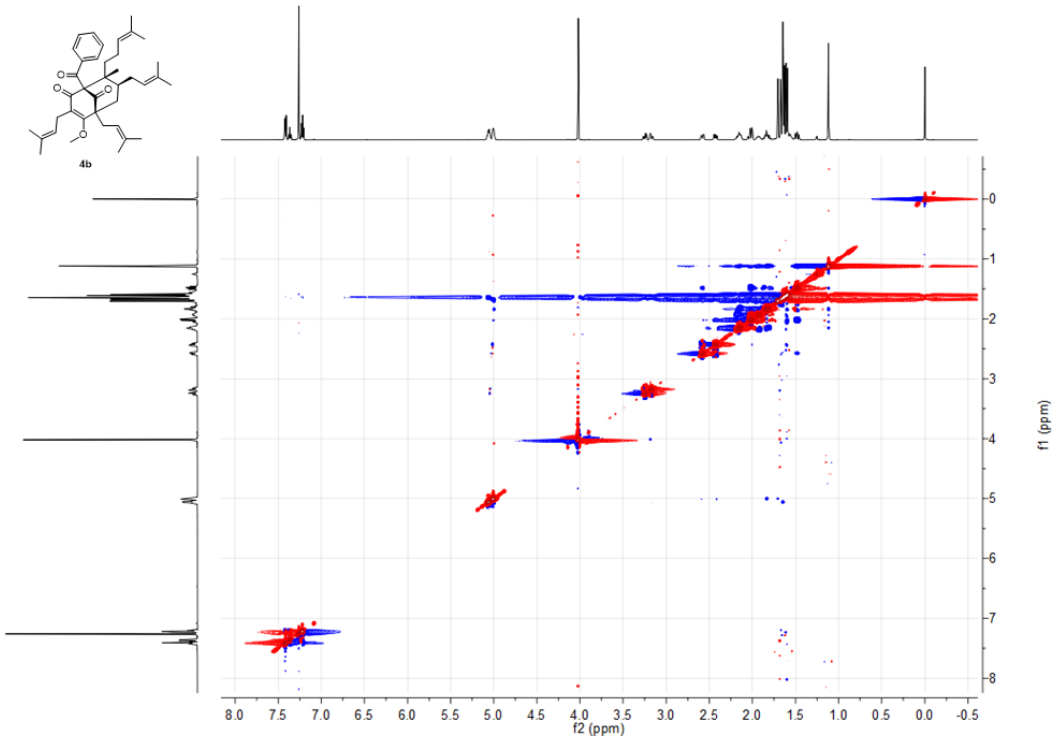
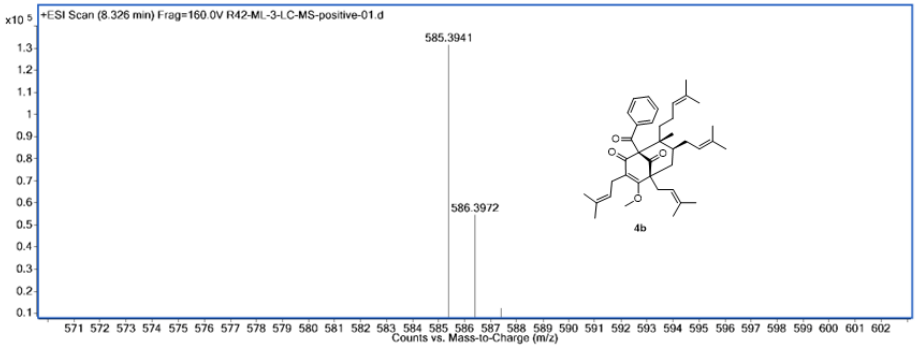


Figure S4-55. ROESY spectrum of **4b** ($CDCl_3$)



Elemental Composition Calculator

Target m/z:	585.3941	**Result type:**	Positive ions	**Species:**	$[M+H]^+$
Elements:		C (0-80); H (0-120); O (0-30)			
Ion Formula		**Calcalated m/z**		**PPM Error**	
C39H53O4		585.3938		-0.51	

Figure S4-56. HRESIMS of **4b**

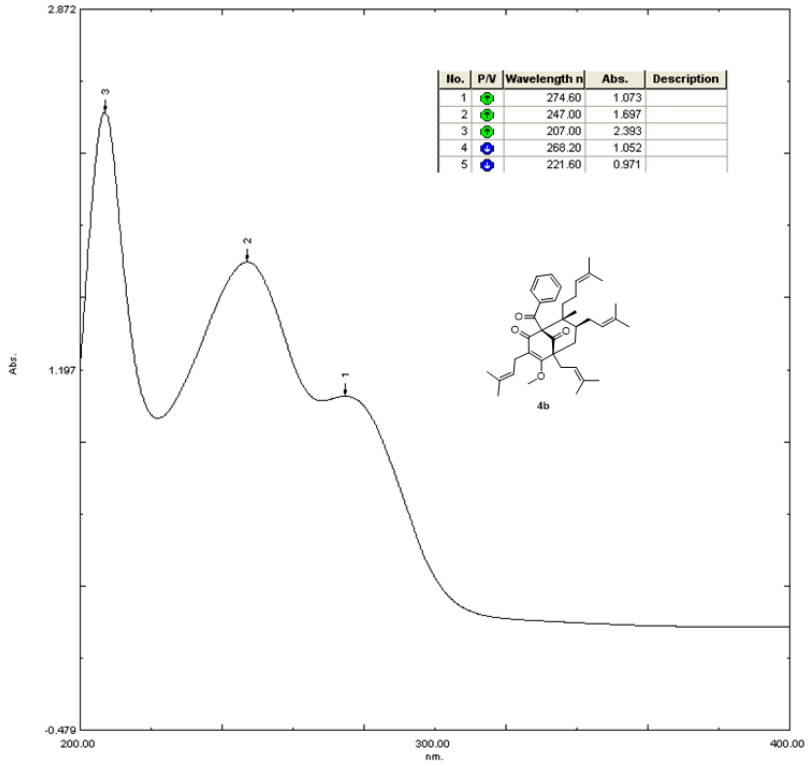


Figure S4-57. UV spectrum of **4b** (MeOH)

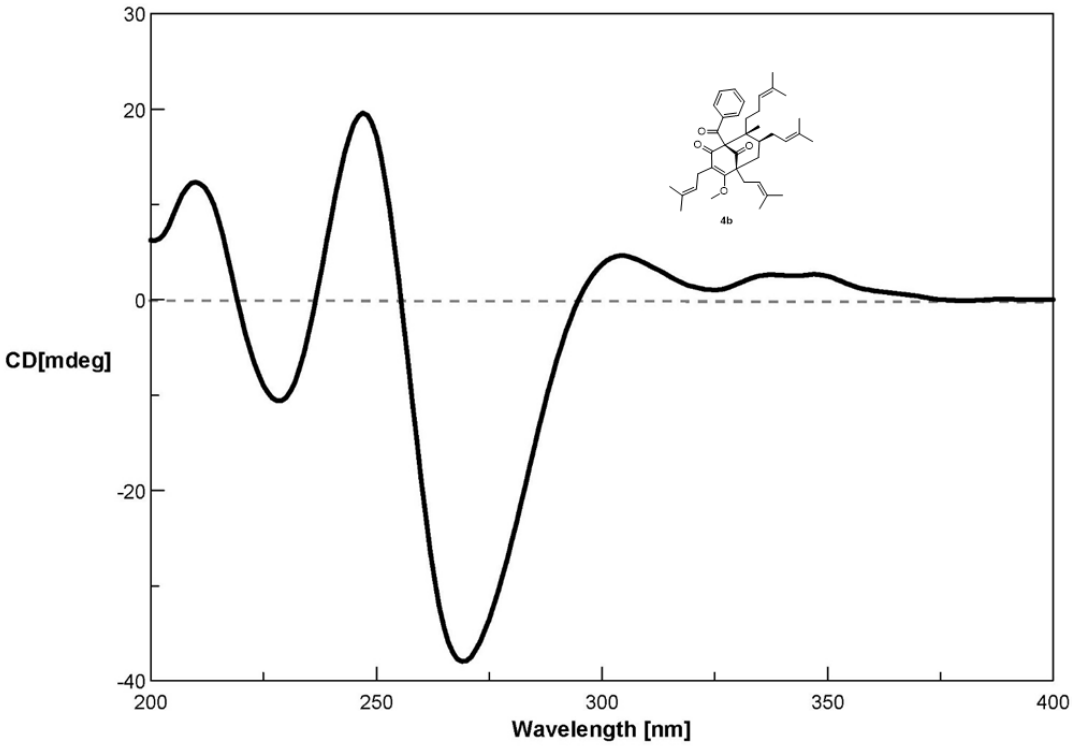


Figure S4-58. ECD spectrum of **4b** (MeOH)