Electronic supplementary information

for

^{13}C CP MAS NMR and DFT studies of 6-chromanyl etheral derivatives.†

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† Dedicated to Prof. Stanisław Witkowski on the occasion of his 70th birthday.

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1. Synthesis and spectroscopic data of ethers **3-5**

2,2,5,7,8-pentamethyl-6-((tetrahydro-2*H*-pyran-2-yl)oxy)chromane (**3**).

The chroman-6-ol (**2**; 1 equiv.) was stirred overnight at room temperature with 3,4-dihydro-2H-pyran (3 equiv.) in diethyl ether solutions containing catalytic amount of PTSA. In next step the reaction mixture was incubated with excess of solid K_2CO_3 and after aqueous work-up the resulted organic fraction was concentrated in vacuum to dryness. The crude ether **3** was purified by MPLC (hexane-ethyl acetate. 15:1 v/v)). Re-crystallization from ethanol gave the desired product **3** with 60% yield.

^1H NMR (δ, 400 MHz, $CDCl_3$): 4.67 (dd, 1H, H-1′, $^3J_{H-H}$ = 6.9 Hz and 2.2 Hz), 4.09 (m, 1H, H-5′$_{ax}$), 3.48 (m, 1H, H-5′$_{eq}$), 2.62 (m, 2H, H-4), 2.21 (s, 3H, H-7a), 2.18 (s, 3H, H8b), 2.11 (s, 3H, H-5a), 1.95 (m, 2H, H-2′$_{ax}$ and 3′$_{ax}$), 1.87 (m, 1H, H-2′$_{eq}$), 1.81 (~t, 2H, H-3, $^3J_{H-H}$ = 7.1 Hz), 1.599 (m, 2H, H-4′ and 3′$_{eq}$), 1.315 (s, 6H, H-2a and 2b) ppm.

^{13}C NMR (δ, 150 MHz, $CDCl_3$): 148.00 (C8a), 147.33 (C6), 128.25 (C7), 126.38 (C5), 122.57 (C8), 117.04 (C4a), 103.73 (C1′), 72.64 (C2), 65.06 (C5′), 32.94 (C3), 31.29 (C2′), 26.86 (C2a), 26.80 (C2b), 25.24 (C4′), 21.16 (C3′), 21.06 (C4), 13.81 (C7a), 12.93 (C5a), 11.86 (C8b) ppm.

IR ($CHCl_3$) ν_{max}/cm^{-1}: 3003,. 2977, 2945, 2855, 1456, 1412, 1382, 1370, 1264, 1167, 1125, 1102, 1077, 1035, 952, 926, 909, 897.

TOF MS ES$^+$: 327 [M + Na]$^+$; HRMS: m/z: calc. for $C_{19}H_{28}O_3Na$ [M + Na]$^+$: 327.1931; found: 327.1938

6-methoxy-2.2.5.7.8-pentamethylchromane (**4**)

The chroman-2-ol (**2**. 1 equiv.) and dimethyl sulfate (excess) were heating with stirring in dry suspension of K_2CO_3 in acetone. The cooled solution was poured into water and extracted with diethyl ether (3 × 50 mL). The combined organic extracts were washed with sodium bicarbonate, dried over anhydrous Na_2SO_4 and concentrated under reduced pressure. The residue was purified by flash column chromatography (hexane/ethyl acetate, 20:1, *v*/*v*) to afford ester **4** as a white solid with 70% yield.

The ^{1}H and ^{13}C NMR spectra were with good similarity to those described in literature. [Byzova. V. N.; Zakharova. E. I.; Zhukova. E. E.; Sarycheva. I. K.; Evstigneeva. R. P.; Journal of Organic Chemistry USSR (English Translation); vol. 24; nb. 11; (1988); p. 2135 - 2140; Zhurnal Organicheskoi Khimii; vol. 24; nb. 11; (1988); p. 2368 - 2374. and Al-Khayat. Isam; Dean. Francis M.; France. Steven N.; Matkin. David A.; Orabi. Mohamed O. A.; et al.; Journal of the Chemical Society. Perkin Transactions 1: Organic and Bio-Organic Chemistry (1972-1999); (1985); p. 1301 – 1310]

^{1}H NMR (δ. 400 MHz. $CDCl_3$): 3.64 (s, 1H, H-1'), 2.63 (t, 2H, H-4, $^3J_{H\text{-}H}$ = 6.8 Hz), 2.20 (s, 3H, H-7a), 2.16 (s, 3H, H8b), 2.10 (s, 3H, H-5a), 1.82 (t, 2H, H-3, $^3J_{H\text{-}H}$ = 6.8 Hz), 1.33 (s, 6H H-2a and 2b) ppm.

^{13}C NMR (δ, 150 MHz, $CDCl_3$): 147.88 (C8a), 149.45 (C6), 127.72 (C7), 125.70 (C5), 122.85 (C8), 117.31 (C4a), 72.71 (C2), 60.35 (C1'), 32.91 (C3), 26.8179 (C2a and 2b), 20.94 (C4), 12.52 (C7a), 11.74 (C8b), 11.66 (C5a) ppm.

TOF MS ES$^+$: 257 [M + Na]$^+$; HRMS: m/z: calc. for $C_{15}H_{22}O_2Na$ [M + Na]$^+$: 257.1512; found: 257.1519

tert-butyl-*di*-methyl((2.2.5.7.8-pentamethylchroman-6-yl)oxy)silane (**5**)

Trimethylamine (1.5 equiv.) under argon atmosphere was added to the chroman-2-ol (**2**, 1 equiv.) in dry THF solution and after 5 min. of stirring the *tert*-butyldimethylsilyl chloride (TBDMSCl, 1.1 equiv.) was added dropwise. The reaction after overnight stirring at room temperature was poured into water and extracted with diethyl ether (3 × 50 mL). The combined organic extracts were washed with sodium bicarbonate, dried over anhydrous Na_2SO_4 and concentrated under reduced pressure. The residue was purified by flash column chromatography (hexane/ethyl acetate, 30:1. v/v) to afford ester **5** with 80% yield.

^{1}H NMR (δ. 400 MHz. $CDCl_3$): 2.58 (t, 2H, H-4, $^3J_{H\text{-}H}$ = 6.8 Hz), 2.11 (s, 3H, H-7a), 2.09 (s, 6H, H-8b), 2.07 (s, 3H, H-5a), 1.80 (t, 2H, H-3, $^3J_{H\text{-}H}$ = 6.8 Hz), 1.30 (s, 6H, H-2a and 2b), 1.06 (s, 9H., H-2'), 0.13 (s, 6H, H-1') ppm.

^{13}C NMR (δ, 150 MHz, $CDCl_3$): 146.05 (C8a), 144.14 (C6), 125.84 (C7), 123.50 (C5), 122.63 (C8), 117.25 (C4a), 72.45 (C2), 33.10 (C3), 26.77 (C2a and 2b) 26.12 (C2''), 21.21 (C4), 18.61 (C2'), 14.33 (C7a), 13.41 (C5a), 11.93 (C8b), -3.21 (C1') ppm.

TOF MS ES$^+$: 357 $[M + Na]^+$; HRMS: m/z: calc. for $C_{20}H_{34}NaO_2Si$ $[M + Na]^+$: 357.2220; found: 357.2226

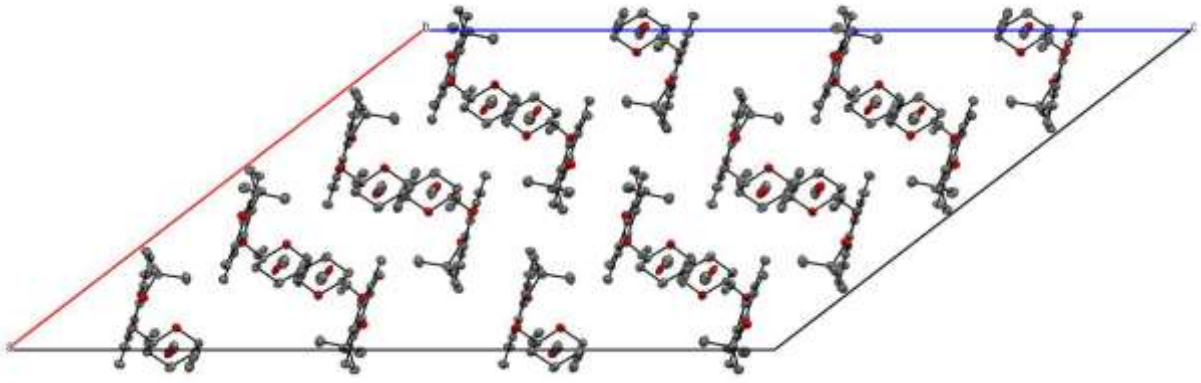

Fig. S1. Crystal packing scheme in **3**. A view of the unit cell in the [010] direction. Hydrogen atoms are omitted for clarity.

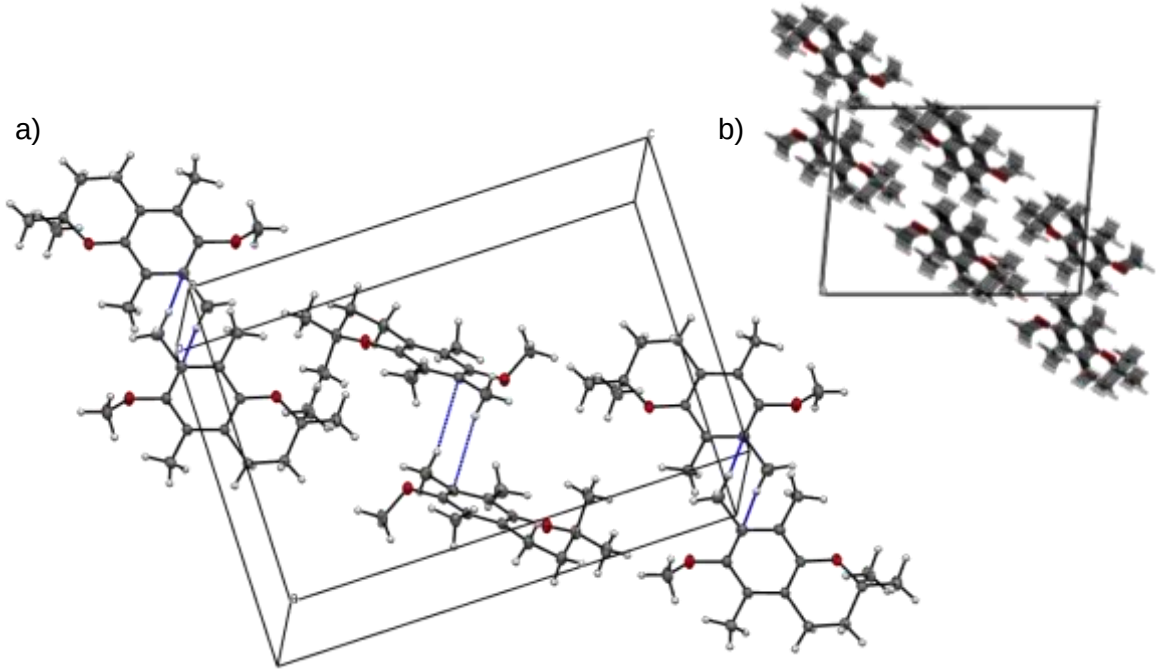

Fig. S2. The dimeric structure formed in crystals of **4** a) and supramolecular structure formed by methyl ether **4** (view of the unit cell in the [010] direction).

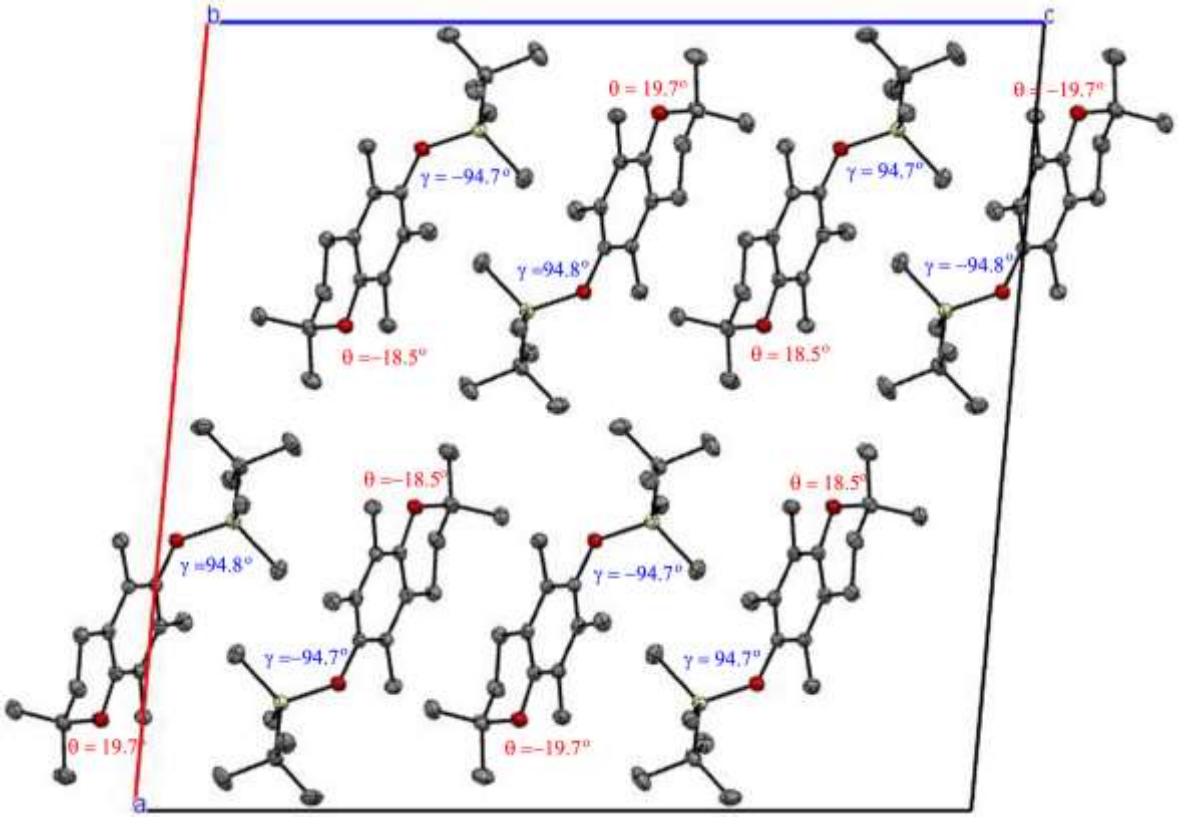

Fig. S3. Crystal packing scheme in **5** with torsion angle θ[°] (red) and γ[°] (blue) values. A view of the unit cell in the [010] direction. Hydrogen atoms are omitted for clarity.

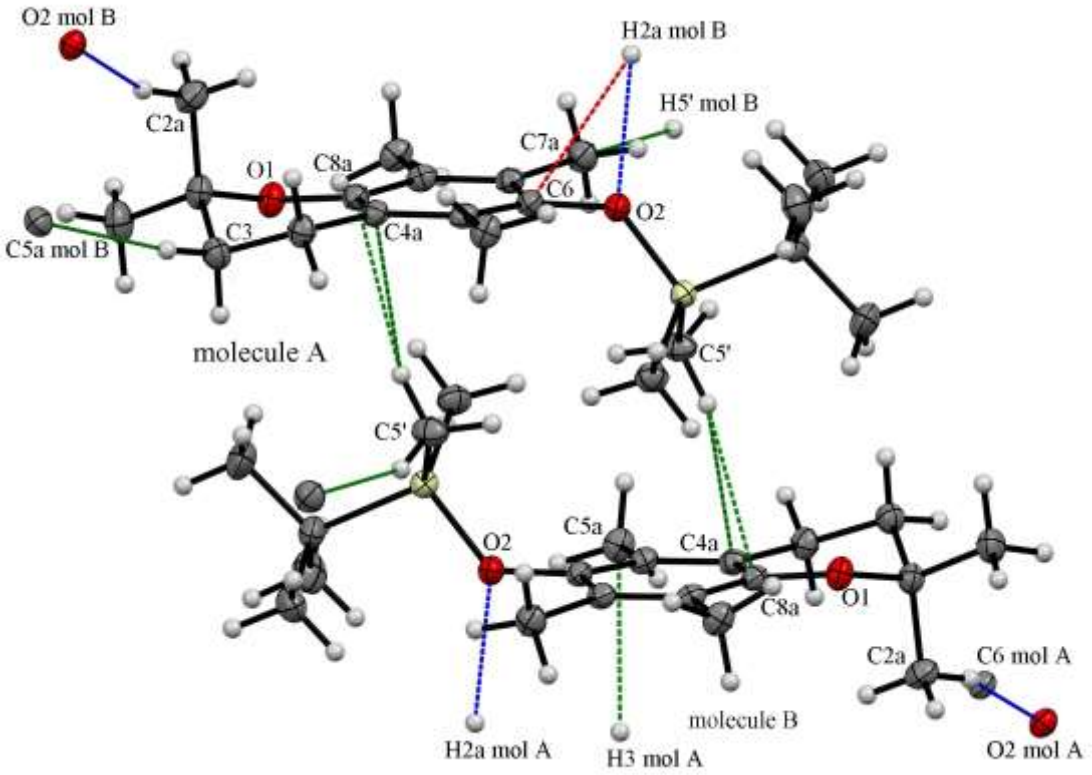

Fig. S4. The short contact in crystal structure of **5**.

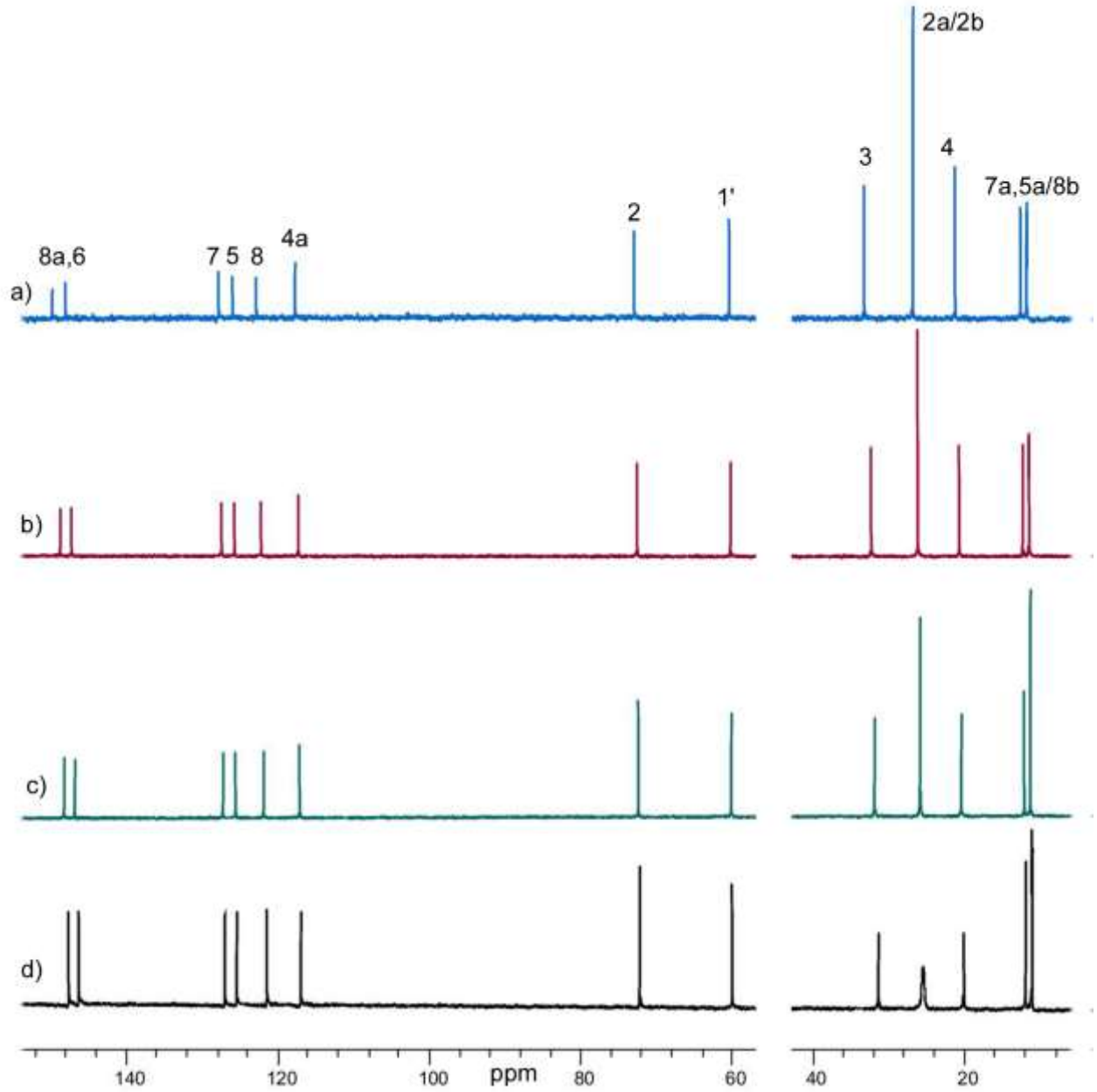

Fig. S5 Dynamic ^{13}C NMR spectra of **4**: **a**) 298.3, **b**) 239.6, **c**) 210.2, **d**) 178.4 K.

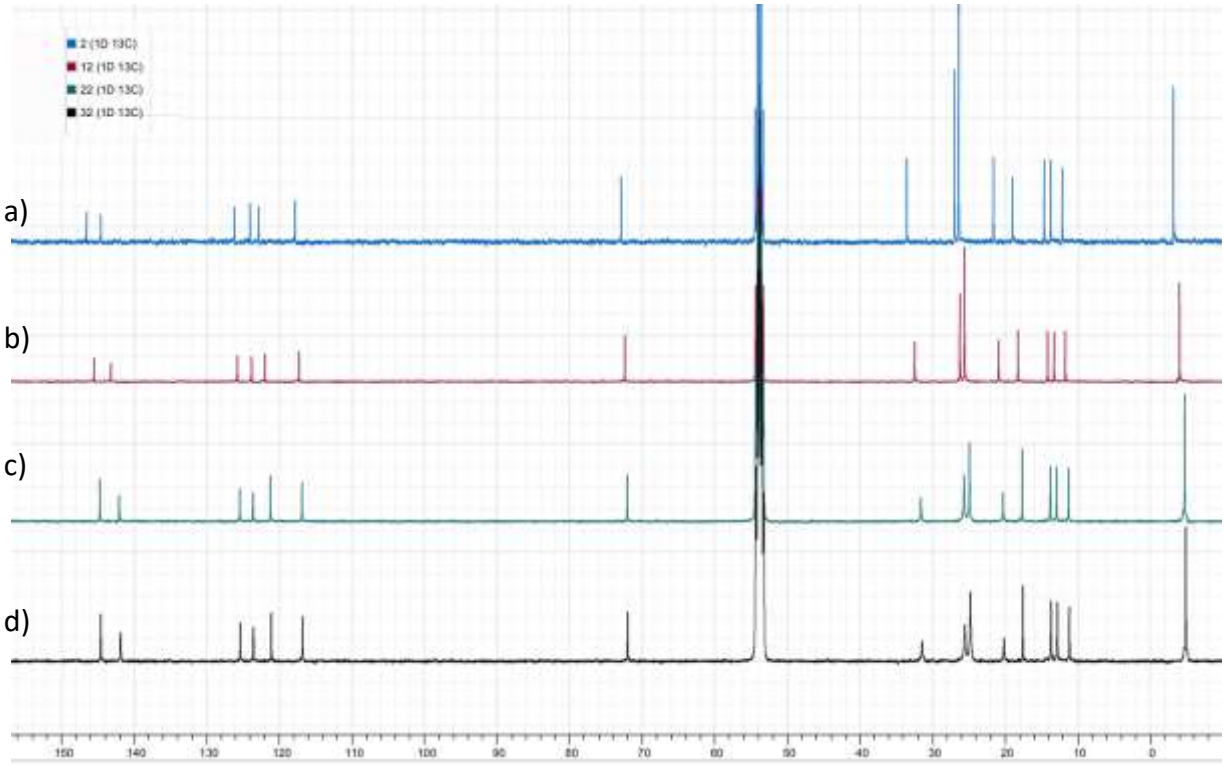

Fig. S6 Dynamic ^{13}C NMR spectra of **5** (eter TBDMS): **a**) 298, **b**) 250, **c**) 200 and **d**) 190 K.

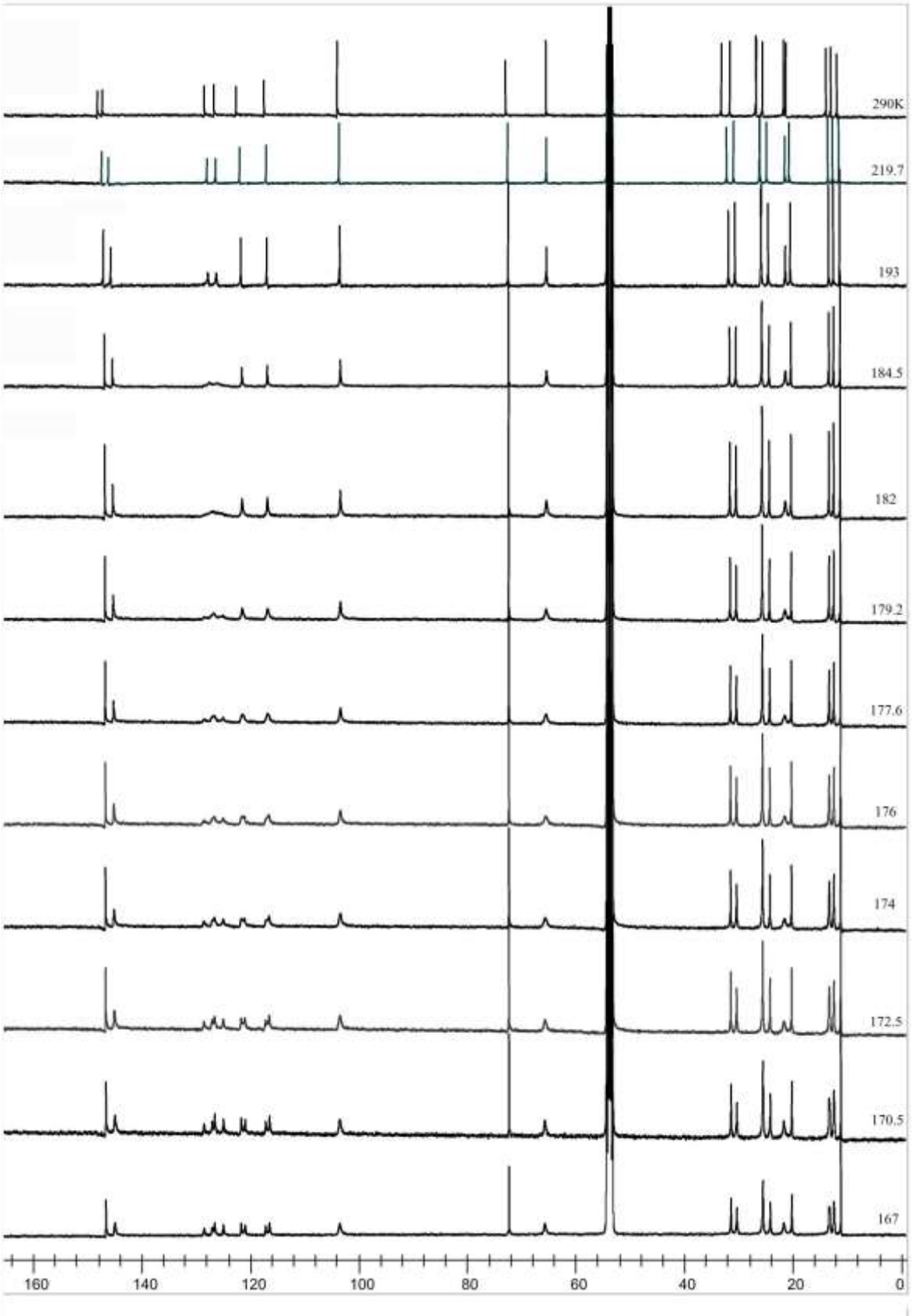

Fig. S7 Dynamic ^{13}C NMR of **3** in differentia temperature of measurement (temp. range 290 – 165 K).

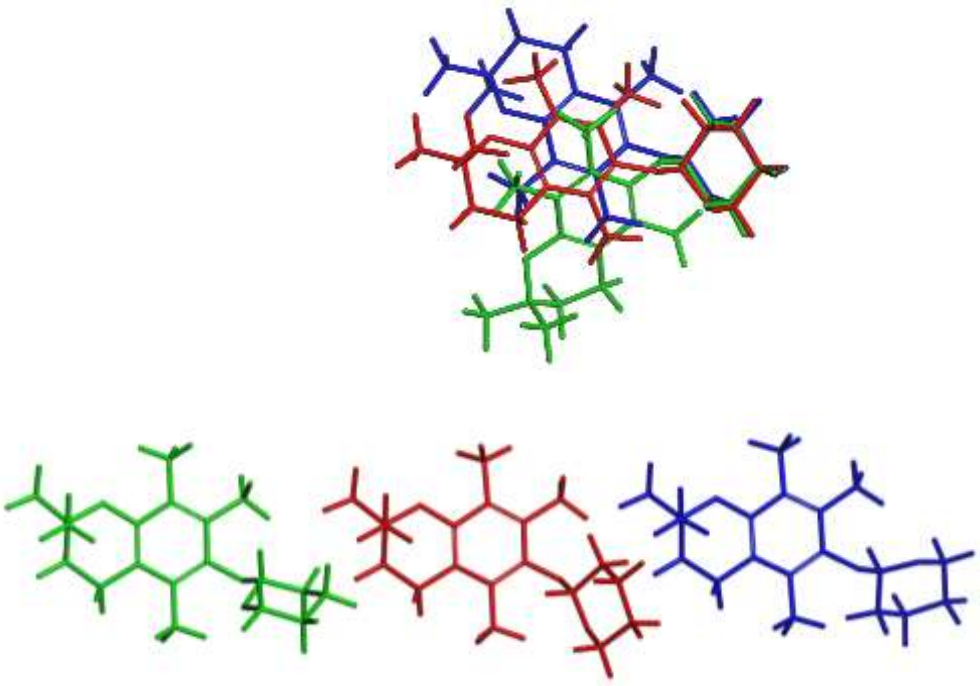

Fig. S8 Conformations of **3**: a (green), TS (red), h (blue).

Table S1. Selected bond lengths [Å] in ethers **3**, **4** and **5** determined by XRD data.

Bond lengths		**3**A	**3**B	**4**	**5**A	**5**B
8a	4a	1.397(2)	1.397(2)	1.399(2)	1.396(2)	1.395(2)
4a	5	1.404(2)	1.406(2)	1.406(2)	1.408(2)	1.407(2)
5	6	1.390(3)	1.391(3)	1.393(2)	1.395(2)	1.395(2)
6	7	1.401(2)	1.401(2)	1.397(2)	1.404(2)	1.404(2)
7	8	1.399(2)	1.400(2)	1.401(2)	1.402(2)	1.405(2)
8	8a	1.404(3)	1.403(3)	1.402(2)	1.397(2)	1.397(2)
8	8b	1.508(2)	1.510(3)	1.508(2)	1.514(2)	1.511(2)
5	5a	1.508(2)	1.508(2)	1.508(2)	1.510(2)	1.510(2)
7	7a	1.507(3)	1.508(3)	1.508(2)	1.508(2)	1.506(2)
O2	6	1.403(2)	1.405(2)	1.399(2)	1.390(1)	1.391(1)
O1	2	1.451(3)	1.453(3)	1.453(2)	1.450(2)	1.453(2)
O1	8a	1.380(2)	1.379(2)	1.383(2)	1.381(1)	1.382(1)
O2	2b	1.517(2)	1.521(4)	1.523(2)	1.521(2)	1.525(2)
O2	2a	1.525(4)	1.522(2)	1.519(2)	1.517(2)	1.517(2)
O2	C1'/Si	1.427(7)	1.418(3)	1.426(2)	1.666(1)	1.667(1)

Table S2. Selected bond angles [°] in ethers **3**, **4** and **5** determined by XRD data.

Bond angle			**3**A	**3**B	**4**	**5**A	**5**B
4a	5	6	118.5(2)	118.9(2)	118.8(1)	119.1(1)	119.2(1)
5	6	7	122.5(2)	122.3(2)	122.4(1)	121.6(1)	121.8(1)
6	7	8	118.9(2)	118.8(2)	118.9(1)	118.9(1)	118.7(1)
7	8	8a	118.6(2)	119.0(2)	118.9(1)	119.2(1)	119.2(1)
8	8a	4a	122.0(2)	121.8(2)	121.9(1)	121.8(1)	121.9(1)
8a	4a	5	119.0(2)	119.1(2)	119.0(1)	119.0(1)	118.9(1)
6	5	5a	121.2(2)	121.4(2)	120.9(1)	120.9(1)	120.9(1)
6	7	7a	120.3(2)	120.7(2)	120.8(1)	120.8(1)	120.9(1)
7	8	8b	121.5(2)	121.5(2)	120.7(1)	121.6(1)	121.6(1)
8	7	7a	120.8(2)	120.5(2)	120.2(1)	120.3(1)	120.5(1)
8b	8	8a	119.9(2)	119.5(2)	120.4(1)	119.1(1)	119.2(1)
O2	6	7	118.6(2)	119.2(2)	119.0(1)	119.1(1)	118.8(1)
O2	6	5	118.8(2)	118.3(2)	118.6(1)	119.2(1)	119.3(1)

Table S3. Selected torsion angles [°] in ethers **3**, **4** and **5** determined by XRD data.

Torsion angle				**4**	**3**A	**3**B	**5**A	**5**B
4a	8a	O1	2	−21.3	16.9	14.2	19.7	−18.5
8b	8	7	7a	2.5	0.6	−3.5	2.3	−2.7
8	8a	4a	5	−1.0	6.5	2.7	−3.7	3.4
8a	4a	5	6	2.6	−1.9	−1.5	−0.8	1.1
4a	5	6	7	−2.3	−3.9	−1.7	5.4	−5.7
5	6	7	8	0.1	5.1	3.5	−5.5	5.8
6	7	8	8a	1.6	−0.5	−2.3	1.0	−1.2
5	6	7	7a	179.2	−175.4	174.8	172.7	−172.5
5a	5	6	7	177.5	175.6	175.8	−174.2	174.4
8b	8	8a	4a	178.8	174.2	178.8	−176	176.4
8a	4a	5	5a	−177.1	178.7	−179	178.8	−179
O2	6	7	7a	−2.2	0.9	−0.4	−3.5	3.4
O2	6	5	5a	−1.1	−0.7	1.3	2.0	−1.5

Table S4. The bonds length comparison in ethers **4**, **3**A-B and **5**A-B and differences in bond lengthens between **4** and ethers **3** and **5** with 3σ values).

Bond		**4**	**3**A	**3**B	**5**A	**5**B	Differences in bond length							
		Length					**4** - **3**A	(**3**σ)	**4** - **3**B	(**3**σ)	**4** - **5**A	(3σ)	**4** - **5**B	(3σ)
C8a	C4a	1.399(2)	1.397(2)	1.397(2)	1.396(2)	1.395(2)	0.002	0.008	0.002	0.008	0.003	0.008	0.004	0.008
C4a	C5	1.406(2)	1.404(2)	1.406(2)	1.408(2)	1.407(2)	0.002	0.008	0	0.008	−0.002	0.008	−0.001	0.008
C5	C6	1.393(2)	1.390(3)	1.391(3)	1.395(2)	1.395(2)	0.003	0.011	0.002	0.011	−0.002	0.008	−0.002	0.008
C6	**C7**	**1.397(2)**	**1.401(2)**	**1.401(2)**	**1.404(2)**	**1.404(2)**	**−0.004**	**0.008**	**−0.004**	**0.008**	**−0.007**	**0.008**	**−0.007**	**0.008**
C7	C8	1.401(2)	1.399(2)	1.400(2)	1.402(2)	1.405(2)	0.002	0.008	0.001	0.008	−0.001	0.008	−0.004	0.008
C8	C8a	1.402(2)	1.404(3)	1.403(3)	1.397(2)	1.397(2)	−0.002	0.011	−0.001	0.011	0.005	0.008	0.005	0.008
C8	C8b	1.508(2)	1.508(2)	1.510(3)	1.514(2)	1.511(2)	0	0.008	−0.002	0.011	−0.006	0.008	−0.003	0.008
C5	C5a	1.508(2)	1.508(2)	1.508(2)	1.510(2)	1.510(2)	0	0.008	0	0.008	−0.002	0.008	−0.002	0.008
C7	C7a	1.508(2)	1.507(3)	1.508(3)	1.508(2)	1.506(2)	0.001	0.011	0	0.011	0	0.008	0.002	0.008
C6	**O2**	**1.399(2)**	**1.403(2)**	**1.405(2)**	**1.390(1)**	**1.391(1)**	−0.004	0.008	−0.006	0.008	**0.009**	**0.007**	**0.008**	**0.007**
O1	C2	1.453(2)	1.451(3)	1.453(3)	1.450(2)	1.453(2)	0.002	0.011	0	0.011	0.003	0.008	0	0.008
O1	C8a	1.383(2)	1.380(2)	1.379(2)	1.381(1)	1.382(1)	0.003	0.008	0.004	0.008	0.002	0.007	0.001	0.007
C2	C2b	1.523(2)	1.525(4)	1.521(4)	1.521(2)	1.525(2)	−0.002	0.022	0.002	0.013	0.002	0.008	−0.002	0.008
C2	C2a	1.519(2)	1.517(2)	1.522(2)	1.517(2)	1.517(2)	0.002	0.008	−0.003	0.008	0.002	0.008	0.002	0.008

Table S5. The bonds length comparison between 4-methoxy−2,3,5,6-tetramethylphenol (4MTP, CCDC MOPHLA) and ethers **4**, **3**A-B and **5**A-B.

bond		**4PMT**	**4**	**3**A	**3**B	**5**A	**5**B	**4**−4PMT	**3**A−4PMT	**3**B−4PMT	**5**A−4PMT	**5**B−4PMT
C8a	**C4a**	**1.382**	**1.399**	**1.397**	**1.397**	**1.396**	**1.395**	**0.017**	**0.015**	**0.015**	**0.014**	**0.013**
C4A	**C5**	**1.394**	**1.406**	**1.404**	**1.406**	**1.408**	**1.407**	**0.012**	**0.010**	**0.012**	**0.014**	**0.013**
C5	C6	1.390	1.393	1.39	1.391	1.395	1.395	0.003	0.000	0.001	0.005	0.005
C6	**C7**	**1.387**	**1.397**	**1.401**	**1.401**	**1.404**	**1.404**	**0.010**	**0.014**	**0.014**	**0.017**	**0.017**
C7	C8	1.398	1.401	1.399	1.4	1.402	1.405	0.003	0.001	0.002	0.004	0.007
C8	**C8a**	**1.387**	**1.402**	**1.404**	**1.403**	**1.397**	**1.397**	**0.015**	**0.017**	**0.016**	**0.010**	**0.010**
C8	C8a	1.509	1.508	1.508	1.51	1.514	1.511	−0.001	−0.001	0.001	0.005	0.002
C5	C5a	1.504	1.508	1.508	1.508	1.51	1.51	0.004	0.004	0.004	0.006	0.006
C7	C7a	1.508	1.508	1.507	1.508	1.508	1.506	0.000	−0.001	0.000	0.000	−0.002
C6	O2	1.409	1.399	1.403	1.405	1.39	1.391	−0.010	−0.006	−0.004	−0.019	−0.018
O1	C2	1.443	1.453	1.451	1.453	1.45	1.453	0.010	0.008	0.010	0.007	0.010
O1	**C8a**	**1.409**	**1.383**	**1.38**	**1.379**	**1.381**	**1.382**	**−0.026**	**−0.029**	**−0.030**	**−0.028**	**−0.027**

Tabela S6. Data for ether **3** from WinNMR.

Temp. [K]	**165.0**	**170.5**	**172.5**	**174.0**	**176.0**	**177.6**	**179.2**	**182.0**	**184.5**	**193.0**	**219.7**
$\Delta G^{\#}_{(ab)}$ [kcal/mol]	8.56	8.56	8.54	8.53	8.46	8.46	8.43	8.39	8.39	8.36	8.14
1/T [x10^{-2}]	0.606	0.586	0.579	0.574	0.568	0.563	0.557	0.549	0.542	0.518	0.455
k*ab*	15.68	37.75	55.189	70.451	116.147	144.011	195.149	315.	437.950	1360.	36800
ln*k*	2.752	3.631	4.011	4.255	4.755	4.97	5.274	5.753	6.082	7.215	10.513

Average $\Delta G^{\#}_{(ab)}$ = 8.44 kcal·mol^{-1}; std. dev. = 0.42 kcal·mol^{-1}

Table S7. Energies [kJ/mol], relative energies [kJ/mol] and calculated NMR isotropic chemical shift values [ppm] of the studied conformations of 3.

Conformation symbol		a	b	c	d	e	f	g	h	i	j
Relative energy [kJ/mol]		0.00	0.00	0.00	0.00	0.00	19.86	20.09	26.25	30.74	30.74
Energy [kJ/mol]		−2513941.28	−2513941.28	−2513941.28	−2513941.28	−2513941.28	−2513921.41	−2513921.19	−2513915.03	2513910.54	2513910.54
Atom number	Exp.	GIAO									
2	72.6	73.65	73.64	73.65	73.65	73.65	73.53	73.53	73.95	73.49	73.49
2a	26.9	25.85	25.85	25.85	25.85	25.85	25.78	25.8	25.83	25.72	25.72
2b	26.8	27.43	27.48	27.43	27.43	27.43	27.38	27.48	27.47	27.53	27.52
3	32.9	30.8	30.8	30.8	30.8	30.8	30.85	30.9	30.8	30.82	30.82
4	21.1	19.66	19.66	19.66	19.67	19.67	19.7	19.67	19.83	19.62	19.62
4a	117	118.48	118.48	118.48	118.48	118.48	118.19	119.15	117.25	118.86	118.86
5	126.4	127.05	126.04	126.05	126.04	126.05	132.79	130.97	124.82	124.09	124.1
5a	11.9	9.52	9.52	9.52	9.52	9.57	9.75	8.51	9.15	7.74	7.74
6	147.3	148.38	148.38	148.38	148.39	148.38	151.03	150.68	149.06	148.38	148.38
7	128.2	129.42	129.42	129.42	129.43	129.42	129.45	131.86	130.89	133.16	133.16
7a	13.8	13.35	13.35	13.35	13.35	13.45	14.05	15.5	12.87	14.56	14.56
8	122.6	124.46	124.46	124.46	124.45	124.46	124.96	123.92	125.5	124.01	124.01
8b	12.9	12.45	12.33	12.34	12.34	12.44	12.38	12.32	12.1	12.19	12.19
8a	148	149.75	149.74	149.75	149.74	149.75	149.59	149.56	149.47	149.52	149.52
1'	103.7	104.95	104.94	104.95	104.95	104.95	102.11	102.49	103.53	103.76	103.75
2'	31.3	30.67	30.67	30.67	30.67	30.67	29.09	29.17	31.06	24.22	24.22
3'	21.2	21.5	21.5	21.5	21.5	21.5	16.49	16.55	21.3	13.84	13.85
4'	25.2	24.11	24.2	24.1	24.11	24.2	24.52	24.56	23.88	20.24	20.24

5'	65.1	65.45	65.45	65.44	65.45	65.45	60.93	61	65.87	56.2	56.2
						Exp. - GIAO					
2	72.6	−1.05	−1.04	−1.05	−1.05	−1.05	−0.93	−0.93	−1.35	−0.89	−0.89
2a	26.9	1.05	1.05	1.05	1.05	1.05	1.12	1.1	1.07	1.18	1.18
2b	26.8	−0.63	−0.68	−0.63	−0.63	−0.63	−0.58	−0.68	−0.67	−0.73	−0.72
3	32.9	2.1	2.1	2.1	2.1	2.1	2.05	2	2.1	2.08	2.08
4	21.1	1.44	1.44	1.44	1.43	1.43	1.4	1.43	1.27	1.48	1.48
4a	117	−1.48	−1.48	−1.48	−1.48	−1.48	−1.19	−2.15	−0.25	−1.86	−1.86
5	126.4	−0.65	0.36	0.35	0.36	0.35	−6.39	−4.57	1.58	2.31	2.3
5a	11.9	2.38	2.38	2.38	2.38	2.33	2.15	3.39	2.75	4.16	4.16
6	147.3	−1.08	−1.08	−1.08	−1.09	−1.08	−3.73	−3.38	−1.76	−1.08	−1.08
7	128.2	−1.22	−1.22	−1.22	−1.23	−1.22	−1.25	−3.66	−2.69	−4.96	−4.96
7a	13.8	0.45	0.45	0.45	0.45	0.35	−0.25	−1.7	0.93	−0.76	−0.76
8	122.6	−1.86	−1.86	−1.86	−1.85	−1.86	−2.36	−1.32	−2.9	−1.41	−1.41
8b	12.9	0.45	0.57	0.56	0.56	0.46	0.52	0.58	0.8	0.71	0.71
8a	148	−1.75	−1.74	−1.75	−1.74	−1.75	−1.59	−1.56	−1.47	−1.52	−1.52
1'	103.7	−1.25	−1.24	−1.25	−1.25	−1.25	1.59	1.21	0.17	−0.06	−0.05
2'	31.3	0.63	0.63	0.63	0.63	0.63	2.21	2.13	0.24	7.08	7.08
3'	21.2	−0.3	−0.3	−0.3	−0.3	−0.3	4.71	4.65	−0.1	7.36	7.35
4'	25.2	1.09	1	1.1	1.09	1	0.68	0.64	1.32	4.96	4.96
5'	65.1	−0.35	−0.35	−0.34	−0.35	−0.35	4.17	4.1	−0.77	8.9	8.9

Conformation symbol	k	l	m	n	o	p	q	r	s	t
Relative energy [kJ/mol]	41.41	41.41	41.41	41.41	41.41	41.41	41.41	41.41	41.41	41.41
Energy	−2513900	−2513900	−2513900	−2513900	−2513900	−2513900	−2513900	−2513900	−2513900	−2513900

[kJ/mol] Atom number	Exp.					GIAO					
2	72.6	73.66	73.66	73.66	73.66	73.66	73.66	73.66	73.66	73.77	73.66
2a	26.9	25.86	25.86	25.86	25.85	25.86	25.86	25.86	25.86	25.86	25.86
2b	26.8	27.45	27.44	27.44	27.44	27.44	27.45	27.44	27.44	27.44	27.44
3	32.9	30.8	30.8	30.8	30.8	30.8	30.8	30.8	30.8	30.8	30.8
4	21.1	19.67	19.67	19.7	19.67	19.67	19.67	19.67	19.67	19.67	19.67
4a	117	118.52	118.6	118.52	118.52	118.52	118.52	118.52	118.51	118.52	118.52
5	126.4	127.47	127.47	127.47	127.47	127.47	127.47	127.46	127.47	127.47	127.46
5a	11.9	9.57	9.57	9.57	9.57	9.57	9.56	9.57	9.57	9.57	9.57
6	147.3	148.37	148.37	148.37	148.37	148.37	148.37	148.37	148.47	148.37	148.37
7	128.2	129.4	129.4	129.4	129.4	129.4	129.4	129.4	129.4	129.4	129.4
7a	13.8	13.01	13	13	13.01	13.01	13	13	13.01	13	13
8	122.6	124.43	124.43	124.43	124.44	124.43	124.43	124.43	124.43	124.43	124.43
8b	12.9	12.3	12.3	12.29	12.29	12.3	12.29	12.3	12.29	12.29	12.3
8a	148	149.76	149.76	149.76	149.76	149.76	149.76	149.76	149.75	149.76	149.76
1'	103.7	101.42	101.42	101.42	101.42	101.42	101.43	101.42	101.42	101.42	101.41
2'	31.3	28.34	28.43	28.34	28.34	28.34	28.33	28.34	28.34	28.34	28.34
3'	21.2	16.35	16.35	16.35	16.45	16.35	16.35	16.35	16.35	16.35	16.35
4'	25.2	19.53	19.53	19.53	19.53	19.53	19.52	19.53	19.53	19.53	19.53
5'	65.1	62.63	62.63	62.63	62.63	62.63	62.63	62.63	62.63	62.63	62.63
						Exp. - GIAO					
2	72.6	−1.06	−1.06	−1.06	−1.06	−1.06	−1.06	−1.06	−1.06	−1.17	−1.06
2a	26.9	1.04	1.04	1.04	1.05	1.04	1.04	1.04	1.04	1.04	1.04
2b	26.8	−0.65	−0.64	−0.64	−0.64	−0.64	−0.65	−0.64	−0.64	−0.64	−0.64
3	32.9	2.1	2.1	2.1	2.1	2.1	2.1	2.1	2.1	2.1	2.1
4	21.1	1.43	1.43	1.4	1.43	1.43	1.43	1.43	1.43	1.43	1.43

4a	117	−1.52	−1.6	−1.52	−1.52	−1.52	−1.52	−1.52	−1.51	−1.52	−1.52
5	126.4	−1.07	−1.07	−1.07	−1.07	−1.07	−1.07	−1.06	−1.07	−1.07	−1.06
5a	11.9	2.33	2.33	2.33	2.33	2.33	2.34	2.33	2.33	2.33	2.33
6	147.3	−1.07	−1.07	−1.07	−1.07	−1.07	−1.07	−1.07	−1.17	−1.07	−1.07
7	128.2	−1.2	−1.2	−1.2	−1.2	−1.2	−1.2	−1.2	−1.2	−1.2	−1.2
7a	13.8	0.79	0.8	0.8	0.79	0.79	0.8	0.8	0.79	0.8	0.8
8	122.6	−1.83	−1.83	−1.83	−1.84	−1.83	−1.83	−1.83	−1.83	−1.83	−1.83
8b	12.9	0.6	0.6	0.61	0.61	0.6	0.61	0.6	0.61	0.61	0.6
8a	148	−1.76	−1.76	−1.76	−1.76	−1.76	−1.76	−1.76	−1.75	−1.76	−1.76
1'	103.7	2.28	2.28	2.28	2.28	2.28	2.27	2.28	2.28	2.28	2.29
2'	31.3	2.96	2.87	2.96	2.96	2.96	2.97	2.96	2.96	2.96	2.96
3'	21.2	4.85	4.85	4.85	4.75	4.85	4.85	4.85	4.85	4.85	4.85
4'	25.2	5.67	5.67	5.67	5.67	5.67	5.68	5.67	5.67	5.67	5.67
5'	65.1	2.47	2.47	2.47	2.47	2.47	2.47	2.47	2.47	2.47	2.47

Conformation symbol		u	v	w	x	y	z
Relative energy [kJ/mol]		42.78	42.78	42.78	42.78	42.78	42.78
Energy [kJ/mol]		−2513899	−2513899	−2513899	−2513899	−2513899	−2513899
Atom number	Exp.			GIAO			
2	72.6	73.52	73.52	73.52	73.52	73.52	73.52
2a	26.9	25.75	25.75	25.75	25.75	25.75	25.75
2b	26.8	27.49	27.48	27.48	27.48	27.48	27.48
3	32.9	30.78	30.77	30.77	30.77	30.77	30.77
4	21.1	19.47	19.47	19.47	19.37	19.47	19.47
4a	117	118.63	118.63	118.63	118.63	118.63	118.63
5	126.4	123.69	123.69	123.69	123.69	123.69	123.69
5a	11.9	7.79	7.79	7.8	7.79	7.79	7.79
6	147.3	148.26	148.25	148.25	148.25	148.26	148.25

7	128.2	133.78	133.78	133.79	133.79	133.78	133.79
7a	13.8	15.1	15.11	15.09	15.1	15.11	15.11
8	122.6	124.15	124.15	124.14	124.15	124.15	124.15
8b	12.9	11.92	11.92	11.91	11.92	11.92	11.92
8a	148	149.39	149.39	149.39	149.39	149.39	149.39
1'	103.7	102.14	102.15	102.15	102.13	102.14	102.15
2'	31.3	28.38	28.37	28.38	28.37	28.38	28.37
3'	21.2	16.33	16.33	16.43	16.33	16.35	16.33
4'	25.2	19.46	19.46	19.46	19.46	19.46	19.46
5'	65.1	62.48	62.48	62.48	62.48	62.49	62.48
			Exp.-GIAO				
2	72.6	−0.92	−0.92	−0.92	−0.92	−0.92	−0.92
2a	26.9	1.15	1.15	1.15	1.15	1.15	1.15
2b	26.8	−0.69	−0.68	−0.68	−0.68	−0.68	−0.68
3	32.9	2.12	2.13	2.13	2.13	2.13	2.13
4	21.1	1.63	1.63	1.63	1.73	1.63	1.63
4a	117	−1.63	−1.63	−1.63	−1.63	−1.63	−1.63
5	126.4	2.71	2.71	2.71	2.71	2.71	2.71
5a	11.9	4.11	4.11	4.1	4.11	4.11	4.11
6	147.3	−0.96	−0.95	−0.95	−0.95	−0.96	−0.95
7	128.2	−5.58	−5.58	−5.59	−5.59	−5.58	−5.59
7a	13.8	−1.3	−1.31	−1.29	−1.3	−1.31	−1.31
8	122.6	−1.55	−1.55	−1.54	−1.55	−1.55	−1.55
8b	12.9	0.98	0.98	0.99	0.98	0.98	0.98
8a	148	−1.39	−1.39	−1.39	−1.39	−1.39	−1.39
1'	103.7	1.56	1.55	1.55	1.57	1.56	1.55
2'	31.3	2.92	2.93	2.92	2.93	2.92	2.93
3'	21.2	4.87	4.87	4.77	4.87	4.85	4.87

4'	25.2	5.74	5.74	5.74	5.74	5.74	5.74
5'	65.1	2.62	2.62	2.62	2.62	2.61	2.62