Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.

Supporting Information-I:

Scaffold diversity-oriented synthesis of limonoid dimers: discovery of an axially chiral agent with *in vivo* anti-breast cancer activity

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^{1}H, ^{13}C NMR data and cytotoxic assay results for 1, 2–4, 2'–4', 5a, and 5b (Tables S1–S6), Optimized coordinates of compounds (Tables S7–S14), Figures S1–S2, and X-ray crystallographic data of 1, 2, 2', 3, 4', 5a and 5b

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Table S1. ^{1}H (400 MHz) and ^{13}C NMR (100 MHz) Data for Compound **1** (δ in ppm, J in Hz)

Position	δ_H[a]	δ_C[a]	δ_H[b]	δ_C[b]
1		90.8 qC		89.9 qC
2		80.4 qC		79.9 qC
3	4.82 s	89.7 CH	5.03 s	90.1 CH
4		43.5 qC		43.1 qC
5	2.76 br s	44.0 CH	2.89 br s	44.7 CH
6	4.47 d (4.0)	70.9 CH	4.49, s	71.8 CH
7		175.6[c] qC		175.1 qC
8		132.0 qC		131.1 qC
9	2.68 m	45.5 CH	2.86 m	46.1 CH
10		48.2 qC		48.0 qC
11α	1.78 m	19.7 CH_2	1.87 m	20.1 CH_2
11β	1.59 m		1.59 m	
12α	1.25 m	30.9 CH_2	1.42 br d (12.0)	30.8 CH_2
12β	1.57 m		1.74 br d (14.0)	
13		38.8 qC		39.1 qC
14		145.1 qC		146.4 qC
15α	3.90 dd (21.2, 4.4)	36.6 CH_2	3.89 br s	36.6 CH_2
15β	3.66 d (21.2)		3.89 br s	
16		168.7 qC		168.6 qC
17	5.37 s	80.1 CH	5.40 s	80.2 CH
18	1.09 s	19.4 CH_3	1.18 s	19.3 CH_3

19	1.25 s	19.3 CH_3	1.37 s	19.3 CH_3
20		120.5 qC		120.2 qC
21	7.76 br s	142.1 CH	7.45 br s	141.1 CH
22	6.56 br s	110.3 CH	6.41 br s	109.6 CH
23	7.75 br s	144.4 CH	7.45 br s	143.5 CH
28	0.90 s	15.5 CH_3	0.97 s	15.2 CH_3
29a	2.59 d (10.4)	42.5 CH_2	2.70 d (10.8)	42.8 CH_2
29b	1.83 d (10.4)		1.92 d (10.8)	
30		198.0 qC		197.9 qC
7-OMe-31	3.57 s	52.5 CH_3	3.76 s	53.3 CH_3
1-isobutyryloxy				
32		175.7 qC		176.8 qC
33	2.50 m	33.7 CH	2.56 m	33.9 CH
34	1.05 d (7.2)	19.2 CH_3	1.14 d (7.2)	18.9 CH_3
35	1.03 d (7.2)	19.6 CH_3	1.13 d (7.2)	19.0 CH_3
3-isobutyryloxy				
36		175.6 [c] qC		175.6 qC
37	2.17 m	33.6 CH	2.27 m	33.8 CH
38	1.01 d (7.2)	20.1 CH_3	1.09 d (7.2)	19.9 CH_3
39	0.95 d (7.2)	18.3 CH_3	1.08 d (7.2)	17.9 CH_3
2-OH	5.54 s		4.49 br s	
6-OH	5.71 d (4.0)		2.92 br s	

[a]Recorded in DMSO-*d*$_6$. [b]Recorded in $CDCl_3$. [c] Overlapped signals assigned by ^1H–^1H COSY, HSQC, and HMBC spectra without designating multiplicity.

Table S2. ^{1}H (400 MHz) and ^{13}C NMR (100 MHz) Data for Compound **2,** and **2′** (δ in ppm, J in Hz)

	2		**2′**	
Position	δ_H	δ_C	δ_H	δ_C
1/1'		91.3 qC		92.1 qC
2/2'		81.4 qC		82.1 qC
3/3'	5.23 s	88.3 CH	5.34 s	86.5 CH
4/4'		43.7 qC		44.3 qC
5/5'	3.09 s	45.1 CH	3.16 d (10.8)	39.3 CH
6a/6a'	4.57 br s	71.9 CH	2.34 dd (16.4, 10.8)	34.0 CH_2
6b/6b'			2.44 d (16.4)	
7/7'		175.5[a] qC		173.8 qC
8/8'		134.8 qC		135.4 qC
9/9'	3.06 m	46.6 CH	2.87 dd (9.2, 6.4)	45.4 CH
10/10'		47.8 qC		47.6 qC
11α/11α'	2.0 m	20.0 CH_2	1.91 m	19.8 CH_2
11β/11β'	2.0 m		1.98 m	
12α/12α'	1.80 m	31.3 CH_2	1.67 m	31.1 CH_2
12β/12β'	1.80 m		1.77 m	
13/13'		40.9 qC		40.8 qC
14/14'		142.9 qC		142.9 qC
15/15'		137.8 qC		137.6 qC
16/16'		160.5 qC		160.6 qC
17/17'	5.76 s	82.0 CH	5.87 s	81.9 CH

18/18'	1.01 s	19.4 CH_3	1.11 s	19.1 CH_3
19/19'	1.36 s	19.3 CH_3	1.07 s	18.5 CH_3
20/20'		120.5 qC		120.1 qC
21/21'	7.52 br s	140.9 CH	7.69 br s	142.1 CH
22/22'	6.40 br s	109.4 CH	6.47 br s	109.6 CH
23/23'	7.45 br s	143.4 CH	7.45 br s	143.3 CH
28/28'	0.96 s	15.2 CH_3	0.86 s	14.5 CH_3
29a/29a'	2.88 d (10.8)	42.2 CH_2	2.52 d (11.2)	40.7 CH_2
29b/29b'	2.15 d (10.8)		2.26 br d (11.2)	
30/30'		192.7 qC		193.7 qC
7,7'-OMe-31,31'	3.74 s	53.3 CH_3	3.67 s	52.0 CH_3
1,1'- *isobutyryloxy*				
32/32'		175.5 [a] qC		175.8 qC
33/33'	2.44 m	34.2 CH	2.42 m	34.3 CH_3
34/34'	1.11 d (6.8)	19.1 CH_3	1.10 d (6.8)	18.9 CH_3
35/35'	1.09 d (6.8)	18.8 CH_3	1.07 d (6.8)	19.2 CH_3
3,3'- *isobutyryloxy*				
36/36'		178.2 qC		178.8 qC
37/37'	2.66 m	33.7 CH	2.71 m	33.9 CH
38/38'	1.13 d (6.8)	20.4 CH_3	1.20 d (6.8)	20.3 CH_3
39/39'	0.91 d (6.8)	17.8 CH_3	0.91 d (6.8)	17.8 CH_3
2-OH/2'-OH	4.41 s		4.33 br s	
6-OH/6'-OH	2.91 br s			

[a] Overlapped signals assigned by ^1H–^1H COSY, HSQC, and HMBC spectra without designating multiplicity.

Table S3. ^{1}H (400 MHz) and ^{13}C NMR (100 MHz) Data for Compound **3,** and **3′** (δ in ppm, J in Hz) in $CDCl_3$

	3		**3′**	
Position	δ_H	δ_C	δ_H	δ_C
1		88.8 qC		89.2 qC
2		78.7 qC		78.6 qC
3	4.92 s	90.5 CH	5.04 s	89.4 CH
4		42.6 qC		43.0 qC
5	2.92 s	45.2 CH	2.97 d (11.6)	39.9 CH
6a	4.50 br s	72.4 CH	2.34 brd (16.4)	35.4 CH_2
6b			2.47 dd (16.4, 11.6)	
7		175.5 qC		172.9 qC
8		131.2 qC		130.9 qC
9	2.77 dd (9.2, 7.2)	43.9 CH	2.71 dd (9.6, 6.4)	43.1 CH
10		46.5 qC		46.2 qC
11α	1.96 m	21.1 CH_2	1.91 m	21.1 CH_2
11β	1.74 m		1.68 m	
12α	1.46 m	30.7 CH_2	1.46 m	30.7 CH_2
12β	1.60 m		1.65 m	
13		40.8 qC		41.0 qC
14		154.5 qC		155.3 qC
15		78.9 qC		78.9 qC
16		170.4 qC		170.1 qC
17	5.86 s	78.3 CH	5.88 s	78.2 CH

18	1.09 s	13.3 CH_3	1.07 s	13.0 CH_3
19	1.31 s	20.3 CH_3	1.01 s	19.5 CH_3
20		121.3 qC		121.3 qC
21	7.43 br s	141.8 CH	7.44 br s	141.8 CH
22	6.38 br s	110.5 CH	6.40 br s	110.5 CH
23	7.40 br s	143.1 CH	7.40 br s	143.0 CH
28	0.93 s	15.4 CH_3	0.84 s	14.8 CH_3
29a	2.70 d (10.4)	42.4 CH_2	2.14 d (11.2)	
29b	1.88 dd (10.4, 1.6)		1.98 dd (11.2, 1.6)	41.4 CH_2
30		192.9 qC		192.7 qC
7-OMe-31	3.78 s	53.3 CH_3	3.65 s	51.9 CH_3
1-isobutyryloxy				
32		175.7 qC		175.8 qC
33	2.41 m	34.3 CH	2.40 m	34.5 CH
34	1.24 d (7.2)	20.1 CH_3	1.24 d (7.2)	19.8 CH_3
35	1.08 d (7.2)	17.9 CH_3	1.06 d (7.2)	18.1 CH_3
3-isobutyryloxy				
36		176.5 qC		177.3 qC
37	2.89 m	33.0 CH	2.97 m	33.0 CH
38	1.18 d (6.8)	19.8 CH_3	1.26 d (7.2)	20.3 CH_3
39	1.16 d (6.8)	18.0 CH_3	1.17 d (7.2)	18.3 CH_3
1'		87.9 qC		88.0 qC
2'		75.7 qC		75.8 qC
3'	4.51 s	88.1 CH	4.67 s	86.6 CH

4'		44.3 qC		44.4 qC
5'	2.81 s	40.2 CH	2.83 dd (10.4, 4.0)	34.3 CH
6a'	4.30 br s	71.6 CH	2.29 d (16.0)	34.4 CH_2
6b'			2.30 dd (16.0, 10.4)	
7'		176.3 qC		173.2 qC
8'		103.1 qC		102.9 qC
9'	2.50 m	36.4 CH	2.43 m	35.3 CH
10'		47.3 qC		46.8 qC
11'α	1.96 m	20.4 CH_2	1.85 m	20.1 CH_2
11'β	1.49 m		1.48 m	
12'α	1.52 m	29.8 CH_2	1.50 m	29.6 CH_2
12'β	1.68 m		1.68 m	
13'		35.7 qC		35.8 qC
14'		156.4 qC		156.2 qC
15'		106.5 qC		106.6 qC
16'		163.3 qC		163.1 qC
17'	5.01 s	79.7 CH	4.99 s	79.8 CH
18'	1.17 s	21.0 CH_3	1.15 s	20.6 CH_3
19'	1.33 s	19.0 CH_3	1.00 s	17.8 CH_3
20'		119.9 qC		119.9 qC
21'	7.40 br s	141.2 CH	7.40 [a]	141.2 CH
22'	6.38 br s	109.9 CH	6.37 br s	109.9 CH
23'	7.40 br s	142.9 CH	7.40 [a]	142.8 CH
28'	1.02 s	15.6 CH_3	0.90 s	14.8 CH_3

29'a	2.94 d (11.2)	39.9 CH_2	2.64 d (11.6)	39.0 CH_2
29'b	2.28 d (11.2)		2.26 d (11.6)	
30'		155.3 qC		154.9 qC
7'-OMe-31'	3.84 s	53.1 CH_3	3.66 s	51.8 CH_3
1'-isobutyryloxy				
32'		177.4[a] qC		177.1 qC
33'	2.96 m	34.1 CH	2.45 m	34.0 CH
34'	1.20 d (6.8)	18.3 CH_3	1.11 d (7.2)	18.9 CH_3
35'	1.17 d (6.8)	20.5 CH_3	1.06 d (7.2)	18.3CH_3
3'-isobutyryloxy				
36'		177.4[a] qC		177.9 qC
37'	2.47 m	34.0 CH	3.08 m	33.9 CH
38'	1.12 d (6.8)	18.9 CH_3	1.23 d (7.2)	20.3 CH_3
39'	1.07 d (6.8)	18.4 CH_3	1.19 d (7.2)	17.9 CH_3
2-OH	4.56 s		4.62 s	
6-OH	3.04 br s		/	
2'-OH	4.03 br s		3.96 br s	
6'-OH	3.00 br s			

[a] **Overlapped signals assigned by ^{1}H–^{1}H COSY, HSQC, and HMBC spectra without designating multiplicity.**

Table S4. ^{1}H NMR (400 MHz) and ^{13}C NMR (100 MHz) Data for Compounds **4,** and **4′** (δ in ppm, *J* in Hz) in $CDCl_3$.

	4		**4′**	
Position	δ_H	δ_C	δ_H	δ_C
1		86.7 qC		86.7 qC
2		77.6 qC		77.5 qC
3	4.76 s	84.6 CH	4.87 s	83.4 CH
4		44.1 qC		44.3 qC
5	2.83 s	42.1 CH	2.82 m	36.4 CH
6a	4.49 br s	72.2 CH_2	2.36 [a]	34.5 CH_2
6b			2.32 (16.8, 11.2)	
7		175.8 qC		173.4 qC
8		107.2 qC		107.1 qC
9	2.54 dd (10.8, 5.2)	36.8 CH	2.45 m	35.9 CH
10		48.0 qC		47.4 qC
11α	1.94 m	19.6 CH_2	1.92 m	19.8 CH_2
11β	1.71 m		1.62 m	
12α	1.35 m	28.9 CH_2	1.35 m	29.1 CH_2
12β	1.40 m		1.48 m	
13		38.8 qC		39.0 qC
14		159.1 qC		159.1 qC
15		122.5 qC		122.6 qC
16		163.1 qC		163.2 qC
17	5.01 s	78.4 CH	5.03 s	78.5 CH

18	1.24 s	17.4 CH_3	1.21 s	17.4 CH_3
19	1.33 s	19.7 CH_3	0.98 s	19.1 CH_3
20		120.2 qC		120.2 qC
21	7.41 br s	140.9 CH	7.41 br s	141.0 CH
22	6.36 br s	109.8 CH	6.37 br s	109.8 CH
23	7.40 br s	142.9 CH	7.40 br s	142.9 CH
28	1.00 s	15.9 CH_3	0.86 s	14.8 CH_3
29a	2.86 d (10.8)	40.2 CH_2	2.51 [a]	39.3 CH_2
29b	2.43 d (10.8)		2.40 [a]	
30		148.1 qC		148.0 qC
7-OMe-31	3.81 s	53.1 CH_3	3.66 s	51.8 CH_3
1-*isobutyryloxy*				
32		177.9 qC		177.5 qC
33	2.77 m	33.9 CH	2.85 m	34.3 CH
34	1.16 d (6.8)	19.8 CH_3	1.13 d (6.8)	19.1 CH_3
35	0.81 d (6.8)	18.2 CH_3	1.07 d (6.8)	18.9 CH_3
3-*isobutyryloxy*				
36		175.2 qC		175.6 qC
37	2.61 m	34.6 CH	2.65 m	34.6 CH
38	1.24 d (6.8)	19.3 CH_3	1.28 d (6.8)	19.3 CH_3
39	1.23 d (6.8)	18.2 CH_3	1.25 d (6.8)	18.3 CH_3
1'		85.7 qC		86.0 qC
2'		80.4 qC		80.2 qC
3'	4.80 s	85.5 CH	4.92 s	84.5 CH

4'		47.3 qC		47.2 qC
5'	2.76 s	45.2 CH	2.80 m	40.8 CH
6a'	4.55 br s	71.6 CH_2	2.43 [a]	33.2 CH_2
6b'			2.50 [a]	
7'		174.8 qC		173.0 qC
8'		127.3 qC		127.3 qC
9'		174.5 qC		175.1 qC
10'		51.4 qC		50.9 qC
11'α	2.74 m	26.3 CH_2	2.58 m	26.2 CH_2
11'β	2.35 br d (19.2)		2.50 m	
12'α	1.42 m	30.1 CH_2	1.40 m	30.1 CH_2
12'β	1.15 [a]		1.22 m	
13'		39.8 qC		39.9 qC
14'		146.6 qC		146.8 qC
15'		124.2 qC		124.2 qC
16'		161.4 qC		161.4 qC
17'	5.19 s	77.2 CH	5.19 s	77.2 CH
18'	1.28 s	17.8 CH_3	1.25 s	17.9 CH_3
19'	1.53 s	17.6 CH_3	1.24 s	17.7 CH_3
20'		119.9 qC		119.8 qC
21'	7.43 br s	141.5 CH	7.42 br s	141.4 CH
22'	6.40 br s	109.7 CH	6.37 br s	109.7 CH
23'	7.41 br s	143.4 CH	7.40 br s	143.3 CH
28'	0.97 s	16.7 CH_3	0.92 s	16.6 CH_3

29'a	3.23 d (11.6)	40.3 CH_2	2.65 [b]	39.1 CH_2
29'b	2.65 br d (11.6)		2.65 [b]	
30'		193.4 qC		193.2 qC
7'-OMe-31'	3.79 s	53.3 CH_3	3.68 s	52.2 CH_3
1′-*isobutyryloxy*				
32'		177.4 qC		177.9 qC
33'	2.85 m	34.2 CH	2.77 m	33.9 CH
34'	1.16 d (6.8)	19.5 CH_3	1.15 d (6.8)	19.7 CH_3
35'	1.08 d (6.8)	18.3 CH_3	0.83 d (6.8)	18.3 CH_3
3′-*isobutyryloxy*				
36'		174.5 qC		174.8 qC
37'	2.57 m	34.3 CH	2.58 m	34.2 CH
38'	1.15 d (6.8)	19.3 CH_3	1.18 d (7.2)	19.3 CH_3
39'	1.08 d (6.8)	18.8 CH_3	1.13 d (6.8)	18.3 CH_3
6-OH	2.90 s		/	/
30-OH	8.66 s		8.61 s	
2'-OH	3.38 br s		3.34 br s	
6'-OH	3.09 br s			

[a] Overlapped signals assigned by ^{1}H–^{1}H COSY, HSQC, and HMBC spectra without designating multiplicity.

Table S5. ^{1}H NMR (400 MHz) and ^{13}C NMR (100 MHz) data for compounds **5a,** and **5b** (δ in ppm, J in Hz) in $CDCl_3$

	5a		5b	
Position	δ_H	δ_C	δ_H	δ_C
1/1'		86.8 qC		87.1 qC
2/2'		77.2 qC		77.9 qC
3/3'	4.80 s	86.5 CH	4.59 s	84.6 CH
4/4'		43.4 qC		43.9 qC
5/5'	2.76 br s	41.6 CH	2.83 s	42.2 CH
6/6'	4.51 br s	72.4 CH	4.46 br s	72.0 CH
7/7'		175.1 qC		175.6 qC
8/8'		103.3 qC		107.7 qC
9/9'	2.57 m	37.1 CH	2.58 m	37.0 CH
10/10'		48.8 qC		47.9 qC
11α/11'α	1.82 m	19.2 CH_2	1.96 m	19.5 CH_2
11β/11'β	1.68 m		1.67 m	
12α/12'α	1.20 m	29.5 CH_2	1.30 m	29.0 CH_2
12β/12'β	1.45 m		1.30 m	
13/13'		40.0 [a] qC		39.2 qC
14/14'		159.6 qC		156.2 qC
15/15'		122.7 qC		122.9 qC
16/16'		166.4 qC		161.5 qC
17/17'	5.19 s	79.5 CH	5.02 s	78.3 CH
18/18'	1.20 s	18.2 CH_3	1.25 s	17.2 CH_3

19/19'	1.33 s	19.8 CH_3	1.34 s	20.1 CH_3
20/20'		119.5 qC		120.2 qC
21/21'	7.46 br s	141.1 CH	7.41 br s	141.2 CH
22/22'	6.37 br s	109.5 CH	6.37 br s	109.8 CH
23/23'	7.43 br s	143.4 CH	7.40 br s	143.1 CH
28/28'	1.01 s	15.6 CH_3	1.01 s	15.9 CH_3
29α/29'α	2.81 d (11.2)	40.0 [a] CH_2	2.91 br d (10.4)	39.8 CH_2
29β/29'β	2.56 d (11.2)		2.27 d (10.4)	
30/30'		148.9 qC		143.7 qC
7,7'-OMe-31,31'	3.79 s	53.2 CH_3	3.81 s	53.2 CH_3
1,1'-isobutyryloxy				
32/32'		177.1 qC		178.5 qC
33/33'	2.50 m	34.7 CH	2.93 m	34.1 CH
34/34'	1.14 d (6.8)	19.3 CH_3	1.18 d (7.2)	18.4 CH_3
35/35'	1.13 d (6.8)	19.3 CH_3	1.00 d (7.2)	18.7 CH_3
3,3'-isobutyryloxy				
36/36'		175.5 qC		176.3 qC
37/37'	2.52 m	34.5 CH	2.65 m	34.7 CH
38/38'	1.25 d (7.2)	19.1 CH_3	1.22 d (7.2)	19.4 CH_3
39/39'	1.23 d (7.2)	19.0 CH_3	1.20 d (7.2)	19.5 CH_3
2-OH/2'-OH	3.49 br s		3.23 br s	
6-OH/6'-OH	3.01 br s		2.93 br s	
30-OH/30'-OH	6.73 s		6.93 s	

[a] Overlapped signals assigned by DEPT135, ^1H–^1H COSY, HSQC, and HMBC spectra without designating multiplicity.

Table S6. Cytotoxic assay results for **1-4, 1′-4′, 5a-5b, 2a-2b** against six human tumor cells. The results are given as IC_{50} values (μM).

Compound	**Cell lines**					
	MDA-MB-231	A375	AGS	HCT-8	HCT-8/T	A549
1	81.46	6.8	82.72	78.85	>100	>100
1′	83.49	55.1	98.6	>100	>100	>100
2	ND	ND	ND	ND	ND	ND
2′	ND	ND	ND	ND	ND	ND
3	88.5	>100	>100	>100	>100	>100
3′	>100	>100	>100	>100	>100	>100
4	>100	>100	>100	>100	>100	>100
4′	>100	>100	>100	>100	>100	>100
5a	>100	>100	>100	>100	>100	>100
5b	5.57	>100	73.1	8.81	39.5	14.59
Cisplatin	6.25	18.12	9.26	21.98	28.15	12.13

Table S7. Optimized coordinates of compound **2** at B3LYP/6-31G(d) level in CH_3CN.

Atom	X	Y	Z	Atom	X	Y	Z	Atom	X	Y	Z
C	3.891	-6.834	-1.02	O	-8.038	-1.909	-1.032	H	6.361	-2.67	0.764
C	2.002	-6.868	-2.724	C	-3.839	1.796	0.789	H	6.104	-3.345	-0.833
C	2.708	-6.055	-1.633	O	0.271	-2.291	2.364	H	-5.337	3.751	-0.267
C	3.222	-4.735	-2.196	C	-4.644	1.709	-0.552	H	-6.5	2.548	0.287
C	3.44	3.918	-1.633	O	-1.815	-1.91	2.901	H	-6.314	2.843	-1.432
C	0.942	4.205	-2.016	C	-4.694	1.348	1.988	H	-5.778	-2.181	3.323
C	2.04	3.285	-1.474	C	4.271	-1.63	2.432	H	0.625	-1.951	-2.26
C	2.001	1.931	-2.162	O	-5.485	-2.665	5.325	H	5.92	3.103	2.099
C	8.52	2.767	-1.189	C	-3.888	1.308	3.28	H	2.689	-0.142	-3.218
C	1.592	-1.278	-0.306	C	4.383	-0.143	2.757	H	-2.396	-1.802	6.024
C	4.528	-2.006	-2.628	O	-0.497	1.438	-0.567	H	2.83	3.359	5.14
C	5.338	0.415	-3.16	C	-2.644	0.409	3.209	H	-4.607	-2.939	7.189
C	4.855	4.14	4.927	C	-1.864	0.64	1.91	H	5.118	4.736	5.787
C	3.745	3.441	4.572	C	-0.539	-0.03	1.962	H	-4.798	-1.272	-4.075
C	5.291	3.271	2.961	C	-0.631	-1.482	2.388	H	-6.332	-0.983	-3.232
C	4.029	2.863	3.282	C	-3.018	-1.098	3.093	H	-5.157	-2.142	-2.579
C	5.593	-3.034	0.079	C	-1.789	0.699	4.463	H	4.92	0.344	-4.17
C	2.448	0.373	4.304	C	-5.767	2.771	-0.491	H	6.397	0.156	-3.209
C	3.149	2.004	2.423	C	-3.777	-1.713	4.227	H	5.249	1.459	-2.839
C	0.685	2.102	2.093	C	-5.066	-2.153	4.136	H	-4.048	1.35	-3.912
C	0.673	0.604	1.889	C	-3.363	-1.989	5.581	H	-5.575	1.758	-3.103
C	1.994	-0.059	1.848	C	-4.432	-2.562	6.193	H	4.033	-2.16	-3.587
C	2.989	0.519	2.866	C	-5.267	-1.178	-3.089	H	5.509	-2.48	-2.653
O	0.372	-1.352	-0.387	C	-4.579	1.341	-2.96	H	-9.358	-3.414	-1.357

O	5.813	4.042	3.955	C	-1.705	1.236	-0.489	H	-8.685	-3.377	0.307
C	4.509	-1.966	-0.194	C	-8.463	-3.263	-0.756	H	-7.679	-3.966	-1.046
O	1.87	2.698	2.345	C	-2.069	-2.402	-1.63	H	9.471	2.742	-1.719
C	3.591	-1.876	1.072	C	-2.075	-3.523	-0.605	H	8.654	3.138	-0.17
O	-0.301	2.811	2.12	C	-3.459	-4.209	-0.594	H	7.798	3.392	-1.718
C	2.369	-0.983	0.92	C	-0.953	-4.528	-0.887	H	-1.92	-3.061	0.375
O	8.059	1.397	-1.162	C	-3.432	4.179	-2.933	H	1.87	3.102	-0.407
C	6.9	1.167	-0.536	C	-2.902	5.568	-2.596	H	-4.258	-3.51	-0.335
O	6.23	2.031	0.001	C	-2.305	6.235	-3.84	H	-3.457	-5.017	0.146
C	6.565	-0.33	-0.484	C	-4.042	6.415	-1.991	H	-3.682	-4.651	-1.572
O	7.362	-1.11	-1.356	H	-8.329	0.178	-1.643	H	-0.045	3.744	-1.928
C	5.063	-0.579	-0.72	H	-3.624	2.867	0.93	H	1.115	4.437	-3.073
O	1.382	1.675	-3.178	H	-0.724	1.522	-2.533	H	0.939	5.146	-1.456
C	4.587	-0.521	-2.216	H	-2.64	-0.568	-3.104	H	0.022	-4.036	-0.93
O	2.787	1.022	-1.524	H	-4.675	-0.452	-0.169	H	-1.117	-5.036	-1.843
C	3.069	-0.22	-2.199	H	-6.945	0.489	0.299	H	-0.928	-5.285	-0.096
O	1.546	-2.095	-2.563	H	5.255	-2.103	2.471	H	4.222	3.295	-1.192
C	2.396	-1.517	-1.601	H	3.669	-2.122	3.206	H	3.456	4.893	-1.133
O	3.606	-4.576	-3.335	H	-3.548	2.321	3.528	H	3.676	4.08	-2.691
C	3.657	-2.432	-1.429	H	-4.522	0.978	4.111	H	-2.126	5.446	-1.833
O	3.245	-3.787	-1.223	H	-1.928	7.231	-3.586	H	2.001	-5.819	-0.831
C	-3.773	2.003	-1.822	H	-3.06	6.341	-4.624	H	1.143	-6.327	-3.133
O	-3.404	3.388	-1.831	H	-1.474	5.648	-4.247	H	1.643	-7.816	-2.309
C	-2.48	1.132	-1.808	H	-5.532	2.038	2.121	H	2.688	-7.088	-3.547
O	-3.864	3.85	-4.017	H	-5.131	0.363	1.795	H	-4.445	5.958	-1.082
C	-3.078	-0.285	-2.147	H	4.979	0.361	1.99	H	-4.861	6.535	-2.71

O	-1.645	1.547	-2.866	H	4.919	0.002	3.701	H	-3.666	7.411	-1.733
C	-4.603	-0.054	-2.298	H	-3.612	-1.228	2.184	H	4.377	-6.265	-0.221
O	-2.79	-1.332	-1.201	H	3.558	1.992	1.408	H	4.642	-7.064	-1.785
C	-5.155	0.241	-0.862	H	-0.972	-0.013	4.61	H	3.534	-7.779	-0.598
O	-1.528	-2.449	-2.719	H	-2.422	0.665	5.355	H	4.567	0.227	-0.178
C	-6.665	0.004	-0.65	H	-1.359	1.701	4.391	H	8.267	-0.759	-1.323
O	-7.431	0.542	-1.712	H	1.485	0.873	4.446	H	6.784	-0.594	0.565
C	-6.96	-1.475	-0.368	H	3.156	0.793	5.023	H	3.155	-2.886	1.134
O	-6.333	-2.146	0.433	H	2.305	-0.685	4.544				
C	-2.448	1.143	0.787	H	5.137	-3.918	0.533				

Table S8. Optimized coordinates of (P)-configured **2** at B3LYP/6-31G(d) level in CH_3CN.

Atom	X	Y	Z	Atom	X	Y	Z	Atom	X	Y	Z
C	2.206	6.779	0.75	O	-8.606	0.288	0.713	H	4.778	2.906	-2.126
C	1.032	6.173	2.925	C	-2.805	1.261	1.092	H	5.076	3.822	-0.663
C	1.64	5.638	1.622	O	-1.344	-3.912	-0.939	H	-3.431	3.856	1.363
C	2.759	4.652	1.927	C	-3.945	2.016	0.325	H	-4.758	2.981	2.13
C	5.54	-3.549	2.288	O	-2.47	-3.392	0.884	H	-5.055	3.889	0.659
C	3.386	-4.264	3.454	C	-3.318	0.675	2.422	H	-5.696	-2.346	2.962
C	4.03	-3.281	2.472	C	2.636	1.039	-2.464	H	1.612	1.344	3.338
C	3.82	-1.845	2.924	O	-5.226	-3.812	4.361	H	5.872	-2.794	-2.747
C	9.279	-1.203	-1.081	C	-2.306	-0.241	3.1	H	4.356	0.5	3.333
C	1.81	0.558	1.252	C	3.12	-0.385	-2.717	H	-2.092	-4.618	3.811
C	4.999	2.575	1.772	O	-0.863	0.159	-1.821	H	2.094	-4.637	-3.837
C	6.721	0.634	2.013	C	-1.804	-1.393	2.215	H	-4.206	-5.269	5.437
C	4.132	-4.718	-4.611	C	-1.405	-0.852	0.815	H	4.185	-5.394	-5.451
C	3.124	-4.313	-3.795	C	-0.608	-1.922	0.167	H	-6.695	1.069	-3.264
C	5.038	-3.327	-3.178	C	-1.463	-3.17	0.016	H	-7.511	1.463	-1.74
C	3.713	-3.391	-2.855	C	-2.947	-2.395	1.85	H	-6.918	-0.183	-2.037
C	4.337	3.205	-1.173	C	-0.686	-2.129	2.988	H	6.798	0.83	3.089
C	1.068	-1.817	-3.09	C	-4.325	3.258	1.166	H	7.535	1.161	1.512
C	3.064	-2.665	-1.714	C	-3.6	-3.15	2.965	H	6.855	-0.443	1.865
C	1.316	-3.387	-0.142	C	-4.904	-2.978	3.336	H	-4.759	2.95	-2.875
C	0.713	-2.001	-0.169	C	-3.084	-4.189	3.822	H	-5.518	3.455	-1.353
C	1.601	-0.944	-0.723	C	-4.106	-4.547	4.642	H	4.964	2.81	2.835
C	2.176	-1.436	-2.083	C	-6.701	0.882	-2.184	H	5.666	3.279	1.274
O	0.851	0.231	1.945	C	-4.872	2.711	-1.818	H	-10.515	-0.396	0.726

O	5.308	-4.121	-4.251	C	-1.829	0.535	-1.16	H	-9.395	-1.331	1.772
C	3.911	1.983	-0.326	C	-9.52	-0.829	0.811	H	-9.334	-1.534	-0.001
O	2.338	-3.682	-0.96	C	-4.335	-1.81	-2.881	H	10.293	-0.81	-1.106
C	2.611	1.382	-0.964	C	-4.488	-3.206	-2.306	H	9.058	-1.765	-1.991
O	0.963	-4.231	0.662	C	-5.969	-3.422	-1.922	H	9.131	-1.841	-0.207
C	1.988	0.237	-0.174	C	-3.998	-4.261	-3.304	H	-3.89	-3.263	-1.393
O	8.42	-0.043	-0.995	C	-2.5	4.645	-1.783	H	3.554	-3.386	1.491
C	7.103	-0.274	-0.951	C	-1.181	5.378	-1.586	H	-6.297	-2.705	-1.164
O	6.603	-1.384	-0.978	C	-0.104	4.696	-2.457	H	-6.097	-4.431	-1.514
C	6.297	1.033	-0.966	C	-1.324	6.867	-1.913	H	-6.618	-3.327	-2.801
O	7.082	2.172	-0.67	H	-8.027	2.393	0.842	H	2.312	-4.08	3.556
C	5.069	0.94	-0.041	H	-2.064	2.035	1.346	H	3.841	-4.181	4.446
O	3.496	-1.494	4.04	H	-1.509	1.308	-3.226	H	3.524	-5.289	3.096
C	5.363	1.102	1.495	H	-4.289	0.565	-3.35	H	-2.936	-4.126	-3.533
O	4.082	-0.965	1.915	H	-4.882	0.037	0.145	H	-4.562	-4.204	-4.24
C	4.198	0.428	2.256	H	-6.122	1.354	1.872	H	-4.129	-5.262	-2.88
O	2.426	1.859	3.164	H	3.247	1.753	-3.021	H	5.973	-2.895	1.525
C	2.937	1.333	1.96	H	1.615	1.143	-2.849	H	5.689	-4.587	1.973
O	3.597	4.819	2.787	H	-1.426	0.338	3.403	H	6.083	-3.4	3.229
C	3.6	2.48	1.133	H	-2.741	-0.66	4.014	H	-0.897	5.255	-0.535
O	2.719	3.605	1.063	H	0.871	5.16	-2.274	H	0.874	5.107	1.048
C	-3.518	2.512	-1.1	H	-0.341	4.807	-3.521	H	0.599	5.364	3.525
O	-2.551	3.557	-0.97	H	-0.031	3.628	-2.233	H	0.239	6.894	2.701
C	-2.898	1.339	-1.911	H	-3.565	1.489	3.11	H	1.796	6.673	3.529
O	-3.371	4.978	-2.556	H	-4.249	0.123	2.255	H	-2.069	7.348	-1.272
C	-4.187	0.508	-2.266	H	4.135	-0.507	-2.326	H	-1.631	7.009	-2.954

O	-2.319	1.844	-3.096	H	3.185	-0.58	-3.792	H	-0.366	7.377	-1.765
C	-5.351	1.263	-1.58	H	-3.73	-1.844	1.322	H	2.621	6.398	-0.189
O	-4.134	-0.883	-1.896	H	3.853	-2.307	-1.044	H	2.997	7.316	1.284
C	-5.168	1.075	-0.036	H	-0.347	-3.044	2.497	H	1.411	7.492	0.508
O	-4.425	-1.524	-4.057	H	-1.068	-2.395	3.977	H	4.683	-0.067	-0.204
C	-6.438	1.273	0.82	H	0.176	-1.477	3.12	H	7.938	2.065	-1.116
O	-7.145	2.438	0.439	H	0.378	-2.568	-2.696	H	5.929	1.087	-2.005
C	-7.303	0.005	0.823	H	1.525	-2.211	-4.001	H	1.883	2.202	-0.857
O	-6.857	-1.116	0.991	H	0.478	-0.938	-3.352				
C	-2.008	0.239	0.271	H	3.464	3.827	-1.391				

Table S9. Optimized coordinates of compound **2′** at B3LYP/6-31G(d) level in CH_3CN.

Atom	X	Y	Z	Atom	X	Y	Z	Atom	X	Y	Z
C	-3.28	2.268	-1.879	C	5.239	-3.315	-0.707	H	-5.118	0.823	1.577
C	3.28	-2.264	-1.883	C	-4.225	-1.497	4.025	H	5.117	-0.825	1.576
O	-2.695	3.577	-1.884	C	4.224	1.49	4.029	H	-4.611	1.255	3.957
O	2.696	-3.573	-1.89	C	-3.929	-1.947	5.281	H	4.611	-1.262	3.955
C	-2.116	1.227	-1.772	C	3.928	1.937	5.286	H	-3.429	2.478	3.515
C	2.116	-1.223	-1.774	C	-5.651	-1.65	3.881	H	3.429	-2.484	3.511
O	-1.164	1.473	-2.782	C	5.65	1.642	3.886	H	-1.245	-0.194	4.654
O	1.165	-1.468	-2.784	C	-6.102	-2.168	5.054	H	1.243	0.184	4.655
C	-2.874	-0.103	-2.135	C	6.1	2.158	5.059	H	-2.662	0.607	5.338
C	2.874	0.107	-2.135	C	-5.098	-0.687	-3.244	H	2.66	-0.617	5.337
O	-1.721	-2.546	-2.564	C	5.098	0.693	-3.242	H	-1.423	1.561	4.504
O	1.721	2.551	-2.559	C	-4.08	1.704	-3.069	H	1.422	-1.57	4.502
C	-4.335	0.335	-2.406	C	4.081	-1.699	-3.072	H	-5.989	3.262	0.089
C	4.335	-0.331	-2.406	C	-1.433	1.306	-0.403	H	5.99	-3.261	0.083
O	-2.815	-1.15	-1.148	C	1.433	-1.305	-0.405	H	-5.773	3.397	-1.652
O	2.816	1.153	-1.146	C	-8.841	-2.157	-1.127	H	5.773	-3.393	-1.658
C	-4.956	0.725	-1.022	C	8.841	2.159	-1.124	H	-4.678	4.244	-0.555
C	4.957	-0.722	-1.023	C	-2.3	-2.355	-1.51	H	4.678	-4.243	-0.562
O	-6.6	-1.436	0.124	C	2.3	2.358	-1.505	H	-6.111	-0.348	-3.479
O	6.601	1.436	0.127	C	-2.605	-3.417	-0.469	H	6.111	0.355	-3.478
C	-6.498	0.719	-0.988	C	2.605	3.417	-0.462	H	-5.176	-1.65	-2.728
C	6.498	-0.717	-0.989	C	-4.014	-3.99	-0.744	H	5.177	1.655	-2.725
O	-8.179	-0.902	-1.397	C	4.014	3.992	-0.736	H	-4.579	-0.86	-4.194
O	8.18	0.905	-1.396	C	-1.539	-4.516	-0.46	H	4.579	0.868	-4.192

C	-7.065	-0.657	-0.691	C	1.538	4.517	-0.45	H	-3.488	1.634	-3.982
C	7.065	0.658	-0.69	C	-2.652	4.383	-2.974	H	3.489	-1.627	-3.985
O	-0.216	1.457	-0.388	C	2.654	-4.378	-2.981	H	-4.996	2.253	-3.293
O	0.216	-1.456	-0.391	C	-1.776	5.602	-2.721	H	4.996	-2.247	-3.296
C	-2.274	1.282	0.815	C	1.778	-5.597	-2.73	H	-9.718	-2.166	-1.773
C	2.273	-1.283	0.813	C	-0.541	5.52	-3.639	H	9.718	2.169	-1.77
O	-0.153	-2.552	2.357	C	0.542	-5.512	-3.648	H	-9.136	-2.212	-0.077
O	0.152	2.547	2.362	C	-2.583	6.887	-2.973	H	9.137	2.213	-0.074
C	-3.572	2.097	0.728	C	2.583	-6.882	-2.986	H	-8.18	-2.993	-1.366
C	3.572	-2.098	0.725	H	-0.316	1.681	-2.337	H	8.18	2.995	-1.362
O	-2.202	-1.926	2.839	H	0.316	-1.677	-2.34	H	-4.238	-4.771	-0.009
O	2.201	1.92	2.844	H	-2.405	-0.472	-3.048	H	4.237	4.771	0.001
C	-4.271	2.111	-0.675	H	2.406	0.478	-3.047	H	-4.063	-4.441	-1.742
C	4.271	-2.11	-0.678	H	-4.642	-0.022	-0.291	H	4.062	4.445	-1.732
O	-5.059	-2.359	5.918	H	4.642	0.022	-0.29	H	-4.787	-3.22	-0.665
O	5.058	2.348	5.924	H	-3.248	3.135	0.908	H	4.787	3.222	-0.659
C	-4.566	1.729	1.847	H	3.248	-3.136	0.903	H	-0.547	-4.102	-0.261
C	4.566	-1.732	1.845	H	-3.834	-0.994	2.014	H	0.547	4.101	-0.252
O	-3.234	4.174	-4.017	H	3.833	0.99	2.017	H	-1.51	-5.041	-1.419
O	3.238	-4.168	-4.023	H	-3.01	-2.061	5.834	H	1.509	5.044	-1.408
C	-3.876	1.529	3.192	H	3.008	2.05	5.838	H	-1.771	-5.246	0.324
C	3.875	-1.535	3.19	H	-6.238	-1.419	3.002	H	1.77	5.244	0.335
C	-2.753	0.479	3.171	H	6.237	1.413	3.006	H	0.047	4.617	-3.441
C	2.752	-0.485	3.171	H	-7.075	-2.453	5.421	H	-0.044	-4.61	-3.448
C	-1.852	0.658	1.95	H	7.074	2.443	5.428	H	0.102	6.391	-3.474
C	1.851	-0.662	1.949	H	-2.628	-2.923	0.506	H	-0.102	-6.383	-3.485

C	-0.65	-0.206	2.029	H	2.628	2.921	0.512	H	-0.847	5.513	-4.691
C	0.65	0.202	2.03	H	-1.448	5.576	-1.677	H	0.848	-5.503	-4.7
C	-0.956	-1.643	2.377	H	1.45	-5.573	-1.687	H	-1.946	7.764	-2.817
C	0.955	1.639	2.381	H	-6.856	1.347	-0.165	H	1.946	-7.759	-2.832
C	-3.303	-0.967	2.969	H	6.856	-1.346	-0.166	H	-3.439	6.964	-2.294
C	3.301	0.961	2.972	H	-6.951	1.119	-1.898	H	3.44	-6.961	-2.307
C	-1.966	0.612	4.494	H	6.951	-1.115	-1.899	H	-2.957	6.909	-4.001
C	1.965	-0.621	4.493	H	-5.311	2.523	1.956	H	2.957	-6.902	-4.014
C	-5.239	3.317	-0.702	H	5.311	-2.526	1.952				

Table S10. Optimized coordinates of (P)-configured **2′** at B3LYP/6-31G(d) level in CH_3CN.

Atom	X	Y	Z	Atom	X	Y	Z	Atom	X	Y	Z
C	3.766	2.545	1.017	C	0.448	4.846	2.308	H	-0.119	-2.685	2.582
O	2.883	3.661	0.886	C	1.8	6.983	1.991	H	-0.829	-2.055	4.076
C	3.058	1.427	1.84	C	-5.273	0.958	0.044	H	0.267	-1.048	3.117
O	2.511	1.982	3.017	C	-6.56	1.047	0.888	H	-4.999	2.909	2.23
C	4.278	0.511	2.216	C	-7.279	-0.286	0.981	H	-5.473	3.737	0.756
O	4.702	-1.463	4.016	C	-2.107	0.371	0.347	H	-3.835	3.928	1.386
C	5.49	1.151	1.496	C	-2.945	1.361	1.171	H	-7.67	1.206	-1.624
O	4.088	-0.882	1.907	C	-4.145	2.01	0.405	H	-6.971	-0.394	-1.919
C	5.273	0.958	-0.044	C	-3.398	0.763	2.515	H	-6.853	0.867	-3.153
O	6.723	-1.359	-1.15	C	-2.298	-0.049	3.186	H	-5.055	2.898	-2.778
C	6.56	1.046	-0.888	C	-1.752	-1.198	2.323	H	-5.834	3.331	-1.25
O	8.611	-0.148	-0.909	C	-1.459	-0.698	0.883	H	-10.428	-1.043	0.986
C	7.279	-0.286	-0.981	C	-0.642	-1.753	0.226	H	-9.189	-1.815	2.029
O	0.895	0.513	1.701	C	-1.385	-3.078	0.224	H	-9.143	-2.063	0.263
C	2.107	0.371	-0.347	C	-2.823	-2.31	2.088	H	-5.513	-4.609	-1.283
O	1.244	-3.891	0.67	C	-0.528	-1.791	3.058	H	-6.432	-3.555	-2.373
C	2.946	1.361	-1.171	C	-4.647	3.211	1.242	H	-5.804	-2.917	-0.836
O	2.31	-3.328	-1.17	C	-3.349	-3.024	3.297	H	-3.008	-3.916	-4.025
C	4.146	2.01	-0.405	C	-2.751	-3.989	4.058	H	-4.743	-4.149	-4.296
O	3.587	-4.398	-5.051	C	-4.658	-2.832	3.868	H	-3.873	-5.196	-3.155
C	3.398	0.763	-2.515	C	-4.744	-3.681	4.925	H	-0.318	3.808	-1.985
O	3.748	4.976	2.537	C	-6.822	0.681	-2.074	H	0.488	5.386	-2.131
C	2.298	-0.049	-3.186	C	-5.136	2.638	-1.723	H	-0.644	4.847	-3.386
O	-2.883	3.661	-0.886	C	-1.931	0.722	-1.074	H	-0.877	7.552	-1.839

C	1.752	-1.198	-2.323	C	-9.387	-1.355	1.058	H	-2.6	7.471	-1.425
O	-2.511	1.982	-3.017	C	-4.374	-1.785	-2.893	H	-2.062	7.029	-3.053
C	1.459	-0.698	-0.884	C	-4.271	-3.212	-2.387	H	6.31	1.297	-1.925
O	-4.704	-1.463	-4.016	C	-5.589	-3.589	-1.673	H	7.249	1.821	-0.543
C	0.642	-1.753	-0.226	C	-3.954	-4.173	-3.538	H	3.697	1.566	-3.194
O	-4.088	-0.882	-1.907	C	-2.873	4.719	-1.739	H	4.284	0.136	-2.368
C	1.385	-3.078	-0.224	C	-1.601	5.532	-1.543	H	2.659	-0.459	-4.136
O	-6.723	-1.358	1.15	C	-0.448	4.846	-2.307	H	1.454	0.607	-3.426
C	2.823	-2.31	-2.088	C	-1.8	6.983	-1.991	H	0.119	-2.684	-2.582
O	-8.611	-0.147	0.908	H	1.623	1.575	3.097	H	0.829	-2.055	-4.076
C	0.528	-1.79	-3.058	H	4.399	0.602	3.295	H	-0.267	-1.048	-3.117
O	-0.894	0.513	-1.701	H	-1.623	1.576	-3.097	H	4.999	2.908	-2.23
C	4.648	3.211	-1.242	H	4.88	-0.049	-0.206	H	5.473	3.737	-0.756
O	-1.244	-3.891	-0.67	H	-4.399	0.602	-3.295	H	3.835	3.928	-1.386
C	3.349	-3.024	-3.297	H	-4.88	-0.049	0.207	H	7.67	1.205	1.624
O	-2.31	-3.328	1.169	H	2.255	2.188	-1.398	H	6.971	-0.394	1.919
C	2.751	-3.989	-4.058	H	-2.254	2.188	1.398	H	6.853	0.867	3.153
O	-3.587	-4.398	5.05	H	-3.678	-1.865	1.57	H	5.056	2.898	2.778
C	4.658	-2.831	-3.868	H	-1.797	-4.489	4.011	H	5.834	3.331	1.25
O	-3.748	4.976	-2.537	H	-5.428	-2.164	3.504	H	10.427	-1.044	-0.987
C	4.744	-3.681	-4.925	H	-5.514	-3.9	5.649	H	9.189	-1.816	-2.03
C	-3.766	2.545	-1.017	H	3.678	-1.865	-1.57	H	9.143	-2.064	-0.263
C	-3.058	1.427	-1.84	H	-3.462	-3.247	-1.652	H	5.512	-4.609	1.284
C	-4.278	0.511	-2.216	H	1.796	-4.489	-4.012	H	6.431	-3.554	2.373
C	-5.49	1.151	-1.496	H	5.428	-2.164	-3.504	H	5.803	-2.917	0.837
C	6.822	0.681	2.074	H	5.513	-3.899	-5.65	H	3.008	-3.916	4.026

C	5.136	2.638	1.723	H	-1.362	5.504	-0.474	H	4.743	-4.149	4.297
C	1.931	0.722	1.074	H	-6.31	1.297	1.925	H	3.873	-5.196	3.156
C	9.386	-1.356	-1.059	H	-7.249	1.821	0.543	H	0.318	3.809	1.985
C	4.374	-1.785	2.893	H	-3.697	1.566	3.194	H	-0.488	5.386	2.131
C	4.271	-3.212	2.388	H	-4.284	0.136	2.368	H	0.644	4.848	3.386
C	5.588	-3.589	1.673	H	-2.659	-0.459	4.136	H	0.877	7.552	1.838
C	3.954	-4.173	3.539	H	3.462	-3.248	1.653	H	2.6	7.471	1.424
C	2.873	4.719	1.739	H	-1.453	0.607	3.426	H	2.062	7.03	3.052
C	1.601	5.532	1.543	H	1.362	5.504	0.473				

Table S11. Optimized coordinates of compound ***4′*** at B3LYP/6-31G(d) level in CH_3CN.

Atom	X	Y	Z	Atom	X	Y	Z	Atom	X	Y	Z
C	4.68	1.333	-0.241	C	3.172	-2.175	4.883	H	-1.026	2.683	-3.931
C	3.398	1.332	0.65	O	4.509	2.053	-1.479	H	-2.216	3.924	-3.508
C	3.998	0.9	2.04	O	2.818	2.63	0.752	H	-2.675	2.214	-3.551
C	5.484	0.604	1.746	O	2.282	1.035	4.161	H	-6.217	1.412	-1.797
C	5.516	-0.674	0.832	O	3.36	-0.244	2.633	H	-6.744	-0.261	-1.571
C	2.49	-0.53	-0.81	O	1.143	0.706	0.777	H	-5.358	0.103	-2.606
C	3.897	-0.911	-1.27	O	-1.7	-1.176	-3.245	H	-0.076	5.779	0.473
C	5.074	-0.135	-0.597	O	-0.749	-2.918	-2.281	H	-0.145	5.378	-3.85
C	4.108	-2.463	-1.215	O	0.324	-7.136	-1.207	H	-0.102	7.988	-2.989
C	2.813	-3.251	-0.977	O	4.625	4.158	-0.636	H	-6.088	-1.8	3.508
C	1.658	-2.726	-1.842	O	-4.288	-2.004	-1.482	H	-7.302	-0.699	2.852
C	1.406	-1.252	-1.484	O	-2.926	-2.758	0.757	H	-5.928	-0.054	3.766
C	0.211	-0.71	-1.878	O	-1.047	-0.835	0.612	H	-6.704	-1.717	0.269
C	-0.804	-1.58	-2.521	O	1.72	1.188	-3.349	H	-5.525	-2.809	1.022
C	0.342	-3.457	-1.478	O	0.869	2.937	-2.315	H	-3.583	-2.898	-3.563
C	2	-2.876	-3.345	O	-0.094	7.149	-1.088	H	-3.492	-4.919	-2.101
C	6.233	-0.134	-1.622	O	-6.367	-2.841	-1.901	H	-3.685	-5.393	-3.795
C	0.309	-4.942	-1.677	H	3.888	1.745	2.721	H	-5.082	-5.441	-2.7
C	0.376	-5.878	-0.687	H	4.767	-1.374	1.204	H	-5.645	-2.367	-4.9
C	0.193	-5.685	-2.908	H	6.938	-2.092	-0.008	H	-6.376	-3.901	-4.393
C	0.207	-6.999	-2.562	H	7.725	-0.76	0.805	H	-4.937	-3.902	-5.433
C	6.328	0.578	3.017	H	3.936	-0.626	-2.329	H	3.51	3.292	0.553
C	5.78	1.752	0.755	H	4.805	-2.733	-0.418	H	0.407	0.09	0.537
C	2.294	0.424	0.144	H	4.573	-2.793	-2.149	H	-2.775	-3.102	-0.141

C	2.535	-0.058	3.694	H	2.984	-4.313	-1.183	H	2.775	-3.084	5.349
C	2.018	-1.379	4.241	H	2.528	-3.176	0.081	H	3.675	-1.591	5.662
C	1.287	-2.207	3.171	H	0.117	-3.234	-0.428	H	3.915	-2.467	4.135
C	4.553	3.393	-1.586	H	2.821	-2.212	-3.628	C	6.861	-1.426	0.86
C	4.52	3.82	-3.044	H	1.148	-2.629	-3.984	C	7.003	-2.338	2.064
C	3.979	5.246	-3.186	H	2.307	-3.904	-3.566	H	-7.07	1.888	0.067
C	5.932	3.679	-3.652	H	5.933	0.407	-2.523	H	-7.731	0.395	0.696
C	-4.595	-1.299	-0.27	H	6.484	-1.155	-1.923	C	8.541	-3.311	3.574
C	-3.338	-1.408	0.62	H	7.147	0.33	-1.241	C	-7.355	1.943	2.134
C	-3.897	-0.965	2.012	H	0.46	-5.811	0.388	O	6.098	-2.97	2.576
C	-5.41	-0.722	1.76	H	0.094	-5.283	-3.906	O	8.281	-2.411	2.477
C	-5.544	0.611	0.941	H	0.142	-7.919	-3.123	H	9.613	-3.243	3.758
C	-2.388	0.575	-0.763	H	5.989	-0.208	3.7	H	8.262	-4.332	3.305
C	-3.674	1.063	-0.784	H	6.244	1.536	3.543	H	7.98	-3.001	4.459
C	-4.909	0.221	-0.476	H	7.389	0.412	2.805	C	-2.548	0.125	3.693
C	-3.915	2.514	-1.107	H	5.632	2.74	1.195	O	-2.259	-0.93	4.216
C	-2.646	3.347	-0.921	H	6.785	1.714	0.329	O	-3.276	0.215	2.541
C	-1.507	2.778	-1.78	H	1.304	-1.101	5.023	C	-6.978	1.164	0.885
C	-1.278	1.3	-1.425	H	0.893	-3.123	3.624	C	-2.223	1.512	4.223
C	-0.112	0.735	-1.861	H	1.969	-2.492	2.364	H	-1.917	2.117	3.361
C	0.893	1.604	-2.558	H	0.447	-1.657	2.735	C	-9.154	2.599	3.521
C	-0.168	3.483	-1.451	H	3.85	3.117	-3.552	O	-6.59	2.619	2.796
C	-1.875	2.909	-3.282	H	3.954	5.528	-4.244	O	-8.669	1.837	2.395
C	-5.871	0.384	-1.681	H	4.616	5.961	-2.655	H	-10.223	2.394	3.57
C	-0.134	4.97	-1.621	H	2.964	5.328	-2.787	H	-8.974	3.665	3.364
C	-0.1	5.877	-0.602	H	6.307	2.654	-3.571	H	-8.659	2.276	4.439

C	-0.14	5.749	-2.835	H	6.641	4.347	-3.15	H	-3.278	3.148	5.182
C	-0.114	7.052	-2.452	H	5.903	3.95	-4.712	H	-3.869	1.549	5.663
C	-6.231	-0.818	3.043	H	-3.732	-1.79	2.707	H	-4.304	2.218	4.074
C	-5.699	-1.786	0.682	H	-4.934	1.382	1.412	H	-0.918	2.472	5.652
C	-2.151	-0.566	0.133	H	-4.303	2.626	-2.127	H	-0.154	1.111	4.82
C	-5.193	-2.742	-2.187	H	-4.71	2.888	-0.452	H	-1.357	0.81	6.09
C	-4.515	-3.434	-3.36	H	-2.359	3.338	0.138	C	-3.504	2.141	4.815
C	-4.174	-4.884	-2.957	H	-2.838	4.388	-1.198	C	-1.092	1.466	5.254
C	-5.426	-3.396	-4.595	H	0.105	3.235	-0.419				

Table S12. Optimized coordinates of (P)-configured **4′** at B3LYP/6-31G(d) level in CH_3CN.

Atom	X	Y	Z	Atom	X	Y	Z	Atom	X	Y	Z
C	2.819	2.069	1.718	C	-2.785	0.785	0.509	H	5.595	-4.311	0.218
O	1.523	2.683	1.908	C	-3.409	1.889	-0.339	H	4.875	-2.712	-0.046
C	2.902	0.591	2.218	C	-3.107	0.846	1.98	H	4.189	-3.805	1.173
O	2.238	0.408	3.462	C	-3.29	-0.568	2.534	H	-0.62	3.797	2.063
C	4.463	0.432	2.394	C	-1.998	-1.379	2.38	H	-1.771	4.836	4.028
O	5.293	-1.762	3.773	C	-1.451	-1.282	0.934	H	-0.352	4.514	5.044
C	5.057	1.726	1.805	C	-0.439	-2.149	0.639	H	-1.307	3.166	4.405
O	5.032	-0.728	1.77	C	-0.155	-3.286	1.567	H	1.099	5.562	1.675
C	4.73	1.745	0.266	C	-2.296	-2.88	2.612	H	1.099	5.956	3.408
O	2.249	-1.628	1.91	C	-0.939	-0.839	3.372	H	-0.353	6.247	2.43
C	1.968	-0.196	-0.02	C	-2.995	3.251	0.264	H	-4.781	-0.206	-3.356
O	-0.621	-4.215	-1.182	C	-2.886	-3.25	3.939	H	-5.241	0.725	0.143
C	2.312	1.149	-0.667	C	-4.188	-3.595	4.159	H	-2.32	1.378	2.529
O	1.169	-3.688	-2.35	C	-2.239	-3.329	5.225	H	-4.021	1.424	2.137
C	3.181	2.119	0.201	C	-3.198	-3.704	6.111	H	-4.116	-1.054	1.998
O	4.558	-3.876	-5.282	C	-6.684	1.434	-2.404	H	-3.573	-0.524	3.59
C	2.958	0.948	-2.082	C	-4.268	2.41	-2.57	H	-2.974	-3.213	1.817
O	1.695	3.001	4.153	C	-2.191	-0.554	-1.421	H	-0.026	-1.437	3.375
C	3.277	-0.513	-2.403	C	-1.535	3.666	-2.654	H	-1.348	-0.814	4.386
O	-1.718	2.427	-2.122	C	-0.115	3.817	-3.175	H	-0.629	0.173	3.104
C	2.012	-1.379	-2.31	C	-0.067	3.251	-4.612	H	-3.312	3.364	1.302
O	-2.474	0.321	-3.628	C	0.342	5.277	-3.119	H	-3.415	4.077	-0.313
C	1.414	-1.257	-0.891	C	7.391	-2.375	1.117	H	-1.906	3.345	0.236
O	-1.805	-1.584	-1.965	C	5.668	2.669	-0.535	H	-5.047	-3.69	3.511

C	0.453	-2.174	-0.557	C	6.998	2.016	-0.869	H	-1.196	-3.15	5.444
O	0.881	-3.939	1.503	C	9.275	2.434	-1.354	H	-3.199	-3.898	7.173
C	0.27	-3.406	-1.375	C	-7.259	2.272	0.549	H	-6.733	1.287	-3.489
O	-1.067	-3.65	2.482	C	-5.041	-2.254	-2.026	H	-7.159	2.395	-2.182
C	2.366	-2.873	-2.488	C	-5.865	2.753	0.183	H	-7.275	0.643	-1.929
O	-4.399	-3.866	5.476	C	-5.427	-3.298	-0.994	H	-4.512	3.441	-2.322
C	0.987	-0.924	-3.378	C	-9.514	2.934	0.812	H	-4.194	2.321	-3.658
O	-2.395	4.518	-2.732	C	-6.911	-3.671	-1.184	H	0.533	3.201	-2.543
C	2.925	3.541	-0.35	C	-4.511	-4.526	-1.127	H	-0.42	2.216	-4.643
O	7.169	0.828	-1.071	H	4.659	0.37	3.465	H	0.961	3.281	-4.988
C	2.995	-3.265	-3.792	H	4.877	0.738	-0.13	H	-0.693	3.85	-5.282
O	7.977	2.932	-0.968	H	5.228	2.925	-1.506	H	0.333	5.661	-2.093
C	4.313	-3.565	-3.978	H	5.853	3.624	-0.037	H	-0.314	5.912	-3.723
O	-4.88	-2.47	-3.21	H	1.355	1.668	-0.818	H	1.362	5.366	-3.507
C	2.375	-3.416	-5.085	H	3.88	1.525	-2.167	H	2.248	1.262	3.939
O	-4.912	-1.018	-1.466	H	2.293	1.349	-2.853	H	1.971	-2.364	1.324
C	3.364	-3.784	-5.941	H	3.701	-0.587	-3.41	H	-2.183	-0.608	-3.72
O	-7.533	1.154	0.943	H	4.041	-0.89	-1.71	H	7.883	-3.205	0.599
C	6.513	1.924	2.217	H	3.046	-3.156	-1.674	H	8.086	-1.989	1.871
O	-8.162	3.26	0.425	H	-5.3	-2.85	-0.004	H	7.197	-1.58	0.39
C	4.044	2.734	2.382	H	0.535	0.036	-3.117	H	-5.436	3.118	1.125
C	2.313	-0.439	1.272	H	0.172	-1.641	-3.479	H	-5.943	3.627	-0.469
C	5.427	-1.757	2.566	H	1.479	-0.816	-4.35	H	9.923	3.309	-1.392
C	6.082	-2.869	1.762	H	1.878	3.816	-0.2	H	9.222	1.952	-2.333
C	5.121	-3.458	0.715	H	3.125	3.586	-1.424	H	9.641	1.718	-0.615
C	1.14	3.218	3.086	H	3.543	4.307	0.127	H	-10.091	3.843	0.644

C	-0.042	4.155	2.92	H	5.164	-3.602	-3.314	H	-9.549	2.646	1.865
C	-0.92	4.165	4.176	H	1.331	-3.282	-5.328	H	-9.897	2.117	0.197
C	0.49	5.566	2.584	H	3.391	-4.015	-6.995	H	-7.201	-4.425	-0.444
C	-3.012	1.87	-1.857	H	7.143	1.114	1.836	H	-7.078	-4.087	-2.183
C	-2.993	0.402	-2.315	H	6.595	1.925	3.31	H	-7.563	-2.8	-1.058
C	-4.535	0.067	-2.329	H	6.922	2.873	1.859	H	-4.783	-5.275	-0.377
C	-5.233	1.389	-1.933	H	4.021	2.729	3.472	H	-3.457	-4.261	-0.984
C	-4.991	1.634	-0.408	H	4.203	3.762	2.049	H	-4.617	-4.977	-2.119
C	-2.062	-0.277	0.023	H	6.32	-3.643	2.499				

Table S13. Optimized coordinates of compound **5a** at B3LYP/6-31G(d) level in CH_3CN.

Atom	X	Y	Z	Atom	X	Y	Z	Atom	X	Y	Z
C	4.74	1.337	-0.17	C	-2.247	-0.473	0.099	H	3.635	3.27	-3.253
C	3.486	1.271	0.748	C	-6.165	3.855	3.538	H	3.32	5.024	-1.515
C	4.087	0.792	2.106	C	-5.183	-3.098	-2.003	H	3.493	5.769	-3.109
C	5.574	0.538	1.777	C	-4.509	-3.834	-3.155	H	4.859	5.784	-1.976
C	5.611	-0.695	0.799	C	-4.5	-2.93	-4.406	H	6.325	4.649	-3.853
C	6.96	-1.452	0.748	C	-5.207	-5.172	-3.421	H	4.903	4.672	-4.917
C	7.203	-2.371	1.951	C	-2.38	-0.055	3.597	H	5.753	3.148	-4.603
C	2.51	-0.495	-0.782	C	-1.807	1.25	4.135	H	3.054	-2.065	4.406
C	3.908	-0.886	-1.256	C	-1.984	2.457	3.209	H	0.392	-1.987	2.877
C	5.113	-0.116	-0.606	C	-2.405	1.506	5.535	H	1.121	-3.423	3.62
C	4.093	-2.442	-1.222	O	4.376	2.199	-1.262	H	1.936	-2.621	2.265
C	2.785	-3.207	-0.97	O	6.406	3.184	-1.583	H	1.818	-0.699	6.166
C	1.626	-2.665	-1.822	O	2.961	2.586	0.987	H	1.188	-2.346	5.976
C	1.397	-1.185	-1.464	O	3.494	-0.386	2.672	H	0.308	-0.983	5.271
C	0.214	-0.626	-1.857	O	1.916	0.83	3.746	H	-3.767	-1.863	2.663
C	-0.786	-1.495	-2.548	O	8.078	-0.594	0.612	H	-4.734	1.274	1.194
C	0.299	-3.37	-1.441	O	8.27	-2.395	2.54	H	-6.83	2.048	0.067
C	1.954	-2.832	-3.326	O	6.17	-3.169	2.22	H	-3.886	0.593	-2.337
C	6.223	-0.085	-1.68	O	-1.598	-1.094	-3.362	H	-4.551	2.747	-2.159
C	0.241	-4.857	-1.616	O	-0.781	-2.824	-2.256	H	-4.846	2.661	-0.441
C	0.292	-5.777	-0.61	O	0.218	-7.042	-1.108	H	-3.05	4.296	-1.097
C	0.111	-5.619	-2.834	O	1.157	0.739	0.75	H	-2.595	3.139	0.15
C	0.103	-6.926	-2.466	O	-4.325	-2.204	-1.443	H	-0.185	3.314	-0.289
C	6.421	0.47	3.045	O	-6.331	-3.263	-1.651	H	-2.306	3.962	-3.473

C	5.842	1.727	0.829	O	-2.838	-2.727	0.701	H	-2.751	2.253	-3.586
C	2.363	0.434	0.183	O	-3.254	0.133	2.581	H	-1.088	2.742	-3.887
C	6.362	-4.129	3.287	O	-2.111	-1.148	4.06	H	-6.465	1.102	-1.91
C	5.236	3.061	-1.874	O	-7.949	0.453	0.741	H	-7.086	-0.427	-1.288
C	4.509	3.855	-2.949	O	-8.073	2.136	2.775	H	-5.867	-0.412	-2.576
C	4.017	5.188	-2.344	O	-5.996	2.953	2.419	H	-0.641	5.86	0.555
C	5.431	4.093	-4.152	O	1.766	1.394	-3.149	H	-0.131	5.417	-3.734
C	2.458	-0.239	3.541	O	0.754	3.06	-2.118	H	-0.298	8.036	-2.911
C	2.101	-1.57	4.181	O	-0.507	7.214	-1.014	H	-7.262	-0.597	2.851
C	1.34	-2.451	3.166	O	-1.088	-0.778	0.72	H	-5.856	0.061	3.713
C	1.306	-1.379	5.476	H	3.978	1.61	2.82	H	-6.059	-1.687	3.556
C	-4.635	-1.404	-0.286	H	4.886	-1.428	1.154	H	-5.487	-2.858	1.132
C	-3.342	-1.398	0.59	H	6.921	-2.142	-0.11	H	-6.715	-1.829	0.359
C	-3.9	-1.01	1.995	H	3.924	-0.594	-2.314	H	-7.022	4.509	3.365
C	-5.394	-0.73	1.738	H	4.536	-2.77	-2.168	H	-5.243	4.431	3.586
C	-5.474	0.558	0.832	H	4.796	-2.739	-0.442	H	-6.313	3.286	4.459
C	-6.828	1.308	0.883	H	2.935	-4.271	-1.179	H	-3.467	-4.011	-2.865
C	-7.029	2.155	2.145	H	2.515	-3.13	0.091	H	-4.056	-3.474	-5.247
C	-2.447	0.517	-0.812	H	0.078	-3.124	-0.396	H	-3.907	-2.028	-4.233
C	-3.863	0.87	-1.275	H	1.109	-2.562	-3.965	H	-5.52	-2.644	-4.69
C	-5.037	0.06	-0.623	H	2.227	-3.87	-3.543	H	-5.197	-5.814	-2.534
C	-4.113	2.416	-1.212	H	2.794	-2.196	-3.617	H	-4.697	-5.701	-4.233
C	-2.852	3.235	-0.913	H	5.869	0.448	-2.567	H	-6.25	-5.016	-3.714
C	-1.657	2.77	-1.758	H	6.473	-1.102	-2	H	-0.735	1.053	4.258
C	-1.363	1.297	-1.433	H	7.14	0.389	-1.331	H	-1.548	2.27	2.223
C	-0.14	0.807	-1.816	H	0.376	-5.693	0.464	H	-1.483	3.329	3.643

C	0.858	1.735	-2.411	H	0.018	-5.232	-3.838	H	-3.041	2.704	3.069
C	-0.38	3.542	-1.344	H	0.021	-7.855	-3.011	H	-1.929	2.381	5.988
C	-1.966	2.942	-3.266	H	7.48	0.353	2.814	H	-2.248	0.647	6.194
C	-6.19	0.074	-1.651	H	6.108	-0.361	3.688	H	-3.482	1.701	5.471
C	-0.398	5.031	-1.518	H	6.298	1.394	3.621	H	2.877	3.01	0.111
C	-0.528	5.947	-0.515	H	5.657	2.699	1.297	H	8.766	-0.963	1.2
C	-0.273	5.798	-2.733	H	6.845	1.712	0.413	H	1.284	1.559	1.274
C	-0.346	7.105	-2.367	H	7.195	-4.793	3.047	H	-2.671	-3.03	-0.21
C	-6.196	-0.731	3.036	H	5.428	-4.685	3.344	H	-8.613	0.783	1.377
C	-5.696	-1.862	0.732	H	6.561	-3.609	4.226	H	-0.382	-0.119	0.544

Table S14. Optimized coordinates of compound **5b** at B3LYP/6-31G(d) level in CH_3CN.

Atom	X	Y	Z	Atom	X	Y	Z	Atom	X	Y	Z
C	2.912	2.075	1.664	C	-8.295	0.49	1.867	H	8.095	-0.88	-2.026
C	2.956	0.611	2.201	C	-5.324	-2.18	-2.098	H	8.851	0.693	-2.442
C	4.513	0.402	2.342	C	-5.842	-3.175	-1.071	H	7.666	-3.292	2.608
C	5.143	1.685	1.762	C	-7.24	-2.743	-0.579	H	7.654	-3.942	0.956
C	4.829	1.707	0.223	C	-5.844	-4.597	-1.638	H	7.785	-2.193	1.218
C	5.775	2.607	-0.611	C	-1.333	3.014	-3.402	H	4.022	-4.25	1.97
C	7.154	1.986	-0.87	C	0.093	3.548	-3.356	H	5.437	-5.153	1.396
C	2.019	-0.216	-0.012	C	0.054	5.025	-2.911	H	5.392	-4.532	3.059
C	2.399	1.1	-0.696	C	0.767	3.393	-4.725	H	-0.529	3.834	1.944
C	3.279	2.087	0.145	O	1.625	2.718	1.825	H	1.206	5.551	1.431
C	3.032	0.838	-2.106	O	1.778	3.104	4.06	H	-0.23	6.297	2.158
C	3.328	-0.638	-2.378	O	2.316	0.483	3.464	H	1.229	6.051	3.136
C	2.048	-1.48	-2.256	O	5.004	-0.769	1.67	H	-0.218	4.726	4.874
C	1.449	-1.284	-0.849	O	5.299	-1.873	3.632	H	-1.646	5.001	3.855
C	0.457	-2.16	-0.496	O	5.966	3.892	-0.048	H	-1.193	3.352	4.327
C	0.228	-3.372	-1.318	O	8.182	2.629	-0.744	H	-2.358	-0.85	-3.682
C	2.381	-2.992	-2.356	O	7.093	0.731	-1.311	H	-6.88	4.133	-0.328
C	1.029	-1.069	-3.346	O	-0.79	-4.054	-1.213	H	-1.898	-2.524	-1.223
C	3.028	3.493	-0.445	O	1.162	-3.774	-2.195	H	-4.818	-0.15	-3.384
C	3	-3.45	-3.644	O	3.253	-4.288	-5.707	H	-4.967	0.745	0.112
C	2.359	-3.98	-4.726	O	2.223	-1.593	1.965	H	-5.264	2.967	1.246
C	4.399	-3.435	-3.986	O	-1.643	2.367	-2.249	H	-1.437	1.715	0.598
C	4.491	-3.948	-5.241	O	-2.09	3.199	-4.331	H	-3.941	1.652	1.993
C	6.601	1.828	2.194	O	-2.419	0.113	-3.559	H	-2.34	1.577	2.662

C	4.149	2.72	2.326	O	-5.049	-0.983	-1.514	H	-3.7	-0.331	3.421
C	2.33	-0.429	1.295	O	-5.188	-2.395	-3.285	H	-4.049	-0.799	1.758
C	8.354	0.113	-1.663	O	-5.941	3.896	-0.461	H	-3.01	-3.031	1.878
C	5.332	-1.854	2.419	O	-8.136	2.792	0.507	H	-1.431	-0.501	4.367
C	5.778	-3.015	1.546	O	-7.046	0.995	1.337	H	-0.104	-1.285	3.482
C	5.114	-4.316	2.023	O	-1.124	-3.478	2.597	H	-0.584	0.336	3.055
C	1.236	3.295	2.982	O	0.796	-3.914	1.606	H	-3.605	4.225	-0.621
C	0.065	4.236	2.772	O	-4.519	-3.489	5.53	H	-3.18	3.683	0.999
C	0.608	5.618	2.345	O	-2.219	-1.818	-1.828	H	-1.937	3.748	-0.252
C	-0.799	4.331	4.034	H	2.324	1.36	3.9	H	-5.124	-3.384	3.546
C	-2.945	1.832	-1.965	H	6.913	4.098	-0.179	H	-1.302	-2.841	5.534
C	-3.012	0.314	-2.28	H	1.937	-2.341	1.4	H	-3.354	-3.471	7.251
C	-4.568	0.083	-2.348	H	4.735	0.307	3.406	H	-7.254	0.772	-1.836
C	-5.182	1.439	-1.941	H	4.968	0.699	-0.172	H	-7.067	2.513	-2.136
C	-4.828	1.681	-0.432	H	5.343	2.714	-1.618	H	-6.746	1.347	-3.428
C	-5.738	2.71	0.286	H	1.453	1.632	-0.862	H	-4.394	3.427	-2.489
C	-7.11	2.161	0.695	H	3.961	1.398	-2.219	H	-4.184	2.198	-3.754
C	-2.01	-0.223	-0.006	H	2.368	1.221	-2.886	H	-8.711	1.202	2.583
C	-2.387	1.171	0.507	H	3.751	-0.75	-3.381	H	-9.007	0.322	1.056
C	-3.273	2.046	-0.449	H	4.081	-1.005	-1.668	H	-8.041	-0.447	2.358
C	-3.007	1.09	1.945	H	3.046	-3.252	-1.522	H	-5.156	-3.122	-0.216
C	-3.289	-0.342	2.406	H	1.515	-1.039	-4.326	H	-7.962	-2.746	-1.404
C	-2.008	-1.189	2.377	H	0.192	-1.768	-3.404	H	-7.596	-3.442	0.184
C	-1.423	-1.176	0.951	H	0.6	-0.085	-3.143	H	-7.216	-1.74	-0.145
C	-0.436	-2.091	0.699	H	3.631	4.267	0.03	H	-4.843	-4.898	-1.964
C	-0.204	-3.202	1.657	H	3.262	3.511	-1.513	H	-6.183	-5.303	-0.873

C	-2.341	-2.673	2.67	H	1.973	3.758	-0.337	H	-6.516	-4.673	-2.499
C	-0.972	-0.631	3.381	H	1.327	-4.213	-4.933	H	0.644	2.975	-2.604
C	-2.989	3.516	-0.066	H	5.219	-3.094	-3.369	H	-0.403	5.137	-1.922
C	-2.963	-2.974	3.999	H	5.315	-4.137	-5.912	H	1.072	5.425	-2.863
C	-4.276	-3.28	4.207	H	7.207	1	1.809	H	-0.518	5.627	-3.625
C	-2.343	-3.009	5.301	H	7.035	2.767	1.85	H	0.211	3.942	-5.492
C	-3.328	-3.325	6.182	H	6.669	1.802	3.287	H	1.788	3.789	-4.688
C	-6.65	1.529	-2.351	H	4.118	2.722	3.417	H	0.819	2.342	-5.031
C	-4.202	2.372	-2.68	H	4.344	3.734	1.977	H	5.466	-2.799	0.519
C	-2.341	-0.591	-1.268	H	8.997	0.047	-0.783	C	7.317	-3.112	1.586

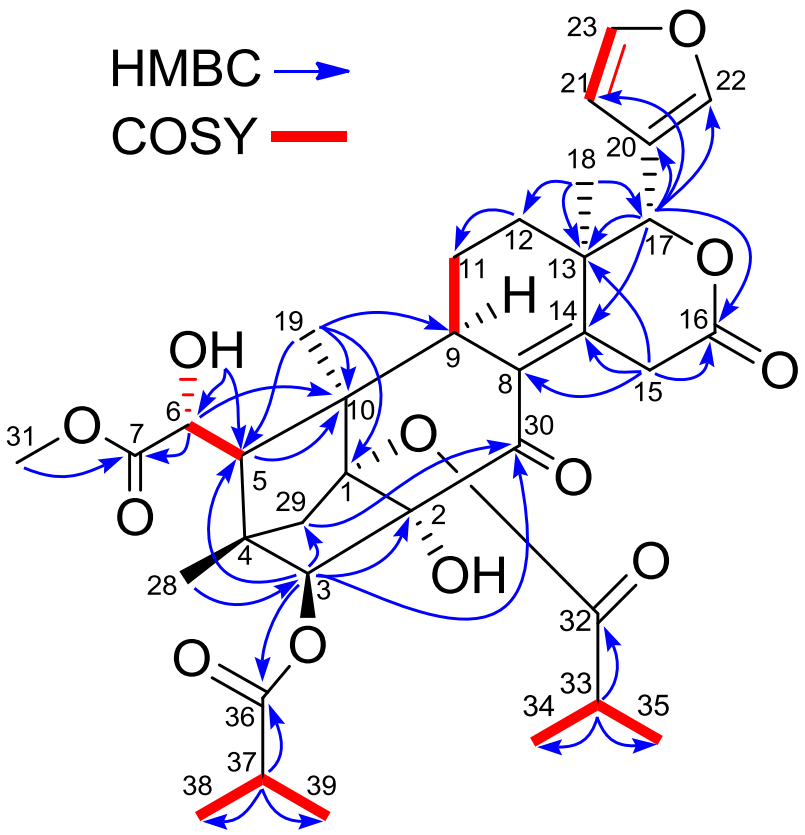

Figure S1. ^{1}H-^{1}H COSY and HMBC correlations of compound **1.**

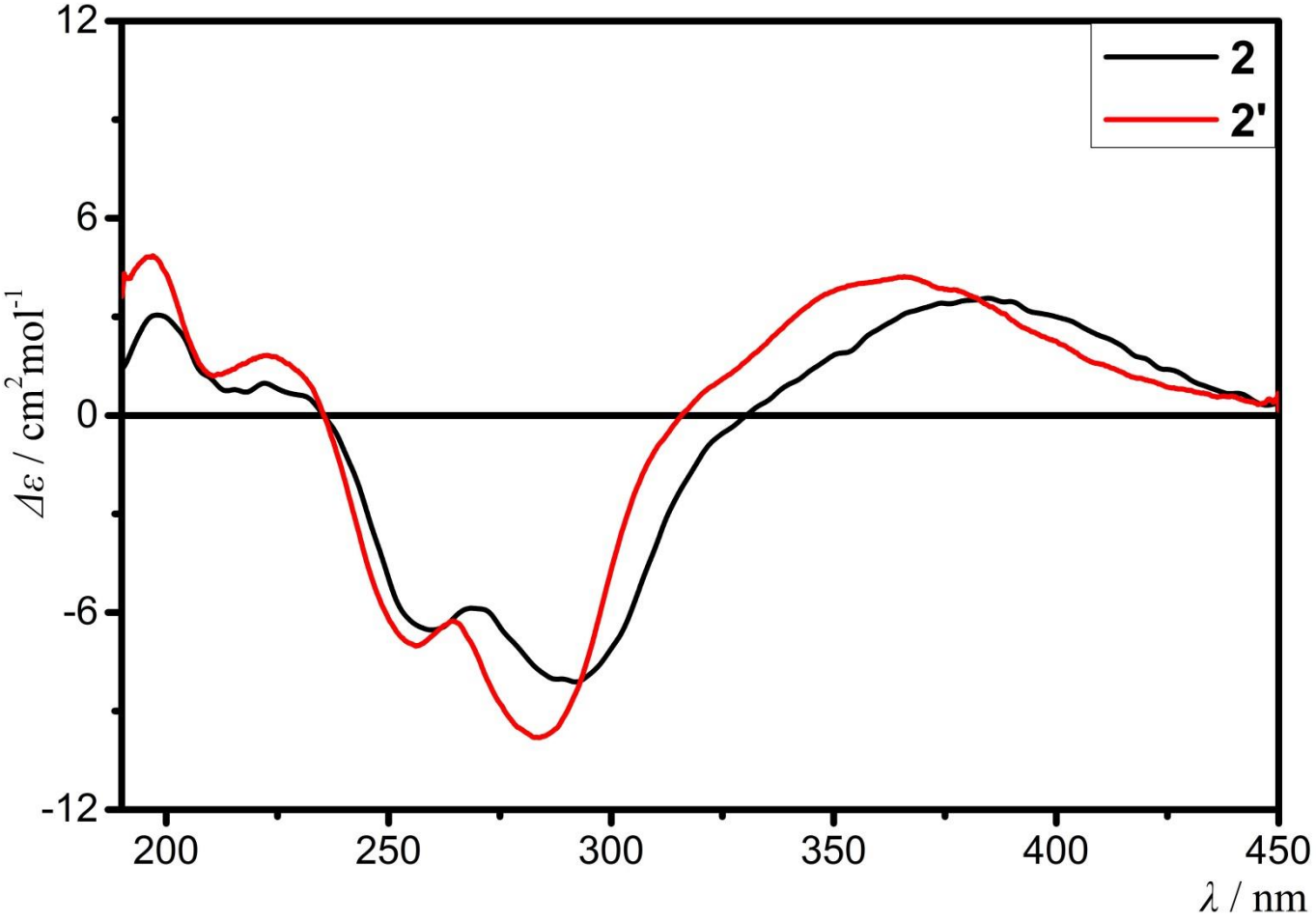

Figure S2. ECD spectra of **2, 2′** measured at the concentration of 250 μg/mL in $CHCl_3$.

X-Ray Crystallographic Data.

6*R*-hydroxymoluccensin A (1): Suitable crystals of **1** were obtained in chloroform/methanol (1:2) at room temperature. The measurement was made on an Agilent Xcalibur Atlas Gemini ultra diffractometer with mirror monochromated Cu-Kα radiation (λ = 1.54184 Å) at 150 K. Orthorhombic, $C_{35}H_{44}O_{12}$, space group P2(1)2(1)2(1) with a = 9.18292(14) Å, b = 12.4621(2) Å, c = 28.4369(5) Å, V = 3254.29(9) Å^3, Z = 4, D_{calcd} = 1.340 Mg/m^3, m = 0.839 mm^{-1} and F(000) = 1400. Crystal size: 0.35 $\times$ 0.30 $\times$ 0.25 mm^3. Independent reflections: 4962 with R_{int} = 0.0193. The structure was solved by direct methods (SHELXS-97) and refined using full-matrix least-squares difference Fourier techniques. All non-hydrogen atoms were refined anisotropically, and all hydrogen atoms were placed in idealized positions and refined as riding atoms with the relative isotropic parameters. The final agreement factors were R1 = 0.0268 and wR2 = 0.0674 [$I > 2\sigma(I)$]. The absolute structure parameter is 0.00(11). CCDC 1818979 contains the supplementary crystallographic data for this paper (excluding structure factors). These data can be obtained free of charge from The Cambridge Crystallographic Data Centre.

Compound 2: Suitable crystals of **2** were obtained in chloroform/ acetonitrile (1:2) at room temperature. The measurement was made on an Agilent Xcalibur Atlas Gemini ultra diffractometer with mirror monochromated Cu-Kα radiation (λ = 1.54184 Å) at 293 K. Triclinic, $C_{77.37}H_{93.10}N_4O_{24}$ [$C_{70}H_{84}O_{24}$, 4(CH_3CN)], space group P1 with a = 10.54064(16) Å, b = 14.6009(3) Å, c = 14.9312(2) Å, V = 1884.09(5) Å^3, Z = 1, D_{calcd} = 1.289 Mg/m^3, m = 0.796 mm^{-1} and F(000) = 777. Crystal size: 0.30 $\times$ 0.20 $\times$ 0.10 mm^3. Independent reflections: 12974 with R_{int} = 0.0333. The structure was solved by direct methods (SHELXS-97) and refined using full-matrix least-squares difference Fourier techniques. All non-hydrogen atoms were refined anisotropically, and all hydrogen atoms were placed in idealized positions and refined as riding atoms with the relative isotropic parameters. The final agreement factors were R1 = 0.0506 and wR2 = 0.1346 [$I > 2\sigma(I)$]. The absolute structure parameter is 0.05(12). CCDC 1818983 contains the supplementary crystallographic data for this paper (excluding structure factors). These data can be obtained free of charge from The Cambridge Crystallographic Data Centre.

Compound 2′: Suitable crystals of **2′** were obtained in chloroform/ acetonitrile (1:2) at room temperature. The measurement was made on an Agilent Xcalibur Atlas Gemini ultra diffractometer with mirror monochromated Cu-Kα radiation (λ = 1.54178 Å) at 150 K. Orthorhombic,

$C_{78}H_{96}N_4O_{22}$ [$C_{70}H_{84}O_{22}$, $4(CH_3CN)$], space group $C222_1$ with a = 10.70154(11) Å, b = 27.4281(3) Å, c = 26.4591(3) Å, V = 7766.36(14) Å^3, Z = 4, D_{calcd} = 1.233 Mg/m^3, m = 0.744 mm^{-1} and F(000) =3072 . Crystal size: 0.35 × 0.35 × 0.30 mm^3. Independent reflections: 6934 with R_{int} = 0.0357. The structure was solved by direct methods (SHELXS-97) and refined using full-matrix least-squares difference Fourier techniques. All non-hydrogen atoms were refined anisotropically, and all hydrogen atoms were placed in idealized positions and refined as riding atoms with the relative isotropic parameters. The final agreement factors were $R1$ = 0.0757 and $wR2$ = 0.2014 [$I > 2\sigma(I)$]. The absolute structure parameter is 0.02(3). CCDC 1818987 contains the supplementary crystallographic data for this paper (excluding structure factors). These data can be obtained free of charge from The Cambridge Crystallographic Data Centre.

Compound 3: Suitable crystals of **3** were obtained in chloroform/methanol (1:3) at room temperature. The measurement was made on an Agilent Xcalibur Atlas Gemini ultra diffractometer with mirror monochromated Cu-Kα radiation (λ = 1.54178 Å) at 293 K. Hexagonal, $C_{70}H_{84}O_{24}$, space group P6(5) with a = 14.7018(1) Å, b = 14.7018(1) Å, c = 53.2893(2) Å, V = 9975.00(7) Å^3, Z = 6, D_{calcd} = 1.308 Mg/m^3, m = 0.821 mm^{-1} and F(000) = 4176 . Crystal size: 0.47 × 0.45 × 0.40 mm^3. Independent reflections: 11839 with R_{int} = 0.0334. The structure was solved by direct methods (SHELXS-97) and refined using full-matrix least-squares difference Fourier techniques. All non-hydrogen atoms were refined anisotropically, and all hydrogen atoms were placed in idealized positions and refined as riding atoms with the relative isotropic parameters. The final agreement factors were $R1$ = 0.0724 and $wR2$ = 0.2119 [$I > 2\sigma(I)$]. The absolute structure parameter is 0.01(2). CCDC 1818988 contains the supplementary crystallographic data for this paper (excluding structure factors). These data can be obtained free of charge from The Cambridge Crystallographic Data Centre.

Compound 4′: Suitable crystals of **1** were obtained in dimethyl sulfoxide at room temperature. The measurement was made on an Agilent Xcalibur Atlas Gemini ultra diffractometer with mirror monochromated Cu-Kα radiation (λ = 1.54178 Å) at 150 K. Monoclinic, $C_{76}H_{104}O_{26}S_3$, [$C_{70}H_{84}O_{22}$, $3(CH_3SOCH_3)$, $1H_2O$] space group $P2(1)$ with a = 13.7347(9) Å, b = 21.9890(14) Å, c = 13.7372 (11) Å, V = 3882.8(5) Å^3, Z = 2, D_{calcd} = 1.308 Mg/m^3, m = 1.531 mm^{-1} and F(000) = 1632.0 Crystal size: 0.30 × 0.20 × 0.15 mm^3. Independent reflections: 10068 with R_{int} = 0.0640. The structure was solved by direct methods (SHELXS-97) and refined using full-matrix least-squares difference Fourier

techniques. All non-hydrogen atoms were refined anisotropically, and all hydrogen atoms were placed in idealized positions and refined as riding atoms with the relative isotropic parameters. The final agreement factors were $R1$ = 0.1161 and $wR2$ = 0.2152 [$I > 2\sigma(I)$]. The absolute structure parameter is 0.04(9). CCDC 1518171 contains the supplementary crystallographic data for this paper (excluding structure factors). These data can be obtained free of charge from The Cambridge Crystallographic Data Centre.

Compound 5a: Suitable crystals of **5a** were obtained in chloroform/ acetonitrile (1:1) at room temperature. The measurement was made on a Bruker Smart 1000 CCD system diffractometer with graphite-monochromated Mo-Kα radiation (λ = 0.71073 Å) at 296 K. Orthorhombic, $C_{74}H_{91}N_2O_{24}$ [$C_{70}H_{86}O_{24}$, $2(CH_3CN)$], space group P2(1)2(1)2(1) with a = 15.2487(11) Å, b = 16.1229(11) Å, c = 29.1352(19) Å, V = 7163.0(9) Å^3, Z = 4, D_{calcd} = 1.291 Mg/m^3, m = 0.096 mm^{-1} and F(000) = 2964. Crystal size: 0.34 $\times$ 0.32 $\times$ 0.28 mm^3. Independent reflections: 15927 with R_{int} = 0.0348. The structure was solved by direct methods (SHELXS-97) and refined using full-matrix least-squares difference Fourier techniques. All non-hydrogen atoms were refined anisotropically, and all hydrogen atoms were placed in idealized positions and refined as riding atoms with the relative isotropic parameters. The final agreement factors were $R1$ = 0.0548 and $wR2$ = 0.1445 [$I > 2\sigma(I)$]. The absolute structure parameter is 0.4(7). CCDC 1818989 contains the supplementary crystallographic data for this paper (excluding structure factors). These data can be obtained free of charge from The Cambridge Crystallographic Data Centre.

Compound 5b: Suitable crystals of **5b** were obtained in chloroform/*n*-hexane (1:1) at room temperature. The measurement was made on an Agilent Xcalibur Atlas Gemini ultra diffractometer with mirror monochromated Cu-Kα radiation (λ = 1.54184 Å) at 123 K. Orthorhombic, $C_{74}H_{90}Cl_{12}O_{24}$ [$C_{70}H_{86}O_{24}$,$4(CHCl_3)$], space group P2(1)2(1)2(1) with a = 15.8696(6) Å, b = 16.1185(5) Å, c = 32.0556(7) Å, V = 8199.6(4) Å^3, Z = 4, D_{calcd} = 1.449 Mg/m^3, m = 4.336 mm^{-1} and F(000) = 3720. Crystal size: 0.42 $\times$ 0.40 $\times$ 0.39 mm^3. Independent reflections: 13583 with R_{int} = 0.1210. The structure was solved by direct methods (SHELXS-97) and refined using full-matrix least-squares difference Fourier techniques. All non-hydrogen atoms were refined anisotropically, and all hydrogen atoms were placed in idealized positions and refined as riding atoms with the relative isotropic parameters. The final agreement factors were $R1$ = 0.0812 and $wR2$ = 0.1738 [$I > 2\sigma(I)$]. The

absolute structure parameter is 0.03(2). CCDC 1818990 contains the supplementary crystallographic data for this paper (excluding structure factors). These data can be obtained free of charge from The Cambridge Crystallographic Data Centre.