Supplementary Material

NMR solution structures of procyanidin B1, B2, and C1

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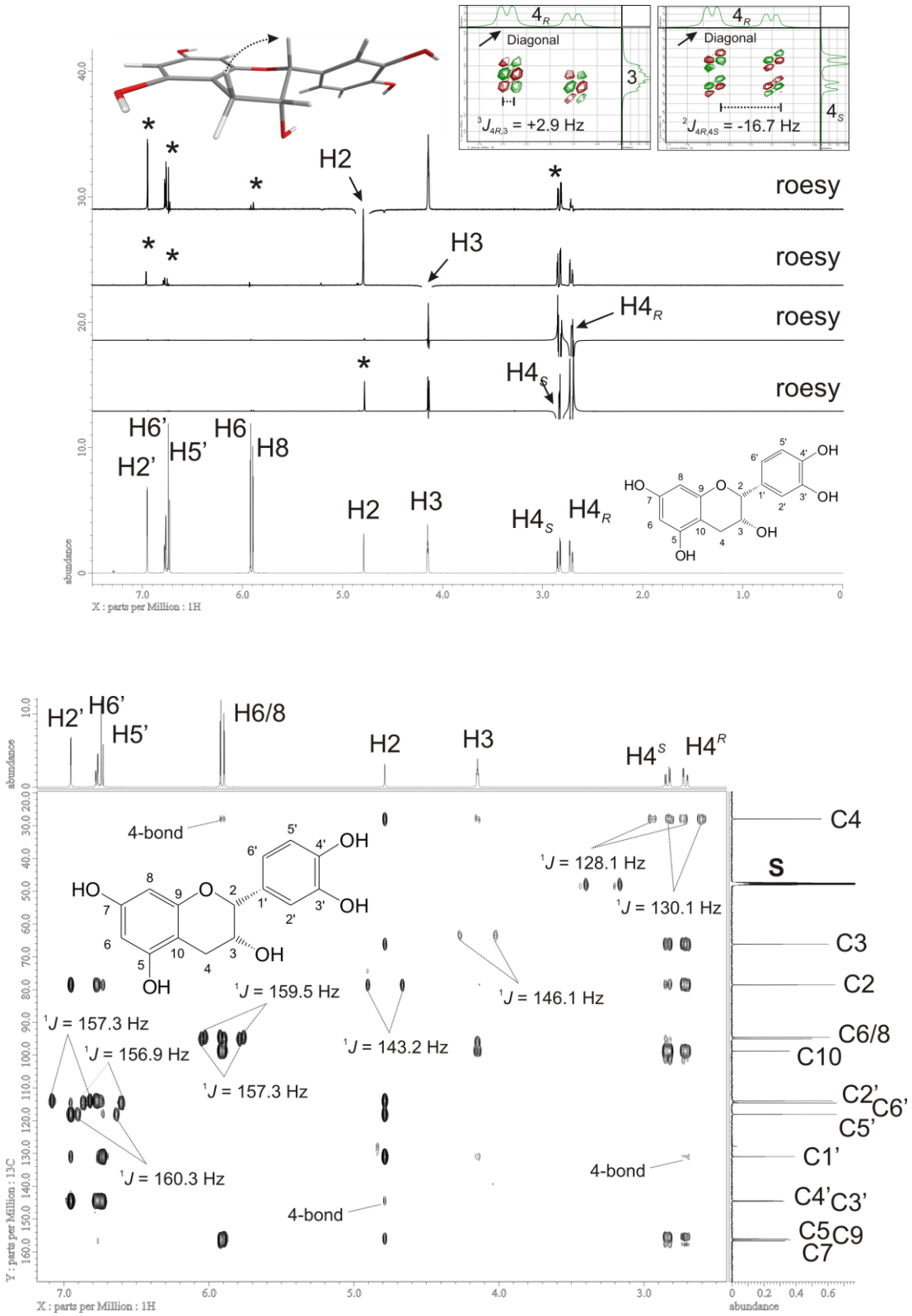


Figure S1. Top: Conformational analysis of (-)-**1b**. Small coupling constants of $^{3}J_{H4R,H3}$ = +4.6 Hz and $^{3}J_{H4S,H3}$ = +2.9 Hz (E-COSY, inset) as well as 1d-pfg-rOe response at H4$_S$ and H2'/H6' upon irradiation of H2 confirmed the preferred tetrahydropyran-$^{2}H_3$ conformation and conformational flexibility of the catechol; bottom: ^{1}H-^{13}C-HMBC spectrum of (**1b**) with $^{3}J_{H3\text{-}C10}$ = 5.5 Hz, $^{3}J_{H4R\text{-}C2}$ = 0.4 Hz, and $^{3}J_{H4S\text{-}C2}$: 5.3 Hz. Identities of all carbons were established from HMQC correlations and typical one-bond ^{1}H-^{13}C-*J*-values were observed.

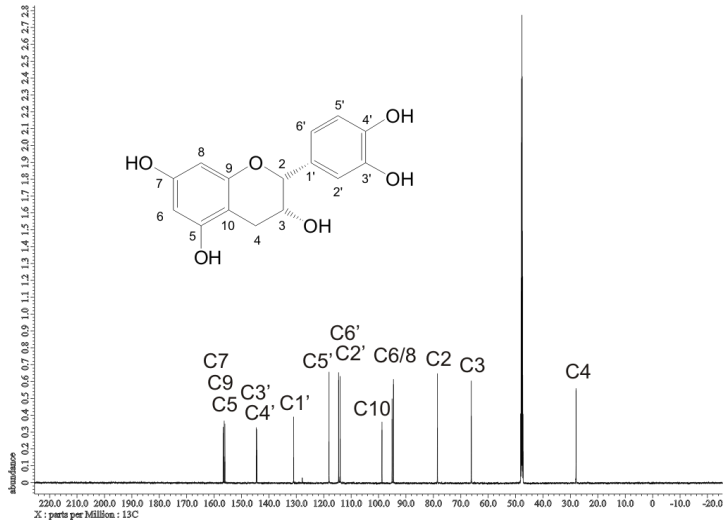


Figure S2. ^{13}C NMR of **compound 1b**

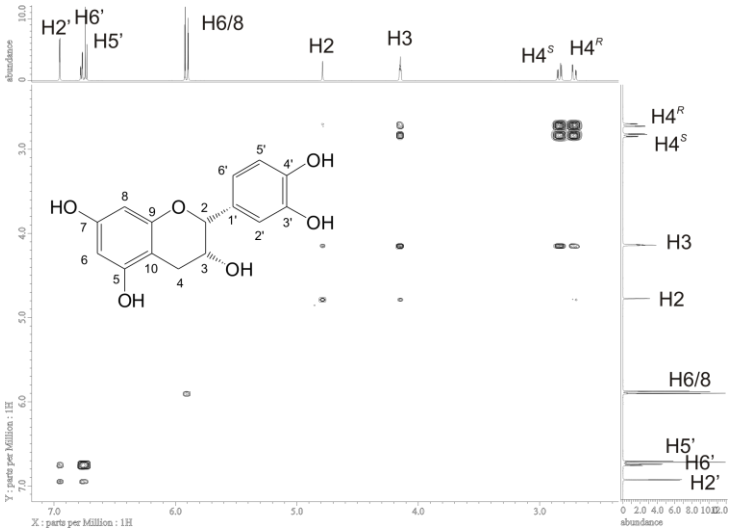


Figure S3. ^{1}H-^{1}H-COSY of **compound 1b**

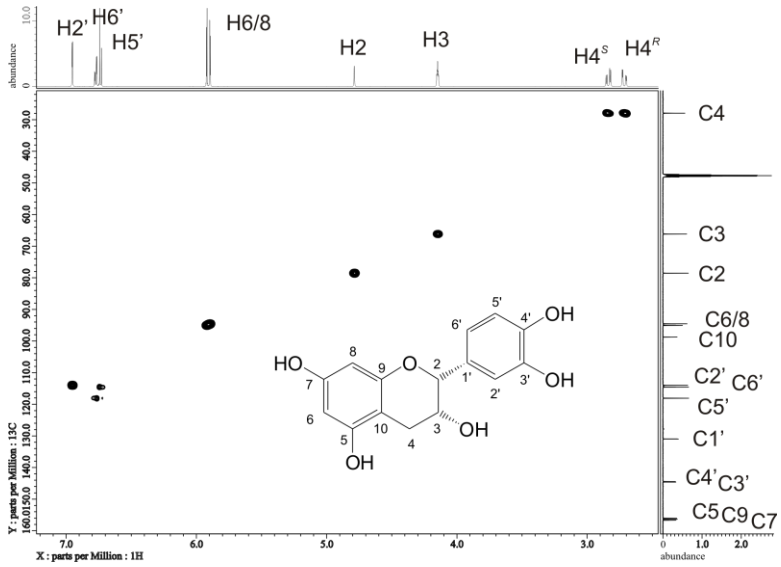


Figure S4. ^{1}H-^{13}C-HMQC of **compound 1b**

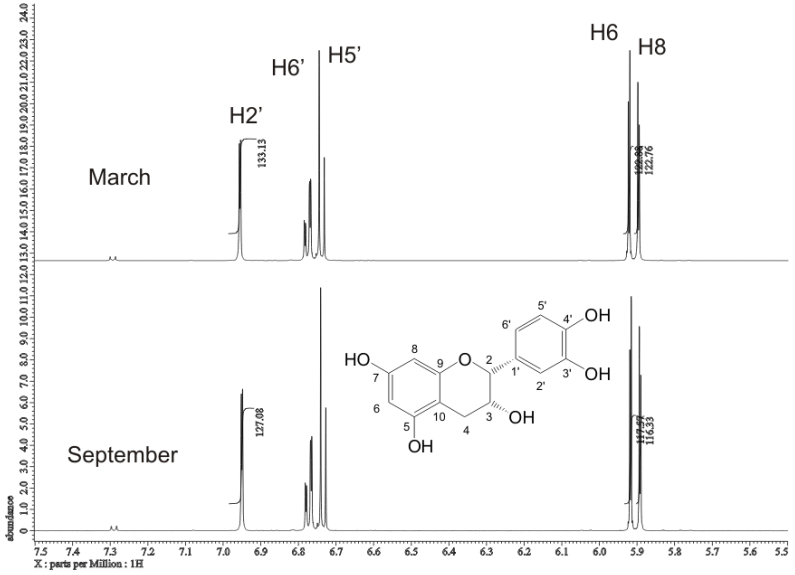


Figure S5. No H/D-exchange in **compound 1b** (H6 and H8). [1]

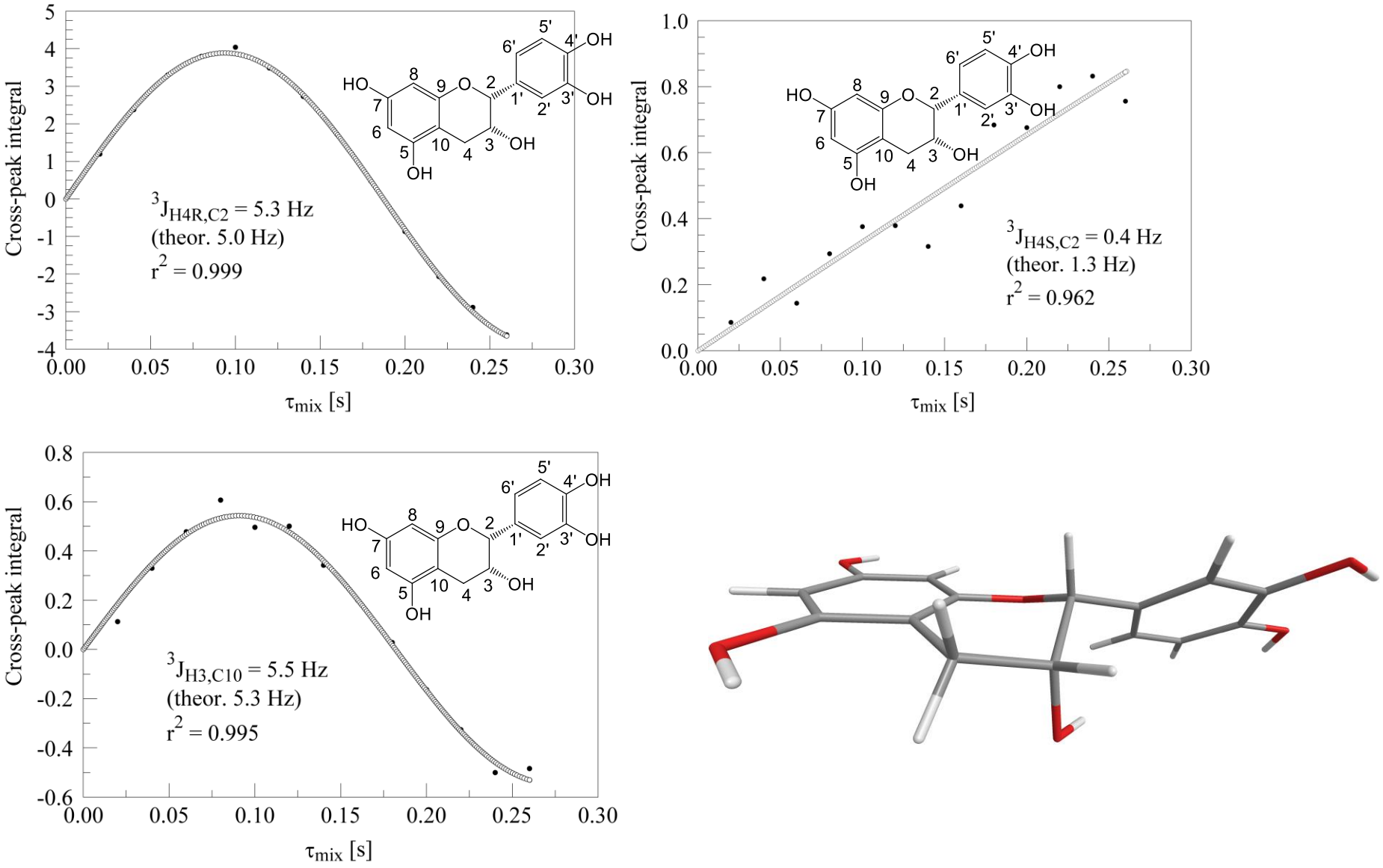


Figure S6. *J*-HMBC fitting of **compound 1b**. Theoretical *J*-values (GIAO, B3LYP/6-311G**(d,p)(u+1s), correction factor[2]) were Boltzmann-weighted by energy differences between $^{2}H_{3}$ and $^{3}H_{2}$ half chair for four conformations at 56:26:11:7 (at rt with thermal correction).

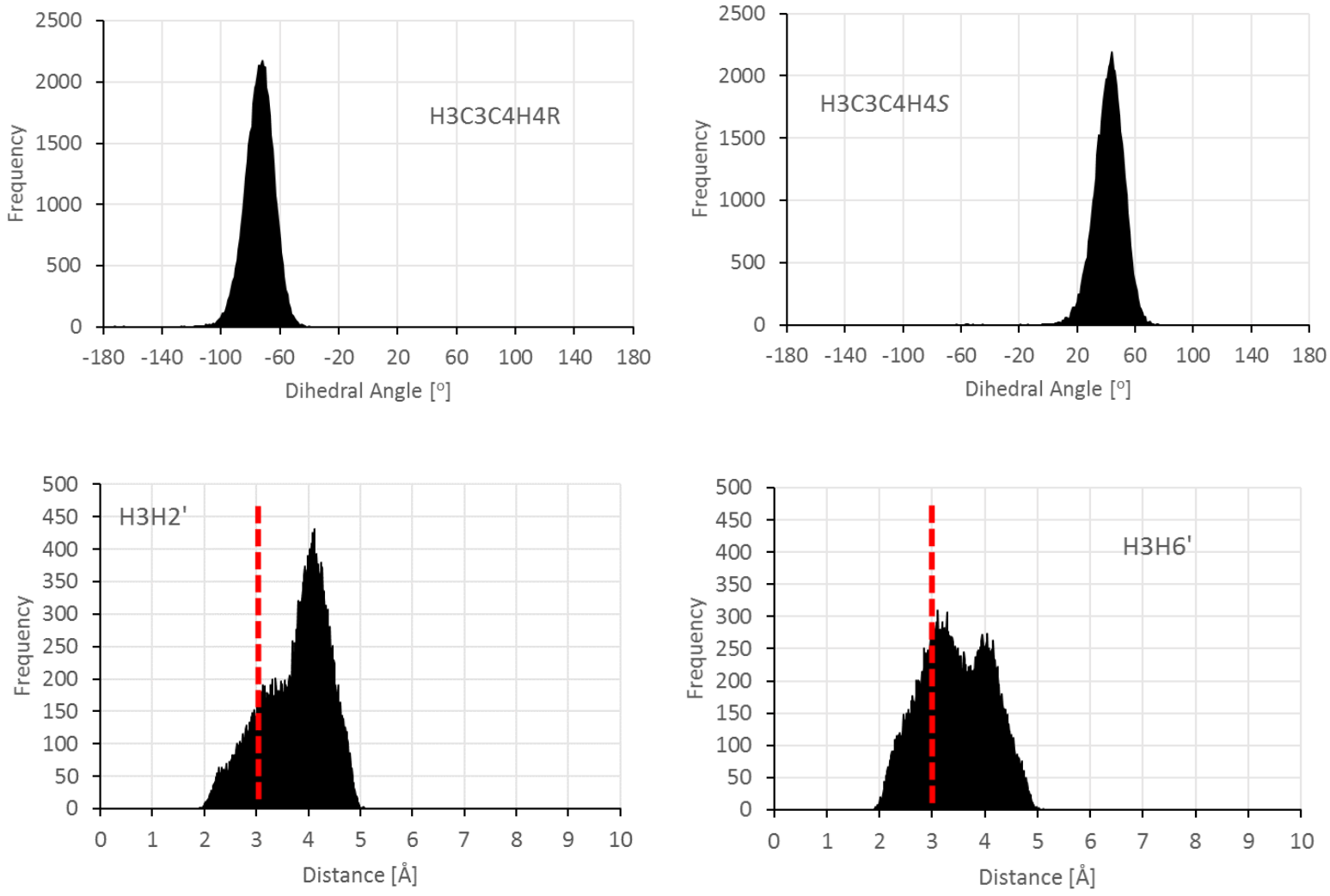


Figure S7. Histograms from GAFF-MD-simulation of **1b** at rt with explicit methanol solvent. Top: Diagnostic half-chair angle; bottom: distance histogram for H3-H2' and H3H6'.

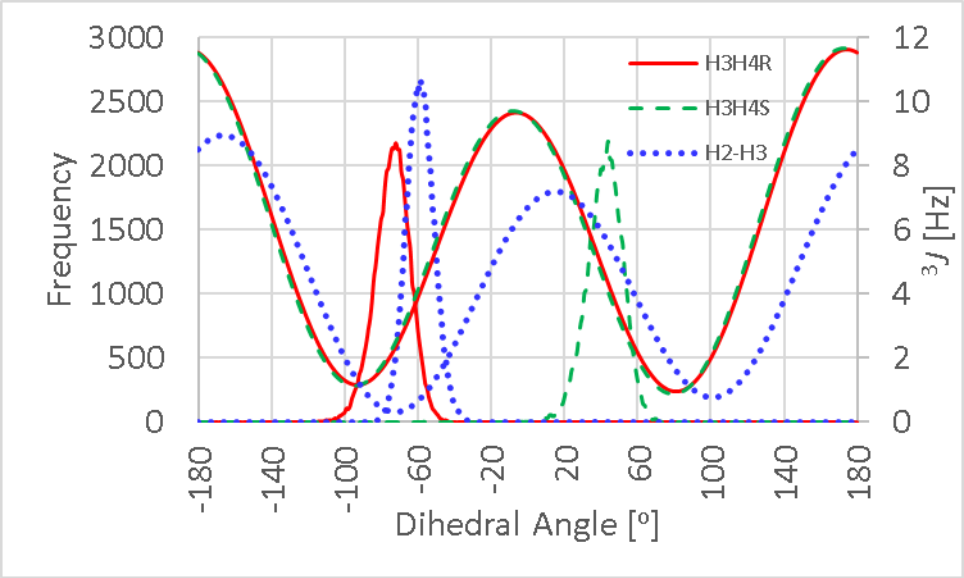


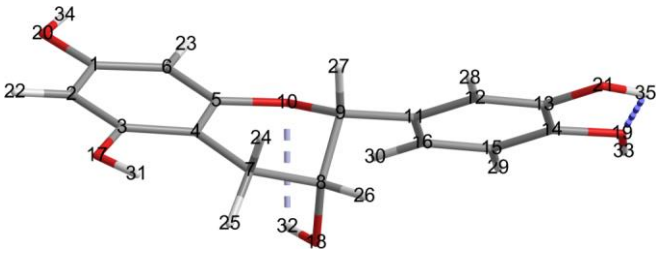
Figure S8. Histogram from MD-simulation of **1b** at rt with corresponding Haasnoot-deLeuw-Altona (HLA) equations[3] overlaid.

Equation for H3-C3-C4-H4*R* (3-substituent system): $13.22*\cos^2(\varphi) - 0.99*\cos(\varphi) + \{[0.4*(0.87 - 2.46*(\cos^2(\varphi + 19.9*0.4)) + 1.3*(0.87 - 2.46*(\cos^2(-\varphi + 19.9*1.3)) + 0.4*(0.87 - 2.46*(\cos^2(\varphi + 19.9*0.4))]\}$.

Equation for H3-C3-C4-H4*S* (3-substituent system): $13.22*\cos^2(\varphi) - 0.99*\cos(\varphi) + \{[0.4*(0.87 - 2.46*(\cos^2(\varphi + 19.9*0.4)) + 1.3*(0.87 - 2.46*(\cos^2(-\varphi + 19.9*1.3)) + 0.4*(0.87 - 2.46*(\cos^2(-\varphi + 19.9*0.4))]\}$.

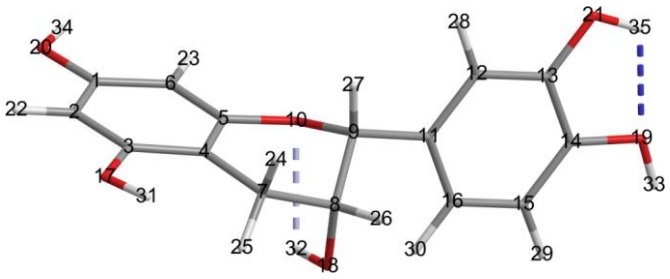
Equation for H2-C2-C3-H3 (4-substituent system): $13.24*\cos^2(\varphi) - 0.91*\cos(\varphi) + \{[1.3*(0.53- 2.41*(\cos^2(\varphi + 15.5*1.3)) + 0.4*(0.53 - 2.41*(\cos^2(-\varphi + 15.5*0.4)) + 1.3*(0.53- 2.41*(\cos^2(\varphi + 15.5*1.3)) + 0.4*(0.53 - 2.41*(\cos^2(-\varphi + 15.5*0.4))]\}$.

Compound 1b: Conformer (I) (0.00 kcal/mol)



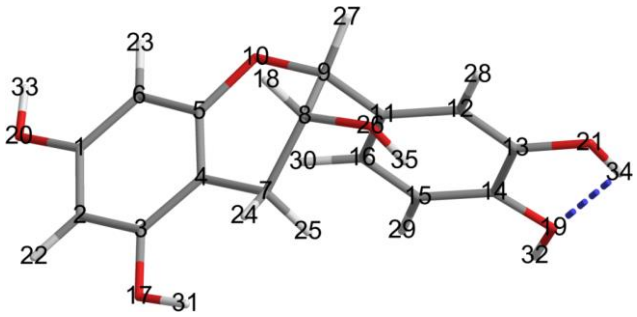
	X	Y	Z
C(1)	4.026	1.477	-0.299
C(2)	4.596	0.207	-0.233
C(3)	3.763	-0.896	-0.1
C(4)	2.368	-0.775	-0.026
C(5)	1.844	0.515	-0.118
C(6)	2.647	1.645	-0.248
C(7)	1.474	-1.978	0.173
C(8)	0.06	-1.537	0.547
C(9)	-0.345	-0.374	-0.364
O(10)	0.493	0.746	-0.048
C(11)	-1.779	0.043	-0.177
C(12)	-2.767	-0.629	-0.903
C(13)	-4.104	-0.322	-0.712
C(14)	-4.466	0.672	0.208
C(15)	-3.489	1.344	0.925
C(16)	-2.143	1.025	0.737
O(17)	4.368	-2.113	-0.035
O(18)	-0.029	-1.144	1.904
O(19)	-5.81	0.899	0.31
O(20)	4.878	2.53	-0.427
O(21)	-5.065	-0.975	-1.421
H(22)	5.668	0.08	-0.285
H(23)	2.184	2.622	-0.312
H(24)	1.432	-2.589	-0.734
H(25)	1.844	-2.61	0.986
H(26)	-0.638	-2.363	0.412
H(27)	-0.171	-0.665	-1.406
H(28)	-2.509	-1.395	-1.626
H(29)	-3.778	2.114	1.631
H(30)	-1.383	1.553	1.295
H(31)	3.708	-2.814	-0.003
H(32)	0.397	-0.281	1.982
H(33)	-5.989	1.586	0.961
H(34)	4.375	3.35	-0.469
H(35)	-5.923	-0.62	-1.153

Compound 1b: Conformer (II) (+0.45kcal/mol)



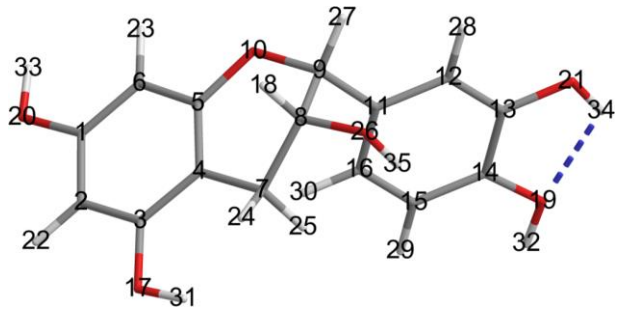
	X	Y	Z
C(1)	-3.906	1.613	-0.329
C(2)	-4.553	0.462	0.116
C(3)	-3.794	-0.657	0.43
C(4)	-2.396	-0.67	0.311
C(5)	-1.792	0.513	-0.118
C(6)	-2.521	1.654	-0.446
C(7)	-1.584	-1.91	0.604
C(8)	-0.156	-1.75	0.082
C(9)	0.345	-0.351	0.456
O(10)	-0.432	0.606	-0.278
C(11)	1.796	-0.139	0.115
C(12)	2.61	0.507	1.049
C(13)	3.965	0.664	0.804
C(14)	4.517	0.177	-0.388
C(15)	3.712	-0.459	-1.319
C(16)	2.349	-0.624	-1.065
O(17)	-4.473	-1.757	0.855
O(18)	-0.083	-1.933	-1.32
O(19)	5.86	0.393	-0.531
O(20)	-4.688	2.685	-0.627
O(21)	4.756	1.296	1.713
H(22)	-5.629	0.438	0.217
H(23)	-1.998	2.542	-0.776
H(24)	-1.552	-2.113	1.679
H(25)	-2.015	-2.786	0.109
H(26)	0.494	-2.499	0.532
H(27)	0.183	-0.193	1.528
H(28)	2.202	0.899	1.974
H(29)	4.147	-0.828	-2.24
H(30)	1.722	-1.117	-1.794
H(31)	-3.858	-2.455	1.103
H(32)	-0.458	-1.145	-1.733
H(33)	6.175	0.03	-1.365
H(34)	-4.135	3.419	-0.916
H(35)	5.657	1.309	1.362

Compound 1b: Conformer (III) (+0.96 kcal/mol)



	X	Y	Z
C(1)	-3.817	-1.142	-0.417
C(2)	-3.883	-0.592	0.861
C(3)	-2.881	0.28	1.266
C(4)	-1.814	0.635	0.427
C(5)	-1.778	0.044	-0.838
C(6)	-2.765	-0.839	-1.274
C(7)	-0.757	1.625	0.847
C(8)	-0.065	2.177	-0.389
C(9)	0.368	1.029	-1.315
O(10)	-0.779	0.287	-1.739
C(11)	1.425	0.139	-0.696
C(12)	2.752	0.59	-0.687
C(13)	3.75	-0.171	-0.098
C(14)	3.431	-1.405	0.485
C(15)	2.125	-1.864	0.464
C(16)	1.121	-1.094	-0.126
O(17)	-2.986	0.788	2.524
H(18)	-0.769	2.794	-0.951
O(19)	4.489	-2.074	1.033
O(20)	-4.817	-1.991	-0.777
O(21)	5.035	0.271	-0.096
H(22)	-4.694	-0.842	1.53
H(23)	-2.69	-1.27	-2.264
H(24)	-1.194	2.466	1.393
H(25)	-0.008	1.155	1.496
O(26)	1.026	3.012	-0.064
H(27)	0.771	1.473	-2.226
H(28)	3.026	1.528	-1.155
H(29)	1.889	-2.825	0.906
H(30)	0.108	-1.472	-0.142
H(31)	-2.2	1.298	2.746
H(32)	4.206	-2.921	1.393
H(33)	-4.669	-2.302	-1.677
H(34)	5.578	-0.397	0.343
H(35)	1.632	2.501	0.488

Compound 1b: Conformer (IV) (+1.24 kcal/mol)



	X	Y	Z
C(1)	-3.743	-1.264	-0.565
C(2)	-3.905	-0.723	0.707
C(3)	-2.966	0.192	1.169
C(4)	-1.871	0.596	0.392
C(5)	-1.738	0.012	-0.869
C(6)	-2.658	-0.912	-1.361
C(7)	-0.884	1.63	0.872
C(8)	-0.148	2.216	-0.322
C(9)	0.387	1.091	-1.223
O(10)	-0.7	0.301	-1.712
C(11)	1.446	0.247	-0.546
C(12)	2.774	0.376	-0.975
C(13)	3.785	-0.346	-0.362
C(14)	3.477	-1.22	0.69
C(15)	2.164	-1.365	1.107
C(16)	1.148	-0.633	0.491
O(17)	-3.166	0.691	2.419
H(18)	-0.845	2.804	-0.923
O(19)	4.547	-1.884	1.22
O(20)	-4.682	-2.156	-0.982
O(21)	5.07	-0.218	-0.785
H(22)	-4.741	-1.01	1.329
H(23)	-2.509	-1.337	-2.345
H(24)	-1.387	2.449	1.394
H(25)	-0.152	1.192	1.562
O(26)	0.885	3.097	0.066
H(27)	0.82	1.555	-2.11
H(28)	3.032	1.026	-1.803
H(29)	1.932	-2.052	1.913
H(30)	0.128	-0.766	0.822
H(31)	-2.417	1.234	2.686
H(32)	4.262	-2.482	1.919
H(33)	-4.47	-2.457	-1.872
H(34)	5.62	-0.805	-0.249
H(35)	1.48	2.611	0.65

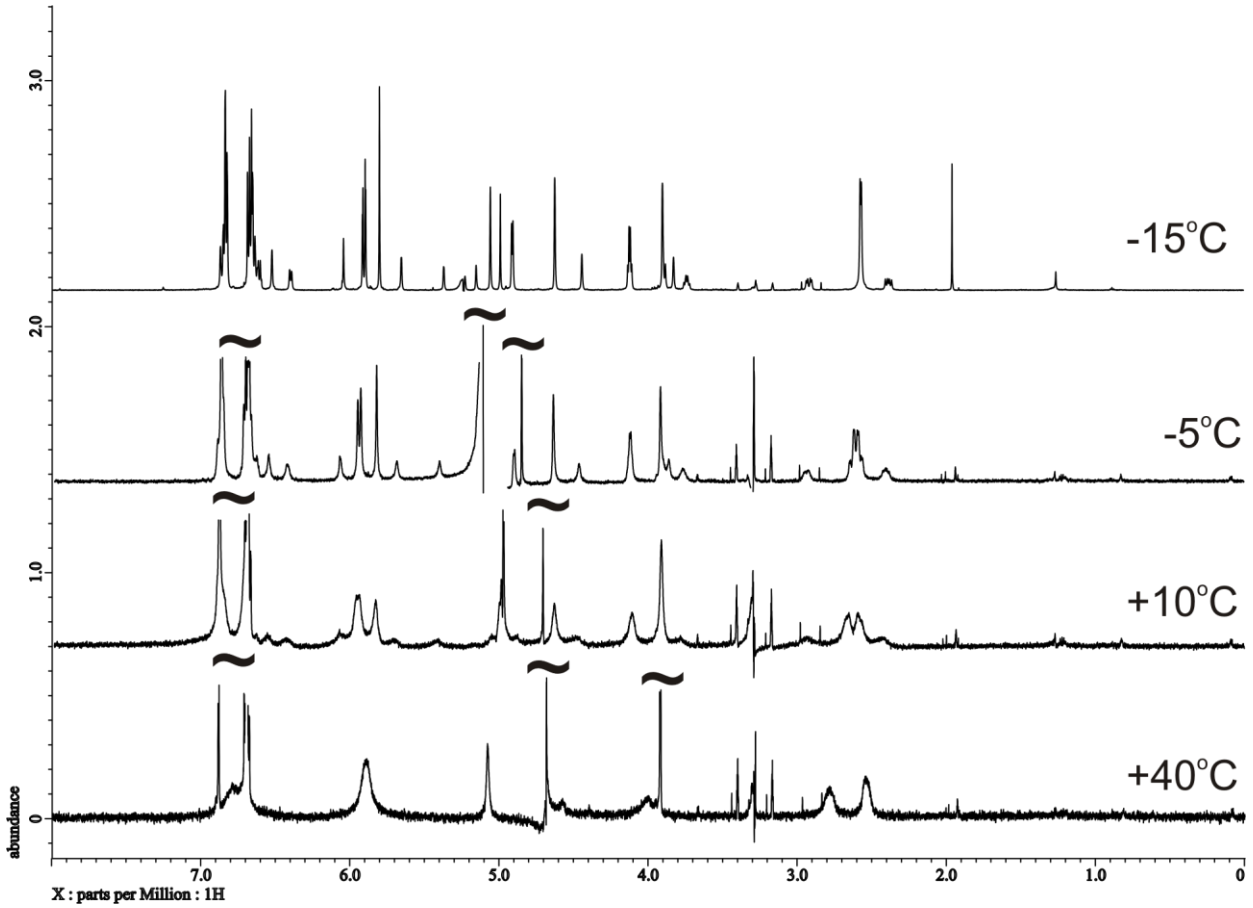


Figure S9. VT-^{1}H-NMR of **compound 2** (methanol-d_4).

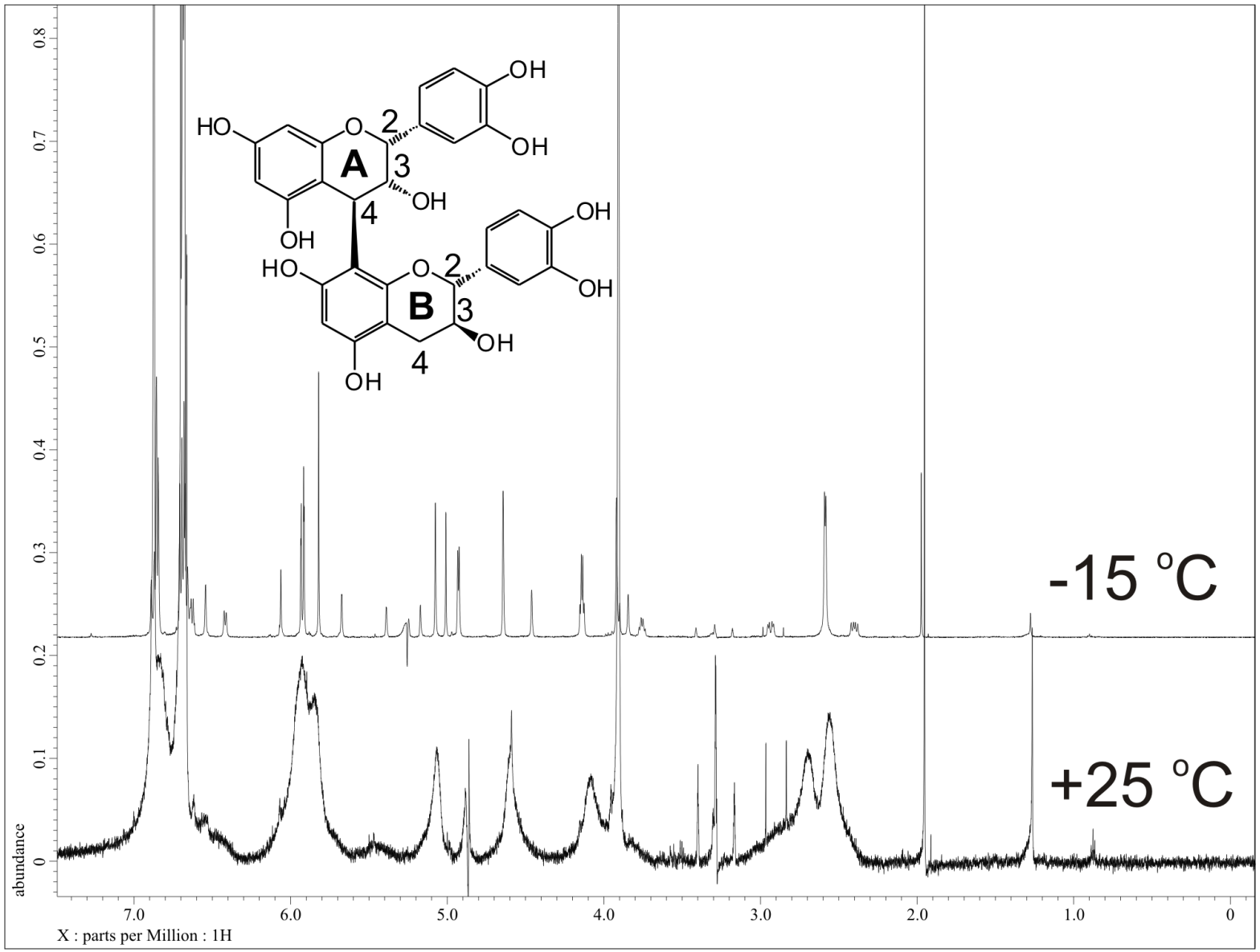


Figure S10. Direct comparison of ^{1}H-spectra of **compound 2** – integration at room temperature leads to unreliable results.

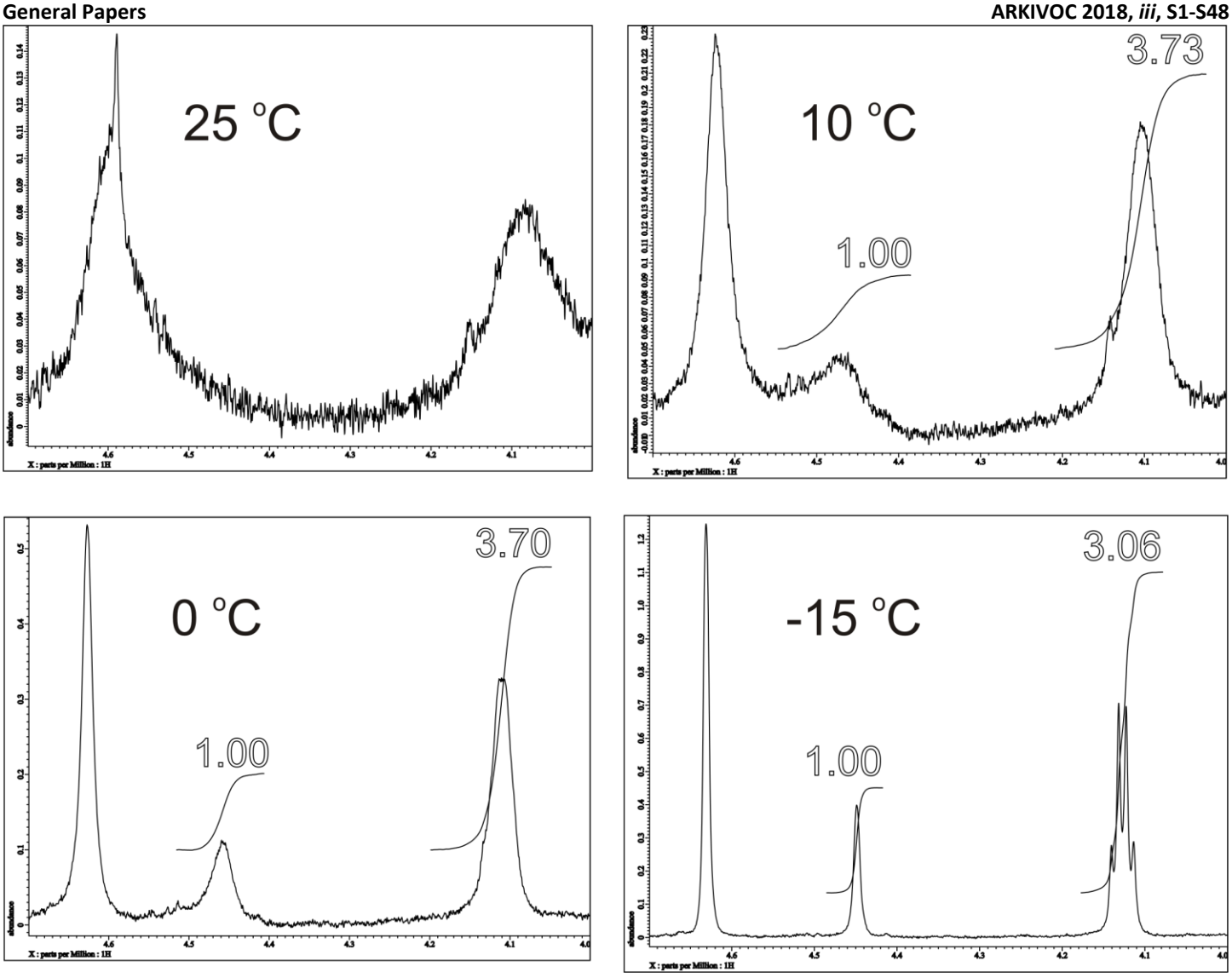


Figure S11. Compound 2. Unreliable integration at rt. No apparent change in abundance of species. Therefore, conformational changes between the two species are mostly enthalpy-driven.

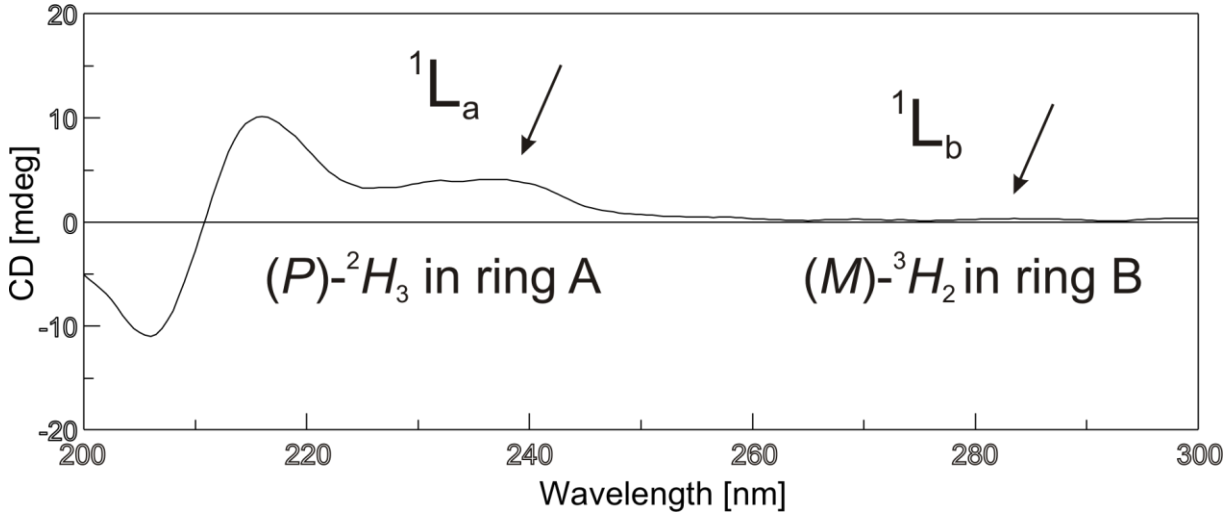


Figure S12. CD-Spectrum of native **2** in methanol at room temperature.

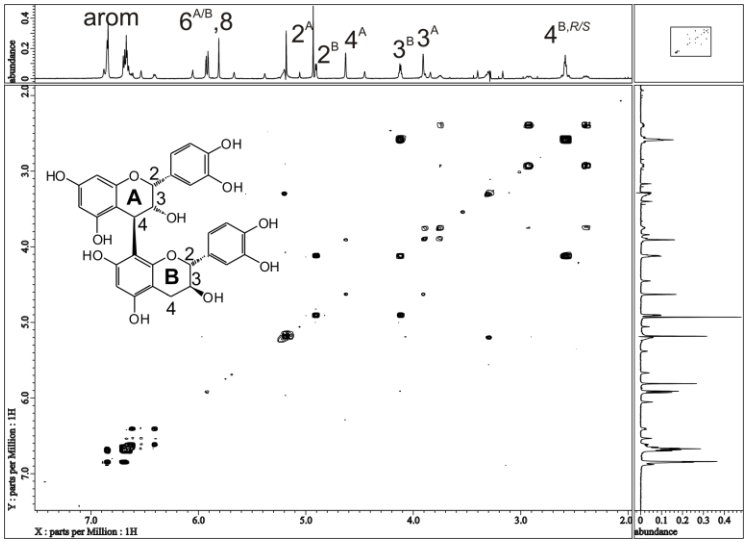


Figure S13. ^{1}H-^{1}H-COSY of **compound 2** at -15 ^{o}C

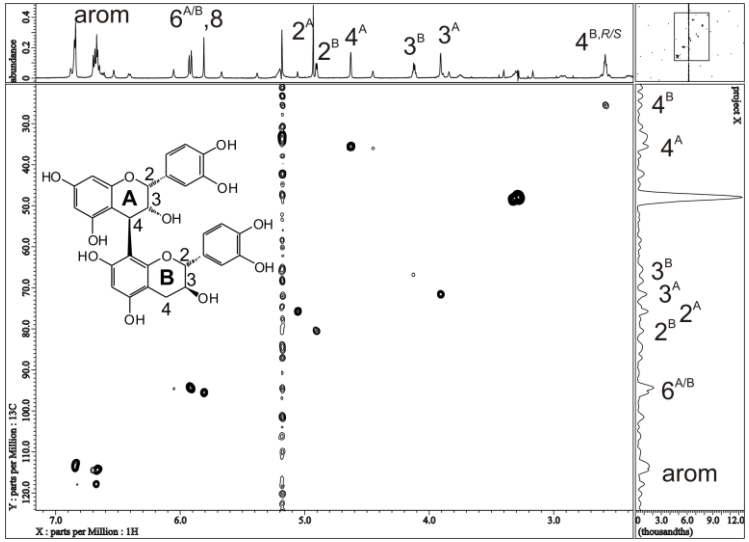


Figure S14. ^{1}H-^{13}C-HMQC of **compound 2** at -15 ^{o}C

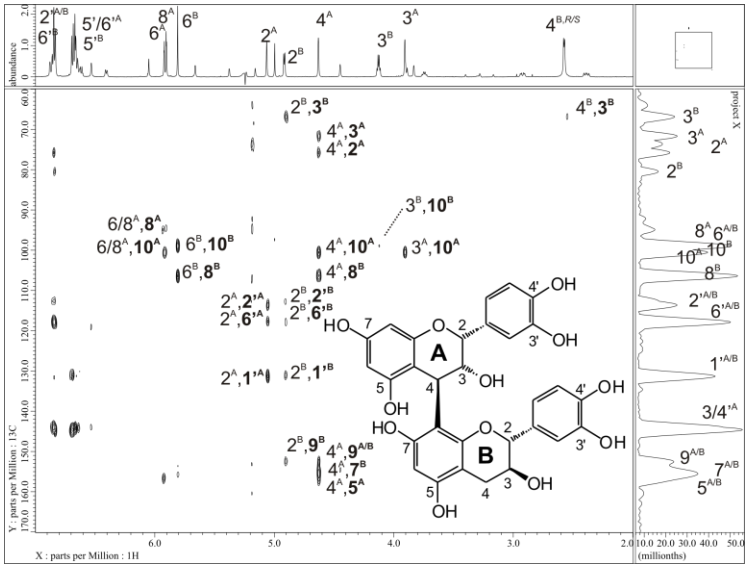


Figure S15. ^{1}H-^{13}C-HMBC of **compound 2** at -15 ^{o}C.

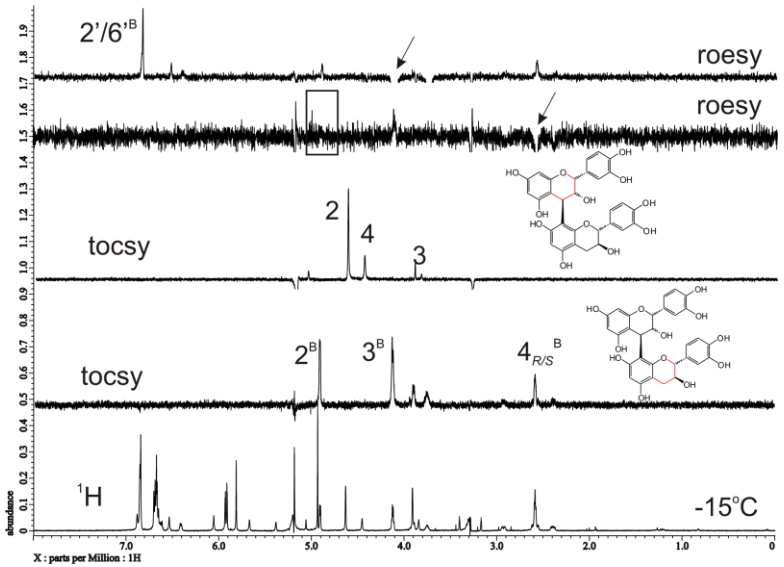


Figure S16. 1d-pfg TOCSY/ROESY of **compound 2** at -15 ^{o}C.

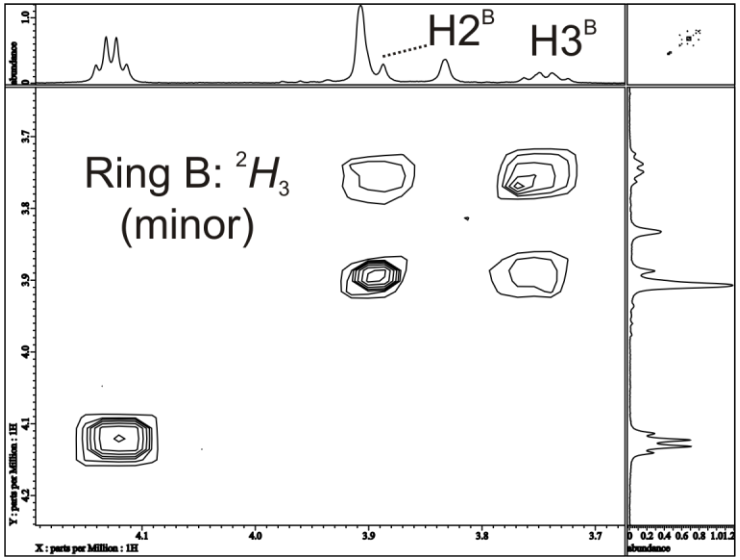


Figure S17. COSY of **compound 2**. Minor conformation, ring B.

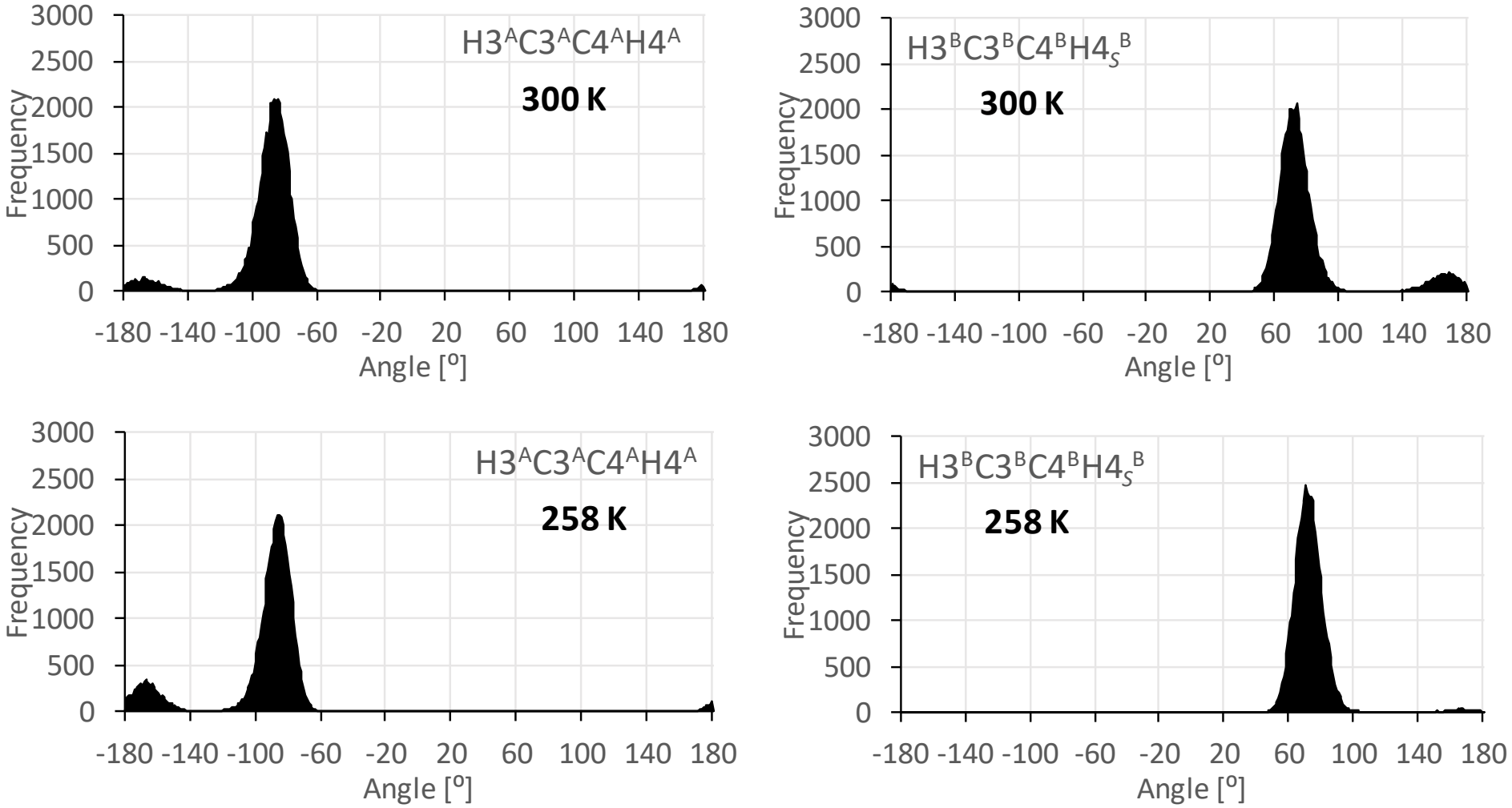


Figure S18. Histograms from MD-simulation of **2**. Top: Diagnostic half-chair dihedral angle in ring A + B at 300 K; bottom: ring A + B at 258 K.

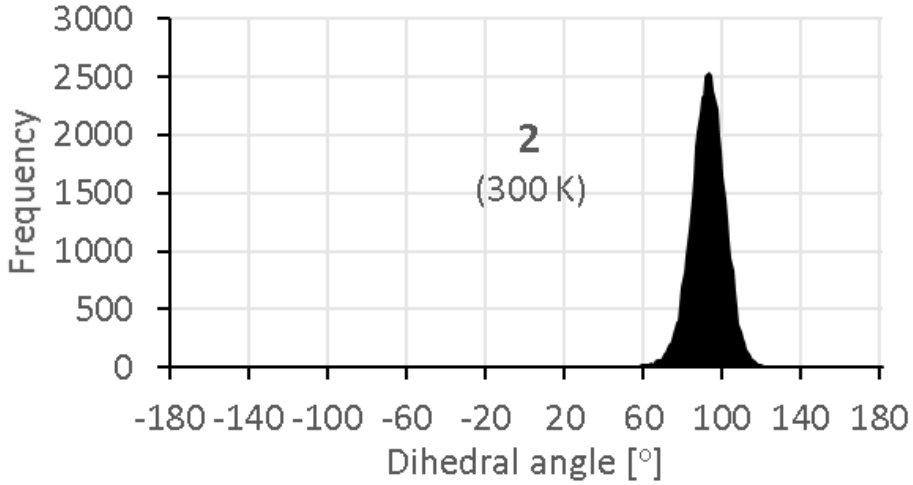


Figure S19. Control experiment: MD-simulation of the (*P*)-**2** atrop isomer at 300 K. No interconversion to the (*M*)-**2** atrop isomer was observed because the rotational barrier was too high. The lowest-energy (*P*)-structure was +3.81 kcal/mol less stable than the most stable (*M*)-structure.

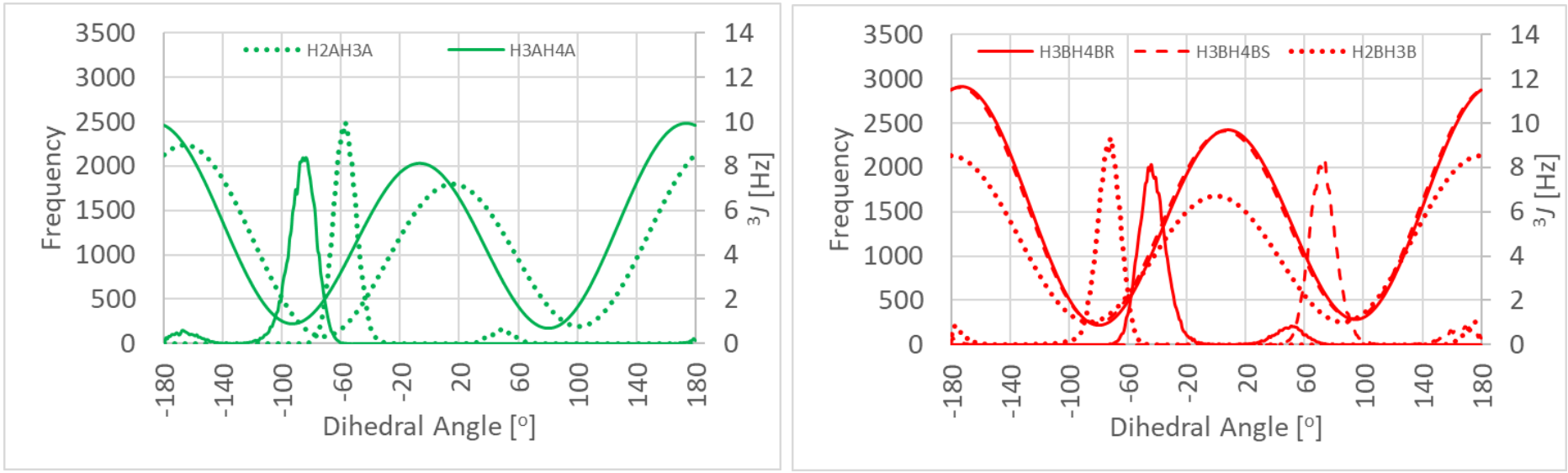


Figure S20. Histogram from MD-simulation of **2** at 258 K (-15 °C) with corresponding Haasnoot-deLeuw-Altona (HLA) equations[3] overlaid.

Equation for $H2^{A}$-$C2^{A}$-$C3^{A}$-$H3^{A}$ (4-substituent system): $13.24*\cos^2(\varphi) - 0.91*\cos(\varphi) + \{[1.3*(0.53- 2.41*(\cos^2(\varphi + 15.5*1.3)) + 0.4*(0.53 - 2.41*(\cos^2(-\varphi + 15.5*0.4)) + 1.3*(0.53- 2.41*(\cos^2(\varphi + 15.5*1.3)) + 0.4*(0.53 - 2.41*(\cos^2(-\varphi + 15.5*0.4))]\}$.

Equation for $H3^{A}$-$C3^{A}$-$C4^{A}$-$H4^{A}$ (4-substituent system): $13.24*\cos^2(\varphi) - 0.91*\cos(\varphi) + \{[0.4*(0.53- 2.41*(\cos^2(\varphi + 15.5*0.4)) + 1.3*(0.53 - 2.41*(\cos^2(-\varphi + 15.5*1.3)) + 0.4*(0.53- 2.41*(\cos^2(\varphi + 15.5*0.4)) + 0.4*(0.53 - 2.41*(\cos^2(-\varphi + 15.5*0.4))]\}$.

Equation for $H2^{B}$-$C2^{B}$-$C3^{B}$-$H3^{B}$ (4-substituent system): $13.24*\cos^2(\varphi) - 0.91*\cos(\varphi) + \{[1.3*(0.53- 2.41*(\cos^2(\varphi + 15.5*1.3)) + 0.4*(0.53 - 2.41*(\cos^2(-\varphi + 15.5*0.4)) + 0.4*(0.53- 2.41*(\cos^2(\varphi + 15.5*0.4)) + 1.3*(0.53 - 2.41*(\cos^2(-\varphi + 15.5*1.3))]\}$.

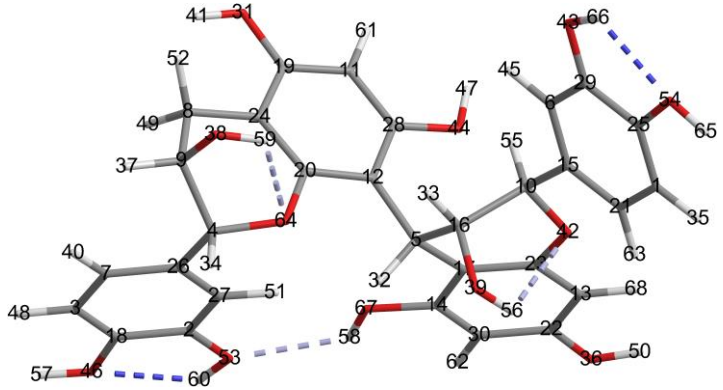
Equation for $H3^{B}$-$C3^{B}$-$C4^{B}$-$H4^{B}$*R* (3-substituent system): $13.22*\cos^2(\varphi) - 0.99*\cos(\varphi) + \{[1.3*(0.87 - 2.46*(\cos^2(\varphi + 19.9*1.3)) + 0.4*(0.87 - 2.46*(\cos^2(-\varphi + 19.9*0.4)) + 0.4*(0.87 - 2.46*(\cos^2(\varphi + 19.9*0.4))]\}$.

Equation for $H3^{B}$-$C3^{B}$-$C4^{B}$-$H4^{B}$*S* (3-substituent system): $13.22*\cos^2(\varphi) - 0.99*\cos(\varphi) + \{[1.3*(0.87 - 2.46*(\cos^2(\varphi + 19.9*1.3)) + 0.4*(0.87 - 2.46*(\cos^2(-\varphi + 19.9*0.4)) + 0.4*(0.87 - 2.46*(\cos^2(-\varphi + 19.9*0.4))]\}$.

```
; Definition of sample heteronuclear spin system
; C-CH2-CH-CH
;
proton   a 2.575      t= 0.3
proton   b 2.596    t= 0.3
proton   c 4.12    t= 0.4
proton   d 4.905    t= 0.3
;
; H-H couplings in Hz
;
couple a b -17.0
couple a c 5.9
couple b c 4.5
couple c d 5
```

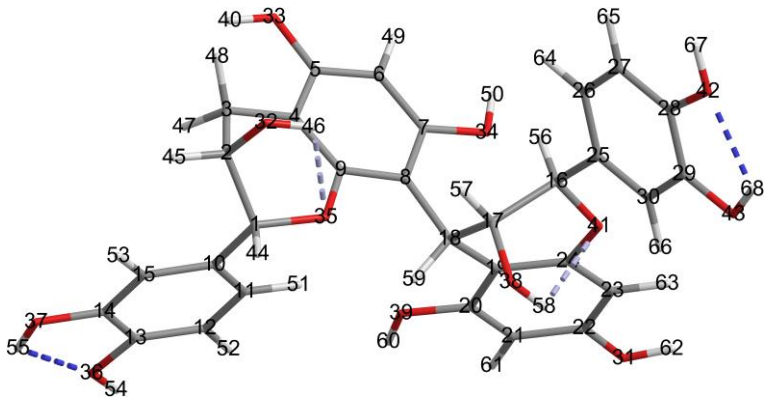
Figure S21. Parameters for the simulation of the spin system H2-H3-H4$_{R/S}$ in NMRSim 6.0 (TopSpin 3.5 pl7) (Bruker).

Compound 2: Conformer (I) (0.00 kcal/mol) – Five H-bonds



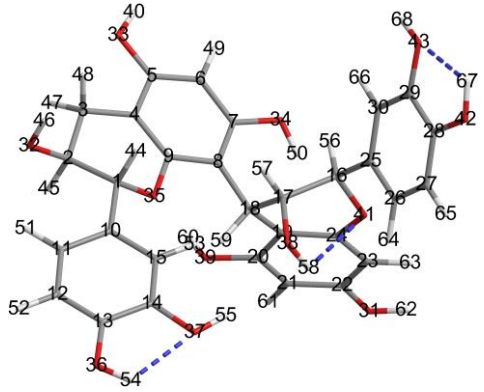
	X	Y	Z		X	Y	Z		X	Y	Z
C(1)	6.223	-0.194	-1.398	C(24)	-1.796	-2.061	1.367	H(47)	0.83	1.022	3.497
C(2)	-4.734	0.82	-0.881	C(25)	6.485	-1.458	-0.895	H(48)	-7.105	-1.532	-1.473
C(3)	-6.122	-1.1	-1.327	C(26)	-3.717	-1.343	-1.212	H(49)	-3.748	-2.942	1.127
C(4)	-2.468	-2.195	-1.33	C(27)	-3.603	0.024	-0.96	H(50)	1.921	6.431	0.677
C(5)	0.337	0.632	-0.335	C(28)	-0.079	0.015	2.15	H(51)	-2.642	0.493	-0.817
C(6)	4.387	-1.429	0.291	C(29)	5.561	-2.081	-0.045	H(52)	-2.466	-4.108	1.491
C(7)	-4.982	-1.9	-1.4	C(30)	-0.407	4.334	0.263	O(53)	-4.611	2.156	-0.627
C(8)	-2.699	-3.193	0.94	O(31)	-2.164	-2.504	3.706	O(54)	7.613	-2.186	-1.155
C(9)	-2.515	-3.503	-0.542	H(32)	-0.34	0.556	-1.187	H(55)	2.509	0.238	1.146
C(10)	2.793	0.48	0.119	H(33)	1.603	-1.053	-0.818	H(56)	2.24	1.352	-2.123
C(11)	-0.717	-0.762	3.114	H(34)	-2.269	-2.431	-2.376	H(57)	-7.884	0.681	-1.122
C(12)	-0.288	-0.191	0.781	H(35)	6.945	0.282	-2.052	H(58)	-2.501	3.024	-0.123
C(13)	1.997	4.024	0.314	O(36)	0.991	6.191	0.601	H(59)	-0.588	-3.613	-0.699
C(14)	-0.559	2.97	0.048	H(37)	-3.332	-4.128	-0.897	H(60)	-5.497	2.541	-0.612
C(15)	4.115	-0.156	-0.22	O(38)	-1.323	-4.232	-0.784	H(61)	-0.558	-0.584	4.17
C(16)	1.669	0.036	-0.82	O(39)	1.957	0.429	-2.15	H(62)	-1.262	4.994	0.331
C(17)	0.536	2.1	-0.039	H(40)	-5.099	-2.954	-1.617	H(63)	4.832	1.444	-1.455
C(18)	-6.002	0.257	-1.065	H(41)	-2.774	-3.148	3.329	O(64)	-1.294	-1.478	-0.914
C(19)	-1.57	-1.782	2.718	O(42)	2.943	1.904	0.004	H(65)	8.196	-1.704	-1.751
C(20)	-1.146	-1.248	0.436	O(43)	5.825	-3.32	0.454	H(66)	6.684	-3.6	0.112
C(21)	5.033	0.456	-1.065	O(44)	0.774	1.006	2.535	O(67)	-1.776	2.388	-0.095
C(22)	0.883	4.85	0.392	H(45)	3.689	-1.925	0.957	H(68)	3.003	4.409	0.418
C(23)	1.803	2.658	0.104	O(46)	-7.047	1.133	-0.968				

Compound 2: Conformer (II) (+0.45 kcal/mol) – Four H-bonds



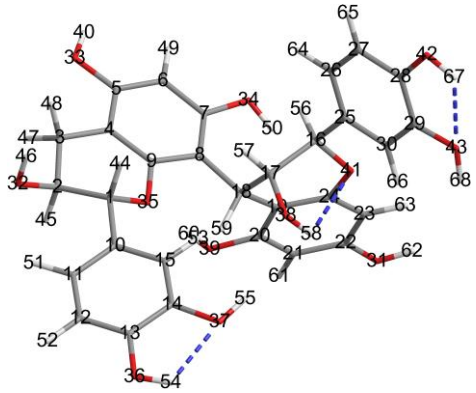
	X	Y	Z		X	Y	Z		X	Y	Z
C(1)	-2.619	-1.904	-1.035	C(24)	2.272	2.429	0.026	H(47)	-4.051	-2.189	1.413
C(2)	-2.82	-3.095	-0.098	C(25)	4.022	-0.779	-0.027	H(48)	-2.947	-3.448	1.993
C(3)	-3.035	-2.587	1.324	C(26)	4.131	-1.976	0.676	H(49)	-0.611	0.04	4.337
C(4)	-2.01	-1.532	1.664	C(27)	5.181	-2.856	0.414	H(50)	0.976	1.383	3.543
C(5)	-1.762	-1.151	2.986	C(28)	6.125	-2.531	-0.546	H(51)	-2.696	0.824	-0.585
C(6)	-0.786	-0.216	3.3	C(29)	6.024	-1.325	-1.253	H(52)	-4.663	2.307	-0.698
C(7)	-0.045	0.377	2.279	C(30)	4.973	-0.459	-0.999	H(53)	-5.204	-2.52	-1.65
C(8)	-0.274	0.07	0.933	O(31)	2.135	6.079	0.229	H(54)	-6.996	2.392	-1.116
C(9)	-1.256	-0.9	0.674	O(32)	-1.699	-3.959	-0.187	H(55)	-8.012	-0.404	-1.82
C(10)	-3.8	-0.959	-1.083	O(33)	-2.45	-1.692	4.028	H(56)	2.514	0.015	1.268
C(11)	-3.66	0.402	-0.83	O(34)	0.932	1.276	2.586	H(57)	1.388	-1.241	-0.602
C(12)	-4.771	1.246	-0.897	O(35)	-1.41	-1.234	-0.651	H(58)	2.365	0.931	-2.1
C(13)	-6.015	0.734	-1.22	O(36)	-7.167	1.464	-1.313	H(59)	-0.245	0.654	-1.089
C(14)	-6.16	-0.634	-1.49	O(37)	-7.381	-1.136	-1.82	H(60)	-1.844	3.631	-0.209
C(15)	-5.059	-1.471	-1.422	O(38)	1.997	0.041	-2.04	H(61)	-0.299	5.304	0.034
C(16)	2.84	0.115	0.23	O(39)	-1.305	2.832	-0.186	H(62)	3.093	6.149	0.298
C(17)	1.651	-0.187	-0.686	H(40)	-3.152	-2.265	3.702	H(63)	3.78	3.944	0.206
C(18)	0.456	0.679	-0.253	O(41)	3.253	1.473	0.003	H(64)	3.398	-2.228	1.433
C(19)	0.922	2.105	-0.085	O(42)	7.201	-3.307	-0.88	H(65)	5.269	-3.787	0.962
C(20)	0.011	3.167	-0.078	O(43)	6.958	-1.009	-2.191	H(66)	4.912	0.469	-1.55
C(21)	0.416	4.492	0.029	H(44)	-2.401	-2.287	-2.033	H(67)	7.221	-4.108	-0.346
C(22)	1.78	4.769	0.128	H(45)	-3.681	-3.679	-0.418	H(68)	7.6	-1.73	-2.224
C(23)	2.719	3.747	0.126	H(46)	-0.908	-3.416	-0.09				

Compound 2: Conformer (III) (+0.70 kcal/mol) – Three H-bonds



	X	Y	Z		X	Y	Z		X	Y	Z
C(1)	3.2	-0.309	-0.969	C(24)	-2.555	1.451	1.654	H(47)	4.005	2.389	-2.963
C(2)	4.173	0.641	-1.684	C(25)	-3.173	-1.467	-0.426	H(48)	3.388	0.869	-3.706
C(3)	3.425	1.451	-2.744	C(26)	-3.443	-2.446	0.535	H(49)	-0.642	3.688	-3.406
C(4)	2.044	1.808	-2.345	C(27)	-4.083	-3.632	0.186	H(50)	-2.129	2.694	-0.468
C(5)	1.269	2.673	-3.144	C(28)	-4.462	-3.847	-1.146	H(51)	5.853	-0.817	-0.294
C(6)	-0.034	3.017	-2.784	C(29)	-4.191	-2.856	-2.116	H(52)	6.657	-2.3	1.542
C(7)	-0.588	2.493	-1.601	C(30)	-3.554	-1.668	-1.758	H(53)	1.743	-1.645	0.823
C(8)	0.142	1.636	-0.76	O(31)	-3.578	4.069	4.032	H(54)	4.42	-3.982	3.695
C(9)	1.456	1.305	-1.18	O(32)	5.251	-0.053	-2.282	H(55)	1.525	-3.07	2.614
C(10)	3.752	-1.153	0.139	O(33)	1.863	3.152	-4.285	H(56)	-2.604	0.571	-0.879
C(11)	5.12	-1.328	0.351	O(34)	-1.892	2.866	-1.393	H(57)	-0.472	-0.851	-0.665
C(12)	5.58	-2.155	1.375	O(35)	2.154	0.468	-0.336	H(58)	-1.224	-0.929	2.055
C(13)	4.665	-2.811	2.207	O(36)	5.168	-3.615	3.2	H(59)	0.57	0.781	1.15
C(14)	3.28	-2.625	2	O(37)	2.434	-3.295	2.861	H(60)	0.98	2.937	1.168
C(15)	2.826	-1.802	0.97	O(38)	-0.728	-1.257	1.292	H(61)	-1.139	4.648	3.381
C(16)	-2.48	-0.194	-0.058	O(39)	0.521	3.49	1.821	H(62)	-4.452	3.66	4.127
C(17)	-0.979	-0.37	0.218	H(40)	1.24	3.755	-4.719	H(63)	-4.396	1.825	2.736
C(18)	-0.345	1.007	0.51	O(41)	-3.132	0.312	1.127	H(64)	-3.139	-2.272	1.579
C(19)	-1.236	1.848	1.361	O(42)	-5.087	-5.031	-1.445	H(65)	-4.298	-4.405	0.938
C(20)	-0.748	3.007	2.005	O(43)	-4.591	-3.146	-3.406	H(66)	-3.357	-0.899	-2.519
C(21)	-1.54	3.748	2.894	H(44)	2.717	-0.981	-1.737	H(67)	-5.294	-5.032	-2.393
C(22)	-2.846	3.312	3.152	H(45)	4.663	1.321	-0.931	H(68)	-4.404	-2.371	-3.955
C(23)	-3.372	2.168	2.536	H(46)	4.882	-0.68	-2.917				

Compound 2: Conformer (IV) (+0.90 kcal/mol) – Three H-bonds



	X	Y	Z		X	Y	Z		X	Y	Z
C(1)	-2.853	3.891	-4.092	C(24)	-0.472	0.504	1.002	H(47)	-4.143	6.726	-2.608
C(2)	-3.254	5.374	-4.058	C(25)	-3.173	-1.467	-0.426	H(48)	-5.247	5.419	-3.171
C(3)	-4.184	5.634	-2.871	C(26)	-4.564	-1.52	-0.556	H(49)	-4.736	4.464	1.635
C(4)	-3.85	4.827	-1.675	C(27)	-5.205	-2.71	-0.892	H(50)	-2.23	2.109	1.748
C(5)	-4.516	5.049	-0.452	C(28)	-4.446	-3.868	-1.102	H(51)	-2.055	5.251	-6.387
C(6)	-4.216	4.295	0.682	C(29)	-3.04	-3.814	-0.972	H(52)	-0.509	4.402	-8.15
C(7)	-3.229	3.294	0.609	C(30)	-2.404	-2.617	-0.64	H(53)	-1.532	1.573	-4.144
C(8)	-2.525	3.037	-0.58	O(31)	2.302	1.059	3.358	H(54)	1.016	1.224	-7.92
C(9)	-2.88	3.82	-1.708	O(32)	-3.882	5.782	-5.258	H(55)	-0.114	0.06	-5.137
C(10)	-1.903	3.46	-5.168	O(33)	-5.468	6.038	-0.444	H(56)	-3.127	0.419	0.635
C(11)	-1.605	4.25	-6.279	O(34)	-3.071	2.594	1.778	H(57)	-3.019	0.891	-1.891
C(12)	-0.742	3.785	-7.27	O(35)	-2.172	3.553	-2.86	H(58)	-0.463	-0.277	-1.642
C(13)	-0.159	2.518	-7.149	O(36)	0.683	2.106	-8.152	H(59)	-0.809	2.338	-1.642
C(14)	-0.452	1.722	-6.019	O(37)	0.164	0.488	-5.96	H(60)	-0.294	4.091	-0.425
C(15)	-1.32	2.19	-5.035	O(38)	-1.227	0.011	-2.159	H(61)	2.022	3.298	2.088
C(16)	-2.48	-0.194	-0.058	O(39)	0.416	4.006	0.232	H(62)	2.225	0.149	3.685
C(17)	-2.107	0.674	-1.27	H(40)	-5.82	6.109	0.457	H(63)	0.487	-0.761	2.478
C(18)	-1.47	1.993	-0.781	O(41)	-1.281	-0.562	0.659	H(64)	-5.155	-0.606	-0.386
C(19)	-0.547	1.76	0.368	O(42)	-5.12	-5.019	-1.427	H(65)	-6.298	-2.757	-0.997
C(20)	0.372	2.751	0.779	O(43)	-2.365	-4.999	-1.189	H(66)	-1.309	-2.583	-0.551
C(21)	1.319	2.51	1.785	H(44)	-3.789	3.262	-4.155	H(67)	-4.467	-5.726	-1.549
C(22)	1.354	1.245	2.384	H(45)	-2.332	6.017	-3.993	H(68)	-1.417	-4.815	-1.13
C(23)	0.462	0.231	2.009	H(46)	-4.668	5.236	-5.381				

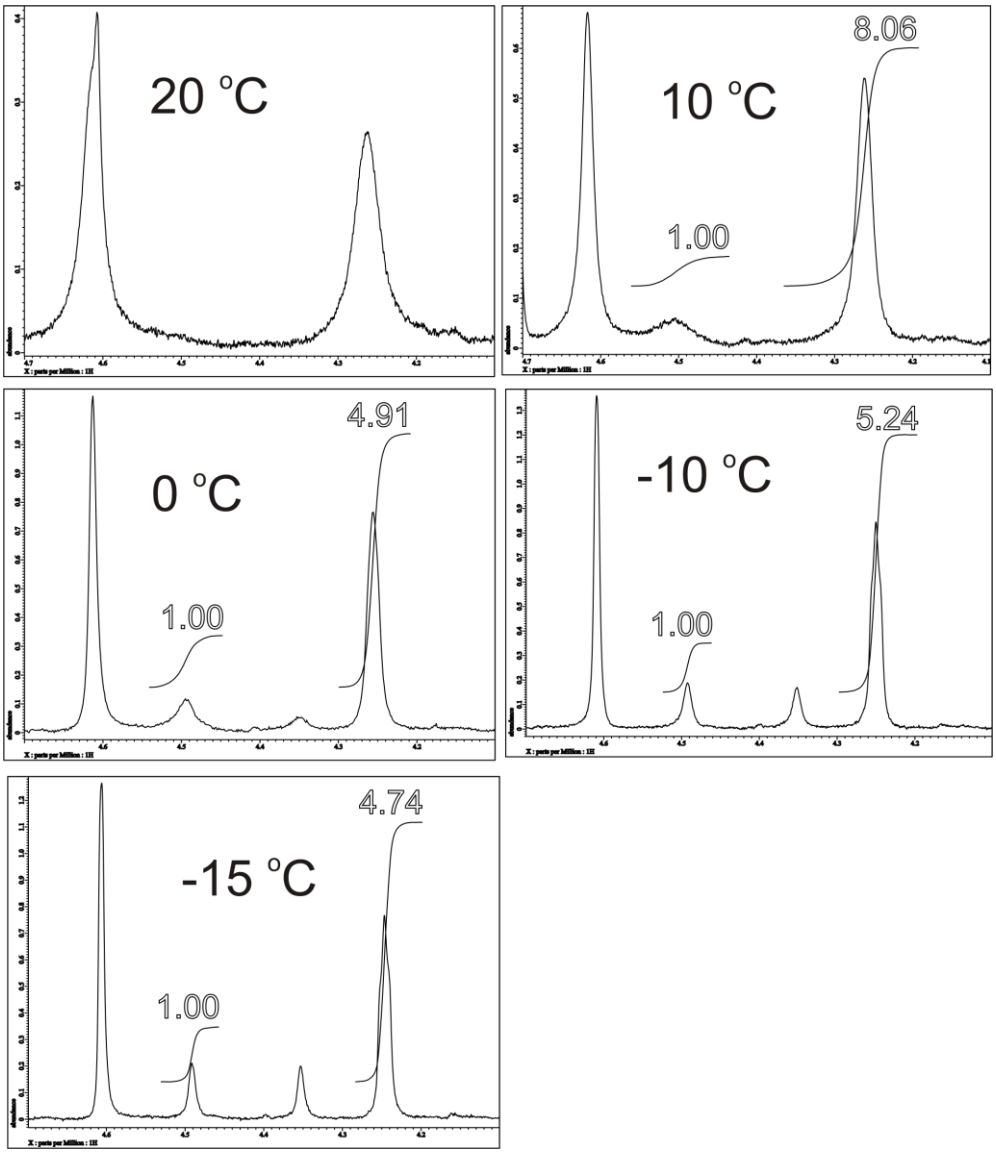


Figure S22. Compound **3**. Unreliable integration at rt. No apparent change in abundance of species. Therefore, conformational changes between the two species are mostly enthalpy-driven.

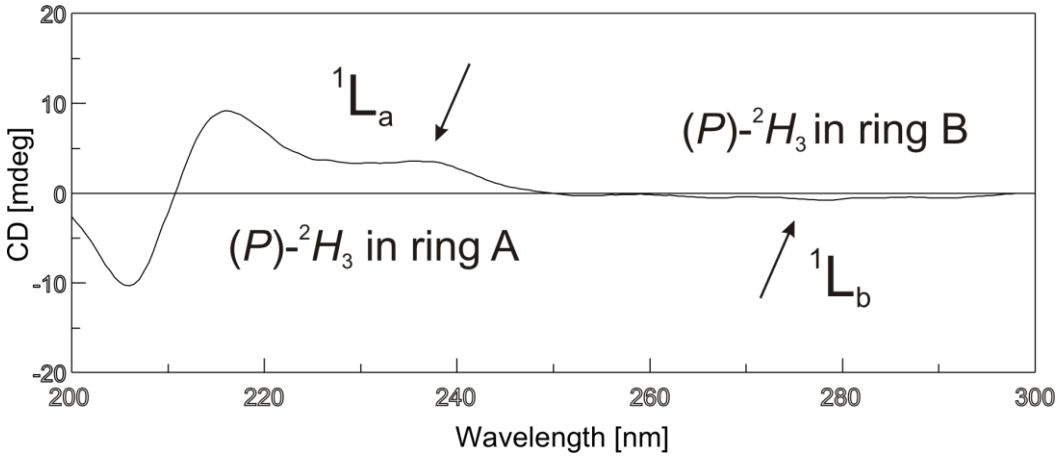


Figure S23. The CD-spectrum of native **3** in methanol at room temperature.

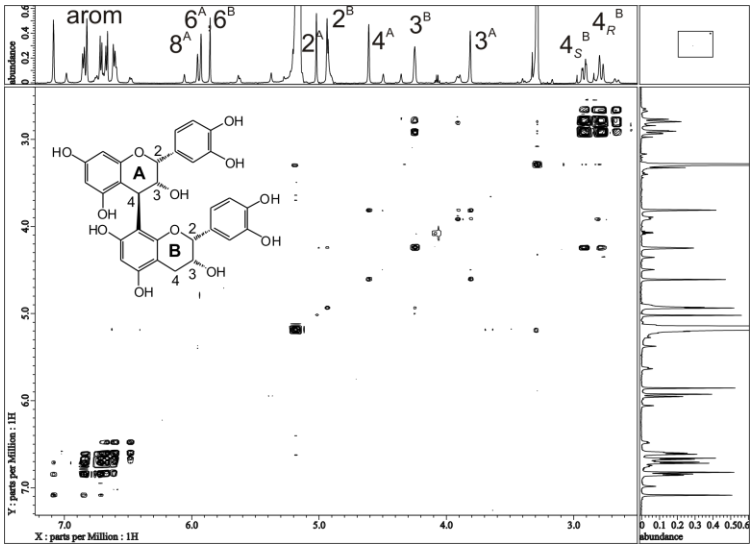


Figure S24. ^{1}H-^{1}H-COSY of **compound 3** at -15 ^{o}C

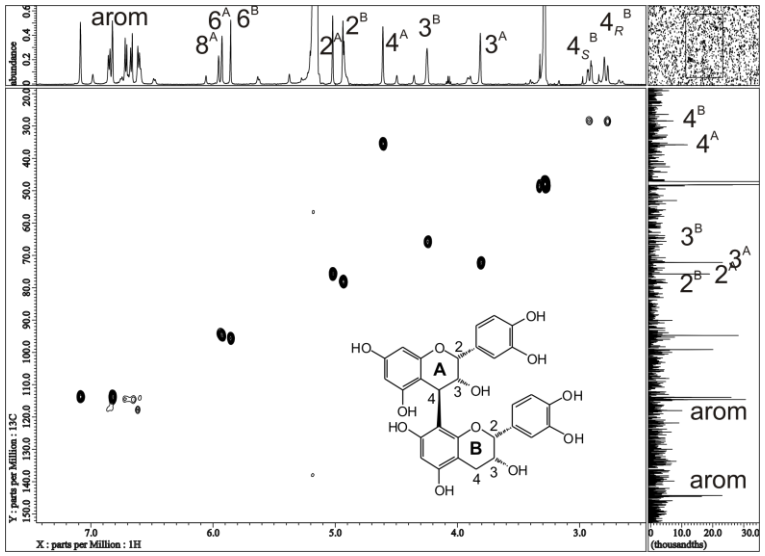


Figure S25. ^{1}H-^{13}C-HMQC of **compound 3** at -15 ^{o}C

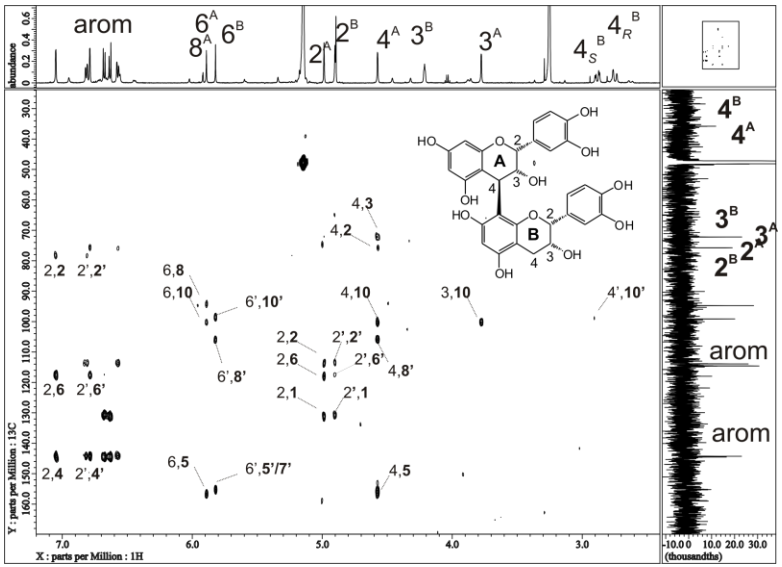


Figure S26. ^{1}H-^{13}C-HMBC of **compound 3** at -15 ^{o}C.

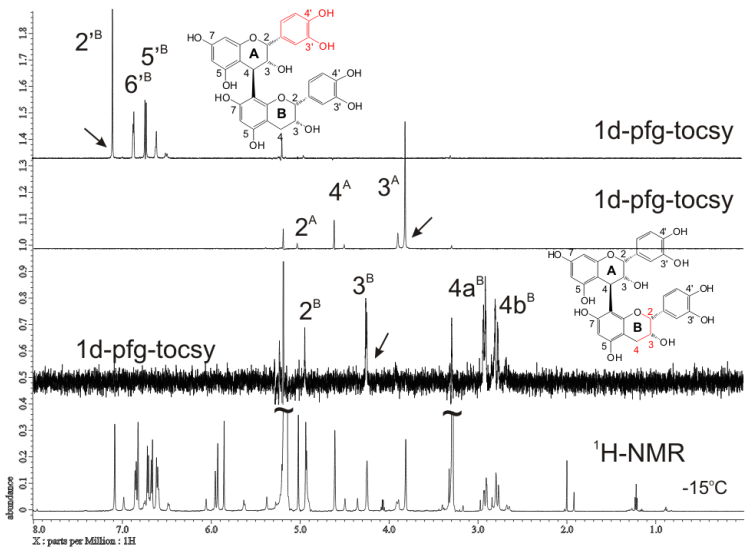


Figure S27. 1d-pfg TOCSY of **compound 3** at -15 ^{o}C.

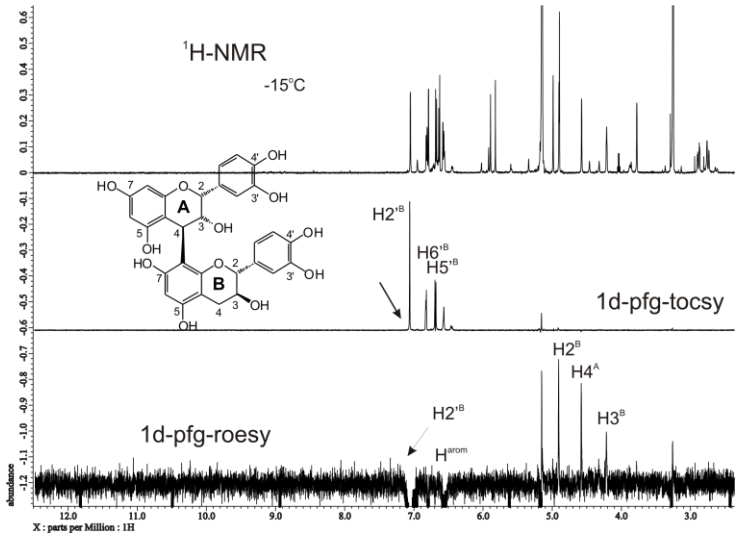


Figure S28. 1d-pfg-TOCSY + ROESY of **compound 3** at -15 ^{o}C

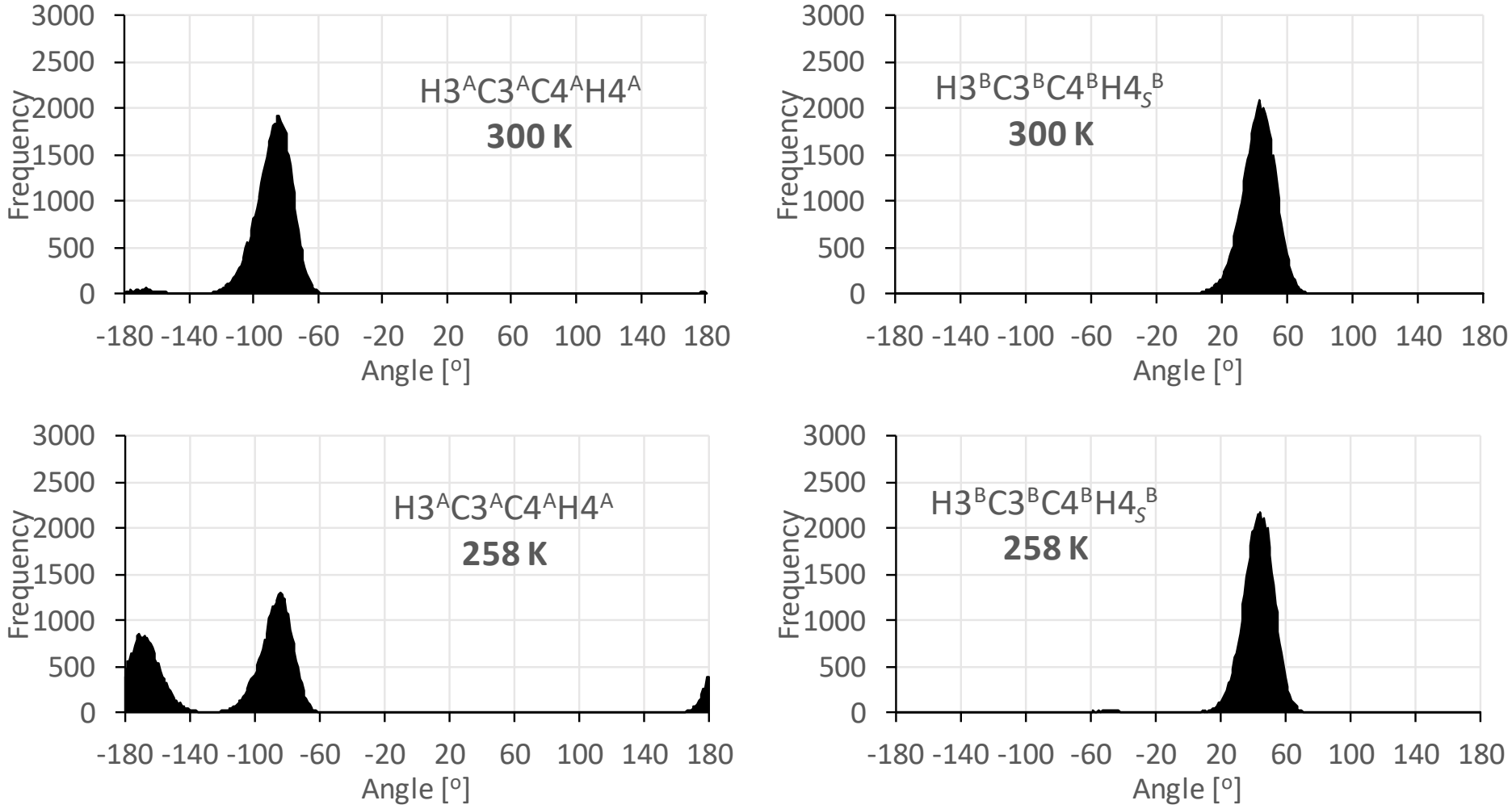


Figure S29. Histograms from MD-simulation of **3**. Top: Diagnostic half-chair dihedral angle in ring A + B at 300 K; bottom: ring A + B at 258 K.

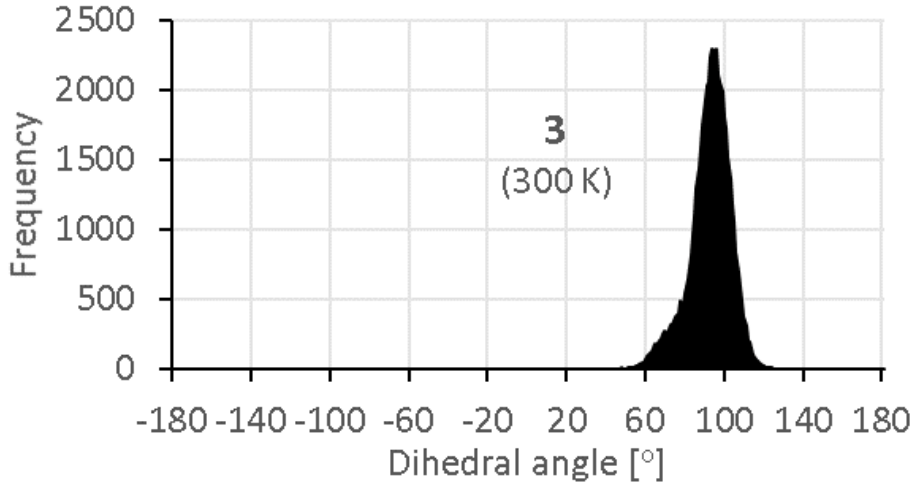


Figure S30. Control experiment: MD-simulation of the (*P*)-**3** atrop isomer at 300 K. No interconversion to the (*M*)-**3** *atrop* isomer was observed because the rotational barrier was too high. The lowest-energy (*P*)-structure was +3.40 kcal/mol less stable than the most stable (*M*)-structure.

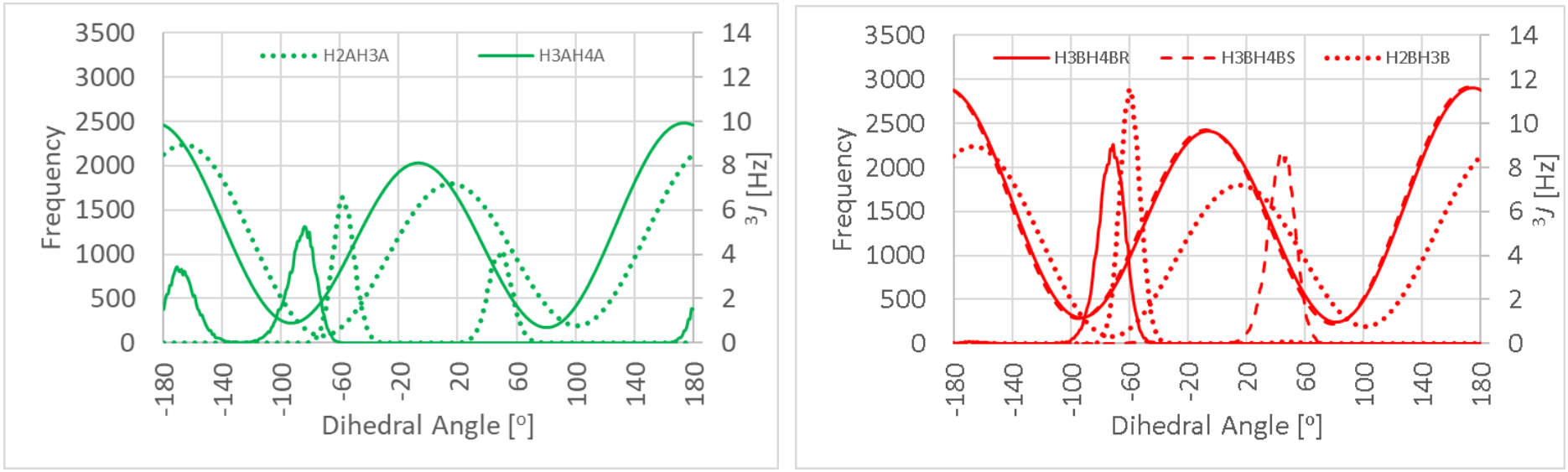


Figure S31. Histogram from MD-simulation of **3** at 258 K (-15 °C) with corresponding Haasnoot-deLeuw-Altona (HLA) equations[3] overlaid.

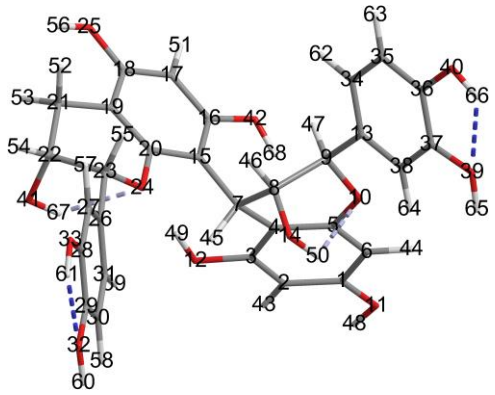
Equation for $H2^{A}$-$C2^{A}$-$C3^{A}$-$H3^{A}$ (4-substituent system) and for $H2^{B}$-$C2^{B}$-$C3^{B}$-$H3^{B}$ (4-substituent system): $13.24*\cos^2(\varphi) - 0.91*\cos(\varphi) + \{[1.3*(0.53- 2.41*(\cos^2(\varphi + 15.5*1.3)) + 0.4*(0.53 - 2.41*(\cos^2(-\varphi + 15.5*0.4)) + 1.3*(0.53- 2.41*(\cos^2(\varphi + 15.5*1.3)) + 0.4*(0.53 - 2.41*(\cos^2(-\varphi + 15.5*0.4))]\}$.

Equation for $H3^{A}$-$C3^{A}$-$C4^{A}$-$H4^{A}$ (4-substituent system): $13.24*\cos^2(\varphi) - 0.91*\cos(\varphi) + \{[0.4*(0.53- 2.41*(\cos^2(\varphi + 15.5*0.4)) + 1.3*(0.53 - 2.41*(\cos^2(-\varphi + 15.5*1.3)) + 0.4*(0.53- 2.41*(\cos^2(\varphi + 15.5*0.4)) + 0.4*(0.53 - 2.41*(\cos^2(-\varphi + 15.5*0.4))]\}$.

Equation for $H3^{B}$-$C3^{B}$-$C4^{B}$-$H4^{B}$*R* (3-substituent system): $13.22*\cos^2(\varphi) - 0.99*\cos(\varphi) + \{[1.3*(0.87 - 2.46*(\cos^2(\varphi + 19.9*1.3)) + 0.4*(0.87 - 2.46*(\cos^2(-\varphi + 19.9*0.4)) + 0.4*(0.87 - 2.46*(\cos^2(\varphi + 19.9*0.4))]\}$.

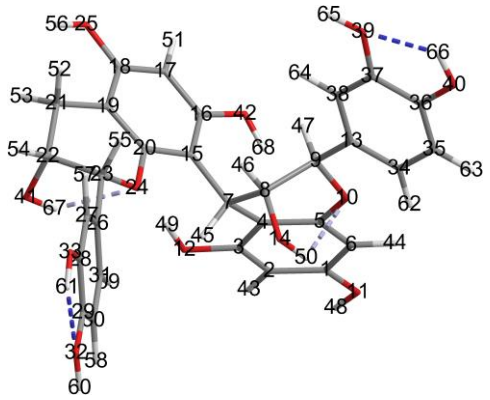
Equation for $H3^{B}$-$C3^{B}$-$C4^{B}$-$H4^{B}$*S* (3-substituent system): $13.22*\cos^2(\varphi) - 0.99*\cos(\varphi) + \{[1.3*(0.87 - 2.46*(\cos^2(\varphi + 19.9*1.3)) + 0.4*(0.87 - 2.46*(\cos^2(-\varphi + 19.9*0.4)) + 0.4*(0.87 - 2.46*(\cos^2(-\varphi + 19.9*0.4))]\}$.

Compound 3: Conformer (I) (0.00 kcal/mol) – Four H-bonds



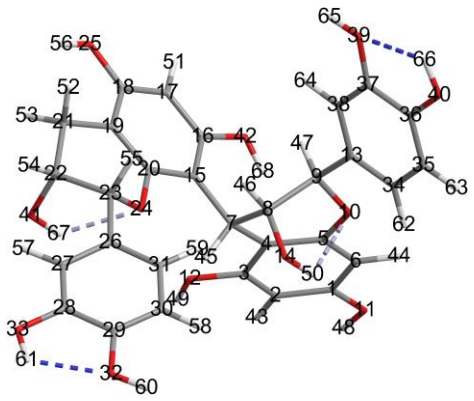
	X	Y	Z		X	Y	Z		X	Y	Z
C(1)	-3.95	-2.783	-2.696	O(24)	1.888	-0.753	0.258	H(47)	-2.553	-0.155	1.146
C(2)	-2.752	-3.486	-2.561	O(25)	1.419	-3.441	4.214	H(48)	-4.752	-4.129	-3.793
C(3)	-1.728	-2.926	-1.809	C(26)	3.752	0.61	-0.318	H(49)	-0.019	-3.262	-1.006
C(4)	-1.864	-1.676	-1.18	C(27)	4.536	1.716	0.022	H(50)	-1.605	1.059	-1.954
C(5)	-3.096	-1.02	-1.324	C(28)	5.216	2.418	-0.96	H(51)	-1.014	-3.679	3.439
C(6)	-4.138	-1.553	-2.072	C(29)	5.111	2.019	-2.299	H(52)	3.365	-1.245	3.419
C(7)	-0.682	-1.025	-0.49	C(30)	4.332	0.925	-2.64	H(53)	3.713	-2.855	2.772
C(8)	-1.002	0.457	-0.212	C(31)	3.656	0.215	-1.648	H(54)	4.917	-0.887	1.658
C(9)	-2.432	0.56	0.325	O(32)	5.815	2.786	-3.184	H(55)	2.809	0.513	1.605
O(10)	-3.325	0.198	-0.744	O(33)	5.976	3.497	-0.629	H(56)	2.342	-3.201	4.352
O(11)	-4.989	-3.274	-3.417	C(34)	-2.591	2.283	2.126	H(57)	4.621	2.048	1.051
O(12)	-0.572	-3.629	-1.709	C(35)	-2.857	3.576	2.575	H(58)	4.254	0.626	-3.679
C(13)	-2.795	1.941	0.793	C(36)	-3.335	4.529	1.69	H(59)	3.046	-0.636	-1.918
O(14)	-0.856	1.246	-1.375	C(37)	-3.547	4.183	0.348	H(60)	5.682	2.473	-4.085
C(15)	-0.181	-1.736	0.761	C(38)	-3.273	2.903	-0.102	H(61)	6.351	3.856	-1.443
C(16)	-0.951	-2.522	1.634	O(39)	-4.029	5.194	-0.436	H(62)	-2.226	1.539	2.825
C(17)	-0.396	-3.081	2.784	O(40)	-3.607	5.791	2.118	H(63)	-2.706	3.854	3.61
C(18)	0.939	-2.865	3.083	O(41)	4.215	-2.253	0.347	H(64)	-3.448	2.647	-1.139
C(19)	1.763	-2.095	2.249	O(42)	-2.275	-2.767	1.45	H(65)	-4.157	4.89	-1.34
C(20)	1.166	-1.536	1.122	H(43)	-2.606	-4.453	-3.023	H(66)	-3.93	6.298	1.361
C(21)	3.231	-1.898	2.551	H(44)	-5.075	-1.023	-2.16	H(67)	3.374	-2.474	-0.072
C(22)	3.953	-1.29	1.35	H(45)	0.145	-1.003	-1.203	H(68)	-2.536	-2.503	0.555
C(23)	3.085	-0.161	0.788	H(46)	-0.302	0.844	0.527				

Compound 3: Conformer (II) (+0.23 kcal/mol) – Four H-bonds



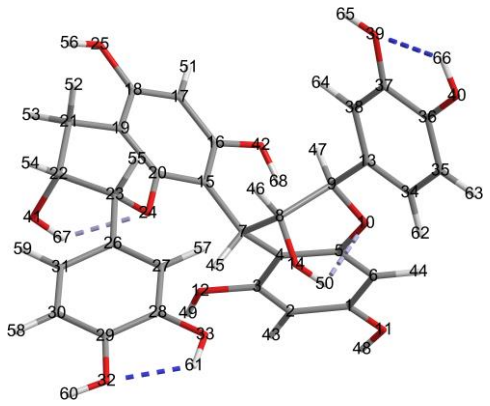
	X	Y	Z		X	Y	Z		X	Y	Z
C(1)	0.513	-1.604	-2.717	O(24)	-2.774	-2.954	3.14	H(47)	-3.279	0.113	-0.207
C(2)	0.247	-2.843	-2.133	O(25)	-6.821	-4.549	1.098	H(48)	1.595	-2.357	-4.102
C(3)	-0.551	-2.891	-0.998	C(26)	-2.273	-2.932	5.467	H(49)	-1.502	-4.057	0.191
C(4)	-1.099	-1.731	-0.423	C(27)	-2.612	-2.433	6.728	H(50)	-0.2	0.303	1.366
C(5)	-0.824	-0.512	-1.061	C(28)	-1.65	-2.326	7.718	H(51)	-5.872	-3.446	-1.014
C(6)	-0.027	-0.431	-2.196	C(29)	-0.33	-2.714	7.451	H(52)	-6.063	-3.908	3.971
C(7)	-1.843	-1.799	0.896	C(30)	0.011	-3.205	6.201	H(53)	-5.533	-5.484	3.367
C(8)	-2.014	-0.376	1.462	C(31)	-0.963	-3.321	5.208	H(54)	-4.411	-4.642	5.511
C(9)	-2.432	0.56	0.325	O(32)	0.538	-2.557	8.495	H(55)	-4.118	-2.311	4.571
O(10)	-1.317	0.669	-0.579	O(33)	-1.98	-1.836	8.944	H(56)	-7.017	-4.858	1.989
O(11)	1.285	-1.488	-3.825	C(34)	-1.905	2.988	0.576	H(57)	-3.624	-2.116	6.951
O(12)	-0.779	-4.111	-0.448	C(35)	-2.241	4.291	0.94	H(58)	1.035	-3.5	6.003
C(13)	-2.795	1.941	0.793	C(36)	-3.468	4.548	1.531	H(59)	-0.692	-3.702	4.234
O(14)	-0.826	0.087	2.069	C(37)	-4.362	3.492	1.757	H(60)	1.428	-2.82	8.239
C(15)	-3.166	-2.555	0.863	C(38)	-4.034	2.199	1.385	H(61)	-1.179	-1.824	9.484
C(16)	-4.018	-2.69	-0.245	O(39)	-5.538	3.853	2.352	H(62)	-0.94	2.792	0.123
C(17)	-5.236	-3.36	-0.144	O(40)	-3.804	5.813	1.9	H(63)	-1.557	5.114	0.78
C(18)	-5.626	-3.906	1.067	O(41)	-3.125	-5.487	4.204	H(64)	-4.731	1.392	1.571
C(19)	-4.819	-3.809	2.21	O(42)	-3.744	-2.164	-1.469	H(65)	-6.102	3.084	2.483
C(20)	-3.62	-3.115	2.073	H(43)	0.643	-3.762	-2.545	H(66)	-4.687	5.784	2.291
C(21)	-5.223	-4.446	3.519	H(44)	0.162	0.524	-2.664	H(67)	-2.655	-5.233	3.4
C(22)	-4.051	-4.459	4.499	H(45)	-1.196	-2.31	1.613	H(68)	-2.818	-1.88	-1.503
C(23)	-3.363	-3.093	4.443	H(46)	-2.784	-0.386	2.233				

Compound 3: Conformer (III) (+0.78 kcal/mol) – Four H-bonds



	X	Y	Z		X	Y	Z		X	Y	Z
C(1)	-3.909	-3.066	-2.583	O(24)	1.821	-0.731	0.413	H(47)	-2.581	0.091	0.897
C(2)	-2.721	-3.757	-2.334	O(25)	0.925	-2.551	4.772	H(48)	-4.711	-4.539	-3.504
C(3)	-1.704	-3.115	-1.639	C(26)	3.645	0.621	-0.245	H(49)	-0.51	-4.606	-1.75
C(4)	-1.841	-1.8	-1.163	C(27)	5.016	0.451	-0.453	H(50)	-1.454	0.778	-2.316
C(5)	-3.051	-1.148	-1.44	C(28)	5.636	1.049	-1.54	H(51)	-1.42	-2.969	3.816
C(6)	-4.086	-1.761	-2.14	C(29)	4.886	1.817	-2.439	H(52)	2.937	-0.535	3.764
C(7)	-0.682	-1.095	-0.49	C(30)	3.522	1.978	-2.245	H(53)	3.372	-2.221	3.455
C(8)	-0.958	0.42	-0.472	C(31)	2.904	1.382	-1.148	H(54)	4.658	-0.44	2.16
C(9)	-2.403	0.653	-0.026	O(32)	5.598	2.356	-3.473	H(55)	2.525	0.816	1.578
O(10)	-3.272	0.144	-1.052	O(33)	6.972	0.881	-1.737	H(56)	1.838	-2.295	4.941
O(11)	-4.939	-3.636	-3.256	C(34)	-3.198	2.911	-0.848	H(57)	5.618	-0.163	0.202
O(12)	-0.519	-3.717	-1.378	C(35)	-3.433	4.269	-0.629	H(58)	2.946	2.568	-2.948
C(13)	-2.728	2.106	0.184	C(36)	-3.188	4.826	0.616	H(59)	1.837	1.502	-1.011
O(14)	-0.724	1.018	-1.731	C(37)	-2.71	4.016	1.655	H(60)	5.02	2.855	-4.059
C(15)	-0.314	-1.573	0.908	C(38)	-2.485	2.667	1.442	H(61)	7.214	1.353	-2.545
C(16)	-1.169	-2.182	1.835	O(39)	-2.509	4.662	2.842	H(62)	-3.396	2.481	-1.82
C(17)	-0.735	-2.503	3.121	O(40)	-3.415	6.15	0.835	H(63)	-3.806	4.907	-1.42
C(18)	0.566	-2.218	3.502	O(41)	4.145	-2.061	1.053	H(64)	-2.12	2.048	2.256
C(19)	1.473	-1.623	2.616	O(42)	-2.475	-2.468	1.571	H(65)	-2.203	4.048	3.518
C(20)	0.995	-1.313	1.346	H(43)	-2.59	-4.775	-2.683	H(66)	-3.195	6.34	1.756
C(21)	2.901	-1.335	3.018	H(44)	-5.008	-1.23	-2.327	H(67)	3.422	-2.259	0.443
C(22)	3.749	-0.931	1.811	H(45)	0.197	-1.237	-1.119	H(68)	-2.632	-2.395	0.619
C(23)	2.933	0.02	0.945	H(46)	-0.281	0.899	0.235				

Compound 3: Conformer (IV) (+ 0.98 kcal/mol) – Four H-bonds



	X	Y	Z		X	Y	Z		X	Y	Z
C(1)	-2.083	6.227	3.203	O(24)	1.88	0.943	1.294	H(47)	1.487	3.438	5.023
C(2)	-2.41	5.164	2.358	O(25)	0.107	-2.222	4.448	H(48)	-3.765	7.103	2.942
C(3)	-1.478	4.15	2.165	C(26)	3.645	0.621	-0.245	H(49)	-2.589	3.186	0.941
C(4)	-0.229	4.153	2.808	C(27)	4.279	1.864	-0.181	H(50)	2.294	5.347	2.236
C(5)	0.051	5.242	3.644	C(28)	4.891	2.393	-1.307	H(51)	-0.986	-0.151	5.498
C(6)	-0.856	6.276	3.853	C(29)	4.885	1.678	-2.51	H(52)	2.543	-2.251	2.662
C(7)	0.799	3.082	2.507	C(30)	4.269	0.437	-2.576	H(53)	1.028	-2.642	1.839
C(8)	2.179	3.561	2.993	C(31)	3.649	-0.089	-1.445	H(54)	3.025	-2.058	0.365
C(9)	2.029	4.154	4.396	O(32)	5.52	2.293	-3.552	H(55)	3.617	-0.043	1.798
O(10)	1.251	5.358	4.29	O(33)	5.507	3.606	-1.238	H(56)	0.61	-2.854	3.924
O(11)	-2.947	7.247	3.432	C(34)	3.939	5.75	4.859	H(57)	4.333	2.428	0.74
O(12)	-1.719	3.098	1.345	C(35)	5.189	6.018	5.416	H(58)	4.273	-0.115	-3.509
C(13)	3.347	4.504	5.032	C(36)	5.855	5.038	6.137	H(59)	3.181	-1.064	-1.502
O(14)	2.755	4.507	2.114	C(37)	5.26	3.78	6.308	H(60)	5.492	1.74	-4.34
C(15)	0.511	1.69	3.05	C(38)	4.015	3.516	5.763	H(61)	5.886	3.795	-2.107
C(16)	-0.261	1.374	4.174	O(39)	5.996	2.891	7.04	H(62)	3.422	6.52	4.303
C(17)	-0.386	0.06	4.625	O(40)	7.074	5.293	6.683	H(63)	5.66	6.985	5.298
C(18)	0.263	-0.964	3.955	O(41)	1.272	-1.248	-0.257	H(64)	3.562	2.54	5.907
C(19)	1.039	-0.715	2.815	O(42)	-0.907	2.312	4.924	H(65)	5.523	2.057	7.138
C(20)	1.142	0.613	2.406	H(43)	-3.369	5.132	1.854	H(66)	7.364	4.497	7.148
C(21)	1.727	-1.831	2.064	H(44)	-0.609	7.096	4.511	H(67)	0.853	-0.384	-0.148
C(22)	2.287	-1.343	0.728	H(45)	0.872	2.995	1.422	H(68)	-0.928	3.15	4.439
C(23)	2.933	0.02	0.945	H(46)	2.861	2.712	3.032				

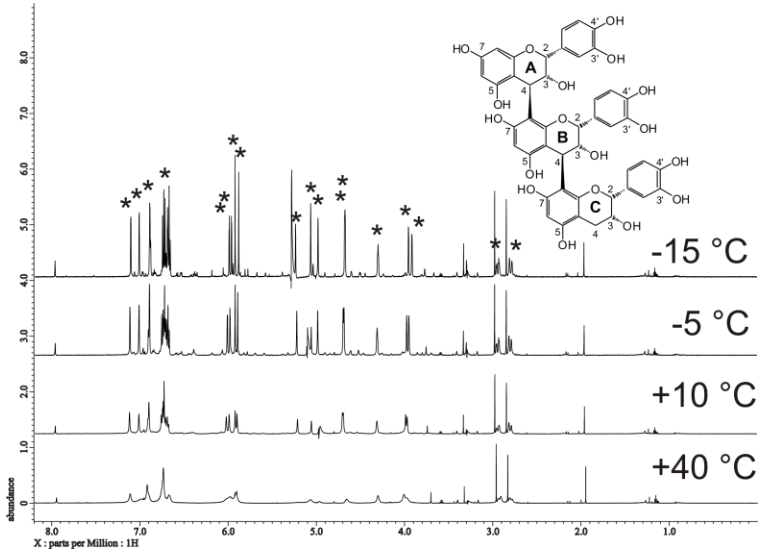


Figure S32. VT-^{1}H-NMR of **compound 4** at -15 ^{o}C.

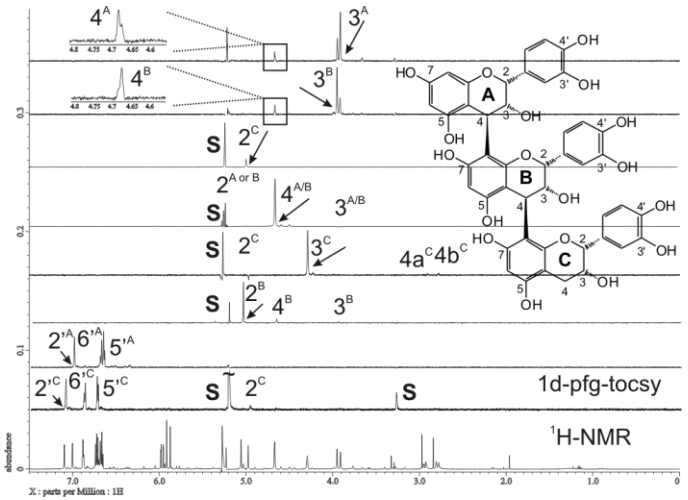


Figure S33. ^{1}H-NMR + 1d-pfg-tocsy of **compound 4** at -15 ^{o}C.

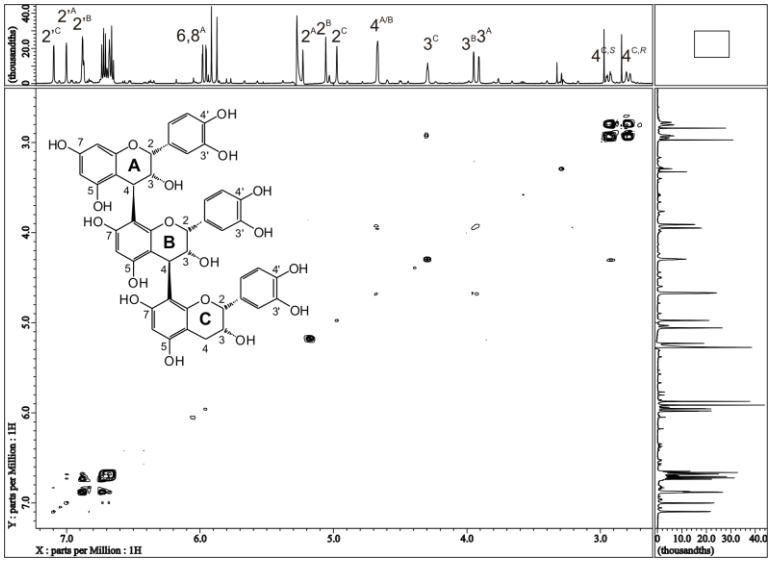


Figure S34. ^{1}H-^{1}H-COSY of **compound 4** at -15 ^{o}C.

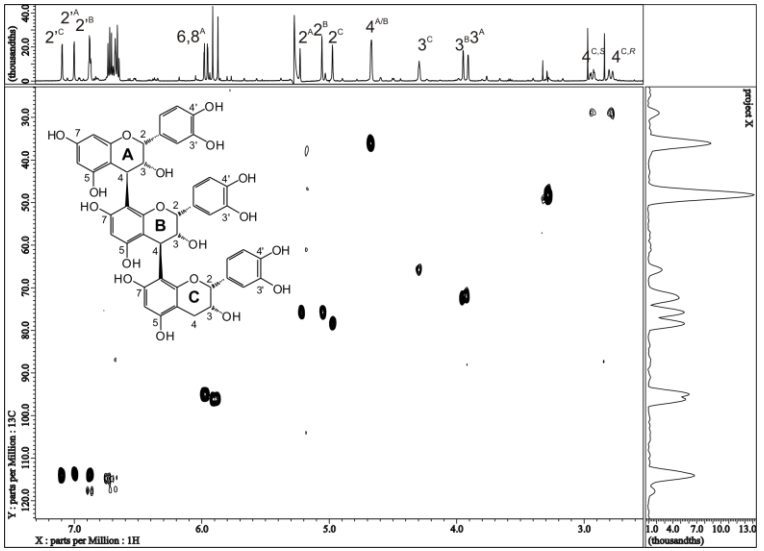


Figure S35. ^{1}H-^{13}C-HMQC of **compound 4** at -15 ^{o}C.

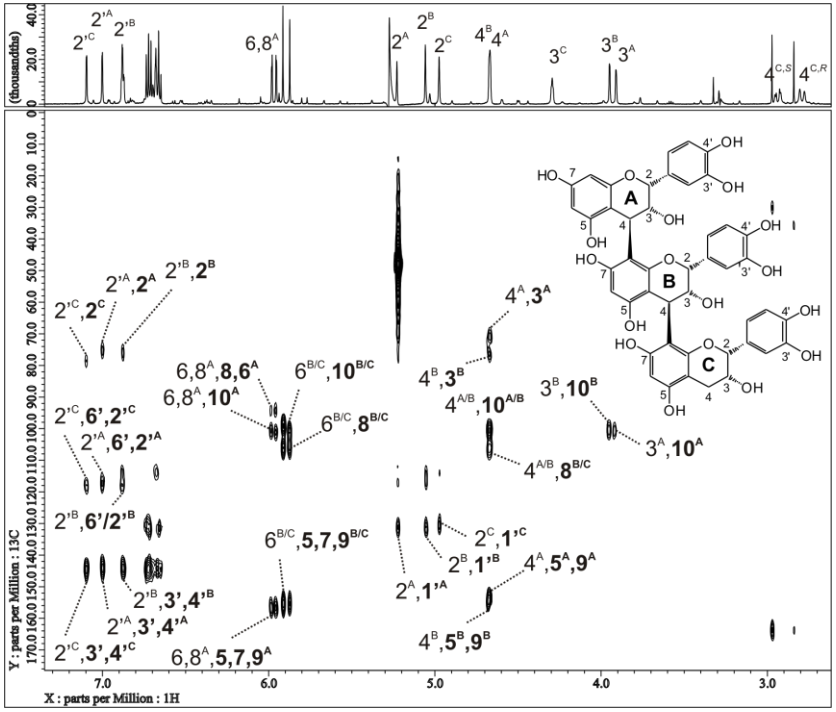


Figure S36. ^{1}H-^{13}C-HMBC of **compound 4** at -15 ^{o}C.

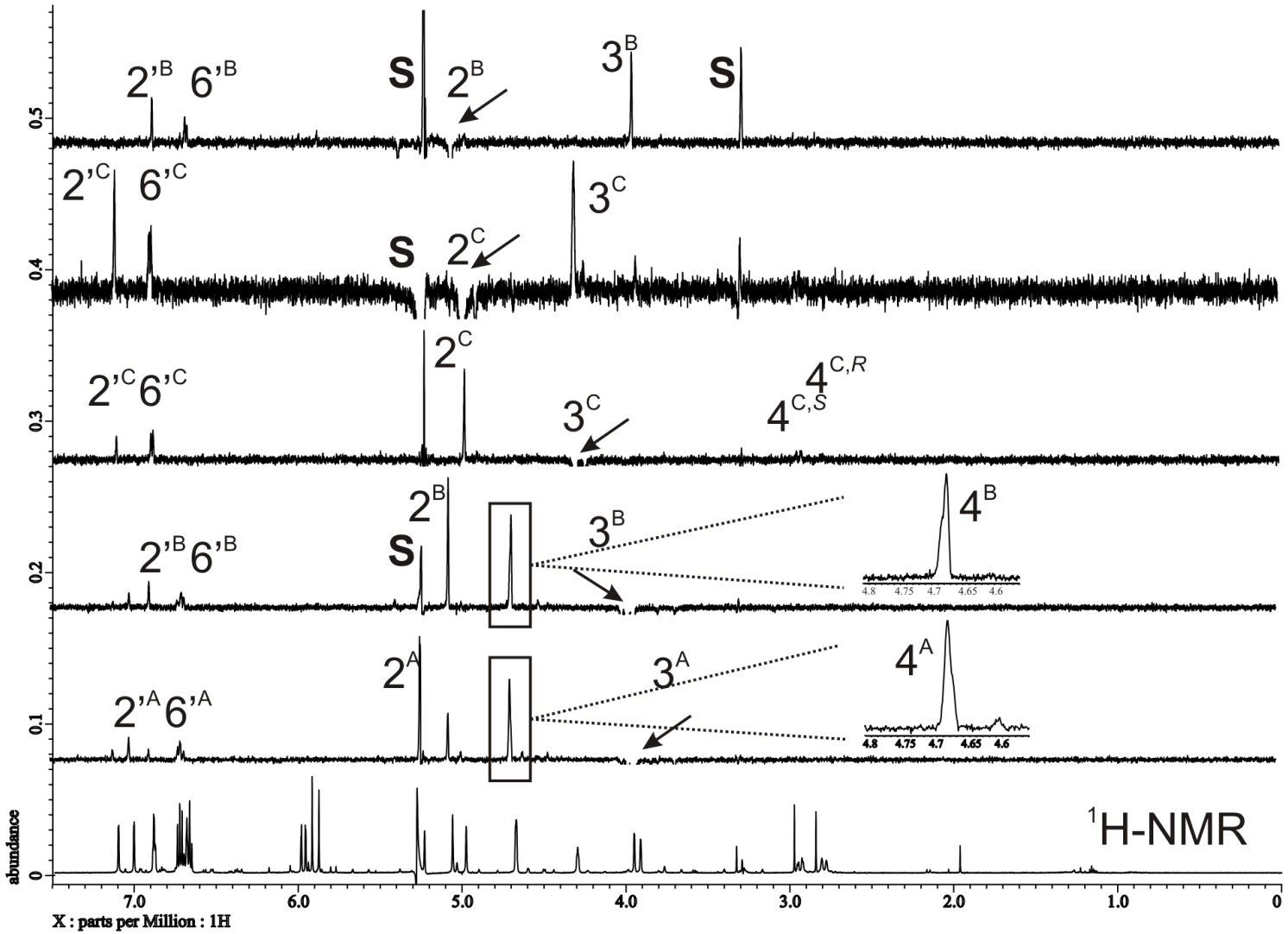


Figure S37. 1d-pfg-ROESY of **compound 4** at -15 ^{o}C (methanol-d_4)

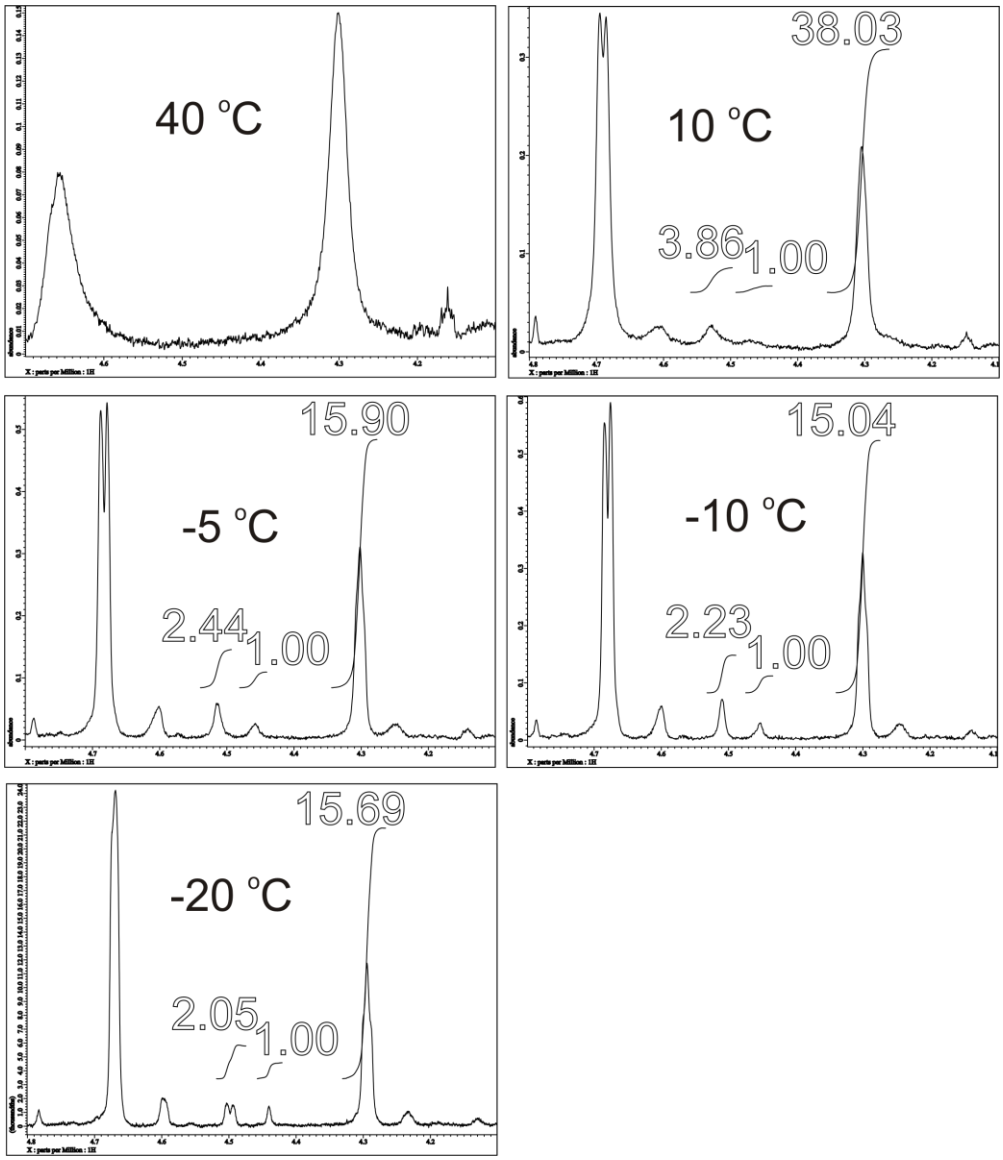


Figure S38. Compound **4**. Unreliable integration at rt. No apparent change in abundance of species. Therefore, conformational changes between the two species are mostly enthalpy-driven.

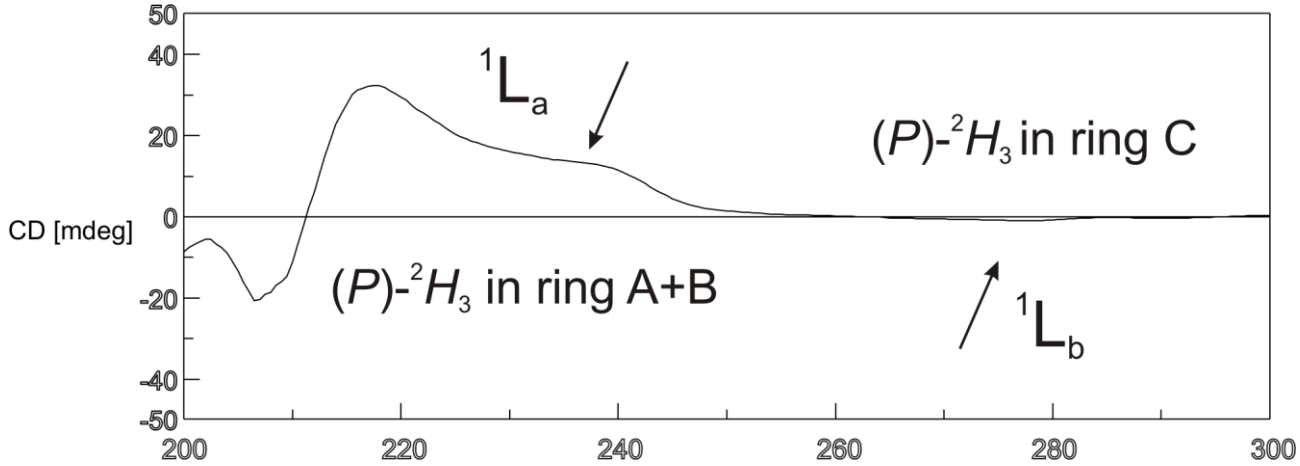


Figure S39. CD-Spectrum of native **4** in methanol at room temperature.

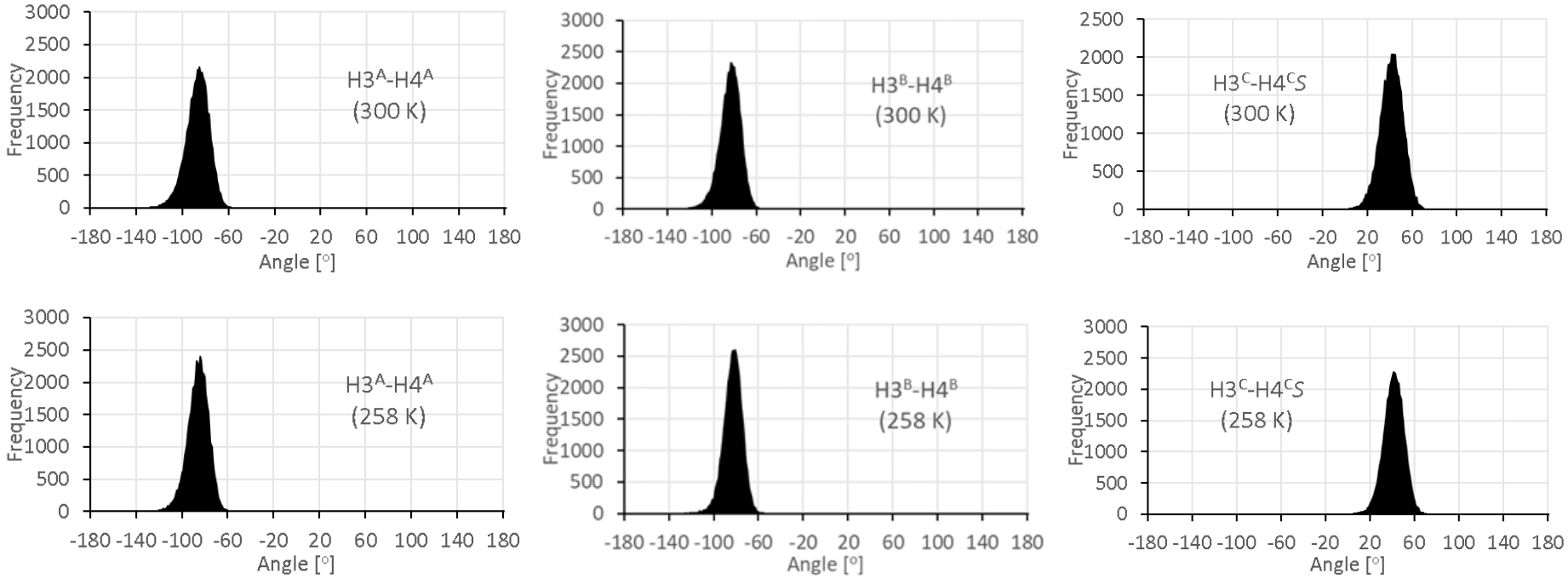


Figure S40. Histograms from MD-simulation of **4**. Top: Diagnostic half-chair dihedral angle in ring A + B + C at 300 K; bottom: ring A + B + C at 258 K.

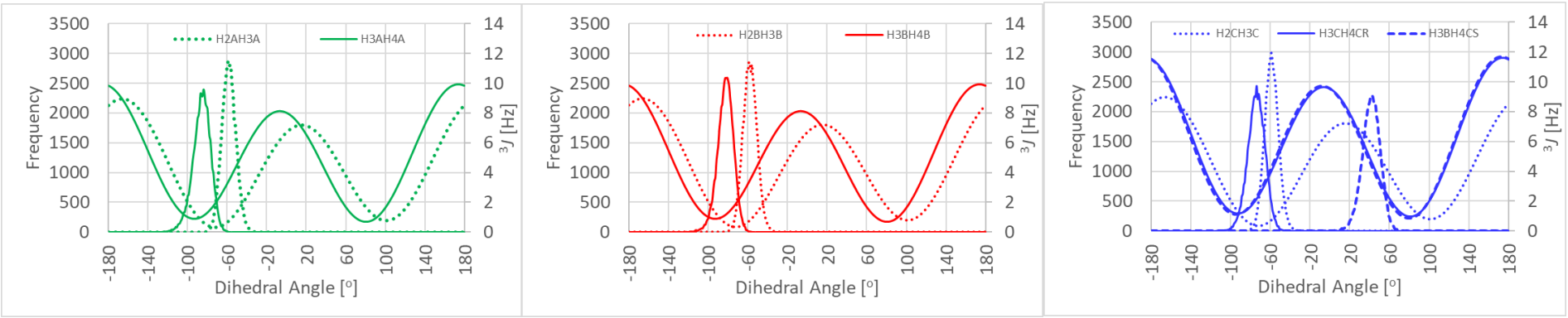


Figure S41. Histogram from MD-simulation of **4** at 258 K (-15 °C) with corresponding Haasnoot-deLeuw-Altona (HLA) equations[3] overlaid.

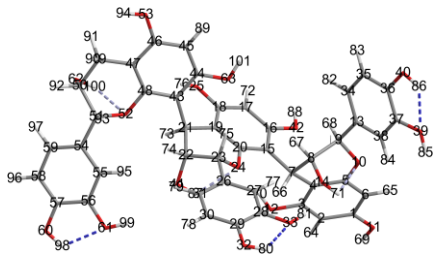
Equation for $H2^A$-$C2^A$-$C3^A$-$H3^A$ (4-substituent system), for $H2^B$-$C2^B$-$C3^B$-$H3^B$ (4-substituent system), and for $H2^C$-$C2^C$-$C3^C$-$H3^C$ (4-substituent system): $13.24*\cos^2(\varphi) - 0.91*\cos(\varphi) + \{[1.3*(0.53- 2.41*(\cos^2(\varphi + 15.5*1.3)) + 0.4*(0.53 - 2.41*(\cos^2(-\varphi + 15.5*0.4)) + 1.3*(0.53- 2.41*(\cos^2(\varphi + 15.5*1.3)) + 0.4*(0.53 - 2.41*(\cos^2(-\varphi + 15.5*0.4))]\}$.

Equation for $H3^A$-$C3^A$-$C4^A$-$H4^A$ (4-substituent system) and for $H3^B$-$C3^B$-$C4^B$-$H4^B$ (4-substituent system): $13.24*\cos^2(\varphi) - 0.91*\cos(\varphi) + \{[0.4*(0.53- 2.41*(\cos^2(\varphi + 15.5*0.4)) + 1.3*(0.53 - 2.41*(\cos^2(-\varphi + 15.5*1.3)) + 0.4*(0.53- 2.41*(\cos^2(\varphi + 15.5*0.4)) + 0.4*(0.53 - 2.41*(\cos^2(-\varphi + 15.5*0.4))]\}$.

Equation for $H3^C$-$C3^C$-$C4^C$-$H4^C$*R* (3-substituent system): $13.22*\cos^2(\varphi) - 0.99*\cos(\varphi) + \{[1.3*(0.87 - 2.46*(\cos^2(\varphi + 19.9*1.3)) + 0.4*(0.87 - 2.46*(\cos^2(-\varphi + 19.9*0.4)) + 0.4*(0.87 - 2.46*(\cos^2(\varphi + 19.9*0.4))]\}$.

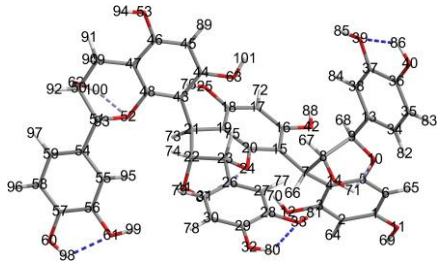
Equation for $H3^C$-$C3^C$-$C4^C$-$H4^C$*S* (3-substituent system): $13.22*\cos^2(\varphi) - 0.99*\cos(\varphi) + \{[1.3*(0.87 - 2.46*(\cos^2(\varphi + 19.9*1.3)) + 0.4*(0.87 - 2.46*(\cos^2(-\varphi + 19.9*0.4)) + 0.4*(0.87 - 2.46*(\cos^2(-\varphi + 19.9*0.4))]\}$.

Compound 4: Conformer (I) (0.00 kcal/mol) – Six H-bonds



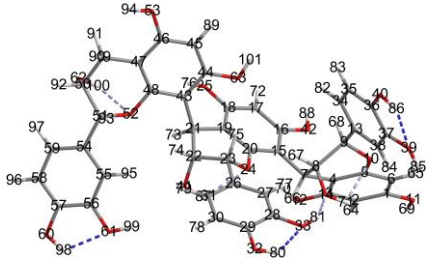
	X	Y	Z		X	Y	Z		X	Y	Z
C(1)	-5.59	4.253	-1.975	C(35)	-5.361	-3.917	-0.401	H(69)	-6.121	5.97	-2.633
C(2)	-4.239	4.591	-1.932	C(36)	-6.421	-3.892	0.492	H(70)	-1.458	3.222	-1.393
C(3)	-3.324	3.641	-1.49	C(37)	-6.908	-2.661	0.954	H(71)	-4.703	1.095	1.311
C(4)	-3.719	2.364	-1.078	C(38)	-6.334	-1.473	0.533	H(72)	-0.65	0.203	-4.616
C(5)	-5.077	2.059	-1.175	O(39)	-7.958	-2.75	1.825	H(73)	2.799	0.444	-1.212
C(6)	-6.022	2.984	-1.607	O(40)	-6.993	-5.052	0.915	H(74)	2.734	-0.416	1.224
C(7)	-2.719	1.396	-0.488	O(41)	2.234	1.529	0.919	H(75)	0.343	-1.224	0.922
C(8)	-3.452	0.19	0.131	O(42)	-2.844	1.091	-3.429	H(76)	2.283	-0.899	-3.108
C(9)	-4.587	-0.231	-0.804	C(43)	2.537	-1.642	-0.995	H(77)	-1.813	0.061	2.371
O(10)	-5.559	0.826	-0.809	C(44)	1.75	-2.792	-1.145	H(78)	1.781	0.302	5.754
O(11)	-6.538	5.135	-2.394	C(45)	2.332	-4.052	-1.281	H(79)	2.372	0.039	3.361
O(12)	-2.014	4.011	-1.453	C(46)	3.714	-4.188	-1.246	H(80)	-1.598	0.544	6.778
C(13)	-5.269	-1.5	-0.371	C(47)	4.553	-3.081	-1.074	H(81)	-3.226	0.37	4.151
O(14)	-3.961	0.488	1.422	C(48)	3.926	-1.846	-0.939	H(82)	-3.967	-2.746	-1.539
C(15)	-1.597	0.944	-1.416	C(49)	6.059	-3.214	-1.018	H(83)	-5.001	-4.874	-0.756
C(16)	-1.672	0.795	-2.807	C(50)	6.761	-1.849	-0.973	H(84)	-6.722	-0.528	0.892
C(17)	-0.582	0.327	-3.542	C(51)	5.942	-0.927	-0.08	H(85)	-8.247	-1.873	2.098
C(18)	0.597	-0.018	-2.896	O(52)	4.677	-0.718	-0.747	H(86)	-7.709	-4.825	1.523
C(19)	0.729	0.103	-1.508	O(53)	4.21	-5.443	-1.38	H(87)	1.401	2.006	0.807
C(20)	-0.385	0.56	-0.816	C(54)	6.48	0.456	0.182	H(88)	-2.754	0.928	-4.375
C(21)	2.031	-0.216	-0.803	C(55)	5.583	1.375	0.739	H(89)	1.718	-4.936	-1.401
C(22)	1.965	0.153	0.7	C(56)	5.979	2.668	1.008	H(90)	6.351	-3.789	-0.133
C(23)	0.58	-0.198	1.22	C(57)	7.297	3.07	0.747	H(91)	6.44	-3.741	-1.898
O(24)	-0.345	0.682	0.547	C(58)	8.191	2.159	0.203	H(92)	7.765	-1.979	-0.571
O(25)	1.619	-0.472	-3.667	C(59)	7.783	0.855	-0.088	H(93)	5.736	-1.44	0.867
C(26)	0.324	0.006	2.693	O(60)	7.687	4.345	1.016	H(94)	5.173	-5.43	-1.34
C(27)	-1.013	0.094	3.099	O(61)	5.149	3.622	1.527	H(95)	4.558	1.091	0.939
C(28)	-1.331	0.258	4.432	O(62)	6.896	-1.281	-2.263	H(96)	9.201	2.487	-0.004
C(29)	-0.318	0.326	5.398	O(63)	0.397	-2.657	-1.134	H(97)	8.486	0.171	-0.543
C(30)	1.007	0.237	5	H(64)	-3.885	5.566	-2.241	H(98)	6.92	4.825	1.356
C(31)	1.331	0.082	3.649	H(65)	-7.067	2.713	-1.663	H(99)	4.246	3.278	1.555
O(32)	-0.636	0.487	6.711	H(66)	-2.238	1.897	0.356	H(100)	6.061	-0.841	-2.466
O(33)	-2.612	0.367	4.897	H(67)	-2.751	-0.637	0.254	H(101)	-0.013	-3.523	-1.241
C(34)	-4.79	-2.721	-0.835	H(68)	-4.179	-0.344	-1.813				

Compound 4: Conformer (II) (0.25 kcal/mol) – Six H-bonds



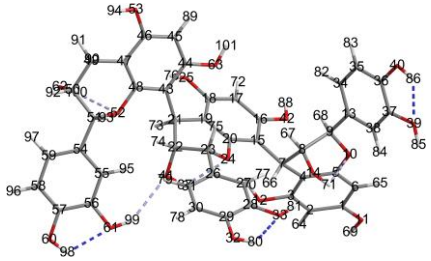
	X	Y	Z		X	Y	Z		X	Y	Z
C(1)	5.718	-4.12	-2.172	C(35)	6.953	2.53	1.368	H(69)	6.277	-5.766	-2.972
C(2)	4.368	-4.466	-2.196	C(36)	6.404	3.769	1.08	H(70)	1.567	-3.16	-1.61
C(3)	3.436	-3.564	-1.696	C(37)	5.303	3.854	0.216	H(71)	4.775	-1.21	1.362
C(4)	3.812	-2.328	-1.158	C(38)	4.766	2.709	-0.348	H(72)	0.83	0.148	-4.564
C(5)	5.17	-2.011	-1.187	O(39)	4.844	5.122	-0.007	H(73)	-2.709	-0.381	-1.282
C(6)	6.133	-2.889	-1.676	O(40)	6.93	4.9	1.623	H(74)	-2.697	0.257	1.223
C(7)	2.791	-1.422	-0.51	O(41)	-2.203	-1.658	0.754	H(75)	-0.295	1.067	1.052
C(8)	3.5	-0.273	0.235	O(42)	2.992	-0.853	-3.408	H(76)	-2.138	1.121	-3.037
C(9)	4.658	0.233	-0.625	C(43)	-2.438	1.675	-0.872	H(77)	1.818	-0.313	2.433
O(10)	5.635	-0.815	-0.696	C(44)	-1.64	2.827	-0.903	H(78)	-1.852	-0.919	5.686
O(11)	6.683	-4.956	-2.645	C(45)	-2.209	4.099	-0.943	H(79)	-2.39	-0.44	3.313
O(12)	2.127	-3.939	-1.73	C(46)	-3.591	4.244	-0.927	H(80)	1.504	-1.219	6.768
C(13)	5.318	1.458	-0.051	C(47)	-4.441	3.134	-0.871	H(81)	3.192	-0.784	4.209
O(14)	3.978	-0.684	1.506	C(48)	-3.826	1.887	-0.829	H(82)	6.843	0.41	1.033
C(15)	1.692	-0.888	-1.422	C(49)	-5.948	3.275	-0.837	H(83)	7.805	2.482	2.034
C(16)	1.804	-0.612	-2.791	C(50)	-6.661	1.918	-0.919	H(84)	3.919	2.788	-1.022
C(17)	0.734	-0.074	-3.508	C(51)	-5.866	0.918	-0.091	H(85)	4.083	5.111	-0.598
C(18)	-0.46	0.215	-2.863	O(52)	-4.59	0.754	-0.75	H(86)	6.414	5.652	1.303
C(19)	-0.629	-0.032	-1.496	O(53)	-4.074	5.511	-0.964	H(87)	-1.37	-2.13	0.624
C(20)	0.465	-0.557	-0.821	C(54)	-6.418	-0.478	0.047	H(88)	2.925	-0.609	-4.338
C(21)	-1.946	0.233	-0.797	C(55)	-5.536	-1.447	0.537	H(89)	-1.587	4.985	-0.97
C(22)	-1.92	-0.27	0.668	C(56)	-5.946	-2.755	0.695	H(90)	-6.255	3.779	0.085
C(23)	-0.546	0.02	1.251	C(57)	-7.263	-3.122	0.386	H(91)	-6.306	3.875	-1.679
O(24)	0.39	-0.803	0.524	C(58)	-8.142	-2.162	-0.092	H(92)	-7.672	2.023	-0.525
O(25)	-1.46	0.745	-3.615	C(59)	-7.721	-0.841	-0.27	H(93)	-5.673	1.348	0.899
C(26)	-0.327	-0.317	2.705	O(60)	-7.667	-4.411	0.545	H(94)	-5.037	5.506	-0.943
C(27)	1.001	-0.426	3.134	O(61)	-5.129	-3.754	1.145	H(95)	-4.511	-1.19	0.771
C(28)	1.29	-0.713	4.453	O(62)	-6.777	1.458	-2.253	H(96)	-9.152	-2.462	-0.338
C(29)	0.255	-0.884	5.383	O(63)	-0.288	2.68	-0.873	H(97)	-8.412	-0.116	-0.676
C(30)	-1.062	-0.774	4.961	H(64)	4.03	-5.41	-2.603	H(98)	-6.909	-4.924	0.856
C(31)	-1.355	-0.496	3.623	H(65)	7.177	-2.61	-1.678	H(99)	-4.225	-3.42	1.215
O(32)	0.543	-1.165	6.681	H(66)	2.291	-1.998	0.273	H(100)	-5.941	1.029	-2.477
O(33)	2.561	-0.851	4.937	H(67)	2.79	0.536	0.411	H(101)	0.129	3.549	-0.89
C(34)	6.407	1.374	0.809	H(68)	4.281	0.436	-1.632				

Compound 4: Conformer (III) (1.22 kcal/mol) – Seven H-bonds



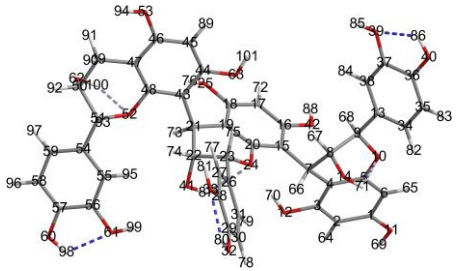
	X	Y	Z		X	Y	Z		X	Y	Z
C(1)	-5.958	3.709	-2.154	C(35)	-4.741	-4.106	0.441	H(69)	-6.708	5.256	-2.995
C(2)	-4.652	4.19	-2.237	C(36)	-5.755	-4.072	1.386	H(70)	-1.714	3.206	-1.694
C(3)	-3.618	3.41	-1.732	C(37)	-6.355	-2.849	1.714	H(71)	-4.572	1.133	1.451
C(4)	-3.847	2.165	-1.136	C(38)	-5.938	-1.675	1.109	H(72)	-0.542	0.519	-4.64
C(5)	-5.166	1.708	-1.111	O(39)	-7.347	-2.93	2.651	H(73)	2.702	-0.069	-1.08
C(6)	-6.227	2.462	-1.601	O(40)	-6.173	-5.219	1.988	H(74)	2.399	-1.222	1.213
C(7)	-2.719	1.396	-0.488	O(41)	2.127	0.79	1.149	H(75)	-0.041	-1.711	0.696
C(8)	-3.282	0.214	0.324	O(42)	-2.698	1.488	-3.446	H(76)	2.162	-1.091	-3.161
C(9)	-4.405	-0.446	-0.479	C(43)	2.209	-2.122	-1.158	H(77)	-2.133	-0.389	2.204
O(10)	-5.489	0.492	-0.562	C(44)	1.315	-3.148	-1.496	H(78)	1.256	-0.99	5.75
O(11)	-7.018	4.422	-2.626	C(45)	1.768	-4.437	-1.774	H(79)	1.96	-1.008	3.372
O(12)	-2.357	3.917	-1.822	C(46)	3.124	-4.731	-1.694	H(80)	-2.134	-0.504	6.641
C(13)	-4.919	-1.71	0.154	C(47)	4.063	-3.756	-1.337	H(81)	-3.61	-0.155	3.943
O(14)	-3.762	0.627	1.595	C(48)	3.563	-2.487	-1.065	H(82)	-3.541	-2.958	-0.921
C(15)	-1.597	0.944	-1.416	C(49)	5.541	-4.064	-1.23	H(83)	-4.293	-5.058	0.191
C(16)	-1.603	0.985	-2.816	C(50)	6.378	-2.804	-0.97	H(84)	-6.413	-0.736	1.367
C(17)	-0.527	0.495	-3.557	C(51)	5.609	-1.919	0	H(85)	-7.72	-2.059	2.825
C(18)	0.569	-0.06	-2.91	O(52)	4.415	-1.485	-0.69	H(86)	-6.881	-4.988	2.604
C(19)	0.629	-0.134	-1.513	O(53)	3.493	-6.006	-1.973	H(87)	1.357	1.368	1.065
C(20)	-0.47	0.352	-0.818	C(54)	6.273	-0.649	0.47	H(88)	-2.568	1.439	-4.401
C(21)	1.845	-0.685	-0.798	C(55)	5.446	0.284	1.104	H(89)	1.074	-5.224	-2.04
C(22)	1.728	-0.508	0.735	C(56)	5.959	1.48	1.563	H(90)	5.716	-4.777	-0.418
C(23)	0.285	-0.765	1.14	C(57)	7.325	1.762	1.419	H(91)	5.916	-4.513	-2.154
O(24)	-0.5	0.292	0.55	C(58)	8.149	0.834	0.799	H(92)	7.338	-3.096	-0.544
O(25)	1.581	-0.523	-3.687	C(59)	7.624	-0.368	0.316	H(93)	5.293	-2.522	0.859
C(26)	-0.036	-0.725	2.614	O(60)	7.83	2.939	1.874	H(94)	4.447	-6.107	-1.888
C(27)	-1.379	-0.54	2.965	O(61)	5.204	2.446	2.167	H(95)	4.386	0.095	1.217
C(28)	-1.758	-0.514	4.292	O(62)	6.651	-2.093	-2.164	H(96)	9.199	1.07	0.684
C(29)	-0.803	-0.685	5.305	O(63)	-0.014	-2.865	-1.53	H(97)	8.278	-1.063	-0.194
C(30)	0.527	-0.87	4.959	H(64)	-4.426	5.146	-2.69	H(98)	7.099	3.454	2.24
C(31)	0.913	-0.885	3.616	H(65)	-7.237	2.078	-1.558	H(99)	4.27	2.205	2.107
O(32)	-1.181	-0.659	6.611	H(66)	-2.259	2.053	0.254	H(100)	5.879	-1.54	-2.345
O(33)	-3.046	-0.323	4.709	H(67)	-2.489	-0.51	0.509	H(101)	-0.506	-3.658	-1.771
C(34)	-4.328	-2.926	-0.176	H(68)	-4.033	-0.651	-1.488				

Compound 4: Conformer (IV) (1.76 kcal/mol) – Seven H-bonds



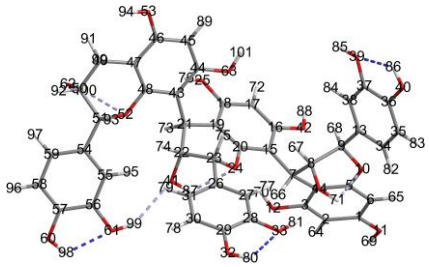
	X	Y	Z		X	Y	Z		X	Y	Z
C(1)	5.729	-4.132	-1.081	C(35)	5.22	3.969	0.764	H(69)	6.359	-5.82	-1.726
C(2)	4.387	-4.475	-1.237	C(36)	6.147	3.911	1.793	H(70)	1.548	-3.136	-1.03
C(3)	3.413	-3.546	-0.888	C(37)	6.576	2.664	2.269	H(71)	4.374	-1.111	2.173
C(4)	3.737	-2.285	-0.376	C(38)	6.075	1.492	1.727	H(72)	1.178	0.071	-4.198
C(5)	5.093	-1.972	-0.274	O(39)	7.496	2.721	3.279	H(73)	-2.724	-0.482	-1.366
C(6)	6.096	-2.877	-0.608	O(40)	6.647	5.055	2.335	H(74)	-3.046	0.215	1.101
C(7)	2.657	-1.344	0.109	O(41)	-2.441	-1.693	0.753	H(75)	-0.665	1.1	1.209
C(8)	3.289	-0.161	0.869	O(42)	3.202	-0.84	-2.756	H(76)	-1.981	0.998	-3.077
C(9)	4.538	0.299	0.116	C(43)	-2.567	1.591	-0.983	H(77)	1.297	-0.225	2.879
O(10)	5.51	-0.754	0.202	C(44)	-1.803	2.727	-1.283	H(78)	-2.744	-0.78	5.669
O(11)	6.732	-4.994	-1.401	C(45)	-2.392	3.986	-1.387	H(79)	-2.986	-0.372	3.235
O(12)	2.113	-3.921	-1.044	C(46)	-3.755	4.137	-1.168	H(80)	0.455	-1.007	7.167
C(13)	5.144	1.552	0.687	C(47)	-4.568	3.046	-0.84	H(81)	2.443	-0.617	4.827
O(14)	3.619	-0.509	2.205	C(48)	-3.935	1.811	-0.745	H(82)	4.004	2.84	-0.599
C(15)	1.669	-0.859	-0.946	C(49)	-6.052	3.196	-0.584	H(83)	4.904	4.938	0.401
C(16)	1.942	-0.616	-2.298	C(50)	-6.747	1.841	-0.391	H(84)	6.418	0.535	2.098
C(17)	0.957	-0.126	-3.156	C(51)	-5.818	0.945	0.417	H(85)	7.753	1.834	3.554
C(18)	-0.315	0.145	-2.672	O(52)	-4.658	0.699	-0.409	H(86)	7.274	4.805	3.027
C(19)	-0.645	-0.071	-1.329	O(53)	-4.26	5.392	-1.281	H(87)	-1.585	-2.14	0.736
C(20)	0.37	-0.546	-0.509	C(54)	-6.322	-0.422	0.803	H(88)	3.246	-0.618	-3.693
C(21)	-2.047	0.168	-0.807	C(55)	-5.361	-1.328	1.267	H(89)	-1.797	4.859	-1.623
C(22)	-2.19	-0.298	0.662	C(56)	-5.723	-2.607	1.637	H(90)	-6.217	3.807	0.31
C(23)	-0.909	0.051	1.404	C(57)	-7.066	-3.005	1.575	H(91)	-6.547	3.694	-1.423
O(24)	0.135	-0.759	0.823	C(58)	-8.021	-2.106	1.125	H(92)	-7.687	1.996	0.14
O(25)	-1.228	0.625	-3.556	C(59)	-7.652	-0.817	0.731	H(93)	-5.482	1.491	1.306
C(26)	-0.865	-0.245	2.883	O(60)	-7.422	-4.264	1.945	H(94)	-5.207	5.39	-1.108
C(27)	0.4	-0.326	3.476	O(61)	-4.833	-3.548	2.073	H(95)	-4.317	-1.048	1.312
C(28)	0.525	-0.571	4.829	O(62)	-7.062	1.226	-1.627	H(96)	-9.053	-2.43	1.071
C(29)	-0.616	-0.728	5.628	O(63)	-0.463	2.579	-1.453	H(97)	-8.407	-0.143	0.35
C(30)	-1.871	-0.645	5.043	H(64)	4.087	-5.438	-1.629	H(98)	-6.618	-4.739	2.194
C(31)	-1.998	-0.409	3.672	H(65)	7.136	-2.601	-0.51	H(99)	-3.934	-3.212	1.964
O(32)	-0.489	-0.969	6.961	H(66)	2.07	-1.879	0.859	H(100)	-6.264	0.771	-1.926
O(33)	1.727	-0.679	5.472	H(67)	2.571	0.657	0.927	H(101)	-0.067	3.436	-1.648
C(34)	4.723	2.79	0.21	H(68)	4.271	0.452	-0.935				

Compound 4: Conformer (V) (2.19 kcal/mol) – Six H-bonds



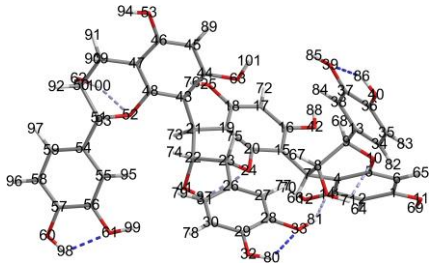
	X	Y	Z		X	Y	Z		X	Y	Z
C(1)	5.65	-4.521	-1.449	C(35)	7.378	2.422	1.186	H(69)	6.089	-6.302	-1.993
C(2)	4.281	-4.78	-1.403	C(36)	6.938	3.652	0.724	H(70)	1.58	-3.226	-0.984
C(3)	3.419	-3.758	-1.024	C(37)	5.848	3.711	-0.154	H(71)	4.995	-1.132	1.607
C(4)	3.881	-2.484	-0.678	C(38)	5.213	2.549	-0.56	H(72)	1.191	-0.243	-4.431
C(5)	5.255	-2.259	-0.778	O(39)	5.499	4.971	-0.556	H(73)	-2.504	-0.413	-1.389
C(6)	6.149	-3.258	-1.148	O(40)	7.562	4.798	1.111	H(74)	-2.695	0.282	1.094
C(7)	2.932	-1.427	-0.163	O(41)	-2.096	-1.615	0.729	H(75)	-0.347	1.217	1.097
C(8)	3.733	-0.254	0.431	O(42)	3.26	-1.173	-3.071	H(76)	-1.825	0.933	-3.156
C(9)	4.897	0.076	-0.506	C(43)	-2.269	1.657	-1.037	H(77)	-1.349	1.865	3.222
O(10)	5.805	-1.038	-0.476	C(44)	-1.471	2.809	-1.064	H(78)	0.055	-2.485	5.127
O(11)	6.55	-5.477	-1.808	C(45)	-2.039	4.077	-1.187	H(79)	0.202	-2.1	2.669
O(12)	2.088	-4.049	-0.983	C(46)	-3.419	4.216	-1.263	H(80)	-1.155	0.045	7.282
C(13)	5.655	1.308	-0.091	C(47)	-4.27	3.105	-1.22	H(81)	-1.818	2.42	5.474
O(14)	4.222	-0.565	1.722	C(48)	-3.657	1.863	-1.093	H(82)	7.088	0.294	1.14
C(15)	1.878	-0.951	-1.154	C(49)	-5.776	3.24	-1.292	H(83)	8.224	2.393	1.86
C(16)	2.055	-0.832	-2.539	C(50)	-6.475	1.877	-1.39	H(84)	4.373	2.608	-1.246
C(17)	1.039	-0.349	-3.364	C(51)	-5.743	0.901	-0.479	H(85)	4.773	4.938	-1.187
C(18)	-0.178	0.02	-2.811	O(52)	-4.42	0.728	-1.031	H(86)	7.12	5.538	0.676
C(19)	-0.417	-0.083	-1.437	O(53)	-3.902	5.479	-1.377	H(87)	-1.28	-2.076	0.499
C(20)	0.634	-0.535	-0.644	C(54)	-6.306	-0.493	-0.357	H(88)	3.238	-1.038	-4.025
C(21)	-1.784	0.222	-0.867	C(55)	-5.454	-1.473	0.166	H(89)	-1.417	4.963	-1.211
C(22)	-1.859	-0.222	0.607	C(56)	-5.893	-2.771	0.327	H(90)	-6.148	3.764	-0.405
C(23)	-0.552	0.162	1.3	C(57)	-7.207	-3.12	-0.018	H(91)	-6.077	3.817	-2.171
O(24)	0.494	-0.631	0.717	C(58)	-8.054	-2.151	-0.534	H(92)	-7.513	1.989	-1.077
O(25)	-1.137	0.476	-3.659	C(59)	-7.605	-0.839	-0.709	H(93)	-5.632	1.354	0.513
C(26)	-0.566	-0.1	2.781	O(60)	-7.637	-4.4	0.143	H(94)	-4.865	5.47	-1.414
C(27)	-1.045	0.905	3.628	O(61)	-5.112	-3.781	0.814	H(95)	-4.431	-1.232	0.424
C(28)	-1.13	0.681	4.992	O(62)	-6.489	1.383	-2.717	H(96)	-9.061	-2.436	-0.807
C(29)	-0.731	-0.549	5.533	O(63)	-0.124	2.667	-0.947	H(97)	-8.275	-0.107	-1.138
C(30)	-0.253	-1.543	4.693	H(64)	3.876	-5.75	-1.663	H(98)	-6.901	-4.92	0.491
C(31)	-0.176	-1.322	3.318	H(65)	7.208	-3.051	-1.207	H(99)	-4.214	-3.455	0.956
O(32)	-0.809	-0.759	6.874	H(66)	2.393	-1.853	0.686	H(100)	-5.637	0.954	-2.868
O(33)	-1.577	1.593	5.906	H(67)	3.08	0.613	0.534	H(101)	0.293	3.536	-0.968
C(34)	6.735	1.251	0.784	H(68)	4.511	0.19	-1.522				

Compound 4: Conformer (VI) (2.22 kcal/mol) – Seven H-bonds



	X	Y	Z		X	Y	Z		X	Y	Z
C(1)	5.889	-4.012	-1.214	C(35)	6.496	2.449	2.806	H(69)	6.581	-5.612	-2.003
C(2)	4.562	-4.361	-1.46	C(36)	5.982	3.7	2.501	H(70)	1.689	-3.099	-1.24
C(3)	3.555	-3.49	-1.061	C(37)	5.024	3.825	1.486	H(71)	4.388	-1.293	2.28
C(4)	3.83	-2.282	-0.41	C(38)	4.592	2.709	0.79	H(72)	1.369	0.355	-4.099
C(5)	5.174	-1.96	-0.217	O(39)	4.589	5.102	1.261	H(73)	-2.62	-0.358	-1.422
C(6)	6.209	-2.806	-0.599	O(40)	6.407	4.803	3.175	H(74)	-2.994	0.148	1.085
C(7)	2.712	-1.415	0.121	O(41)	-2.412	-1.737	0.599	H(75)	-0.603	0.976	1.322
C(8)	3.287	-0.305	1.022	O(42)	3.342	-0.695	-2.68	H(76)	-1.807	1.236	-2.992
C(9)	4.556	0.251	0.374	C(43)	-2.438	1.675	-0.872	H(77)	1.292	-0.467	2.934
O(10)	5.545	-0.789	0.398	C(44)	-1.649	2.815	-1.084	H(78)	-2.82	-1.254	5.558
O(11)	6.923	-4.819	-1.577	C(45)	-2.213	4.09	-1.103	H(79)	-2.998	-0.653	3.159
O(12)	2.271	-3.868	-1.312	C(46)	-3.575	4.252	-0.887	H(80)	0.338	-1.597	7.12
C(13)	5.107	1.446	1.103	C(47)	-4.412	3.156	-0.644	H(81)	2.388	-1.023	4.872
O(14)	3.572	-0.779	2.328	C(48)	-3.803	1.905	-0.63	H(82)	6.463	0.35	2.351
C(15)	1.758	-0.839	-0.919	C(49)	-5.896	3.316	-0.391	H(83)	7.239	2.371	3.59
C(16)	2.072	-0.492	-2.24	C(50)	-6.618	1.965	-0.292	H(84)	3.856	2.819	0
C(17)	1.117	0.078	-3.083	C(51)	-5.711	1	0.457	H(85)	3.926	5.118	0.563
C(18)	-0.165	0.329	-2.612	O(52)	-4.55	0.787	-0.378	H(86)	5.937	5.568	2.819
C(19)	-0.535	0.01	-1.301	O(53)	-4.054	5.521	-0.916	H(87)	-1.563	-2.198	0.573
C(20)	0.451	-0.545	-0.495	C(54)	-6.241	-0.381	0.75	H(88)	3.414	-0.404	-3.596
C(21)	-1.946	0.233	-0.796	C(55)	-5.299	-1.334	1.151	H(89)	-1.598	4.965	-1.27
C(22)	-2.136	-0.345	0.627	C(56)	-5.686	-2.627	1.437	H(90)	-6.058	3.87	0.54
C(23)	-0.87	-0.08	1.426	C(57)	-7.036	-2.994	1.35	H(91)	-6.374	3.877	-1.199
O(24)	0.176	-0.861	0.809	C(58)	-7.973	-2.049	0.961	H(92)	-7.557	2.103	0.243
O(25)	-1.045	0.893	-3.479	C(59)	-7.579	-0.744	0.652	H(93)	-5.369	1.477	1.382
C(26)	-0.869	-0.492	2.878	O(60)	-7.416	-4.268	1.635	H(94)	-5.002	5.528	-0.749
C(27)	0.38	-0.618	3.497	O(61)	-4.814	-3.612	1.81	H(95)	-4.25	-1.078	1.214
C(28)	0.47	-0.972	4.828	O(62)	-6.937	1.44	-1.568	H(96)	-9.011	-2.349	0.886
C(29)	-0.692	-1.195	5.58	O(63)	-0.31	2.653	-1.251	H(97)	-8.321	-0.032	0.318
C(30)	-1.931	-1.068	4.97	H(64)	4.3	-5.284	-1.961	H(98)	-6.622	-4.773	1.854
C(31)	-2.022	-0.722	3.619	H(65)	7.238	-2.524	-0.429	H(99)	-3.908	-3.285	1.725
O(32)	-0.6	-1.542	6.892	H(66)	2.107	-2.033	0.788	H(100)	-6.147	0.99	-1.893
O(33)	1.654	-1.131	5.492	H(67)	2.549	0.491	1.129	H(101)	0.104	3.515	-1.376
C(34)	6.055	1.322	2.113	H(68)	4.333	0.504	-0.667				

Compound 4: Conformer (VII) (2.63 kcal/mol) – Seven H-bonds



	X	Y	Z		X	Y	Z		X	Y	Z
C(1)	6.05	-3.625	-2.281	C(35)	6.443	2.648	2.051	H(69)	6.807	-5.108	-3.225
C(2)	4.743	-4.088	-2.427	C(36)	5.79	3.857	1.87	H(70)	1.801	-3.124	-1.871
C(3)	3.703	-3.341	-1.886	C(37)	4.731	3.942	0.955	H(71)	4.648	-1.25	1.492
C(4)	3.928	-2.148	-1.191	C(38)	4.34	2.825	0.234	H(72)	0.738	-0.132	-4.616
C(5)	5.248	-1.706	-1.102	O(39)	4.162	5.18	0.847	H(73)	-2.627	0.063	-1.121
C(6)	6.315	-2.427	-1.626	O(40)	6.175	4.96	2.568	H(74)	-2.402	0.973	1.288
C(7)	2.791	-1.422	-0.51	O(41)	-2.117	-1.021	1.023	H(75)	0.049	1.519	0.902
C(8)	3.345	-0.308	0.401	O(42)	2.865	-1.204	-3.461	H(76)	-2.028	1.295	-3.067
C(9)	4.49	0.4	-0.324	C(43)	-2.143	2.115	-0.971	H(77)	2.106	0.099	2.328
O(10)	5.567	-0.538	-0.452	C(44)	-1.245	3.172	-1.177	H(78)	-1.397	0.231	5.809
O(11)	7.114	-4.308	-2.785	C(45)	-1.696	4.482	-1.337	H(79)	-2.033	0.491	3.426
O(12)	2.441	-3.829	-2.042	C(46)	-3.055	4.763	-1.269	H(80)	1.976	-0.276	6.749
C(13)	4.996	1.604	0.423	C(47)	-3.999	3.755	-1.04	H(81)	3.537	-0.301	4.076
O(14)	3.796	-0.82	1.645	C(48)	-3.5	2.466	-0.882	H(82)	6.559	0.582	1.475
C(15)	1.692	-0.888	-1.422	C(49)	-5.482	4.047	-0.947	H(83)	7.261	2.602	2.758
C(16)	1.744	-0.78	-2.818	C(50)	-6.32	2.766	-0.833	H(84)	3.524	2.905	-0.478
C(17)	0.687	-0.223	-3.539	C(51)	-5.571	1.792	0.066	H(85)	3.437	5.168	0.214
C(18)	-0.434	0.253	-2.873	O(52)	-4.359	1.43	-0.633	H(86)	5.604	5.693	2.303
C(19)	-0.541	0.179	-1.479	O(53)	-3.421	6.059	-1.43	H(87)	-1.34	-1.584	0.907
C(20)	0.54	-0.372	-0.803	C(54)	-6.24	0.482	0.395	H(88)	2.764	-1.062	-4.409
C(21)	-1.782	0.649	-0.751	C(55)	-5.423	-0.508	0.95	H(89)	-0.998	5.293	-1.499
C(22)	-1.713	0.314	0.76	C(56)	-5.941	-1.743	1.281	H(90)	-5.684	4.679	-0.076
C(23)	-0.285	0.531	1.235	C(57)	-7.303	-2.011	1.084	H(91)	-5.833	4.582	-1.835
O(24)	0.525	-0.457	0.564	C(58)	-8.118	-1.029	0.541	H(92)	-7.291	3.014	-0.404
O(25)	-1.424	0.791	-3.631	C(59)	-7.588	0.216	0.188	H(93)	-5.28	2.31	0.987
C(26)	-0.009	0.34	2.706	O(60)	-7.814	-3.228	1.414	H(94)	-4.377	6.151	-1.36
C(27)	1.327	0.148	3.077	O(61)	-5.194	-2.762	1.804	H(95)	-4.367	-0.329	1.101
C(28)	1.669	-0.016	4.404	O(62)	-6.56	2.174	-2.096	H(96)	-9.165	-1.254	0.383
C(29)	0.681	0.022	5.399	O(63)	0.086	2.897	-1.198	H(97)	-8.233	0.956	-0.266
C(30)	-0.643	0.215	5.033	H(64)	4.52	-5.006	-2.957	H(98)	-7.089	-3.775	1.744
C(31)	-0.991	0.368	3.689	H(65)	7.326	-2.056	-1.533	H(99)	-4.26	-2.512	1.789
O(32)	1.021	-0.138	6.706	H(66)	2.312	-2.129	0.172	H(100)	-5.782	1.642	-2.311
O(33)	2.948	-0.224	4.837	H(67)	2.551	0.406	0.623	H(101)	0.58	3.713	-1.338
C(34)	6.043	1.521	1.334	H(68)	4.145	0.684	-1.323				

Table 1. ^{13}C-NMR chemical shifts in ppm for (-)-epicatechin (**1**), procyanidin B1 (**2**), B2 (**3**), and C1 (**4**) in MeOD. Compound **1** was measured at rt; compounds **2**-**4** were measured at -15 ^{o}C. $^{a}\delta$ = 155-157 ppm (C5^{A,B}, C7^{A,B}, C9^{A,B}; not resolved, ambiguous), $^{b}\delta$ = 143-145 ppm (C3'^{A,B}, C4'^{A,B}; not resolved, ambiguous), $^{c}\delta$ = 154-157 ppm (C5^{A,B,C}, C7^{A,B,C}, C9^{A,B,C}; not resolved, ambiguous), $^{d}\delta$ = 143-145 ppm (C3'^{A,B,C}, C4'^{A,B,C}; not resolved, ambiguous).

1b	**2**		**3**		**4**		
	A	**B**	**A**	**B**	**A**	**B**	**C**
2	75.8	78.1	75.8	80.5	75.3	75.7	78.4
3	72.3	65.7	71.1	66.8	72.0	72.4	65.7
4	35.5	28.5	35.6	25.5	36.2	36.2	28.8
5	a	a	a	a	c	c	c
6	94.8	95.8	94.5	95.5	95.0	96.0	96.3
7	a	a	a	a	c	c	c
8	94.1	106.0	94.3	105.9	95.0	104.5	106.9
9	a	a	a	a	c	c	c
10	100.3	98.6	100.4	96.1	101.2	100.5	100.5
1'	131.1	130.7	131.2	130.8	131.2	131.2	130.5
2'	113.9	113.7	112.9	113.4	113.8	113.9	114.1
3'	b	b	b	b	d	d	d
4'	b	b	b	b	d	d	d
5'	114.7	114.5	114.2	114.5	114.7	114.8	114.9
6'	117.6	117.2	117.7	117.7	116.8	117.5	117.7

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