Supplementary Data

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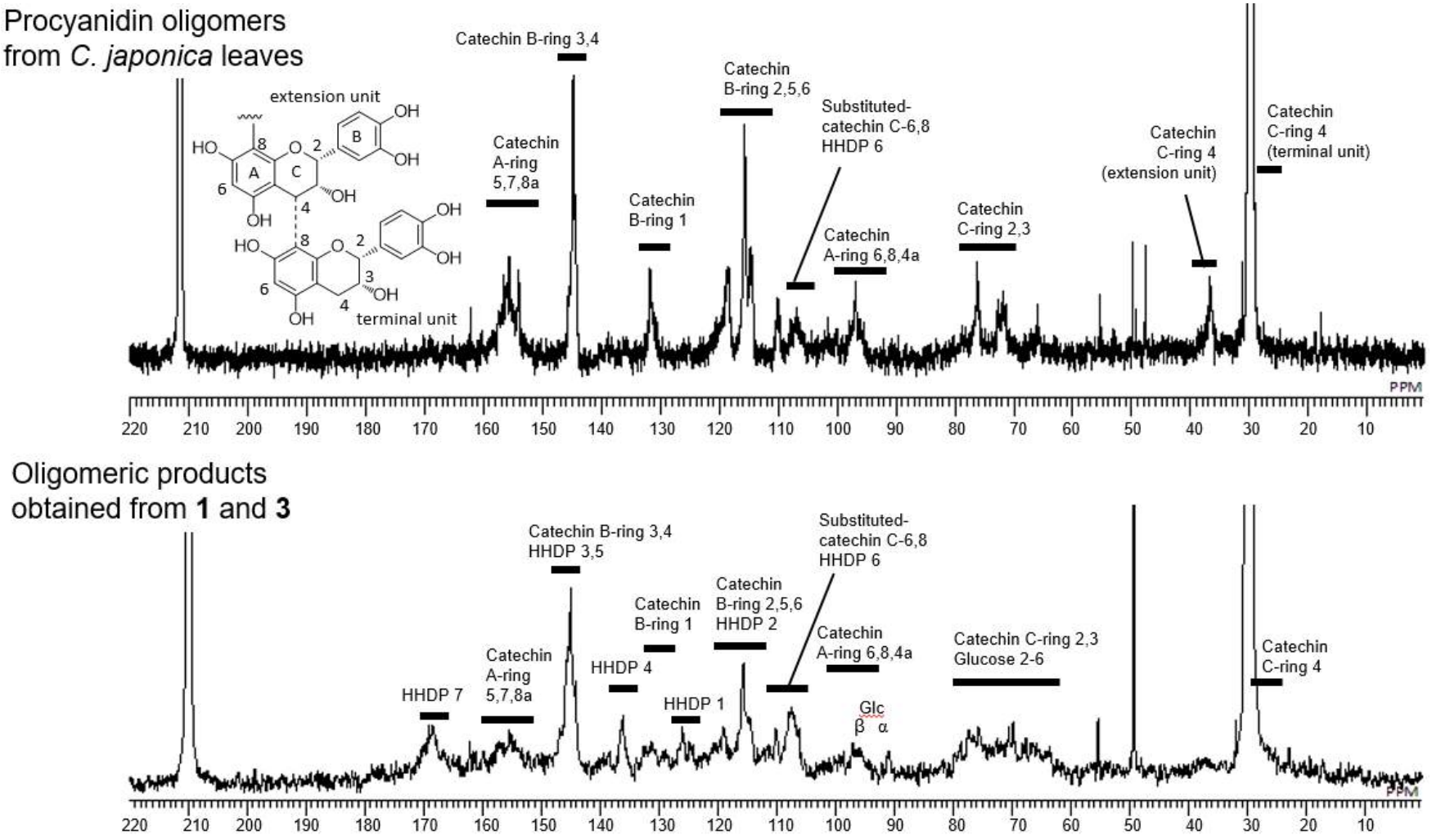
Table of contents

Fig. S1. ^{13}C NMR spectra of a mixture of procyanidin oligomers obtained from April leaves of *C. japonica* and oligomeric oxidation products obtained from **1** and **3**



Scheme S1. Possible production mechanism for **6** and **7** from **1**.

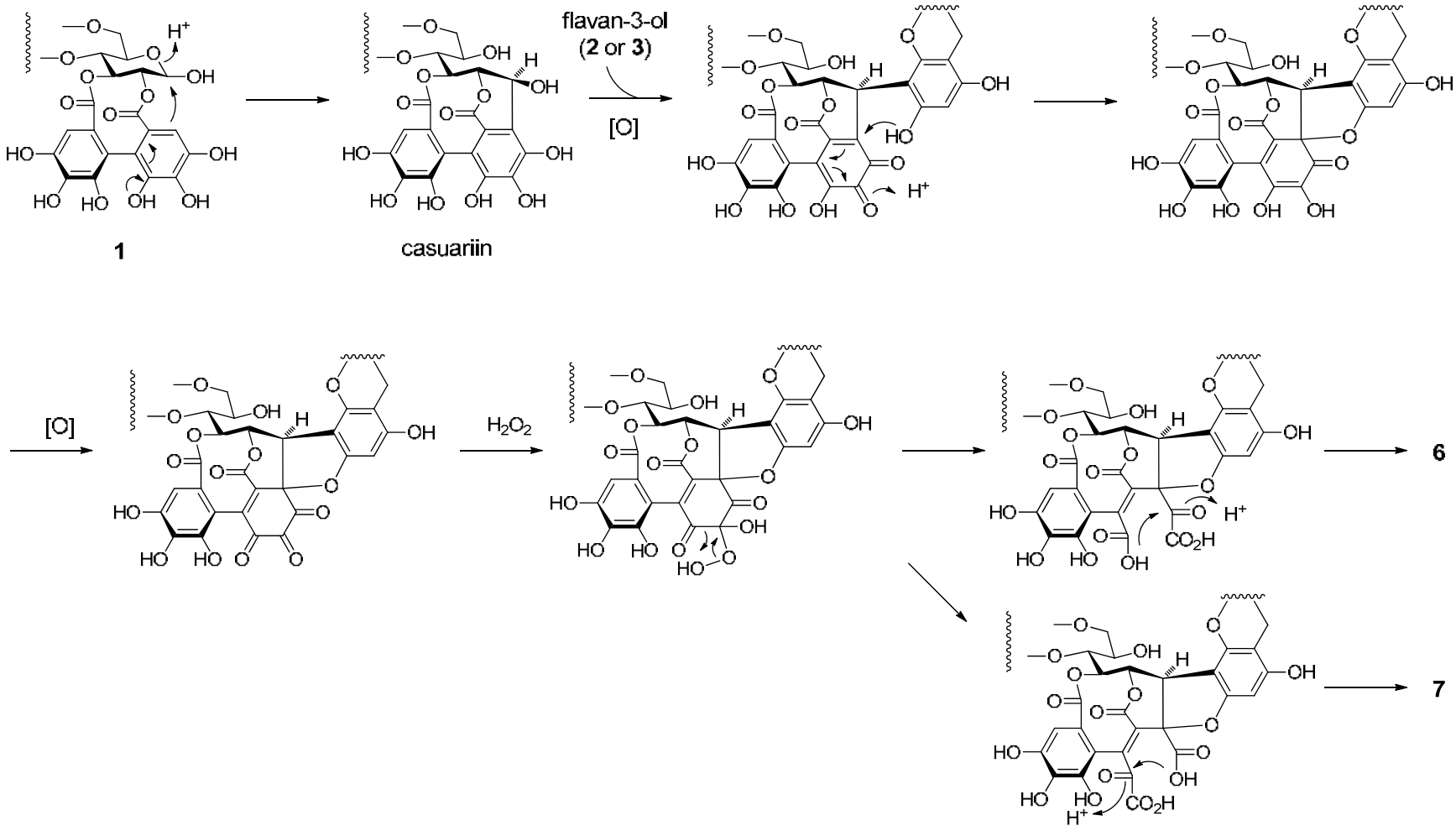


Fig. S2. ^{13}C NMR spectra of oligomeric oxidation products obtained from **1** and **3** and oligomeric polyphenol fraction obtained from August leaves of *C. japonica*.

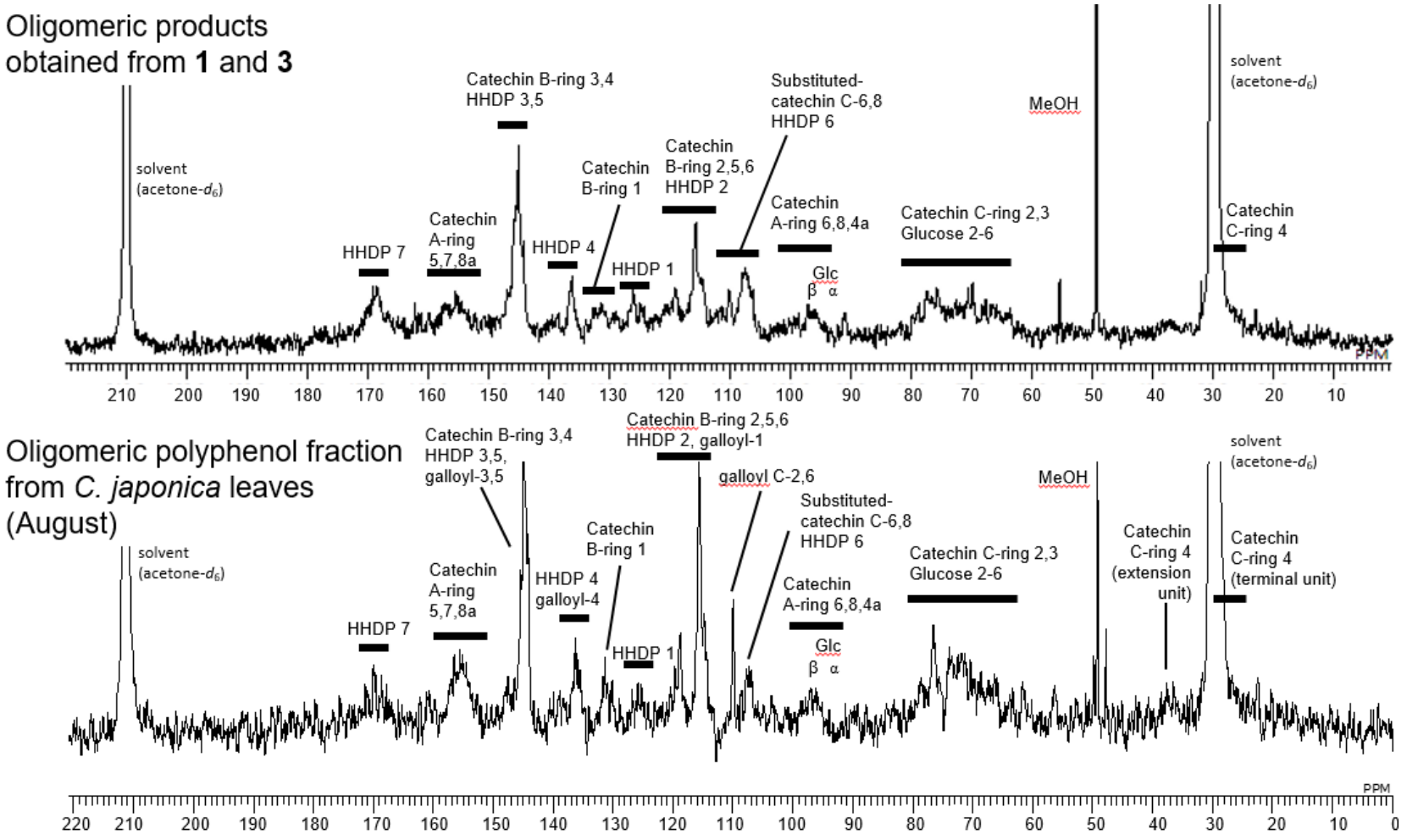
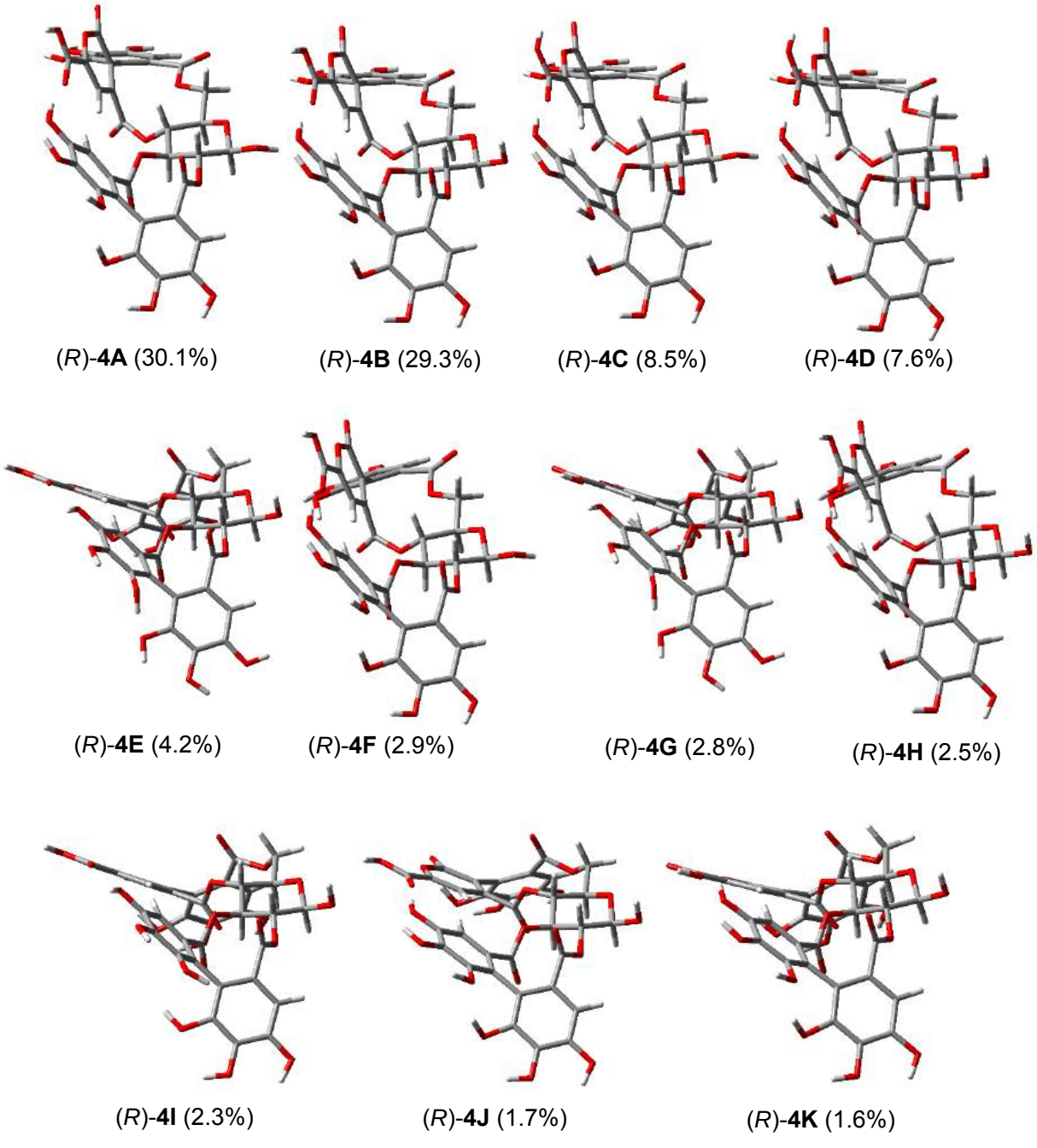
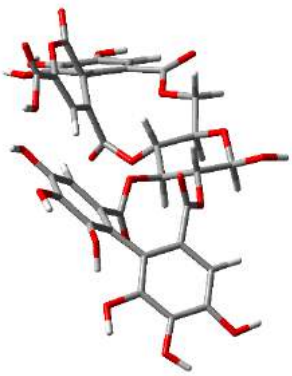
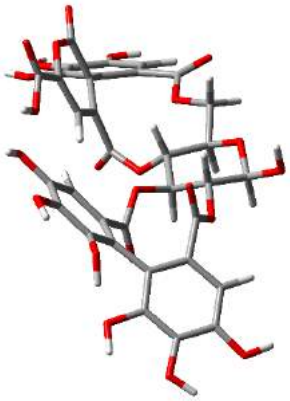


Fig. S3. Optimized conformers of (*R*)-**4** at the B3LYP/6-31G(d,p) level in acetone (PCM) with populations greater than 1% calculated from their relative Gibbs free energies (ΔG).

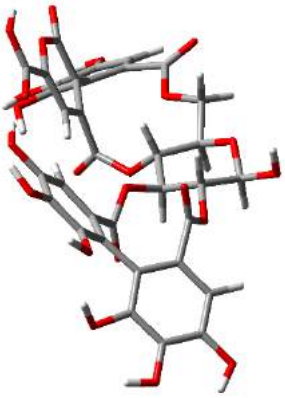




(*R*)-**4L** (1.1%)

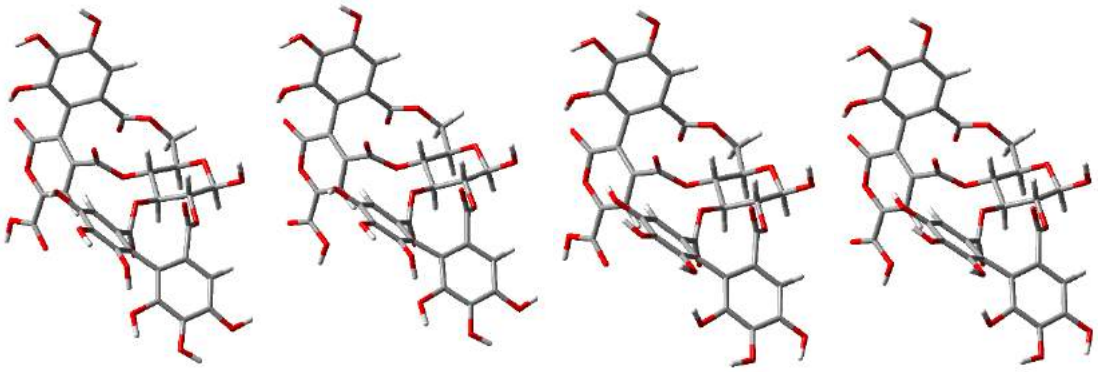


(*R*)-**4M** (1.1%)

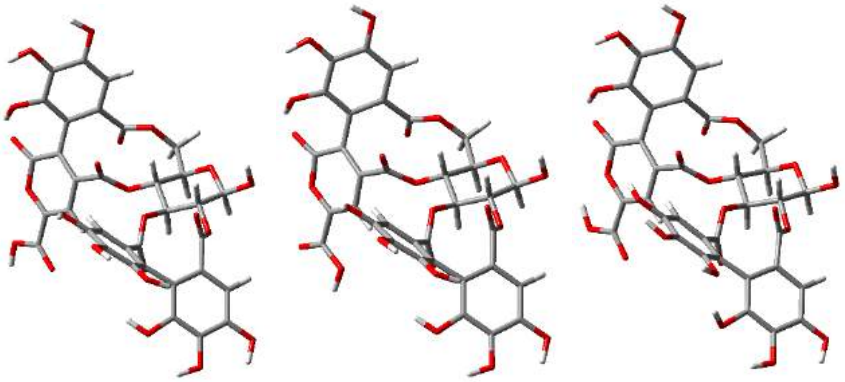


(*R*)-**4N** (1.0%)

Fig. S4. Optimized conformers of (*S*)-**4** at the B3LYP/6-31G(d,p) level in acetone (PCM) with populations greater than 1% calculated from their relative Gibbs free energies (ΔG).

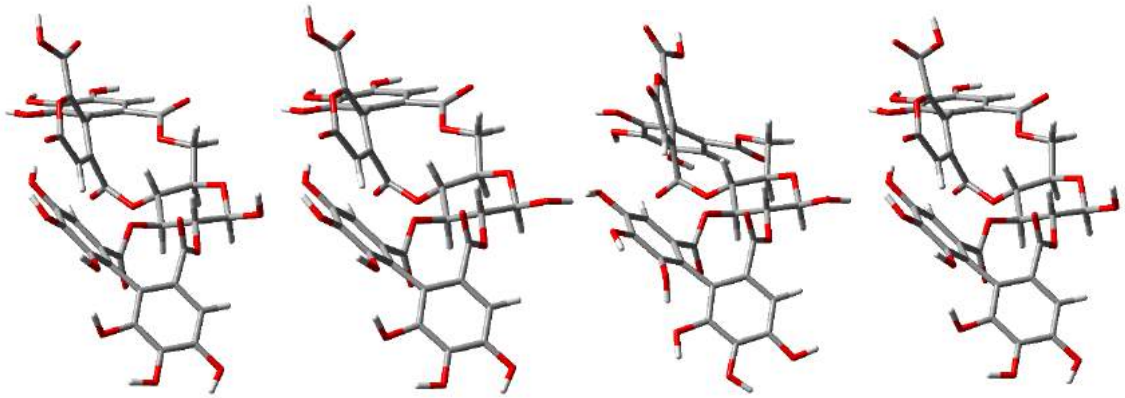


(*S*)-**4A** (28.3%) (*S*)-**4B** (21.5%) (*S*)-**4C** (20.1%) (*S*)-**4D** (17.4%)

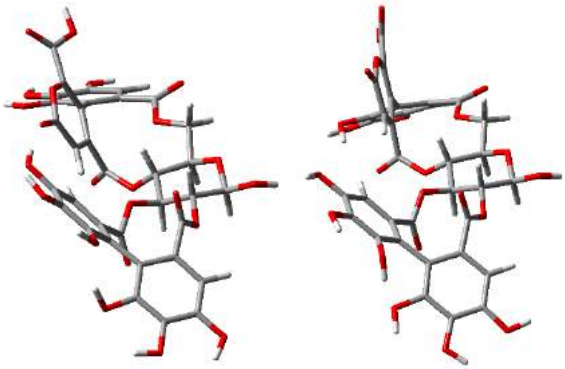


(*S*)-**4E** (4.9%) (*S*)-**4F** (3.5%) (*S*)-**4G** (1.5%)

Fig. S5. Optimized conformers of (*R*)-**4a** at the B3LYP/6-31G(d,p) level in acetone (PCM) with populations greater than 1% calculated from their relative Gibbs free energies (ΔG).

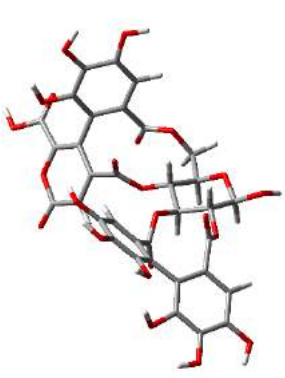


(*R*)-**4aA** (30.6%) (*R*)-**4aB** (30.5%) (*R*)-**4aC** (11.5%) (*R*)-**4aD** (10.6%)



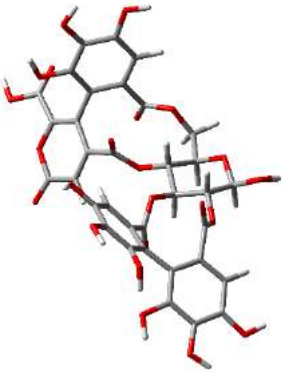
(*R*)-**4aE** (10.2%) (*R*)-**4aF** (1.5%)

Fig. S6. Optimized conformers of (*S*)-**4a** at the B3LYP/6-31G(d,p) level in acetone (PCM) with populations greater than 1% calculated from their relative Gibbs free energies (ΔG).

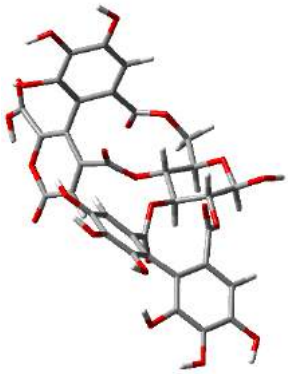


(*S*)-**4aA** (27.0%)

(*S*)-**4aB** (15.9%)

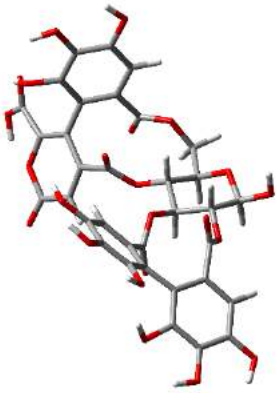


(*S*)-**4aC** (8.2%)

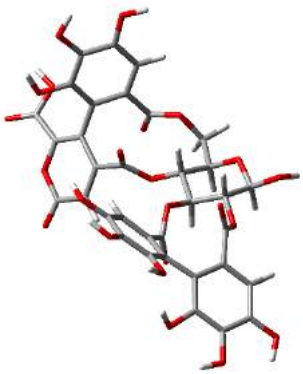


(*S*)-**4aD** (8.0%)

(*S*)-**4aE** (7.1%)

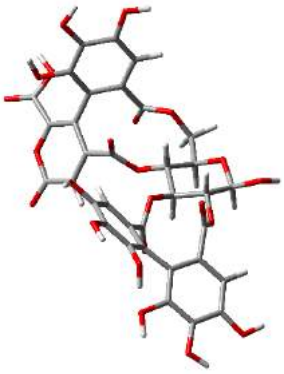


(*S*)-**4aF** (6.9%)

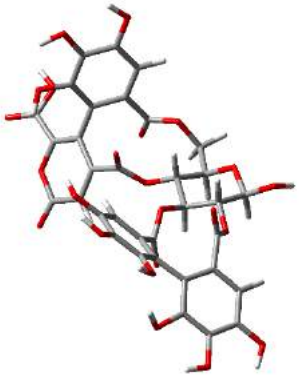


(*S*)-**4aG** (6.5%)

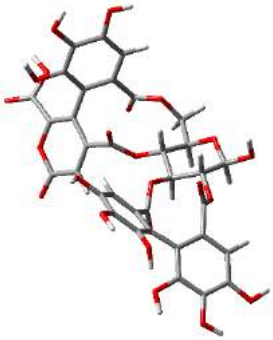
(*S*)-**4aH** (4.7%)



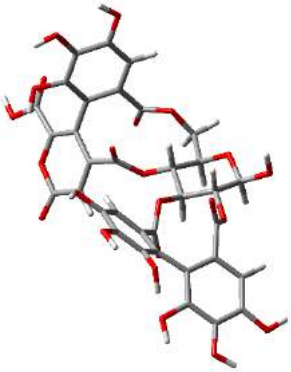
(*S*)-**4aI** (2.5%)



(*S*)-**4aJ** (2.2%)



(*S*)-**4aK** (2.1%)



(*S*)-**4aL** (1.3%)

(*S*)-**4aM** (1.0%)

Table S1. Calculated ^{1}H NMR chemical shifts of (*R*)-**4**.

	calculated[a]																experimental[b]
Position	(*R*)-**4A**	(*R*)-**4B**	(*R*)-**4C**	(*R*)-**4D**	(*R*)-**4E**	(*R*)-**4F**	(*R*)-**4G**	(*R*)-**4H**	(*R*)-**4I**	(*R*)-**4J**	(*R*)-**4K**	(*R*)-**4L**	(*R*)-**4M**	(*R*)-**4N**	averaged-(*R*)-**4**	averaged-(*R*)-**4** (corrected)	**4**
Glucose-1	5.47	5.15	5.47	5.15	5.24	5.46	5.24	5.15	5.21	5.34	5.26	5.45	5.13	5.15	5.30	4.95	5.04
2	5.41	5.24	5.42	5.25	5.19	5.41	5.19	5.24	5.11	5.19	5.19	5.42	5.24	5.25	5.31	4.95	4.82
3	5.86	5.86	5.87	5.88	6.53	5.86	6.53	5.87	6.46	6.28	6.53	5.89	5.89	5.88	5.94	5.42	5.23
4	5.16	5.15	5.14	5.13	4.68	5.14	4.68	5.13	4.63	4.54	4.66	5.23	5.21	5.12	5.09	4.79	4.97
5	4.27	4.30	4.29	4.32	4.91	4.32	4.91	4.36	4.89	4.89	4.92	4.27	4.30	4.37	4.37	4.27	4.30
6a	5.48	5.50	5.45	5.47	4.37	5.02	4.37	5.04	4.36	4.42	4.37	5.40	5.41	5.05	5.31	4.95	5.35
6b	3.87	3.84	3.88	3.85	5.60	3.97	5.61	3.94	5.59	5.55	5.61	3.86	3.83	3.95	4.09	4.06	3.92
A-Ring 6	7.20	7.22	7.20	7.22	7.09	7.18	7.10	7.20	7.16	7.30	7.23	7.08	7.09	7.19	7.20	6.34	6.59
B-Ring 6	8.10	8.08	8.20	8.18	7.49	7.95	7.45	7.94	7.43	7.51	7.25	8.09	8.08	8.03	8.01	6.93	6.36
C-Ring 6	8.14	8.14	8.10	8.09	8.31	8.17	8.21	8.17	8.29	8.35	8.16	8.04	8.03	8.13	8.15	7.03	6.97
D-Ring 6	7.50	7.51	7.52	7.53	7.39	7.73	7.40	7.74	7.39	7.55	7.40	7.48	7.49	7.74	7.51	6.57	6.71

[a] Calculated using the GIAO method at the mPW1PW91/6-311+G(2d,p) level in acetone (PCM). [b] Measured in acetone-d_6 + D_2O. [c] Averaged according to the Boltzmann distribution theory at 298 K based on relative Gibbs free energies. [d] Linearly corrected for the experimental data.

Table S2. Calculated ^{1}H NMR chemical shifts of (*S*)-**4**.

Position	calculated[a]									experimental[b]
	(*S*)-**4A**	(*S*)-**4B**	(*S*)-**4C**	(*S*)-**4D**	(*S*)-**4E**	(*S*)-**4F**	(*S*)-**4G**	averaged-(*S*)-**4**	averaged-(*S*)-**4** (corrected)	**4**
Glucose-1	5.13	5.14	5.16	5.16	5.13	5.13	5.16	5.14	4.73	5.04
2	5.22	5.23	5.22	5.23	5.19	5.20	5.22	5.22	4.80	4.82
3	5.90	5.90	5.90	5.89	5.94	5.91	5.90	5.90	5.37	5.23
4	5.60	5.61	5.56	5.57	5.63	5.63	5.55	5.59	5.11	4.97
5	4.46	4.47	4.47	4.49	4.46	4.47	4.48	4.47	4.17	4.30
6a	6.18	6.20	6.19	6.21	6.10	6.16	6.19	6.19	5.61	5.35
6b	4.23	4.23	4.23	4.22	4.23	4.24	4.23	4.23	3.97	3.92
A-Ring 6	7.10	7.11	7.34	7.34	7.21	7.23	7.34	7.21	6.47	6.59
B-Ring 6	7.02	7.03	6.82	6.84	6.92	6.95	6.83	6.94	6.24	6.36
C-Ring 6	7.98	7.86	7.97	7.85	7.95	7.85	7.90	7.92	7.07	6.97
D-Ring 6	7.48	7.48	7.50	7.49	7.50	7.48	7.51	7.49	6.71	6.71

[a] Calculated using the GIAO method at the mPW1PW91/6-311+G(2d,p) level in acetone (PCM). [b] Measured in acetone-d_6 + D_2O. [c] Averaged according to the Boltzmann distribution theory at 298 K based on relative Gibbs free energies. [d] Linearly corrected for the experimental data.

Table S3. Calculated ^{1}H NMR chemical shifts of (*R*)-**4a**.

Position	calculated[a]								experimental[b]
	(*R*)-**4aA**	(*R*)-**4aB**	(*R*)-**4aC**	(*R*)-**4aD**	(*R*)-**4aE**	(*R*)-**4aF**	averaged-(*R*)-**4a**	averaged-(*R*)-**4a** (corrected)	**4**
Glucose-1	5.19	5.50	5.43	5.21	5.51	5.41	5.36	4.99	5.04
2	5.29	5.46	5.37	5.30	5.47	5.39	5.37	5.00	4.82
3	5.83	5.83	5.82	5.85	5.84	5.90	5.83	5.35	5.23
4	5.28	5.29	5.37	5.31	5.32	5.42	5.30	4.95	4.97
5	4.37	4.33	4.34	4.39	4.36	4.13	4.35	4.22	4.30
6a	5.62	5.61	5.55	5.66	5.64	5.43	5.61	5.18	5.35
6b	3.85	3.88	3.94	3.89	3.91	3.80	3.88	3.86	3.92
A-Ring 6	7.36	7.35	7.22	7.36	7.35	7.14	7.34	6.49	6.59
B-Ring 6	7.79	7.80	7.42	7.79	7.80	7.40	7.74	6.80	6.36
C-Ring 6	7.78	7.78	7.12	7.73	7.74	7.16	7.68	6.75	6.97
D-Ring 6	7.49	7.48	8.06	7.50	7.50	7.83	7.56	6.67	6.71

[a] Calculated using the GIAO method at the mPW1PW91/6-311+G(2d,p) level in acetone (PCM). [b] Measured in acetone-d_6 + D_2O. [c] Averaged according to the Boltzmann distribution theory at 298 K based on relative Gibbs free energies. [d] Linearly corrected for the experimental data.

Table S4. Calculated ^{1}H NMR chemical shifts of (*S*)-**4a**.

	calculated[a]															experimental[b]
Position	(*S*)-**4aA**	(*S*)-**4aB**	(*S*)-**4aC**	(*S*)-**4aD**	(*S*)-**4aE**	(*S*)-**4aF**	(*S*)-**4aG**	(*S*)-**4aH**	(*S*)-**4aI**	(*S*)-**4aJ**	(*S*)-**4aK**	(*S*)-**4aL**	(*S*)-**4aM**	averaged-(*S*)-**4a**	averaged-(*S*)-**4a** (corrected)	**4**
Glucose-1	5.43	5.13	5.42	5.43	6.51	5.11	5.44	5.14	5.43	5.12	5.09	5.44	5.14	5.41	4.94	5.04
2	5.42	5.22	5.42	5.40	6.98	5.20	5.42	5.22	5.42	5.22	5.21	5.42	5.23	5.46	5.00	4.82
3	5.81	5.82	5.84	5.76	7.00	5.76	5.82	5.82	5.84	5.84	5.80	5.82	5.82	5.90	5.44	5.23
4	5.46	5.44	5.49	5.33	7.04	5.31	5.48	5.46	5.50	5.48	5.40	5.47	5.45	5.56	5.09	4.97
5	4.33	4.36	4.32	4.28	6.50	4.31	4.34	4.38	4.34	4.37	4.33	4.35	4.38	4.50	4.02	4.30
6a	6.04	6.06	6.05	5.95	5.21	5.96	6.08	6.10	6.08	6.10	6.01	6.07	6.10	5.98	5.52	5.35
6b	4.14	4.18	4.14	4.20	5.11	4.23	4.17	4.20	4.16	4.19	4.19	4.19	4.23	4.24	3.76	3.92
A-Ring 6	7.27	7.29	7.03	7.26	5.85	7.28	7.28	7.30	7.03	7.04	7.03	7.28	7.30	7.13	6.68	6.59
B-Ring 6	6.96	6.95	7.20	6.90	7.14	6.89	6.95	6.94	7.19	7.19	7.17	6.95	6.94	7.00	6.55	6.36
C-Ring 6	6.98	6.98	6.98	6.95	7.25	6.95	6.93	6.93	6.93	6.93	7.01	7.02	7.02	6.99	6.54	6.97
D-Ring 6	7.24	7.25	7.26	7.68	5.10	7.67	7.27	7.27	7.27	7.27	7.38	7.45	7.45	7.16	6.72	6.71

[a] *Calculated using the GIAO method at the mPW1PW91/6-311+G(2d,p) level in acetone (PCM).* [b] *Measured in acetone-d_6 + D_2O.* [c] *Averaged according to the Boltzmann distribution theory at 298 K based on relative Gibbs free energies.*

[d] *Linearly corrected for the experimental data.*

Table S5. Calculated ^{13}C NMR chemical shifts of (*R*)-**4**.

	calculated[a]																experimental[b]
Position	(*R*)-**4A**	(*R*)-**4B**	(*R*)-**4C**	(*R*)-**4D**	(*R*)-**4E**	(*R*)-**4F**	(*R*)-**4G**	(*R*)-**4H**	(*R*)-**4I**	(*R*)-**4J**	(*R*)-**4K**	(*R*)-**4L**	(*R*)-**4M**	(*R*)-**4N**	averaged-(*R*)-**4**	averaged-(*R*)-**4** (corrected)	**4**
Glucose-1	93.1	93.0	93.1	93.0	95.2	92.9	95.2	92.8	95.3	95.6	95.3	93.0	92.9	92.7	93.4	92.0	94.7
2	75.4	77.3	75.4	77.3	79.6	75.1	79.6	77.0	79.2	78.8	79.5	75.5	77.4	77.0	76.7	75.5	77.5
3	78.3	78.3	78.4	78.3	73.7	78.7	73.7	78.7	73.5	72.0	74.1	78.2	78.1	78.8	77.7	76.5	77.2
4	79.2	79.1	79.3	79.2	77.6	80.8	77.6	80.6	77.5	77.0	77.7	79.1	79.0	80.7	79.1	77.8	70.8
5	69.0	69.8	69.0	69.8	70.6	69.1	70.6	69.9	70.5	69.1	70.5	69.2	70.0	69.9	69.5	68.3	71.3
6	63.3	63.3	63.5	63.5	62.7	64.7	62.7	64.7	62.7	62.1	62.8	63.2	63.2	64.9	63.4	62.2	63.6
A-Ring 1	128.4	128.2	128.3	128.1	127.2	128.4	127.2	128.1	127.2	126.2	126.1	128.9	128.6	128.1	128.1	126.4	126.0 [e]
2	118.5	118.4	118.5	118.4	116.0	118.6	115.9	118.5	108.7	116.4	117.5	115.8	115.8	118.5	117.9	116.3	114.4
3	143.8	143.8	143.8	143.8	142.4	143.9	142.4	143.9	142.8	143.2	143.2	142.4	142.4	143.9	143.6	141.8	145.0
4	140.7	140.7	140.7	140.8	134.8	140.7	134.7	140.8	138.0	138.5	139.5	135.7	135.7	140.8	140.0	138.2	136.1
5	146.4	146.4	146.4	146.4	143.3	146.3	143.3	146.3	147.8	144.2	145.6	144.2	144.1	146.4	146.1	144.2	144.1
6	108.3	108.4	108.2	108.3	105.9	108.2	106.0	108.3	107.6	108.8	108.8	106.3	106.4	108.2	108.1	106.6	107.4
7	174.1	174.3	174.2	174.4	173.6	174.1	173.7	174.3	173.4	174.3	174.1	173.4	173.6	174.4	174.2	172.0	169.0
B-Ring 1	127.0	127.0	127.0	126.9	126.6	126.8	126.6	126.8	128.6	127.7	127.7	126.4	126.3	126.7	127.0	125.3	126.0 [e]
2	115.1	115.1	115.0	115.0	117.4	115.6	117.5	115.6	109.9	115.1	115.6	118.3	118.3	115.4	115.3	113.6	114.3
3	141.7	141.7	141.7	141.7	143.5	141.9	143.4	141.9	142.3	142.5	142.3	142.5	142.5	141.9	141.9	140.1	145.0
4	136.6	136.7	136.7	136.7	140.1	136.9	140.1	137.0	137.0	135.5	135.4	140.3	140.3	137.0	137.0	135.2	136.0
5	146.0	146.0	146.2	146.2	146.3	146.0	146.2	146.0	147.9	145.3	143.6	144.9	144.8	146.1	146.0	144.1	144.1
6	111.2	111.2	111.2	111.3	109.7	111.0	109.6	111.0	108.8	108.2	107.0	111.8	111.8	111.1	110.9	109.3	107.2
7	173.3	173.2	173.3	173.2	174.2	173.1	174.2	173.0	173.7	173.3	173.8	173.5	173.4	173.0	173.3	171.2	169.3
C-Ring 1	147.7	147.6	148.2	148.2	149.6	149.9	150.3	149.9	149.5	150.0	150.2	147.9	147.8	150.7	148.2	146.3	143.8
2	137.8	137.8	137.4	137.5	132.2	134.8	132.2	134.9	132.3	131.1	132.4	135.4	135.4	134.8	136.7	134.9	129.2
3	162.4	162.4	161.2	161.1	165.9	161.7	166.5	161.7	165.9	166.5	166.4	163.2	163.2	160.5	162.6	160.6	159.3
4	164.2	164.2	163.2	163.2	162.4	163.8	161.3	163.8	162.4	163.2	161.3	161.2	161.2	162.6	163.7	161.6	160.6
5	150.5	150.5	149.1	149.1	150.1	152.1	149.1	152.1	0.0	149.8	149.0	152.0	152.0	150.6	146.8	144.9	149.6
6	111.8	111.7	110.3	110.2	115.6	110.6	115.4	110.5	115.6	118.6	115.3	110.0	109.9	109.1	111.9	110.3	108.0
7	168.0	168.0	167.8	167.7	168.0	171.2	168.1	171.1	168.1	167.6	168.0	168.5	168.4	170.6	168.2	166.1	163.8
D-Ring 1	122.1	122.1	122.1	122.1	126.9	123.9	127.0	123.8	126.9	129.9	127.0	122.3	122.3	123.6	122.9	121.2	124.6 [e]
2	115.1	115.0	114.6	114.5	114.9	117.1	114.8	117.1	114.9	113.8	114.8	115.5	115.4	116.5	115.1	113.5	112.1
3	145.5	145.5	145.3	145.3	147.5	143.9	147.5	143.8	147.4	146.6	147.5	145.6	145.6	143.8	145.6	143.7	146.9
4	137.0	137.1	137.1	137.1	141.8	141.0	141.7	141.1	141.8	140.5	141.8	137.0	137.1	141.2	137.9	136.1	136.5
5	144.6	144.6	144.7	144.7	149.0	147.2	149.0	147.2	149.0	147.8	149.1	144.4	144.5	147.5	145.3	143.4	145.5
6	109.3	109.4	109.6	109.7	112.7	113.5	112.8	113.5	112.7	113.4	112.8	109.0	109.0	113.7	110.1	108.6	107.8
7	168.8	168.7	168.7	168.7	170.8	169.4	170.7	169.4	170.8	171.4	170.7	169.0	168.9	169.4	169.1	167.0	168.1

[a] Calculated using the GIAO method at the mPW1PW91/6-311+G(2d,p) level in acetone (PCM). [b] Measured in acetone-d_6 + D_2O. [c] Averaged according to the Boltzmann distribution theory at 298 K based on relative Gibbs free energies. [d] Linearly corrected for the experimental data. [e] May be interchanged in each column.

Table S6. Calculated ^{13}C NMR chemical shifts of (*S*)-**4**.

	calculated[a]									experimental[b]
Position	(*S*)-**4A**	(*S*)-**4B**	(*S*)-**4C**	(*S*)-**4D**	(*S*)-**4E**	(*S*)-**4F**	(*S*)-**4G**	averaged-(*S*)-**4**	averaged-(*S*)-**4** (corrected)	**4**
Glucose-1	94.3	94.3	94.4	94.4	94.5	94.4	94.4	94.4	93.5	94.7
2	78.6	78.5	78.2	78.1	78.3	78.2	78.1	78.4	78.1	77.5
3	76.3	76.3	76.5	76.6	76.1	76.2	76.5	76.4	76.1	77.2
4	70.0	69.9	70.1	70.0	69.9	69.9	70.2	70.0	69.9	70.8
5	71.8	71.9	71.8	71.9	71.5	71.4	71.9	71.8	71.7	71.3
6	61.5	61.5	61.6	61.5	61.6	61.6	61.6	61.5	61.8	63.6
A-Ring 1	129.2	129.2	128.6	128.6	128.0	128.2	128.5	128.8	126.8	126.0 [e]
2	115.7	115.7	117.7	117.6	108.7	108.4	117.6	115.9	114.3	114.4
3	142.0	142.0	142.7	142.8	141.9	142.0	142.8	142.3	139.8	145.0
4	134.3	134.3	138.6	138.6	135.9	135.8	138.6	136.2	133.9	136.1
5	142.9	142.9	145.3	145.4	146.9	146.8	145.4	144.2	141.7	144.1
6	106.9	107.0	109.6	109.5	108.1	108.1	109.5	108.1	106.8	107.4
7	173.6	173.6	174.1	174.1	173.3	173.3	174.1	173.8	170.3	169.0
B-Ring 1	127.7	127.7	128.4	128.4	128.4	128.9	128.4	128.1	126.1	124.6 [e]
2	117.9	117.7	116.1	116.1	110.0	110.3	116.1	116.4	114.9	114.3
3	144.1	144.1	142.8	142.8	142.4	142.6	142.8	143.4	141.0	145.0
4	139.4	139.4	135.0	135.0	135.9	135.8	135.0	137.3	135.0	136.0
5	145.6	145.7	143.7	143.7	147.0	147.0	143.7	145.0	142.5	144.1
6	109.6	109.6	107.1	107.1	108.2	108.3	107.1	108.5	107.2	107.2
7	174.1	174.2	173.6	173.7	173.5	173.6	173.6	173.9	170.4	169.3
C-Ring 1	151.3	151.4	151.3	151.4	150.8	151.0	151.8	151.3	148.6	143.8
2	132.9	133.0	132.9	133.1	132.4	132.6	132.9	132.9	130.8	129.2
3	166.2	166.7	166.2	166.8	165.9	166.5	165.0	166.4	163.2	159.3
4	162.4	161.4	162.4	161.4	162.4	161.4	160.9	161.9	158.9	160.6
5	151.0	150.0	151.0	150.0	151.2	150.1	149.8	150.6	147.9	149.6
6	114.2	113.7	114.0	113.5	114.9	114.2	112.4	113.9	112.4	108.0
7	168.8	168.8	169.0	169.0	168.8	168.7	168.8	168.9	165.6	163.8
D-Ring 1	129.0	129.1	129.1	129.2	128.8	129.0	129.1	129.1	127.1	126.0 [e]
2	115.3	115.2	115.3	115.3	115.6	115.2	115.3	115.3	113.8	112.1
3	145.9	145.8	145.8	145.8	146.8	146.4	145.6	145.9	143.4	146.9
4	138.6	138.5	138.5	138.5	139.9	139.1	138.7	138.6	136.3	136.5
5	148.5	148.5	148.5	148.5	148.4	148.5	148.6	148.5	145.8	145.5
6	112.3	112.4	112.5	112.4	112.0	112.1	112.7	112.4	110.9	107.8
7	171.9	171.9	172.0	172.0	171.4	171.6	171.9	171.9	168.5	168.1

[a] Calculated using the GIAO method at the mPW1PW91/6-311+G(2d,p) level in acetone (PCM). [b] Measured in acetone-d_6 + D_2O. [c] Averaged according to the Boltzmann distribution theory at 298 K based on relative Gibbs free energies. [d] Linearly corrected for the experimental data. [e] May be interchanged in each column.

Table S7. Calculated ^{13}C NMR chemical shifts of (*R*)-**4a**.

Position	calculated[a]								experimental[b]	
	(*R*)-**4aA**	(*R*)-**4aB**	(*R*)-**4aC**	(*R*)-**4aD**	(*R*)-**4aE**	(*R*)-**4aF**	averaged-(*R*)-**4a**	averaged-(*R*)-**4a** (corrected)	**4**	
Glucose-1	92.5	92.5	93.3	92.5	92.5	93.2	92.6	91.3	94.7	
2	76.6	74.7	75.1	76.5	74.7	75.0	75.6	74.5	77.5	
3	77.4	77.5	76.8	77.4	77.5	76.5	77.4	76.3	77.2	
4	79.8	79.9	79.3	79.8	79.9	81.1	79.8	78.7	70.8	
5	69.0	68.2	66.4	69.0	68.3	68.7	68.4	67.3	71.3	
6	64.8	64.7	62.5	64.8	64.8	62.6	64.4	63.5	63.6	
A-Ring 1	128.3	128.5	129.1	128.3	128.5	128.7	128.5	126.9	126.0	[e]
2	117.6	117.6	116.1	117.5	117.6	116.1	117.4	115.9	114.4	
3	143.2	143.2	141.8	143.2	143.3	142.1	143.0	141.3	145.0	
4	139.9	139.8	134.8	139.9	139.8	135.4	139.2	137.5	136.1	
5	146.7	146.7	143.9	146.7	146.7	144.0	146.3	144.6	144.1	
6	109.8	109.8	107.9	109.8	109.8	107.0	109.5	108.1	107.4	
7	174.8	174.6	173.2	174.8	174.6	173.2	174.5	172.5	169.0	
B-Ring 1	126.9	127.0	126.8	127.0	127.0	126.7	126.9	125.4	126.0	[e]
2	115.5	115.5	117.6	115.5	115.5	117.6	115.7	114.3	114.3	
3	142.1	142.1	141.8	142.1	142.1	142.0	142.0	140.3	145.0	
4	135.1	135.2	139.7	135.1	135.2	140.3	135.8	134.1	136.0	
5	144.6	144.7	145.8	144.7	144.7	146.1	144.8	143.1	144.1	
6	109.7	109.7	109.6	109.8	109.8	109.7	109.7	108.3	107.2	
7	172.3	172.4	174.0	172.3	172.4	173.9	172.6	170.6	169.3	
C-Ring 1	151.5	151.5	151.6	151.6	151.5	151.0	151.5	149.7	143.8	
2	124.7	124.7	123.7	122.9	122.9	124.3	124.2	122.6	129.2	
3	154.8	154.8	152.6	155.9	155.9	152.4	154.8	152.9	149.6	
4	162.3	162.3	163.8	163.2	163.2	162.2	162.7	160.8	160.6	
5	162.8	162.8	161.1	163.3	163.3	160.5	162.7	160.8	159.3	
6	119.0	119.0	118.2	118.2	118.2	117.5	118.7	117.2	108.0	
7	167.9	167.9	167.7	168.1	168.2	171.8	168.0	166.0	163.8	
D-Ring 1	122.8	122.8	119.1	123.3	123.3	125.0	122.5	121.0	124.6	[e]
2	113.6	113.6	115.7	113.0	113.0	118.0	113.8	112.4	112.1	
3	145.0	144.9	145.6	145.5	145.5	145.4	145.1	143.4	146.9	
4	136.9	136.8	137.9	136.5	136.4	141.4	137.0	135.3	136.5	
5	144.3	144.3	143.8	144.4	144.3	148.0	144.3	142.6	145.5	
6	109.7	109.6	111.4	109.8	109.8	113.8	110.0	108.5	107.8	
7	169.0	169.1	168.1	169.0	169.1	168.6	168.9	167.0	168.1	

[a] *Calculated using the GIAO method at the mPW1PW91/6-311+G(2d,p) level in acetone (PCM).* [b] *Measured in acetone-d_6 + D_2O.* [c] *Averaged according to the Boltzmann distribution theory at 298 K based on relative Gibbs free energies.* [d] *Linearly corrected for the experimental data.*
[e] *May be interchanged in each column.*

Table S8. Calculated ^{13}C NMR chemical shifts of (*S*)-**4a**.

	calculated[a]															experimental[b]
Position	(*S*)-**4aA**	(*S*)-**4aB**	(*S*)-**4aC**	(*S*)-**4aD**	(*S*)-**4aE**	(*S*)-**4aF**	(*S*)-**4aG**	(*S*)-**4aH**	(*S*)-**4aI**	(*S*)-**4aJ**	(*S*)-**4aK**	(*S*)-**4aL**	(*S*)-**4aM**	averaged-(*S*)-**4a**	averaged-(*S*)-**4a** (corrected)	**4**
Glucose-1	94.7	94.7	94.7	94.6	94.6	94.6	94.7	94.7	94.7	94.6	94.6	94.7	94.7	94.7	93.9	94.7
2	76.2	78.1	76.4	76.0	78.3	78.0	76.2	78.1	76.4	78.3	78.3	76.2	78.1	77.0	76.7	77.5
3	76.8	76.6	76.5	76.6	76.3	76.4	76.7	76.5	76.4	76.3	76.3	76.8	76.6	76.6	76.3	77.2
4	70.4	70.3	70.2	71.1	70.1	71.0	70.3	70.2	70.2	70.1	70.6	70.6	70.5	70.4	70.3	70.8
5	71.8	72.7	71.9	71.7	72.8	72.6	71.8	72.7	71.9	72.8	72.8	71.7	72.7	72.2	72.0	71.3
6	61.5	61.6	61.5	61.7	61.6	61.7	61.6	61.6	61.6	61.6	61.6	61.6	61.7	61.6	61.6	63.6
A-Ring 1	128.5	128.3	128.8	128.3	128.7	128.2	128.5	128.4	128.8	128.7	128.6	128.4	128.3	128.5	126.8	126.0 [e]
2	117.2	117.0	115.7	117.4	115.6	117.3	117.2	117.0	115.6	115.6	115.6	117.2	117.1	116.8	115.4	114.4
3	143.7	143.8	142.5	143.7	142.5	143.7	143.7	143.8	142.5	142.5	142.7	143.7	143.8	143.4	141.4	145.0
4	139.7	139.8	135.0	139.8	135.1	139.9	139.7	139.8	135.0	135.1	135.3	139.7	139.9	138.7	136.7	136.1
5	145.3	145.5	144.2	145.4	144.4	145.6	145.4	145.5	144.2	144.4	144.5	145.4	145.5	145.2	143.1	144.1
6	109.5	109.7	107.7	109.7	107.8	109.8	109.5	109.7	107.7	107.8	107.7	109.6	109.7	109.2	108.0	107.4
7	173.9	174.0	173.2	173.9	173.4	174.0	173.9	174.0	173.2	173.4	173.4	173.8	174.0	173.8	171.0	169.0
B-Ring 1	128.3	128.3	127.3	128.1	127.3	128.1	128.3	128.3	127.3	127.3	127.3	128.3	128.3	128.1	126.4	126.0 [e]
2	116.6	116.6	118.3	116.4	118.4	116.4	116.6	116.7	118.3	118.4	118.5	116.7	116.7	117.0	115.6	114.3
3	142.5	142.5	143.0	142.5	143.0	142.5	142.5	142.4	143.0	143.0	143.1	142.5	142.5	142.6	140.6	145.0
4	135.5	135.5	139.9	135.4	140.0	135.4	135.5	135.5	139.9	140.0	140.1	135.6	135.6	136.5	134.7	136.0
5	143.9	144.0	145.8	143.6	145.8	143.6	143.9	144.0	145.8	145.8	145.8	143.9	144.0	144.3	142.3	144.1
6	107.8	108.0	109.9	107.6	109.9	107.7	107.8	108.0	109.9	109.9	109.8	107.7	107.9	108.3	107.2	107.2
7	173.6	173.5	174.1	173.5	174.0	173.4	173.6	173.5	174.1	174.0	173.9	173.6	173.5	173.6	170.8	169.3
C-Ring 1	154.5	154.5	154.6	155.5	154.6	155.4	154.9	154.8	154.9	154.9	154.4	154.6	154.5	154.7	152.4	143.8
2	122.6	122.6	122.7	124.7	122.7	124.7	121.4	121.5	121.5	121.4	121.9	120.1	120.1	122.7	121.2	129.2
3	152.2	152.2	152.1	148.1	152.1	148.1	152.8	152.9	152.8	152.8	150.4	152.5	152.6	151.6	149.3	149.6
4	163.7	163.7	163.8	166.1	163.8	166.1	164.6	164.6	164.6	164.6	161.9	163.5	163.5	164.2	161.6	160.6
5	161.1	161.1	161.2	159.3	161.2	159.3	161.4	161.4	161.5	161.5	160.5	161.0	161.0	160.9	158.4	159.3
6	119.8	119.8	119.9	121.6	120.0	121.6	119.1	119.1	119.2	119.2	121.4	119.8	119.9	120.1	118.6	108.0
7	168.4	168.5	168.3	167.7	168.3	167.7	168.6	168.6	168.4	168.4	167.6	168.2	168.2	168.3	165.6	163.8
D-Ring 1	125.1	125.2	125.4	125.7	125.4	125.7	125.6	125.6	125.7	125.8	123.7	124.5	124.7	125.3	123.7	124.6 [e]
2	115.4	115.4	115.4	117.1	115.4	117.1	115.1	115.1	115.1	115.1	112.9	114.8	114.8	115.6	114.2	112.1
3	145.3	145.2	145.4	145.4	145.3	145.4	145.4	145.4	145.5	145.5	143.2	142.7	142.6	145.2	143.1	146.9
4	136.9	136.7	136.8	143.3	136.7	143.3	136.2	136.1	136.2	136.1	138.5	138.5	138.3	137.8	135.9	136.5
5	145.2	145.1	145.0	148.4	145.0	148.3	144.7	144.7	144.6	144.6	148.1	147.4	147.4	145.7	143.6	145.5
6	107.9	107.8	107.8	114.2	107.7	114.1	107.7	107.7	107.6	107.6	110.3	110.6	110.6	108.9	107.8	107.8
7	171.3	171.4	171.5	171.3	171.5	171.3	171.3	171.3	171.4	171.4	171.6	171.5	171.6	171.4	168.6	168.1

[a] *Calculated using the GIAO method at the mPW1PW91/6-311+G(2d,p) level in acetone (PCM).* [b] *Measured in acetone-d_6 + D_2O.* [c] *Averaged according to the Boltzmann distribution theory at 298 K based on relative Gibbs free energies.* [d] *Linearly corrected for the experimental data.* [e] *May be interchanged in each column.*

Fig. S7. Correlation plots of experimental ^{1}H NMR chemical shifts versus corresponding calculated ^{1}H NMR chemical shifts of **4**.

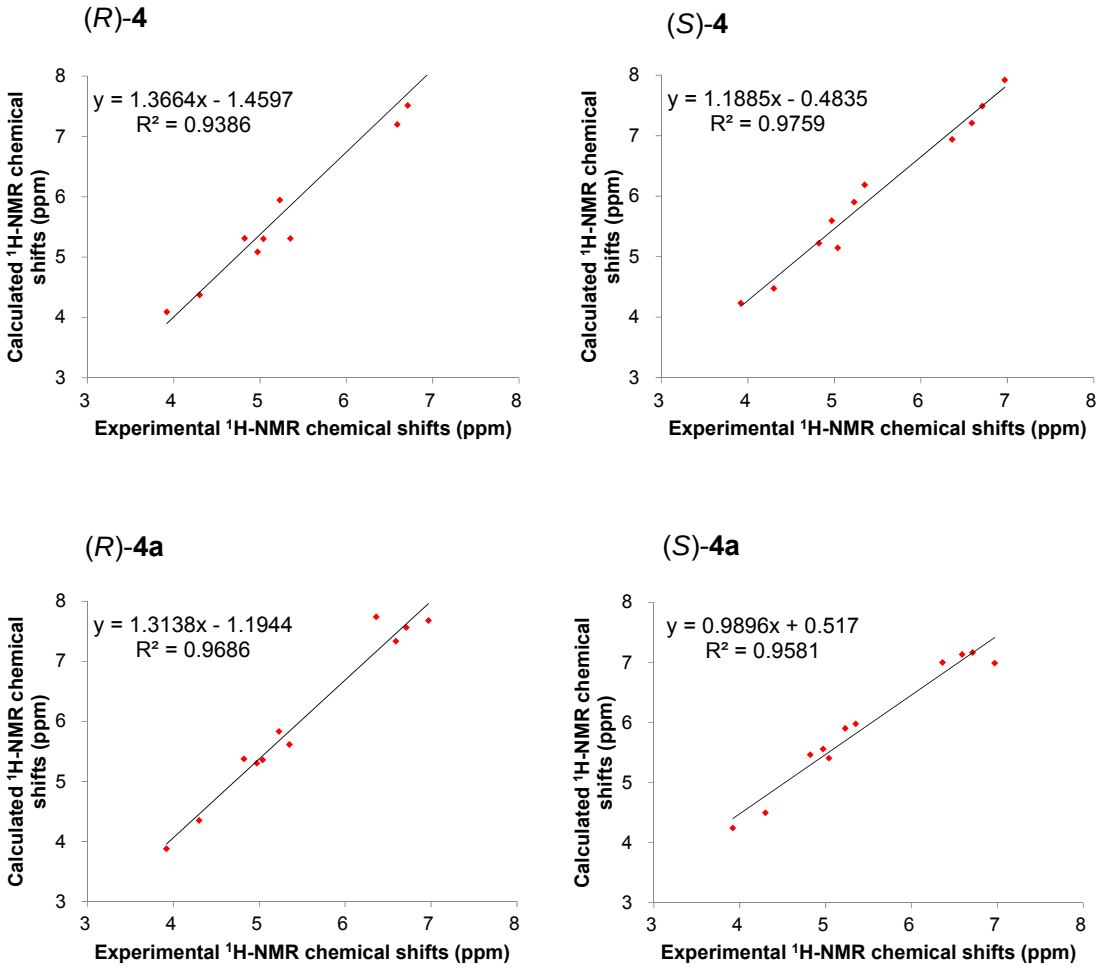


Fig. S8. Correlation plots of experimental ^{13}C NMR chemical shifts versus corresponding calculated ^{13}C NMR chemical shifts of **4**.

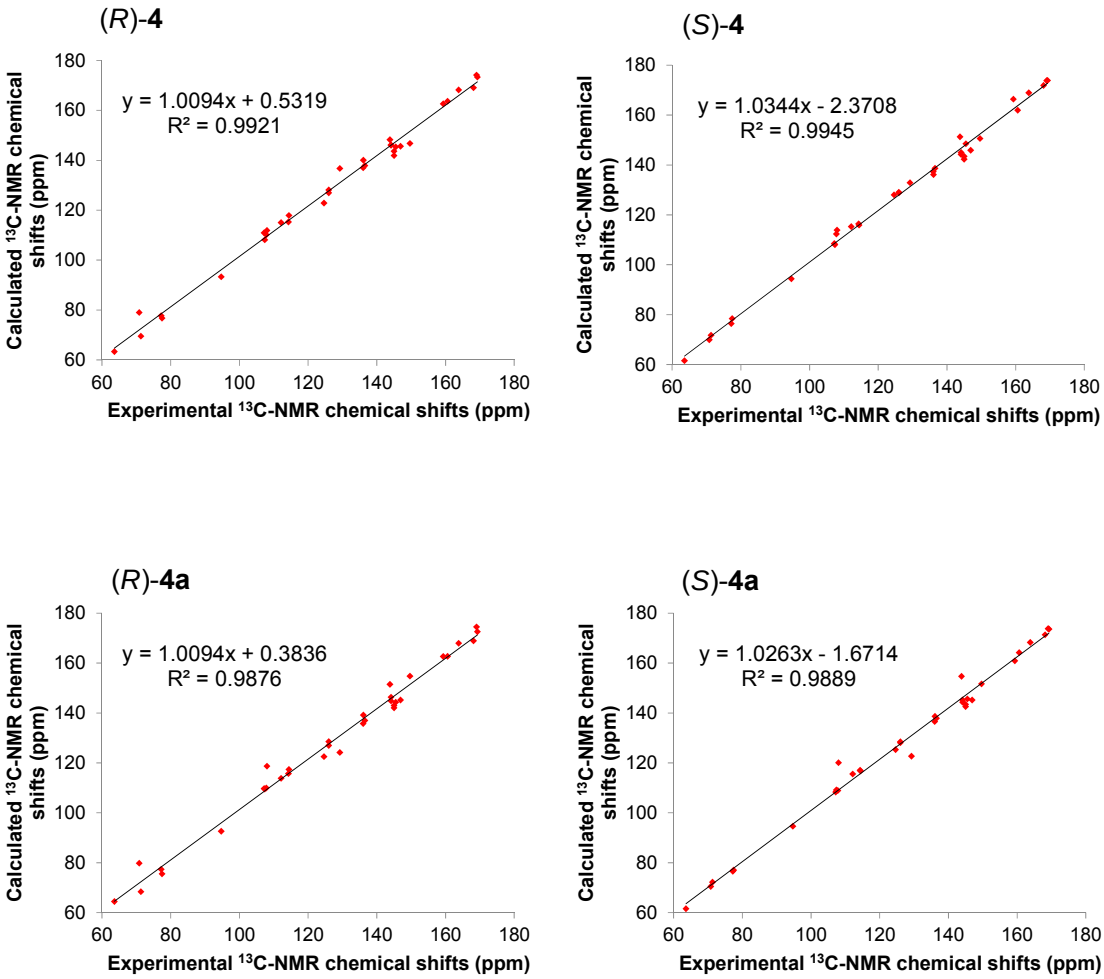


Table S9. Statistical parameters of calculated ^{1}H NMR chemical shifts of **4** (ppm).

	R^2	CMaxErr	CMAE
(*R*)-**4**	0.9386	0.57	0.20
(*S*)-**4**	0.9759	0.31	0.13
(*R*)-**4a**	0.9686	0.44	0.13
(*S*)-**4a**	0.9581	0.43	0.18

R^2: coefficient of determination; CMaxErr: corrected maximum absolute error with respect to the linear fit; CMAE: corrected mean absolute error with respect to the linear fit

Table S10. Statistical parameters of calculated ^{13}C NMR chemical shifts of **4** (ppm).

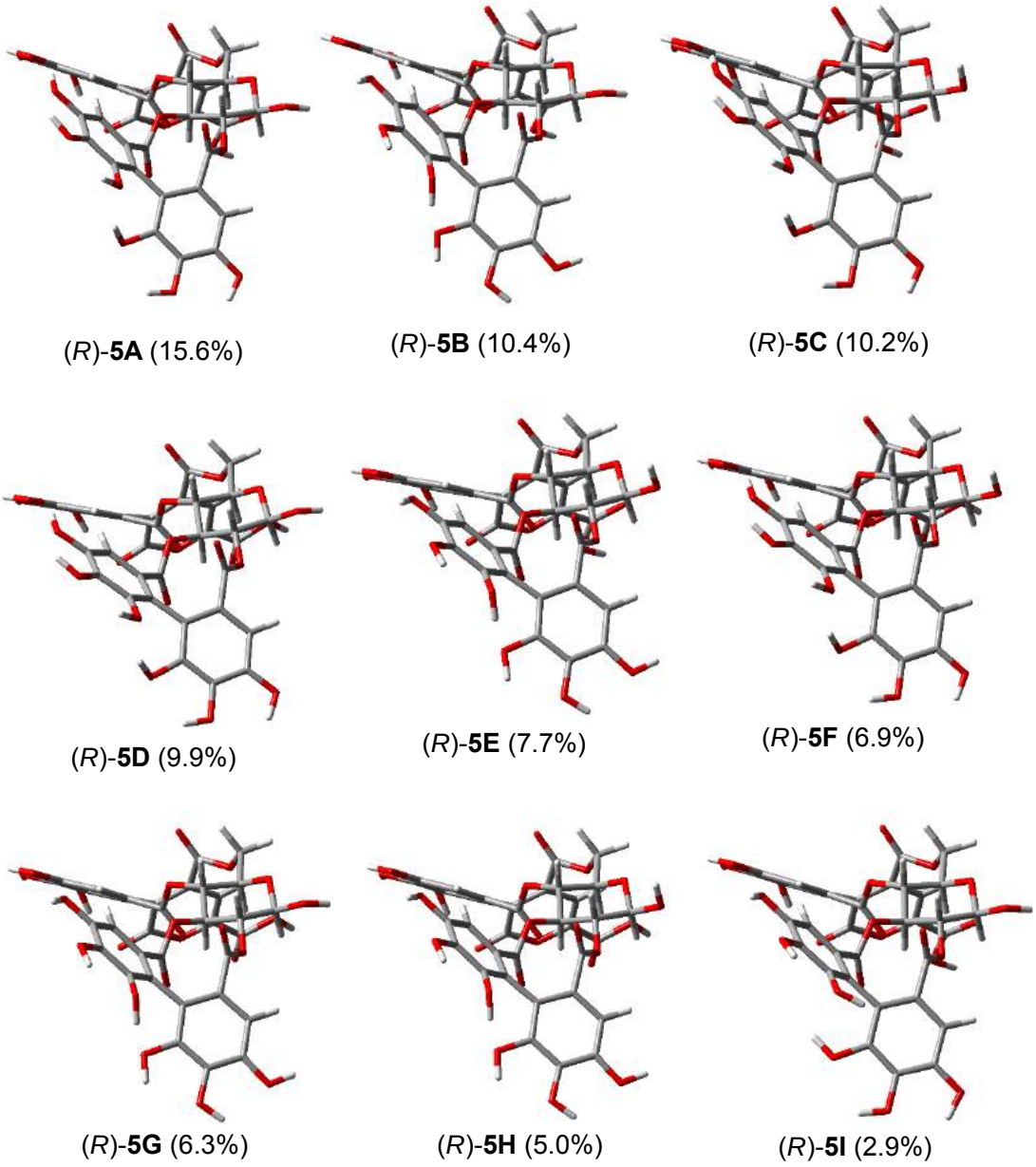
	R^2	CMaxErr	CMAE
(*R*)-**4**	0.9921	7.0	2.1
(*S*)-**4**	0.9945	5.2	1.7
(*R*)-**4a**	0.9876	9.2	2.5
(*S*)-**4a**	0.9889	10.6	2.0

R^2: coefficient of determination; CMaxErr: corrected maximum absolute error with respect to the linear fit; CMAE: corrected mean absolute error with respect to the linear fit

Table S11. The DP4 and DP4+ probability analysis of **4**.

	(*R*)-**4**	(*S*)-**4**	(*R*)-**4a**	(*S*)-**4a**
DP4 (^{1}H)	0.1%	70.9%	27.6%	1.4%
DP4 (^{13}C)	0.0%	99.9%	0.0%	0.0%
DP4 (^{1}H + ^{13}C)	0.0%	100.0%	0.0%	0.0%
sDP4+ (^{1}H)	0.30%	56.09%	42.74%	0.87%
sDP4+ (^{13}C)	0.08%	99.59%	0.00%	0.33%
sDP4+ (^{1}H + ^{13}C)	0.00%	99.99%	0.00%	0.01%
uDP4+ (^{1}H)	1.97%	3.71%	2.44%	91.88%
uDP4+ (^{13}C)	0.00%	100.00%	0.00%	0.00%
uDP4+ (^{1}H + ^{13}C)	0.00%	100.00%	0.00%	0.00%
DP4+ (^{1}H)	0.15%	53.00%	26.57%	20.28%
DP4+ (^{13}C)	0.00%	100.00%	0.00%	0.00%
DP4+ (^{1}H + ^{13}C)	0.00%	100.00%	0.00%	0.00%

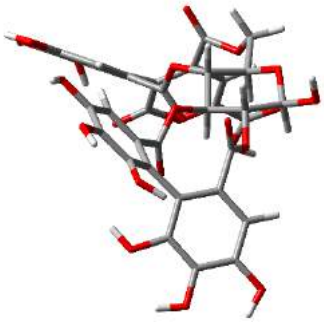
Fig. S9. Optimized conformers of (*R*)-**5** at the B3LYP/6-31G(d,p) level in acetone (PCM) with populations greater than 1% calculated from their relative Gibbs free energies (ΔG).



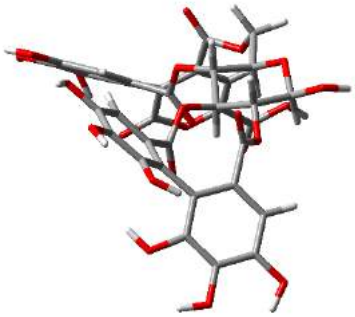
(*R*)-**5A** (15.6%) (*R*)-**5B** (10.4%) (*R*)-**5C** (10.2%)

(*R*)-**5D** (9.9%) (*R*)-**5E** (7.7%) (*R*)-**5F** (6.9%)

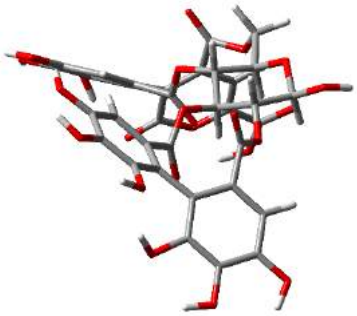
(*R*)-**5G** (6.3%) (*R*)-**5H** (5.0%) (*R*)-**5I** (2.9%)



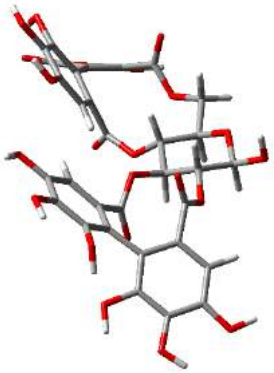
(*R*)-**5J** (1.9%)



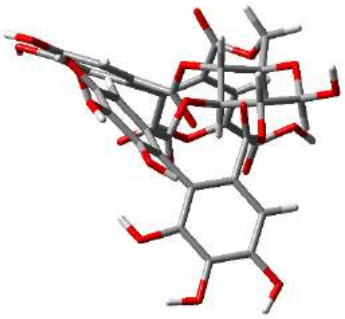
(*R*)-**5K** (1.9%)



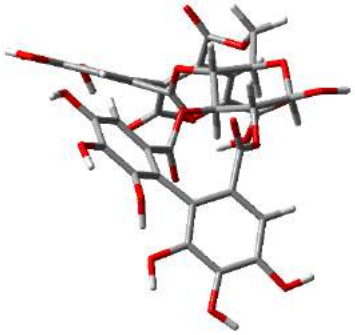
(*R*)-**5L** (1.5%)



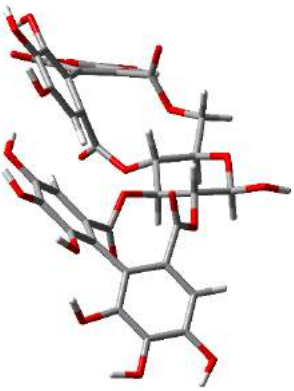
(*R*)-**5M** (1.4%)



(*R*)-**5N** (1.3%)

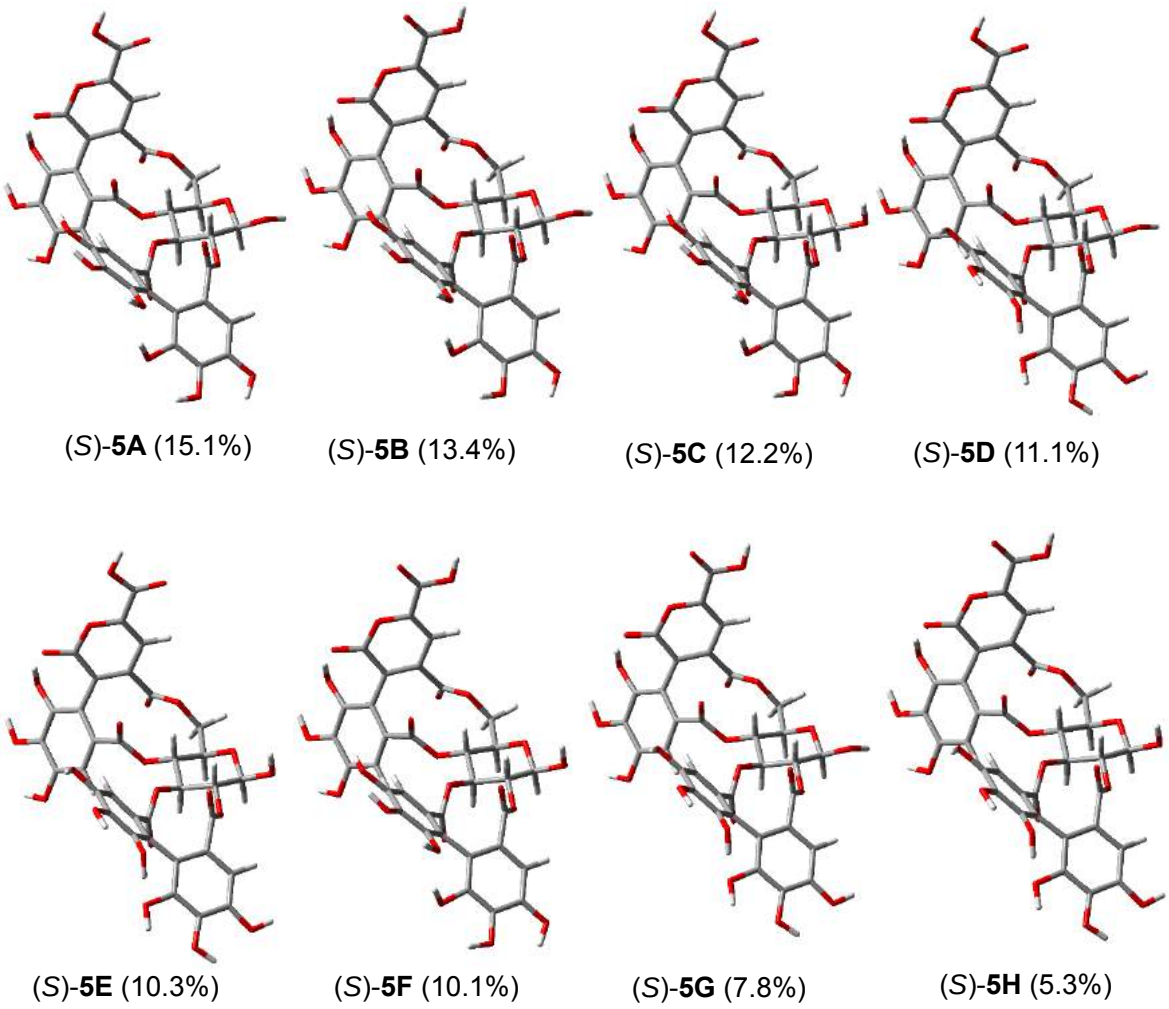


(*R*)-**5O** (1.1%)



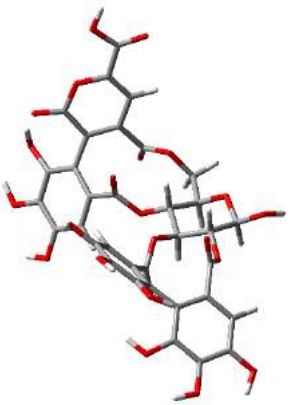
(*R*)-**5P** (1.1%)

Fig. S10.Optimized conformers of (*S*)-**5** at the B3LYP/6-31G(d,p) level in acetone (PCM) with populations greater than 1% calculated from their relative Gibbs free energies (Δ*G*).



(*S*)-**5A** (15.1%) (*S*)-**5B** (13.4%) (*S*)-**5C** (12.2%) (*S*)-**5D** (11.1%)

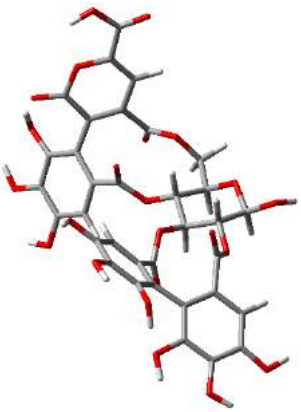
(*S*)-**5E** (10.3%) (*S*)-**5F** (10.1%) (*S*)-**5G** (7.8%) (*S*)-**5H** (5.3%)



(*S*)-**5I** (2.4%)

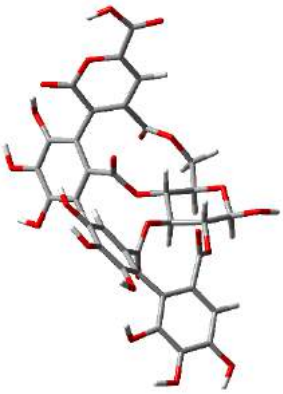
(*S*)-**5J** (1.6%)

(*S*)-**5K** (1.6%)

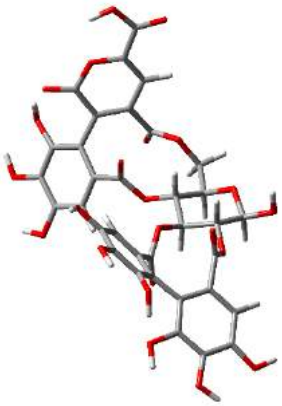


(*S*)-**5L** (1.4%)

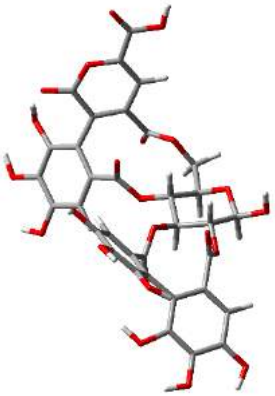
(*S*)-**5M** (1.4%)



(*S*)-**5N** (1.4%)

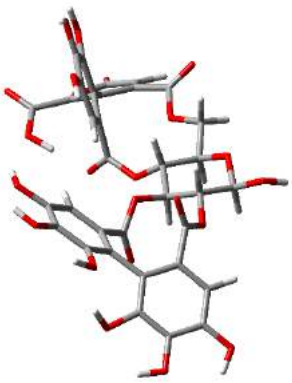


(*S*)-**5O** (1.2%)

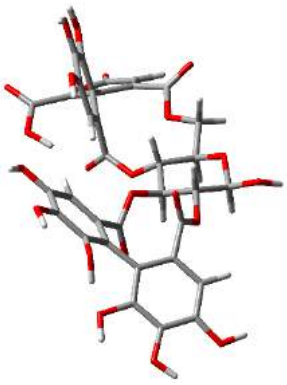


(*S*)-**5P** (1.0%)

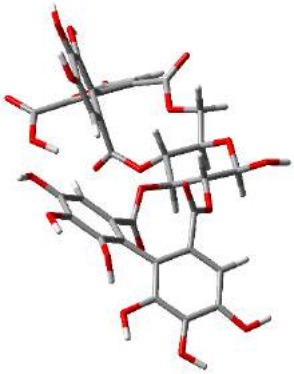
Fig. S11. Optimized conformers of (*R*)-**5a** at the B3LYP/6-31G(d,p) level in acetone (PCM) with populations greater than 1% calculated from their relative Gibbs free energies (ΔG).



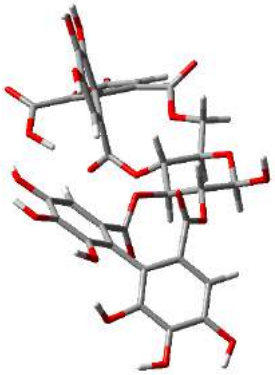
(*R*)-**5aA** (24.3%)



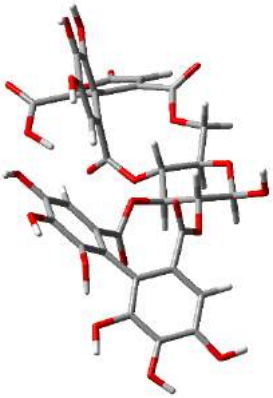
(*R*)-**5aA** (18.1%)



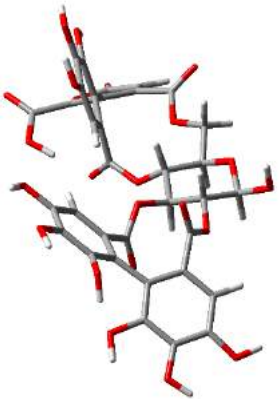
(*R*)-**5aA** (11.5%)



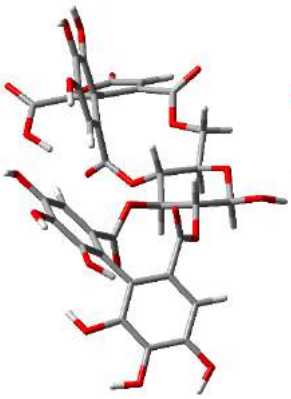
(*R*)-**5aA** (10.5%)



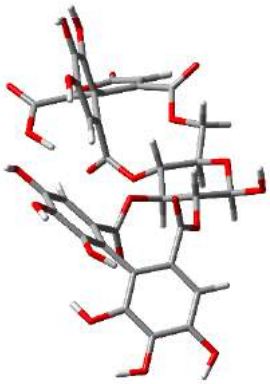
(*R*)-**5aA** (10.0%)



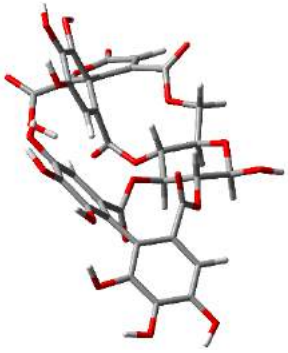
(*R*)-**5aA** (9.1%)



(*R*)-**5aA** (1.7%)

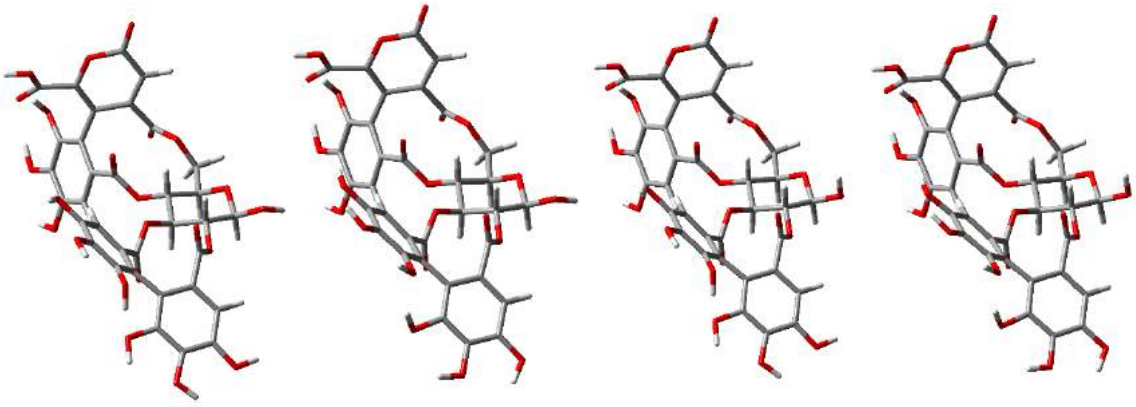


(*R*)-**5aA** (1.3%)

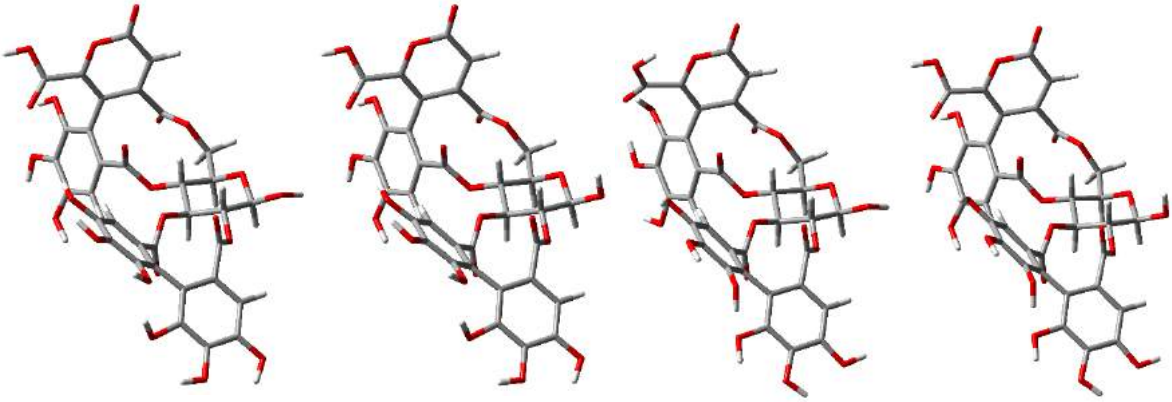


(*R*)-**5aA** (1.4%)

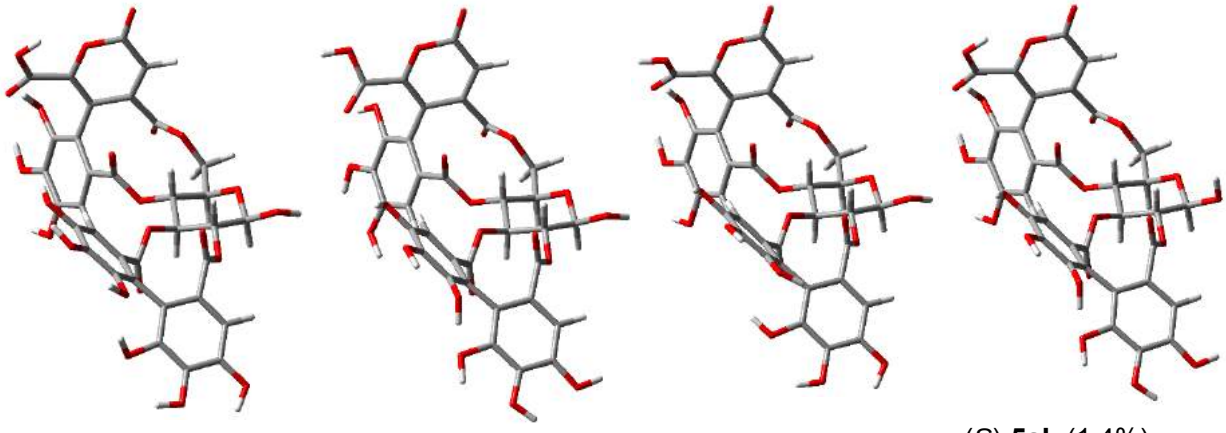
Fig. S12. Optimized conformers of (*S*)-**5a** at the B3LYP/6-31G(d,p) level in acetone (PCM) with populations greater than 1% calculated from their relative Gibbs free energies (ΔG).



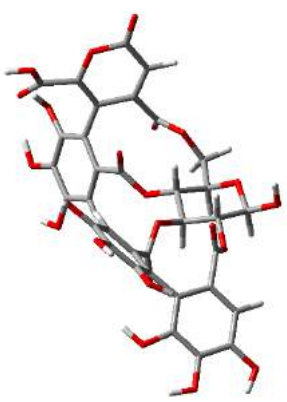
(*S*)-**5aA** (1.4%) (*S*)-**5aB** (1.4%) (*S*)-**5aC** (1.4%) (*S*)-**5aD** (1.4%)



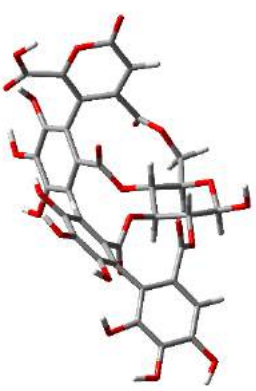
(*S*)-**5aE** (1.4%) (*S*)-**5aF** (1.4%) (*S*)-**5aG** (1.4%) (*S*)-**5aH** (1.4%)



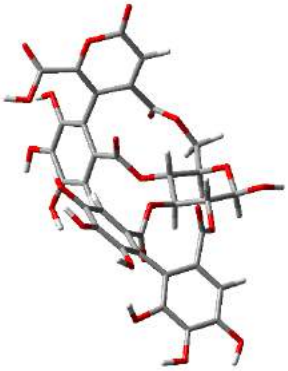
(*S*)-**5aI** (1.4%) (*S*)-**5aJ** (1.4%) (*S*)-**5aK** (1.4%) (*S*)-**5aL** (1.4%)



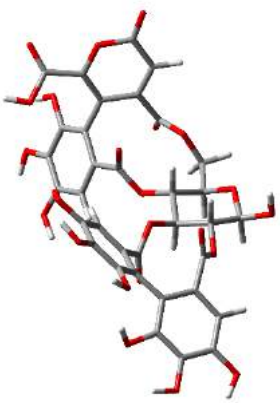
(*S*)-**5aM** (1.4%)



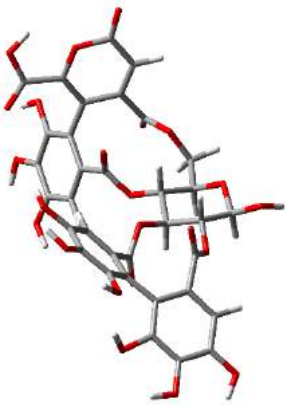
(*S*)-**5aN** (1.4%)



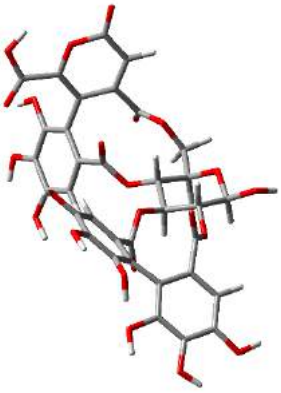
(*S*)-**5aO** (1.4%)



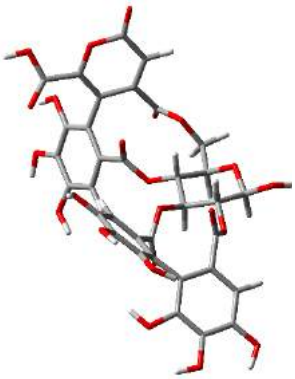
(*S*)-**5aP** (1.4%)



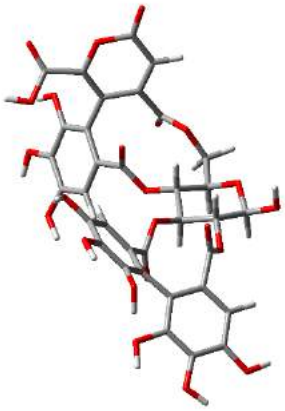
(*S*)-**5aQ** (1.4%)



(*S*)-**5aR** (1.4%)



(*S*)-**5aS** (1.4%)



(*S*)-**5aT** (1.4%)

Table S12. Calculated ^{1}H NMR chemical shifts of (*R*)-**5**.

	calculated[a]																		experimental[b]
Position	(*R*)-**5A**	(*R*)-**5B**	(*R*)-**5C**	(*R*)-**5D**	(*R*)-**5E**	(*R*)-**5F**	(*R*)-**5G**	(*R*)-**5H**	(*R*)-**5I**	(*R*)-**5J**	(*R*)-**5K**	(*R*)-**5L**	(*R*)-**5M**	(*R*)-**5N**	(*R*)-**5O**	(*R*)-**5P**	averaged-(*R*)-**5**	averaged-(*R*)-**5** (corrected)	**5**
Glucose-1	5.55	5.54	5.23	5.56	5.22	5.24	5.55	5.23	5.51	5.19	5.52	5.55	5.16	5.20	5.54	5.51	5.42	4.90	4.97
2	5.35	5.36	5.17	5.36	5.17	5.17	5.36	5.17	5.28	5.10	5.29	5.35	5.28	5.10	5.36	5.47	5.28	4.79	4.79
3	6.48	6.49	6.48	6.49	6.49	6.49	6.49	6.49	6.42	6.42	6.42	6.48	5.94	6.42	6.48	5.83	6.46	5.75	5.19
4	4.57	4.59	4.54	4.57	4.57	4.55	4.60	4.57	4.54	4.52	4.54	4.57	5.49	4.52	4.59	5.37	4.59	4.23	5.08
5	5.04	5.04	5.05	5.06	5.05	5.06	5.06	5.07	5.01	5.02	5.03	5.04	4.44	5.04	5.04	4.44	5.03	4.58	4.55
6a	4.44	4.44	4.46	4.44	4.46	4.46	4.44	4.46	4.43	4.46	4.43	4.45	4.33	4.46	4.44	4.36	4.44	4.11	4.02
6b	5.73	5.74	5.72	5.73	5.73	5.72	5.74	5.73	5.73	5.73	5.73	5.73	5.38	5.73	5.74	5.58	5.72	5.15	4.98
A-Ring 6	7.24	7.03	7.26	7.24	7.05	7.26	7.03	7.05	7.16	7.18	7.16	7.24	7.23	7.17	7.04	7.33	7.17	6.33	6.57
B-Ring 6	7.27	7.46	7.27	7.27	7.46	7.27	7.47	7.46	7.43	7.43	7.43	7.27	7.73	7.43	7.46	7.55	7.37	6.49	6.33
C-Ring 6	7.62	7.65	7.62	7.63	7.64	7.63	7.65	7.65	7.63	7.63	7.64	7.62	7.98	7.64	7.65	8.26	7.65	6.72	6.55
D-Ring 6	8.02	8.01	8.03	7.96	8.02	7.97	7.96	7.97	8.01	8.01	7.95	7.96	7.84	7.96	7.96	7.89	7.99	7.00	7.02

[a] Calculated using the GIAO method at the mPW1PW91/6-311+G(2d,p) level in acetone (PCM). [b] Measured in acetone-d_6 + D_2O. [c] Averaged according to the Boltzmann distribution theory at 298 K based on relative Gibbs free energies. [d] Linearly corrected for the experimental data.

Table S13. Calculated ^{1}H NMR chemical shifts of (*S*)-**5**.

	calculated[a]																		experimental[b]
Position	(*S*)-**5A**	(*S*)-**5B**	(*S*)-**5C**	(*S*)-**5D**	(*S*)-**5E**	(*S*)-**5F**	(*S*)-**5G**	(*S*)-**5H**	(*S*)-**5I**	(*S*)-**5J**	(*S*)-**5K**	(*S*)-**5L**	(*S*)-**5M**	(*S*)-**5N**	(*S*)-**5O**	(*S*)-**5P**	averaged-(*S*)-**5**	averaged-(*S*)-**5** (corrected)	**5**
Glucose-1	5.47	5.49	5.17	5.47	5.16	5.18	5.48	5.16	5.46	5.46	5.15	5.46	5.17	5.46	5.17	5.15	5.34	4.83	4.97
2	5.39	5.39	5.23	5.39	5.22	5.21	5.39	5.21	5.35	5.36	5.15	5.40	5.24	5.40	5.24	5.16	5.31	4.81	4.79
3	5.90	5.94	5.91	5.92	5.93	5.94	5.96	5.96	5.92	5.97	5.92	5.90	5.90	5.89	5.91	5.97	5.93	5.33	5.19
4	5.77	5.78	5.76	5.80	5.80	5.77	5.80	5.80	5.77	5.77	5.76	5.80	5.76	5.77	5.79	5.76	5.78	5.21	5.08
5	4.46	4.47	4.50	4.46	4.50	4.51	4.46	4.50	4.46	4.44	4.49	4.46	4.49	4.45	4.50	4.47	4.48	4.11	4.55
6a	4.34	4.34	4.37	4.34	4.38	4.37	4.33	4.36	4.33	4.31	4.36	4.36	4.37	4.34	4.39	4.34	4.35	4.01	4.02
6b	6.13	6.12	6.15	6.13	6.15	6.15	6.10	6.12	6.10	6.03	6.12	6.12	6.12	6.11	6.13	6.05	6.13	5.50	4.98
A-Ring 6	7.36	7.35	7.38	7.18	7.20	7.37	7.16	7.18	7.23	7.20	7.26	7.17	7.38	7.36	7.19	7.22	7.29	6.47	6.57
B-Ring 6	6.85	6.81	6.85	7.04	7.04	6.81	7.01	7.00	6.98	6.97	6.97	7.07	6.88	6.88	7.07	6.96	6.92	6.16	6.33
C-Ring 6	7.27	7.27	7.28	7.28	7.28	7.27	7.28	7.28	7.29	7.30	7.29	7.30	7.31	7.30	7.31	7.30	7.28	6.46	6.55
D-Ring 6	8.15	8.07	8.15	8.16	8.16	8.06	8.05	8.04	8.13	8.00	8.13	8.09	8.06	8.06	8.09	7.99	8.11	7.16	7.02

[a] Calculated using the GIAO method at the mPW1PW91/6-311+G(2d,p) level in acetone (PCM). [b] Measured in acetone-d_6 + D_2O. [c] Averaged according to the Boltzmann distribution theory at 298 K based on relative Gibbs free energies. [d] Linearly corrected for the experimental data.

Table S14. Calculated ^{1}H NMR chemical shifts of (*R*)-**5a**.

	calculated[a]											experimental[b]
Position	(*R*)-**5aA**	(*R*)-**5aB**	(*R*)-**5aC**	(*R*)-**5aD**	(*R*)-**5aE**	(*R*)-**5aF**	(*R*)-**5aG**	(*R*)-**5aH**	(*R*)-**5aI**	averaged-(*R*)-**5a**	averaged-(*R*)-**5a** (corrected)	**5**
Glucose-1	5.49	5.46	5.46	5.19	5.16	5.15	5.42	5.12	5.52	5.36	5.07	4.97
2	5.39	5.38	5.41	5.22	5.20	5.23	5.30	5.13	5.43	5.32	5.04	4.79
3	6.00	6.01	6.03	6.00	6.01	6.03	5.95	5.94	5.92	6.01	5.60	5.19
4	5.64	5.64	5.70	5.63	5.63	5.69	5.57	5.56	5.43	5.65	5.30	5.08
5	4.40	4.39	4.37	4.44	4.43	4.41	4.37	4.41	4.49	4.40	4.28	4.55
6a	3.88	3.90	3.92	3.86	3.89	3.89	3.89	3.87	4.01	3.89	3.86	4.02
6b	4.61	4.56	4.59	4.62	4.56	4.61	4.54	4.55	4.51	4.59	4.43	4.98
A-Ring 6	7.32	7.12	7.11	7.34	7.14	7.13	7.28	7.29	7.34	7.21	6.58	6.57
B-Ring 6	7.16	7.46	7.51	7.15	7.45	7.50	7.34	7.33	7.63	7.35	6.69	6.33
C-Ring 6	7.33	7.41	7.59	7.32	7.42	7.58	7.33	7.34	8.05	7.42	6.76	6.55
D-Ring 6	7.03	7.06	7.03	7.05	7.09	7.06	7.02	7.05	7.10	7.05	6.45	7.02

[a] Calculated using the GIAO method at the mPW1PW91/6-311+G(2d,p) level in acetone (PCM). [b] Measured in acetone-d_6 + D_2O. [c] Averaged according to the Boltzmann distribution theory at 298 K based on relative Gibbs free energies. [d] Linearly corrected for the experimental data.

Table S15. Calculated ^{1}H NMR chemical shifts of (*S*)-**5a**.

	calculated[a]																					experimental[b]
Position	(*S*)-**5aA**	(*S*)-**5aB**	(*S*)-**5aC**	(*S*)-**5aD**	(*S*)-**5aE**	(*S*)-**5aF**	(*S*)-**5aG**	(*S*)-**5aH**	(*S*)-**5aI**	(*S*)-**5aJ**	(*S*)-**5aK**	(*S*)-**5aL**	(*S*)-**5aM**	(*S*)-**5aN**	(*S*)-**5aO**	(*S*)-**5aP**	(*S*)-**5aQ**	(*S*)-**5aR**	(*S*)-**5aS**	(*S*)-**5aT**	averaged-(*S*)-**5a**	averaged-(*S*)-**5a** (corrected)	**5**
Glucose-1	5.49	5.50	5.17	5.19	5.48	5.16	5.49	5.14	5.50	5.46	5.45	5.17	5.14	5.18	5.49	5.17	5.48	5.46	5.44	5.14	5.35	4.88	4.97
2	5.48	5.46	5.28	5.27	5.45	5.25	5.47	5.25	5.45	5.45	5.38	5.27	5.18	5.26	5.48	5.28	5.45	5.45	5.36	5.28	5.37	4.90	4.79
3	5.93	5.90	5.93	5.90	5.86	5.86	5.93	5.88	5.90	5.89	5.86	5.92	5.86	5.90	5.87	5.87	5.86	5.89	5.83	5.89	5.90	5.40	5.19
4	5.82	5.79	5.80	5.78	5.84	5.83	5.82	5.85	5.79	5.86	5.78	5.80	5.76	5.78	5.91	5.90	5.83	5.85	5.81	5.92	5.81	5.32	5.08
5	4.37	4.37	4.40	4.41	4.31	4.35	4.37	4.34	4.37	4.31	4.35	4.40	4.38	4.40	4.34	4.38	4.31	4.31	4.29	4.37	4.37	3.95	4.55
6a	4.36	4.36	4.39	4.39	4.28	4.31	4.37	4.31	4.37	4.28	4.35	4.40	4.38	4.40	4.32	4.35	4.28	4.28	4.27	4.35	4.36	3.94	4.02
6b	5.76	5.76	5.76	5.76	5.59	5.59	5.77	5.60	5.76	5.61	5.72	5.78	5.73	5.77	5.68	5.68	5.57	5.58	5.61	5.70	5.72	5.23	4.98
A-Ring 6	7.08	7.34	7.09	7.36	7.31	7.32	7.07	7.05	7.34	7.04	7.24	7.08	7.25	7.36	7.31	7.32	7.32	7.05	7.23	7.05	7.21	6.64	6.57
B-Ring 6	7.19	6.98	7.19	6.98	7.00	7.00	7.17	7.22	6.96	7.23	7.10	7.16	7.09	6.95	7.03	7.03	7.00	7.22	7.11	7.27	7.09	6.53	6.33
C-Ring 6	7.51	7.50	7.52	7.51	7.16	7.16	7.53	7.16	7.52	7.16	7.51	7.53	7.51	7.53	7.20	7.20	7.15	7.15	7.16	7.20	7.42	6.84	6.55
D-Ring 6	7.02	7.03	7.01	7.02	6.84	6.84	7.10	6.85	7.09	6.85	7.08	7.08	7.06	7.08	6.77	6.77	6.88	6.89	6.86	6.77	6.98	6.43	7.02

[a] Calculated using the GIAO method at the mPW1PW91/6-311+G(2d,p) level in acetone (PCM). [b] Measured in acetone-d_6 + D_2O. [c] Averaged according to the Boltzmann distribution theory at 298 K based on relative Gibbs free energies. [d] Linearly corrected for the experimental data.

Table S16. Calculated ^{13}C NMR chemical shifts of (*R*)-**5**.

	calculated[a]																		experimental[b]
Position	(*R*)-**5A**	(*R*)-**5B**	(*R*)-**5C**	(*R*)-**5D**	(*R*)-**5E**	(*R*)-**5F**	(*R*)-**5G**	(*R*)-**5H**	(*R*)-**5I**	(*R*)-**5J**	(*R*)-**5K**	(*R*)-**5L**	(*R*)-**5M**	(*R*)-**5N**	(*R*)-**5O**	(*R*)-**5P**	averaged-(*R*)-**5**	averaged-(*R*)-**5** (corrected)	**5**
Glucose-1	95.4	95.4	95.4	95.5	95.3	95.4	95.4	95.4	95.4	95.3	95.4	95.4	93.6	95.4	95.4	93.5	95.4	93.2	94.5
2	77.6	77.9	79.8	77.6	80.1	79.7	77.9	80.1	77.4	79.7	77.4	77.6	77.5	79.6	77.9	74.8	78.5	76.2	77.6
3	74.2	73.9	74.0	74.2	73.8	74.0	73.9	73.8	73.7	73.5	73.7	74.2	77.8	73.5	73.9	77.0	74.1	71.7	76.8
4	76.2	76.3	76.1	76.3	76.1	76.1	76.3	76.1	76.2	76.1	76.2	76.3	78.4	76.1	76.3	78.5	76.3	73.9	69.7
5	69.7	69.7	70.4	69.7	70.5	70.4	69.7	70.5	69.6	70.4	69.6	69.7	70.0	70.4	69.7	69.2	70.0	67.6	66.2
6	64.6	64.6	64.5	64.6	64.5	64.5	64.6	64.5	64.5	64.4	64.5	64.6	63.1	64.4	64.6	62.6	64.5	62.0	65.0
A-Ring 1	126.9	127.8	126.7	126.8	127.6	126.6	127.7	127.6	127.6	127.4	127.6	126.8	129.1	127.4	127.8	128.3	127.2	125.4	124.1 [e]
2	116.9	115.1	116.9	116.9	115.2	116.9	115.2	115.2	108.0	107.9	108.1	116.9	116.1	108.0	115.1	117.9	115.4	113.4	114.3
3	142.0	142.4	142.0	142.0	142.4	141.9	142.4	142.3	142.8	142.8	142.7	142.1	141.9	142.7	142.4	143.4	142.2	140.5	144.0
4	138.9	135.0	138.9	138.9	135.0	138.8	134.9	134.9	136.8	136.9	136.8	138.9	135.2	136.9	135.0	140.4	137.2	135.4	136.0
5	145.4	143.7	145.4	145.4	143.6	145.4	143.6	143.6	147.6	147.6	147.6	145.4	144.1	147.6	143.7	146.6	145.0	143.3	144.8
6	109.2	106.2	109.3	109.2	106.3	109.3	106.2	106.3	107.6	107.7	107.5	109.2	107.6	107.6	106.2	109.2	108.0	105.9	107.2
7	173.9	173.4	174.1	173.9	173.7	174.2	173.4	173.7	173.3	173.5	173.3	173.9	173.4	173.5	173.4	174.1	173.8	172.3	169.1
B-Ring 1	128.3	127.4	128.3	128.3	127.3	128.2	127.4	127.3	129.6	129.6	129.7	128.3	126.8	129.6	127.3	127.3	128.0	126.2	125.7 [e]
2	115.9	118.2	115.9	115.9	118.2	115.8	118.2	118.2	110.0	110.0	110.0	115.9	117.8	110.0	118.2	115.4	116.2	114.2	114.1
3	142.7	144.0	142.7	142.8	144.0	142.7	144.1	144.1	143.2	143.1	143.2	142.7	141.9	143.2	144.0	141.7	143.2	141.5	144.0
4	135.5	140.1	135.6	135.6	140.2	135.7	140.2	140.2	136.7	136.8	136.8	135.5	140.0	136.8	140.1	135.3	137.4	135.6	135.9
5	144.0	146.3	144.0	144.1	146.3	144.0	146.3	146.4	147.9	148.0	148.0	144.0	146.0	148.0	146.3	144.3	145.3	143.5	144.8
6	106.6	109.6	106.6	106.7	109.6	106.7	109.6	109.6	108.8	108.9	108.9	106.6	110.1	108.9	109.5	110.1	108.0	106.0	106.9
7	173.9	174.3	173.8	173.9	174.2	173.8	174.3	174.2	173.7	173.5	173.7	173.9	173.8	173.5	174.3	172.7	173.9	172.5	169.7
C-Ring 1	128.0	128.1	128.0	128.1	128.1	128.1	128.2	128.1	127.9	127.9	128.0	128.0	123.4	127.9	128.1	124.3	127.9	126.1	125.6 [e]
2	114.3	114.2	114.3	114.2	114.3	114.3	114.2	114.2	114.3	114.4	114.2	114.2	116.7	114.3	114.2	119.2	114.4	112.4	112.1
3	145.0	144.9	145.1	145.1	145.0	145.1	145.0	145.0	144.9	144.9	144.9	144.8	148.3	145.0	144.7	149.1	145.1	143.4	145.1
4	139.9	140.0	140.0	140.0	140.0	140.0	140.0	140.1	139.9	139.9	140.0	140.1	141.7	140.0	140.1	142.2	140.0	138.3	136.5
5	146.9	147.1	146.9	146.9	147.0	146.9	147.1	147.1	147.1	147.0	147.1	147.0	148.5	147.1	147.2	147.1	147.0	145.3	146.5
6	112.6	112.6	112.5	112.6	112.6	112.6	112.7	112.6	112.7	112.6	112.7	112.7	113.9	112.7	112.8	113.2	112.6	110.6	106.9
7	171.3	171.6	171.3	171.3	171.6	171.2	171.6	171.5	171.6	171.5	171.5	171.3	170.4	171.5	171.6	170.3	171.4	169.9	168.1
D-Ring 1	149.3	149.1	149.3	149.2	149.2	149.3	149.0	149.1	149.2	149.3	149.1	149.7	151.2	149.2	149.5	151.7	149.3	147.6	146.0
2	130.1	129.9	130.0	130.2	129.8	130.1	129.9	129.9	129.7	129.6	129.7	129.9	131.5	129.6	129.6	132.4	130.0	128.2	125.1
3	165.6	165.5	165.6	166.1	165.5	166.1	166.0	166.0	165.5	165.5	166.0	164.4	165.1	166.0	164.4	165.3	165.7	164.2	161.9
4	162.4	162.4	162.4	161.5	162.4	161.5	161.5	161.6	162.4	162.4	161.5	161.0	162.4	161.5	161.0	162.3	162.0	160.5	163.5
5	150.3	150.3	150.4	149.4	150.3	149.5	149.3	149.4	150.3	150.3	149.4	149.0	151.6	149.4	149.0	151.7	150.0	148.3	155.6
6	115.4	115.4	115.4	114.9	115.4	114.9	114.9	114.9	115.4	115.4	114.9	113.8	113.9	114.9	113.8	114.1	115.1	113.1	105.8
7	167.6	167.6	167.5	167.5	167.6	167.5	167.6	167.6	167.6	167.6	167.6	167.3	168.8	167.6	167.4	169.0	167.6	166.1	165.1

[a] Calculated using the GIAO method at the mPW1PW91/6-311+G(2d,p) level in acetone (PCM). [b] Measured in acetone-d_6 + D_2O. [c] Averaged according to the Boltzmann distribution theory at 298 K based on relative Gibbs free energies. [d] Linearly corrected for the experimental data. [e] May be interchanged in each column.

Table S17. Calculated ^{13}C NMR chemical shifts of (*S*)-**5**.

	calculated[a]																		experimental[b]
Position	(*S*)-**5A**	(*S*)-**5B**	(*S*)-**5C**	(*S*)-**5D**	(*S*)-**5E**	(*S*)-**5F**	(*S*)-**5G**	(*S*)-**5H**	(*S*)-**5I**	(*S*)-**5J**	(*S*)-**5K**	(*S*)-**5L**	(*S*)-**5M**	(*S*)-**5N**	(*S*)-**5O**	(*S*)-**5P**	averaged-(*S*)-**5**	averaged-(*S*)-**5** (corrected)	**5**
Glucose-1	94.5	94.5	94.5	94.5	94.5	94.6	94.5	94.5	94.6	94.6	94.6	94.5	94.6	94.5	94.5	94.7	94.5	92.8	94.5
2	76.4	76.5	78.4	76.7	78.7	78.5	76.9	78.8	76.4	76.4	78.4	76.6	78.3	76.3	78.6	78.4	77.4	75.8	77.6
3	76.7	76.6	76.6	76.3	76.2	76.5	76.3	76.2	76.1	76.1	76.0	76.3	76.6	76.8	76.2	75.9	76.4	74.8	76.8
4	68.5	68.5	68.4	68.4	68.3	68.4	68.4	68.3	68.3	68.3	68.2	68.5	68.4	68.5	68.4	68.2	68.4	66.9	69.7
5	70.6	70.7	71.5	70.8	71.6	71.5	70.8	71.6	70.6	70.7	71.4	70.8	71.5	70.6	71.7	71.5	71.1	69.5	66.2
6	63.9	64.0	64.0	63.9	64.0	64.1	63.9	64.0	63.9	63.9	64.0	64.1	64.2	64.1	64.2	64.0	64.0	62.5	65.0
A-Ring 1	128.8	128.6	128.7	129.4	129.3	128.5	129.3	129.1	128.5	128.2	128.4	129.4	128.6	128.8	129.3	128.1	128.9	126.9	125.6 [e]
2	118.2	118.3	118.2	115.9	115.9	118.4	115.9	115.9	108.2	108.5	108.2	115.8	117.9	117.9	115.8	108.6	116.7	114.8	114.3
3	143.0	142.7	143.1	142.3	142.3	142.7	142.1	142.1	141.9	141.7	141.9	142.5	143.3	143.2	142.6	141.7	142.6	140.5	144.0
4	138.5	138.3	138.7	134.0	134.0	138.4	133.9	133.9	135.3	135.3	135.3	134.2	138.9	138.7	134.2	135.4	136.6	134.5	136.0
5	145.2	145.0	145.2	142.7	142.7	145.0	142.6	142.6	146.7	146.6	146.7	142.9	145.3	145.3	143.0	146.6	144.3	142.2	144.8
6	109.5	109.6	109.6	107.3	107.4	109.6	107.3	107.4	107.7	107.8	107.9	107.3	109.6	109.5	107.4	107.9	108.6	106.8	107.2
7	174.0	174.0	174.3	173.5	173.8	174.2	173.4	173.7	173.3	173.2	173.5	173.5	174.3	174.1	173.8	173.4	173.9	171.5	169.1
B-Ring 1	128.5	128.4	128.5	127.7	127.7	128.4	127.6	127.6	128.7	128.3	128.6	127.7	128.5	128.5	127.6	128.3	128.2	126.2	124.1 [e]
2	116.0	116.0	116.0	117.7	117.8	115.9	117.9	117.9	110.7	110.5	110.6	117.7	116.1	116.1	117.8	110.4	116.3	114.4	114.1
3	143.0	143.1	143.0	144.8	144.9	143.1	145.0	145.1	143.0	142.4	143.1	144.6	142.9	142.9	144.7	142.5	143.7	141.6	144.0
4	135.3	135.3	135.4	139.9	140.0	135.4	139.9	140.0	135.9	135.7	135.9	139.8	135.4	135.3	139.9	135.7	137.1	135.1	135.9
5	143.8	143.7	143.8	145.8	145.8	143.7	145.7	145.8	147.1	147.0	147.1	145.9	143.9	143.8	145.9	147.0	144.8	142.7	144.8
6	107.0	106.9	107.0	109.5	109.5	106.9	109.5	109.4	108.5	108.4	108.4	109.6	107.1	107.1	109.6	108.3	108.0	106.2	106.9
7	173.9	173.8	173.7	174.4	174.3	173.7	174.3	174.2	173.7	173.6	173.6	174.4	173.7	173.8	174.3	173.4	174.0	171.6	169.7
C-Ring 1	129.9	129.9	129.9	129.8	129.8	129.9	129.6	129.6	129.6	129.2	129.6	129.9	129.8	129.9	129.8	129.2	129.8	127.8	125.7 [e]
2	115.7	115.1	115.8	115.5	115.5	115.1	114.8	114.7	115.0	114.2	115.0	115.8	115.9	115.9	115.8	114.1	115.3	113.4	112.1
3	145.7	145.5	145.6	145.6	145.6	145.5	145.5	145.6	145.5	145.7	145.6	145.4	145.5	145.5	145.4	145.7	145.6	143.5	145.1
4	137.9	138.2	137.9	138.1	138.1	138.2	138.5	138.5	138.5	139.2	138.5	138.0	138.0	138.0	138.1	139.3	138.1	136.1	136.5
5	147.7	147.8	147.6	147.7	147.7	147.8	147.9	148.0	147.8	148.2	147.9	147.8	147.7	147.8	147.8	148.2	147.8	145.6	146.5
6	110.4	110.4	110.5	110.5	110.6	110.5	110.6	110.6	110.5	110.7	110.5	110.8	110.8	110.7	110.9	110.8	110.5	108.7	106.9
7	171.5	171.6	171.5	171.5	171.5	171.6	171.5	171.5	171.7	171.7	171.7	171.4	171.4	171.4	171.4	171.6	171.6	169.2	168.1
D-Ring 1	151.9	151.9	151.9	151.9	151.9	151.9	151.8	151.8	151.7	151.4	151.7	152.5	152.4	152.4	152.4	151.4	151.9	149.7	146.0
2	132.6	132.6	132.6	132.7	132.7	132.6	132.7	132.8	132.7	133.2	132.7	132.5	132.4	132.4	132.6	133.2	132.6	130.6	125.1
3	166.2	166.7	166.2	166.2	166.2	166.7	166.7	166.6	166.1	166.6	166.1	165.0	164.9	164.9	165.0	166.6	166.3	164.0	161.9
4	162.4	161.4	162.4	162.4	162.4	161.4	161.4	161.4	162.5	161.4	162.5	160.9	160.8	160.8	160.9	161.4	161.9	159.7	163.5
5	151.2	150.1	151.2	151.2	151.1	150.1	150.0	150.0	151.0	149.9	151.0	149.9	149.9	149.9	149.9	149.9	150.6	148.5	155.6
6	114.7	114.7	114.6	114.9	114.9	114.7	114.8	114.8	115.2	114.8	115.1	113.3	113.1	113.2	113.3	114.8	114.7	112.8	105.8
7	169.4	169.4	169.4	169.5	169.5	169.4	169.5	169.5	169.6	169.4	169.5	169.2	169.0	169.1	169.2	169.4	169.4	167.1	165.1

[a] *Calculated using the GIAO method at the mPW1PW91/6-311+G(2d,p) level in acetone (PCM).* [b] *Measured in acetone-d_6 + D_2O.* [c] *Averaged according to the Boltzmann distribution theory at 298 K based on relative Gibbs free energies.* [d] *Linearly corrected for the experimental data.* [e] *May be interchanged in each column.*

Table S18. Calculated ^{13}C NMR chemical shifts of (*R*)-**5a**.

	calculated[a]											experimental[b]
Position	(*R*)-**5aA**	(*R*)-**5aB**	(*R*)-**5aC**	(*R*)-**5aD**	(*R*)-**5aE**	(*R*)-**5aF**	(*R*)-**5aG**	(*R*)-**5aH**	(*R*)-**5aI**	averaged-(*R*)-**5a**	averaged-(*R*)-**5a** (corrected)	**5**
Glucose-1	93.4	93.2	93.4	93.5	93.3	93.4	93.2	93.2	92.8	93.4	92.1	94.5
2	74.0	74.3	74.6	75.7	75.9	76.3	74.0	75.6	74.0	74.8	73.8	77.6
3	76.4	76.4	76.5	76.2	76.2	76.2	76.4	76.1	76.8	76.4	75.3	76.8
4	78.9	79.3	79.5	78.8	79.1	79.3	79.5	79.3	80.4	79.1	78.1	69.7
5	68.6	68.7	68.7	69.3	69.4	69.4	68.7	69.4	68.6	68.9	68.0	66.2
6	65.7	65.7	65.7	65.6	65.7	65.7	65.7	65.7	66.6	65.7	64.8	65.0
A-Ring 1	127.4	128.3	128.5	127.2	128.1	128.3	129.4	129.2	128.3	127.9	126.4	125.7 [e]
2	117.7	116.1	116.2	117.7	116.0	116.2	108.3	108.3	117.3	116.5	115.0	114.3
3	143.5	142.8	142.7	143.4	142.8	142.7	143.2	143.4	143.8	143.1	141.3	144.0
4	140.9	136.5	136.4	140.9	136.5	136.4	137.3	137.4	140.2	138.3	136.6	136.0
5	146.7	144.6	144.6	146.7	144.6	144.5	148.9	148.9	146.7	145.6	143.8	144.8
6	109.3	106.9	106.7	109.5	107.1	106.9	108.8	108.9	109.9	108.0	106.6	107.2
7	174.0	173.5	173.4	174.2	173.7	173.6	173.5	173.6	174.4	173.8	171.7	169.1
B-Ring 1	127.7	126.9	126.8	127.7	126.9	126.8	128.3	128.3	127.4	127.3	125.7	125.6 [e]
2	115.6	117.2	117.1	115.6	117.2	117.0	110.0	109.9	116.2	116.3	114.8	114.1
3	141.6	142.5	142.3	141.5	142.5	142.2	142.2	142.1	142.4	142.1	140.3	144.0
4	135.0	139.8	140.1	134.9	139.7	140.0	136.1	135.8	135.8	137.8	136.1	135.9
5	144.3	146.0	146.2	144.2	145.9	146.1	147.2	147.1	144.2	145.3	143.6	144.8
6	107.0	109.4	110.0	107.0	109.4	109.9	108.1	107.9	109.9	108.5	107.2	106.9
7	173.3	173.7	173.9	173.2	173.6	173.8	173.2	173.0	172.4	173.5	171.5	169.7
C-Ring 1	123.1	122.8	122.6	123.1	122.7	122.7	122.6	122.6	122.3	122.8	121.3	124.1 [e]
2	111.6	111.1	108.6	111.7	111.1	108.6	111.0	111.0	110.5	110.7	109.3	112.1
3	148.0	148.2	146.1	148.0	148.1	145.9	148.4	148.3	145.8	147.6	145.8	145.1
4	136.0	136.0	136.4	136.0	136.0	136.4	136.3	136.2	137.7	136.1	134.5	136.5
5	144.7	144.9	147.5	144.7	144.9	147.5	144.9	144.9	146.2	145.4	143.7	146.5
6	105.4	105.8	109.2	105.4	105.8	109.1	105.8	105.8	109.0	106.5	105.1	106.9
7	178.1	178.3	178.5	178.1	178.2	178.4	178.2	178.2	178.0	178.2	176.1	168.1
D-Ring 1	151.6	151.2	151.5	151.6	151.2	151.5	151.3	151.3	152.8	151.5	149.6	146.0
2	113.8	114.4	109.8	113.7	114.3	109.7	114.9	114.8	110.1	113.0	111.6	125.1
3	159.0	158.8	161.3	158.9	158.8	161.1	158.7	158.6	160.5	159.5	157.5	155.6
4	164.9	164.9	164.4	164.8	164.9	164.3	164.9	164.9	164.4	164.7	162.8	163.5
5	162.0	162.4	161.5	162.0	162.5	161.5	162.4	162.5	161.3	162.0	160.1	161.9
6	119.0	119.1	119.3	119.1	119.2	119.3	119.2	119.3	120.1	119.2	117.7	105.8
7	168.4	168.6	167.9	168.4	168.6	167.9	168.7	168.7	168.7	168.4	166.4	165.1

[a] *Calculated using the GIAO method at the mPW1PW91/6-311+G(2d,p) level in acetone (PCM).* [b] *Measured in acetone-d_6 + D_2O.* [c] *Averaged according to the Boltzmann distribution theory at 298 K based on relative Gibbs free energies.* [d] *Linearly corrected for the experimental data.* [e] *May be interchanged in each column.*

Table S19. Calculated ^{13}C NMR chemical shifts of (*S*)-**5a**.

	calculated[a]																					experimental[b]
Position	(*S*)-**5aA**	(*S*)-**5aB**	(*S*)-**5aC**	(*S*)-**5aD**	(*S*)-**5aE**	(*S*)-**5aF**	(*S*)-**5aG**	(*S*)-**5aH**	(*S*)-**5aI**	(*S*)-**5aJ**	(*S*)-**5aK**	(*S*)-**5aL**	(*S*)-**5aM**	(*S*)-**5aN**	(*S*)-**5aO**	(*S*)-**5aP**	(*S*)-**5aQ**	(*S*)-**5aR**	(*S*)-**5aS**	(*S*)-**5aT**	averaged-(*S*)-**5a**	averaged-(*S*)-**5a** (corrected)	**5**
Glucose-1	94.8	94.8	94.8	94.8	94.7	94.7	94.8	94.7	94.9	94.7	94.9	94.8	94.9	94.8	94.8	94.7	94.8	94.7	94.8	94.7	94.8	92.9	94.5
2	76.5	76.2	78.6	78.3	76.2	78.3	76.5	78.6	76.2	76.5	76.0	78.6	78.1	78.3	76.3	78.3	76.2	76.4	76.0	78.6	77.2	75.3	77.6
3	76.2	76.6	76.0	76.4	76.4	76.2	76.1	75.9	76.5	76.1	76.0	76.0	75.8	76.3	76.4	76.3	76.4	76.1	75.9	76.0	76.2	74.3	76.8
4	68.8	68.9	68.7	68.8	68.5	68.4	68.8	68.3	68.9	68.4	68.7	68.7	68.6	68.8	68.5	68.4	68.6	68.5	68.4	68.3	68.7	66.7	69.7
5	71.6	71.5	72.5	72.4	71.5	72.4	71.6	72.5	71.5	71.6	71.5	72.5	72.4	72.4	71.5	72.4	71.5	71.6	71.5	72.5	71.9	70.0	66.2
6	64.8	64.9	64.9	64.9	64.5	64.5	65.0	64.5	65.0	64.4	64.8	65.1	64.9	65.1	64.4	64.4	64.7	64.6	64.4	64.4	64.8	62.8	65.0
A-Ring 1	128.8	128.3	128.7	128.2	128.4	128.3	128.8	128.6	128.3	128.8	129.4	128.6	129.2	128.2	128.5	128.3	128.4	128.7	129.7	128.6	128.6	126.7	125.7 [e]
2	116.2	117.7	116.2	117.7	117.4	117.4	116.2	115.8	117.7	115.9	109.1	116.2	109.1	117.6	117.4	117.3	117.6	116.0	109.6	115.7	116.3	114.4	114.3
3	143.3	143.7	143.3	143.6	143.9	143.9	143.4	143.1	143.6	143.0	142.9	143.4	143.0	143.6	143.9	143.9	143.8	143.2	142.4	142.9	143.5	141.5	144.0
4	136.2	140.1	136.2	140.1	140.0	140.1	136.2	135.7	140.1	135.6	136.8	136.3	137.0	140.1	139.9	140.1	140.1	135.8	135.8	135.5	138.0	136.1	136.0
5	144.8	146.1	144.9	146.2	145.7	145.8	144.8	144.8	146.1	144.7	147.6	144.9	147.7	146.2	145.6	145.7	145.9	144.8	146.9	144.8	145.6	143.7	144.8
6	107.2	109.7	107.3	109.9	109.8	109.9	107.1	107.6	109.8	107.5	108.3	107.2	108.5	109.9	109.7	109.8	109.8	107.4	108.3	107.7	108.5	106.6	107.2
7	173.6	174.1	173.7	174.3	174.0	174.2	173.6	173.6	174.1	173.4	173.4	173.8	173.6	174.3	174.0	174.1	174.0	173.5	173.3	173.5	173.9	172.0	169.1
B-Ring 1	127.4	128.4	127.4	128.4	128.6	128.6	127.3	127.6	128.3	127.6	129.7	127.4	129.7	128.3	128.6	128.6	128.5	127.6	129.9	127.6	128.1	126.2	125.6 [e]
2	118.1	116.0	118.1	116.0	116.4	116.4	118.1	118.5	116.0	118.5	110.1	118.1	110.1	116.0	116.7	116.6	116.3	118.3	109.8	118.6	116.6	114.7	114.1
3	143.2	142.4	143.1	142.3	142.5	142.5	143.2	143.1	142.3	143.1	141.6	143.1	141.5	142.3	142.6	142.5	142.4	143.2	141.8	143.1	142.7	140.8	144.0
4	139.7	135.0	139.7	134.9	135.3	135.2	139.7	140.0	134.9	140.0	134.9	139.7	134.7	134.9	135.5	135.4	135.1	139.9	135.6	140.0	137.2	135.3	135.9
5	145.6	143.5	145.6	143.4	143.7	143.7	145.6	145.7	143.4	145.7	146.8	145.6	146.8	143.4	143.8	143.8	143.6	145.7	147.1	145.8	144.7	142.8	144.8
6	109.6	107.5	109.6	107.4	107.7	107.7	109.6	109.8	107.4	109.8	108.6	109.6	108.6	107.4	107.7	107.8	107.6	109.8	108.8	109.9	108.6	106.7	106.9
7	174.4	173.8	174.2	173.7	173.9	173.8	174.3	174.3	173.8	174.4	173.8	174.2	173.7	173.7	173.9	173.8	173.9	174.4	173.9	174.3	174.0	172.1	169.7
C-Ring 1	124.4	124.4	124.3	124.3	122.6	122.5	124.0	122.5	124.0	122.6	124.3	123.9	124.2	123.9	123.3	123.3	122.5	122.6	122.7	123.3	123.8	121.9	124.1 [e]
2	117.5	117.5	117.5	117.5	115.1	115.1	117.3	115.2	117.2	115.2	117.7	117.3	117.7	117.2	114.8	114.8	114.7	114.7	115.2	114.9	116.8	114.9	112.1
3	143.7	143.8	143.7	143.7	143.6	143.6	144.3	143.7	144.3	143.6	144.2	144.2	144.1	144.2	144.3	144.3	144.5	144.6	143.6	144.4	143.9	142.0	145.1
4	141.7	141.6	141.7	141.6	137.0	137.1	141.7	137.0	141.7	136.9	141.7	141.8	141.7	141.8	137.1	137.2	136.7	136.6	136.8	137.1	140.4	138.5	136.5
5	146.8	146.8	146.8	146.8	144.9	144.9	146.9	144.9	146.9	144.9	146.8	146.9	146.8	146.9	144.9	144.9	144.9	144.9	144.8	144.9	146.3	144.4	146.5
6	112.2	112.3	112.3	112.3	105.9	105.9	112.7	105.9	112.8	105.9	112.5	112.7	112.5	112.8	106.2	106.2	105.9	105.9	106.0	106.2	110.6	108.7	106.9
7	171.5	171.7	171.5	171.6	171.6	171.5	171.5	171.4	171.6	171.4	171.5	171.4	171.5	171.6	171.7	171.7	171.5	171.3	171.4	171.6	171.5	169.6	168.1
D-Ring 1	155.2	155.2	155.1	155.2	155.1	155.2	156.4	155.3	156.3	155.2	155.8	156.3	155.7	156.3	155.4	155.4	155.3	155.4	154.9	155.6	155.4	153.5	146.0
2	125.5	125.6	125.5	125.6	122.7	122.6	126.4	122.8	126.5	122.8	125.3	126.4	125.3	126.5	120.7	120.7	122.7	122.6	122.8	120.6	124.8	122.8	125.1
3	149.1	149.0	149.0	148.9	152.4	152.3	147.3	152.3	147.1	152.4	149.5	147.2	149.4	147.0	153.1	153.1	150.2	150.2	152.5	153.2	149.7	147.8	155.6
4	167.9	167.9	167.9	167.9	163.3	163.3	166.1	163.2	166.0	163.2	168.0	166.0	167.9	166.0	164.1	164.1	161.2	161.1	163.2	164.1	166.3	164.4	163.5
5	160.7	160.6	160.7	160.6	161.2	161.2	159.7	161.2	159.6	161.2	160.6	159.7	160.6	159.6	161.4	161.4	159.9	160.0	161.2	161.4	160.6	158.7	161.9
6	120.7	120.8	120.7	120.7	119.5	119.4	121.7	119.4	121.7	119.5	121.0	121.6	120.9	121.6	118.8	118.7	119.6	119.6	119.5	118.7	120.5	118.6	105.8
7	169.0	168.9	169.0	168.9	168.8	168.8	168.9	168.8	168.8	168.8	169.0	168.9	168.9	168.8	169.2	169.2	168.5	168.6	168.9	169.3	168.9	167.0	165.1

[a] Calculated using the GIAO method at the mPW1PW91/6-311+G(2d,p) level in acetone (PCM). [b] Measured in acetone-d_6 + D_2O. [c] Averaged according to the Boltzmann distribution theory at 298 K based on relative Gibbs free energies. [d] Linearly corrected for the experimental data. [e] May be interchanged in each column.

Fig. S13. Correlation plots of experimental ^{1}H NMR chemical shifts versus corresponding calculated ^{1}H NMR chemical shifts of **5**.

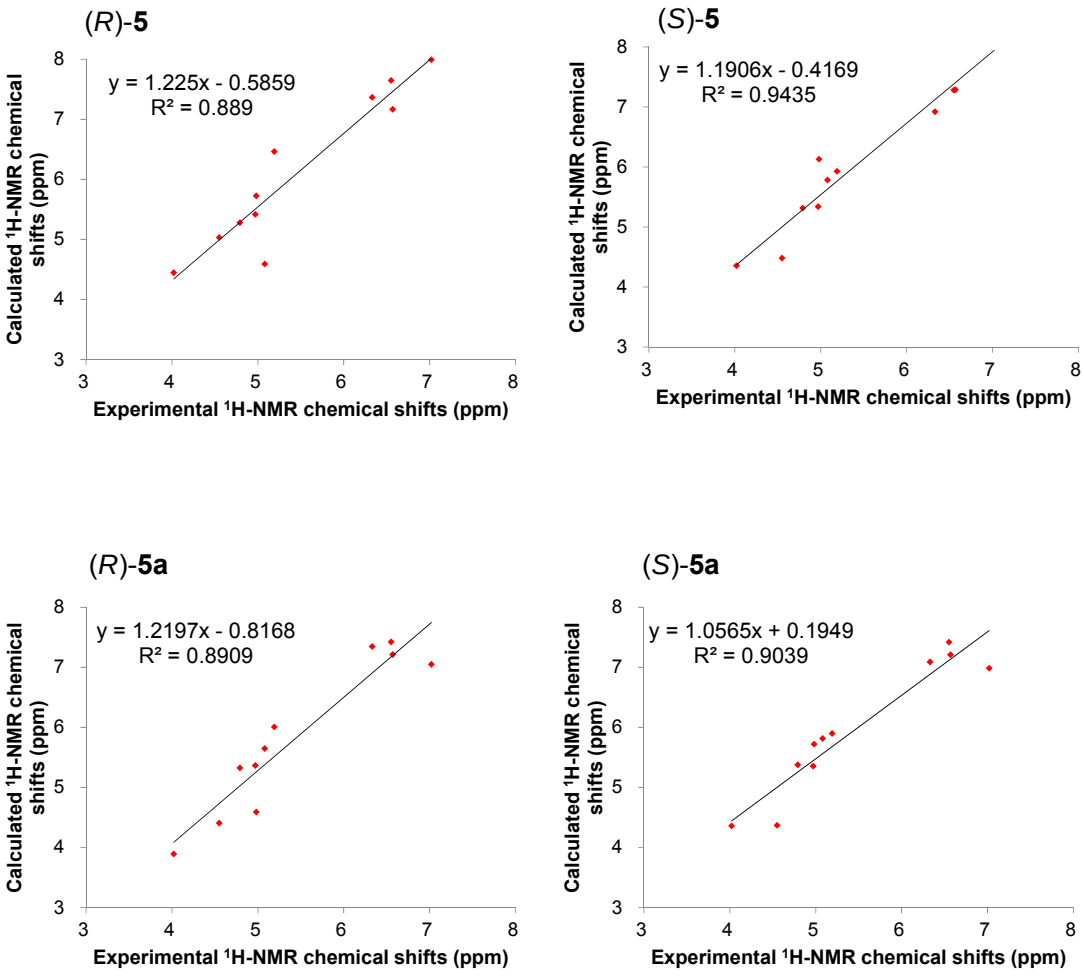


Fig. S14. Correlation plots of experimental ^{13}C NMR chemical shifts versus corresponding calculated ^{13}C NMR chemical shifts of **5**.

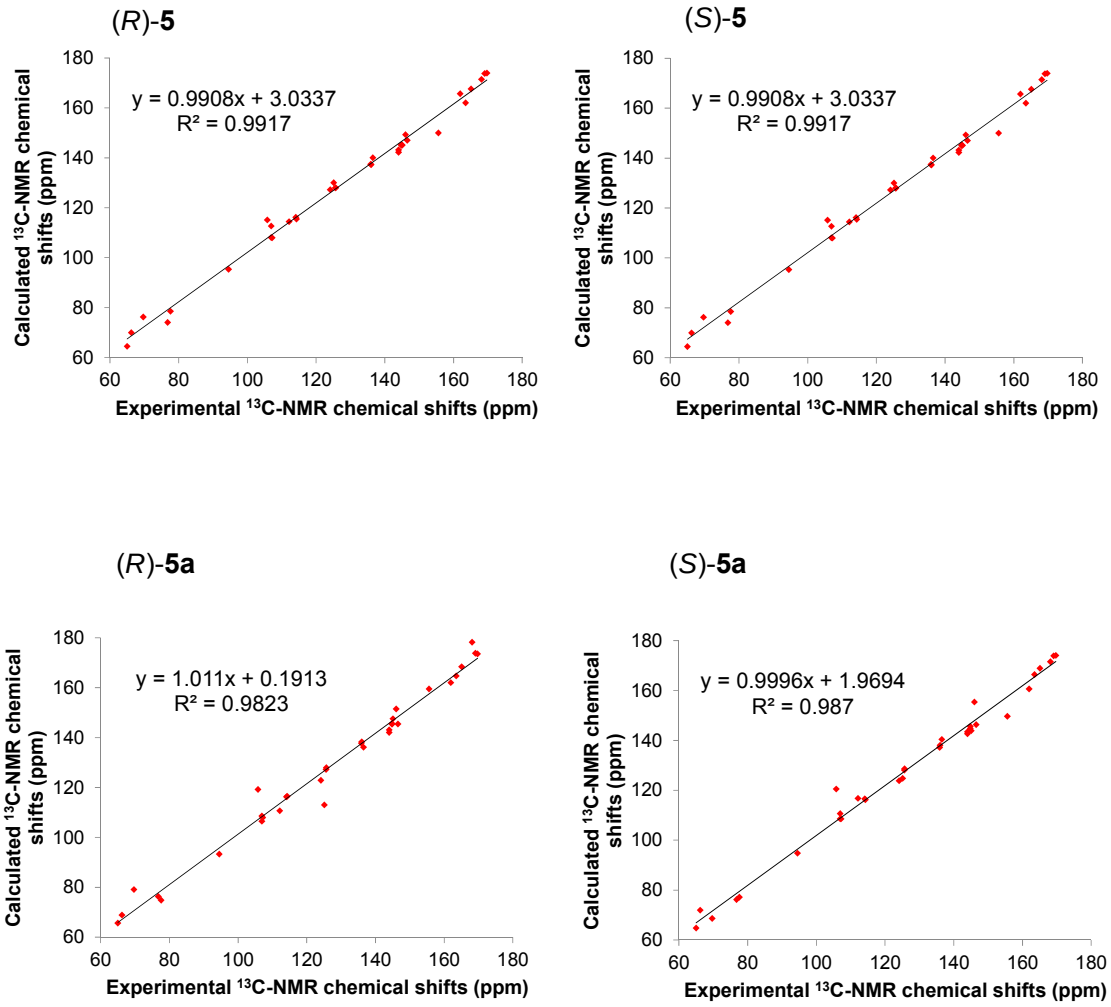


Table S20. Statistical parameters of calculated ^{1}H NMR chemical shifts of **5** (ppm).

	R^2	CMaxErr	CMAE
(*R*)-**5**	0.8890	0.85	0.22
(*S*)-**5**	0.9435	0.52	0.17
(*R*)-**5a**	0.8909	0.57	0.28
(*S*)-**5a**	0.9039	0.60	0.25

R^2: coefficient of determination; CMaxErr: corrected maximum absolute error with respect to the linear fit; CMAE: corrected mean absolute error with respect to the linear fit

Table S21. Statistical parameters of calculated ^{13}C NMR chemical shifts of **5** (ppm).

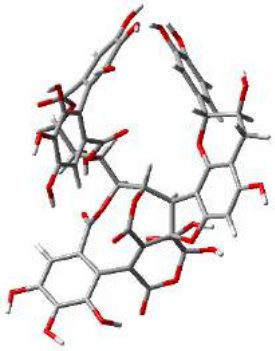
	R^2	CMaxErr	CMAE
(*R*)-**5**	0.9917	7.3	2.2
(*S*)-**5**	0.9917	7.1	2.3
(*R*)-**5a**	0.9823	13.5	2.7
(*S*)-**5a**	0.9870	12.8	2.5

R^2: coefficient of determination; CMaxErr: corrected maximum absolute error with respect to the linear fit; CMAE: corrected mean absolute error with respect to the linear fit

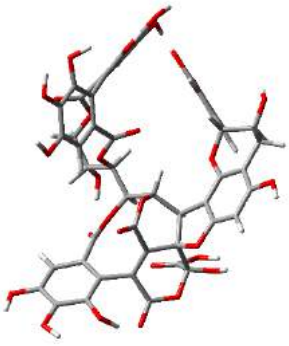
Table S22. The DP4 and DP4+ probability analysis of **5**.

	(*R*)-**5**	(*S*)-**5**	(*R*)-**5a**	(*S*)-**5a**
DP4 (^{1}H)	0.7%	99.2%	0.1%	0.0%
DP4 (^{13}C)	79.5%	20.5%	0.0%	0.0%
DP4 (^{1}H + ^{13}C)	2.6%	97.4%	0.0%	0.0%
sDP4+ (^{1}H)	18.69%	80.99%	0.02%	0.30%
sDP4+ (^{13}C)	93.72%	6.23%	0.00%	0.05%
sDP4+ (^{1}H + ^{13}C)	77.64%	22.36%	0.00%	0.00%
uDP4+ (^{1}H)	0.01%	7.94%	83.26%	8.79%
uDP4+ (^{13}C)	0.45%	99.55%	0.00%	0.00%
uDP4+ (^{1}H + ^{13}C)	0.00%	100.00%	0.00%	0.00%
DP4+ (^{1}H)	0.03%	99.30%	0.25%	0.41%
DP4+ (^{13}C)	6.35%	93.65%	0.00%	0.00%
DP4+ (^{1}H + ^{13}C)	0.00%	100.00%	0.00%	0.00%

Fig. S15. Optimized conformers of (5*R*)-**6** at the B3LYP/6-31G(d,p) level in MeOH (PCM) with populations greater than 1% calculated from their relative Gibbs free energies (ΔG).

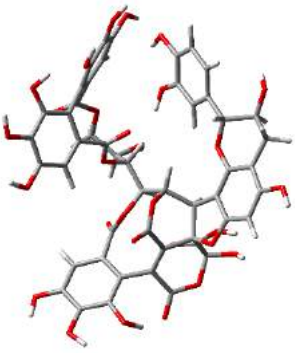


(5*R*)-**6A** (36.9%)

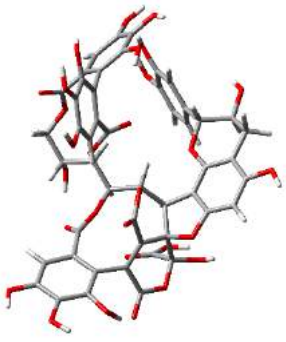


(5*R*)-**6B** (27.3%)

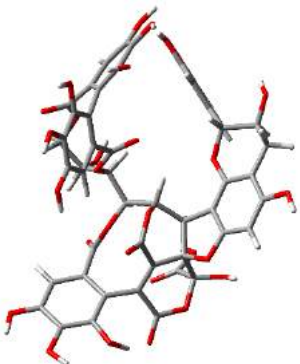
(5*R*)-**6C** (8.7%)



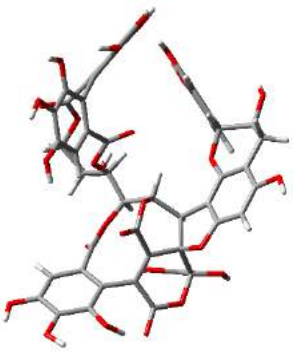
(5*R*)-**6D** (4.3%)



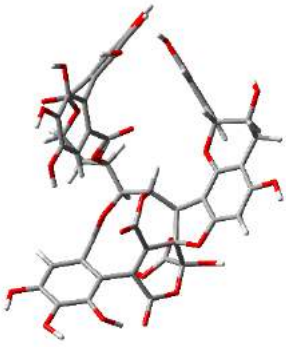
(5*R*)-**6E** (3.8%)



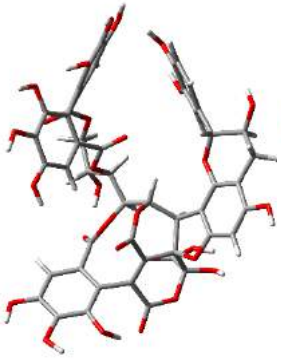
(5*R*)-**6F** (2.7%)



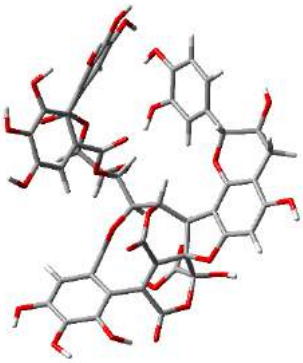
(5*R*)-**6G** (2.5%)



(5*R*)-**6H** (2.3%)

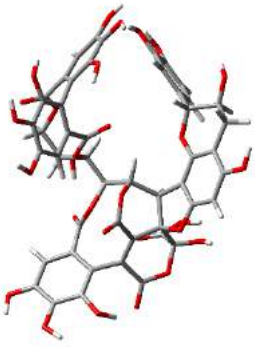


(5*R*)-**6I** (2.2%)



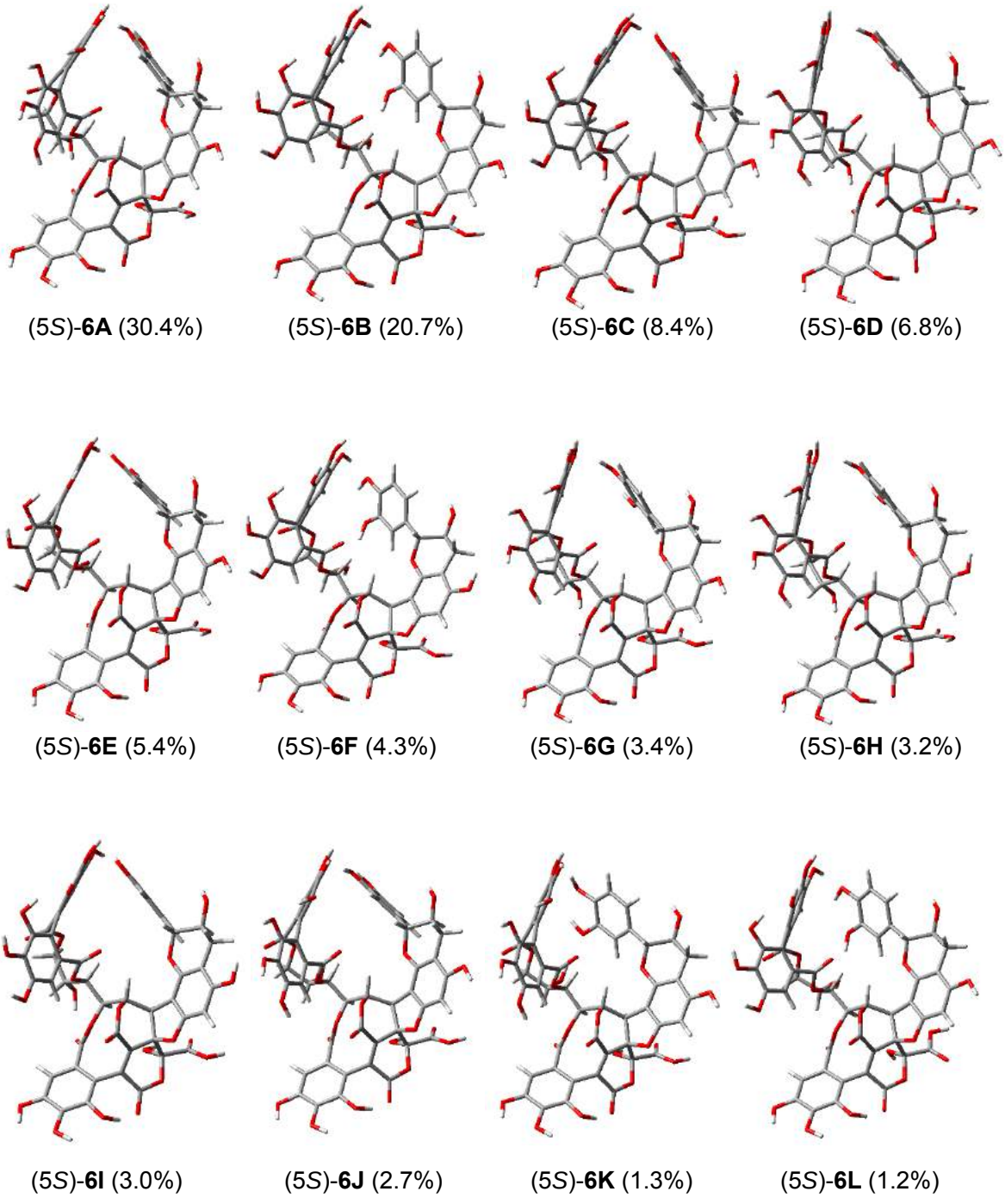
(5*R*)-**6J** (1.3%)

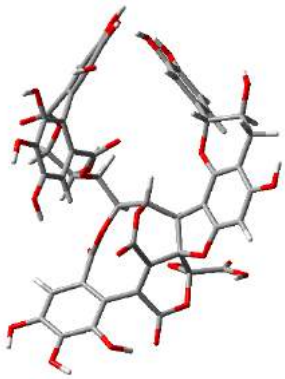
(5*R*)-**6K** (1.1%)



(5*R*)-**6L** (1.1%)

Fig. S16. Optimized conformers of (5*S*)-**6** at the B3LYP/6-31G(d,p) level in MeOH (PCM) with populations greater than 1% calculated from their relative Gibbs free energies (ΔG).





(5*S*)-**6M** (1.1%)

(5*S*)-**6N** (1.0%)

Table S23. Important thermodynamic parameters and conformational analysis of (5*R*)-**6** at the B3LYP/6-31G(d,p) level in MeOH (PCM).

conformers	*E* (a.u.)	*E′* (a.u.)	*H* (a.u.)	*G* (a.u.)	Δ*G* (kcal/mol)	P_G (%)
(5*R*)-**6A**	-4069.283560	-4068.479046	-4068.412180	-4068.578230	0.00	36.9
(5*R*)-**6B**	-4069.282745	-4068.478279	-4068.411396	-4068.577946	0.18	27.3
(5*R*)-**6C**	-4069.282187	-4068.477695	-4068.410810	-4068.576867	0.86	8.7
(5*R*)-**6D**	-4069.285477	-4068.479733	-4068.413680	-4068.576203	1.27	4.3
(5*R*)-**6E**	-4069.279494	-4068.475940	-4068.408544	-4068.576087	1.34	3.8
(5*R*)-**6F**	-4069.279648	-4068.475985	-4068.408799	-4068.575761	1.55	2.7
(5*R*)-**6G**	-4069.279858	-4068.476288	-4068.409120	-4068.575677	1.60	2.5
(5*R*)-**6H**	-4069.278440	-4068.475073	-4068.407795	-4068.575603	1.65	2.3
(5*R*)-**6I**	-4069.281675	-4068.476855	-4068.410158	-4068.575583	1.66	2.2
(5*R*)-**6J**	-4069.284049	-4068.478587	-4068.412466	-4068.575053	1.99	1.3
(5*R*)-**6K**	-4069.284131	-4068.478426	-4068.412321	-4068.574921	2.08	1.1
(5*R*)-**6L**	-4069.278077	-4068.474669	-4068.407211	-4068.574881	2.10	1.1

E: total energy; E': total energy with zero point energy; H: enthalpy; G: Gibbs free energy; ΔG: relative Gibbs free energy at the B3LYP/6-31G(d,p) level in MeOH (PCM). P_G: conformational distribution calculated from relative Gibbs free energy.

Table S24. Important thermodynamic parameters and conformational analysis of (5*S*)-**6** at the B3LYP/6-31G(d,p) level in MeOH (PCM).

conformers	*E* (a.u.)	*E′* (a.u.)	*H* (a.u.)	*G* (a.u.)	Δ*G* (kcal/mol)	P_G (%)
(5*S*)-**6A**	-4069.285372	-4068.481432	-4068.414419	-4068.581557	0.00	30.4
(5*S*)-**6B**	-4069.288121	-4068.483082	-4068.416640	-4068.581193	0.23	20.7
(5*S*)-**6C**	-4069.284331	-4068.480035	-4068.413041	-4068.580347	0.76	8.4
(5*S*)-**6D**	-4069.285617	-4068.480933	-4068.414215	-4068.580144	0.89	6.8
(5*S*)-**6E**	-4069.281948	-4068.478876	-4068.411340	-4068.579933	1.02	5.4
(5*S*)-**6F**	-4069.286746	-4068.481705	-4068.415231	-4068.579713	1.16	4.3
(5*S*)-**6G**	-4069.284910	-4068.480280	-4068.413439	-4068.579497	1.29	3.4
(5*S*)-**6H**	-4069.284251	-4068.479841	-4068.412969	-4068.579435	1.33	3.2
(5*S*)-**6I**	-4069.282826	-4068.478738	-4068.411631	-4068.579365	1.38	3.0
(5*S*)-**6J**	-4069.282333	-4068.478855	-4068.411467	-4068.579271	1.43	2.7
(5*S*)-**6K**	-4069.285108	-4068.480312	-4068.413567	-4068.578562	1.88	1.3
(5*S*)-**6L**	-4069.285240	-4068.480370	-4068.413765	-4068.578492	1.92	1.2
(5*S*)-**6M**	-4069.281422	-4068.478002	-4068.410675	-4068.578394	1.98	1.1
(5*S*)-**6N**	-4069.285580	-4068.480523	-4068.413955	-4068.578379	1.99	1.0

E: total energy; E': total energy with zero point energy; H: enthalpy; G: Gibbs free energy; ΔG: relative Gibbs free energy at the B3LYP/6-31G(d,p) level in MeOH (PCM). P_G: conformational distribution calculated from relative Gibbs free energy.

Table S25. Calculated ^{13}C NMR chemical shifts of (5*R*)-**6**.

	calculated[a]														experimental[b]
Position	(5*R*)-**6A**	(5*R*)-**6B**	(5*R*)-**6C**	(5*R*)-**6D**	(5*R*)-**6E**	(5*R*)-**6F**	(5*R*)-**6G**	(5*R*)-**6H**	(5*R*)-**6I**	(5*R*)-**6J**	(5*R*)-**6K**	(5*R*)-**6L**	averaged-(5*R*)-**6**	averaged-(5*R*)-**6** (corrected)	**6**
Glucose-1	50.5	50.7	50.5	51.1	50.5	48.7	50.9	47.1	50.6	47.6	51.1	50.5	50.4	51.6	50.6
2	78.0	78.3	78.0	78.6	78.3	79.3	79.7	78.3	76.8	77.8	78.6	78.4	78.2	78.7	78.7
3	74.5	74.5	74.5	75.4	74.4	72.8	73.7	72.8	74.9	74.9	75.4	74.5	74.4	75.1	75.5
4	76.6	76.5	76.6	74.9	76.7	77.5	77.7	77.0	76.9	75.0	74.9	76.7	76.5	77.1	77.3
5	65.1	64.7	65.1	72.7	65.7	69.0	69.2	68.8	64.1	72.5	72.7	65.7	65.8	66.7	69.3
6	64.7	64.3	64.7	63.9	65.8	66.3	66.3	66.3	64.2	64.0	63.9	65.8	64.7	65.6	68.4
Catechin C-ring 2	81.5	81.3	81.0	78.9	81.3	81.6	81.6	81.7	82.6	78.7	78.6	80.9	81.2	81.6	82.2
3	68.0	66.8	67.7	67.8	67.6	67.2	67.1	67.2	67.1	67.8	67.7	67.3	67.5	68.3	68.0
4	26.2	26.2	24.8	27.9	26.0	26.4	26.3	25.8	27.5	27.5	26.2	24.7	26.2	28.0	27.3
A-ring 4a	103.8	104.1	101.5	106.7	103.7	103.7	102.4	103.8	106.0	106.1	105.6	101.3	103.8	103.7	103.0
5	158.9	159.0	159.5	160.4	158.9	158.7	158.8	158.9	160.0	160.1	161.5	159.4	159.1	157.6	158.6
6	87.2	87.8	87.7	88.5	87.5	87.3	87.5	87.4	88.3	88.9	89.5	87.8	87.6	87.9	90.8
7	159.9	159.9	160.6	160.1	159.8	160.0	161.4	159.2	159.6	160.5	160.8	160.5	160.0	158.5	159.2
8	103.8	104.3	103.7	103.6	104.1	104.7	104.6	104.2	102.9	104.3	103.5	103.8	104.0	103.8	104.9
8a	154.6	154.3	154.3	153.6	154.4	154.6	154.2	153.9	155.4	153.1	153.3	154.0	154.4	153.0	152.1
B-ring 1	129.2	131.7	128.9	133.0	129.2	129.7	129.7	129.9	130.3	133.3	132.6	128.9	130.2	129.4	131.7
2	116.0	117.8	115.9	111.9	115.8	116.1	116.2	116.1	110.9	112.1	112.0	115.8	116.1	115.6	114.1
3	145.8	143.9	145.8	146.6	145.4	145.2	145.2	145.4	148.8	146.5	146.7	145.4	145.3	144.1	146.1
4	148.7	145.4	148.8	145.5	148.6	148.3	148.3	148.4	146.2	145.5	145.5	148.7	147.4	146.2	146.1
5	115.5	114.8	115.5	115.2	115.5	115.1	114.9	115.1	114.7	115.2	115.3	115.5	115.2	114.8	116.5
6	119.8	120.6	119.8	119.5	119.6	118.9	118.8	119.5	120.1	119.6	119.5	119.8	120.0	119.4	120.9
D-Ring 1	139.1	139.0	139.1	140.0	138.9	138.8	140.2	137.2	138.9	138.1	140.1	138.7	139.1	138.1	137.9
2	135.1	135.4	135.2	137.9	135.4	136.0	134.4	139.0	136.6	140.4	137.9	135.7	135.6	134.7	132.1
3	168.8	168.7	168.8	168.7	168.9	170.3	170.2	171.8	168.5	171.4	168.7	168.9	169.0	167.2	162.7
4	170.1	170.2	170.1	170.2	170.0	170.7	170.3	169.3	170.4	170.0	170.2	169.9	170.1	168.3	168.5
5	99.2	99.2	99.2	99.5	99.2	100.8	99.7	101.1	99.5	100.9	99.4	99.1	99.4	99.3	100.1
6	87.3	87.3	87.3	87.2	87.4	88.3	86.3	88.7	86.8	88.4	87.1	87.5	87.4	87.6	86.8
7	167.8	167.6	167.8	167.8	167.7	168.0	168.2	167.4	167.6	167.2	167.7	167.7	167.7	166.0	166.4
E-Ring 1	125.1	125.1	125.1	126.7	125.2	126.4	126.2	126.2	126.1	126.3	126.7	125.1	125.3	124.6	125.1 [f]
2	118.0	117.8	118.0	117.0	118.1	116.1	116.8	115.4	117.1	114.3	117.0	118.1	117.7	117.2	112.4
3	144.3	144.6	144.3	145.0	144.2	145.4	144.6	145.7	144.4	145.9	145.1	144.2	144.5	143.4	146.9 [g]
4	140.6	140.7	140.7	142.1	140.3	140.7	139.7	139.5	141.8	141.4	142.1	140.5	140.7	139.7	137.2
5	147.2	147.3	147.2	148.4	147.0	148.4	147.4	148.7	148.1	149.7	148.4	147.1	147.4	146.2	147.9 [g]
6	112.8	112.6	112.8	112.7	112.6	111.4	111.5	109.2	111.6	110.0	112.7	112.7	112.5	112.1	106.4
7	173.3	173.5	173.2	170.4	173.2	171.1	172.6	173.9	173.3	174.5	170.4	173.1	173.1	171.2	168.5
F-Ring 1	128.3	128.0	128.3	127.1	128.3	128.1	128.1	128.0	128.3	127.1	127.1	128.3	128.1	127.4	125.7 [f]
2	117.6	119.4	117.6	118.9	110.5	117.5	117.6	117.6	115.7	118.9	118.9	110.4	117.8	117.3	116.0
3	142.1	142.7	142.1	142.5	142.9	142.4	142.6	142.5	141.7	142.6	142.5	142.9	142.4	141.3	144.7 [h]
4	135.4	139.6	135.4	139.2	137.1	135.8	136.1	136.0	134.6	139.1	139.2	137.1	137.0	136.0	137.0
5	143.9	146.0	144.0	145.2	147.6	144.5	144.8	144.6	143.4	145.3	145.2	147.7	144.9	143.7	145.8 [h]
6	107.9	110.4	107.9	110.7	109.6	108.0	108.2	108.1	108.0	110.6	110.7	109.6	108.9	108.6	107.7
7	172.9	172.9	172.8	172.0	173.2	172.3	172.3	172.2	171.7	171.9	172.0	173.2	172.7	170.9	169.1
G-Ring 1	129.6	130.1	129.6	129.1	130.5	130.2	130.4	130.2	126.6	128.9	129.1	130.6	129.7	128.9	127.2 [f]
2	120.5	117.7	120.5	116.6	112.8	120.7	120.7	120.7	119.6	116.8	116.6	112.8	119.0	118.5	116.5
3	143.9	143.5	143.9	143.2	143.9	143.0	142.7	142.9	144.2	143.2	143.2	143.9	143.6	142.5	145.8 [e]
4	139.5	137.9	139.5	136.4	136.7	138.4	138.2	138.4	140.0	136.7	136.4	136.7	138.6	137.6	137.6
5	142.9	143.6	142.9	145.2	144.5	142.6	142.6	142.6	143.4	145.3	145.2	144.5	143.3	142.2	144.8 [e]
6	110.5	110.7	110.5	110.6	108.7	110.5	110.5	110.5	111.9	110.7	110.5	108.7	110.5	110.2	109.1
7	172.4	172.3	172.3	172.8	172.4	173.0	173.1	173.0	171.8	172.7	172.8	172.4	172.4	170.5	170.9

[a] *Calculated using the GIAO method at the mPW1PW91/6-311+G(2d,p) level in MeOH (PCM).* [b] *Measured in CD_3OD.* [c] *Averaged according to the Boltzmann distribution theory at 298 K based on relative Gibbs free energies.* [d] *Linearly corrected for the experimental data.* [e–h] *May be interchanged in each column.*

Table S26. Calculated ^{13}C NMR chemical shifts of (5*S*)-**6**.

	calculated[a]																experimental[b]
Position	(5*S*)-**6A**	(5*S*)-**6B**	(5*S*)-**6C**	(5*S*)-**6D**	(5*S*)-**6E**	(5*S*)-**6F**	(5*S*)-**6G**	(5*S*)-**6H**	(5*S*)-**6I**	(5*S*)-**6J**	(5*S*)-**6K**	(5*S*)-**6L**	(5*S*)-**6M**	(5*S*)-**6N**	averaged-(5*S*)-**6**	averaged-(5*S*)-**6** (corrected)	**6**
Glucose-1	49.0	49.4	49.2	48.3	48.9	49.4	48.8	48.3	49.1	48.7	49.0	50.0	48.7	48.8	49.0	50.5	50.6
2	77.8	78.9	78.8	75.9	79.5	78.9	76.6	75.9	78.8	79.3	78.5	78.7	78.9	78.0	78.1	78.8	78.7
3	74.7	75.6	74.7	75.5	73.2	75.6	76.1	75.5	74.7	73.4	75.1	75.6	73.1	74.8	74.9	75.7	75.5
4	76.0	75.1	76.1	76.3	76.1	75.1	76.1	76.3	76.1	77.6	78.2	75.1	77.6	78.1	75.9	76.6	77.3
5	64.5	72.8	64.5	63.8	68.3	72.8	63.7	63.8	64.5	69.0	69.8	72.8	69.0	70.0	67.3	68.2	69.3
6	64.1	64.0	63.4	64.1	67.2	64.0	63.9	64.1	63.4	66.5	65.4	64.0	66.4	65.4	64.3	65.3	68.4
Catechin C-ring 2	81.5	78.5	81.3	82.4	81.6	78.1	82.2	82.0	80.7	81.7	78.6	78.5	81.4	78.7	80.6	81.2	82.2
3	67.3	67.7	67.1	67.1	66.9	67.4	67.2	66.8	66.9	66.9	67.4	67.8	66.8	67.0	67.3	68.2	68.0
4	25.6	27.3	25.9	26.6	25.7	26.1	26.9	25.4	24.5	25.7	27.2	27.4	24.6	27.0	26.2	28.3	27.3
A-ring 4a	105.0	105.7	104.3	105.8	105.7	105.5	104.9	104.7	103.0	103.6	105.3	105.1	103.7	107.0	105.1	105.0	103.0
5	159.5	160.6	159.9	159.8	159.9	161.8	159.9	160.6	161.0	159.4	160.4	160.3	160.4	160.6	160.1	158.4	158.6
6	88.8	88.9	89.9	89.3	89.6	89.9	88.4	90.5	91.0	89.6	88.4	88.6	89.7	89.1	89.2	89.5	90.8
7	157.4	159.9	160.0	158.6	157.7	160.6	160.6	159.4	160.7	160.1	160.0	159.4	158.1	158.4	158.9	157.3	159.2
8	102.9	102.3	102.8	102.6	103.1	102.8	102.6	102.6	103.1	103.3	102.9	103.0	103.3	102.5	102.7	102.7	104.9
8a	154.2	153.3	153.5	155.4	153.5	153.2	155.0	155.2	153.2	153.9	153.3	153.9	153.9	153.3	153.9	152.4	152.1
B-ring 1	129.5	133.1	131.9	130.7	132.0	132.8	130.8	130.1	131.5	129.6	133.1	133.1	129.3	132.9	131.2	130.3	131.7
2	116.3	111.9	117.2	111.9	117.6	111.9	111.7	111.8	117.2	116.4	111.3	112.0	116.4	111.3	114.5	114.1	114.1
3	145.3	147.2	143.5	148.9	143.5	147.2	148.8	149.0	143.7	144.9	147.9	147.2	145.2	148.1	146.1	144.8	146.1
4	148.6	145.9	145.3	145.8	145.1	146.0	146.0	145.9	145.4	148.4	144.3	146.0	148.5	144.5	146.8	145.5	146.1
5	115.3	115.3	114.8	114.8	114.6	115.4	114.8	114.8	114.9	114.9	116.8	115.3	115.0	116.8	115.1	114.7	116.5
6	119.6	119.5	121.0	119.8	120.7	119.5	120.5	120.0	121.1	118.9	119.4	119.6	119.2	119.4	119.8	119.3	120.9
D-Ring 1	140.1	140.5	140.8	139.5	140.0	140.5	140.2	139.5	140.8	140.7	139.9	139.2	139.5	139.3	140.2	139.1	137.9
2	134.9	136.2	134.5	136.6	135.6	136.2	135.5	136.7	134.5	135.0	136.7	136.4	135.7	137.3	135.5	134.6	132.1
3	170.8	171.3	171.3	170.1	170.9	171.3	170.8	170.1	171.2	171.4	171.4	170.9	170.9	170.7	170.9	169.0	162.7
4	170.0	171.1	171.2	170.1	170.2	171.1	171.1	170.2	171.2	171.1	171.0	167.2	170.2	170.0	170.5	168.6	168.5
5	96.0	97.2	97.2	96.6	96.4	97.2	97.3	96.6	97.2	97.2	97.4	99.5	96.4	96.9	96.7	96.8	100.1
6	89.5	88.9	88.9	88.4	89.6	88.9	88.0	88.3	88.9	88.7	88.8	88.4	89.4	89.3	89.1	89.4	86.8
7	167.2	167.9	167.4	167.6	167.0	167.9	167.7	167.6	167.3	167.7	168.1	168.0	167.3	167.8	167.5	165.6	166.4
E-Ring 1	124.6	128.2	124.9	126.4	126.5	128.2	126.4	126.4	124.9	126.5	128.6	128.2	126.3	128.5	126.2	125.5	125.1 [f]
2	116.6	115.8	115.7	116.6	115.0	115.7	116.5	116.6	115.7	115.3	115.7	115.8	115.3	115.5	116.1	115.7	112.4
3	144.9	145.5	144.7	144.9	144.7	145.5	145.2	145.0	144.7	145.0	145.3	145.5	144.9	145.4	145.1	143.8	146.9 [h]
4	141.0	140.9	140.8	141.8	140.5	140.9	141.7	141.8	140.9	140.2	140.6	140.9	140.4	140.8	141.0	139.9	137.2
5	148.0	149.1	148.0	148.6	148.7	149.2	148.6	148.6	148.0	148.7	149.1	149.1	148.8	149.2	148.5	147.2	147.9 [h]
6	112.1	111.4	111.8	111.3	111.0	111.3	111.2	111.4	111.8	110.7	111.1	111.3	110.8	111.2	111.6	111.3	106.4
7	173.6	172.0	173.9	173.9	171.6	172.0	174.6	174.0	173.9	171.8	172.2	172.2	171.3	171.7	173.0	171.0	168.5
F-Ring 1	128.2	126.6	128.5	128.2	127.0	126.7	128.2	128.2	128.5	128.0	128.2	126.7	127.9	128.0	127.7	127.0	125.7 [f]
2	117.4	118.9	118.6	115.6	119.9	118.9	115.7	115.6	118.5	117.6	117.2	118.9	117.6	117.2	117.8	117.4	116.0
3	141.8	142.5	143.8	141.5	143.0	142.6	141.5	141.5	143.8	142.1	142.3	142.6	142.1	142.4	142.3	141.1	144.7 [g]
4	135.1	139.3	140.1	134.5	139.7	139.3	134.4	134.4	140.1	135.5	135.0	139.3	135.4	135.2	137.1	136.1	137.0
5	143.6	145.1	146.5	143.1	145.9	145.2	143.1	143.2	146.5	144.3	143.4	145.2	144.1	143.6	144.5	143.3	145.8 [g]
6	107.6	110.6	110.2	107.6	110.5	110.6	107.4	107.7	110.2	107.9	107.5	110.6	107.8	107.7	108.9	108.7	107.7
7	172.6	172.1	172.2	171.8	172.4	172.1	172.0	171.7	172.2	172.2	171.5	172.0	172.3	171.4	172.2	170.2	169.1
G-Ring 1	129.9	128.6	130.5	126.9	131.8	128.6	127.3	126.9	130.5	130.6	129.2	128.7	130.5	129.2	129.3	128.5	127.2 [f]
2	120.8	116.8	117.0	120.4	117.1	116.9	120.8	120.4	117.0	120.8	120.2	116.9	120.8	120.1	118.9	118.4	116.5
3	143.9	142.9	141.0	144.1	142.3	142.9	144.0	144.2	141.0	143.5	143.3	143.0	143.7	143.3	143.2	142.0	144.8 [e]
4	139.4	137.2	136.3	140.4	136.0	137.2	140.5	140.5	136.3	138.5	139.9	137.2	138.7	139.9	138.3	137.3	137.6
5	142.7	145.1	144.3	143.5	143.7	145.1	143.6	143.4	144.3	142.5	144.2	145.1	142.5	144.2	143.8	142.6	145.8 [e]
6	110.9	110.8	112.8	111.6	111.2	110.8	111.4	111.6	112.8	110.6	110.7	110.9	110.6	110.7	111.2	110.9	109.1
7	172.4	172.8	171.6	171.8	173.9	172.8	171.9	171.9	171.6	173.3	173.1	172.8	173.3	173.1	172.5	170.5	170.9

[a] Calculated using the GIAO method at the mPW1PW91/6-311+G(2d,p) level in MeOH (PCM). [b] Measured in CD_3OD. [c] Averaged according to the Boltzmann distribution theory at 298 K based on relative Gibbs free energies. [d] Linearly corrected for the experimental data. [e–h] May be interchanged in each column.

Fig. S17. Correlation plots of experimental ^{13}C NMR chemical shifts versus corresponding calculated ^{13}C NMR chemical shifts of **6**.

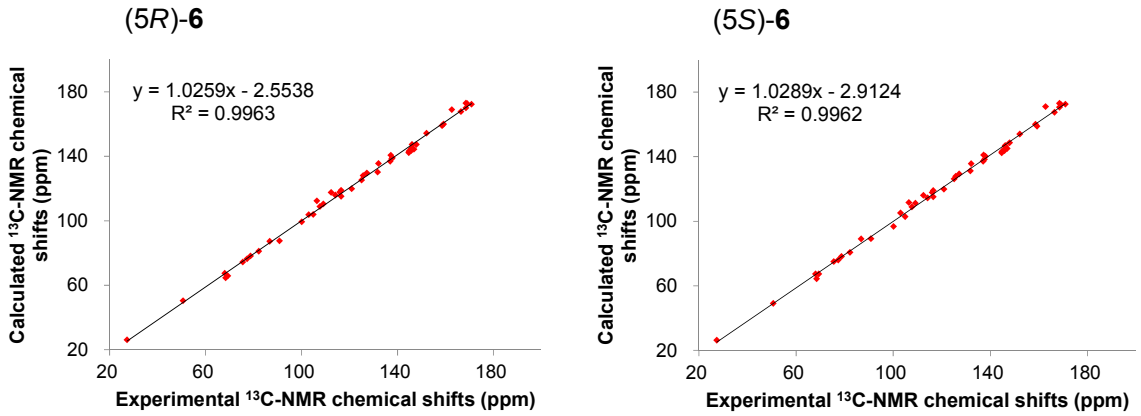


Fig. S18. Differences between experimental and calculated ^{13}C NMR chemical shifts of **6**. $\Delta\delta$ (ppm) = $\delta_{calcd.} - \delta_{exptl.}$ Calculations of NMR chemical shifts were performed at the mPW1PW91/6-311+G(2d,p) level in MeOH (PCM) and linearly corrected for the experimental data.

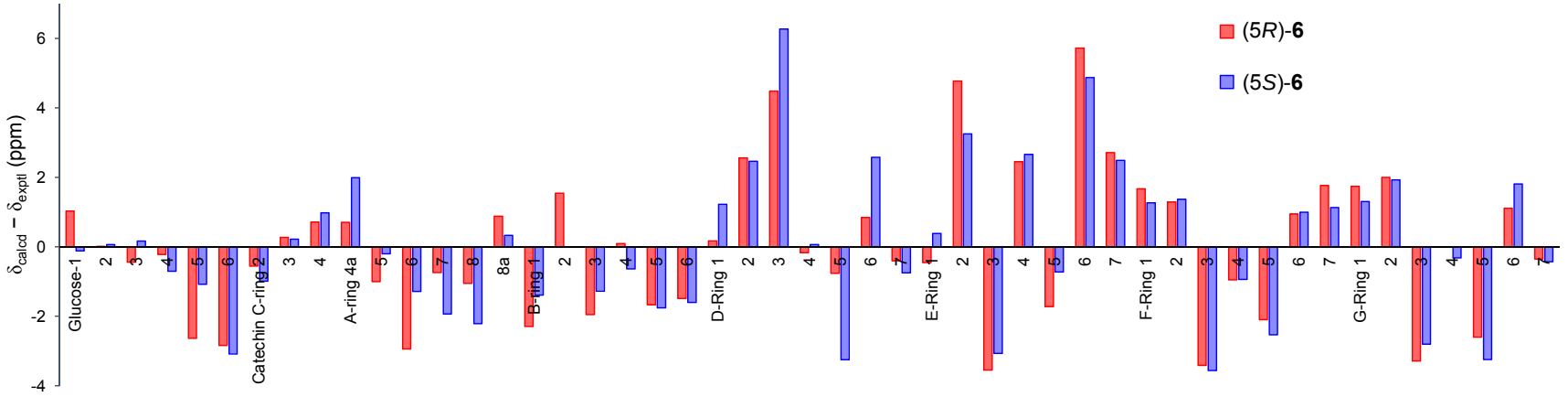


Table S27. Statistical parameters of calculated ^{13}C NMR chemical shifts of **6** (ppm).

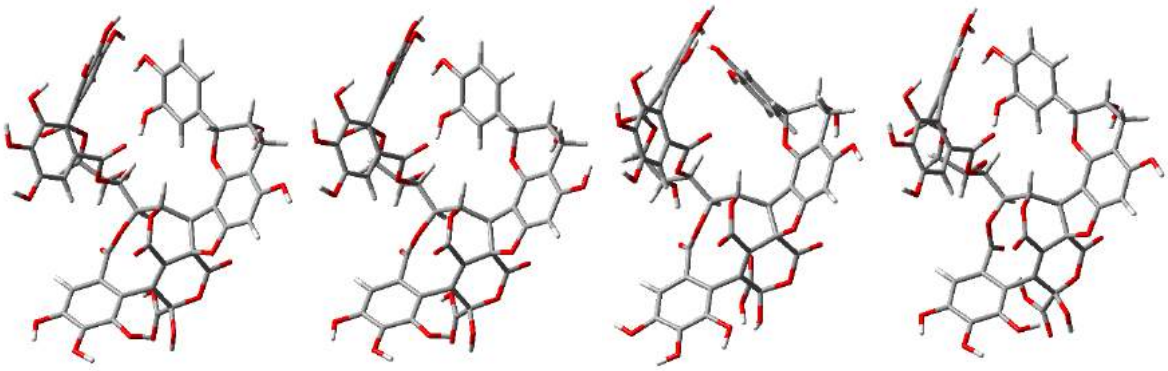
	R^2	CMaxErr	CMAE
(5*R*)-**6**	0.9963	5.7	1.6
(5*S*)-**6**	0.9962	6.3	1.6

R^2: coefficient of determination; CMaxErr: corrected maximum absolute error with respect to the linear fit; CMAE: corrected mean absolute error with respect to the linear fit

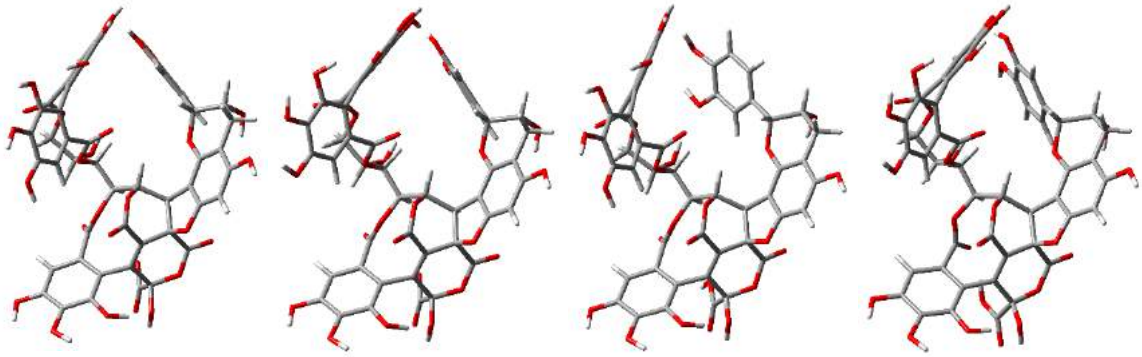
Table S28. The DP4 and DP4+ probability analysis of **6**.

	(5*R*)-**6**	(5*S*)-**6**
DP4 (^{13}C)	61.0%	39.0%
sDP4+ (^{13}C)	59.82%	40.18%
uDP4+ (^{13}C)	50.69%	49.31%
DP4+ (^{13}C)	60.48%	39.52%

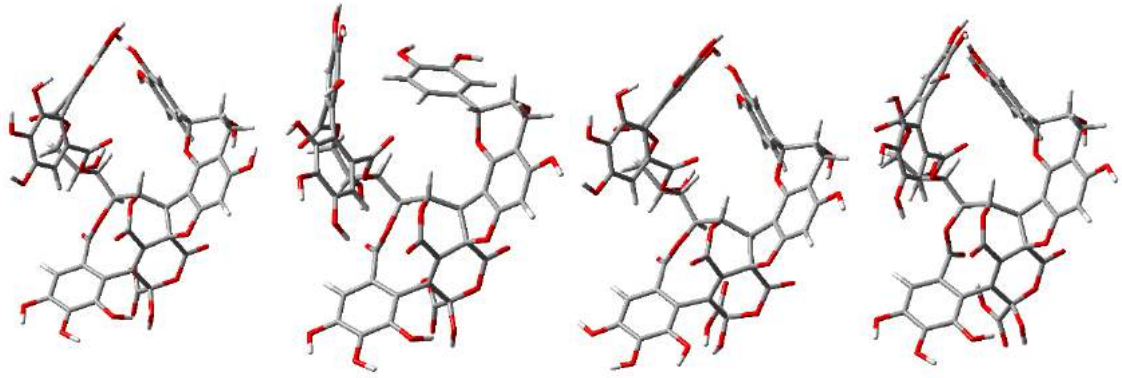
Fig. S19. Optimized conformers of (3*S*)-**7** at the B3LYP/6-31G(d,p) level in acetone (PCM) with populations greater than 1% calculated from their relative Gibbs free energies (ΔG).



(3*S*)-**7A** (38.3%) (3*S*)-**7B** (32.8%) (3*S*)-**7C** (4.3%) (3*S*)-**7D** (3.5%)



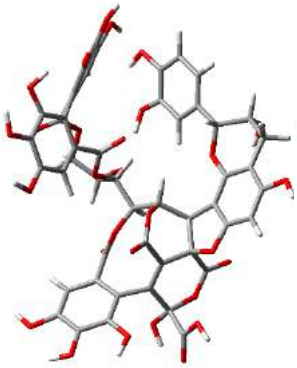
(3*S*)-**7E** (2.9%) (3*S*)-**7F** (2.9%) (3*S*)-**7G** (2.0%) (3*S*)-**7H** (1.4%)



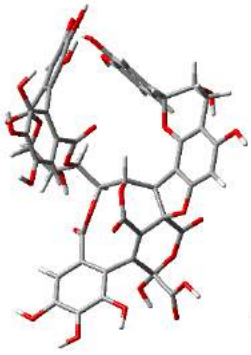
(3*S*)-**7I** (1.2%) (3*S*)-**7J** (1.2%) (3*S*)-**7K** (1.1%) (3*S*)-**7L** (1.1%)

(3*S*)-**7M** (1.0%)

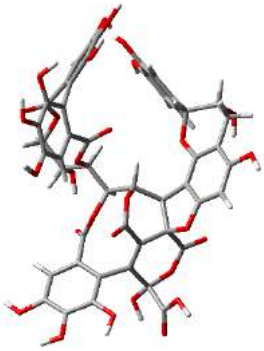
Fig. S20. Optimized conformers of (3*R*)-**7** at the B3LYP/6-31G(d,p) level in acetone (PCM) with populations greater than 1% calculated from their relative Gibbs free energies (ΔG).



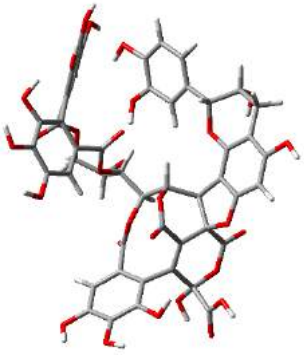
(3*R*)-**7A** (22.1%)



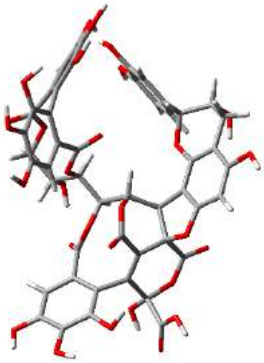
(3*R*)-**7B** (21.1%)



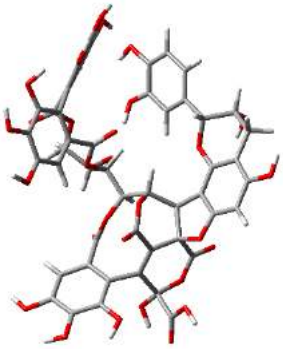
(3*R*)-**7C** (20.0%)



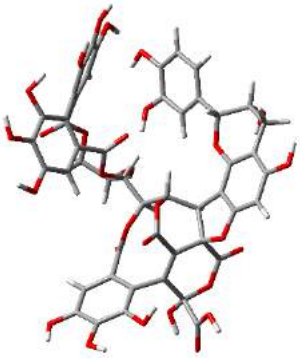
(3*R*)-**7D** (8.2%)



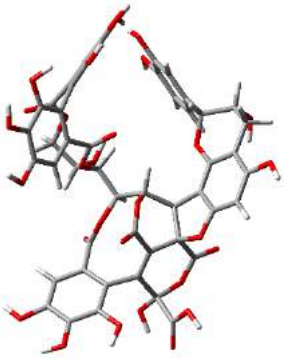
(3*R*)-**7E** (6.1%)



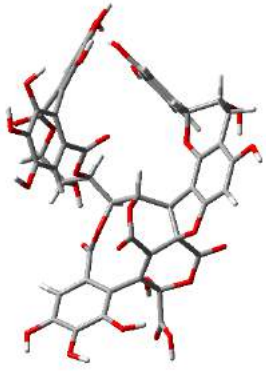
(3*R*)-**7F** (6.0%)



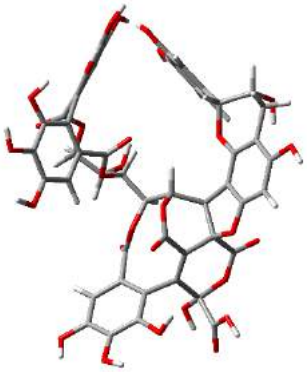
(3*R*)-**7G** (2.2%)



(3*R*)-**7H** (1.6%)



(3*R*)-**7I** (1.2%)



(3*R*)-**7J** (1.1%)

Table S29. Important thermodynamic parameters and conformational analysis of (3*S*)-**7** at the B3LYP/6-31G(d,p) level in acetone (PCM).

conformers	*E* (a.u.)	*E′* (a.u.)	*H* (a.u.)	*G* (a.u.)	Δ*G* (kcal/mol)	P_G (%)
(3*S*)-7**A**	-4069.279667	-4068.474482	-4068.407913	-4068.573138	0.00	38.3
(3*S*)-7**B**	-4069.278287	-4068.473423	-4068.406713	-4068.572992	0.09	32.8
(3*S*)-7**C**	-4069.276056	-4068.471573	-4068.404366	-4068.571069	1.30	4.3
(3*S*)-7**D**	-4069.279517	-4068.474139	-4068.407989	-4068.570868	1.42	3.5
(3*S*)-7**E**	-4069.273696	-4068.469902	-4068.402518	-4068.570717	1.52	2.9
(3*S*)-7**F**	-4069.273693	-4068.469909	-4068.402459	-4068.570694	1.53	2.9
(3*S*)-7**G**	-4069.276020	-4068.471513	-4068.404565	-4068.570348	1.75	2.0
(3*S*)-7**H**	-4069.274514	-4068.470569	-4068.403497	-4068.570033	1.95	1.4
(3*S*)-7**I**	-4069.272169	-4068.468624	-4068.401063	-4068.569899	2.03	1.2
(3*S*)-7**J**	-4069.270798	-4068.467334	-4068.399637	-4068.569881	2.04	1.2
(3*S*)-7**K**	-4069.272894	-4068.469115	-4068.401562	-4068.569783	2.11	1.1
(3*S*)-7**L**	-4069.274408	-4068.470220	-4068.403234	-4068.569781	2.11	1.1
(3*S*)-7**M**	-4069.274576	-4068.470178	-4068.402906	-4068.569712	2.15	1.0

E: total energy; E': total energy with zero point energy; H: enthalpy; G: Gibbs free energy; ΔG: relative Gibbs free energy at the B3LYP/6-31G(d,p) level in acetone (PCM). P_G*: conformational distribution calculated from relative Gibbs free energy.*

Table S30. Important thermodynamic parameters and conformational analysis of (3*R*)-**7** at the B3LYP/6-31G(d,p) level in acetone (PCM).

conformers	*E* (a.u.)	*E′* (a.u.)	*H* (a.u.)	*G* (a.u.)	Δ*G* (kcal/mol)	P_G (%)
(3*R*)-7**A**	-4069.276287	-4068.472176	-4068.404955	-4068.571399	0.00	22.1
(3*R*)-7**B**	-4069.272686	-4068.469474	-4068.401592	-4068.571355	0.03	21.1
(3*R*)-7**C**	-4069.272685	-4068.469464	-4068.401589	-4068.571304	0.06	20.0
(3*R*)-7**D**	-4069.275144	-4068.470800	-4068.403680	-4068.570463	0.59	8.2
(3*R*)-7**E**	-4069.271632	-4068.468137	-4068.400422	-4068.570188	0.76	6.1
(3*R*)-7**F**	-4069.274948	-4068.470915	-4068.403646	-4068.570175	0.77	6.0
(3*R*)-7**G**	-4069.273832	-4068.469560	-4068.402398	-4068.569236	1.36	2.2
(3*R*)-7**H**	-4069.269779	-4068.466974	-4068.398864	-4068.568928	1.55	1.6
(3*R*)-7**I**	-4069.271537	-4068.468019	-4068.400366	-4068.568633	1.74	1.2
(3*R*)-7**J**	-4069.268650	-4068.465849	-4068.397742	-4068.568559	1.78	1.1

E: total energy; E': total energy with zero point energy; H: enthalpy; G: Gibbs free energy; ΔG: relative Gibbs free energy at the B3LYP/6-31G(d,p) level in acetone (PCM). P_G*: conformational distribution calculated from relative Gibbs free energy.*

Table S31. Calculated ^{13}C NMR chemical shifts of (3*S*)-**7**.

	calculated[a]															experimental[b]
Position	(3*S*)-**7A**	(3*S*)-**7B**	(3*S*)-**7C**	(3*S*)-**7D**	(3*S*)-**7E**	(3*S*)-**7F**	(3*S*)-**7G**	(3*S*)-**7H**	(3*S*)-**7I**	(3*S*)-**7J**	(3*S*)-**7K**	(3*S*)-**7L**	(3*S*)-**7M**	averaged-(3*S*)-**7**	averaged-(3*S*)-**7** (corrected)	**7**
Glucose-1	53.5	53.4	53.3	53.9	52.4	53.0	52.5	53.2	52.9	52.5	53.0	52.8	53.3	53.3	53.7	50.2
2	80.0	79.8	80.8	79.5	81.0	81.3	79.3	81.7	81.5	80.9	82.3	81.3	80.8	80.1	79.9	76.4
3	76.4	76.3	76.2	77.6	74.2	74.3	75.7	76.4	74.3	75.6	75.2	76.3	76.2	76.2	76.0	75.8
4	75.1	75.4	77.0	74.1	78.2	78.0	78.3	76.2	77.9	76.5	78.1	76.3	77.0	75.6	75.5	75.7
5	72.6	72.4	65.4	71.8	69.2	69.6	69.4	68.8	69.6	63.7	69.7	68.7	65.4	71.5	71.5	69.0
6	63.9	63.9	64.9	63.8	66.2	66.4	65.4	66.1	66.4	64.3	66.3	66.0	64.9	64.2	64.3	67.4
epicatechin C-ring 2	78.1	77.9	79.1	78.0	79.4	79.3	78.8	79.0	78.9	79.4	79.3	79.2	78.8	78.2	78.0	79.3
3	65.9	65.7	66.4	65.9	66.3	65.9	66.3	66.3	66.0	65.4	66.2	66.3	66.2	65.9	66.0	66.4
4	29.4	26.9	27.9	29.2	28.0	27.9	29.9	27.7	25.7	30.2	28.1	27.7	25.8	28.2	29.2	28.2
A-ring 4a	104.2	100.8	100.2	103.9	100.1	100.4	104.1	100.7	97.2	103.2	100.2	100.1	97.0	102.2	101.5	102.4
5	159.6	160.0	159.6	159.7	159.6	159.7	159.3	159.5	159.9	160.3	159.5	159.5	159.9	159.8	157.7	158.2
6	89.3	90.4	89.0	89.4	88.4	89.4	89.9	89.5	90.3	89.8	89.2	88.6	90.3	89.7	89.2	90.6
7	160.3	161.3	161.4	160.1	160.5	161.3	160.3	160.9	162.1	160.7	161.6	160.2	162.2	160.8	158.7	158.5
8	107.3	107.6	108.1	107.0	107.2	108.1	108.0	108.9	108.2	107.1	108.8	107.6	108.2	107.5	106.7	104.9
8a	153.7	153.4	154.3	153.7	154.9	154.0	154.5	154.0	153.5	155.1	154.4	154.7	153.8	153.7	151.8	152.0
B-ring 1	133.8	133.4	132.6	134.1	131.2	134.6	134.6	134.6	134.5	130.8	134.9	130.5	132.3	133.5	132.0	131.1
2	112.1	112.1	114.6	112.5	113.5	115.0	111.4	114.3	114.7	113.4	114.4	112.9	114.4	112.5	111.5	114.9
3	145.6	145.6	143.2	146.1	143.8	143.1	146.7	143.7	143.4	144.3	143.4	144.7	143.2	145.3	143.5	145.2 [e]
4	143.7	143.9	144.7	144.4	147.6	144.3	142.8	144.5	144.4	147.8	144.3	147.6	144.7	144.1	142.4	145.0 [e]
5	115.6	115.5	113.7	115.5	113.6	113.1	117.4	114.2	113.6	115.7	114.0	113.6	113.8	115.2	114.2	115.8
6	117.5	117.4	122.8	117.9	121.3	123.8	118.1	122.1	123.7	127.3	123.2	121.9	122.5	118.5	117.4	119.4
D-Ring 1	139.1	138.9	141.1	136.8	139.1	139.7	138.6	136.6	139.8	139.9	140.6	136.6	141.1	139.0	137.4	137.8
2	138.7	139.1	138.1	144.0	138.2	138.5	139.6	144.1	138.6	139.2	138.7	143.8	138.2	139.1	137.5	131.0
3	97.8	97.9	100.2	97.4	98.0	98.0	97.8	96.9	98.1	97.5	100.4	96.8	100.2	98.0	97.3	99.2
4	170.5	170.5	171.9	170.4	170.8	170.7	170.5	170.5	170.7	170.4	172.6	170.6	171.9	170.6	168.3	166.8
5	167.5	167.4	168.9	167.3	167.8	167.7	167.5	167.4	167.7	167.5	169.0	167.5	168.9	167.6	165.3	161.5
6	81.4	81.4	83.4	81.9	82.1	82.4	81.6	82.5	82.4	81.4	83.7	81.8	83.4	81.7	81.4	86.6
7	167.4	167.3	168.2	166.6	168.0	167.8	167.5	167.5	167.8	168.7	168.3	167.8	168.2	167.4	165.2	164.2
E-Ring 1	126.2	126.5	124.4	123.6	126.9	126.8	127.1	126.0	126.7	123.7	125.3	125.3	124.3	126.1	124.8	125.1 [f]
2	111.4	110.8	112.9	107.3	113.5	112.8	110.3	110.8	112.8	112.8	112.3	110.5	112.9	111.2	110.3	112.1
3	144.4	143.6	143.2	143.2	146.2	144.3	143.2	145.1	144.3	146.9	142.9	144.9	143.2	144.1	142.3	145.0 [g]
4	139.2	138.4	135.0	137.5	138.5	136.8	137.3	138.8	137.0	142.3	134.1	139.4	135.0	138.5	136.9	136.0
5	148.6	148.5	144.5	150.2	146.7	146.1	148.0	151.0	146.1	149.0	144.1	151.2	144.5	148.2	146.4	146.9 [g]
6	110.9	111.3	110.1	104.6	111.5	111.3	111.5	106.1	111.4	112.0	109.9	105.9	110.1	110.7	109.7	105.8
7	172.0	172.3	173.1	183.1	172.3	172.3	172.3	183.7	172.4	174.6	170.6	183.3	173.1	172.9	170.5	167.2
F-Ring 1	127.4	127.5	127.6	126.8	128.4	127.0	128.1	126.0	126.8	128.3	126.7	127.9	127.6	127.4	126.1	125.8 [f]
2	118.6	118.6	119.4	118.8	117.6	119.8	117.0	119.7	119.7	115.8	119.6	117.6	119.4	118.6	117.5	115.9
3	142.7	142.7	142.7	143.2	142.8	143.8	141.8	143.1	143.8	141.4	143.5	142.6	142.7	142.7	141.0	144.2 [g]
4	139.1	138.9	139.4	139.1	136.2	139.9	134.3	139.7	139.9	134.5	139.7	136.1	139.4	138.8	137.2	136.4
5	145.4	145.3	145.8	145.5	145.1	146.2	142.7	145.8	146.2	143.4	145.9	145.3	145.8	145.3	143.6	146.9 [g]
6	110.5	110.3	110.7	110.3	108.4	110.5	107.2	110.9	110.5	109.3	110.5	108.7	110.7	110.3	109.3	108.6
7	172.0	172.0	173.3	172.1	172.3	172.6	171.7	172.9	172.6	172.6	172.7	172.5	173.3	172.2	169.8	167.5
G-Ring 1	128.7	128.8	129.5	129.0	130.5	130.2	128.6	129.4	130.1	126.9	129.7	130.3	129.5	128.9	127.5	127.3 [f]
2	116.8	117.1	117.2	117.1	120.7	116.7	121.0	116.5	116.6	117.7	116.5	120.7	117.2	117.2	116.1	115.3
3	143.3	143.1	143.3	142.8	142.8	141.7	143.8	142.1	141.5	141.6	141.8	143.8	143.3	143.1	141.4	144.2 [g]
4	136.5	136.5	137.8	136.6	137.9	135.2	139.3	135.7	135.1	138.6	135.3	138.5	137.7	136.6	135.1	135.6
5	145.5	145.3	144.7	145.3	142.5	143.9	143.3	144.1	144.1	144.5	144.1	142.2	144.6	145.1	143.3	145.3 [g]
6	110.0	110.0	109.7	110.7	110.5	109.8	109.8	109.5	109.8	111.1	109.3	110.4	109.6	110.0	109.1	107.1
7	172.6	172.6	172.4	172.6	173.0	173.1	172.9	173.1	173.1	173.3	173.0	173.0	172.4	172.7	170.3	169.1

[a] Calculated using the GIAO method at the mPW1PW91/6-311+G(2d,p) level in acetone (PCM). [b] Measured in acetone-d_6 + D_2O (ref. 6c). [c] Averaged according to the Boltzmann distribution theory at 298 K based on relative Gibbs free energies. [d] Linearly corrected for the experimental data. [e–g] May be interchanged in each column.

Table S32. Calculated ^{13}C NMR chemical shifts of (3*R*)-**7**.

	calculated[a]												experimental[b]
Position	(3*R*)-**7A**	(3*R*)-**7B**	(3*R*)-**7C**	(3*R*)-**7D**	(3*R*)-**7E**	(3*R*)-**7F**	(3*R*)-**7G**	(3*R*)-**7H**	(3*R*)-**7I**	(3*R*)-**7J**	averaged-(3*R*)-**7**	averaged-(3*R*)-**7** (corrected)	**7**
Glucose-1	55.3	55.7	55.7	55.4	55.7	55.3	55.3	55.6	55.0	55.7	55.5	56.0	50.2
2	79.2	79.4	79.4	79.9	80.2	79.2	79.9	80.7	80.8	81.5	79.5	79.3	76.4
3	75.4	75.1	75.1	75.1	74.7	75.4	75.1	73.5	75.1	73.3	75.1	75.0	75.8
4	75.5	76.3	76.3	75.6	76.5	75.5	75.6	77.7	77.0	77.9	76.0	75.9	75.7
5	72.4	65.2	65.1	72.4	65.3	72.4	72.4	69.5	65.6	69.5	68.4	68.5	69.0
6	63.8	64.6	64.5	63.8	64.8	63.8	63.8	66.4	65.2	66.4	64.3	64.5	67.4
epicatechin C-ring 2	78.0	79.0	79.0	78.0	79.1	77.7	77.7	78.9	79.2	79.1	78.5	78.3	79.3
3	66.0	66.0	66.0	66.1	66.0	65.9	65.9	66.1	66.4	66.0	66.0	66.2	66.4
4	29.0	27.7	27.7	28.9	27.7	26.8	26.8	28.0	27.9	27.9	28.1	29.2	28.2
A-ring 4a	104.4	100.2	100.2	104.7	100.4	102.7	103.1	101.2	100.2	101.5	101.9	101.1	102.4
5	159.7	159.6	159.6	159.9	159.7	160.6	160.9	160.0	159.8	160.2	159.8	157.4	158.2
6	88.6	89.2	89.2	88.6	89.0	89.2	89.1	90.1	88.8	90.0	89.0	88.5	90.6
7	160.9	162.5	162.5	160.7	162.3	161.6	161.4	162.4	161.9	162.3	161.8	159.3	158.5
8	106.4	107.3	107.3	106.1	107.0	106.4	106.1	107.2	106.9	106.9	106.8	105.9	104.9
8a	153.1	153.9	153.9	153.2	154.0	152.7	152.8	153.3	154.7	153.4	153.5	151.3	152.0
B-ring 1	133.6	133.7	133.7	133.5	133.5	133.2	133.1	135.4	132.7	135.4	133.7	131.9	131.1
2	112.1	115.4	115.4	112.1	115.3	112.2	112.1	114.6	114.8	114.5	114.0	112.8	114.9
3	145.6	143.1	143.1	145.7	143.1	145.7	145.7	143.1	143.2	143.1	144.2	142.2	145.0 [e]
4	144.2	144.4	144.4	144.1	144.4	144.2	144.2	144.1	144.7	144.2	144.3	142.3	145.2 [e]
5	115.5	113.4	113.3	115.6	113.4	115.6	115.7	113.2	113.6	113.3	114.3	113.1	115.8
6	117.5	123.0	123.0	117.5	122.9	117.5	117.5	124.2	122.5	124.1	120.6	119.3	119.4
D-Ring 1	136.4	138.2	138.2	139.9	141.8	136.3	139.9	137.9	143.7	141.5	138.2	136.3	137.8
2	145.6	144.4	144.4	142.8	141.6	145.6	142.8	145.1	136.7	141.5	144.3	142.3	131.0
3	98.2	97.9	97.8	98.0	97.6	98.2	98.0	98.2	97.1	97.9	98.0	97.2	99.2
4	171.4	172.1	172.1	171.0	171.2	171.4	171.0	172.1	169.6	171.1	171.6	168.9	166.8
5	170.2	170.5	170.5	169.1	169.4	170.2	169.1	170.5	169.3	169.3	170.2	167.5	161.5
6	81.7	83.2	83.2	80.6	82.0	81.7	80.6	83.0	81.4	81.7	82.3	82.0	86.6
7	168.4	168.8	168.8	169.1	169.4	168.4	169.1	168.8	167.1	169.4	168.8	166.1	164.2
E-Ring 1	126.2	124.8	124.8	126.2	125.3	126.1	126.2	126.2	128.0	126.7	125.5	124.0	125.1 [f]
2	115.3	116.1	116.1	116.9	117.2	115.3	116.8	115.3	111.9	116.4	115.9	114.7	112.1
3	144.8	145.2	145.2	140.6	141.8	144.8	140.6	144.8	143.1	141.0	144.2	142.2	145.0 [g]
4	136.8	135.1	135.1	139.6	138.5	136.8	139.6	134.6	136.5	137.3	136.4	134.6	136.0
5	146.3	144.6	144.6	148.3	147.2	146.3	148.3	144.8	146.3	146.7	145.8	143.8	146.9 [g]
6	106.8	106.7	106.7	111.6	112.8	106.8	111.6	106.1	112.0	111.0	107.8	106.8	105.8
7	172.7	174.3	174.3	171.8	174.0	172.7	171.9	172.0	174.2	171.6	173.4	170.7	167.2
F-Ring 1	127.2	127.4	127.5	127.2	127.3	127.2	127.2	126.8	127.4	126.4	127.3	125.8	125.8 [f]
2	118.8	119.6	119.6	118.9	119.6	118.8	118.8	119.8	119.5	119.8	119.3	117.9	115.9
3	142.3	142.1	142.1	142.3	142.3	142.3	142.3	143.3	142.6	143.7	142.3	140.3	144.2 [g]
4	138.7	139.2	139.2	138.8	139.3	138.7	138.9	139.8	139.4	139.9	139.0	137.2	136.4
5	145.0	145.5	145.5	145.0	145.6	145.1	145.0	145.8	145.8	146.0	145.3	143.3	146.9 [g]
6	110.1	110.4	110.4	110.3	110.5	110.1	110.4	110.5	110.7	110.5	110.3	109.2	108.6
7	171.7	172.6	172.6	171.8	172.8	171.7	171.8	172.2	173.2	172.3	172.3	169.5	167.5
G-Ring 1	129.3	130.9	130.9	129.3	131.0	129.3	129.3	130.5	130.0	130.4	130.2	128.6	127.3 [f]
2	117.4	117.9	117.9	117.1	117.7	117.4	117.1	116.7	117.4	116.4	117.6	116.3	115.3
3	142.8	143.3	143.3	142.9	143.2	142.8	142.9	142.1	143.3	141.7	143.1	141.1	144.2 [g]
4	136.6	137.3	137.3	136.5	137.1	136.6	136.5	135.7	137.6	135.5	136.9	135.1	135.6
5	145.1	143.7	143.7	145.1	143.7	145.1	145.1	144.1	144.5	144.5	144.3	142.3	145.3 [g]
6	110.5	110.4	110.5	110.5	110.3	110.5	110.4	110.2	109.8	110.2	110.4	109.4	107.1
7	172.8	172.6	172.6	172.8	172.7	172.8	172.8	173.4	172.6	173.3	172.7	170.0	169.1

[a] Calculated using the GIAO method at the mPW1PW91/6-311+G(2d,p) level in acetone (PCM). [b] Measured in acetone-d_6 + D_2O (ref. 6c). [c] Averaged according to the Boltzmann distribution theory at 298 K based on relative Gibbs free energies. [d] Linearly corrected for the experimental data. [e–g] May be interchanged in each column.

Fig. S21. Correlation plots of experimental ^{13}C NMR chemical shifts versus corresponding calculated ^{13}C NMR chemical shifts of **7**.

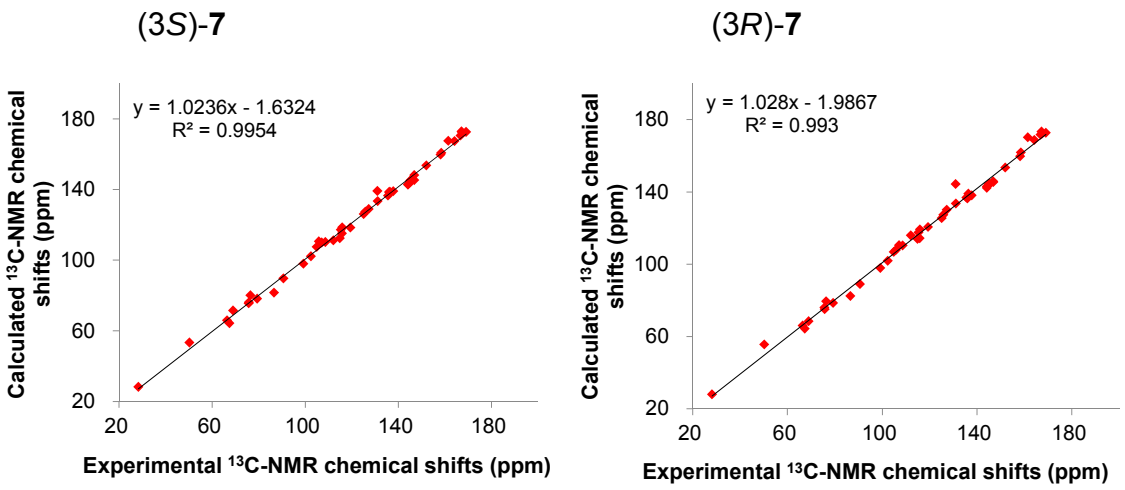


Fig. S22. Differences between experimental and calculated ^{13}C NMR chemical shifts of **7**. $\Delta\delta$ (ppm) = $\delta_{calcd.} - \delta_{exptl}$. Calculations of NMR chemical shifts were performed at the mPW1PW91/6-311+G(2d,p) level in acetone (PCM) and linearly corrected for the experimental data.

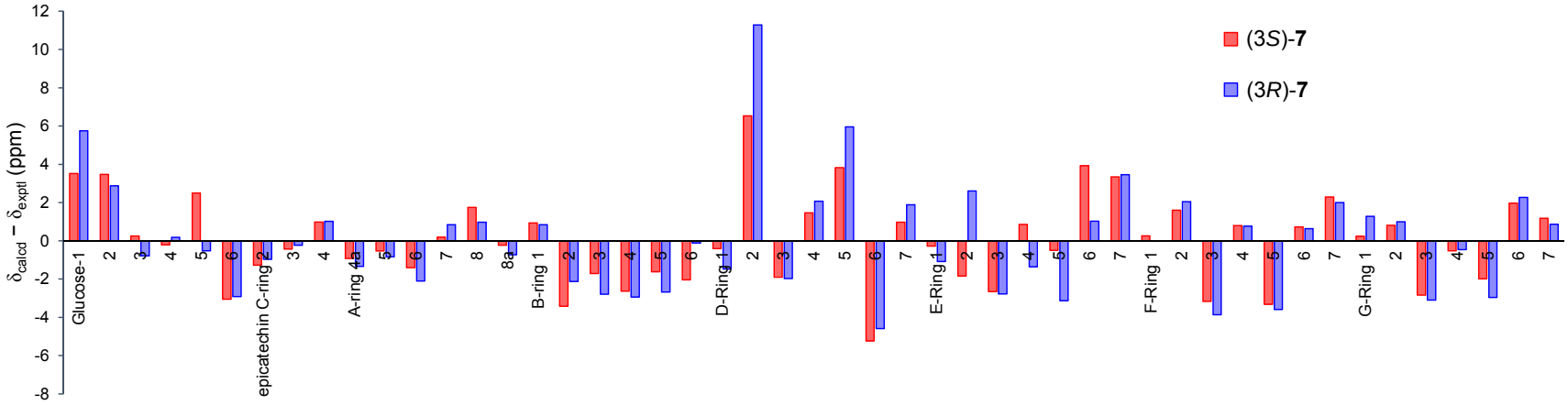


Table S33. Statistical parameters of calculated ^{13}C NMR chemical shifts of **7** (ppm).

	R^2	CMaxErr	CMAE
(3*S*)-**7**	0.9954	6.5	1.8
(3*R*)-**7**	0.9930	11.3	2.1

R^2: coefficient of determination; CMaxErr: corrected maximum absolute error with respect to the linear fit; CMAE: corrected mean absolute error with respect to the linear fit

Table S34. The DP4 and DP4+ probability analysis of **7**.

	(3*S*)-**7**	(3*R*)-**7**
DP4 (^{13}C)	100.0%	0.0%
sDP4+ (^{13}C)	100.00%	0.00%
uDP4+ (^{13}C)	98.88%	1.12%
DP4+ (^{13}C)	100.00%	0.00%

Fig. S23. ^{1}H NMR spectrum of **4** (500 MHz for ^{1}H and 125 MHz for ^{13}C, acetone-d_6 + D_2O).

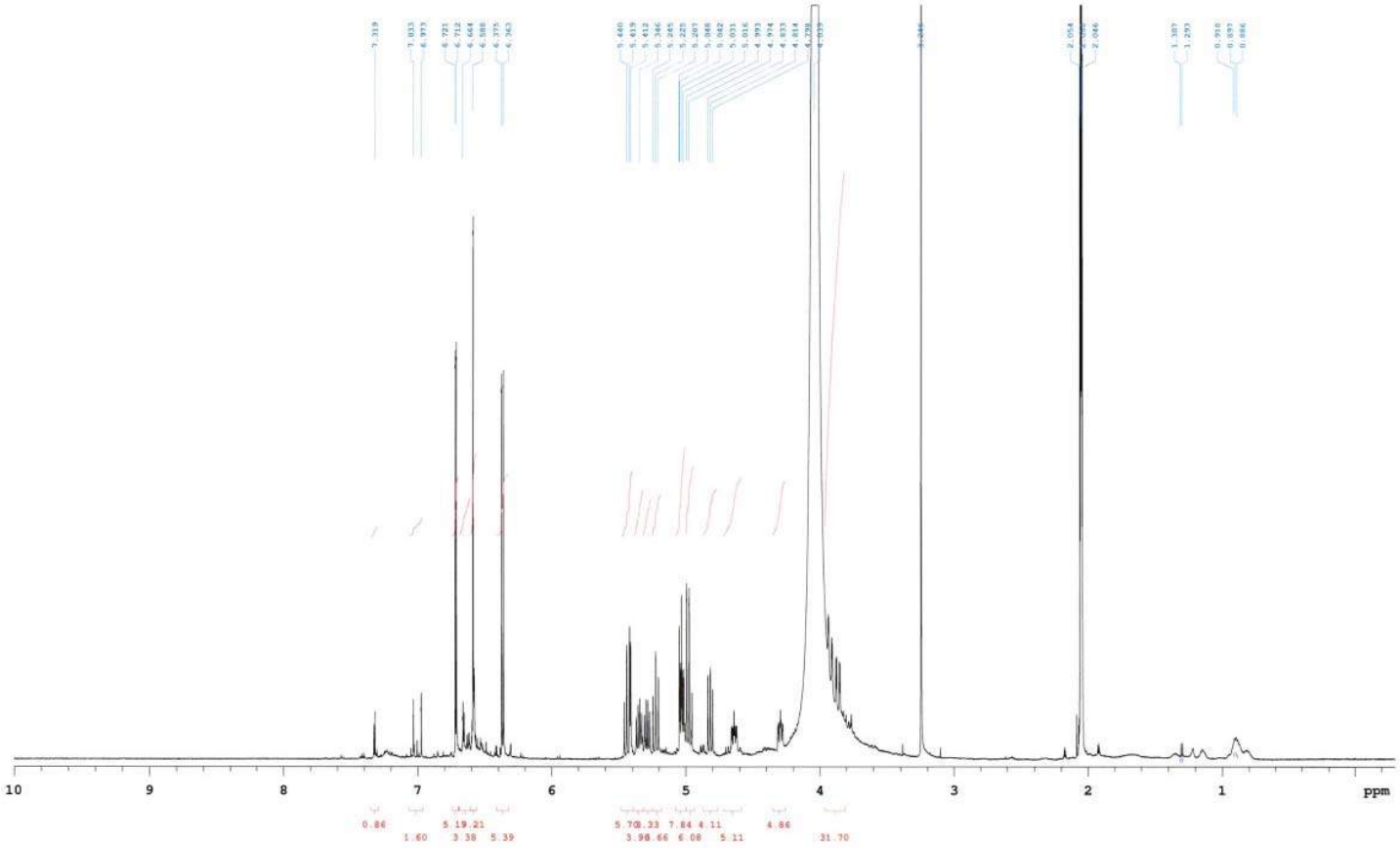


Fig. S24. ^{13}C NMR spectrum of **4** (500 MHz for ^{1}H and 125 MHz for ^{13}C, acetone-d_6 + D_2O).

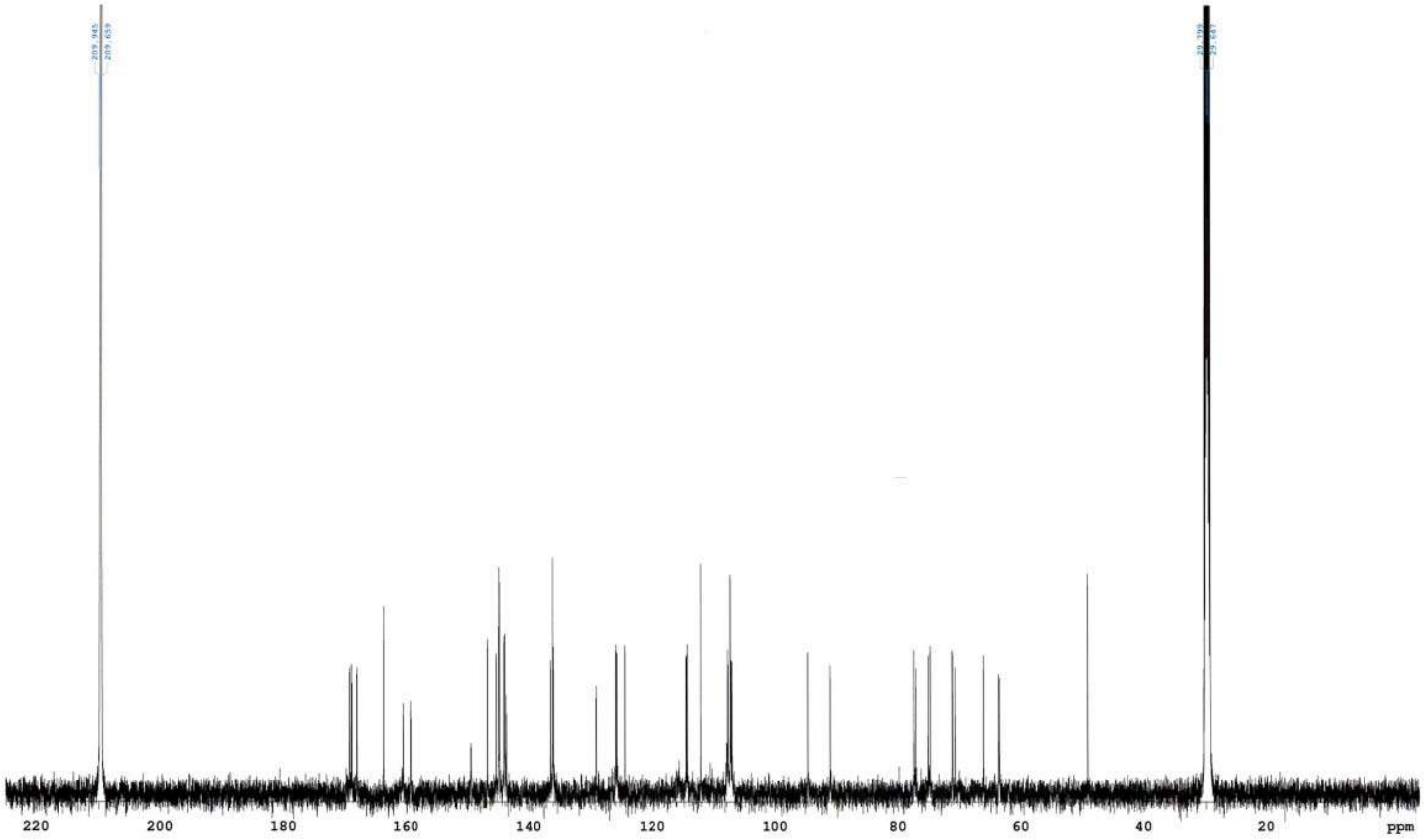


Fig. S25. ^{1}H-^{1}H COSY spectrum of **4** (500 MHz, acetone-d_6 + D_2O).

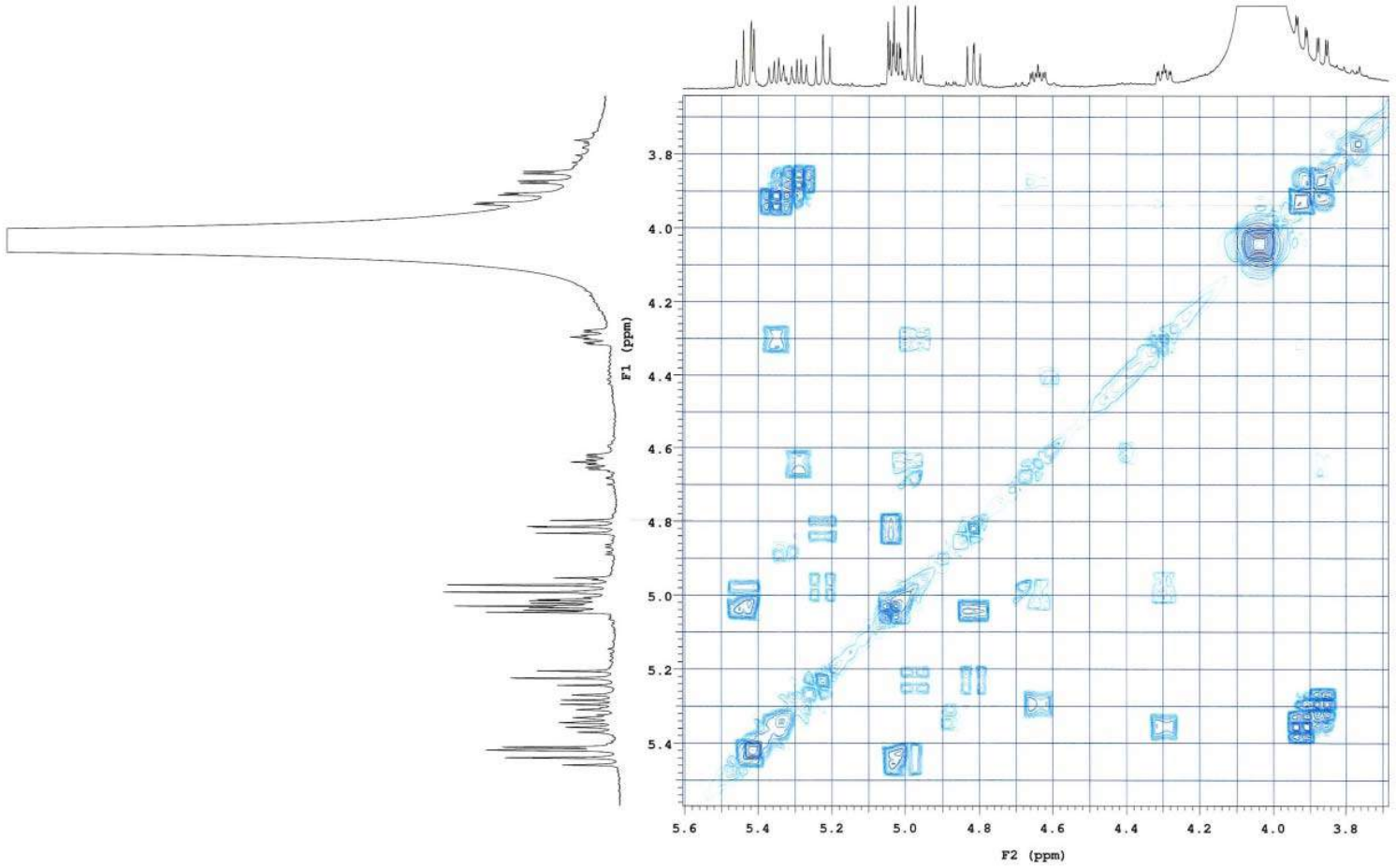


Fig. S26. HSQC spectrum of **4** (500 MHz, acetone-d_6 + D_2O).

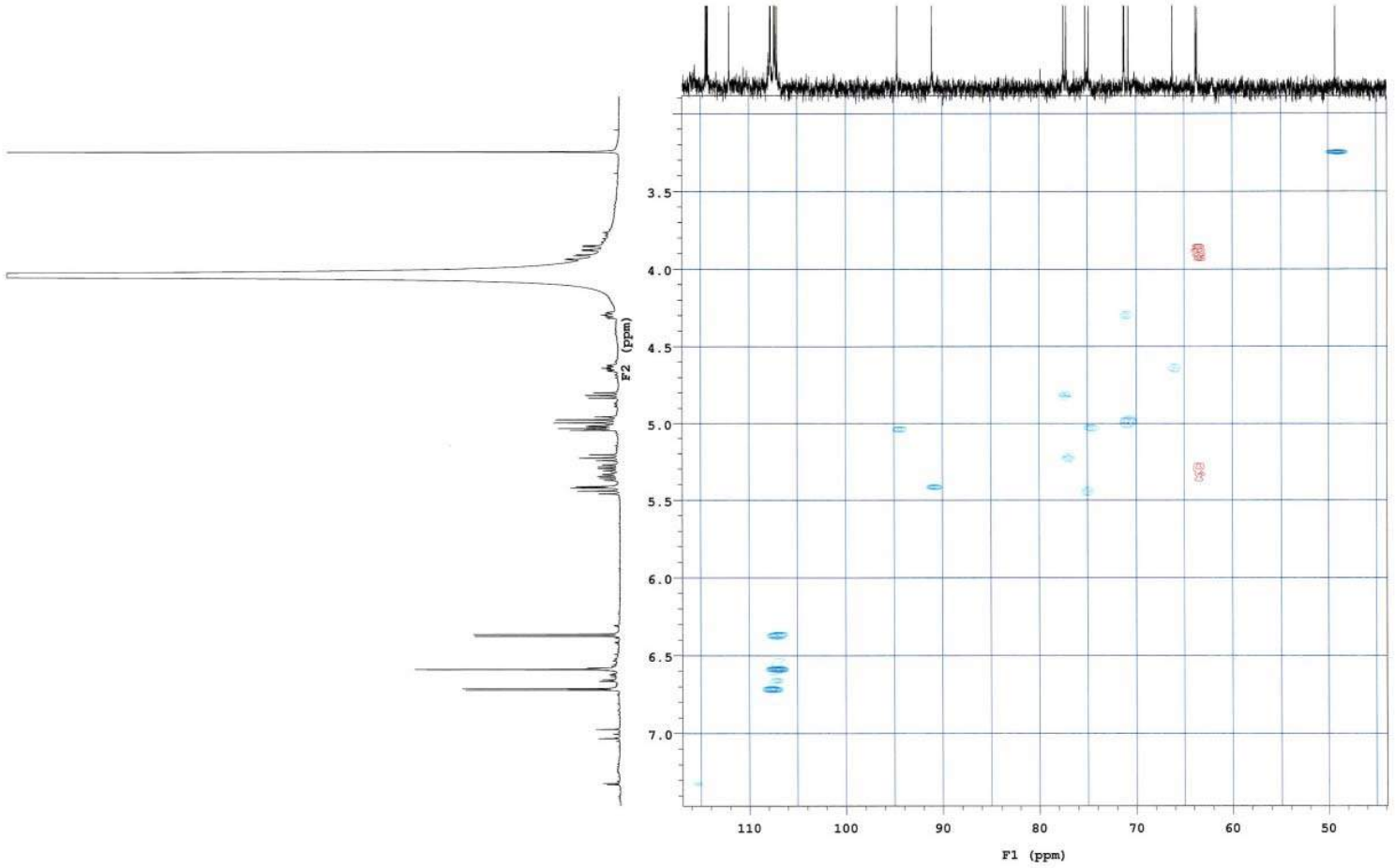


Fig. S27. HMBC spectrum of **4** (500 MHz, acetone-d_6 + D_2O).

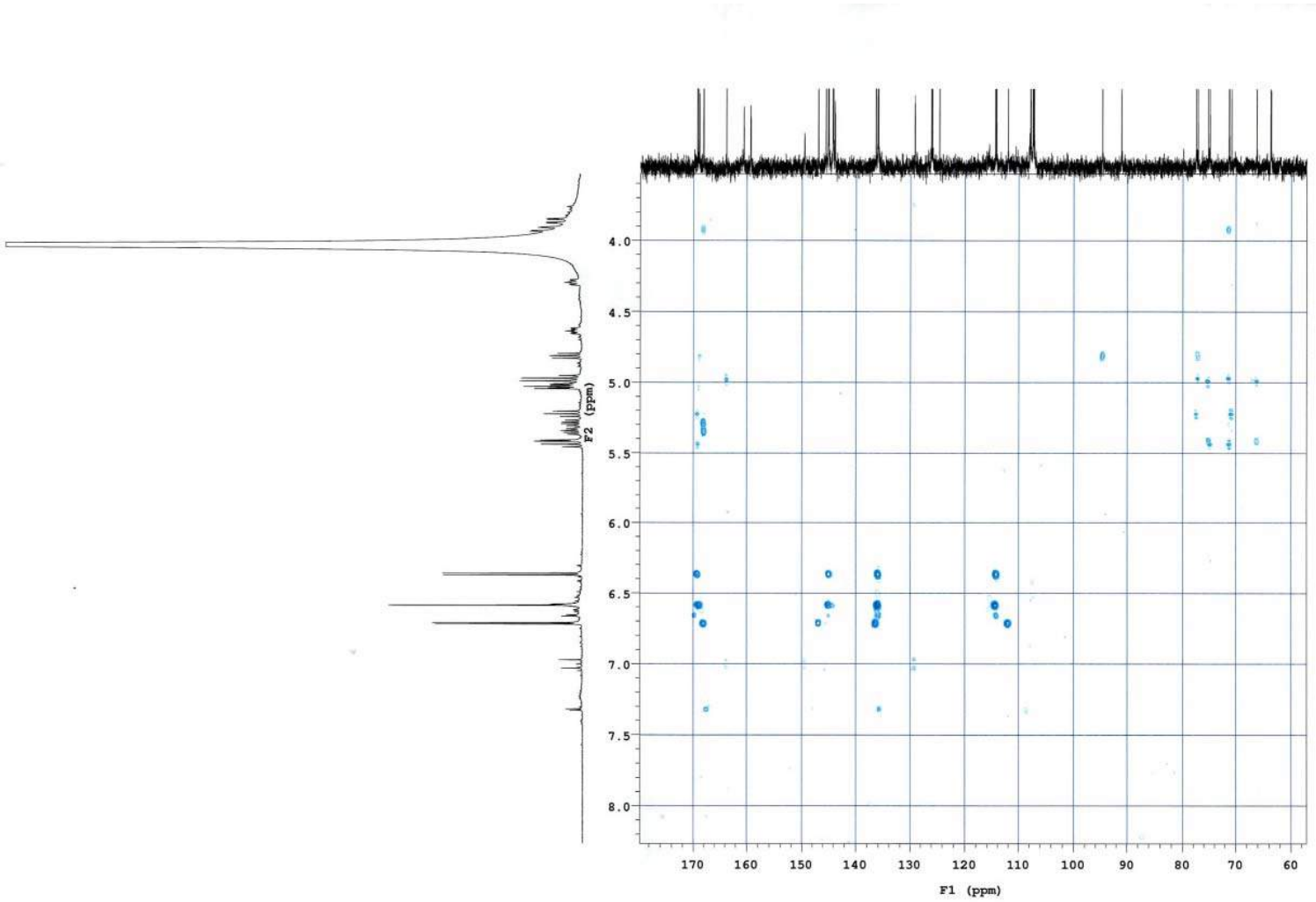


Fig. S28. ^{1}H NMR spectrum of **5** (500 MHz, acetone-*d*6+D_2O).

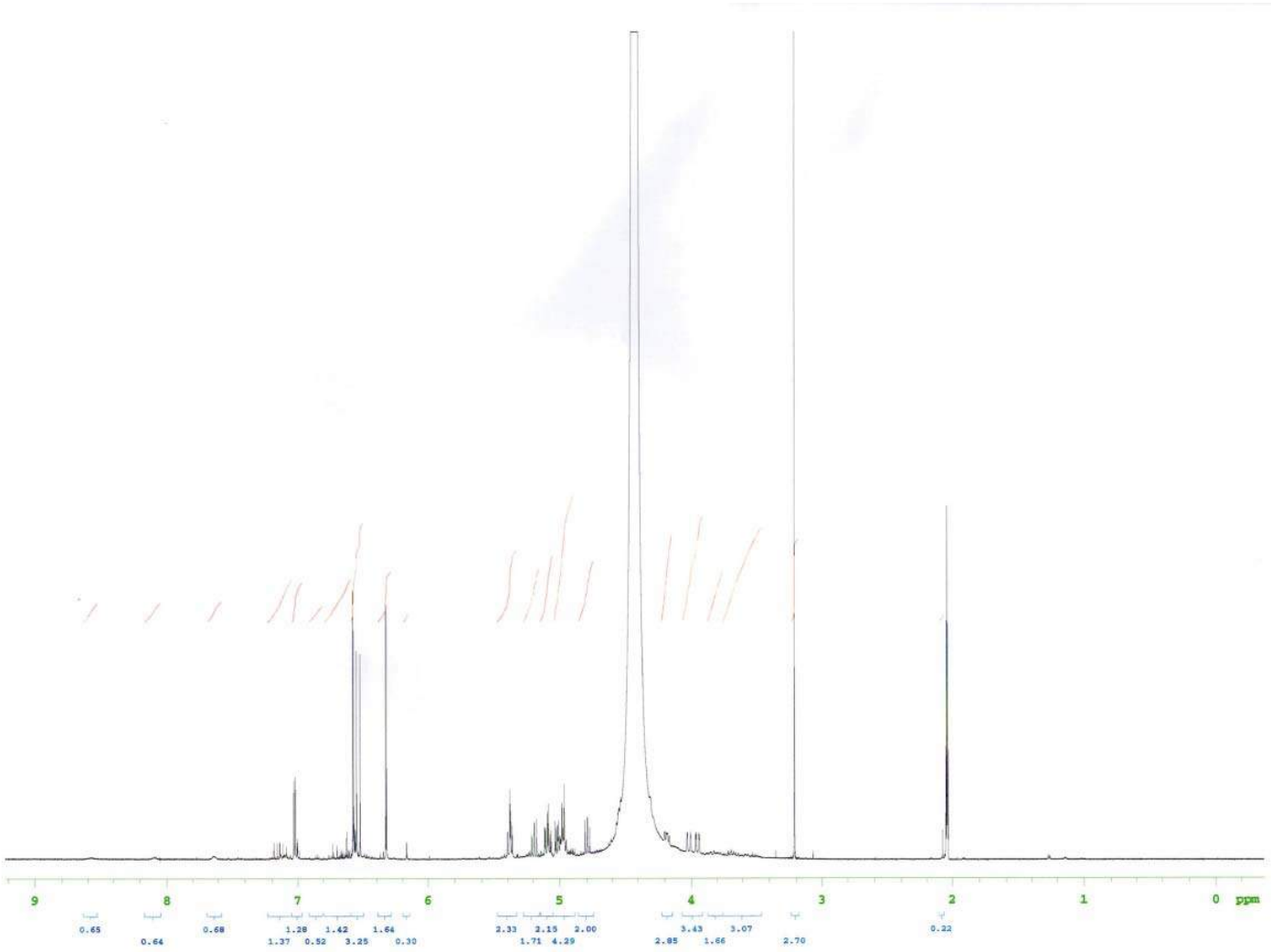
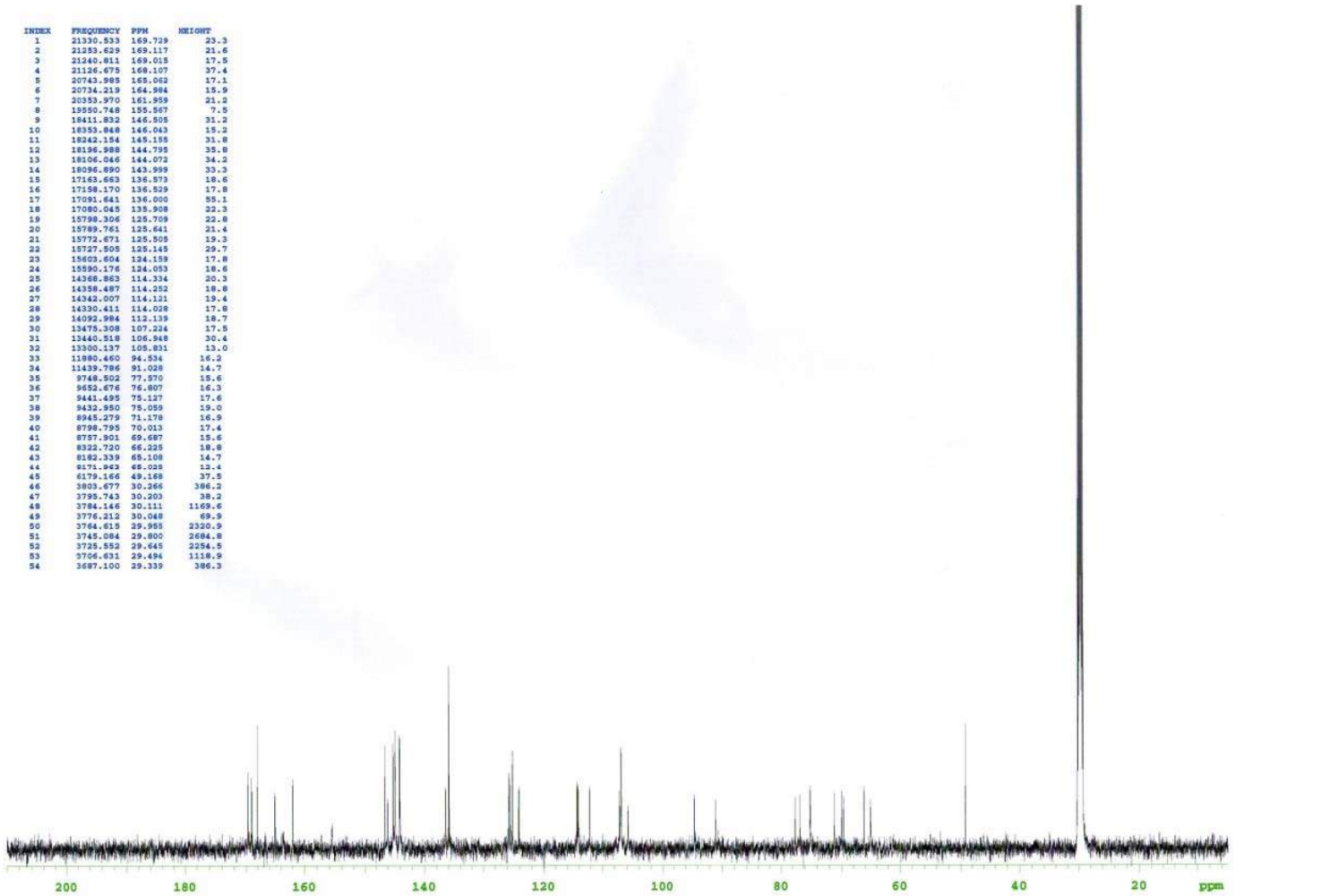


Fig. S29. ^{13}C NMR spectrum of **5** (125 MHz, acetone-*d*6+D_2O).



INDEX	FREQUENCY	PPM	HEIGHT
1	21330.533	169.729	23.3
2	21253.629	169.117	21.6
3	21240.811	169.015	17.5
4	21126.675	168.107	37.4
5	20743.985	165.062	17.1
6	20734.219	164.984	15.9
7	20353.970	161.959	21.2
8	19550.748	155.567	7.5
9	18411.832	146.505	31.2
10	18353.848	146.043	15.2
11	18242.154	145.155	31.8
12	18196.988	144.795	35.8
13	18106.046	144.072	34.2
14	18096.890	143.999	33.3
15	17163.663	136.573	18.6
16	17158.170	136.529	17.8
17	17091.641	136.000	55.1
18	17080.045	135.908	22.3
19	15798.306	125.709	22.8
20	15789.761	125.641	21.4
21	15772.671	125.505	19.3
22	15727.505	125.145	29.7
23	15603.604	124.159	17.8
24	15590.176	124.053	18.6
25	14368.863	114.334	20.3
26	14358.487	114.252	18.8
27	14342.007	114.121	19.4
28	14330.411	114.028	17.8
29	14092.984	112.139	18.7
30	13475.308	107.224	17.5
31	13440.518	106.948	30.4
32	13300.137	105.831	13.0
33	11890.460	94.634	16.2
34	11439.786	91.028	14.7
35	9748.502	77.570	15.6
36	9652.676	76.807	16.3
37	9441.495	75.127	17.6
38	9432.950	75.059	19.0
39	8945.279	71.178	16.9
40	8798.795	70.013	17.4
41	8757.901	69.687	15.6
42	8322.720	66.225	18.8
43	8182.339	65.108	14.7
44	8171.943	65.025	12.4
45	6179.166	49.168	37.5
46	3803.677	30.266	386.2
47	3795.743	30.203	38.2
48	3784.146	30.111	1169.6
49	3776.212	30.048	69.9
50	3764.615	29.955	2320.9
51	3745.084	29.800	2684.8
52	3725.552	29.645	2254.5
53	3706.631	29.494	1118.9
54	3687.100	29.339	386.3

Fig. S30. ^{1}H-^{1}H COSY spectrum of **5** (500 MHz, acetone-*d*6+D_2O).

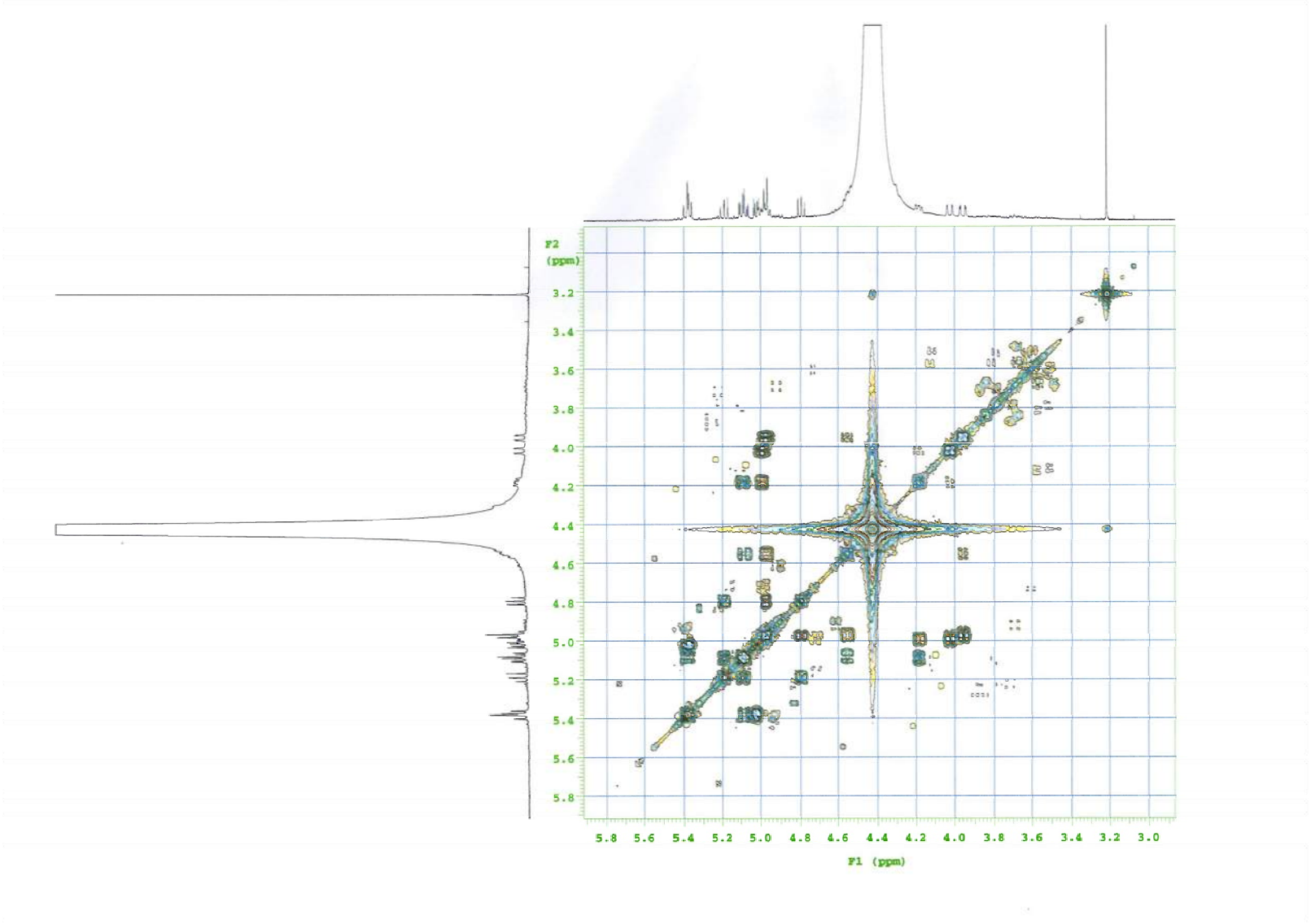


Fig. S31. HSQC spectrum of **5** (500 MHz, acetone-*d*6+D_2O).

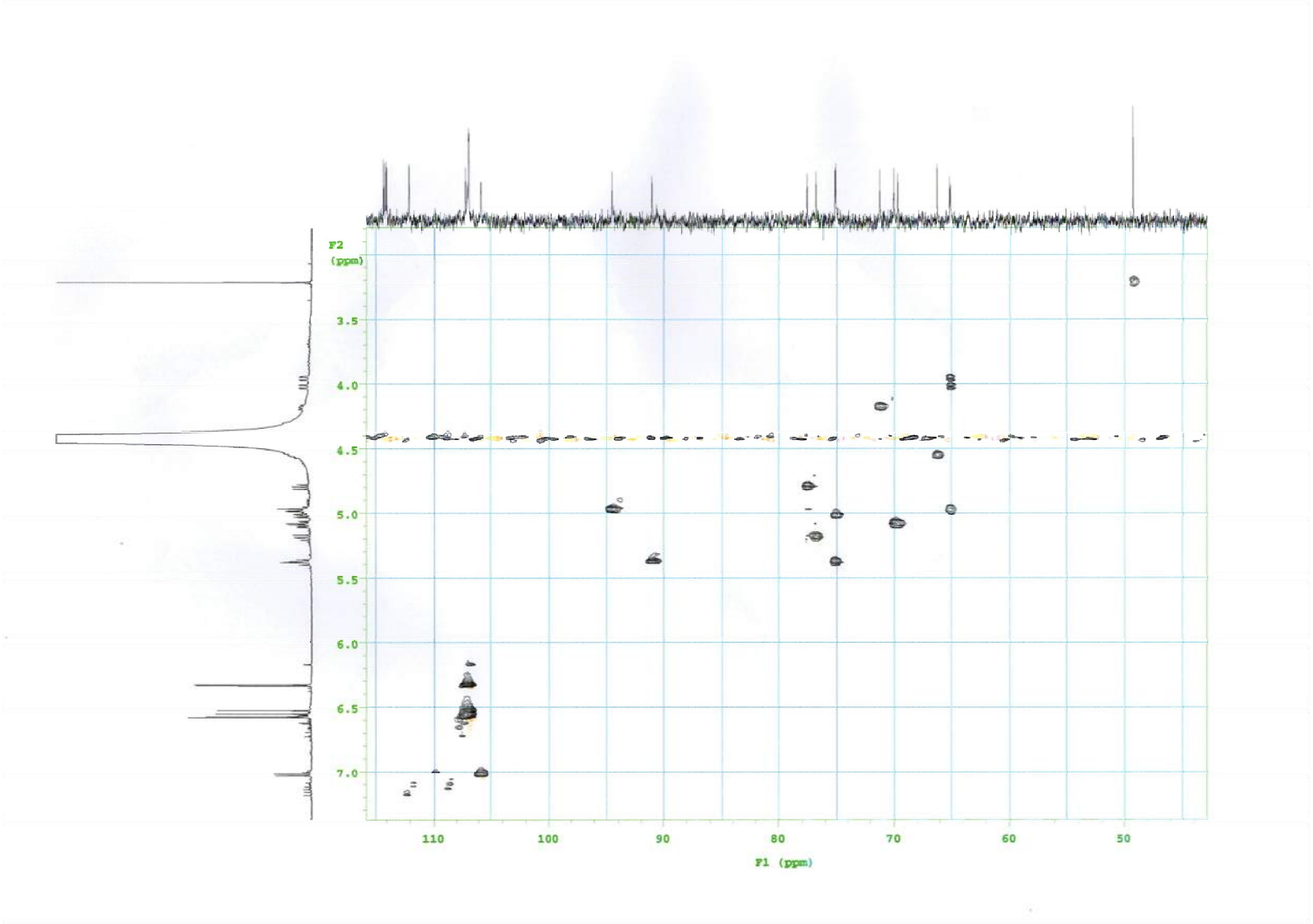


Fig. S32. HMBC spectrum of **5** (500 MHz, acetone-*d*6+D_2O).

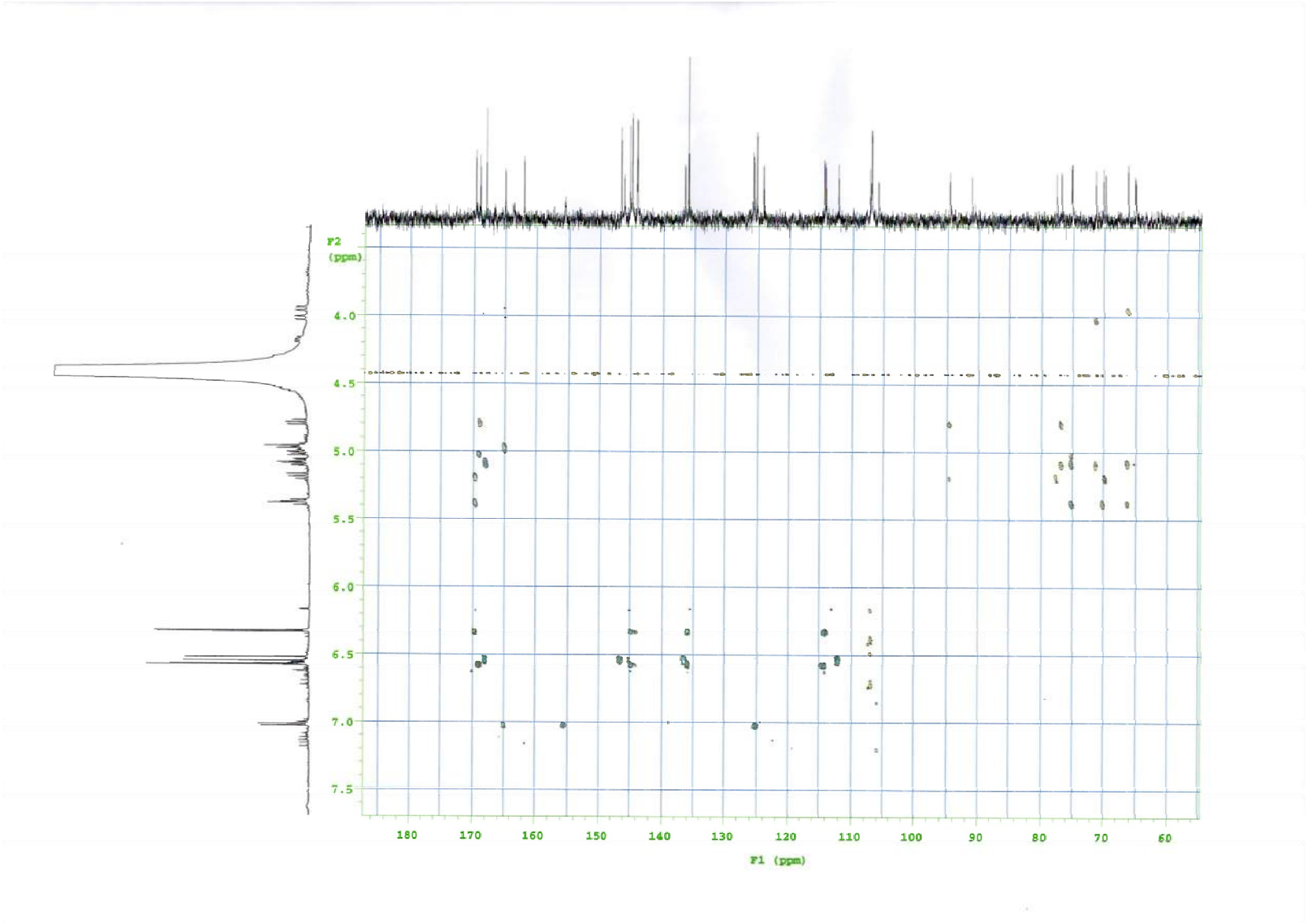


Fig. S33. ^{1}H NMR spectrum of **6** (500 MHz, acetone-*d*6+D_2O).

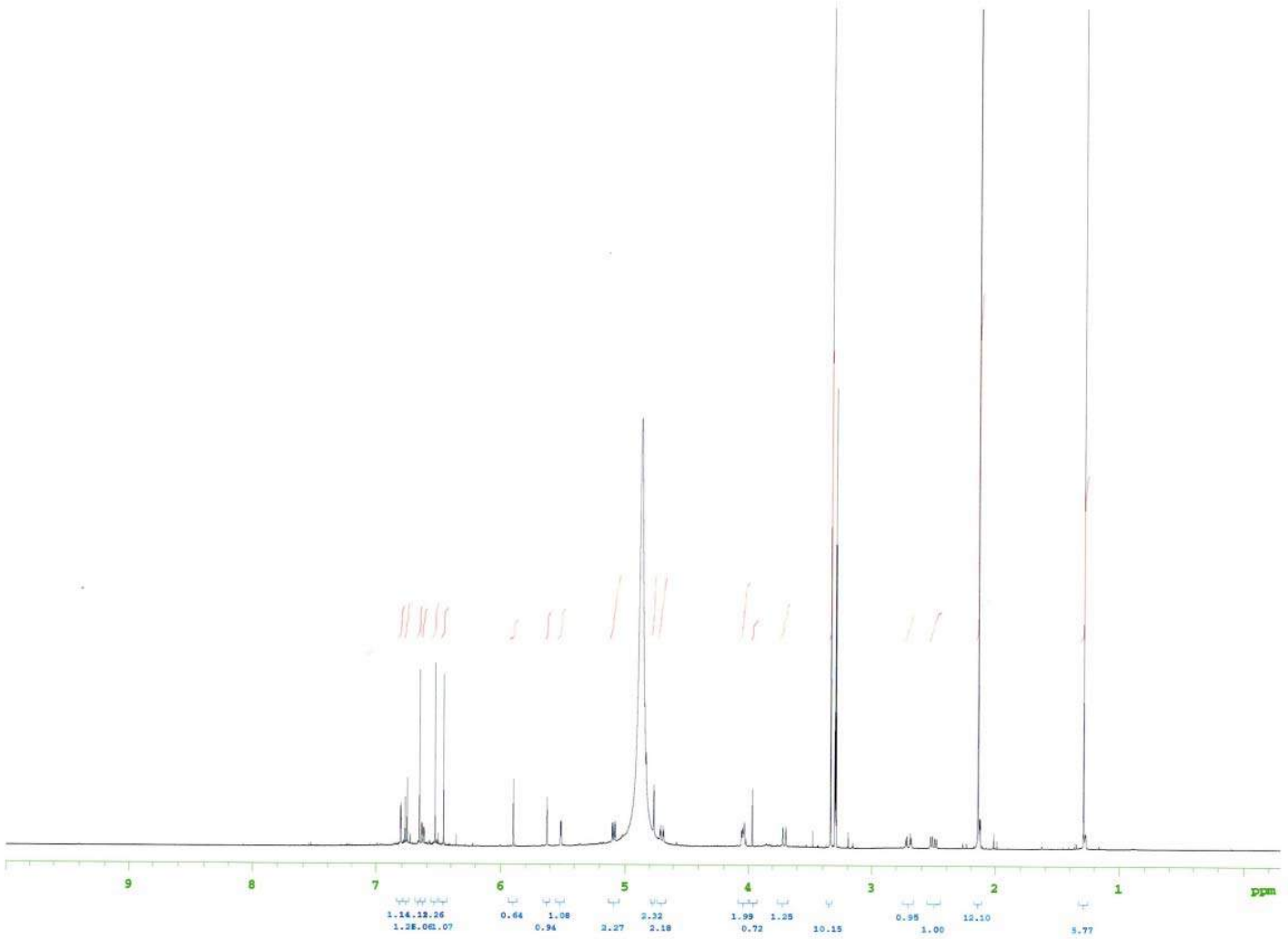


Fig. S34. ^{13}C NMR spectrum of **6 (**125 MHz, acetone-*d*6+D_2O).

INDEX	FREQUENCY	PPM	HEIGHT	INDEX	FREQUENCY	PPM	HEIGHT
1	26433.206	210.335	36.757		6179.300	49.170	7626.7
2	21477.151	170.898	37.658		6157.937	49.000	9000.0
3	21247.049	169.067	35.359		6136.575	48.830	8347.4
4	21173.196	168.480	35.360		6123.758	48.728	101.1
5	21169.534	168.450	33.561		6115.213	48.660	4293.4
6	20918.679	166.454	31.462		6102.395	48.558	72.1
7	20447.488	162.705	28.963		6093.850	48.490	1403.3
8	20014.138	159.257	19.864		6081.033	48.388	26.8
9	20007.425	159.203	11.465		6034.036	48.014	12.3
10	19939.676	158.664	21.866		6012.674	47.844	13.9
11	19113.870	152.093	24.767		5990.701	47.669	11.8
12	18581.643	147.858	35.368		3856.302	30.685	209.3
13	18463.845	146.921	34.369		3429.666	27.291	22.9
14	18372.293	146.192	39.570		3039.651	24.187	161.3
15	18365.579	146.139	39.2				
16	18327.737	145.838	44.8				
17	18324.685	145.813	53.2				
18	18196.511	144.793	39.8				
19	18189.798	144.740	39.1				
20	17335.916	137.946	28.3				
21	17290.139	137.581	35.5				
22	17242.532	137.202	34.3				
23	17215.066	136.984	39.9				
24	16599.221	132.083	33.8				
25	16557.718	131.753	35.8				
26	15985.818	127.203	33.7				
27	15794.168	125.678	36.0				
28	15717.263	125.066	34.1				
29	15194.192	120.903	34.3				
30	14638.772	116.484	52.9				
31	14581.399	116.027	35.5				
32	14337.869	114.089	35.3				
33	14121.194	112.365	33.0				
34	13713.479	109.121	30.7				
35	13535.867	107.708	31.4				
36	13375.344	106.430	28.0				
37	13181.253	104.886	31.0				
38	12950.540	103.050	32.0				
39	12577.615	100.083	26.1				
40	11413.064	90.816	20.8				
41	10911.966	86.829	24.5				
42	10335.794	82.244	37.8				
43	9887.796	78.679	30.7				
44	9709.573	77.261	32.8				
45	9483.743	75.464	34.0				
46	8714.700	69.345	36.7				
47	8602.395	68.451	28.1				
48	8553.346	68.053	32.7				
49	6932.473	55.163	10.3				
50	6353.860	50.559	34.1				
51	6264.749	49.850	194.9				
52	6236.673	49.627	33.2				
53	6222.635	49.515	1373.1				
54	6215.310	49.457	80.0				
55	6201.272	49.345	4100.3				
56	6193.948	49.287	163.4				

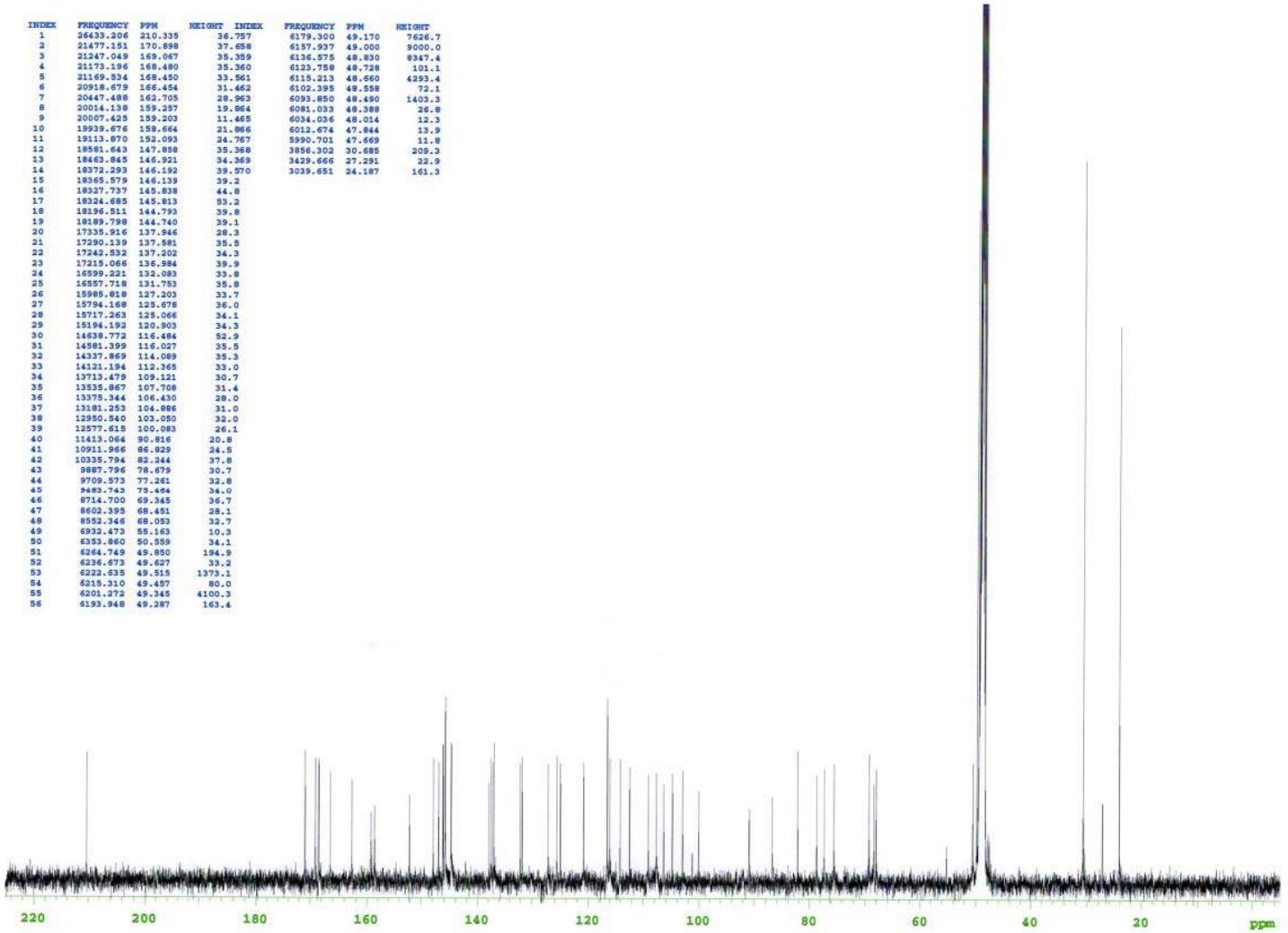


Fig. S35. ^{1}H-^{1}H COSY (500 MHz, acetone-*d*6+D_2O) spectrum of **6**.

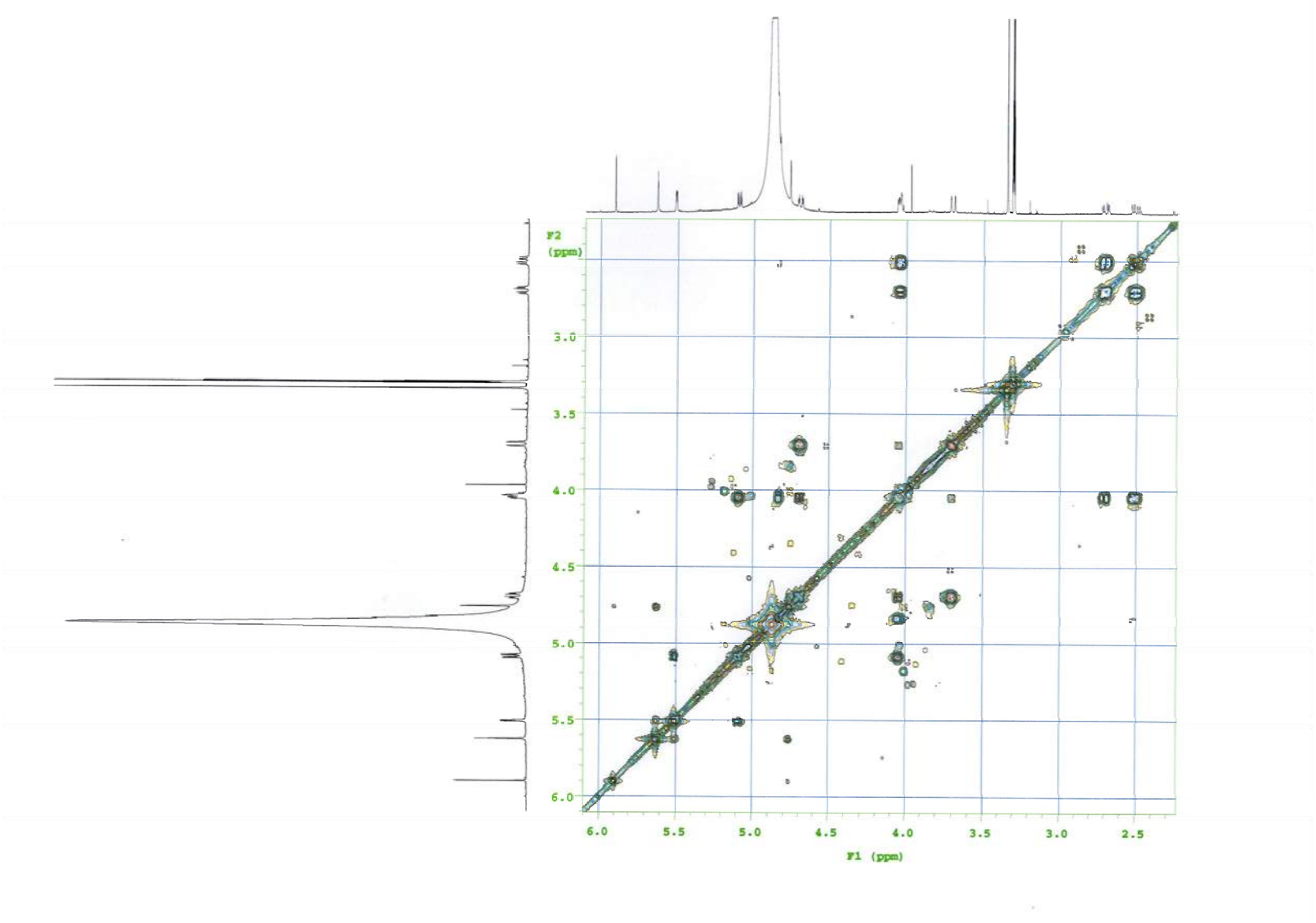


Fig. S36. HSQC (500 MHz, acetone-*d*6+D_2O) spectrum of **6**.

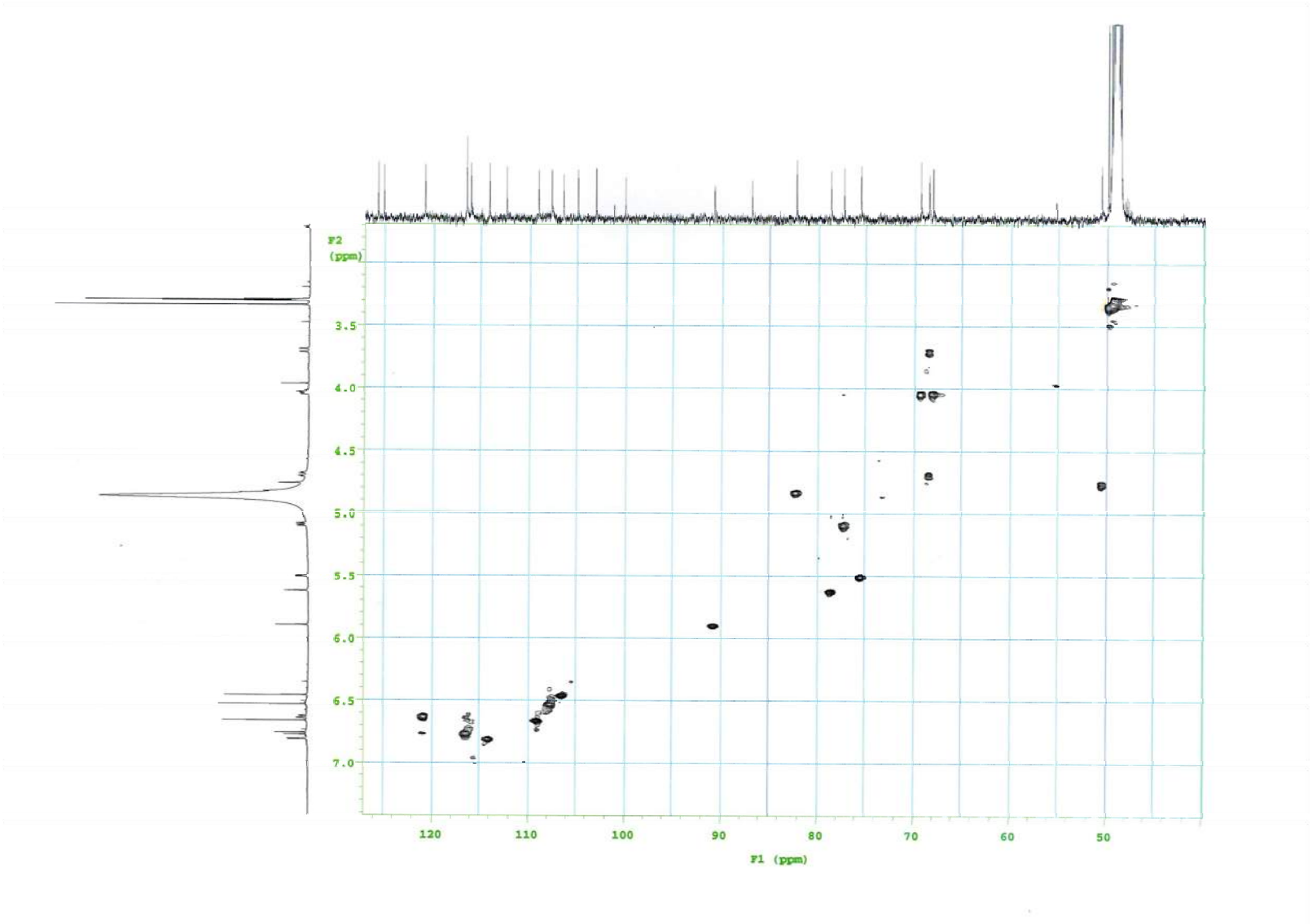
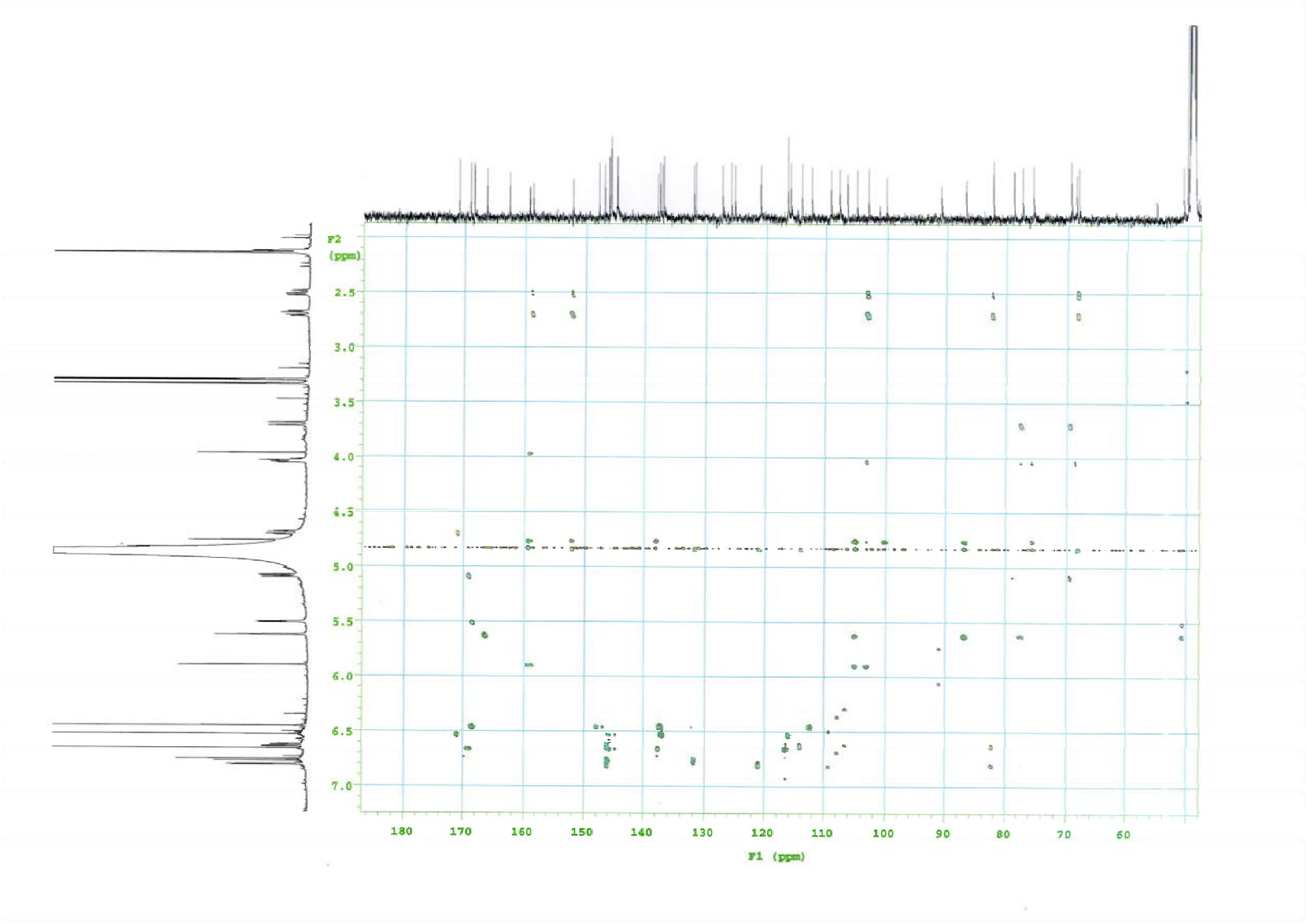


Fig. S37. HMBC (500 MHz, acetone-*d*6+D_2O) spectrum of **6**.



Cartesian coordinates of the lowest-energy conformer of (*R*)-**4** [(*R*)-**4A**] at the B3LYP/6-31G(d,p) level in acetone (PCM).

C	-0.81337000	-1.40735800	-0.40229100
C	0.69230600	-1.49035400	-0.14164400
C	1.47724500	-2.14969500	-1.28760400
C	0.85166800	-3.49142500	-1.64563200
O	-0.49579300	-3.20894800	-2.03727300
C	-1.34315100	-2.74303500	-0.99354500
O	1.52371000	-4.02145000	-2.73169900
O	2.81868500	-2.32369100	-0.80738300
O	1.21959700	-0.16014100	0.01821900
C	2.27808500	0.00481600	0.88574400
C	3.09364000	1.18514300	0.47251300
C	3.74437300	-1.37734800	-1.16134300
C	4.88382500	-1.37903500	-0.19584900
C	5.26532400	-0.18221100	0.46228200
C	6.38289700	-0.26151600	1.31456600
C	7.06115500	-1.46687500	1.52197600
C	6.63615200	-2.64258200	0.89618300
C	5.53946400	-2.59160000	0.04069400
C	2.40237200	2.36985700	0.20341200
C	3.08614800	3.51970700	-0.17772500
C	4.47988600	3.47690600	-0.26839200
C	5.16235300	2.28170400	-0.02980800
C	4.50113600	1.09532700	0.33193100
O	7.29439400	-3.81706200	1.09930500
O	8.14687600	-1.53467900	2.34303100
O	6.87772600	0.79767300	2.03613100
O	6.53119400	2.27614000	-0.17292400
O	5.22504900	4.56231000	-0.62689200
O	2.50230200	4.71494400	-0.46731500
O	3.61149200	-0.63066300	-2.10610000
O	2.49547900	-0.73355000	1.81884300
O	-1.40314100	-1.20432500	0.90544000
C	-2.70039100	-2.61928300	-1.68517100
O	-3.58312500	-1.87570400	-0.83064800
C	-4.91173600	-2.11510600	-0.93132000
C	-5.70999100	-1.25914300	-0.01387100
O	-5.37742300	-2.97351100	-1.65627300
C	-2.46087300	-0.41872700	1.21125000
C	-2.87196200	0.68618600	0.27147500
O	-3.00000500	-0.56629000	2.28304800
C	-6.91033800	-1.83839100	0.42441700
C	-7.74029700	-1.16193300	1.30916800
C	-7.37840300	0.11227700	1.75565100
C	-6.19889000	0.70642100	1.29844700
C	-5.33911100	0.03840700	0.40939700
C	-4.18554900	0.85017400	-0.07884400
C	-4.55688100	1.97480300	-0.95521200
O	-3.54563800	2.88821400	-1.26313000
C	-2.27476100	2.73155100	-0.83718200
C	-1.88592900	1.65199600	-0.11999600
O	-5.87053400	1.95607500	1.72360000
O	-8.14078300	0.83130200	2.62557500
O	-8.91632300	-1.63714100	1.81070100
O	-5.64723800	2.18432000	-1.43404400
C	-1.34709400	3.84132600	-1.19131400
O	-0.19439900	3.87313900	-0.78942200
O	-1.90701800	4.76816200	-1.96273900
H	-1.03567400	-0.57733800	-1.07740100
H	0.86007000	-2.05400400	0.78010000
H	1.48065600	-1.51849100	-2.17864600
H	0.84457800	-4.17648200	-0.78277700
H	-1.39428600	-3.47167000	-0.17151800
H	1.23907700	-4.93873400	-2.85195800
H	5.21610100	-3.49934800	-0.45551700
H	1.32585200	2.40755900	0.29120800
H	8.02747300	-3.64918100	1.71226800
H	8.31655700	-0.62993400	2.65818300
H	6.97820000	1.55273900	1.42047600
H	6.81310800	3.16524100	-0.44585800
H	4.62016900	5.28699300	-0.85262800
H	1.54215700	4.59238500	-0.59526000
H	-3.11837100	-3.60408900	-1.89409600

H	-2.57789000	-2.07583200	-2.62713700
H	-7.17606000	-2.82689600	0.06692100
H	-0.85496200	1.55759800	0.19067500
H	-6.59430500	2.28920100	2.27799800
H	-8.93727100	0.32066600	2.84023200
H	-9.10694600	-2.51707700	1.45682700
H	-1.24472900	5.45978700	-2.14066400

Cartesian coordinates of the lowest-energy conformer of (*S*)-**4** [(*S*)-**4A**] at the B3LYP/6-31G(d,p) level in acetone (PCM).

C	0.67051000	1.81652900	0.22854700
C	-0.80856100	1.51691600	0.42646400
C	-1.65765900	2.60912800	-0.25309500
C	-1.25075200	4.01120800	0.21862000
O	0.15433100	4.14958500	-0.01114100
C	0.95033000	3.24026100	0.75368100
O	-1.91560200	5.02765700	-0.44477500
O	-3.02519900	2.34886300	0.09850700
O	-1.15426600	0.27167600	-0.19846600
C	-2.15301500	-0.46888300	0.38191300
C	-2.78225200	-1.36436000	-0.63128500
C	-3.77314000	1.60518600	-0.77634300
C	-4.91892800	0.96762400	-0.05829900
C	-5.11749700	-0.43426000	-0.11192500
C	-6.24411900	-0.92510800	0.57016100
C	-7.12182800	-0.08866100	1.26154100
C	-6.88096900	1.28578200	1.32044200
C	-5.76992600	1.80942900	0.66718300
C	-1.93233400	-2.16421400	-1.40347500
C	-2.45714400	-3.05287300	-2.33627800
C	-3.84410800	-3.11985900	-2.49828000
C	-4.69190600	-2.29122800	-1.75605000
C	-4.18946800	-1.37894900	-0.80765000
O	-7.79564300	2.00435000	2.03351900
O	-8.18766200	-0.67759900	1.87685000
O	-6.51131900	-2.27456100	0.55733300
O	-6.02320500	-2.42475800	-2.06776400
O	-4.34046600	-4.00474600	-3.40737900
O	-1.63083200	-3.85494500	-3.06193100
O	-3.50669100	1.47748100	-1.95014100
O	-2.47532700	-0.36365600	1.54509500
O	1.48944900	0.89039900	0.97779700
C	2.42015700	3.68817900	0.66567700
O	3.16793100	2.89461900	-0.28001500
C	4.13204000	2.07893100	0.22926100
C	4.69992900	1.18595500	-0.82245200
O	4.47142000	2.07685100	1.39560200
C	2.12343400	-0.08100900	0.27866900
C	3.18013200	-0.73053800	1.13336700
O	1.89044800	-0.38453000	-0.86702000
C	5.01779600	1.75164100	-2.05761700
C	5.68034100	0.99958600	-3.02744200
C	6.03404500	-0.32177600	-2.74001800
C	5.69867100	-0.90375600	-1.51148700
C	4.99727400	-0.17437100	-0.53091700
C	4.48593800	-0.83383600	0.69599600
C	5.41587700	-1.61601200	1.51110800
O	4.97680700	-2.06153400	2.73527200
C	3.70950700	-1.87271500	3.16997600
C	2.78809200	-1.24016700	2.40693500
O	6.06024700	-2.21444500	-1.39360000
O	6.70467800	-1.02332500	-3.69218100
O	6.00747800	1.56302400	-4.21713100
O	6.55877500	-1.92839200	1.19759900
C	3.40486200	-2.40858700	4.52652200
O	2.30034700	-2.32265900	5.02453900
O	4.46725900	-2.97807700	5.10752500
H	0.93888100	1.74686500	-0.82637600
H	-1.04652600	1.46156800	1.49243100
H	-1.53809700	2.54415000	-1.33850900
H	-1.47300800	4.13764600	1.28701100
H	0.64508600	3.29632900	1.80922000
H	-1.76988700	4.92263500	-1.39778600
H	-5.57297600	2.87568100	0.70365400

H	-0.85784500	-2.10973700	-1.27213300
H	-7.56298400	2.94322100	2.04146500
H	-8.69333200	0.00314000	2.34769800
H	-7.31458600	-2.43084100	1.08198800
H	-6.51436800	-2.52007400	-1.22579500
H	-5.31012400	-3.93502600	-3.36526800
H	-2.17846100	-4.39980800	-3.64889500
H	2.90216400	3.61492500	1.63919100
H	2.44694700	4.72164000	0.31675200
H	4.78582200	2.78938200	-2.26329200
H	1.77860700	-1.12844300	2.77775400
H	6.40703900	-2.34066300	-0.48044300
H	6.91079900	-1.89643400	-3.31568900
H	6.47469900	0.90083300	-4.75137000
H	4.18651700	-3.29838700	5.98293200

Cartesian coordinates of the lowest-energy conformer of (*R*)-**4a** [(*R*)-**4aA**] at the B3LYP/6-31G(d,p) level in acetone (PCM).

C	-0.60357400	-1.62767500	-0.10344600
C	0.89856700	-1.64720400	0.17538700
C	1.67474800	-2.29135900	-0.98352300
C	1.13593800	-3.69867200	-1.24930200
O	-0.22248900	-3.51325000	-1.66029000
C	-1.11329500	-2.97097000	-0.68888900
O	1.80988000	-4.37756600	-2.24711600
O	3.05784600	-2.31290600	-0.60550600
O	1.34035200	-0.28273800	0.27918400
C	2.44635100	0.00711200	1.04692100
C	3.07143700	1.25873600	0.52266200
C	3.84388300	-1.29495100	-1.08671100
C	5.06066400	-1.11446800	-0.24183500
C	5.37380300	0.16069700	0.29569300
C	6.58356700	0.26423400	1.00720400
C	7.41494200	-0.84388900	1.20133800
C	7.05765000	-2.10105300	0.70481800
C	5.87258300	-2.23002800	-0.01434600
C	2.21205300	2.33576400	0.29267400
C	2.68068900	3.52758000	-0.24281100
C	4.04606000	3.64957500	-0.51533000
C	4.90106000	2.56420000	-0.29974900
C	4.44818500	1.33012200	0.20087700
O	7.86463700	-3.18049900	0.89631100
O	8.58835300	-0.73586700	1.88571800
O	7.03230000	1.41954600	1.59835000
O	6.23171200	2.71304600	-0.61603700
O	4.59788000	4.78567500	-1.03095000
O	1.89182500	4.60107800	-0.52194600
O	3.54709800	-0.62287100	-2.05034500
O	2.82115300	-0.67793400	1.96923900
O	-1.25500500	-1.41775900	1.17334900
C	-2.41516100	-2.80250600	-1.47900600
O	-3.29933200	-1.93381000	-0.74411100
C	-4.63357100	-2.14506100	-0.87228900
C	-5.44515900	-1.23321200	-0.02224300
O	-5.09546600	-3.03236100	-1.56340700
C	-2.30078200	-0.58890700	1.39675900
C	-2.53668600	0.56767300	0.46062900
O	-2.96086900	-0.72703500	2.39920200
C	-6.66405000	-1.78459300	0.40055000
C	-7.50826400	-1.07343400	1.24290700
C	-7.14160100	0.20871600	1.65912400
C	-5.94483000	0.77760300	1.21415900
C	-5.07250600	0.07431500	0.36499700
C	-3.85587100	0.82641700	-0.07681700
C	-3.95316400	1.92310900	-0.88878400
O	-2.91251500	2.76176800	-1.13016100
C	-1.66470300	2.61836100	-0.55303100
C	-1.50246100	1.42276800	0.23410100
O	-5.63366200	2.04567800	1.60095300
O	-7.91746300	0.96286600	2.48689500
O	-8.70228000	-1.52052100	1.72736500
C	-5.19365700	2.35204900	-1.61815800
H	-0.52219900	1.22586300	0.64202000
O	-6.15393400	1.63552200	-1.80391600

O	-5.10325500	3.61744900	-2.05169100
H	-5.92921900	3.81569200	-2.52725700
H	-0.82302200	-0.81233900	-0.79503000
H	1.10779800	-2.17642200	1.10929300
H	1.55760500	-1.69619600	-1.89324000
H	1.18579900	-4.32904800	-0.35192200
H	-1.24698100	-3.67021400	0.14801900
H	1.82707100	-3.82397700	-3.04323300
H	5.60360500	-3.19973300	-0.41707600
H	1.16273100	2.26107500	0.53339700
H	8.63730300	-2.89211500	1.40736000
H	8.69072300	0.20231800	2.12210600
H	6.95906800	2.13897000	0.93786500
H	6.36457400	3.60922600	-0.96794600
H	3.88540900	5.41454800	-1.22707000
H	0.95660600	4.31919900	-0.53430400
H	-2.89762800	-3.76350000	-1.65387400
H	-2.18637500	-2.33493100	-2.44122000
H	-6.93026400	-2.78193600	0.06955100
H	-6.35399800	2.37342100	2.16325000
H	-8.72043500	0.46410400	2.70520200
H	-8.89628000	-2.40639200	1.39041100
O	-0.83538400	3.48450300	-0.77652600

Cartesian coordinates of the lowest-energy conformer of (*S*)-**4a** [(*S*)-**4aA**] at the B3LYP/6-31G(d,p) level in acetone (PCM).

C	0.54198500	1.85460500	-0.04379100
C	-0.94374900	1.60364400	0.17747300
C	-1.78032900	2.47237400	-0.78351100
C	-1.37989500	3.94356400	-0.68589400
O	0.03506200	4.02926300	-0.89977300
C	0.79463300	3.36978700	0.11487000
O	-2.02385600	4.63932400	-1.69395300
O	-3.15229500	2.30215300	-0.39900600
O	-1.27757600	0.23631000	-0.10962200
C	-2.26635400	-0.34287500	0.64124000
C	-2.86773200	-1.48895300	-0.10551600
C	-3.87433800	1.33578000	-1.05177800
C	-5.02427500	0.89370800	-0.20875100
C	-5.22395000	-0.48094200	0.07874800
C	-6.35956800	-0.80137800	0.84829500
C	-7.22925700	0.18669600	1.32084300
C	-6.98661800	1.53769800	1.05670800
C	-5.87481700	1.88368600	0.29531300
C	-1.99330100	-2.47410400	-0.57942300
C	-2.49334300	-3.59170500	-1.23970800
C	-3.87069200	-3.70546800	-1.44231600
C	-4.72915900	-2.69475100	-1.00673700
C	-4.26554300	-1.55574000	-0.32618200
O	-7.83095200	2.50122400	1.51696700
O	-8.32961900	-0.13441800	2.05737900
O	-6.69401100	-2.07677000	1.23490200
O	-6.07502200	-2.83737000	-1.25309600
O	-4.43632100	-4.76942400	-2.08234600
O	-1.74896600	-4.62824900	-1.72232500
O	-3.57681000	0.89646200	-2.14066900
O	-2.60053500	0.05092000	1.73626300
O	1.34251000	1.15331600	0.93592600
C	2.26337800	3.80476000	-0.00108400
O	3.03911600	2.86295800	-0.77057700
C	3.98142400	2.15084100	-0.09198700
C	4.51196100	1.03104400	-0.91495700
O	4.30220000	2.37703100	1.05845400
C	1.94594600	0.00844600	0.54122000
C	2.99591200	-0.41017900	1.53724600
O	1.71168600	-0.59259400	-0.48082600
C	4.74925200	1.23808000	-2.27923900
C	5.26760300	0.20563000	-3.05386300
C	5.52253400	-1.03915400	-2.46949200
C	5.25685100	-1.25506100	-1.11358700
C	4.76442700	-0.21831100	-0.30539800
C	4.37955200	-0.51962700	1.10362100
C	5.26361400	-0.94806300	2.05110000
O	4.88548600	-1.29582400	3.30600200

C	3.57576100	-1.20262300	3.77498400
C	2.62027000	-0.71057700	2.80743800
O	5.47319300	-2.48723700	-0.58075200
O	6.01095300	-2.09495600	-3.18059000
O	5.56137600	0.28825200	-4.38338400
C	6.74743100	-1.04917400	1.86157700
H	1.59483500	-0.61425600	3.14233500
H	-6.67031200	-2.64255100	0.43575000
H	-0.92493500	-2.36967900	-0.42075000
H	0.84583600	1.53014600	-1.04007100
H	-1.21143900	1.82452700	1.21445000
H	-1.63969300	2.13968000	-1.81458600
H	-1.61484800	4.34480300	0.31348100
H	0.43558900	3.69076600	1.10474000
H	-1.91905100	5.58709600	-1.52801600
H	-5.68876200	2.92963000	0.08088200
H	-8.54183400	2.06662500	2.01404400
H	-8.35512900	-1.10555600	2.11326600
H	-6.20969900	-3.66720500	-1.74098900
H	-3.73307500	-5.37208400	-2.37054100
H	-0.80671300	-4.47331600	-1.56797300
H	2.71177800	3.90010600	0.98649500
H	2.30191700	4.76484200	-0.51844400
H	4.54180900	2.20441100	-2.72459900
H	5.79499700	-3.06933800	-1.28787700
H	6.10227800	-1.83115500	-4.10962900
H	5.33668500	1.16354300	-4.72870200
O	7.36265100	-0.47822000	0.98599300
O	7.31704000	-1.83093600	2.79150800
H	8.27467500	-1.82808700	2.61710800
O	3.36186200	-1.53157200	4.92163300

Cartesian coordinates of the lowest-energy conformer of (*R*)-**5** [(*R*)-**5A**] at the B3LYP/6-31G(d,p) level in acetone (PCM).

C	-0.53332400	-0.51262600	-1.92492000
C	0.71023900	-0.84273900	-1.10718400
C	1.54362900	-1.90058600	-1.86084100
C	0.69893000	-3.11712500	-2.24250900
O	-0.44383000	-2.65100400	-2.97774400
C	-1.30069700	-1.82964000	-2.18665800
O	1.45521200	-3.92864800	-3.06857300
O	2.60927500	-2.28845400	-0.98215000
O	1.54688200	0.32186800	-0.97730700
C	2.28567700	0.43739600	0.17138500
C	3.47675200	1.30899500	-0.06651600
C	3.80624800	-1.63433400	-1.12217500
C	4.58510800	-1.70378600	0.14891600
C	5.08492000	-0.52161200	0.75225000
C	5.84282600	-0.69012000	1.92760100
C	6.06883200	-1.95495300	2.47989300
C	5.52962900	-3.10041400	1.88733200
C	4.78077500	-2.96466300	0.72270000
C	3.24732600	2.57736100	-0.61261200
C	4.30710700	3.45585600	-0.81329800
C	5.60180600	3.04827200	-0.48473700
C	5.82583000	1.76583800	0.01870400
C	4.78155600	0.85344100	0.24720400
O	5.74733300	-4.33195300	2.42501600
O	6.81078600	-2.10846600	3.61232500
O	6.38551400	0.34457100	2.65063700
O	7.12077400	1.40144100	0.30631200
O	6.69302100	3.84983900	-0.65225800
O	4.20646300	4.72215900	-1.31083600
O	4.14075600	-1.05646400	-2.13309300
O	2.00780600	-0.11903600	1.21009700
O	-1.32859300	0.56035500	-1.38380800
C	-2.62883100	-1.65039400	-2.93472300
O	-3.66910600	-1.60858200	-1.92960700
C	-4.34383600	-0.46547600	-1.69998700
C	-5.02973900	-0.58753800	-0.36058900
O	-4.38465700	0.49462300	-2.43322900
C	-2.02309900	0.43180800	-0.22386100
C	-2.80799900	1.67674300	0.03015300
O	-2.00840600	-0.56382400	0.47314800

C	-4.94334600	0.38957500	0.61189900
C	-6.35297800	-1.98854400	1.07001000
O	-6.31838400	-1.03982400	2.03231200
C	-5.67277400	0.16149300	1.86610500
C	-4.14906400	1.64266500	0.50213700
C	-4.75173700	2.88681800	0.78955400
C	-4.06878600	4.09233000	0.59231500
C	-2.76265700	4.10133100	0.09781100
C	-2.14175400	2.88679600	-0.18158000
O	-5.77154100	0.95504500	2.79486100
O	-6.03980400	3.04595600	1.22091400
C	-5.74266300	-1.80248700	-0.12147300
C	-7.09608100	-3.23395300	1.41261700
H	-1.12178800	2.89084600	-0.54487200
H	-5.53592200	5.09212900	1.23636200
H	-0.22860300	-0.11463900	-2.89652900
H	0.44086300	-1.20332800	-0.11304200
H	1.95813300	-1.46866800	-2.77492000
H	0.34870500	-3.64783500	-1.34286100
H	-1.52620400	-2.32791500	-1.23626600
H	1.00867200	-4.78320400	-3.15321300
H	4.36869000	-3.85144100	0.25547200
H	2.23710900	2.88392300	-0.86239400
H	6.29052600	-4.22097000	3.22118900
H	7.12551500	-1.22234900	3.86260700
H	6.87832700	0.91393700	2.02439200
H	7.70431900	2.14455700	0.07786000
H	6.40759000	4.69232200	-1.03901100
H	3.28684900	4.93584200	-1.52131500
H	-2.81509300	-2.53249900	-3.54845600
H	-2.66961900	-0.75023200	-3.54963300
H	-2.67816900	5.99833500	0.17134300
O	-4.65528900	5.28633200	0.86990000
O	-7.22156200	-4.15116400	0.62634400
O	-7.59101500	-3.21471500	2.65564400
H	-8.05493000	-4.05833800	2.79999600
O	-2.09443300	5.26740600	-0.08774000
H	-5.79653700	-2.57987500	-0.87029800
H	-6.17302100	2.41534700	1.96474700

Cartesian coordinates of the lowest-energy conformer of (*S*)-**5** [(*S*)-**5A**] at the B3LYP/6-31G(d,p) level in acetone (PCM).

C	-0.57752500	1.67658600	-0.45015700
C	0.92325400	1.45766600	-0.56172700
C	1.67764800	2.53925800	0.23677700
C	1.22286700	3.94098700	-0.16943600
O	-0.20238600	4.00323200	-0.01957400
C	-0.89221000	3.11671500	-0.90182000
O	1.79956700	4.85517000	0.69448700
O	3.07355900	2.36201400	-0.04800800
O	1.28271300	0.19133600	0.01667800
C	2.32935900	-0.48697500	-0.54778000
C	2.92793000	-1.42353100	0.45076600
C	3.79559400	1.57990300	0.81707700
C	4.99565800	1.01734000	0.12995200
C	5.25510300	-0.37720100	0.15558800
C	6.43588500	-0.80732200	-0.48099000
C	7.29224900	0.09209600	-1.12408700
C	6.99110200	1.45622800	-1.17098900
C	5.83447400	1.91065400	-0.54537900
C	2.06405000	-2.32498700	1.08352000
C	2.56593500	-3.25609600	1.98698400
C	3.93372800	-3.26351600	2.26979100
C	4.77905700	-2.32988900	1.66809200
C	4.31359500	-1.38120900	0.74151500
O	7.82258400	2.33230800	-1.79906000
O	8.43617100	-0.33213300	-1.73074500
O	6.83082900	-2.12025900	-0.56771900
O	6.11448500	-2.35931500	1.99716700
O	4.50131300	-4.14369000	3.14441900
O	1.83246100	-4.20028500	2.64421200
O	3.46313000	1.36298600	1.96163500
O	2.71177300	-0.31490200	-1.68370500
O	-1.30177800	0.76632200	-1.29684800

C	-2.38532900	3.47481700	-0.90665100
O	-3.14325900	2.59919300	-0.03092000
C	-4.16118900	1.90677200	-0.58498900
C	-4.72232400	0.90968600	0.39754200
O	-4.59321800	2.06402900	-1.70412900
C	-2.05425600	-0.18241400	-0.66747700
C	-3.03262900	-0.80664800	-1.60264400
O	-1.95356000	-0.44653000	0.51240900
C	-5.09125000	1.39345600	1.68850200
C	-5.66632800	0.54144600	2.56863200
O	-5.93346700	-0.74301400	2.23641800
C	-5.62798800	-1.26818800	1.00372500
C	-4.90315000	-0.41742300	0.05947300
C	-4.37186800	-1.03249200	-1.18189200
C	-5.19959000	-1.77734000	-2.04538100
C	-4.72961700	-2.22031400	-3.28751500
C	-3.42576600	-1.93547400	-3.70475900
C	-2.57753100	-1.23006500	-2.85127800
O	-6.00724200	-2.41445500	0.79229200
C	-6.05030700	0.94561100	3.95042500
H	-0.90260000	1.53492600	0.58098200
H	1.23691100	1.47369200	-1.60910800
H	1.49884200	2.41326000	1.30708600
H	1.47980100	4.14276900	-1.22210900
H	-0.52019700	3.26144200	-1.92751600
H	1.66793100	5.74374700	0.33392600
H	5.60374100	2.96922600	-0.57108100
H	1.00285900	-2.30480400	0.85852800
H	8.56890800	1.83034500	-2.16289000
H	8.49845400	-1.29020700	-1.57227500
H	6.78729400	-2.50112500	0.33361000
H	6.25056400	-3.06012200	2.65694700
H	3.80400500	-4.69870600	3.52721100
H	0.89477800	-4.12201400	2.41974600
H	-2.80000900	3.39529000	-1.90988200
H	-2.50882100	4.49481800	-0.53906900
H	-1.55392100	-1.04909800	-3.15639800
O	-5.89130700	2.07704100	4.36262700
O	-6.57463300	-0.06249100	4.65707200
H	-4.91655000	2.41957300	1.98095800
O	-5.52515300	-2.93306200	-4.12909400
H	-6.36956900	-3.08335800	-3.66991400
O	-2.97273300	-2.36854900	-4.90734500
H	-3.68916700	-2.85453100	-5.34652600
O	-6.50566500	-2.08341700	-1.79509600
H	-6.56437500	-2.35795000	-0.85096200
H	-6.79415500	0.28178100	5.54087300

Cartesian coordinates of the lowest-energy conformer of (*R*)-**5a** [(*R*)-**5aA**] at the B3LYP/6-31G(d,p) level in acetone (PCM).

C	0.69855000	-1.47127200	0.27826600
C	-0.80829200	-1.48875700	0.03745500
C	-1.56742600	-2.24484800	1.13755700
C	-0.99424200	-3.65196700	1.26942500
O	0.39625500	-3.50372100	1.58361400
C	1.20253800	-2.90796900	0.57089000
O	-1.61418300	-4.28796900	2.32842300
O	-2.93877400	-2.30332100	0.72497600
O	-1.30567500	-0.13726200	0.01139100
C	-2.32559000	0.14034300	-0.86834800
C	-3.07625700	1.35349000	-0.42140500
C	-3.76907900	-1.30193600	1.15832200
C	-4.94982100	-1.19054100	0.25369000
C	-5.29569900	0.05327700	-0.33254700
C	-6.44544300	0.06171100	-1.14750300
C	-7.19077400	-1.09877100	-1.37896900
C	-6.80484000	-2.31991800	-0.81869100
C	-5.67522500	-2.35816000	-0.00804900
C	-2.34405300	2.53266000	-0.23827700
C	-2.98826100	3.70650800	0.13979600
C	-4.36716500	3.68659100	0.35898600
C	-5.08340400	2.49828300	0.20690500
C	-4.47356100	1.29579100	-0.19196100
O	-7.52796500	-3.45066000	-1.04394500

O	-8.30529400	-1.07733300	-2.16166100
O	-6.91251500	1.17031500	-1.81170600
O	-6.43795700	2.52619900	0.44271500
O	-5.07083700	4.79232100	0.73639600
O	-2.38865700	4.91800900	0.32245600
O	-3.53134300	-0.60040100	2.11698000
O	-2.57688100	-0.53703200	-1.83795600
O	1.26185000	-0.98629700	-0.96438400
C	2.60056900	-2.97473100	1.18519600
O	3.50629300	-2.21906300	0.35709600
C	4.79892200	-2.20853200	0.72962700
C	5.59607500	-1.34790700	-0.21104700
O	5.25737800	-2.84396200	1.65200400
C	2.24331000	-0.08166700	-1.08874300
C	2.76195200	0.68818100	0.07433900
O	2.68911900	0.09162600	-2.21901700
C	5.16693700	-0.00796500	-0.55605300
C	7.46895300	-1.19370400	-1.77897300
O	6.94128600	0.05055700	-2.15168600
C	5.86614100	0.60404100	-1.55146500
C	4.16036200	0.75018800	0.25631400
C	4.65449100	1.54461600	1.30404600
C	3.78198600	2.28044800	2.11751400
C	2.40295600	2.22595800	1.90380800
C	1.88894900	1.42418400	0.88447400
C	5.58366700	1.97724300	-2.12336200
C	6.70373100	-1.89958800	-0.77545000
O	5.99071200	1.60255900	1.53050000
O	8.47561400	-1.56455800	-2.34022000
H	0.81837800	1.39775700	0.71127300
O	6.47289800	2.78652900	-2.27945500
H	3.64013700	3.48409700	3.59562900
O	4.32177000	2.22295100	-2.46021400
H	0.95169600	-0.81321200	1.10939400
H	-1.01259500	-1.95482800	-0.93038800
H	-1.48603600	-1.73606800	2.10045300
H	-1.09609600	-4.21200200	0.32677400
H	1.16218700	-3.48537200	-0.36385700
H	-1.39184100	-5.22949000	2.29689500
H	-5.37612800	-3.30143800	0.43384600
H	-1.27471500	2.54193100	-0.42140400
H	-8.27146900	-3.22267700	-1.62411700
H	-8.43570100	-0.15312300	-2.43710500
H	-6.97989300	1.89729800	-1.15914800
H	-6.68145000	3.42660900	0.71663600
H	-4.46270000	5.54483400	0.80499100
H	-1.44777300	4.87180700	0.10322800
H	2.93388900	-4.01201000	1.25220800
H	2.58305300	-2.54409200	2.18984300
H	0.71517200	2.88253500	2.58222000
O	4.34328500	3.03252600	3.10254400
O	1.66158500	2.99887800	2.74472800
H	7.03772700	-2.89651700	-0.51617500
H	6.14780400	2.19591000	2.28298300
H	3.73689300	1.41924300	-2.37740900

Cartesian coordinates of the lowest-energy conformer of (*S*)-**5a** [(*S*)-**5aA**] at the B3LYP/6-31G(d,p) level in acetone (PCM).

C	-0.53510900	-1.71919100	-0.29140100
C	0.95019400	-1.53263000	-0.02755600
C	1.76961900	-2.25516200	-1.11574800
C	1.33894400	-3.71490200	-1.26602300
O	-0.07692900	-3.74103000	-1.49315400
C	-0.81886200	-3.23363100	-0.38366300
O	1.97634100	-4.24415100	-2.37465300
O	3.14646200	-2.18031600	-0.71064100
O	1.30161700	-0.14118700	-0.10243700
C	2.31390000	0.29394700	0.71353000
C	2.94638700	1.51872500	0.14318900
C	3.89395700	-1.14801100	-1.21235700
C	5.05488100	-0.86814200	-0.31255400
C	5.27202000	0.43338600	0.20391300
C	6.41005800	0.59536700	1.01256300

C	7.28180700	-0.45729300	1.29527500
C	7.02261300	-1.73549900	0.79592800
C	5.90032000	-1.93921000	-0.00057100
C	2.10214700	2.57406000	-0.21945100
C	2.63194700	3.76020500	-0.71719300
C	4.01791700	3.87159700	-0.86176500
C	4.85933700	2.80262200	-0.53721400
C	4.35174200	1.58838700	-0.03530800
O	7.93188800	-2.69033800	1.14729200
O	8.36000200	-0.17798000	2.08369900
O	6.69405800	1.83149800	1.54540700
O	6.18958600	3.03767300	-0.78874600
O	4.51989500	5.04552200	-1.33747100
O	1.81196600	4.79868300	-1.03694600
O	3.61709000	-0.54385300	-2.22407300
O	2.64839800	-0.27550000	1.72964500
O	-1.33175700	-1.17215500	0.77181900
C	-2.29855700	-3.59258300	-0.54363000
O	-3.01269400	-2.52162100	-1.21361800
C	-4.17986900	-2.12437900	-0.66834000
C	-4.66156300	-0.85004000	-1.31577700
O	-4.77420400	-2.69412700	0.21837200
C	-2.16806000	-0.14306600	0.43984700
C	-3.27700600	-0.01203800	1.42012600
O	-2.04462800	0.51968800	-0.57017300
C	-4.89298400	-0.85690800	-2.65327800
C	-5.42457000	0.30262900	-3.33416000
O	-5.63191000	1.41068900	-2.51357400
C	-5.38127500	1.41820000	-1.18055200
C	-4.91046600	0.33235500	-0.49757200
C	-4.58120000	0.30920600	0.96153200
C	-5.59603600	0.40484700	1.92654700
C	-5.32622900	0.19840300	3.28436100
C	-4.03676100	-0.13123300	3.71717200
C	-3.01758100	-0.23760800	2.77637600
C	-5.64573800	2.77173600	-0.60375600
H	1.02850700	2.48420600	-0.10144400
O	-5.69772200	0.41053000	-4.50858000
H	-0.81559700	-1.23691800	-1.22825100
H	1.21482800	-1.91410300	0.96245600
H	1.64081600	-1.75528300	-2.07858400
H	1.56204000	-4.28287200	-0.34809000
H	-0.47311000	-3.72338700	0.53991500
H	1.85401400	-5.20431500	-2.36943000
H	5.68998800	-2.92689100	-0.39741300
H	-5.57548600	4.59802400	-1.02608300
H	7.68628500	-3.54950000	0.77709200
H	8.86228200	-0.99495200	2.22861100
H	7.50169300	1.75420900	2.08079800
H	6.69068700	2.77928200	0.01207800
H	5.48858000	4.95312000	-1.34373200
H	2.36273400	5.52821100	-1.36212700
H	-2.76257800	-3.75783900	0.42792500
H	-2.38971000	-4.49813200	-1.14664600
H	-2.01763100	-0.48820900	3.10863600
H	-4.69807900	-1.73008500	-3.26345200
O	-6.30589100	0.30484700	4.21834500
H	-7.12004000	0.55431700	3.74574300
O	-3.77377400	-0.32776100	5.03513800
H	-4.59839100	-0.20783700	5.53239500
O	-6.90676100	0.67681300	1.63220600
H	-6.90469400	1.55331900	1.18574700
O	-6.08852700	2.96345500	0.51993000
O	-5.35534100	3.75071800	-1.45417400

Cartesian coordinates of the lowest-energy conformer of (5*R*)-**6** [(5*R*)-**6A**] at the B3LYP/6-31G(d,p) level in MeOH (PCM).

C	0.01965000	0.86484900	-1.64605800
C	-1.15359700	-0.04684400	-1.26333800
C	-0.91500900	-0.73606300	0.11147100
C	-1.50816800	-2.14566500	0.35084500
O	-0.35861100	0.57636900	-4.00877300

C	-0.16170300	1.56652100	-3.00827200
C	1.03634000	2.46021100	-3.40162000
O	0.21212400	1.90628900	-0.66034800
O	-1.32955000	0.15194200	1.17269700
O	-2.37103400	0.71157200	-1.11314800
C	-3.31740000	0.81748100	-2.07097400
C	-4.57552400	1.36767400	-1.48802900
O	-3.12409400	0.57559500	-3.24859700
C	-5.10214000	2.48310800	-2.14629300
C	-6.23682800	3.12349000	-1.65595100
C	-6.87232700	2.60499000	-0.52158000
C	-6.38657100	1.45381600	0.10663900
C	-5.21072200	0.82345800	-0.33505400
C	-4.76547100	-0.48041700	0.23574400
C	-5.74042400	-1.61302400	0.18700000
O	-5.29006700	-2.87153300	0.35361500
C	-2.99226300	-2.12422400	0.89020500
C	-3.55851100	-0.72933300	0.79051800
C	-2.66297500	0.35130000	1.32888000
O	-3.06349400	1.29265600	1.97287000
O	-7.12929100	1.03269200	1.17896500
O	-7.99440400	3.22956200	-0.08076600
O	-6.72632400	4.22021500	-2.28596800
O	2.24279800	2.10522600	-2.68600000
C	2.79310200	3.06368900	-1.89153700
C	3.88456000	2.51011600	-1.03545200
O	2.42825200	4.22242800	-1.87697000
C	4.83598300	1.67159000	-1.62458900
C	5.91268900	1.21399100	-0.87428300
C	6.05709900	1.61722900	0.45310900
C	5.08744100	2.43060300	1.05211500
C	3.95890300	2.86321300	0.33613700
C	2.82453500	3.51773300	1.05080300
C	3.01889700	4.66285000	1.83492100
C	1.96114200	5.30169300	2.48496800
C	0.65824800	4.81185400	2.35227000
C	0.42740900	3.67346200	1.58479200
C	1.50051700	3.02612300	0.96212700
O	-0.29423400	5.51641500	3.02866500
O	2.26104700	6.40506100	3.22771400
O	4.28934000	5.16789300	1.98470200
O	7.14315500	1.17664200	1.14367500
O	6.84622900	0.37639900	-1.43950600
O	5.30980800	2.69457900	2.37777600
C	1.22452200	1.75212800	0.23566300
O	1.82626700	0.70948800	0.39858300
C	-0.79903200	-2.81850100	1.49507500
H	-1.42265600	-2.71679900	-0.57779300
C	-1.64810200	-2.95326100	2.57540600
C	-1.25632400	-3.46336300	3.80306100
C	0.08943100	-3.85062100	3.90876600
C	0.99867800	-3.74314200	2.83688500
C	0.53389300	-3.21509000	1.62425400
C	2.43616900	-4.18579100	2.97329200
C	3.08123700	-4.37341100	1.60321500
C	2.75616300	-3.17888400	0.68255400
O	1.31782800	-3.06654400	0.51765900
C	3.35661100	-3.31171400	-0.69775800
O	4.48351300	-4.47918000	1.80156500
C	4.42919700	-2.49194400	-1.08693200
C	5.00180600	-2.63425600	-2.34963000
C	4.50482600	-3.60626800	-3.24072000
C	3.44281100	-4.42050400	-2.85711300
C	2.87405200	-4.27614400	-1.59058400
O	-2.93421900	-2.51454600	2.29246600
O	0.59295600	-4.36271600	5.06650300
O	5.06245000	-3.73834500	-4.47783400
O	6.04161500	-1.89720000	-2.83752000
C	-3.89412700	-3.18138900	0.17567200
O	-3.69256500	-4.44693500	0.67444800
O	-6.94738600	-1.44538300	0.13135500
C	-3.65257300	-3.24522400	-1.36022900
O	-3.93647000	-2.31769600	-2.08360600
O	-3.11131000	-4.37368800	-1.80629800
H	0.91647700	0.24235200	-1.68466500
H	-1.27432700	-0.79318700	-2.05228500
H	0.16240800	-0.82668600	0.23523100
H	-1.31639700	0.40142800	-4.02668900

H	-1.03845800	2.22254600	-2.95118100
H	0.82148300	3.50934500	-3.20564200
H	1.23046500	2.31752900	-4.46614200
H	-4.61599700	2.87151200	-3.03348300
H	-7.31260600	0.08055400	1.03666500
H	-8.35090900	2.69659400	0.65169100
H	-7.52347200	4.51360000	-1.81616100
H	4.75067900	1.38541400	-2.66606500
H	-0.57399800	3.26239500	1.50705300
H	-1.16879800	5.12576300	2.89297800
H	1.44176900	6.75927900	3.60770000
H	4.24407800	5.94920200	2.56106000
H	7.10541900	1.57966700	2.02825800
H	7.54431400	0.20805500	-0.78481500
H	5.10938900	3.64039600	2.53493200
H	-1.94506000	-3.55308000	4.63538000
H	3.02201900	-3.44278400	3.53098000
H	2.49719500	-5.11849900	3.54189100
H	2.68048800	-5.28207700	1.12890100
H	3.11943800	-2.26262300	1.16508300
H	4.88783100	-4.65544100	0.93943300
H	4.81336100	-1.73548100	-0.40831800
H	3.06826100	-5.15839600	-3.55926100
H	2.03778900	-4.90618800	-1.30595600
H	-0.10600600	-4.41567800	5.73357100
H	5.75867200	-3.06454300	-4.54896800
H	6.27750000	-1.14681900	-2.25407000
H	-3.64046200	-4.39699200	1.64476600
H	-3.01121600	-4.99699500	-1.05983700

Cartesian coordinates of the lowest-energy conformer of (5*S*)-**6** [(5*S*)-**6A**] at the B3LYP/6-31G(d,p) level in MeOH (PCM).

C	-0.11401000	0.94183400	1.67796300
C	1.09475700	0.06276200	1.33919100
C	0.89663300	-0.70005000	-0.00209500
C	1.55275300	-2.09122500	-0.14558600
O	0.28726900	0.73495900	4.05260400
C	0.02183700	1.68149300	3.02598700
C	-1.24205200	2.49036200	3.41131000
O	-0.30955400	1.96007800	0.66945600
O	1.29117400	0.14792500	-1.10299600
O	2.27683500	0.87386300	1.16364900
C	3.23056100	1.01963700	2.10733000
C	4.45860400	1.62767600	1.51206300
O	3.06544600	0.75837700	3.28547700
C	4.91479500	2.79288400	2.13336400
C	6.02026300	3.47437200	1.62932300
C	6.69872600	2.94872400	0.52349200
C	6.28639900	1.74883600	-0.06563200
C	5.13874000	1.07535400	0.38786600
C	4.75720100	-0.27104900	-0.12011000
C	5.77475300	-1.36360600	-0.03187300
O	5.34495300	-2.64284500	0.00381300
C	3.05510700	-2.03601400	-0.59931100
C	3.55147200	-0.60694200	-0.63627900
C	2.61608900	0.39603500	-1.25048700
O	2.98768600	1.31484200	-1.94365200
O	7.06362200	1.33205600	-1.11183200
O	7.79078600	3.61784100	0.07217100
O	6.44154600	4.61869000	2.22153500
O	-2.39998800	2.11256100	2.63125300
C	-2.92800800	3.05591200	1.80371800
C	-3.98456600	2.47943100	0.91882700
O	-2.57258600	4.21744000	1.78711200
C	-4.93718100	1.62677000	1.48627000
C	-5.98327900	1.14338600	0.70942000
C	-6.09870000	1.53659200	-0.62373800
C	-5.12798100	2.36443700	-1.20061600
C	-4.02764500	2.82236500	-0.45681800
C	-2.88554300	3.48820500	-1.14781100
C	-3.07680500	4.62024200	-1.95165400
C	-2.01281500	5.26489800	-2.58537700
C	-0.70696800	4.79497500	-2.41534900

C	-0.47895900	3.67094800	-1.62606400
C	-1.55765500	3.01712900	-1.02025100
O	0.25169600	5.50336400	-3.07894600
O	-2.31000900	6.35384600	-3.35038700
O	-4.35009500	5.10573800	-2.13814900
O	-7.15565300	1.07049900	-1.34188800
O	-6.91502200	0.28996400	1.25324900
O	-5.31780900	2.61439600	-2.53405800
C	-1.28024100	1.76115700	-0.26239900
O	-1.84817000	0.70072200	-0.42886800
C	0.93541900	-2.86305400	-1.27974900
H	1.46744300	-2.60563600	0.81482300
C	1.85986300	-3.08038200	-2.28157700
C	1.56326200	-3.70592500	-3.48213500
C	0.23357000	-4.12773000	-3.64479900
C	-0.74962600	-3.94550300	-2.65060400
C	-0.37805500	-3.30499500	-1.46102100
C	-2.16705300	-4.43177300	-2.83840700
C	-2.87850400	-4.55643200	-1.49427900
C	-2.65412000	-3.29249100	-0.63883500
O	-1.23259400	-3.08738600	-0.42109700
C	-3.30473300	-3.37623800	0.72321900
O	-4.26295200	-4.73406600	-1.75631700
C	-4.41124000	-2.56928500	1.03716700
C	-5.02399000	-2.67064900	2.28503200
C	-4.53316600	-3.58694200	3.23666300
C	-3.43651600	-4.38707700	2.92837800
C	-2.82769100	-4.28389300	1.67679800
O	3.12363900	-2.60284900	-1.94610100
O	-0.18106400	-4.74801200	-4.78433900
O	-5.13133500	-3.67826800	4.45833200
O	-6.10138500	-1.94494600	2.70379300
C	3.95483600	-2.86424500	0.35566500
O	3.70884600	-2.47866700	1.65106100
O	6.97489000	-1.16242100	-0.10035600
C	3.82543200	-4.41216300	0.24344100
O	3.59368900	-5.05627100	1.24298200
O	4.04409400	-4.96331700	-0.94046900
H	-0.99343400	0.29480300	1.70867500
H	1.24504500	-0.64351800	2.15873800
H	-0.17456900	-0.83979100	-0.13466800
H	1.25222000	0.60356900	4.06127800
H	0.85174800	2.39414100	2.94545200
H	-1.07750300	3.55898500	3.28395800
H	-1.47343700	2.27435600	4.45551800
H	4.39939900	3.18842500	3.00067300
H	7.24795600	0.37878500	-0.97110800
H	8.18943800	3.07767900	-0.63247100
H	7.22758900	4.93727600	1.74927600
H	-4.87534900	1.34782300	2.53128900
H	0.52605000	3.27574100	-1.51789500
H	1.12816300	5.12768000	-2.91603400
H	-1.48702800	6.71329500	-3.71713000
H	-4.30154900	5.88129800	-2.72196900
H	-7.09768500	1.46490800	-2.22926500
H	-7.59000100	0.10288400	0.57974300
H	-5.13159100	3.56279600	-2.69359300
H	2.31005700	-3.85732200	-4.25345600
H	-2.73864700	-3.73802400	-3.46965100
H	-2.17508000	-5.39759700	-3.35185900
H	-2.46847500	-5.41552800	-0.94223200
H	-3.04469700	-2.42910300	-1.19200200
H	-4.70567700	-4.87164700	-0.90609000
H	-4.79018600	-1.85452100	0.31196500
H	-3.06711200	-5.08116200	3.67638600
H	-1.96455800	-4.90147200	1.45115100
H	0.56490400	-4.85292000	-5.39158900
H	-5.84575900	-3.02002600	4.47385500
H	-6.33069200	-1.21719600	2.09009800
H	3.73121500	-3.29072800	2.19608600
H	4.12431200	-4.26567800	-1.62198700

Cartesian coordinates of the lowest-energy conformer of (3*S*)-**7** [(3*S*)-**7A**] at the B3LYP/6-31G(d,p) level in acetone (PCM).

C	0.34432900	-0.54440200	1.40915600
C	-1.03770200	0.04356600	1.07039700

C	-0.99631900	0.98703100	-0.18008100
C	-1.81781500	2.29476200	-0.06758100
O	0.77989100	0.35699600	3.52455100
C	0.48692300	-0.91383200	2.90311700
C	1.55281700	-1.96011300	3.19771000
O	0.63638600	-1.67839300	0.57488400
O	-1.35105200	0.26914000	-1.38148000
O	-1.99751200	-0.98089900	0.75539800
C	-2.85205700	-1.51713700	1.66125600
C	-4.01473000	-2.13909200	0.95400400
O	-2.66157700	-1.52619500	2.85901200
C	-4.25215100	-3.49072900	1.20970300
C	-5.27298600	-4.16220400	0.53807500
C	-6.07346300	-3.46121900	-0.36911200
C	-5.87532100	-2.09264300	-0.59166700
C	-4.83381500	-1.40432400	0.05375100
C	-4.67221900	0.07841900	-0.08774400
C	-5.73618000	0.91334800	0.61145700
O	-5.45740300	2.32356800	0.70642900
C	-3.31457700	2.12510200	-0.52396000
C	-3.64218700	0.67333500	-0.70416100
C	-2.65309200	-0.07694100	-1.55274300
O	-2.96229000	-0.86931400	-2.41008400
O	-6.73665700	-1.53886600	-1.49279000
O	-7.06602500	-4.14555700	-0.99992700
O	-5.48833600	-5.48112500	0.77489800
O	2.76564100	-1.61087800	2.50228000
C	3.35238200	-2.58361200	1.75508900
C	4.39918900	-2.00207400	0.86548400
O	3.04590700	-3.75654300	1.81450500
C	5.33328500	-1.14066200	1.44773400
C	6.38627300	-0.63241300	0.69201300
C	6.50761600	-1.01721600	-0.64684800
C	5.54722900	-1.84745200	-1.23103000
C	4.45504300	-2.34674900	-0.50579100
C	3.36919300	-3.12008600	-1.17533900
C	3.65919800	-4.27642600	-1.91861700
C	2.64048000	-5.08752700	-2.43125100
C	1.29625500	-4.77565100	-2.20443200
C	0.98037300	-3.62097800	-1.49289700
C	1.99859200	-2.79111300	-1.01191800
O	0.30565100	-5.56802700	-2.69905700
O	2.92451200	-6.20752000	-3.15341000
O	4.92983000	-4.73172100	-2.16807200
O	7.52067000	-0.57126200	-1.44449800
O	7.34562000	0.21304900	1.16321000
O	5.67263600	-2.16433900	-2.56376000
C	1.60173900	-1.50000300	-0.38218900
O	2.06254300	-0.41256600	-0.66213500
C	-1.35009300	3.35232800	-1.03211500
H	-1.78331600	2.64489100	0.96818500
C	-2.33258100	3.60696100	-1.97408000
C	-2.19426500	4.54029700	-2.99059000
C	-0.98408300	5.24940300	-3.02663100
C	0.05333100	5.02596200	-2.09962200
C	-0.14396500	4.04294600	-1.11968500
C	1.33692900	5.82649600	-2.14195400
C	2.23807200	5.53656900	-0.92780100
C	2.17983000	4.02751800	-0.63083500
O	0.82984500	3.73241900	-0.20013500
C	3.15134700	3.51295500	0.41149300
O	1.87167200	6.28561700	0.22540500
C	2.72142200	2.81404600	1.54757100
C	3.65245500	2.24682500	2.41944200
C	5.02421400	2.40478400	2.16805000
C	5.45896800	3.12289800	1.06148200
C	4.52318600	3.66809100	0.18184700
O	-3.44491000	2.81040500	-1.80719600
O	-0.74453500	6.20639000	-3.96708800
O	5.94353600	1.80112500	3.00380000
O	3.34086200	1.52964800	3.53927300
C	-4.26709500	2.88944900	0.39898000
O	-4.03239200	4.00936200	0.77895100
O	-6.94084900	0.76627800	-0.06750600
C	-5.96865600	0.49660400	2.08941400
O	-7.07159100	0.20182800	2.49411800
O	-4.85229100	0.56451900	2.80131300
H	1.09427200	0.22358400	1.21045400

H	-1.37635300	0.60802700	1.94467900
H	0.04204200	1.27105100	-0.34401900
H	0.46312000	0.33885500	4.43866000
H	-0.46194800	-1.29080200	3.29513100
H	1.22312300	-2.94862700	2.87614300
H	1.75925900	-1.98573000	4.27153000
H	-3.62956400	-4.03509600	1.91009300
H	-6.91033500	-0.60937000	-1.24063900
H	-7.57482000	-3.50775500	-1.52833500
H	-6.23599600	-5.77132600	0.22821500
H	5.23948500	-0.87278900	2.49278200
H	-0.06053800	-3.35547900	-1.34934900
H	0.71888800	-6.30652200	-3.17352700
H	3.89198300	-6.24535600	-3.24758300
H	5.46986900	-3.96774100	-2.45761400
H	8.03253600	0.08382500	-0.94288300
H	7.00030300	0.69877000	1.94249100
H	6.46786800	-1.72654300	-2.91030000
H	-2.98128500	4.71674700	-3.71529600
H	1.88942200	5.60192400	-3.06357300
H	1.11971000	6.89932600	-2.16816000
H	3.26397700	5.83092100	-1.16355300
H	2.35495400	3.48531500	-1.57056000
H	1.09402800	5.85608300	0.61228500
H	1.66379700	2.69389000	1.74932600
H	6.52349800	3.22359100	0.87809500
H	4.87548700	4.19618200	-0.69869500
H	-1.51684200	6.29925700	-4.54254900
H	5.43962500	1.37559900	3.71913600
H	2.44239200	1.13479600	3.48213300
H	-7.64286700	0.67323800	0.60905100
H	-5.02993900	0.29957800	3.72184200

Cartesian coordinates of the lowest-energy conformer of (3*R*)-**7** [(3*R*)-**7A**] at the B3LYP/6-31G(d,p) level in acetone (PCM).

C	0.47093600	-0.60712500	1.48042700
C	-0.93416600	-0.04807400	1.21539100
C	-0.97653800	0.89469100	-0.03130100
C	-1.83302500	2.17398600	0.12265700
O	0.93796700	0.18219400	3.63080900
C	0.66072000	-1.05771600	2.94610600
C	1.75762900	-2.09328700	3.15323200
O	0.77264900	-1.68196400	0.57291000
O	-1.35568400	0.16635300	-1.21638300
O	-1.87542500	-1.10786200	0.96035000
C	-2.75195400	-1.54295800	1.89972200
C	-3.89158300	-2.25608600	1.24370200
O	-2.59978400	-1.39134900	3.09331000
C	-4.11062300	-3.59165300	1.59454000
C	-5.16006500	-4.29653500	1.00802200
C	-6.00967000	-3.65571600	0.09894700
C	-5.81550200	-2.30736300	-0.21102900
C	-4.74702000	-1.58878600	0.33700100
C	-4.65650200	-0.11241700	0.15313600
C	-5.76127900	0.70173900	0.81640900
O	-5.32820000	2.04295500	1.21608200
C	-3.34433400	1.96972000	-0.28161700
C	-3.63808100	0.50894200	-0.46310700
C	-2.65224400	-0.22450100	-1.32742500
O	-2.96259700	-1.04504100	-2.15904800
O	-6.67069700	-1.66842900	-1.05502500
O	-7.06032000	-4.28811100	-0.49558000
O	-5.45905400	-5.60524800	1.24501900
O	2.94381400	-1.67271700	2.45121800
C	3.53581000	-2.58622900	1.63603500
C	4.54675700	-1.92983200	0.75703200
O	3.25835000	-3.76796100	1.63444600
C	5.47334700	-1.07645200	1.36288400
C	6.49220000	-0.49855600	0.61024000
C	6.58997600	-0.80724000	-0.74993700
C	5.63650200	-1.63017300	-1.35544400
C	4.57602100	-2.19644800	-0.63257500
C	3.49072900	-2.95451200	-1.32047400

C	3.78624500	-4.05801400	-2.13829900
C	2.77207200	-4.85610600	-2.67943100
C	1.42720700	-4.58333600	-2.40978300
C	1.10514800	-3.48065700	-1.62264400
C	2.11816700	-2.66316600	-1.11026700
O	0.44123200	-5.36236500	-2.93424800
O	3.06128300	-5.92473300	-3.47384800
O	5.05966700	-4.47218400	-2.44025100
O	7.56981900	-0.29053300	-1.54602500
O	7.43968600	0.34817200	1.10393600
O	5.73484200	-1.87010100	-2.70634400
C	1.71100300	-1.42240500	-0.39186400
O	2.14329700	-0.31004600	-0.61336900
C	-1.42803600	3.25365700	-0.84256300
H	-1.77008400	2.51445300	1.16017000
C	-2.45100800	3.49768300	-1.74315100
C	-2.36532700	4.44554000	-2.75319800
C	-1.17032500	5.17802500	-2.82451800
C	-0.09639500	4.96721700	-1.93677100
C	-0.24127400	3.97082400	-0.96170500
C	1.16982400	5.79240600	-2.01303500
C	2.11195100	5.51333200	-0.82744700
C	2.09638800	4.00135800	-0.53878600
O	0.76640100	3.67213600	-0.07448400
C	3.10649200	3.50377800	0.47556000
O	1.76282800	6.24669000	0.34122500
C	2.72294600	2.78382300	1.61558400
C	3.68954000	2.23373400	2.45930800
C	5.05018200	2.43279900	2.17827700
C	5.43886000	3.17225400	1.06855500
C	4.46787500	3.69832000	0.21576600
O	-3.53954200	2.67904500	-1.54309400
O	-0.98154700	6.14808100	-3.76396300
O	6.00398700	1.84817900	2.98813400
O	3.42637700	1.49814700	3.58027900
C	-4.25155600	2.68593600	0.72689700
O	-4.02323000	3.81530200	1.09269100
O	-6.22218900	0.07480200	1.94103800
C	-6.97479800	1.00879200	-0.11250800
O	-8.10900000	0.87736000	0.29394800
O	-6.61354200	1.50304500	-1.28869600
H	1.19119400	0.19439500	1.30622400
H	-1.23822600	0.50603000	2.10837300
H	0.04497500	1.21281300	-0.23523500
H	0.66060600	0.10155800	4.55431800
H	-0.26879100	-1.47874500	3.34172000
H	1.44274100	-3.06826400	2.77954400
H	1.99144700	-2.17965200	4.21824700
H	-3.45533100	-4.07933800	2.30850000
H	-7.39656700	-2.27300800	-1.27858900
H	-7.10597900	-5.19810200	-0.16250400
H	-4.83101000	-5.99516200	1.86904300
H	5.40187000	-0.86914800	2.42342200
H	0.06274600	-3.24225700	-1.44579000
H	0.85807700	-6.05850800	-3.46612000
H	4.02703900	-5.93765000	-3.58986000
H	5.57765900	-3.68176700	-2.69722900
H	8.07532800	0.35185200	-1.02184500
H	7.08836900	0.80298600	1.89919200
H	6.50758300	-1.39061100	-3.04854400
H	-3.18073300	4.61538000	-3.44776100
H	1.69931500	5.58335300	-2.95168800
H	0.93215600	6.86114000	-2.02625400
H	3.12374500	5.83202900	-1.09102200
H	2.25996500	3.46866500	-1.48608400
H	1.00685800	5.79693300	0.74762400
H	1.67382400	2.63452900	1.84126100
H	6.49554700	3.30409600	0.86109600
H	4.78530900	4.24290100	-0.66798600
H	-1.77357900	6.22843900	-4.31374400
H	5.52674000	1.39832800	3.70713400
H	2.54722700	1.06109400	3.53676500
H	-7.17739400	0.26927800	1.99883800
H	-7.41306500	1.74215200	-1.79079400